

# Insurance, biases, discrimination & fairness

Arthur Charpentier

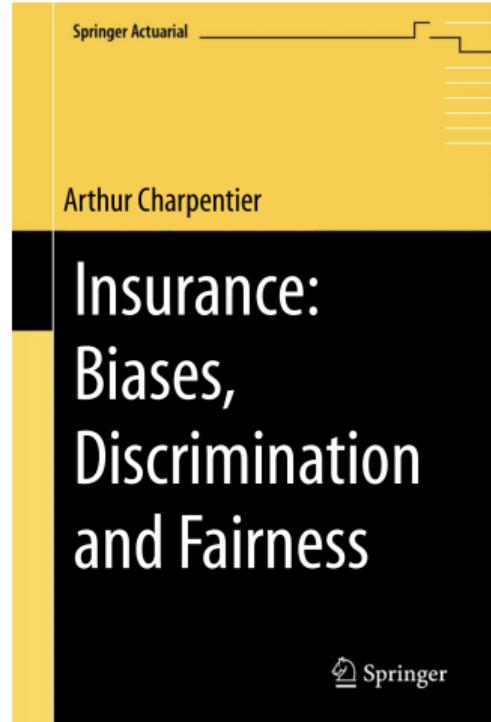
2024

# Reference book

Insurance, Biases, Discrimination and Fairness

ISBN : 978-3-031-49782-7

**Pitch:** Discrimination and fairness of predictive models, in insurance, in the context of data enrichment ("big data") and opaque models ("machine learning", not to say "artificial intelligence").

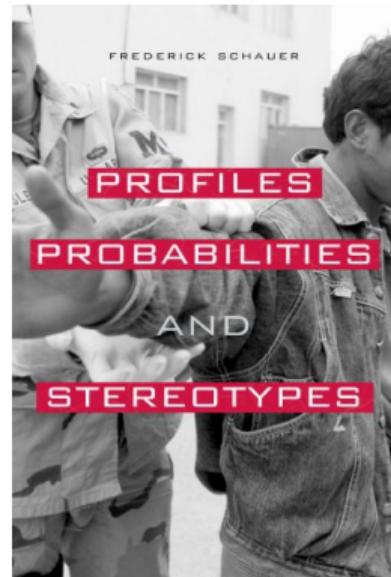


# Preliminaries

## Definition 1.1: Actuaries, Schauer (2006)

To be an **actuary** is to be a specialist in generalization, and actuaries engage in a form of decision making that is sometimes called actuarial. Actuaries guide insurance companies in making decisions about large categories that have the effect of attributing to the entire category certain characteristics that are probabilistically indicated by membership in the **category**, but that still may not be possessed by a particular member of the category.

See **Barry and Charpentier (2020)** on personalization of insurance prices.



# Preliminaries

...

- *Tu la troubles, reprit cette bête cruelle,  
Et je sais que de moi tu médis l'an passé.*
- *Comment l'aurais-je fait si je n'étais pas né ?  
Reprit l'Agneau, je tette encor ma mère.*
- *Si ce n'est toi, c'est donc ton frère.*
- *Je n'en ai point.*
- *C'est donc quelqu'un des tiens.*

...

de La Fontaine (1668), *Le Loup et l'Agneau*.



# Preliminaries

## Definition 1.2: Discrimination, Merriam-Webster (2022)

Discrimination is the act, practice, or an instance of separating or distinguishing categorically rather than individually.

## Definition 1.3: Prejudice, Merriam-Webster (2022)

Prejudice is (1) preconceived judgment or opinion, or an adverse opinion or leaning formed without just grounds or before sufficient knowledge; (2) an instance of such judgment or opinion; (3) an irrational attitude of hostility directed against an individual, a group, a race, or their supposed characteristics.

# Preliminaries

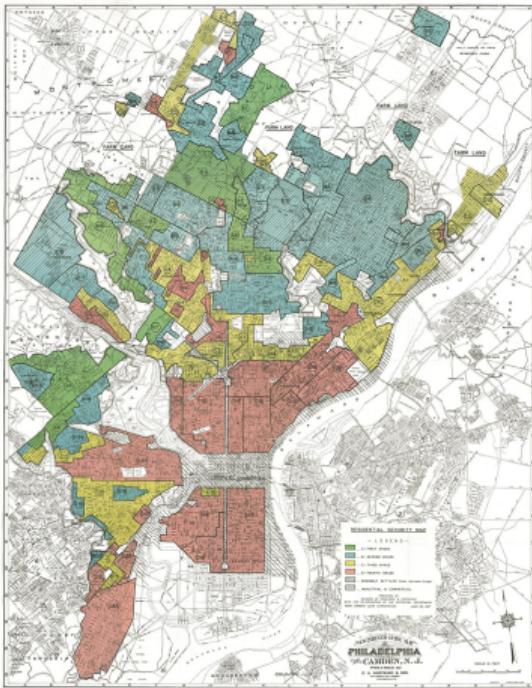
## Definition 1.4: Disparate treatment, Merriam-Webster (2022)

Disparate treatment corresponds to the treatment of an individual (as an employee or prospective juror) that is less favorable than treatment of others for discriminatory reasons (as race, religion, national origin, sex, or disability).

## Definition 1.5: Disparate impact, Merriam-Webster (2022)

Disparate impact corresponds to an unnecessary discriminatory effect on a protected class caused by a practice or policy (as in employment or housing) that appears to be nondiscriminatory.

# Motivation (1. Redlining)



1937 HOLC (Home Owners' Loan Corporation)  
"residential security" map of Philadelphia

## RESIDENTIAL SECURITY MAP

### — L E G E N D —

- [Green Box] .....A - FIRST GRADE
- [Light Blue Box] .....B - SECOND GRADE
- [Yellow Box] .....C - THIRD GRADE
- [Red Box] .....D - FOURTH GRADE
- [Diagonal Hatching Box] .....SPARSELY SETTLED (Color Indicates Grade)
- [Cross-Hatching Box] .....INDUSTRIAL & COMMERCIAL

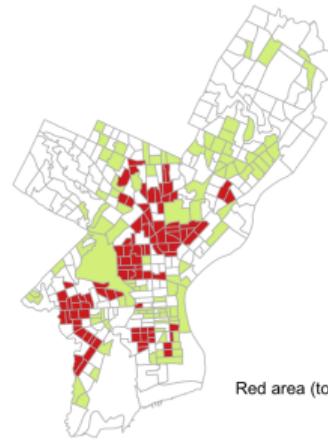
PREPARED BY  
DIVISION OF RESEARCH & STATISTICS  
WITH THE CO-OPERATION OF THE APPRAISAL DEPARTMENT  
HOME OWNERS' LOAN CORPORATION JUNE 25, 1937

HS FORM-B  
2-3-37

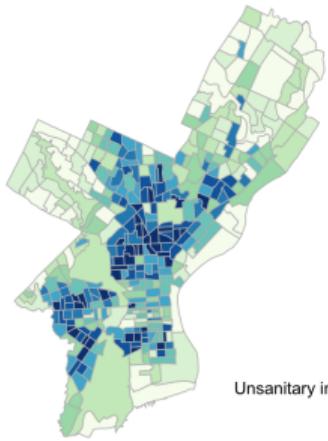
AREA DESCRIPTION  
(For Instructions see Reverse Side)

1. NAME OF CITY Philadelphia, Pa. SECURITY GRADE C AREA NO. 6
2. DESCRIPTION OF TERRAIN. Level
3. FAVORABLE INFLUENCES. Good transportation, particularly in eastern part, -Near to industrial plants of major consequence to entire Philadelphia areas.
4. DETRIMENTAL INFLUENCES. Nominal
5. INHABITANTS:  
a. Type Skilled labor; b. Estimated annual family income \$1,500 - \$1,800.  
c. Foreign-born nominal; d. Negro No (Yes or No); \$  
e. Infiltration of No; f. Relief families moderate  
g. Population is increasing decreasing; static.
6. BUILDINGS:  
a. Type or types predominately; b. Type of construction brick  
c. Average age 20 - 40; d. Repair Fair

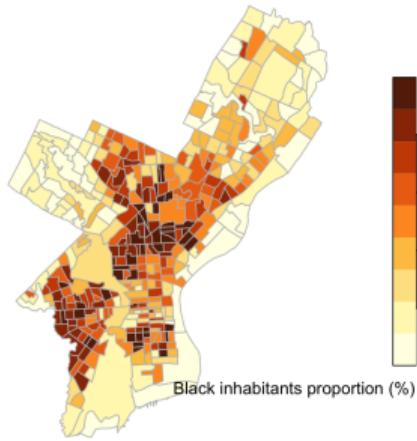
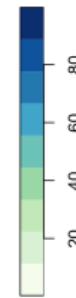
## Motivation (1. Redlining)



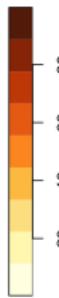
Red area (too risky)



Unsanitary index (0-100)



Black inhabitants proportion (%)



(Fictitious maps, inspired by a Home Owners' Loan Corporation map from 1937)

- ▶ Federal Home Loan Bank Board (FHLBB) "*residential security maps*" (for real-estate investments), [Crossney \(2016\)](#) and [Rhynhart \(2020\)](#)
- ▶ Unsanitary index and proportion of Black inhabitants

## Motivation (1. Redlining)

### Definition 2.1: Redline, Merriam-Webster (2022)

To **redline** is (1) to withhold home-loan funds or insurance from neighborhoods considered poor economic risks; (2) to discriminate against in housing or insurance.

See <https://evolutionofraceandinsurance.org/> for some historical perspective, Squires and Velez (1988), or more recently Squires (2003)

... but still a concern see, e.g., Li (1996) about homosexuals.

## Motivation (2. "Gender directive", 2004/113/EC)

Treaty on European Union (26.10.2012, C326)

### – Article 2 –

The Union is founded on the values of respect for human dignity, freedom, democracy, equality, the rule of law and respect for human rights, including the rights of persons belonging to minorities. These values are common to the Member States in a society in which pluralism, non-discrimination, tolerance, justice, solidarity and equality between women and men prevail.

### – Article 3 –

(...) It shall combat social exclusion and discrimination, and shall promote social justice and protection, equality between women and men, solidarity between generations and protection of the rights of the child.



## Motivation (2. "Gender directive", 2004/113/EC)

Charter of Fundamental Rights of the European Union (18.12.2000 , C364)

### – Article 21 (Non discrimination) –

Any discrimination based on any ground such as sex, race, colour, ethnic or social origin, genetic features, language, religion or belief, political or any other opinion, membership of a national minority, property, birth, disability, age or sexual orientation shall be prohibited.

### – Article 23 (Equality between men and women) –

Equality between men and women must be ensured in all areas, including employment, work and pay.

The principle of equality shall not prevent the maintenance or adoption of measures providing for specific advantages in favour of the under-represented sex.

## Motivation (2. “Gender directive”, 2004/113/EC)

EU Directive ([2004/113/EC](#)), 2004 version

### – Article 5 (Actuarial factors) –

1. Member States shall ensure that in all new contracts concluded after 21 December 2007 at the latest, the use of sex as a factor in the calculation of premiums and benefits for the purposes of insurance and related financial services shall not result in differences in individuals' premiums and benefits.
2. Notwithstanding paragraph 1, Member States may decide before 21 December 2007 to permit proportionate differences in individuals' premiums and benefits where the use of sex is a determining factor in the assessment of risk based on relevant and accurate actuarial and statistical data. The Member States concerned shall inform the Commission and ensure that accurate data relevant to the use of sex as a determining actuarial factor are compiled, published and regularly updated.

## Motivation (2. "Gender directive", 2004/113/EC)

- There was initially (2004) an **opt-out clause** (Article 5(2)).
- Where gender is a determining factor in the assessment of risk based on relevant and accurate actuarial and statistical data then proportionate differences in individual premiums or benefits are allowed.
- March 2011, the European Court of Justice issued its judgement into the "Test-Achats case". The ECJ ruled Article 5(2) was invalid.
- Insurers were no longer able to use gender as a risk factor when pricing policies, "**unisex pricing**".

*"Machine learning won't give you anything like gender neutrality 'for free' that you didn't explicitly ask for"*, Kearns and Roth (2019)

## Motivation (2. “Gender directive”, 2004/113/EC)

“Ten Oever” judgement (*Gerardus Cornelis Ten Oever v Stichting Bedrijfspensioenfonds voor het Glazenwassers – en Schoonmaakbedrijf*, in April 1993), the Advocate General Van Gerven argued that “*the fact that women generally live longer than men has no significance at all for the life expectancy of a specific individual and it is not acceptable for an individual to be penalized on account of assumptions which are not certain to be true in his specific case*,” as mentioned in De Baere and Goessens (2011).

Schanze (2013) used the term “*injustice by generalization*,” from Britz (2008) (“Generalisierungsunrecht”)



# Motivation (2. “Gender directive”, 2004/113/EC)

The Telegraph News Sport Money Business Opinion

## Men are still charged more than women for car insurance, despite EU rule change

Car insurers are dodging European equality laws by making gender judgements based on people's jobs, an economist has found

By Kate Palmer  
10 April 2015 • 12:33pm



Insurers will price by occupation, and female-dominated jobs tend to attract cheaper premiums | CREDIT: Photo: Rex Features

### CAR COSTS: Insurance according to job

Job	Proportion of men	Approximate average premium for a Fiat 500 driver
Dental Nurse	Less than 1pc male	£840
Solicitor	59pc male	£848
Sports and leisure assistants	56pc male	£880
Civil engineer	92pc male	£910
Social worker	21pc male	£920
Plasterer	98pc male	£950

McDonald, 'Indirect Gender Discrimination' (2015); ONS occupation data (2008)

(data source: McDonald (2015))

## Motivation (3. Québec)

Au Québec, Charte des droits et libertés de la personne ([C-12](#))

### – Article 10 –

Toute personne a droit à la reconnaissance et à l'exercice, en pleine égalité, des droits et libertés de la personne, sans distinction, exclusion ou préférence fondée sur la race, la couleur, le sexe, l'identité ou l'expression de genre, la grossesse, l'orientation sexuelle, l'état civil, l'âge sauf dans la mesure prévue par la loi, la religion, les convictions politiques, la langue, l'origine ethnique ou nationale, la condition sociale, le handicap ou l'utilisation d'un moyen pour pallier ce handicap.

Il y a **discrimination** lorsqu'une telle distinction, exclusion ou préférence a pour effet de détruire ou de compromettre ce droit.



## Motivation (3. Québec)

Au Québec, Charte des droits et libertés de la personne ([C-12](#))

– Article 20.1 –

Dans un **contrat d'assurance** ou de rente, un régime d'avantages sociaux, de retraite, de rentes ou d'assurance ou un régime universel de rentes ou d'assurance, une distinction, exclusion ou préférence fondée sur l'âge, le sexe ou l'état civil est **réputée non discriminatoire lorsque son utilisation est légitime et que le motif qui la fonde constitue un facteur de détermination de risque, basé sur des données actuarielles.**



# Motivation (4. Colorado)

Andrus et al. (2021), "*What we can't measure, we can't understand*"



First Regular Session | 74th General Assembly

Colorado General Assembly

September 27, 2023, the Colorado Division of Insurance exposed a new proposed regulation entitled **Concerning Quantitative Testing of External Consumer Data and Information Sources, Algorithms, and Predictive Models Used for Life Insurance Underwriting for Unfairly Discriminatory Outcomes**



## Motivation (4. Colorado)

### – Section 4 (Definitions) –

**Bayesian Improved First Name Surname Geocoding**, or “BIFSG” means, for the purposes of this regulation, the statistical methodology developed by the RAND corporation for estimating race and ethnicity.

**External Consumer Data and Information Source**, or “ECDIS” means, for the purposes of this regulation, a data source or an information source that is used by a life insurer to supplement or supplant traditional underwriting factors. This term includes credit scores, credit history, social media habits, purchasing habits, home ownership, educational attainment, licensures, civil judgments, court records, occupation that does not have a direct relationship to mortality, morbidity or longevity risk, consumer-generated Internet of Things data, biometric data, and any insurance risk scores derived by the insurer or third-party from the above listed or similar data and/or information source.

## Motivation (4. Colorado)

### – Section 5 (Estimating Race and Ethnicity) –

Insurers shall estimate the race or ethnicity of all proposed insureds that have applied for coverage on or after the insurer's initial adoption of the use of ECDIS, or algorithms and predictive models that use ECDIS, including a third party acting on behalf of the insurer that used ECDIS, or algorithms and predictive models that used ECDIS, in the underwriting decision-making process, by utilizing:

1. BIFSG and the insureds' or proposed insureds' name and geolocation (information included in the applications) for life insurance shall be used to estimate the race and ethnicity of each insured or proposed insured.
2. For the purposes of BIFSG, the following racial and ethnic categories shall be used: Hispanic, Black, Asian Pacific Islander (API), and White.

## Motivation (4. Colorado)

### – Section 6 (Application Approval Decision Testing Requirements) –

Using the BIFSG estimated race and ethnicity of proposed insureds and the following methodology, insurers shall calculate whether Hispanic, Black, and API proposed insureds are disapproved at a statistically significant different rate relative to White applicants for whom the insurer, or a third party acting on behalf of the insurer, used ECDIS, or an algorithm or predictive model that used ECDIS, in the underwriting decision-making process.

1. Logistic regression shall be used to model the binary underwriting outcome of either approved or denied.
2. The following factors may be accounted for as control variables in the regression model: policy type, face amount, age, gender, and tobacco use.
3. The estimated race or ethnicity of the proposed insureds shall be accounted for by including Hispanic, Black, and Asian Pacific Islander (API) as separate dummy variables in the regression model.

## Motivation (4. Colorado)

4. Determine if there is a statistically significant difference in approval rates for each BIFSG estimated race or ethnicity variable as indicated by a *p*-value of less than .05.
  - a. If there is not a statistically significant difference in approval rates, no further testing is required.
  - b. If there is a statistically significant difference in approval rates, the insurer shall determine whether the difference in approval rates is five (5) percentage points or greater as indicated by the marginal effects value of each BIFSG estimated race or ethnicity variable. (...)

## Motivation (4. Colorado)

### – Section 7 (Premium Rate Testing Requirements) –

Using the insureds' BIFSG estimated race and ethnicity, insurers shall determine if there is a statistically significant difference in the premium rate per \$1,000 of face amount for policies issued to Hispanic, Black, and API insureds relative to White insureds for whom the insurer, or a third party acting on behalf of the insurer, used ECDIS, or an algorithm or predictive model that used ECDIS, in the underwriting decision-making process.

1. Linear regression shall be used to model the continuous numerical outcome of premium rate per \$1,000 of face amount.
2. The following factors may be accounted for as control variables in the regression model: policy type, face amount, age, gender, and tobacco use.
3. The estimated race or ethnicity of the proposed insureds shall be accounted for by including Hispanic, Black, and Asian Pacific Islander (API) as separate dummy variables in the regression model.

## Motivation (4. Colorado)

4. Determine if there is a statistically significant difference in the premium rate per \$1,000 of face amount for each BIFSG estimated race or ethnicity variable as indicated by a p-value of less than .05.
  - a. If there is not a statistically significant difference in premium rate per \$1,000 of face amount, no further testing is required.
  - b. If there is a statistically significant difference in premium rate per \$1,000 of face amount, determine whether the premium rate per \$1,000 of face amount is at least 5% more than the average premium rate per \$1,000 for all policies.
    - i. If the difference in premium rate per \$1,000 of face amount is less than 5%, no further testing is required.
    - ii. If the difference in premium rate per \$1,000 of face amount is 5% or greater, further testing is required as described in Section 8.

## Motivation (4. Colorado)

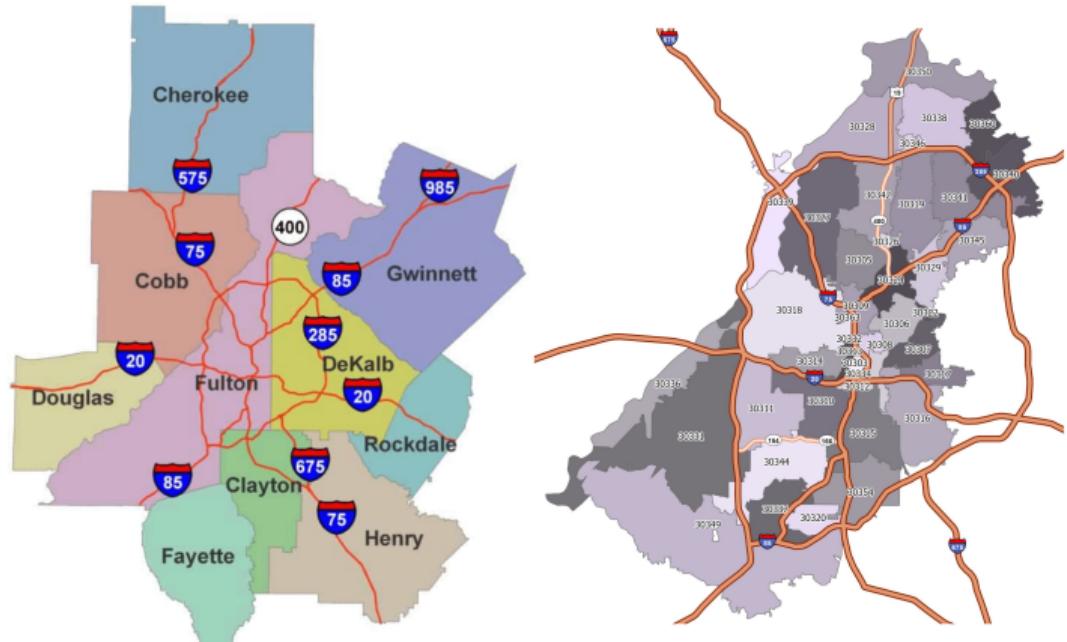
In Elliott et al. (2009), BIFSG<sup>1</sup>, `library(eiCompare)`. , consider 12 people living near Atlanta, GA (Fulton & Gwinnett counties), and `eiCompare::wru_predict_race_wrapper`

	last	first	county	city	zipcode	whi	bla	his	asi
1	LOCKLER	GABRIELLA	Fulton	Atlanta	30318	0	0	0	0
2	RADLEY	OLIVIA	Fulton	Fairburn	30213	14	83	1	0
3	BOORSE	KEISHA	Fulton	Atlanta	30331	97	0	3	0
4	MAZ	SAVANNAH	Gwinnett	Norcross	30093	5	6	76	13
5	GAULE	NATASHIA	Gwinnett	Snellville	30078	67	19	14	0
6	MCMELLEN	ISMAEL	Gwinnett	Lilburn	30047	73	15	6	3
7	RIDEOUT	LUQMAN	Gwinnett	Snellville	30078	77	18	2	0
8	WASHINGTON	BRYN	Gwinnett	Norcross	30093	0	95	3	0
9	KULENOVIC	EVELYN	Gwinnett	Buford	30518	100	0	0	0
10	HERNANDEZ	SAMANTHA	Gwinnett	Duluth	30096	3	1	94	1
11	LONG	BESSIE	Gwinnett	Duluth	30096	53	39	1	1
12	HE	JOSE	Gwinnett	Lawrenceville	30045	2	3	4	89

<sup>1</sup>Bayesian Improved First Name Surname Geocoding

## Motivation (3. Colorado)

We have 12 people,  
in two counties near Atlanta  
(about 10 zip-codes)



## Motivation (3. Colorado)

- Use `eiCompare::wru_predict_race_wrapper` on a revised dataset with the same name “Savannah Maz”

1	last	first	county	city	zipcode	whi	bla	his	asi
2 1	MAZ	SAVANNAH	Fulton	Atlanta	30318	0	0	0	100
3 2	MAZ	SAVANNAH	Fulton	Fairburn	30213	13	61	22	3
4 3	MAZ	SAVANNAH	Fulton	Atlanta	30331	3	77	19	1
5 4	MAZ	SAVANNAH	Gwinnett	Norcross	30093	5	6	76	13
6 5	MAZ	SAVANNAH	Gwinnett	Snellville	30078	13	18	69	0
7 6	MAZ	SAVANNAH	Gwinnett	Lilburn	30047	28	22	34	16
8 7	MAZ	SAVANNAH	Gwinnett	Snellville	30078	53	3	40	3
9 8	MAZ	SAVANNAH	Gwinnett	Norcross	30093	5	6	76	13
10 9	MAZ	SAVANNAH	Gwinnett	Buford	30518	79	4	14	2
11 10	MAZ	SAVANNAH	Gwinnett	Duluth	30096	32	8	38	22
12 11	MAZ	SAVANNAH	Gwinnett	Duluth	30096	55	19	22	5
13 12	MAZ	SAVANNAH	Gwinnett	Lawrenceville	30045	15	19	62	4

## Motivation (3. Colorado)

- Use `eiCompare::wru_predict_race_wrapper` on a revised dataset with the same name “Bryn Washington”

1	last	first	county	city	zipcode	whi	bla	his	asi
2 1	WASHINGTON	BRYN	Fulton	Atlanta	30318	0	0	0	100
3 2	WASHINGTON	BRYN	Fulton	Fairburn	30213	0	99	0	0
4 3	WASHINGTON	BRYN	Fulton	Atlanta	30331	0	99	0	0
5 4	WASHINGTON	BRYN	Gwinnett	Norcross	30093	0	95	3	0
6 5	WASHINGTON	BRYN	Gwinnett	Snellville	30078	0	96	1	0
7 6	WASHINGTON	BRYN	Gwinnett	Lilburn	30047	1	98	0	0
8 7	WASHINGTON	BRYN	Gwinnett	Snellville	30078	6	87	2	0
9 8	WASHINGTON	BRYN	Gwinnett	Norcross	30093	0	95	3	0
10 9	WASHINGTON	BRYN	Gwinnett	Buford	30518	7	92	1	0
11 10	WASHINGTON	BRYN	Gwinnett	Duluth	30096	2	96	1	0
12 11	WASHINGTON	BRYN	Gwinnett	Duluth	30096	1	96	0	0
13 12	WASHINGTON	BRYN	Gwinnett	Lawrenceville	30045	0	98	1	0

## Motivation (3. Colorado)

- Use `eiCompare::wru_predict_race_wrapper` on a revised dataset with the same name "Samantha Hernandez"

	last	first	county	city	zipcode	whi	bla	his	asi
1	HERNANDEZ	SAMANTHA	Fulton	Atlanta	30318	0	0	0	100
2	HERNANDEZ	SAMANTHA	Fulton	Fairburn	30213	2	12	85	0
3	HERNANDEZ	SAMANTHA	Fulton	Atlanta	30331	0	16	81	0
4	HERNANDEZ	SAMANTHA	Gwinnett	Norcross	30093	0	0	99	0
5	HERNANDEZ	SAMANTHA	Gwinnett	Snellville	30078	1	1	97	0
6	HERNANDEZ	SAMANTHA	Gwinnett	Lilburn	30047	3	3	92	1
7	HERNANDEZ	SAMANTHA	Gwinnett	Snellville	30078	5	0	94	0
8	HERNANDEZ	SAMANTHA	Gwinnett	Norcross	30093	0	0	99	0
9	HERNANDEZ	SAMANTHA	Gwinnett	Buford	30518	17	1	81	0
10	HERNANDEZ	SAMANTHA	Gwinnett	Duluth	30096	3	1	94	1
11	HERNANDEZ	SAMANTHA	Gwinnett	Duluth	30096	8	4	86	0
12	HERNANDEZ	SAMANTHA	Gwinnett	Lawrenceville	30045	1	2	97	0

## Motivation (3. Colorado)

- Use `eiCompare::wru_predict_race_wrapper` on a revised dataset with the same name “Jose He”

1	last	first	county	city	zipcode	whi	bla	his	asi
2	1	HE	JOSE	Fulton	Atlanta	30318	0	0	0 100
3	2	HE	JOSE	Fulton	Fairburn	30213	2	9	2 84
4	3	HE	JOSE	Fulton	Atlanta	30331	1	27	3 55
5	4	HE	JOSE	Gwinnett	Norcross	30093	0	0	2 98
6	5	HE	JOSE	Gwinnett	Snellville	30078	13	18	30 0
7	6	HE	JOSE	Gwinnett	Lilburn	30047	1	1	1 97
8	7	HE	JOSE	Gwinnett	Snellville	30078	8	1	3 86
9	8	HE	JOSE	Gwinnett	Norcross	30093	0	0	2 98
10	9	HE	JOSE	Gwinnett	Buford	30518	19	1	2 78
11	10	HE	JOSE	Gwinnett	Duluth	30096	1	0	0 98
12	11	HE	JOSE	Gwinnett	Duluth	30096	6	2	1 85
13	12	HE	JOSE	Gwinnett	Lawrenceville	30045	2	3	4 89

# Motivation (5. Motor Insurance in the U.S.)

## via The Zebra (2022),

### California

**Allowed (with applicable limitations):** driving experience, marital status, address/zip code  
**Prohibited (or effectively prohibited):** gender, age, credit history, education, occupation, employment status, residential status, insurance history

**Notes & Clarifications:** California's insurance commissioner banned gender as of January 2019. Occupation and education are permitted for use in group plans (i.e. for alumni associations and other membership programs).

### Georgia

**Allowed (with applicable limitations):** gender, age, years of driving experience, credit history, marital status, residential status, address/zip code, insurance history

**Prohibited (or effectively prohibited):** occupation, education, and employment status

**Notes & Clarifications:** none

### Hawaii

**Allowed (with applicable limitations):** address/zip code, insurance history

**Prohibited (or effectively prohibited):** gender, age, years of driving experience, credit history, education, occupation, employment status, marital status, residential status

**Notes & Clarifications:** none

### Illinois

**Allowed (with applicable limitations):** gender, age, years of driving experience, credit history, education, occupation, employment status, marital status, residential status, address/zip code, insurance history

**Prohibited (or effectively prohibited):** none

**Notes & Clarifications:** none

### Massachusetts

**Allowed (with applicable limitations):** years of driving experience, address/zip code, insurance history

**Prohibited (or effectively prohibited):** gender, age, credit history, education, occupation, employment status, marital status, residential status

**Notes & Clarifications:** none

### Michigan

**Allowed (with applicable limitations):** gender (group-rated policies), age, years of driving experience, credit history, education, occupation, employment status, marital status (group-rated policies), residential status, address/zip code, insurance history

**Prohibited (or effectively prohibited):** gender (non-group policies), marital status (non-group policies)

**Notes & Clarifications:** Gender and marital status are permitted only in rate-making for group plans (i.e. for alumni associations and other membership programs). UPDATE:[Michigan lawmakers approved a major insurance reform bill](#) in May 2019 that will ban insurers in the state from using gender, marital status, address/zipcode, residential status, education and occupation in rate setting. The ban will be enforced starting in July 2020. Insurers will be permitted to use "territory" as approved by the state regulators instead of zip code.

### New York

**Allowed (with applicable limitations):** gender, age, years of driving experience, credit history, marital status, residential status, address/zip code, insurance history

**Prohibited (or effectively prohibited):** occupation, education, employment status

**Notes & Clarifications:** none

see also → Avraham et al. (2013)

# Motivation (6. Admission in Graduate Program, UC Berkeley)

## Sex Bias in Graduate Admissions: Data from Berkeley

Measuring bias is harder than is usually assumed, and the evidence is sometimes contrary to expectation.

P. J. Bickel, E. A. Hammel, J. W. O'Connell

Determining whether discrimination because of sex or ethnicity is being practiced against persons seeking graduate education is important. It is also another issue that is an important problem in our society today. Is it legally important and morally important? It is also another issue that is an important problem in our society today. The study of measurement and assessment involved in one example of an individual problem is by means of which we hope to shed some light on the difficulties. We will proceed in a straightforward and simple manner over the course of time, and have undertaken an unanticipated approach to the problem. We do this because we think it quite likely that there will be a great deal of confusion in the chain of actions that lead to a decision on an individual problem. We can, however, say that if the admissions decision and the sex of the applicants are statistically associated, then there is a sex bias. In this paper, we may judge that bias existed, and we may then seek to find whether alternative causation existed. By examining the evidence for a causal association between a particular decision and a particular sex of an applicant, and a particular sex of an application, we can determine whether there is sex bias.

We are interested in the validity of assumption 1, that the probability of admission is independent of the sex of the applicant when that is consistent with the qualifications for entry.

The simplest approach would be to examine the aggregate data for the campus. The approach for that quarter, in the admissions cycle for that quarter, in the academic year 1973, involved approximately 15,000 applications, some of which were later withdrawn or transferred to other departments or to other universities. The applications finally remaining for the fall 1973 cycle, 12,763 were thoroughly compiled to permit a

decision to admit or to deny admissions. The question we wish to pursue is whether the decision to admit or to deny was made independently of the sex of the applicant.

We must first make clear two assumptions. One is that the academic qualifications of the students are the sole basis for admission. Now, the outcome of an application for admission to graduate school depends mainly on the academic faculty of the department with which the prospective student applies. Let us then examine each of the departments for which there are data. In the 101 departments we find that 16 did not have no women applicants or denied admission to no applicants of either sex. Of the remaining 85, 10 did not have any women applicants to occur at least once. Then the distribution of applicants is anything but random among the departments. In examining the various procedures we did in our initial approach, we found data from these very different independent decision-making units, and aggregating those statistics, the evidence for campus-wide bias in favor of men was strong. However, in the 101 departments placed in the opposite direction, at the same probability levels, there was a solid case for sex bias in favor of women.

Assumption 2 is that the sex ratio of applicants in the various fields of study and research is the same as is associated with any other factors in admissions. We shall have reason to challenge this assumption. After all, it is the first step in our analysis, which is the investigation of bias in the aggregate data.

## Some Underlying Dependencies

We have started out with a paradox, namely that in the Berkeley data in this context (1) the proportion of men and women applicants have equal chances of admission to the university, while in the basic data of assumption 1 and 2), this contradicts what is given in Table 1, gives the data for all 12,763 applications in the 101 graduate departments and the total number to which applications were made for fall 1973 (we shall refer to this as "all the departments"). There were 3,777 men and 2,770 women applicants. About 44 percent of the males and about 35 percent of the females were admitted. This kind of evidence, under certain assumptions, leads to a paradox. We should on this evidence judge

that bias existed in the fall 1973 admissions. On that account, we are of the opinion that in this naive approach, there is no room for statistical evidence of them for didactic reasons.

We must first make clear two assumptions. One is that the academic qualifications of the students are the sole basis for admission. Now, the outcome of an application for admission to graduate school depends mainly on the academic faculty of the department with which the prospective student applies. Let us then examine each of the departments for which there are data. In the 101 departments we find that 16 did not have no women applicants or denied admission to no applicants of either sex. Of the remaining 85, 10 did not have any women applicants to occur at least once. Then the distribution of applicants is anything but random among the departments. In examining the various procedures we did in our initial approach, we found data from these very different independent decision-making units, and aggregating those statistics, the evidence for campus-wide bias in favor of men was strong. However, in the 101 departments placed in the opposite direction, at the same probability levels, there was a solid case for sex bias in favor of women.

Assumption 2 is that the sex ratio of applicants in the various fields of study and research is the same as is associated with any other factors in admissions. We shall have reason to challenge this assumption. After all, it is the first step in our analysis, which is the investigation of bias in the aggregate data.

Let us first examine an alternative to aggregating the data across the 101 departments. If we apply the decision rule "admit or deny," we find that this table has a chi-square value of 2395, with 10 degrees of freedom. The probability of obtaining such a value by chance alone is 1 in 10,000 (5). This is consistent with the evidence of bias in sense of aggregation procedures shown by Table 1. We can give a more detailed picture to a prior linkage, that between sex of applicant and department to which she or he applied. First, we turn to the distribution of bias, the picture changes. For instance, if we apply Fisher's exact test to the data in Table 1, we find that the association of sex of an application with the sex of the student is marked. For example, in our data analysis, we find that the probability of getting a chi-square value of 2395 or larger by chance alone is 1 in 100 (6).

However, if we apply the weighted chi-square statistic (7) as a measure of the relationship for all 85 departments, we find that the probability of getting a chi-square value of 2395 or larger by chance alone is 1 in 100 (6). When we apply the same measure to the 17 departments with the largest numbers of applicants (accounting for two-

Table 1. Decisions on applications to Graduate Division for fall 1973, by sex of applicant—observed frequencies. Observed frequencies calculated from the marginal totals of the observed data. Chi-square = 2395, D.F. = 10, P = 0.0001. Contingency 12 and 23 given in the text. N = 12,763;  $\chi^2 = 118.6$ , D.F. = 1, P = 0.0001.

Applicants	Outcome						Difference
	Observed		Expected		Actual		
	Admit	Deny	Admit	Deny	Admit	Deny	
Men	3738	4764	3448.7	4801.3	2773	2773	-277.3
Women	1894	2877	1773.3	2847.7	-277.3	-277.3	277.3

thirds of the total population of applicants) we obtain  $\chi^2 = 45.6$ , while the remaining 85 departments have a corresponding  $\chi^2 = 38.3$ . The value of  $\chi^2$  under the hypothesis of no association can be calculated. All three values are significantly significant.

The effect may be gauged by means of an analogy. You take a wheat field with two different mesh sizes. A school of fish,

example that illustrates the danger of incisive pooling of data, consider two departments of a hypothetical university. In one, there are 400 men and 400 women; these are admitted on an equal basis. In the other, there are 200 men and 200 women. To social workers they apply 150 men and 450 women; these are admitted in exactly equal proportions. Of the 150 men, 120 are applied to mechanics and 30 to social work; of the 450 women, 300 are applied to mechanics and 27 percent to social work, while about 69 percent of the women applied to social work are admitted on an equal basis. In mechanization, there is a 20 percent deficit of women. When these two departments are pooled and expected frequencies are computed, we find that the overall sex ratio is 1.5. The difference in standard on each department separately, and aggregating those statistics, the evidence for campus-wide bias in favor of men is strong. However, in the 101 departments placed in the opposite direction, at the same probability levels, there is evidence of bias in favor of women.

It is not surprising that the results of this analysis are not as dramatic as is another fact: not all departments are equally easy to enter. We find that the data across the 101 departments, when aggregated to admit or deny, we find that this table has a chi-square value of 2395, with 10 degrees of freedom. The probability of obtaining such a value by chance alone is 1 in 10,000 (5). This is a deficit of about 21 women (Table 2). A discrepancy is that direction that large number of women applicants has that 2 percent of the bias by chance; yet both departments were seen to have been absolutely fair in dealing with women applicants.

The creation of bias is our original situation is, of course, much more complex, since we have aggregating many variables, and from the interactions of the three factors, choice of department, sex, and admissions status, which better conditions are suggested by sex, but which cannot be described in any simple way.

In any case, aggregation in a single unit of analysis is not always (see Approach A) an unbiased method. More sophisticated methods of aggregation that do not rely on assumption 2 are legitimate but have their difficulties. We shall have reason to say on this later.

## Disaggregation

The most radical alternative to approach A is to consider the individual graduate applications as separate cases. However, this approach (which we call approach B) also poses difficulties. The first difficulty is that it is clearly from the different departments, or we must take account of the probability of obtaining unequal ratios of men to women in the 101 departments of independently conducted independent experiments. That is, in examining 85 separate departments, we are controlling for evidence of bias we are controlling 85 separate experiments,

Table 2. Admissions data by sex of applicant for two hypothetical departments. For small,  $\chi^2 = 5.76$ ;  $\chi^2 = 1.7$ ,  $P = 0.19$  (continued).

Applicants	Outcome						Difference
	Observed		Expected		Actual		
	Admit	Deny	Admit	Deny	Admit	Deny	
Men	200	230	200	200	8	0	0
Women	100	130	100	100	0	0	0
Men	50	80	100	100	0	0	-100
Women	30	300	150	300	0	0	-300
Men	250	380	218.2	218.8	-20.8	-20.8	-20.8
Women	250	400	279.8	279.3	-28.8	-28.8	-28.8

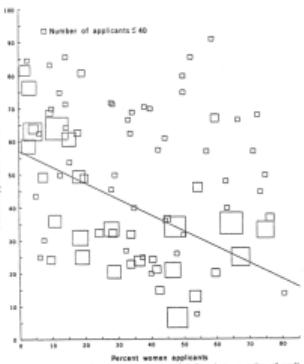


Fig. 1. Proportion of applicants that are women plotted against proportion of applicants admitted, in 85 departments. Size of box indicates relative number of applicants to the department.

## Data and Assumption

The particular body of data chosen for examination consists of applications received in the Graduate Division of the University of California, Berkeley, for the fall 1973 quarter. In the admissions cycle for that quarter, in the academic year 1973, involved approximately 15,000 applications, some of which were later withdrawn or transferred to other departments or to other universities. The applications finally remaining for the fall 1973 cycle, 12,763 were thoroughly compiled to permit a

(a) Ratio is estimate of average. The estimate of proportion of ethnicity and race is based on the data from the 1970 U.S. Census. The estimate of the data from the 1970 U.S. Census is a measure of the fraction of the population of the United States, Berkeley, California.

# Bickel et al. (1975)

## Motivation (6. Admission in Graduate Program, UC Berkeley)

	Total	Men	Women	Proportions
Total	5233/12763 ~ 41%	3714/8442 ~ <b>44%</b>	1512/4321 ~ 35%	66%-34%
Top 6	1745/4526 ~ 39%	1198/2691 ~ <b>45%</b>	557/1835 ~ 30%	59%-41%
A	597/933 ~ 64%	512/825 ~ 62%	89/108 ~ <b>82%</b>	88%-12%
B	369/585 ~ 63%	353/560 ~ 63%	17/ 25 ~ <b>68%</b>	96% - 4%
C	321/918 ~ 35%	120/325 ~ <b>37%</b>	202/593 ~ 34%	35%-65%
D	269/792 ~ 34%	138/417 ~ 33%	131/375 ~ <b>35%</b>	53%-47%
E	146/584 ~ 25%	53/191 ~ <b>28%</b>	94/393 ~ 24%	33%-67%
F	43/714 ~ 6%	22/373 ~ 6%	24/341 ~ <b>7%</b>	52%-48%

Data from [Bickel et al. \(1975\)](#) (discussed as an illustration of "[Simpson's paradox](#)")

Formalize the later,  $S$  is the (binary) genre,  $Y$  the admission and  $X$  the program (category),

## Motivation (6. Admission in Graduate Program, UC Berkeley)

$$\begin{aligned} \mathbb{P}[ Y = \text{yes} | S = \text{men} ] &\geq \mathbb{P}[ Y = \text{yes} | S = \text{women} ] \\ \mathbb{P}[ Y = \text{yes} | X = x, S = \text{men} ] &\leq \mathbb{P}[ Y = \text{yes} | X = x, S = \text{women} ], \forall x. \end{aligned}$$

overall admission

conditional on program

*"the bias in the aggregated data stems not from any pattern of discrimination on the part of admissions committees, which seems quite fair on the whole, but apparently from prior screening at earlier levels of the educational system. Women are shunted by their socialization and education toward fields of graduate study that are generally more crowded, less productive of completed degrees, and less well funded, and that frequently offer poorer professional employment prospects,"* Bickel et al. (1975)

## Motivation (6'. Admission in hospitals)

Consider the following mortality rates in two hospitals (fake data)

	Total	Healthy	Pre-condition	Proportions
Hospital A	$800/1000 = 80\%$	$590/600 \sim 98\%$	$210/400 \sim 53\%$	60%-40%
Hospital B	$900/1000 = 90\%$	$870/900 \sim 97\%$	$30/100 \sim 30\%$	90%-10%

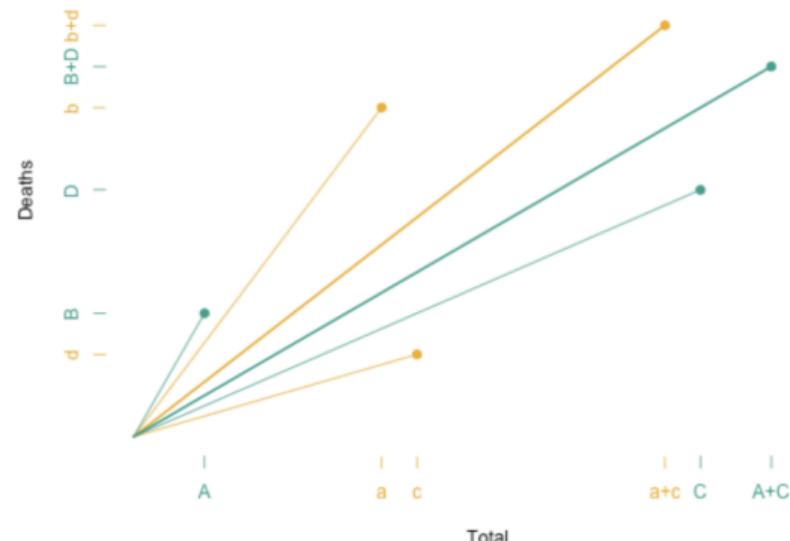
There is no mathematical "paradox", *per se*.

We could have

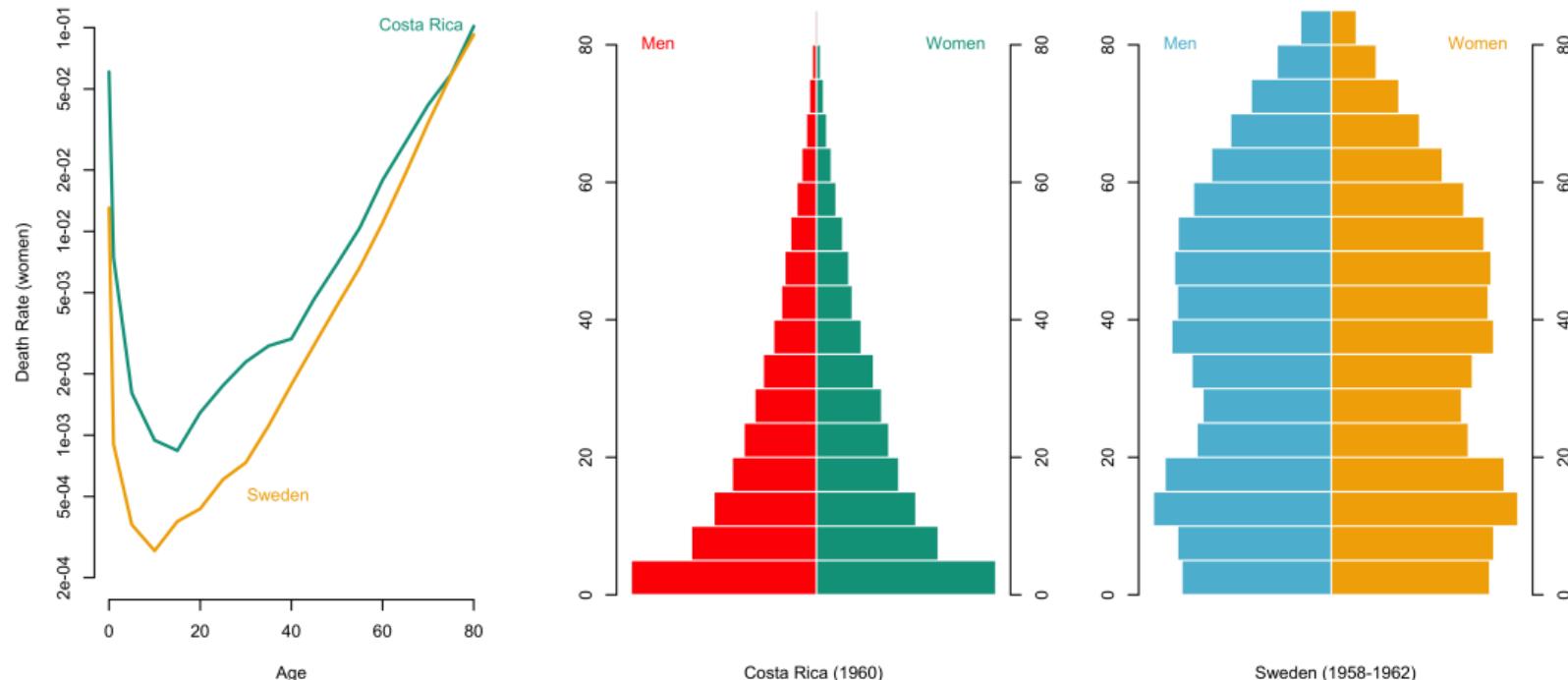
$$\frac{A}{B} \geq \frac{a}{b} \text{ and } \frac{C}{D} \geq \frac{c}{d}$$

and at the same time

$$\frac{A+C}{B+D} \leq \frac{a+c}{b+d}$$



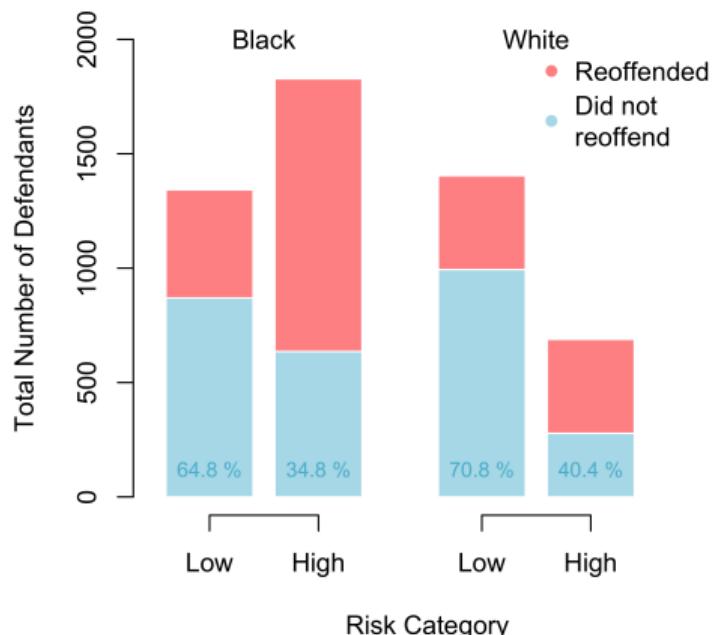
## Motivation (6". Mortality in Costa Rica and Sweden)



Overall mortality rate for women, 8.12% in Costa Rica, against 9.29% in Sweden.

# Motivation (7. Propublica, Actuarial Justice)

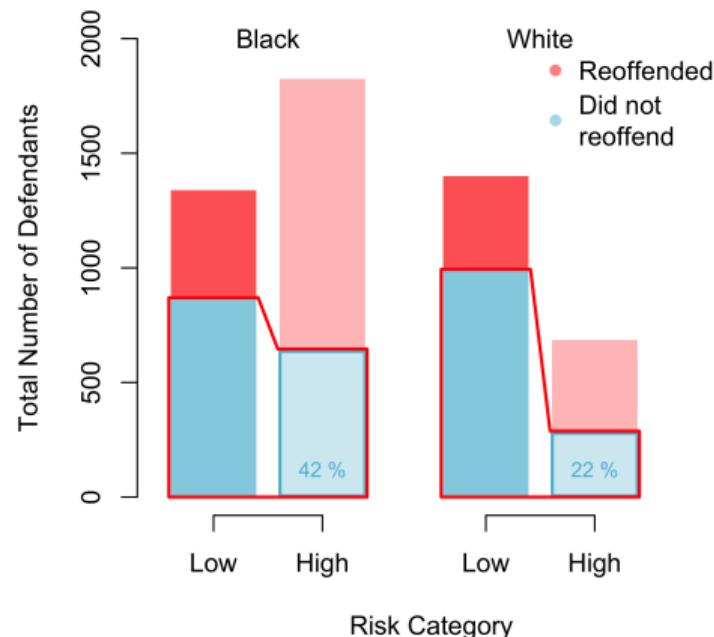
- Concept of "actuarial justice" as coined in Feeley and Simon (1994)
- Correctional Offender Management Profiling for Alternative Sanctions (COMPAS), Perry (2013)



- <https://github.com/propublica/compas-analysis>
- Angwin et al. (2016) Machine Bias  
Dressel and Farid (2018)

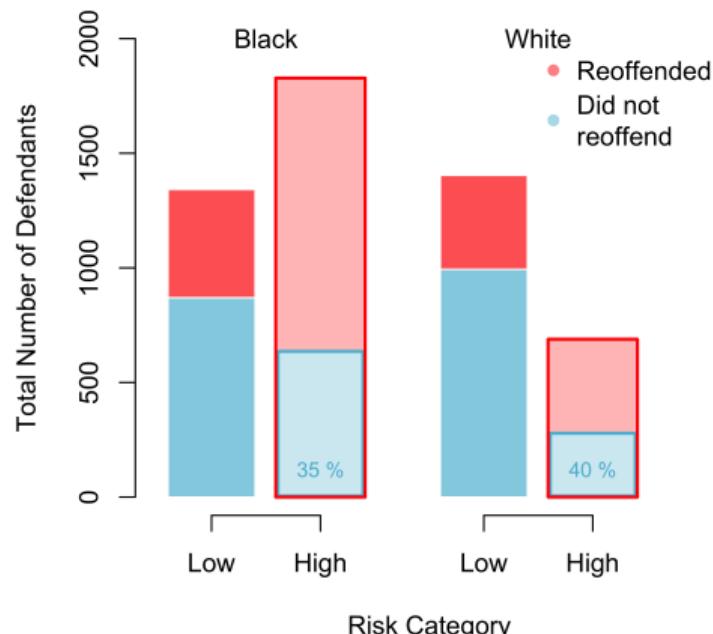
## Motivation (7. Propublica, Actuarial Justice)

- From Feller et al. (2016),
  - ▶ for White people, among those who did not re-offend, 22% were wrongly classified,
  - ▶ for Black people, among those who did not re-offend, 42% were wrongly classified,
  - ▶ problem, since  $42\% \gg 22\%$



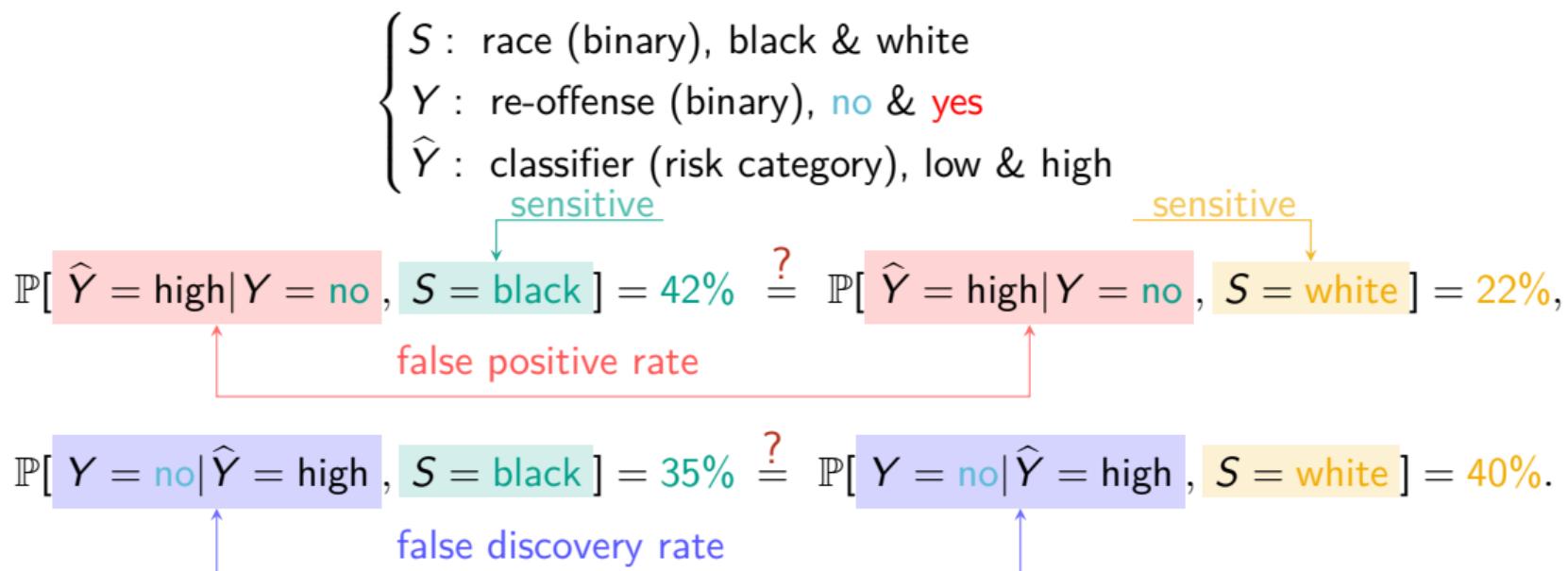
## Motivation (7. Propublica, Actuarial Justice)

- From Dieterich et al. (2016),
  - ▶ for White people, among those who were classified as high risk, 40% did not re-offend,
  - ▶ for Black people, among those who were classified as high risk, 35% did not re-offend,
  - ▶ no problem, since  $40\% \approx 35\%$

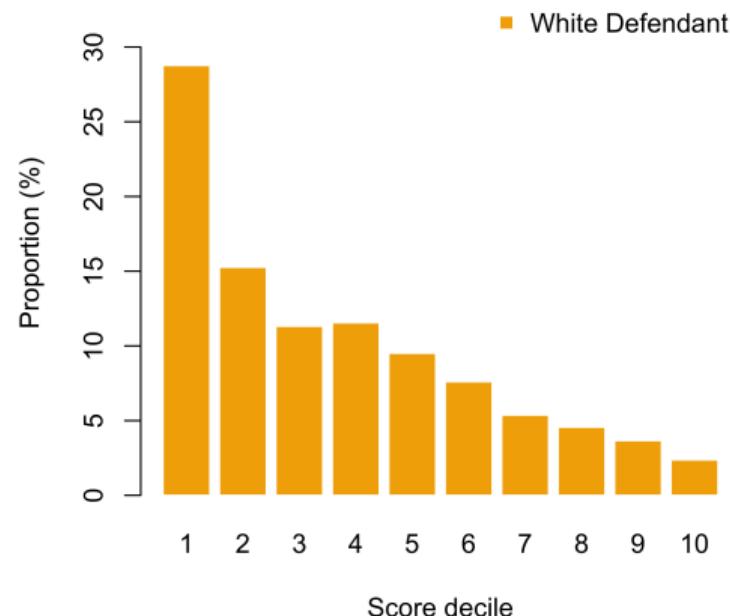
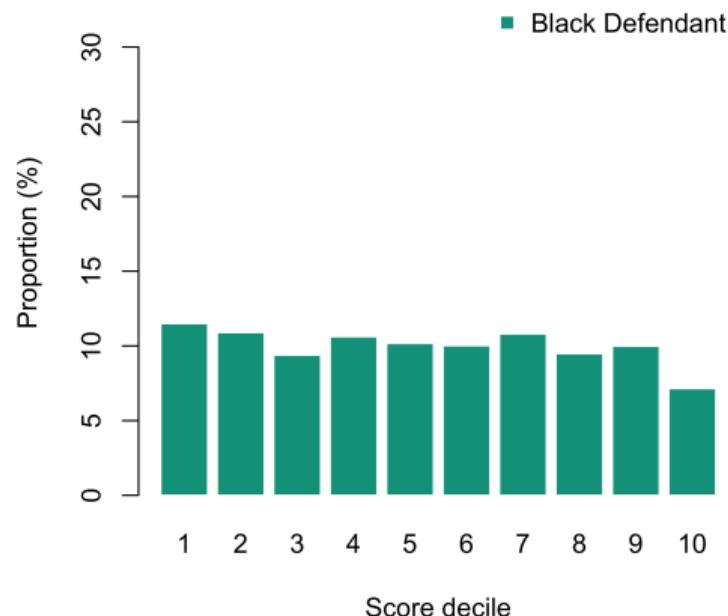


## Motivation (7. Propublica, Actuarial Justice)

Formalize the later,

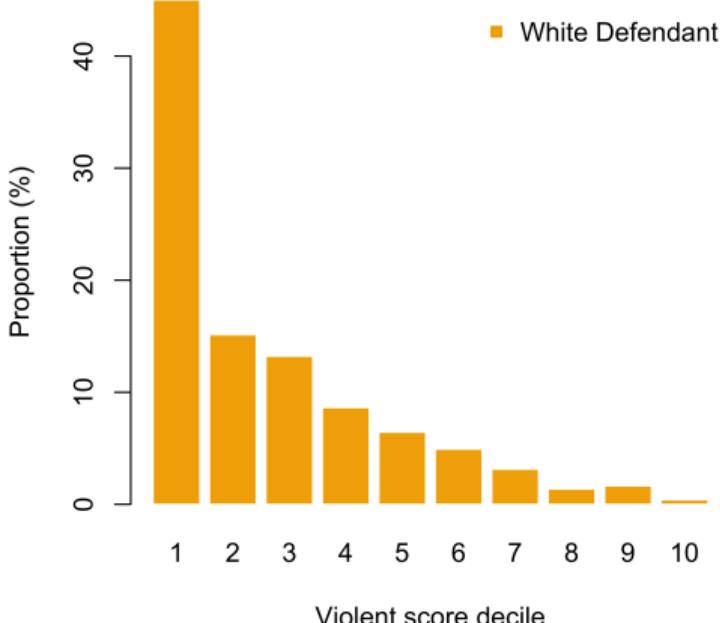
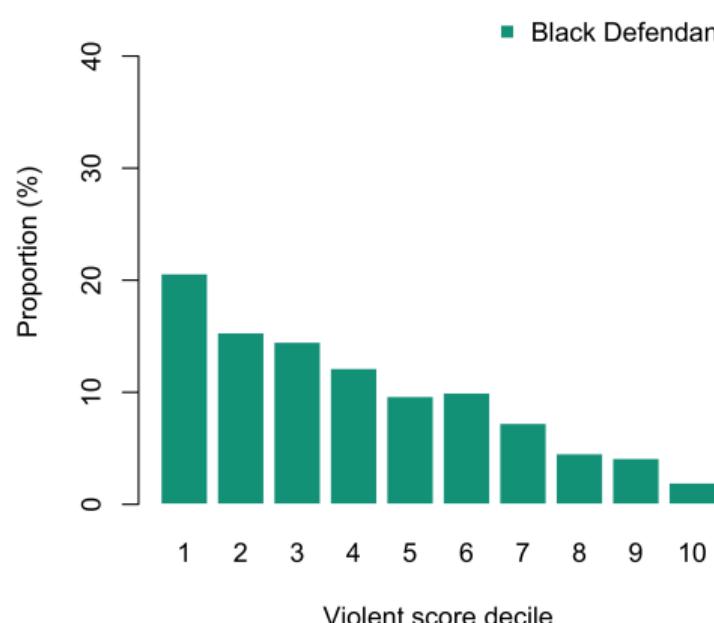


## Motivation (7. Propublica, Actuarial Justice)



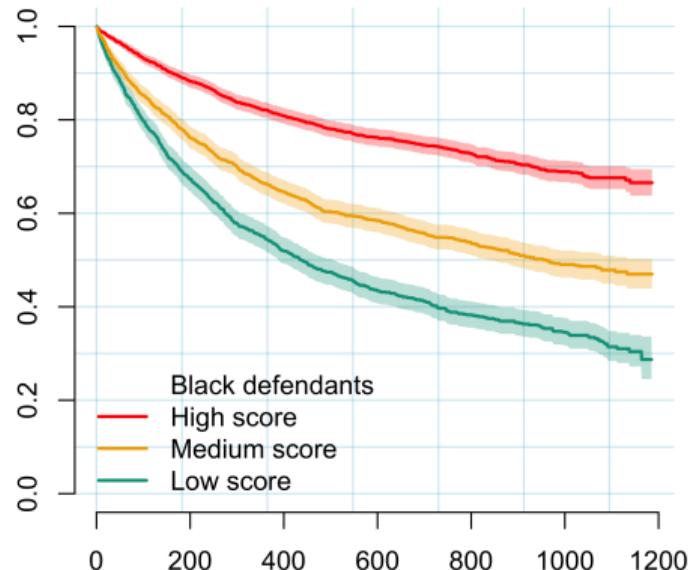
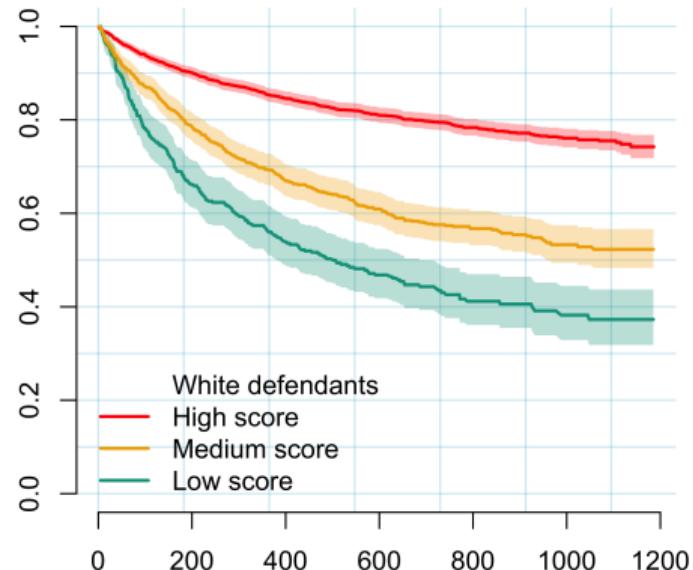
Look at score distributions, black and white defendant, Larson et al. (2016)

## Motivation (7. Propublica, Actuarial Justice)



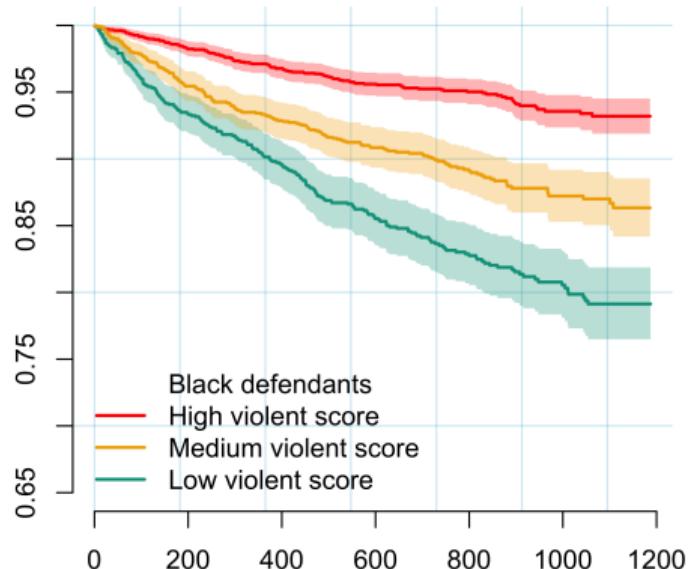
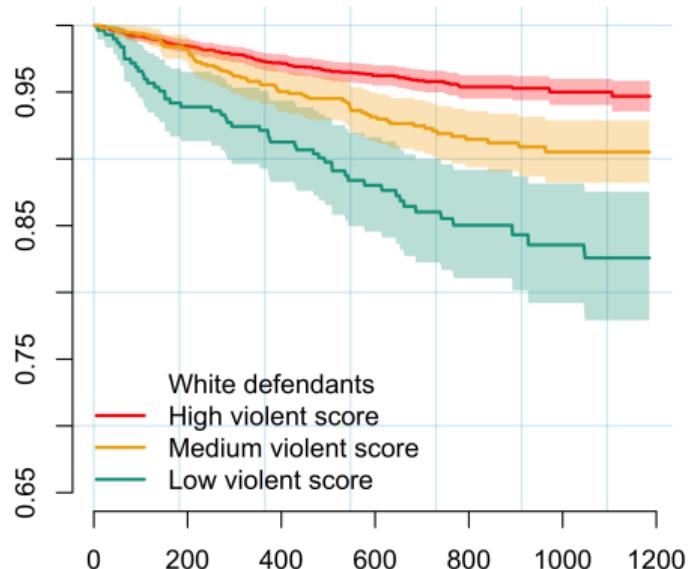
Look at score distributions, black and white defendant, Larson et al. (2016)

## Motivation (7. Propublica, Actuarial Justice)



Cox Proportional Hazards model, **black** and **white** defendant, Larson et al. (2016)

## Motivation (7. Propublica, Actuarial Justice)



Cox Proportional Hazards model, **black** and **white** defendant, Larson et al. (2016)

## Motivation (8. Intention)

En France, Loi n° 2008-496 du 27 mai 2008

### – Article 1 –

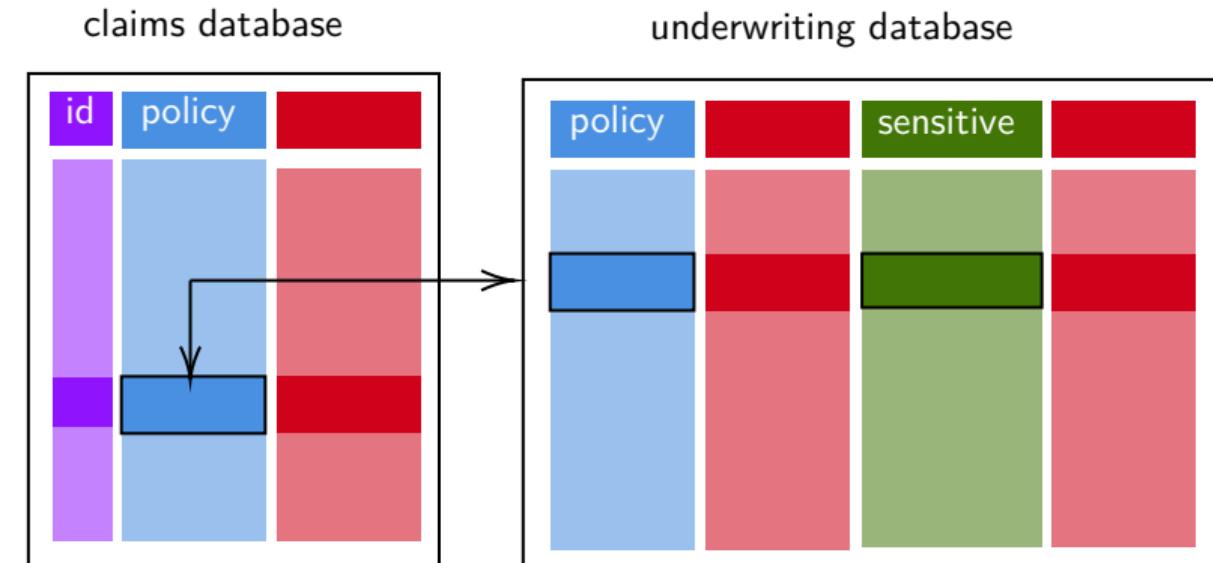
Constitue une **discrimination indirecte** une disposition, un critère ou une pratique neutre en apparence, mais susceptible d'entraîner, pour l'un des motifs mentionnés au premier alinéa, un désavantage particulier pour des personnes par rapport à d'autres personnes, à moins que cette disposition, ce critère ou cette pratique ne soit objectivement justifié par un but légitime et que les moyens pour réaliser ce but ne soient nécessaires et appropriés.

Extention de la "Loi n° 72-546 du 1 juillet 1972", qui supprima l'exigence de l'intention spécifique.

"*Technology is neither good nor bad; nor is it neutral*" , Kranzberg (1986)

## Motivation (9. Biases, biases everywhere...)

- underwriters biases
- commercial discounts
- inferred data
- multiple decisions
  
- claims biases
- fraud detection
- sexist mechanic
- ageist manager

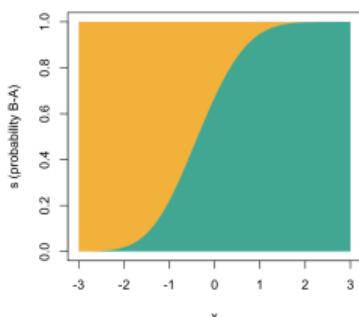
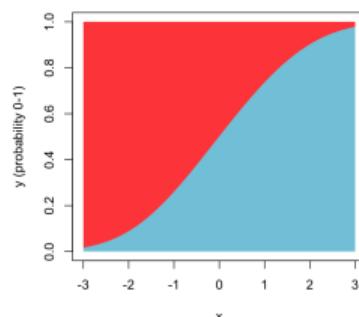
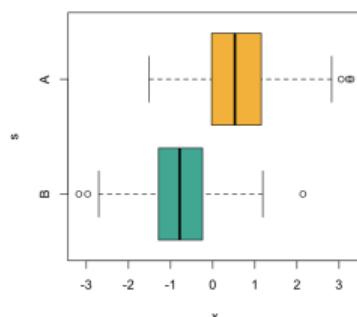
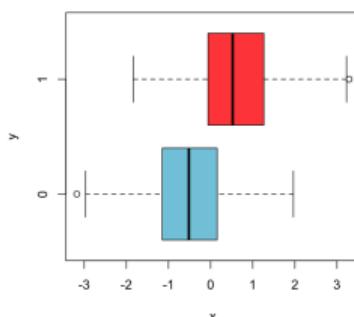


# Datasets

## ▶ toydata1

Consider a confounding Gaussian variable  $X_0$ ,  $X_0 \sim \mathcal{N}(0, 1)$ , and

$$\begin{cases} X = X_0 + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1/2^2), \\ S = \mathbf{1}(X_0 + \eta > 0), \quad \eta \sim \mathcal{N}(0, 1/2^2), \quad s \in \{\text{A, B}\}, \\ Y = \mathbf{1}(X_0 + \nu > 0), \quad \nu \sim \mathcal{N}(0, 1/2^2), \quad y \in \{0, 1\}. \end{cases}$$

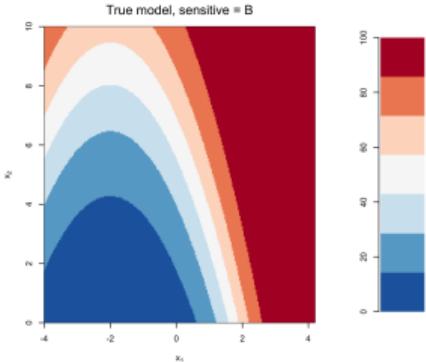
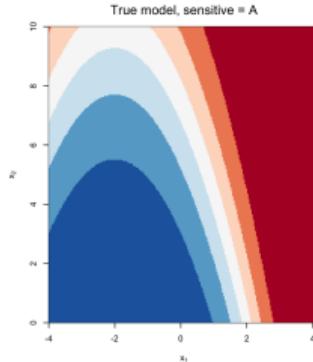
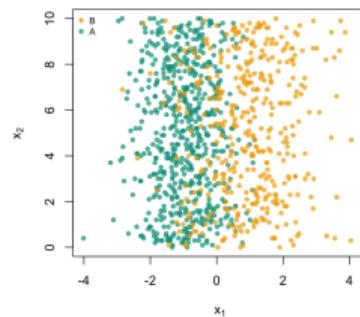
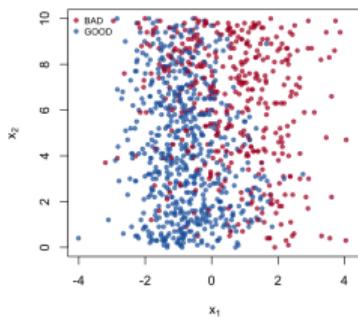


$x \mapsto \mathbb{P}[Y = 0 | X = x]$  (left-hand side) and  $x \mapsto \mathbb{P}[S = \text{A} | X = x]$  (right-hand side)

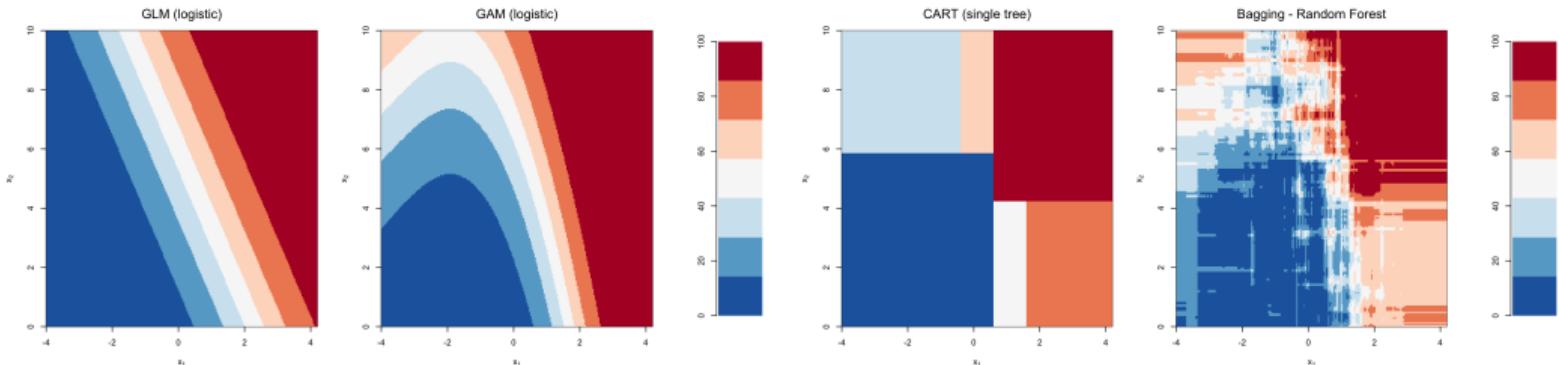
# Datasets

## ▶ toydata2

- ▶ binary sensitive attribute,  $s \in \{A, B\}$ , (60% and 40%)
- ▶  $(x_1, x_3) \sim \mathcal{N}(\mu_s, \Sigma_s)$ ,  $r_{s=A} = 0.4$  and  $r_{s=B} = 0.7$
- ▶  $x_2 \sim \mathcal{U}([0, 10])$ , independent of  $x_1$  and  $x_3$
- ▶  $\eta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 \mathbf{1}_B(s)$ , that does not depend on  $x_3$
- ▶  $y \sim \mathcal{B}(p)$  where  $p = \exp(\eta)/[1 + \exp(\eta)] = \mu(x_1, x_2, s)$ .

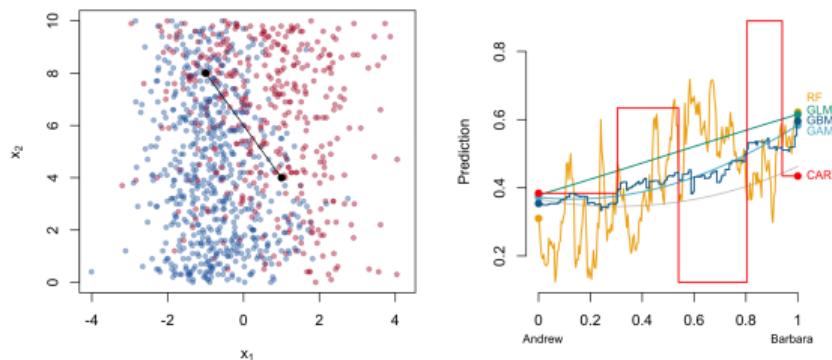


# Datasets



Five models are considered

- ▶ plain GLM (logistic)
- ▶ GAM (cubic splines)
- ▶ CART (classification tree)
- ▶ RF (random forest)
- ▶ GBM (gradient boosting)



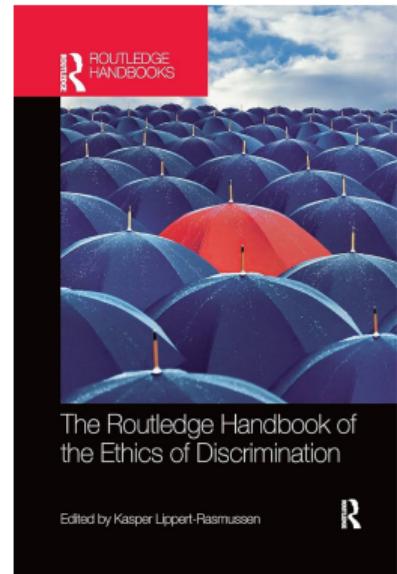
## Datasets

- **GermanCredit**,  $m = 1,000$ 
  - ▶ binary sensitive attribute,  $s \in \{A, B\}$ , (64% and 36%) corresponding to gender
  - ▶  $y$  denotes a default (30%)
  - ▶  $x_1, \dots, x_k$  denote legitimate credit variables (Duration, Purpose, Credit\_amount, Age, Housing, Existing\_credits, Foreign\_worker, Resident\_since, etc)
- **FrenchMotor** (policy observe over one year),  $n = 12,437$ 
  - ▶ binary sensitive attribute,  $s \in \{A, B\}$ , (31% and 69%) corresponding to gender
  - ▶  $y$  denotes the occurrence of a car accident (8.67%, unbalanced data)
  - ▶  $x_1, \dots, x_k$  denote legitimate credit variables (MariStat, VehAge, SocioCateg, DrivAge, VehBody, VehEnergy, VehMaxSpeed, Garage, VehUsage, etc)

– Part 1 –  
Insurance

# Discrimination and Insurance

*"What is unique about insurance is that even statistical discrimination which by definition is absent of any malicious intentions, poses significant moral and legal challenges. Why? Because on the one hand, policy makers would like insurers to treat their insureds equally, without discriminating based on race, gender, age, or other characteristics, even if it makes statistical sense to discriminate (...) On the other hand, at the core of insurance business lies discrimination between risky and non-risky insureds. But riskiness often statistically correlates with the same characteristics policy makers would like to prohibit insurers from taking into account."* Avraham (2017)



# Discrimination and Insurance

## Definition 2.2: Mutuality, Wilkie (1997)

**Mutuality** is considered as the normal form of commercial private insurance, where participants contribute to the risk pool through a premium that relates to their particular risk at the time of the application, i.e., the higher the risk that they bring to the pool, the higher the premium required.

## Definition 2.3: Solidarity, Wilkie (1997)

**Solidarity** is the basis of most national or social insurance schemes. Participation in such state-run schemes is generally compulsory and individuals have no discretion over their level of cover. All participants normally have the same level of cover. In solidarity schemes the contributions are not based on the expected risk of each participant.

# Insurance Pricing and Predictive Modeling

*“Humans think in stories rather than facts, numbers or equations - and the simpler the story, the better,” Harari (2018).* For insurers, it is often a mixture of both.

For Glenn (2000), insurer's risk selection process has two sides:

- › the one presented to regulators and policyholders (numbers, statistics and objectivity),
- › the other presented to underwriters (stories, character and subjective judgment).

The rhetoric of insurance exclusion – numbers, objectivity and statistics – forms what Brian Glenn calls “*the myth of the actuary*,” “*a powerful rhetorical situation in which decisions appear to be based on objectively determined criteria when they are also largely based on subjective ones*” or “*the subjective nature of a seemingly objective process*”.

Glenn (2003) claimed that there are many ways to rate accurately. Insurers can rate risks in many different ways depending on the stories they tell on which characteristics

# Insurance Pricing and Predictive Modeling

are important and which are not. “*The fact that the selection of risk factors is subjective and contingent upon narratives of risk and responsibility has in the past played a far larger role than whether or not someone with a wood stove is charged higher premiums.*” Going further, “*virtually every aspect of the insurance industry is predicated on stories first and then numbers.*”

“*all models are wrong but some models are useful,*” Box et al. (2011) (in other words, any model is at best a useful fable).

# Insurance Pricing and Predictive Modeling

## Definition 3.1: Pure premium (homogeneous risks)

Let  $Y$  be the non-negative random variable corresponding to the total annual loss associated with a given policy, then the **pure premium** is  $\mathbb{E}[Y]$ .

## Proposition 3.1: Law of Large Numbers (2)

Consider an infinite collection of i.i.d. random variables  $Y, Y_1, Y_2, \dots, Y_n, \dots$  in a probabilistic space  $(\Omega, \mathcal{F}, \mathbb{P})$ , with finite expected value, then

$$\underbrace{\frac{1}{n} \sum_{i=1}^n Y_i}_{(\text{empirical}) \text{ average}} \xrightarrow{\text{a.s.}} \underbrace{\mathbb{E}(Y)}_{\text{expected value}}, \text{ as } n \rightarrow \infty.$$

freakonometrics

[freakonometrics.hypotheses.org](https://freakonometrics.hypotheses.org)

– Arthur Charpentier, 2024 (UQAM Course)

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# Insurance Pricing and Predictive Modeling

More realistically, population is heterogeneous (with respect to risks), with some covariates  $\mathbf{x}$  (legitimate, or not).

## Definition 3.2: Pure premium (heterogeneous risks)

Let  $Y$  be the non-negative random variable corresponding to the total annual loss associated with a given policy, with covariates  $\mathbf{x}$ , then the **pure premium** is  $\mu(\mathbf{x}) = \mathbb{E}[Y | \mathbf{X} = \mathbf{x}]$ .

In this general setting,  $\mathbf{x}$  consist in numeric or categorical variables.

# Insurance Pricing and Predictive Modeling

## Proposition 3.2: Law of Large Numbers (2')

Consider an infinite collection of i.i.d. random pairs  $(\mathbf{X}, Y)$ ,  $(\mathbf{X}_1, Y_1)$ ,  $(\mathbf{X}_2, Y_2), \dots, (\mathbf{X}_n, Y_n), \dots$  in a probabilistic space  $(\Omega, \mathcal{F}, \mathbb{P})$ , with finite expected value, then for any  $\mathcal{A} \subset \mathcal{X}$  such that  $\mathbb{P}[\mathbf{X} \in \mathcal{A}] > 0$ ,

$$\frac{\sum_{i=1}^n Y_i \mathbf{1}(\mathbf{X}_i \in \mathcal{A})}{\sum_{i=1}^n \mathbf{1}(\mathbf{X}_i \in \mathcal{A})} = \underbrace{\frac{1}{n_{\mathcal{A}}} \sum_{i \in \mathcal{I}_n(\mathcal{A})} Y_i}_{\text{conditional average}} \xrightarrow{\text{a.s.}} \underbrace{\mathbb{E}(Y | \mathbf{X} \in \mathcal{A})}_{\text{conditional expected value}}, \text{ as } n \rightarrow \infty,$$

where  $\mathcal{I}_n(\mathcal{A}) = \{i : \mathbf{X}_i \in \mathcal{A}\} \subset \{1, 2, \dots, n\}$  and  $n_{\mathcal{A}} = \text{Card}(\mathcal{I}_n(\mathcal{A}))$ .

# Insurance Pricing and Predictive Modeling

- Excerpt from the Men and Women life tables in 1720 (source: [Struyck \(1912\)](#)). Mortality, as a function of the **age** and the **gender** of the individual.



Table des Hommes.

Années	Per- sonnes								
5	710	20	607	35	474	50	313	65	142
6	697	21	599	36	464	51	301	66	132
7	688	22	591	37	454	52	289	67	123
8	681	23	583	38	444	53	277	68	114
9	675	24	575	39	434	54	265	69	105
10	670	25	567	40	424	55	253	70	97
11	665	26	558	41	414	56	241	71	89
12	660	27	549	42	404	57	229	72	82
13	654	28	540	43	393	58	217	73	75
14	648	29	531	44	382	59	206	74	68
15	642	30	522	45	371	60	195	75	61
16	635	31	513	46	360	61	184	76	54
17	628	32	504	47	349	62	173	77	48
18	621	33	494	48	337	63	162	78	43
19	614	34	484	49	325	64	152	79	38

Table des femmes.

Années	Per- sonnes								
5	711	20	624	35	508	50	373	65	205
6	700	21	617	36	500	51	362	66	194
7	692	22	610	37	492	52	351	67	183
8	685	23	603	38	484	53	340	68	172
9	679	24	590	39	476	54	329	69	161
10	674	25	588	40	468	55	318	70	150
11	669	26	580	41	459	56	306	71	140
12	664	27	572	42	450	57	294	72	130
13	660	28	564	43	441	58	282	73	120
14	650	29	556	44	432	59	271	74	110
15	652	30	548	45	423	60	260	75	100
16	647	31	540	46	414	61	249	76	90
17	642	32	532	47	404	62	238	77	81
18	636	33	524	48	394	63	227	78	72
19	630	34	516	49	384	64	216	79	63

# Insurance Pricing and Predictive Modeling

- Excerpt from the Men and Women life tables in 1720 (source: [Struyck \(1912\)](#))  
Mortality, as a function of the **age** and the **gender** of the individual.

men		
$x$	$L_x$	$5P_x$
0	1000	29.0%
5	710	5.6%
10	670	4.2%
15	642	5.5%
20	607	6.6%
25	567	7.9%
30	522	9.2%
35	474	10.5%
40	424	12.5%
45	371	16.6%
50	313	19.2%
55	253	22.9%
60	195	27.2%
65	142	31.7%
70	97	37.1%
75	61	45.9%
80	33	51.5%
85	16	

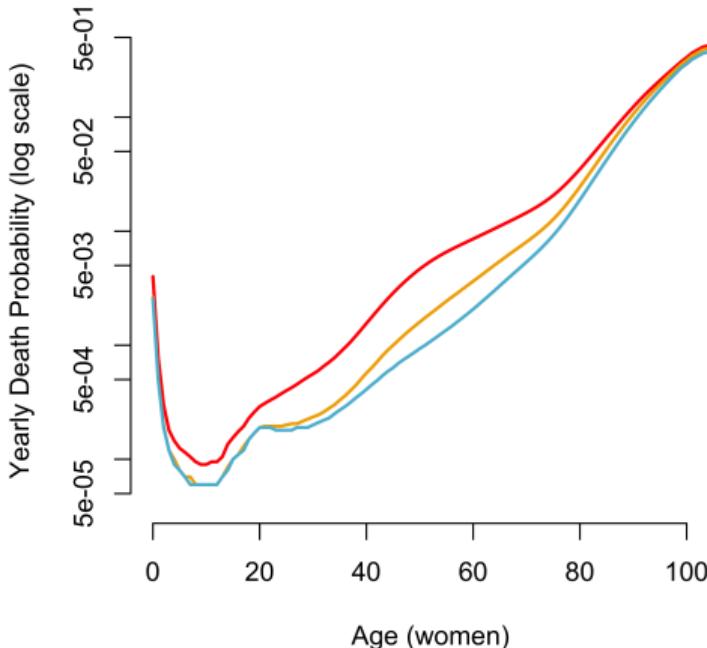
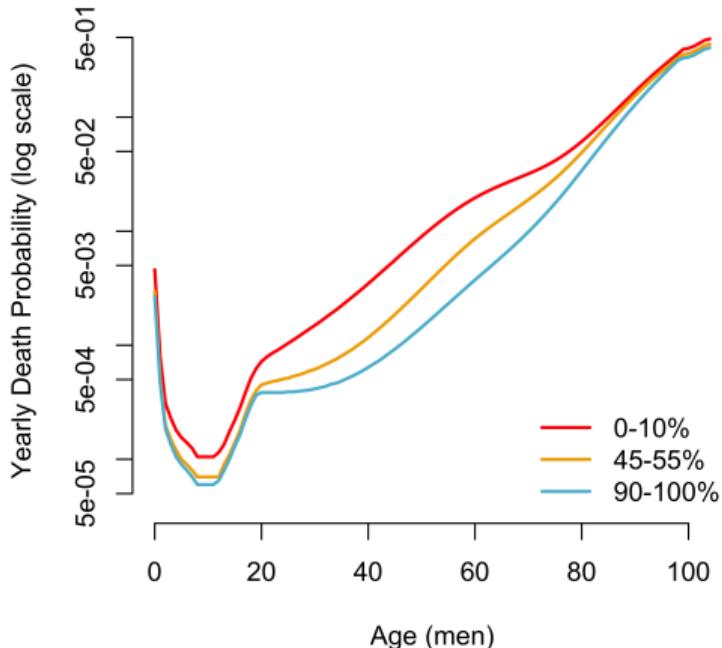
women		
$x$	$L_x$	$5P_x$
0	1000	28.9%
5	711	5.2%
10	674	3.3%
15	652	4.3%
20	624	5.8%
25	588	6.8%
30	548	7.3%
35	508	7.9%
40	468	9.6%
45	423	11.8%
50	373	14.7%
55	318	18.2%
60	260	21.2%
65	205	26.8%
70	150	33.3%
75	100	45.0%
80	55	56.4%
85	24	

# Insurance Pricing and Predictive Modeling

- Excerpt from the Men and Women life tables in 2016 (source: [Blanpain \(2018\)](#))  
Mortality, as a function of the **age**, the **gender** and the **wealth** of the individual.

men				women			
x	0-5%	45-50%	95-100%	x	0-5%	45-50%	95-100%
0	100000	100000	100000	0	100000	100000	100000
10	99299	99566	99619	10	99385	99608	99623
20	99024	99396	99469	20	99227	99506	99526
30	97930	98878	99094	30	98814	99302	99340
40	95595	98058	98627	40	97893	98960	99074
50	90031	96172	97757	50	95021	97959	98472
60	77943	91050	95649	60	88786	95543	97192
70	59824	79805	90399	70	79037	90408	94146
80	38548	59103	76115	80	63224	79117	85825
90	13337	23526	38837	90	31190	45750	55918
100	530	1308	3231	100	2935	5433	8717

# Insurance Pricing and Predictive Modeling



Force of mortality (log scale) for various income quantile, in France, [Blanpain \(2018\)](#).

# Insurance Pricing and Predictive Modeling

U.S. DECENTNIAL LIFE TABLES FOR 1969-71

Volume I, Number 1



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TABLE 10. LIFE TABLE FOR THE NEGRO POPULATION: UNITED STATES, 1969-71

AGE INTERVAL PERIOD OF LIFE BETWEEN TWO AGES	PROPORTION DYING	OF 100,000 BORN ALIVE		STATIONARY POPULATION		AVERAGE REMAINING LIFETIME
		NUMBER LIVING AT BEGINNING OF AGE INTERVAL	NUMBER DYING DURING AGE INTERVAL	IN THE AGE INTERVAL	IN FIVES AND ALL SUBSEQUENT AGE INTERVALS	
					AVERAGE NUMBER OF YEARS OF LIFE REMAINING AT BEGINNING OF AGE INTERVAL	
(1)	(2)	(3)	(4)	(5)	(6)	(7)
$x$ to $x + t$	$t_x$	$I_x$	$t'_x$	$t_x^L$	$T_x$	$\bar{x}$
DAYS						
0-1.....	.001348	100,000	1,348	272	6,411,264	64.11
1-7.....	.00648	95,652	659	1,616	6,410,992	64.59
7-14.....	.00243	95,093	243	5,021	6,410,748	64.51
28-365.....	.01037	97,744	1,013	89,778	6,403,745	65.52

Mortality, gender and “race”

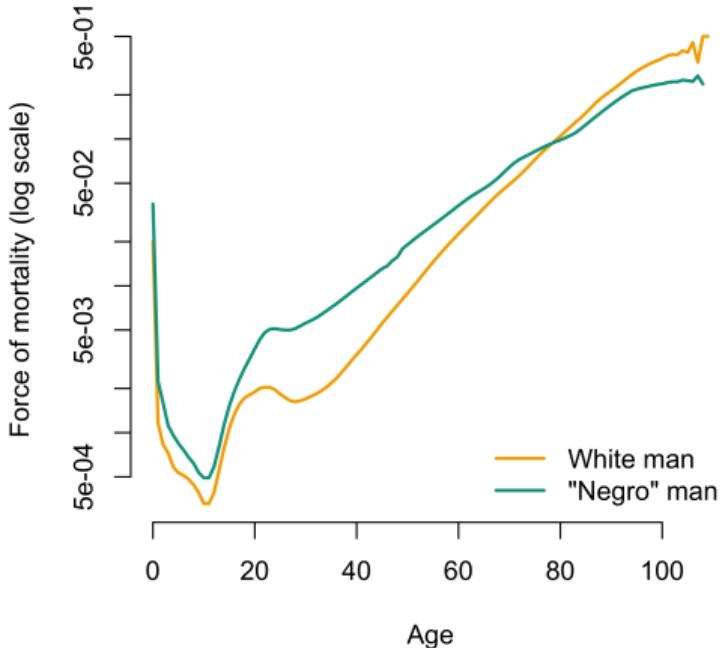
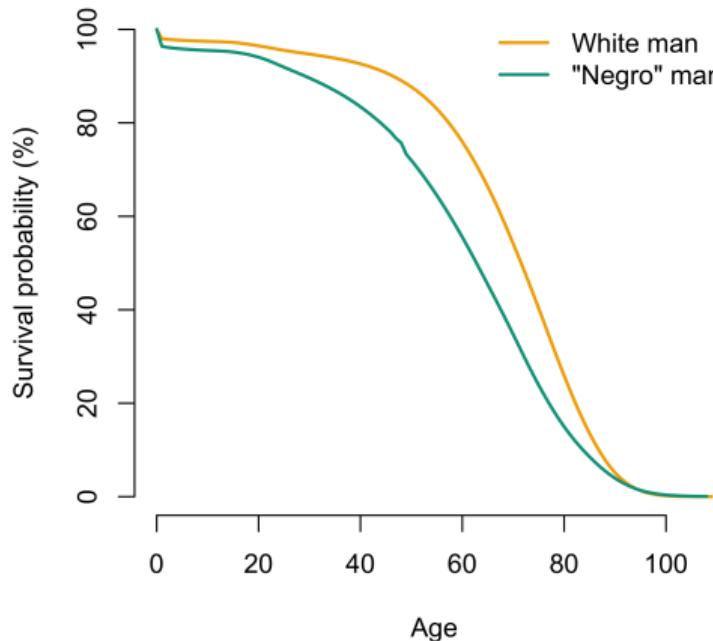


Frederick L. Hoffman  
Hoffman (1896, 1918, 1931)

# Insurance Pricing and Predictive Modeling

White, men			“Negro”, men		
x	$L_x$	$5p_x$	x	$L_x$	$5p_x$
0	100000	2.3%	55	83001	8.5%
5	97671	0.2%	60	75969	12.7%
10	97441	0.2%	65	66343	18.4%
15	97208	0.7%	70	54138	25.5%
20	96480	1.0%	75	40324	35.8%
25	95524	0.8%	80	25885	47.7%
30	94716	0.9%	85	13527	62.1%
35	93843	1.3%	90	5125	75.1%
40	92631	2.1%	95	1274	85.2%
45	90725	3.3%	100	189	90.5%
50	87690	5.3%	105	18	100.0%

# Insurance Pricing and Predictive Modeling



Force of mortality (log scale) white men and "Negro" men, 1968-71, U.S.

# Insurance Pricing and Predictive Modeling

## Definition 3.3: Balance Property

A pricing function  $m$  satisfies the **balance property** if  $\mathbb{E}_{\mathbf{X}}[m(\mathbf{X})] = \mathbb{E}_Y[Y]$ .

## Proposition 3.3: Law of total expectations

$$\mathbb{E}_Y[Y] = \mathbb{E}_{\mathbf{X}}[\mathbb{E}_{Y|\mathbf{X}}[Y|\mathbf{X}]] = \mathbb{E}_{\mathbf{X}}[\mu(\mathbf{X})].$$

**Proof** Since  $\mathbb{E}(Y) = \int yf_y(y)dy$  and  $\mathbb{E}(Y|\mathbf{X} = \mathbf{x}) = \int yf_{y|\mathbf{x}}(y|\mathbf{x})dy$ ,

$$\begin{aligned}\mathbb{E}(\mathbb{E}(X|Y)) &= \int \left( \int x \mathbb{P}[X = x | Y = y] dx \right) \mathbb{P}[Y = y] dy = \int \int x \mathbb{P}[X = x, Y = y] dx dy \\ &= \int x \left( \int \mathbb{P}[X = x, Y = y] dy \right) dx = \int x \mathbb{P}[X = x] dx = \mathbb{E}(X).\end{aligned}$$

# Insurance Pricing and Predictive Modeling

Homogeneous risk sharing

	Policyholder	Insurer
Loss	$\mathbb{E}[Y]$	$Y - \mathbb{E}[Y]$
Average loss	$\mathbb{E}[Y]$	0
Variance	0	$\text{Var}[Y]$

$\mathbb{E}[Y]$  is the premium paid, and  $Y$  the total loss,  
from De Wit and Van Eeghen (1984) and Denuit and Charpentier (2004)

# Insurance Pricing and Predictive Modeling

Heterogeneous risk sharing, with perfect information

	Policyholder	Insurer
Loss	$\mathbb{E}[Y \Theta]$	$Y - \mathbb{E}[Y \Theta]$
Average loss	$\mathbb{E}[Y]$	0
Variance	$\text{Var}[\mathbb{E}[Y \Theta]]$	$\text{Var}[Y - \mathbb{E}[Y \Theta]]$

where  $\Theta$  denotes the heterogeneous risk factor.

The term on the bottom right is  $\mathbb{E}[\text{Var}[Y|\Theta]]$ , corresponding to the standard **variance decomposition** (or Pythagoras theorem)

$$\text{Var}[Y] = \text{Var}[\mathbb{E}[Y|\Theta]] + \mathbb{E}[\text{Var}[Y|\Theta]].$$

to go further → (for more details on Lebesgue spaces, and  $L^2$ )



## Proposition 3.4: Variance decomposition (1)

For any measurable random variable  $Y$  with finite variance

$$\text{Var}[Y] = \underbrace{\mathbb{E}[\text{Var}[Y|\Theta]]}_{\rightarrow \text{insurer}} + \underbrace{\text{Var}[\mathbb{E}[Y|\Theta]]}_{\rightarrow \text{policyholder}}.$$

**Proof:**

$$\begin{aligned}\text{Var}[Y] &= \mathbb{E}[Y^2] - \mathbb{E}[Y]^2 = \mathbb{E}[\text{Var}[Y|\Theta] + \mathbb{E}[Y|\Theta]^2] - \mathbb{E}[\mathbb{E}[Y|\Theta]]^2 \\ &= (\mathbb{E}[\text{Var}[Y|\Theta]]) + (\mathbb{E}[\mathbb{E}[Y|\Theta]^2] - \mathbb{E}[\mathbb{E}[Y|\Theta]]^2) = \mathbb{E}[\text{Var}[Y|\Theta]] + \text{Var}[\mathbb{E}[Y|\Theta]].\end{aligned}$$

# Insurance Pricing and Predictive Modeling

Heterogeneous risk sharing, with imperfect information

	Policyholder	Insurer
Loss	$\mathbb{E}[Y \mathbf{X}]$	$Y - \mathbb{E}[Y \mathbf{X}]$
Average loss	$\mathbb{E}[Y]$	0
Variance	$\text{Var}[\mathbb{E}[Y \mathbf{X}]]$	$\mathbb{E}[\text{Var}[Y \mathbf{X}]]$

$$\mathbb{E}[\text{Var}[Y|\mathbf{X}]] = \underbrace{\mathbb{E}[\text{Var}[Y|\Theta]]}_{\text{perfect ratemaking}} + \underbrace{\mathbb{E}\{\text{Var}[\mathbb{E}[Y|\Theta]|\mathbf{X}]\}}_{\text{misclassification}}$$

This “misclassification” term (on the right) is called “*subsidierende solidariteit*” in De Pril and Dhaene (1996), or “*subsidiary solidarity*”, as opposed to “*kanssolidariteit*” or “*random solidarity*” term (on the left).

# Insurance Pricing and Predictive Modeling

## Proposition 3.5: Variance decomposition (2)

For any measurable random variable  $Y$  with finite variance

$$\text{Var}[Y] = \underbrace{\mathbb{E}[\text{Var}[Y|\mathbf{X}]]}_{\rightarrow \text{insurer}} + \underbrace{\text{Var}[\mathbb{E}[Y|\mathbf{X}]]}_{\rightarrow \text{policyholder}},$$

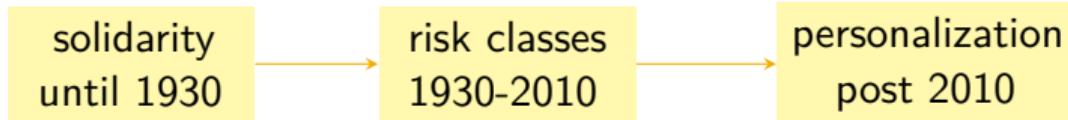
where

$$\begin{aligned}\mathbb{E}[\text{Var}[Y|\mathbf{X}]] &= \mathbb{E}[\mathbb{E}[\text{Var}[Y|\Theta]|\mathbf{X}]] + \mathbb{E}[\text{Var}[\mathbb{E}[Y|\Theta]|\mathbf{X}]] \\ &= \underbrace{\mathbb{E}[\text{Var}[Y|\Theta]]}_{\text{perfect ratemaking}} + \underbrace{\mathbb{E}\{\text{Var}[\mathbb{E}[Y|\Theta]|\mathbf{X}]\}}_{\text{misclassification}}.\end{aligned}$$

## Clubs, Group and Categories

- Groups, or risk classes, are built on the basis of available data, and exist primarily as the product of actuarial models.
- For example, as mentioned in [Bailey and Simon \(1959\)](#), in motor insurance five risk classes can be considered, with rate surcharges relative to the first class (used here as a reference)
  - ▶ “*pleasure, no male operator under 25,*” (reference),
  - ▶ “*pleasure, non-principal male operator under 25,*” +65%,
  - ▶ “*business use,*” +65%,
  - ▶ “*married owner or principal operator under 25,*” +65%,
  - ▶ “*unmarried owner or principal operator under 25,*” +140%.
- There is no “physical basis” for group members to identify other members of *their* group, in the sense that they usually don’t share anything, except some common characteristics, [Gandy \(2016\)](#).

# Clubs, Group and Categories



- In ancient Rome, a *collegium* (plural *collegia*) was an association, such as military *collegia*, [Verboven \(2011\)](#).
- As explained in [Ginsburg \(1940\)](#), upon the completion of his service a veteran had the right to join one of the many *collegia veteranorum* in each legion.
- In case of retirement, upon the completion of his term of service, the soldier would receive a lump sum which helped him somewhat to arrange the rest of his life. The membership in a *collegium* gave him a mutual insurance against “*unforeseen risks*.” These *collegia*, besides being cooperative insurance companies, had other functions.



# Clubs, Group and Categories

- › In the early 1660th, the [Pirate's Code](#) was supposedly written by Portuguese buccaneer Bartolomeu Português.
- › A section is explicitly dedicated to insurance and benefits: “*a standard compensation is provided for maimed and mutilated buccaneers. Thus they order for the loss of a right arm six hundred pieces of eight, or six slaves; for the loss of a left arm five hundred pieces of eight, or five slaves; for a right leg five hundred pieces of eight, or five slaves; for the left leg four hundred pieces of eight, or four slaves; for an eye one hundred pieces of eight, or one slave; for a finger of the hand the same reward as for the eye,*” see [Barbour \(1911\)](#) (or more recently [Leeson \(2009\)](#) and [Fox \(2013\)](#) about this piratical schemes).



## Clubs, Group and Categories

- In the XIX-th century, in Europe, mutual aid societies involved a group of individuals who made regular payments into a common fund in order to provide for themselves in later, unforeseeable moments of financial hardship or of old age. As mentioned by [Garrioch \(2011\)](#), in 1848, there were in Paris 280 mutual aidsocieties with well over 20,000 members.
- For example, the *Société des Arts Graphiques*, was created in 1808. It admitted only men over twenty and under fifty, and it charged much higher admission and annual fees for those who joined at a more advanced age. In return, they received benefits if they were unable to work, reducing over a period of time, but in case of serious illness the Society would pay the admission fee for a hospice. In England, there were “friendly societies,” as described in [Ismay \(2018\)](#).



## Clubs, Group and Categories

- The money collected through contributions came to the rescue of unfortunate workers, who would no longer have any reason to radicalize. It was proposed that insurance should become compulsory (Bismark proposed this in Germany in 1883), but the idea was rejected in favor of giving workers the freedom to contribute, as the only way to moralize the working classes, as [Da Silva \(2023\)](#) explains.
- In 1852, of the 236 mutual funds created, 21 were on a professional basis, while the other 215 were on a territorial basis. And from 1870 onwards, mutual funds diversified the professional profile of contributors beyond blue-collar workers, and expanded to include employees, civil servants, the self-employed and artists.
- The amount of the premium is not linked to the risk.



## Clubs, Group and Categories

- › As Da Silva (2023) puts it, “*mutual insurers see in the actuarial figure the programmed end of solidarity.*” For mutual funds, solidarity is essential, with everyone contributing according to their means and receiving according to their needs. Around the same time, in France, the first insurance companies appeared, based on risk selection, and the first mathematical approaches to calculating premiums.
- › Hubbard (1852) advocates the introduction of an “*English-style scientific organization*” in their management. For its members, they had to be able to know “*the probable average of the claims*” that they should cover, like insurance companies. The development of tables should lead insurers to adopt the principle of contributions varying according to the age of entry and the specialization of contributions and funds (health/retirement).
- › For Stone (1993) and Gowri (2014) the defining feature of “modern insurance” is its reliance on **segmenting the risk pool into distinct categories**, each receiving a price

## Clubs, Group and Categories

corresponding to the particular risk that the individuals assigned to that category are expected to represent (as accurately as can be estimated by actuaries).

- Once heterogeneity with respect to the risk was observed in portfolios, insurers have operated by categorizing individuals into **risk classes** and assigning corresponding tariffs. This ongoing process of categorization ensures that the sums collected, on average, are sufficient to address the realized risks within specific groups.
- The aim of **risk classification**, as explained in **Wortham (1986)**, is to identify the specific characteristics that are supposed to determine an individual's propensity to suffer an adverse event, forming groups within which the risk is (approximately) equally shared. The problem, of course, is that the characteristics associated with various types of risk are almost infinite; as they cannot all be identified and priced in every risk classification system, there will necessarily be unpriced sources of heterogeneity between individuals in a given risk class.

## Clubs, Group and Categories

- In 1915, as mentioned in [Rothstein \(2003\)](#), the president of the Association of Life Insurance Medical Directors of America noted that the question asked almost universally of the Medical Examiner was “*What is your opinion of the risk? Good, bad, first-class, second-class, or not acceptable?*” Historically, insurance prices were a (finite) collection of prices (maybe more than than the two classes mentioned, “first-class” and “second-class”).
- In the early 1920's, Albert Henry Mowbray, who worked for New York Life Insurance Company and later Liberty Mutual (and was also an actuary for state-level insurance commissions in New Carolina and California, and the National Council on Workmen's Insurance) gives his perspective on insurance rate making. See [Mowbray \(1921\)](#).



## Clubs, Group and Categories

*"Classification of risks in some manner forms the basis of rate making in practically all branches of insurance. It would appear therefore that there should be some fundamental principle to which a correct system of classification in any branch of insurance should conform (...) As long ago as the days of ancient Greece and Rome the gradual transition of natural phenomena was observed and set down in the Latin maxim, 'natura non agit per altum'. If each risk, therefore is to be precisely rated, it would be necessary to recognize very minute differences and precisely measure them. (...) Since we are not capable of covering a large field fully and at the same time recognizing small differences in all parts of the field, it is natural that we resort to subdivision of the field by means of classification, thereby concentrating our attention on a smaller interval which may again be subdivided by further classification, and the system so carried on to the limit to which we find it necessary or desirable to go. But however far we may go in any system of classification, whether in the field of pure or applied science including the business or insurance, we shall always find difficulties presented by the borderline case, difficulties which arise from the continuous character*

## Clubs, Group and Categories

*of natural phenomena which we are attempting to place in more or less arbitrary divisions. While thus acknowledging that classification will never completely solve the problem of recognizing differences between individuals, nevertheless classification seems to be necessary at least as a preliminary step toward such recognition in any field of study. The fact that a complete and final solution cannot be made is, therefore, no justification for completely discarding classification as a method of approach. Since it is insurance hazards that we undertake to measure and classify, the preliminary step in studying classification theory may well be to ask what is an insurance hazard and how it may be determined. It must be evident to the members of this Society that an insurance hazard is what is termed "a mathematical expectation," that is a product of a sum at risk and the probability of loss from the conditions insured against, e.g., the destruction of a piece of property by fire, the death of an individual, etc. If the net premiums collected are so determined on the basis of the true natural probability and there is a sufficient spread then the sums collected will just cover the losses and this is what should be," Mowbray (1921).*

## Clubs, Group and Categories

- “1. *The classification should bring together risks which have inherent in their operation the same causes of loss.*
2. *The variation from risk to risk in the strength of each cause or at least of the more important should not be greater than can be handled by the formula by which the classification is subdivided, i.e., the Schedule and / or Experience Rating Plan used.*
3. *The classification should not cover risks which include, as important elements of their hazard, causes which are not common to all.*
4. *The classification system and the formula for its extension (Schedule and / or Experience Rating Plans) should be harmonious.*
5. *The basis throughout should be the outward, recognizable indicia of the presence and potency of the several inherent causes of loss including extent as well as occurrence of loss,” Mowbray (1921).*

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## Clubs, Group and Categories

- Several articles and textbooks in sociology tried to understand how classification mechanisms establish symbolic boundaries that reinforce group identities, such as [Bourdieu \(2018\)](#), [Massey \(2007\)](#), [Fourcade and Healy \(2013\)](#).
- But here, those “groups” or “classes” do not share any identity, and [Simon \(1988\)](#) or [Harcourt \(2015\)](#) use the term “[actuarial classification](#)” (where “actuarial” designates any decision-making technique that relies on predictive statistical methods, replacing more holistic or subjective forms of judgment). In those class-based systems, based on insurance rating table (or grid), results are determined by assigning individuals to a group in which each person is positioned as “average” or “typical”.
- [Most] “*actuaries cannot think of individuals except as members of groups*” claimed [Brilmayer et al. \(1979\)](#). Each individual is assigned the same value as all other members of the group to which it is assigned.



## Clubs, Group and Categories

- Simon (1987, 1988), and then Feeley and Simon (1992), defined “actuarialism,” that designate the use of statistics to guide “*class-based decision-making*,” used to price pensions and insurance. As explained in Harcourt (2015), this “actuarial classification” is the constitution of groups with no experienced social significance for the participants. A person classified as a particular risk by an insurance company shares nothing with the other people so classified, apart from a series of formal characteristics (e.g. age, sex, marital status, etc.).
- For Austin (1983) and Simon (1988), categories used by the insurance company when grouping risks are “*singularly sterile*,” resulting in inert, immobile and deactivated communities, corresponding to “*artificial*” groups. These are not groups organized around a shared history, common experiences or active commitment, forming some “*aggregates*” – living only in the imagination of the actuary who calculates and tabulates, not in any lived form of human association.



## Clubs, Group and Categories

- If Hacking (1990) observed that standard classes creates coherent group identities (causing possible stereotypes and discrimination, Simon (1988), provocatively suggests that actuarial classifications can in turn “*undo people's identity*.”)
- As mentioned in Abraham (1986), the goal for actuaries is to create groups, or “*classes*” made up of individuals who share a series of common characteristics and are therefore presumed to represent the same risk. Following François (2022), we could claim that actuarial techniques reduce individuals to a series of formal roles that have no “*moral density*” and therefore do not grant an “*identity*” that organizes a coherent sense of self. And the inclusion of nominally “*demoralized categories*,” such as gender, in class-based rating systems makes their total demoralization difficult to achieve – and is in itself an issue of struggle. Heimer (1985) used the term “*community of fate*.”
- Rovroy et al. (2013) and Cheney-Lippold (2017) point out that scoring technologies are continually swapping predictors, “*shuffling the cards*,” so that there is no stable basis for constructing group memberships, or a coherent sense.

## Clubs, Group and Categories

*"The price which a person pays for automobile insurance depends on age, sex, marital status, place of residence and other factors. This risk classification system produces widely differing prices for the same coverage for different people. Questions have been raised about the fairness of this system, and especially about its reliability as a predictor of risk for a particular individual. While we have not tried to judge the propriety of these groupings, and the resulting price differences, we believe that the questions about them warrant careful consideration by the State insurance departments. In most States the authority to examine classification plans is based on the requirement that insurance rates are neither inadequate, excessive, nor unfairly discriminatory. The only criterion for approving classifications in most States is that the classifications be statistically justified – that is, that they reasonably reflect loss experience. Relative rates with respect to age, sex, and marital status are based on the analysis of national data. A youthful male driver, for example, is charged twice as much as an older driver all over the country (...) It has also been claimed that insurance companies engage in redlining – the arbitrary denial of insurance to everyone*

## Clubs, Group and Categories

*living in a particular neighborhood. Community groups and others have complained that State regulators have not been diligent in preventing redlining and other forms of improper discrimination that make insurance unavailable in certain areas. In addition to outright refusals to insure, geographic discrimination can include such practices as: selective placement of agents to reduce business in some areas, terminating agents and not renewing their book of business, pricing insurance at un-affordable levels, and instructing agents to avoid certain areas. We reviewed what the State insurance departments were doing in response to these problem. To determine if redlining exists, it is necessary to collect data on a geographic oasis. Such data should include current insurance policies, new policies being written, cancellations, and non-renewals. It is also important to examine data on losses by neighborhoods within existing rating territories because marked discrepancies within territories would cast doubt on the validity of territorial boundaries. Yet, not even a fifth of the States collect anything other than loss data, and that data is gathered on a territory-wide basis," Havens (1979)*

## Clubs, Group and Categories

*“On the other hand, the opinion that distinctions based on sex, or any other group variable, necessarily violate individual rights reflects ignorance of the basic rules of logical inference in that it would arbitrarily forbid the use of relevant information. It would be equally fallacious to reject a classification system based on socially acceptable variables because the results appear discriminatory. For example, a classification system may be built on use of car, mileage, merit rating, and other variables, excluding sex. However, when verifying the average rates according to sex one may discover significant differences between males and females. Refusing to allow such differences would be attempting to distort reality by choosing to be selectively blind. The use of rating territories is a case in point. Geographical divisions, however designed, are often correlated with socio-demographic factors such as income level and race because of natural aggregation or forced segregation according to these factors. Again we conclude that insurance companies should be free to delineate territories and assess territorial differences as well as they can. At the same time, insurance companies should recognize that it is in their best interest to be objective and use clearly relevant*

## Clubs, Group and Categories

*factors to define territories lest they be accused of invidious discrimination by the public. (...) " Casey et al. (1976)*

*"One possible standard does exist for exception to the counsel that particular rating variables should not be proscribed. What we have called 'equal treatment' standard of fairness may precipitate a societal decision that the process of differentiating among individuals on the basis of certain variables is discriminatory and intolerable. This type of decision should be made on a specific, statutory basis. Once taken, it must be adhered to in private and public transactions alike and enforced by the insurance regulator. This is, in effect, a standard for conduct that by design transcends and preempts economic considerations. Because it is not applied without economic cost, however, insurance regulators and the industry should participate in and inform legislative deliberations that would ban the, use of particular rating variables as discriminatory." Casey et al. (1976)*

## Price Optimization

- › Decision theory under uncertainty (see [Charpentier \(2014\)](#)),

$$X \preceq Y \iff \mathcal{R}(X) \leq \mathcal{R}(Y),$$

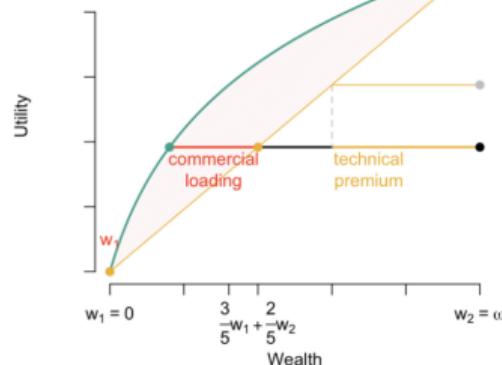
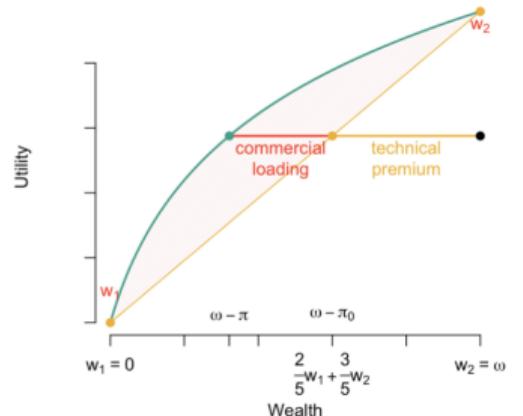
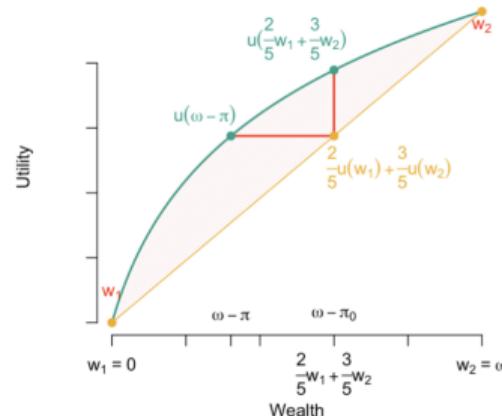
- › A classical representation is  $\mathcal{R}(Y) = \mathbb{E}[u(\omega - Y)]$ , as in [Neumann and Morgenstern \(1947\)](#), where  $\omega$  is the initial wealth.
- ›  $u$  denotes the utility of the agent
- › Let  $\pi$  denote the premium asked to transfer risk (loss)  $Y$ ,

$$\begin{cases} u(\omega - \pi) > \mathbb{E}[u(\omega - Y)] : & \text{purchases insurance} \\ u(\omega - \pi) < \mathbb{E}[u(\omega - Y)] : & \text{does not purchase insurance} \end{cases}$$

# Price Optimization

## Definition 3.4: Indifference utility principle

Let  $Y$  be the non-negative random variable corresponding to the total annual loss associated with a given policy, for a policyholder with utility  $u$  and wealth  $w$ , the **indifference premium** is  $\pi = \omega - u^{-1}(\mathbb{E}[u(\omega - Y)])$ .



– Part 2 –

# Machine Learning

## Proposition 4.1: Law of Large Numbers (1)

Consider an infinite collection of i.i.d. random variables  $Y, Y_1, Y_2, \dots, Y_n, \dots$  in a probabilistic space  $(\Omega, \mathcal{F}, \mathbb{P})$ , then

$$\underbrace{\frac{1}{n} \sum_{i=1}^n \mathbf{1}(Y_i \in \mathcal{A})}_{\text{(empirical) frequency}} \xrightarrow{\text{a.s.}} \underbrace{\mathbb{P}(\{Y \in \mathcal{A}\})}_{\text{probability}} = \mathbb{P}[Y \in \mathcal{A}], \text{ as } n \rightarrow \infty.$$

“*law of the unconscious statistician*” (Ross (2014) and Casella and Berger (1990)),  
“*statisticians make liberal use of conditioning arguments to shorten what would otherwise be long proofs,*” Proschan and Presnell (1998)

$$\mathbb{P}(Y \in \mathcal{A}|X = x) = \lim_{\epsilon \rightarrow 0} \frac{\mathbb{P}(\{Y \in \mathcal{A}\} \cap \{|X - x| \leq \epsilon\})}{\mathbb{P}(\{|X - x| \leq \epsilon\})} = \lim_{\epsilon \rightarrow 0} \mathbb{P}(Y \in \mathcal{A}| |X - x| \leq \epsilon).$$

# Statistical Learning

This frequentist approach is unable to make sense of the probability of a "single singular event", as noted by [von Mises \(1928, 1939\)](#).

*"When we speak of the 'probability of death', the exact meaning of this expression can be defined in the following way only. We must not think of an individual, but of a certain class as a whole, e.g., 'all insured men forty-one years old living in a given country and not engaged in certain dangerous occupations'. A probability of death is attached to the class of men or to another class that can be defined in a similar way. We can say nothing about the probability of death of an individual even if we know his condition of life and health in detail. The phrase 'probability of death', when it refers to a single person, has no meaning for us at all."*



## Definition 4.1: Loss $\ell$

A **loss function**  $\ell$  is a function defined on  $\mathcal{Y} \times \mathcal{Y}$  such that  $\ell(y, y') \geq 0$  and  $\ell(y, y) = 0$ .

## Definition 4.2: Risk $\mathcal{R}$

For a fitted model  $\hat{m}$ , its **risk** is

$$\mathcal{R}(\hat{m}) = \mathbb{E}_{\mathbb{P}}[\ell(Y, \hat{m}(\mathbf{X}))] = \int \ell(y, \hat{m}(\mathbf{x})) d\mathbb{P}(y, \mathbf{x}).$$

## Definition 4.3: Empirical risk $\hat{\mathcal{R}}_n$

Given a sample  $\{(y_i, \mathbf{x}_i), i = 1, \dots, n\}$ , define the empirical risk

$$\hat{\mathcal{R}}_n(\hat{m}) = \frac{1}{n} \sum_{i=1}^n \ell(\hat{m}(\mathbf{x}_i), y_i).$$

- Following Vapnik (1991), the "empirical risk minimization principle" states that the learning algorithm  $\hat{m}^*$  is

$$\hat{m}^* = \operatorname*{argmin}_{\hat{m} \in \mathcal{M}} \{\hat{\mathcal{R}}_n(\hat{m})\}.$$

# Statistical Learning

## Proposition 4.2: Optimal Decision, "*Bayes decision rule*"

For each  $\mathbf{x}$  choose the prediction  $m_{\mathbf{x}}^*$  that minimizes the conditional expected loss,

$$m_{\mathbf{x}}^* \in \operatorname{argmin}_{z \in \mathcal{Y}} \left\{ \int \ell(y, z) d\mathbb{P}_{Y|\mathbf{X}}(y|\mathbf{x}) \right\}$$

- It is straightforward since  $d\mathbb{P}_{Y,\mathbf{X}}(y, \mathbf{x}) = d\mathbb{P}_{Y|\mathbf{X}}(y|\mathbf{x}) \cdot d\mathbb{P}_{\mathbf{X}}(\mathbf{x})$ ,

$$\mathcal{R}(\hat{m}) = \int \left[ \int \ell(y, \hat{m}(\mathbf{x})) d\mathbb{P}_{Y|\mathbf{X}}(y|\mathbf{x}) \right] d\mathbb{P}_{\mathbf{X}}(\mathbf{x}).$$

by definition,  $m_{\mathbf{x}}^*$  minimizes the term in blue, i.e., for any  $\hat{m}$

$$\mathcal{R}(\hat{m}) \geq \int \left[ \int \ell(y, m_{\mathbf{x}}^*) d\mathbb{P}_{Y|\mathbf{X}}(y|\mathbf{x}) \right] d\mathbb{P}_{\mathbf{X}}(\mathbf{x}) = \mathcal{R}(m^*).$$



# Statistical Learning

- It is coined "Bayes decision rule" because the conditional distribution  $Y|\mathbf{X}$  is sometimes referred to as the "posterior" distribution of  $Y$  given data  $\mathbf{X}$ .

## Definition 4.4: Misclassification loss, $\ell_{0/1}$

$$\ell_{0/1}(y, \hat{y}) = \mathbf{1}(y \neq \hat{y}).$$

In the case of a binary classifier, observe that

$$\begin{aligned}\mathcal{R}(\hat{m}) &= \mathbb{E}[\ell(\hat{m}(\mathbf{X}), Y)] = \mathbb{E}[\mathbb{E}[\ell(\hat{m}(\mathbf{X}), Y) | \mathbf{X}]] \\ &= \mathbb{E}[\ell(\hat{m}(\mathbf{X}), 1) \cdot \mathbb{P}(Y = 1 | \mathbf{X}) + \ell(\hat{m}(\mathbf{X}), 0) \cdot \mathbb{P}(Y = 0 | \mathbf{X})] \\ &= \mathbb{E}[\mathbf{1}[\hat{m}(\mathbf{X}) \neq 1] \cdot \mu(\mathbf{X}) + \mathbf{1}[\hat{m}(\mathbf{X}) \neq 0] \cdot (1 - \mu(\mathbf{X}))] \\ &= \mathbb{E}[\mathbf{1}[\hat{m}(\mathbf{X}) \neq 1] \cdot \mu(\mathbf{X}) + (1 - \mathbf{1}[\hat{m}(\mathbf{X}) \neq 1]) \cdot (1 - \mu(\mathbf{X}))] \\ &= \mathbb{E}[\mathbf{1}[\hat{m}(\mathbf{X}) \neq 1] \cdot (2\mu(\mathbf{X}) - 1) + 1 - \mu(\mathbf{X})].\end{aligned}$$

# Statistical Learning

Since  $\hat{m} : \mathcal{X} \rightarrow \{0, 1\}$ , this expectation is minimized by choosing  $\hat{m} = m^*$ , where

$$m^*(\mathbf{x}) = \mathbf{1}(\mu(\mathbf{x}) > 1/2) = \begin{cases} 1 & \text{if } \mu(\mathbf{x}) > 1/2 \\ 0 & \text{if } \mu(\mathbf{x}) \leq 1/2 \end{cases}$$

The optimal risk ("Bayes risk") is  $\mathcal{R}(m^*) = \inf_m \{\mathcal{R}(m)\}$ .

## Definition 4.5: Excess of risk of $\hat{m}$

For any model  $\hat{m}$ , the excess of risk is  $\mathcal{R}(\hat{m}) - \mathcal{R}(m^*)$ .

For a classifier

$$\mathcal{R}(\hat{m}) - \mathcal{R}(m^*) = \mathbb{E}[|2\mu(\mathbf{X}) - 1| \cdot \mathbf{1}(\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X}))].$$

Since we do not know  $\mu$  consider a classifier based on  $\hat{m}$  .....

## Definition 4.6: Plug-in Estimator

Estimate  $\hat{\mu}$  and use, as a classifier,  $\mathbf{1}(\hat{\mu}(\mathbf{x}) > 1/2)$ .

## Proposition 4.3

For any model  $\hat{\mu}$ , the risk of the plug-in classifier  $\hat{m}(\mathbf{x}) = \mathbf{1}(\hat{\mu}(\mathbf{x}) > 1/2)$  satisfies

$$\mathcal{R}(\hat{m}) - \mathcal{R}(m^*) \leq 2\mathbb{E}|\mu(\mathbf{X}) - \hat{\mu}(\mathbf{X})|.$$

**Proof** We have seen that

$$\mathcal{R}(\hat{m}) - \mathcal{R}(m^*) = \mathbb{E}(1[\hat{m}(\mathbf{X}) \neq 1] - 1[m^*(\mathbf{X}) \neq 1]) \cdot (2\mu(\mathbf{X}) - 1).$$

# Statistical Learning

But

$$\begin{aligned} & (\mathbf{1}[\hat{m}(\mathbf{X}) \neq 1] - \mathbf{1}[m^*(\mathbf{X}) \neq 1])(2\mu(\mathbf{X}) - 1) \\ &= \mathbf{1}[\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X})](1[\hat{m}(\mathbf{X}) \neq 1] - 1[m^*(\mathbf{X}) \neq 1])(2\mu(\mathbf{X}) - 1) \\ &= \begin{cases} \mathbf{1}[\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X})](2\mu(\mathbf{X}) - 1) & \text{if } 2\mu(\mathbf{X}) - 1 > 0, \\ \mathbf{1}[\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X})](-1)(2\mu(\mathbf{X}) - 1) & \text{if } 2\mu(\mathbf{X}) - 1 \leq 0. \end{cases} \end{aligned}$$

(from the definition of  $m^*$  )

$$= \mathbf{1}[\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X})] \cdot |2\mu(\mathbf{X}) - 1|,$$

$$\mathcal{R}(\hat{m}) - \mathcal{R}(m^*) = \mathbb{E}(\mathbf{1}[\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X})]) \cdot 2|\mu(\mathbf{X}) - 1/2|.$$

If  $\hat{m}(\mathbf{x}) \neq m^*(\mathbf{x})$ , it means that  $\hat{\mu}(\mathbf{x})$  and  $\mu(\mathbf{x})$  lie on opposite sides of  $1/2$ ,

$$|\hat{\mu}(\mathbf{x}) - \mu(\mathbf{x})| = |\hat{\mu}(\mathbf{x}) - 1/2| + \underbrace{|1/2 - \mu(\mathbf{x})|}_{\geq 0} \geq |\hat{\mu}(\mathbf{x}) - 1/2|$$

# Statistical Learning

i.e.

$$|\hat{\mu}(\mathbf{x}) - \mu(\mathbf{x})| \geq |\hat{\mu}(\mathbf{x}) - 1/2| \cdot \mathbf{1}[\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X})]$$

which is also valid when  $\hat{m}(\mathbf{x}) = m^*(\mathbf{x})$ , thus

$$\mathcal{R}(\hat{m}) - \mathcal{R}(m^*) = 2\mathbb{E}(\mathbf{1}[\hat{m}(\mathbf{X}) \neq m^*(\mathbf{X})]) \cdot |\mu(\mathbf{X}) - 1/2| \leq 2\mathbb{E}[|\hat{\mu}(\mathbf{X}) - \mu(\mathbf{X})|].$$

- This  $\ell_{0/1}$  loss function may be difficult to directly optimize, as shown in [Bartlett et al. \(2006\)](#). One could consider some [surrogate loss](#)  $\tilde{\ell}$  which is easier to optimize.

## Definition 4.7: Elicitation, Brier (1950), Good (1952)

A statistical functional  $\mathcal{I}(Y)$  is said to be elicitable if it minimizes expected loss for some loss function  $s$ , in the sense that

$$\mathcal{I}(Y) = \operatorname{argmin}_{y \in \mathbb{R}} \{\mathbb{E}[s(Y, y)]\}$$

- Important properties for risk measures and backtesting. "*The elicitability of a risk measure means that the risk measure can be obtained by minimizing the expectation of a forecasting objective function. Elicitability is closely related to backtesting, whose objective is to evaluate the performance of a risk forecasting model. If a risk measure is elicitable, then the sample average forecasting error based on the objective function can be used for backtesting the risk measure,*" He et al. (2022)

# Loss Functions

- In a regression problem, a quadratic loss function  $\ell_2$  is used

## Definition 4.8: Quadratic loss, $\ell_2$

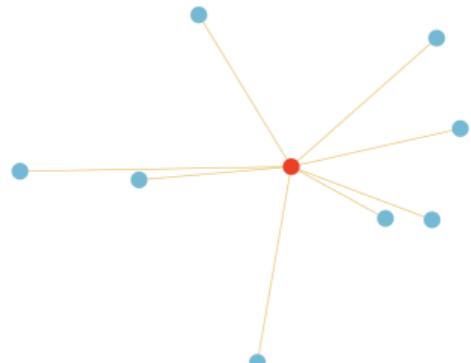
$$\ell_2(y, \hat{y}) = (y - \hat{y})^2, \text{ and the risk is then } \mathcal{R}_2(\hat{m}) = \mathbb{E}\left[(Y - \hat{m}(\mathbf{X}))^2\right].$$

- Observe that

$$\mathbb{E}[Y] = \operatorname{argmin}_{m \in \mathbb{R}} \{\mathcal{R}_2(m)\} = \operatorname{argmin}_{m \in \mathbb{R}} \left\{ \mathbb{E}\left[\ell_2(Y, m)\right] \right\}.$$

The expected value is “ellicitable” (for the  $s = \ell_2$  loss).

The empirical risk minimizer is the “least-square” estimate.



## Loss Functions

- See [Huttegger \(2013\)](#), explaining why the expected value is also called “best estimate”.
- Up to a monotonic transformation (the square root function), the distance here is the expectation of the quadratic loss function. With the terminology of [Angrist and Pischke \(2009\)](#), the regression function  $\mu$  is the function of  $\mathbf{x}$  that serves as “*the best predictor of  $y$ , in the mean-squared error sense.*”

### Proposition 4.4: Optimal Decision, “*Bayes decision rule*”

For the quadratic loss  $\ell_2$ , Bayes decision rule is the (conditional) expected value,  
 $m_{\mathbf{x}}^* = \mathbb{E}[Y|\mathbf{X} = \mathbf{x}] = \mu(\mathbf{x})$ .

# Loss Functions

## Definition 4.9: Inner product

An **inner product** on  $\mathcal{H}$  is the application  $(f, g) \mapsto \langle f, g \rangle_{\mathcal{H}}$  (taking value in  $\mathbb{R}$ ) bilinear, symmetric, definite positive:

- ▶  $\langle f, g \rangle_{\mathcal{H}} = \langle g, f \rangle_{\mathcal{H}}$
- ▶  $\langle \alpha f + \beta g, h \rangle_{\mathcal{H}} = \alpha \langle f, h \rangle_{\mathcal{H}} + \beta \langle g, h \rangle_{\mathcal{H}}$
- ▶  $\langle f, f \rangle_{\mathcal{H}} \geq 0$  and  $\langle f, f \rangle_{\mathcal{H}} = 0$  if and only if  $f = 0$ .

**Example** :  $\mathcal{H} = \mathbb{R}^n$ ,  $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\top \mathbf{y}$

**Example** :  $\mathcal{H} = \mathbb{R}^n$ , let  $\Sigma$  denote some symmetric  $n \times n$  positive definite matrix. Then

$\langle \mathbf{x}, \mathbf{y} \rangle_{\Sigma} = \mathbf{x}^\top \Sigma^{-1} \mathbf{y}$  is an inner product on  $\mathbb{R}^n$ .

**Example** :  $\mathcal{H} = \ell^2 = \left\{ u : \sum_{i=1}^{\infty} u_i^2 < \infty \right\}$ ,  $\langle u, v \rangle = \sum_{i=1}^{\infty} u_i v_i$

# Loss Functions

**Example** :  $\mathcal{H} = L^2(\mu) = \left\{ f : \int f(x)^2 d\mu(x) < \infty \right\}$ ,  $\langle f, g \rangle = \int f(x)g(x)d\mu(x)$

**Example** : Consider the vector space  $\mathcal{V}$  that consists of all real-valued random variables defined on  $(\Omega, \mathcal{F}, \mathbb{P})$ . Given  $k \in [1, \infty)$ , define

$$\|X\|_k = \left[ \mathbb{E}(|X|^k) \right]^{1/k}.$$

to go further  (for more details on Lebesgue spaces, and  $L^2$ )

# Loss Functions

A **norm**  $\|\cdot\|$ , in  $\mathbb{R}^n$ , satisfies

- ▶ homogeneity,  $\|a\vec{u}\| = |a| \cdot \|\vec{u}\|, \forall a$
- ▶ triangle inequality,  $\|\vec{u} + \vec{v}\| \leq \|\vec{u}\| + \|\vec{v}\|$
- ▶ positivity,  $\|\vec{u}\| \geq 0$
- ▶ definiteness,  $\|\vec{u}\| = 0 \iff \vec{u} = \vec{0}$

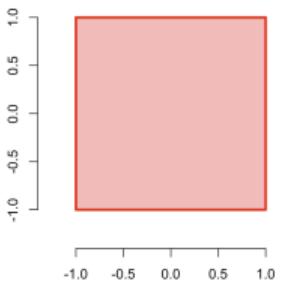
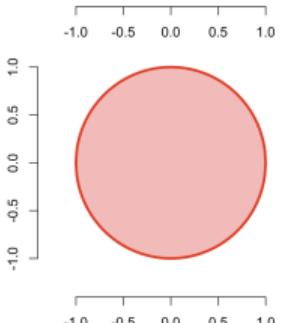
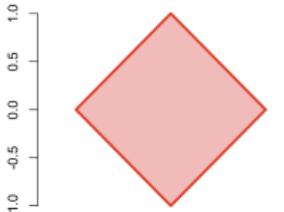
$\ell_1$  norm:  $\|\mathbf{x}\|_{\ell_1} = |x_1| + \cdots + |x_n|,$

$\ell_2$  norm:  $\|\mathbf{x}\|_{\ell_2} = \sqrt{x_1^2 + \cdots + x_n^2},$

$\ell_p$  norm: with  $p \geq 1$ ,  $\|\mathbf{x}\|_{\ell_p} = (|x_1|^p + \cdots + |x_n|^p)^{1/p}$

$\ell_\infty$  norm:  $\|\mathbf{x}\|_{\ell_\infty} = \max\{x_i\}$

Unit balls ( $\|\mathbf{x}\|_{\ell_p} \leq 1$ ) are convex sets



# Loss Functions

## Proposition 4.5: Gradient of $\ell_p$ norms

$$\frac{\partial}{\partial x_j} \|\mathbf{x}\|_{\ell_p} = \frac{1}{p} \left( \sum_i |x_i|^p \right)^{\frac{1}{p}-1} \cdot p|x_j|^{p-1} \operatorname{sign}(x_j) = \left( \frac{|x_j|}{\|\mathbf{x}\|_{\ell_p}} \right)^{p-1} \operatorname{sign}(x_j).$$

$$\begin{aligned} \frac{\partial}{\partial x_j} \|\mathbf{x}\|_{\ell_p} &= \frac{\partial}{\partial x_j} \left( \sum_{i=1}^n |x_i|^p \right)^{1/p} = \frac{1}{p} \left( \sum_{i=1}^n |x_i|^p \right)^{(1/p)-1} \frac{\partial}{\partial x_j} \left( \sum_{i=1}^n |x_i|^p \right) \\ &= \left[ \left( \sum_{i=1}^n |x_i|^p \right)^{\frac{1}{p}} \right]^{1-p} \sum_{i=1}^n |x_i|^{p-1} \delta_{ij} \frac{x_i}{|x_i|} = \left( \frac{|x_j|}{\|\mathbf{x}\|_{\ell_p}} \right)^{p-1} \operatorname{sign}(x_j). \end{aligned}$$

# Loss Functions

## Definition 4.10: Quantile loss, $\ell_{q,\alpha}$

The quantile loss  $\ell_{q,\alpha}$  for some  $\alpha \in (0, 1)$  is

$$\ell_{q,\alpha}(y, \hat{y}) = \max \{ \alpha(y - \hat{y}), (1 - \alpha)(\hat{y} - y) \} = (y - \hat{y})(\alpha - \mathbf{1}_{(y < \hat{y})}).$$

- This loss is not symmetric  $\ell_{q,\alpha}(y, \hat{y}) \neq \ell_{q,\alpha}(\hat{y}, y)$  (if  $\alpha \neq 1/2$ ).
- It is called “quantile” loss since

$$Q(\alpha) = F^{-1}(\alpha) \in \operatorname{argmin}_{q \in \mathbb{R}} \left\{ \mathbb{E} \left[ \ell_{q,\alpha}(Y, q) \right] \right\},$$

(quantiles are also “ellicitable” functionals, elicited by  
 $s(y, \hat{y}) = \alpha(y - \hat{y})_+ + (1 - \alpha)(y - \hat{y})_-$ )

## Loss Functions

- Indeed, the first order condition of

$$\min_{q \in \mathbb{R}} \left\{ (\alpha - 1) \int_{-\infty}^q (y - q) dF_Y(y) + \alpha \int_q^{\infty} (y - q) dF_Y(y) \right\},$$

can be written, using Leibniz integral rule,

$$(1 - \alpha) \int_{-\infty}^{q^*} dF_Y(y) - \alpha \int_{q^*}^{\infty} dF_Y(y) = 0$$

i.e.  $F_Y(q^*) - \alpha = 0$ .

# Loss Functions

## Definition 4.11: Expectile loss, $\ell_{e,\alpha}$

The **expectile loss**  $\ell_{e,\alpha}$ , for some  $\alpha \in (0, 1)$  is

$$\ell_{e,\alpha}(y, \hat{y}) = (y - \hat{y})^2 \cdot (\alpha - \mathbf{1}_{(y < \hat{y})})$$

$$E(\alpha) = \underset{e \in \mathbb{R}}{\operatorname{argmin}} \left\{ \mathbb{E} \left[ \ell_{e,\alpha}(Y, e) \right] \right\},$$

(expectiles are elicited by  $s(x, y) = \alpha(y - x)_+^2 + (1 - \alpha)(y - x)_-^2$ ).

*“Expectiles have properties that are similar to quantiles”* Newey and Powell (1987)

# Loss Functions

Portnoy and Koenker (1997), “*The Gaussian Hare and the Laplacian Tortoise*”



to go further (for more details on optimization issues)

## Loss and Generalized Linear Models

- In GLM, the scaled deviance ( $-2 \times$  the log-likelihood) of the exponential model is

$$D^* = \sum_{i=1}^n d^*(y_i, \hat{y}_i), \text{ where } d^*(y_i, \hat{y}_i) = 2(\log \mathcal{L}_i(y_i) - \log \mathcal{L}_i(\hat{y}_i)).$$

that can be related to in-sample empirical risk

$$\widehat{\mathcal{R}}_n(\hat{m}) = \sum_{i=1}^n \ell(y_i, \hat{m}(\mathbf{x}_i)),$$

- For the Poisson distribution (with a log-link), the loss would be

$$\ell(y_i, \hat{y}_i) = \begin{cases} 2(y_i \log y_i - y_i \log \hat{y}_i - y_i + \hat{y}_i) & y_i > 0 \\ 2\hat{y}_i & y_i = 0, \end{cases}$$

while for a logistic regression, we have the standard binary cross-entropy loss

$$\ell(y_i, \hat{y}_i) = -(y_i \log[\hat{y}_i] + (1 - y_i) \log[1 - \hat{y}_i]).$$

# Distance Between Distributions

## Definition 4.12: Distance (or metric)

A distance  $d$  on a set  $E$  is a function  $E \times E \rightarrow \mathbb{R}_+$  such that

- ▶  $d$  is symmetric,  $\forall (a, b) \in E^2$ ,  $d(a, b) = d(b, a)$ ,
- ▶  $d$  is separable,  $\forall (a, b) \in E^2$ ,  $d(a, b) = 0 \Leftrightarrow a = b$ ,
- ▶  $d$  satisfies  $\forall (a, b, c) \in E^3$ ,  $d(a, c) \leq d(a, b) + d(b, c)$

In a vector space, with norm  $\|\cdot\|$  the induced distance is  $d(x, y) = \|y - x\|$ .

Conversely, if

- ▶  $d$  invariant by translation,  $d(x, y) = d(x + a, y + a)$
- ▶  $d$  is homogeneous,  $d(\alpha x, \alpha y) = |\alpha|d(x, y)$

# Distance Between Distributions

then  $\|x\| = d(x, 0)$  is a norm.

## Proposition 4.6

If  $d$  is a distance on  $E$ , and if  $\psi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$  is an increasing function such that  $\psi(0) = 0$  and  $\psi(t) > 0$  for all  $t > 0$ . If  $\psi$  is subadditive ( $\psi(s+t) \leq \psi(s) + \psi(t)$ ), then  $\delta(a, b) = \psi(d(a, b))$  is also a distance on  $E$ .

## Proposition 4.7:

If  $d$  is a distance on  $E$ , then  $d^2$  is not necessarily a distance.

## Distance Between Distributions

- Consider the Euclidean distance in  $E = \mathbb{R}^2$ , i.e.

$d(\mathbf{z}_1, \mathbf{z}_2) = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$ .  $d^2$  is not a distance, see

$$\begin{cases} d^2(-\mathbf{1}, +\mathbf{1}) = 2^2 + 2^2 = 8 \\ d^2(-\mathbf{1}, \mathbf{0}) = 1^2 + 1^2 = 2 \\ d^2(\mathbf{0}, +\mathbf{1}) = 1^2 + 1^2 = 2 \end{cases}$$

i.e.  $d^2$  does not satisfy the triangular inequality

$$d^2(-\mathbf{1}, +\mathbf{1}) > d^2(-\mathbf{1}, \mathbf{0}) + d^2(\mathbf{0}, +\mathbf{1}),$$

while

$$d(-\mathbf{1}, +\mathbf{1}) \leq d(-\mathbf{1}, \mathbf{0}) + d(\mathbf{0}, +\mathbf{1}).$$

(functions that generalize squared distance are sometimes referred to as divergences)

## Distance Between Distributions

- In addition to "distance", similar terms are used, including "dissimilarity", "deviance", "deviation", "discrepancy", "discrimination", and "divergence" (... all denoted " $d$ ", or " $D$ ")
- A fundamental problem in statistics and machine learning is to come up with useful measures of "distance" between pairs of probability distributions. Two desirable properties of a distance function are symmetry and the triangle inequality.
- Unfortunately, many notions of "distance" between probability distributions do not satisfy these properties. Weaker notions of distance are often used, such as dissimilarity measures and divergences.
- See [Cha \(2007\)](#) for a comprehensive list of distances...

# Distance Between Distributions

## Definition 4.13: Dissimilarity measure

A dissimilarity measure  $D$  on a set  $E$  is a function  $E \times E \rightarrow \mathbb{R}_+$  such that  $D$  is positive and separable, i.e.,  $\forall (a, b) \in E^2$ ,  $D(a, b) = 0 \Leftrightarrow a = b$ ,

## Definition 4.14: Divergence on $\mathbb{R}^n$

A divergence  $D$  on a set  $E \subset \mathbb{R}^n$  is a function  $E \times E \rightarrow \mathbb{R}_+$  such that

- ▶  $D$  is separable,  $\forall (\mathbf{x}, \mathbf{y}) \in E^2$ ,  $D(\mathbf{x}, \mathbf{y}) = 0 \Leftrightarrow \mathbf{x} = \mathbf{y}$ ,
- ▶  $D$  admits development

$$\forall (\mathbf{x}, \mathbf{x} + \boldsymbol{\epsilon}) \in E^2, D(\mathbf{x}, \mathbf{x} + \boldsymbol{\epsilon}) = \frac{1}{2} \sum A_{i,j}(\boldsymbol{\epsilon}) \epsilon_i \epsilon_j + O(|\boldsymbol{\epsilon}|^3),$$

where  $A(\boldsymbol{\epsilon})$  is definite positive.

# Distance Between Distributions

## Definition 4.15: Scale sensitive divergence, Zolotarev (1976)

A divergence  $D$  is scale sensitive (of order  $\beta > 0$ ) if  $D(cx, cy) \leq |c|^\beta D(x, y)$

## Definition 4.16: Bregman Divergence, Bregman (1967)

Let  $\psi : \mathcal{X} \rightarrow \mathbb{R}$  be a strictly convex function that is continuously differentiable. Then the Bregman divergence  $D_\psi(x, y)$  is defined as

$$D_\psi(x, y) = \psi(x) - \psi(y) - \langle \nabla \psi(y), x - y \rangle.$$

- » If  $\psi(x) = \frac{1}{2}\|x\|^2$  (strictly convex), then  $D_\psi(x, y) = \frac{1}{2}\|x - y\|^2$ .  
(recall that  $\nabla\|x\|^2 = 2x$ )

## Proposition 4.8: Bregman Divergence

Let  $\psi : \mathcal{X} \rightarrow \mathbb{R}$  be a strictly convex function that is continuously differentiable. Then **Bregman divergence**  $D_\psi(\mathbf{x}, \mathbf{y})$  is

- ▶ strictly convex in  $\mathbf{x}$ ,
- ▶ (generally) non-convex in  $\mathbf{y}$ ,
- ▶ non-negative  $D_\psi(\mathbf{x}, \mathbf{y}) \geq 0$ ,
- ▶ separable,  $D_\psi(\mathbf{x}, \mathbf{y}) = 0$  if and only if  $\mathbf{x} = \mathbf{y}$ ,
- ▶ (generally) asymmetric.

## Distance Between Distributions

- › If  $\mathcal{X} = \mathbb{R}^n$ , and  $\psi(\mathbf{x}) = \frac{1}{2} \sum_{ij} A_{ij} x_i x_j = \frac{1}{2} \mathbf{x}^\top A \mathbf{x}$  for some  $n \times n$  matrix  $A$  definite positive, then

$$D_\psi(\mathbf{x}, \mathbf{y}) = \frac{1}{2} \sum_{ij} A_{ij} (x_i - y_i)(x_j - y_j) = (\mathbf{x} - \mathbf{y})^\top A (\mathbf{x} - \mathbf{y})$$

(see Mahalanobis distance).

- › If  $\mathcal{X} = \mathbb{R}^n$ , and  $\psi(\mathbf{x}) = -\sum_i \log(x_i)$  then

$$D_\psi(\mathbf{x}, \mathbf{y}) = \sum_i \frac{x_i}{y_i} - \log \frac{x_i}{y_i} - 1$$

See [Banerjee et al. \(2005\)](#) for more examples.

# Distance Between Distributions

We have defined norms

- › on  $\mathbb{R}^n$ , e.g.,

$$\|\mathbf{x}\|_{\ell_2} = \left( |x_1|^2 + \cdots + |x_n|^2 \right)^{1/2} = \left( \sum_{i=1}^n |x_i|^2 \right)^{1/2}$$

that could be extended

- › on  $\mathbb{R}$ -valued random variables, e.g.,

$$\|X\|_2 = \left( \mathbb{E} [|X|^2] \right)^{1/2} = \left( \sum |x|^2 p(x) \right)^{1/2} = \left( \int |x|^2 f(x) dx \right)^{1/2}$$

We can also define "distances", "dissimilarity" measures, and "divergences"

- › on  $\mathbb{R}^n$ , e.g.,

$$\ell_2(\mathbf{x}, \mathbf{y}) = d(\mathbf{x}, \mathbf{y}) = \left( |x_1 - y_1|^2 + \cdots + |x_n - y_n|^2 \right)^{1/2} = \left( \sum_{i=1}^n |x_i - y_i|^2 \right)^{1/2}$$

## Distance Between Distributions

that could be extended

- › on  $\mathbb{R}$ -valued random variables as components of a random vector, e.g.,

$$D(X, Y) = \left( \mathbb{E} [|X - Y|^2] \right)^{1/2} = \left( \sum |x - y|^2 p(x, y) \right)^{1/2} = \left( \int |x - y|^2 f(x, y) dx dy \right)^{1/2}$$

where  $p$  or  $f$  is the joint distribution of  $(X, Y)$ , e.g., for a Gaussian vector

$$D(X, Y) = (\mu_x - \mu_y)^2 + (\sigma_x - \sigma_y)^2 + 2\sigma_x\sigma_y(1 - \rho).$$

- › on  $\mathbb{R}$ -valued random variables assuming that random variables are independent, e.g.,

$$D_{\perp}(X, Y) = \left( \sum |x - y|^2 p_x(x)p_y(y) \right)^{1/2} = \left( \int |x - y|^2 f_x(x)f_y(y) dx dy \right)^{1/2}$$

e.g., for two Gaussian distributions

$$D_{\perp}(X, Y) = (\mu_x - \mu_y)^2 + \sigma_x^2 + \sigma_y^2.$$

# Distance Between Distributions

and one can consider some distance

- on  $\mathbb{R}$ -valued distributions, e.g.,

$$D(\mathcal{N}(\mu_x, \sigma_x^2), \mathcal{N}(\mu_y, \sigma_y^2)) = (\mu_x - \mu_y)^2 + (\sigma_x - \sigma_y)^2.$$

In the context of "probabilistic forecasts" (as in Gneiting et al. (2007)), a "distance"

- on pairs  $\mathbb{R} \times \mathbb{R}$ -valued distributions, e.g.,

$$D(x, \mathcal{N}(\mu_y, \sigma_y^2)) = (x - \mu_y)^2 + \sigma_y^2.$$

# Distance Between Distributions

## Definition 4.17: Sum invariant divergence, Zolotarev (1976)

A divergence  $D$  is sum invariant if  $D(X + Z, Y + Z) \leq D(X, Y)$  whenever  $Z \perp\!\!\!\perp X, Y$

**Example:** if  $D$  is 1-scale sensitive,  $D(\mathbf{1}_0, \mathbf{1}_1) \leq \frac{1}{2}D(\mathbf{1}_0, \mathbf{1}_2)$

**Example:** if  $D$  is sum invariant,  $D(\mathbf{1}_0, \mathbf{1}_1) = D(\mathbf{1}_1, \mathbf{1}_2)$

See Bellemare et al. (2017a).

# Distance Between Distributions

Consider sample  $\{x_1, \dots, x_n\}$  an i.i.d. sample, with empirical measure  $\hat{p}_n = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{x_i}$

## Definition 4.18: Divergence based inference

Consider some parametric family  $\mathcal{Q} = \{q_\theta, \theta \in \Theta\}$ . Given a divergence  $D$ , we want to find

$$\theta^* = \operatorname{argmin}_{\theta \in \Theta} \{D(p, q_\theta)\}$$

or its empirical version

$$\theta^* = \operatorname{argmin}_{\theta \in \Theta} \{D(p, q_\theta)\}$$

$$\hat{\theta}_n = \operatorname{argmin}_{\theta \in \Theta} \{D(\hat{p}_n, q_\theta)\}$$

# Distance Between Distributions

## Definition 4.19: Unbiased sample gradients, [Bellemare et al. \(2017a\)](#)

A divergence  $D$  has **unbiased sample gradients** when the expected gradient of the sample loss equals the gradient of the true loss for all  $p$  and  $n$ ,

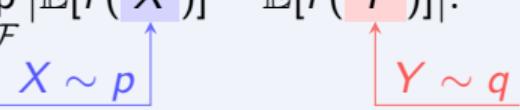
$$\mathbb{E}(\nabla_{\theta}D(\hat{p}_n, q_{\theta})) = \nabla_{\theta}D(p, q_{\theta}).$$

- › Then  $D$  is a **proper scoring rule** (see [Gneiting and Raftery \(2007\)](#)).
- › If this is not satisfied, stochastic gradient descent may not converge...

# Distance Between Distributions

## Definition 4.20: Integral probability metric, Müller (1997)

Integral probability metrics (IPMs) are distances on the space of distributions over a set  $\mathcal{X}$ , defined by a class  $\mathcal{F}$  of real-valued functions on  $\mathcal{X}$  as

$$D_{\mathcal{F}}(p, q) = \sup_{f \in \mathcal{F}} |\mathbb{E}[f(X)] - \mathbb{E}[f(Y)]|.$$


The diagram shows two arrows pointing upwards from the labels  $X \sim p$  and  $Y \sim q$  to the respective terms  $\mathbb{E}[f(X)]$  and  $\mathbb{E}[f(Y)]$  in the formula, indicating that these terms are being compared across all functions in the class  $\mathcal{F}$ .

Discussed also in Dedecker and Merlevède (2007)

# Distance Between Distributions

- Note that it is still possible to define projections with deviance (that will not be "orthogonal" projections since divergence are not related to inner products)

## Definition 4.21: Projection, Bregman (1967), Bauschke et al. (1997)

Given a strictly convex function continuously differentiable  $\psi$  and the associated Bregman divergence  $D_\psi$ , a closed closed convex  $K \subset \mathcal{X}$  and a point  $x \in \mathcal{X}$ . The Bregman projection of  $x$  onto  $K$  is

$$x^* = \operatorname{argmin}_{y \in K} \{D_\psi(x, y)\}$$

- If  $\psi(x) = \|x\|_{\ell_2}^2$ , Bregman projection is the standard orthogonal projection onto a convex set,

$$x^* = \operatorname{argmin}_{y \in K} \{\|x - y\|_{\ell_2}^2\}$$

## Distance Between Distributions

- With Bregman divergence  $D_\psi$ , we have a generalized version of the Pythagorean theorem

$$D_\psi(\mathbf{x}, \mathbf{y}) \geq D_\psi(\mathbf{x}, \mathbf{x}^*) + D_\psi(\mathbf{x}^*, \mathbf{y})$$

Numerically, one can use (cyclical) Dykstra algorithm with Bregman projections (see [Censor and Reich \(1998\)](#), [Bauschke and Lewis \(2000\)](#)) to compute  $\mathbf{x}^*$ : suppose that

$K = \bigcap_{i=1}^m K_i$  where  $K_i$ 's are convex sets (e.g. half-planes - when  $K$  is some polyhedral).

Let  $P_i^\psi$  denote the orthogonal on  $K_i$  based on  $D_\psi$ ,

$$P_i^\psi : \mathbf{x} \mapsto \operatorname{argmin}_{\mathbf{y} \in K_i} \{\|\mathbf{x} - \mathbf{y}\|_{\ell_2}^2\}$$

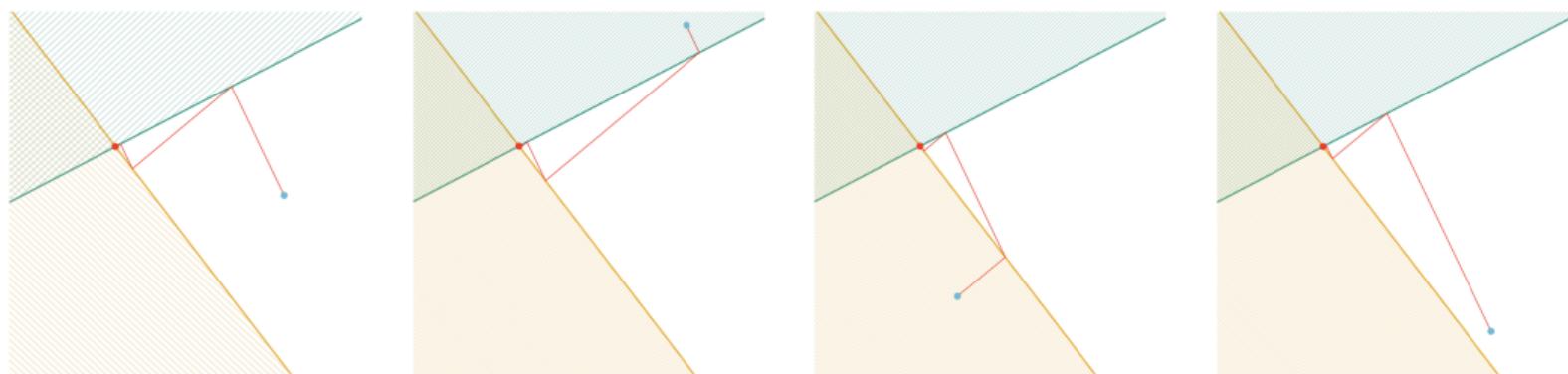
and consider the following iterative sequence of projections, until some  $\mathbf{x}_j \in K$ ,

$$\mathbf{x}_0 \xrightarrow{P_1^\psi} \mathbf{x}_1 \xrightarrow{P_2^\psi} \mathbf{x}_2 \xrightarrow{P_3^\psi} \cdots \xrightarrow{P_{m-1}^\psi} \mathbf{x}_{m-1} \xrightarrow{P_m^\psi} \mathbf{x}_m \xrightarrow{P_1^\psi} \mathbf{x}_{m+1} \xrightarrow{P_2^\psi} \mathbf{x}_{m+2} \cdots$$

# Distance Between Distributions

$$x_0 \xrightarrow{P_1^\psi} x_1 \xrightarrow{P_2^\psi} x_2 \xrightarrow{P_3^\psi} \cdots \xrightarrow{P_{m-1}^\psi} x_{m-1} \xrightarrow{P_m^\psi} x_m \xrightarrow{P_1^\psi} x_{m+1} \xrightarrow{P_2^\psi} x_{m+2} \cdots$$

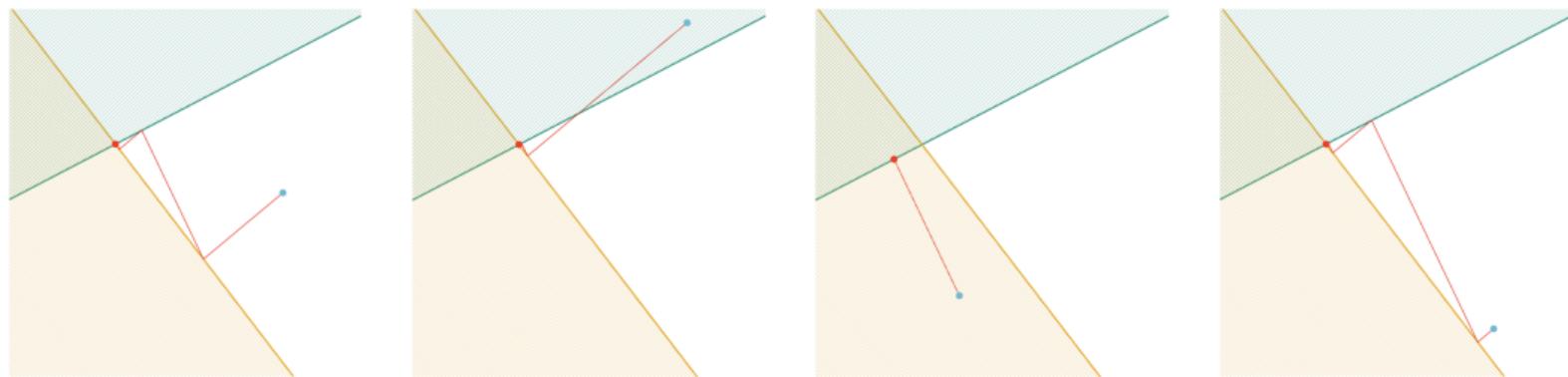
until some  $x_j \in K$ , see Boyle and Dykstra (1986) for the original idea



# Distance Between Distributions

$$x_0 \xrightarrow{P_1^\psi} x_1 \xrightarrow{P_2^\psi} x_2 \xrightarrow{P_3^\psi} \cdots \xrightarrow{P_{m-1}^\psi} x_{m-1} \xrightarrow{P_m^\psi} x_m \xrightarrow{P_1^\psi} x_{m+1} \xrightarrow{P_2^\psi} x_{m+2} \cdots$$

until some  $x_j \in K$ , see Boyle and Dykstra (1986) for the original idea



with half spaces,  $\|x_j - x^*\|_{\ell_2} \leq cr^j \|x - x^*\|_{\ell_2}$  for some  $r \in (0, 1)$  and  $c > 0$  (or "linear convergence" since  $\|x_j - x^*\|_{\ell_2} \leq r\|x_{j-1} - x^*\|_{\ell_2}$ ).

# Distance Between Distributions

## Definition 4.22: Hellinger distance, Hellinger (1909)

For two discrete distributions  $p$  and  $q$ , Hellinger distance is

$$d_H(p, q)^2 = \frac{1}{2} \sum_i \left( \sqrt{p(i)} - \sqrt{q(i)} \right)^2 = 1 - \sum_i \sqrt{p(i)q(i)} \in [0, 1],$$

and for absolutely continuous distributions, if  $p$  and  $q$  are densities,

$$d_H(p, q)^2 = \frac{1}{2} \int_{\mathbb{R}} \left( \sqrt{p(x)} - \sqrt{q(x)} \right)^2 dx \text{ or } \frac{1}{2} \int_{\mathbb{R}^k} \left( \sqrt{p(\mathbf{x})} - \sqrt{q(\mathbf{x})} \right)^2 d\mathbf{x}$$

See Pardo (2018).

# Distance Between Distributions

## Proposition 4.9: Distance between Beta variables

Consider two Beta distribution, then  $d_H^2(\mathcal{B}(a_1, b_1), \mathcal{B}(a_2, b_2))$  is

$$1 - \frac{1}{\sqrt{B(a_1, b_1)B(a_2, b_2)}} B\left(\frac{a_1 + a_2}{2}, \frac{b_1 + b_2}{2}\right)$$

### Proof

$$1 - \int_0^1 \sqrt{f_1(t)f_2(t)} dt = 1 - \frac{1}{\sqrt{B(a_1, b_1)B(a_2, b_2)}} \int_0^1 t^{(a_1+a_2)/2-1} (1-t)^{(b_1+b_2)/2-1} dt,$$

$$\text{then use } B(a, b) = \Gamma(a)\Gamma(b) / \Gamma(a+b).$$

# Distance Between Distributions

## Proposition 4.10: Distance between Gaussian vectors

Consider two Gaussian distributions, then  $d_H^2(\mathcal{N}(\mu_1, \Sigma_1), \mathcal{N}(\mu_2, \Sigma_2))$  is

$$2 - 2 \frac{|\Sigma_1|^{\frac{1}{4}} |\Sigma_2|^{\frac{1}{4}}}{|\bar{\Sigma}|^{\frac{1}{2}}} \exp\left(-\frac{1}{8} (\mu_1 - \mu_2)^\top \bar{\Sigma}^{-1} (\mu_1 - \mu_2)\right)$$

where  $\bar{\Sigma} = \frac{1}{2}(\Sigma_1 + \Sigma_2)$ .

Note that it is a Bregman divergence  $D_\psi$  with  $\psi(x) = \sum_{i=1}^n x_i^2$

# Distance Between Distributions

**Definition 4.23: Pearson/Neyman  $\chi$ -square divergences** Nielsen and Nock (2013)

For two discrete distributions  $p$  and  $q$ , Pearson chi-square divergence is

$$d_{P\chi}(p\|q)^2 = \sum_i \frac{[p(i) - q(i)]^2}{q(i)},$$

while Neyman chi-square divergence is

$$d_{N\chi}(p\|q)^2 = \sum_i \frac{[(i) - q(i)]^2}{p(i)} = d_{P\chi}(q\|p),$$

## Distance Between Distributions

- Note that both are Bregman divergences  $D_\psi$  with  $\psi_P(\mathbf{x}) = -2 \sum_{i=1} \sqrt{x_i}$  and  $\psi_N(\mathbf{x}) = \sum_{i=1} x_i^{-1}$ .
- $d_\chi$  can be extended to the case of continuous distributions, e.g.,

$$d_{P\chi}(p\|q)^2 = \int \left( \frac{p(x)}{q(x)} - 1 \right)^2 p(x) dx$$

# Distance Between Distributions

**Definition 4.24: Total Variation, Jordan (1881); Rudin (1966)**

For two distributions  $p$  and  $q$ , the **total variation distance** between  $p$  and  $q$  is

$$d_{\text{TV}}(p, q) = \sup_{\mathcal{A}} \{|p(\mathcal{A}) - q(\mathcal{A})|\}.$$

**Proposition 4.11: Total Variation**

For two univariate distributions  $p$  and  $q$ , the **total variation distance** between  $p$  and  $q$  is

$$d_{\text{TV}}(p, q) = \frac{1}{2} \sum_i |p(i) - q(i)| = \frac{1}{2} \|p - q\|_{\ell_1} = \sum_{i:p(i) \geq q(i)} (p(i) - q(i))$$

See Proposition 4.2 in [Levin and Peres \(2017\)](#).

# Distance Between Distributions

- Equivalently,

$$d_{\text{TV}}(p, q) = \frac{1}{2} \sup_{f: \mathbb{R}^k \rightarrow \{0,1\}} \left\{ \int f d\mu - \int f d\nu \right\}$$

(see e.g. <https://djalil.chafai.net/blog/>, with  $f : \mathbb{R}^k \rightarrow \{-1, 1\}$ ,  $f = \mathbf{1}_{\mathcal{A}} - \mathbf{1}_{\mathcal{A}^c}$ )

- It is an IPM with  $\mathcal{F} = \{f : \mathcal{X} \rightarrow \{0, 1\}\}$ , so that  $\mathcal{F}$  is a set of indicator functions for any event.
- For Gaussian distributions, the distance has no explicit formula, see, e.g., [Devroye et al. \(2018\)](#).

# Distance Between Distributions

## Proposition 4.12: Total Variation, Scheffé theorem, Billingsley (2017)

For two distributions  $p$  and  $q$  on  $\mathbb{R}^k$ ,

$$d_{\text{TV}}(p, q) = \frac{1}{2} \int_{\mathbb{R}^d} |p(\mathbf{x}) - q(\mathbf{x})| d\mathbf{x},$$

$$d_{\text{TV}}(p, q) = 1 - \int_{\mathbb{R}^d} \min \{p(\mathbf{x}) - q(\mathbf{x})\} d\mathbf{x},$$

$$d_{\text{TV}}(p, q) = p(\mathcal{A}) - q(\mathcal{A}) \text{ where } \mathcal{A} = \{\mathbf{x} : p(\mathbf{x}) \geq q(\mathbf{x})\}.$$

# Distance Between Distributions

In the univariate case, we can restrict  $\mathcal{A}$  to half-lines  $(-\infty, t]$

**Definition 4.25: Kolmogorov-Smirnov, Kolmogorov (1933); Smirnov (1948)**

For two distributions  $p$  and  $q$ , **Kolmogorov-Smirnov distance** between  $p$  and  $q$  is

$$d_{KS}(p, q) = \sup_{t \in \mathbb{R}} \{|p((-\infty, t]) - q((-\infty, t])|\} = \sup_{t \in \mathbb{R}} \{|F_p(t) - F_q(t)|\} = \|F_p - F_q\|_\infty,$$

where  $F_p$  and  $F_q$  are the respective cumulative distribution functions.

# Distance Between Distributions

## Definition 4.26: Entropy, Shannon (1948)

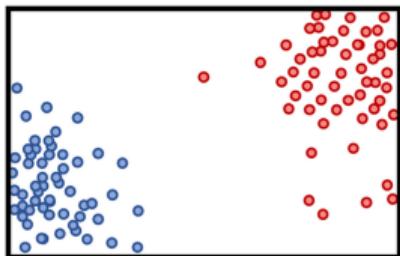
The entropy associated with distribution  $p$  is

$$\mathcal{E}_p(p) = - \sum_i p(i) \log p(i) = \mathbb{E}_p[-\log p(X)].$$

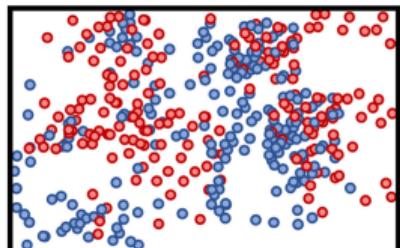
and define cross-entropy (of  $q$  relative to  $p$ ) as

$$\mathcal{E}_q(p) = - \sum_i p(i) \log q(i) = \mathbb{E}_p[-\log q(X)].$$

See Amari (2016) or Chambert-Loir (2023) for more details.



Low Entropy



High Entropy

# Distance Between Distributions

## Definition 4.27: Kullback–Leibler, [Kullback and Leibler \(1951\)](#)

For two discrete distributions  $p$  and  $q$ , Kullback–Leibler divergence of  $p$ , with respect to  $q$  is

$$D_{\text{KL}}(p\|q) = \sum_i p(i) \log \frac{p(i)}{q(i)},$$

and for absolutely continuous distributions,

$$D_{\text{KL}}(p\|q) = \int_{\mathbb{R}} p(x) \log \frac{p(x)}{q(x)} dx \text{ or } \int_{\mathbb{R}^k} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})} d\mathbf{x},$$

in higher dimension.

Also called relative entropy, since  $D_{\text{KL}}(p\|q) = \mathcal{E}_q(p) - \mathcal{E}_p(p)$ .

# Distance Between Distributions

## Proposition 4.13: Divergence for Gaussian vectors

Consider two Gaussian distributions, then  $D_{\text{KL}}(\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \| \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2))$  is

$$\frac{1}{2} \left[ (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top \boldsymbol{\Sigma}_2^{-1} (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1) + \text{tr}(\boldsymbol{\Sigma}_2^{-1} \boldsymbol{\Sigma}_1) - \log \frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_2|} - k \right]$$

where  $k$  is the dimension, see [Polyanskiy and Wu \(2022\)](#).

# Distance Between Distributions

The entropy of  $X$  according to  $p$  is smaller than or equal to the cross-entropy of  $p$  and  $q$ , or equivalently

## Proposition 4.14: Gibbs' inequality

$D_{\text{KL}}(p\|q)$  is positive and separable, i.e.  $D_{\text{KL}}(p\|q) \geq 0$  and  $D_{\text{KL}}(p\|q) = 0$  if and only if  $p = q$ .

**Proof:**  $\sum_{x \in I} p(x) \log \frac{p(x)}{q(x)} \geq 0$  where  $I$  is the set of all  $x$  for which  $p(x) > 0$ . Recall that  $\log x \leq x - 1$  (with equality only when  $x = 1$ ), thus  $\log(1/x) \geq 1 - x$ , and

$$\sum_{x \in I} p(x) \ln \frac{p(x)}{q(x)} \geq \sum_{x \in I} p(x) \left(1 - \frac{q(x)}{p(x)}\right) = \sum_{x \in I} p(x) - \sum_{x \in I} q(x) \geq 0.$$

# Distance Between Distributions

## Proposition 4.15: Additivity for independence distributions

$D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q}) = D_{\text{KL}}(p_x \parallel q_x) + D_{\text{KL}}(p_y \parallel q_y)$  if  $\mathbf{p}(x, y) = p_x(x)p_y(y)$  and  $\mathbf{q}(x, y) = q_x(x)q_y(y)$ .

**Proof** By definition

$$D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q}) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \frac{p(x, y)}{q(x, y)} dy dx .$$

and since  $\mathbf{p}(x, y) = p_x(x)p_y(y)$  and  $\mathbf{q}(x, y) = q_x(x)q_y(y)$ ,

$$D_{\text{KL}}(\mathbf{p} \parallel \mathbf{q}) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \log \frac{p_1(x) p_2(y)}{q_1(x) q_2(y)} dy dx .$$

## Distance Between Distributions

$$\begin{aligned} D_{\text{KL}}(\mathbf{p} \| \mathbf{q}) &= \int_{\mathcal{X}} \int_{\mathcal{Y}} p_x(x) p_y(y) \cdot \left( \log \frac{p_x(x)}{q_x(x)} + \log \frac{p_y(y)}{q_y(y)} \right) dy dx \\ &= \int_{\mathcal{X}} \int_{\mathcal{Y}} p_x(x) p_y(y) \cdot \log \frac{p_x(x)}{q_x(x)} dy dx + \int_{\mathcal{X}} \int_{\mathcal{Y}} p_x(x) p_y(y) \cdot \log \frac{p_y(y)}{q_y(y)} dy dx \\ &= \int_{\mathcal{X}} p_x(x) \cdot \log \frac{p_x(x)}{q_x(x)} \int_{\mathcal{Y}} p_y(y) dy dx + \int_{\mathcal{Y}} p_y(y) \cdot \log \frac{p_y(y)}{q_y(y)} \int_{\mathcal{X}} p_x(x) dx dy \\ &= \int_{\mathcal{X}} p_x(x) \cdot \log \frac{p_x(x)}{q_x(x)} dx + \int_{\mathcal{Y}} p_y(y) \cdot \log \frac{p_y(y)}{q_y(y)} dy \\ &= D_{\text{KL}}(p_x \| q_x) + D_{\text{KL}}(p_y \| q_y). \end{aligned}$$

But for other distances,

$$\begin{cases} d_{\text{H}}(\mathbf{p}, \mathbf{q})^2 \leq d_{\text{H}}(p_x, q_x)^2 + d_{\text{H}}(p_y, q_y)^2 \\ d_{\text{TV}}(\mathbf{p}, \mathbf{q}) \leq d_{\text{TV}}(p_x, q_x) + d_{\text{TV}}(p_y, q_y). \end{cases}$$

# Distance Between Distributions

- It is only defined in this way if, for all  $x$ ,  $q(x) = 0$  implies  $p(x) = 0$  (“absolute continuity” with respect to  $p$ ).

## Proposition 4.16

The KL divergence has unbiased sample gradients, but is not scale sensitive.

### Proof Bellemare et al. (2017b).

- In a Bayesian setting,  $D_{\text{KL}}(p\|q)$  is a measure of the information gained by revising one’s beliefs from the prior probability distribution  $q$  to the posterior probability distribution  $p$  (it is the amount of information lost when  $q$  is used to approximate  $p$ ).
- If  $\psi(\mathbf{x}) = \sum x_i \log(x_i)$  (strictly convex), then Bregman divergence is

$$D_\psi(\mathbf{x}, \mathbf{y}) = \sum x_i \log \frac{x_i}{y_i} = D_{\text{KL}}(\mathbf{x}\|\mathbf{y})$$

## Distance Between Distributions

$$D_{\text{KL}}(\mathcal{B}(p) \parallel \mathcal{B}(q)) = p \log \frac{p}{q} + (1 - p) \log \frac{1 - p}{1 - q}$$

$$D_{\text{KL}}(\mathcal{B}(n, p) \parallel \mathcal{B}(n, q)) = np \log \frac{p}{q} + n(1 - p) \log \frac{1 - p}{1 - q} = n D_{\text{KL}}(\mathcal{B}(p) \parallel \mathcal{B}(q))$$

$$D_{\text{KL}}(\mathcal{U}([a_1, b_1]) \parallel \mathcal{U}([a_2, b_2])) = \log \frac{b_2 - a_2}{b_1 - a_1}$$

$$D_{\text{KL}}(\mathcal{N}(\mu_1, \sigma_1^2) \parallel \mathcal{N}(\mu_2, \sigma_2^2)) = \frac{1}{2} \left[ \frac{(\mu_1 - \mu_2)^2}{\sigma_2^2} + \frac{\sigma_1^2}{\sigma_2^2} - \log \frac{\sigma_1^2}{\sigma_2^2} - 1 \right]$$

$$D_{\text{KL}}(\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \parallel \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)) = \frac{1}{2} \left[ (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top \boldsymbol{\Sigma}_2^{-1} (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1) + \text{tr}(\boldsymbol{\Sigma}_2^{-1} \boldsymbol{\Sigma}_1) - \log \frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_2|} - n \right]$$

# Distance Between Distributions

- Consider some distribution  $p_\theta$ , as in Nielsen (2022). Using Taylor expansion,

$$D_{\text{KL}}(p_\theta \| p_{\theta + d\theta}) = \frac{1}{2} d\theta^\top I(\theta) d\theta \approx \frac{1}{2} ds_\theta^2.$$

## Definition 4.28: Jeffreys (symmetric) divergence Jeffreys (1946)

The Jeffrey divergence is a symmetric divergence induced by Kullback-Liebler divergence,

$$D_J(p_1, p_2) = \frac{1}{2} D_{\text{KL}}(p_1 \| p_2) + \frac{1}{2} D_{\text{KL}}(p_2 \| p_1).$$

# Distance Between Distributions

## Definition 4.29: Jensen-Shannon, Lin (1991)

The **Jensen-Shannon divergence** is a symmetric divergence induced by Kullback-Liebler divergence,

$$D_{JS}(p_1, p_2) = \frac{1}{2}D_{KL}(p_1\|q) + \frac{1}{2}D_{KL}(p_2\|q),$$

where  $q = \frac{1}{2}(p_1 + p_2)$ .

Endres and Schindelin (2003) proved that  $\sqrt{D_{JS}(p_1, p_2)}$  is a proper distance.

- See **philentropy** package.

## Distance Between Distributions

**Definition 4.30:** *f*-divergence, Rényi (1961), Ali and Silvey (1966)

Given a continuous convex function  $f : [0, \infty) \rightarrow \overline{\mathbb{R}}$ , define

$$D_f(p\|q) = \sum_i q(i) \cdot f\left(\frac{p(i)}{q(i)}\right)$$

and for absolutely continuous function

$$D_f(p\|q) = \int_{\mathbb{R}} q(x)f\left(\log \frac{p(x)}{q(x)}\right) dx \text{ or } \int_{\mathbb{R}^k} q(\mathbf{x})f\left(\frac{p(\mathbf{x})}{q(\mathbf{x})}\right) d\mathbf{x},$$

- $D_f(p\|q)$  is properly defined when  $p \ll q$ , see also Csiszár (1964, 1967).  
If  $f(u) = u \log u$ ,  $D_f(p\|q) = D_{\text{KL}}(p, q)$   
If  $f(u) = |u - 1|$ ,  $D_f(p\|q) = d_{\text{TV}}(p, q)$

# Distance Between Distributions

If  $f(u) = \frac{1}{2}(\sqrt{u} - 1)^2$ ,  $D_f(p\|q) = d_H(p, q)^2$

If  $f(u) = \frac{1}{2} \left( u \log u - (u + 1) \log \left( \frac{u + 1}{2} \right) \right)$ ,  $D_f(p\|q) = d_{JS}(p, q)$

► One can define  $D_f(p\|q)$  when  $p \ll q$ : Since  $f$  is convex, and  $f(1) = 0$ , the function  $\frac{f(x)}{x - 1}$  must nondecrease, so there exists  $f'(\infty) := \lim_{x \rightarrow \infty} f(x)/x$ , taking value in  $(-\infty, +\infty]$ . And since for any  $p(x) > 0$ , we have  $\lim_{q(x) \rightarrow 0} q(x)f\left(\frac{p(x)}{q(x)}\right) = p(x)f'(\infty)$ .

## Proposition 4.17

$D_f(p\|q)$  is linear in  $f$ ,  $D_{af+bg}(p\|q) = aD_f(p, q) + bD_g(p\|q)$ .

# Distance Between Distributions

## Proposition 4.18

$D_f = D_g$  if and only if  $f(x) = g(x) + c(x - 1)$  for some  $c \in \mathbb{R}$ .

- › The only  $f$ -divergence that is also a Bregman  $\psi$ -divergence is the KL divergence
- › The only  $f$ -divergence that is also an integral probability metric is the total variation.
- › There is a [variational representation](#) of  $D_f$ , in [Polyanskiy and Wu \(2022\)](#).

## Distance Between Distributions

- Since  $f$  is convex, let  $f^*$  be the convex conjugate of  $f$ . Let  $\text{effdom}(f^*)$  be the effective domain of  $f^*$  (i.e.,  $\text{effdom}(f^*) = \{y : f^*(y) < \infty\}$ )

$$D_f(p; q) = \sup_{g: \Omega \rightarrow \text{effdom}(f^*)} \mathbb{E}_p[g] - \mathbb{E}_q[f^* \circ g]$$

- For example, with the total variation,  $f(x) = \frac{1}{2}|x - 1|$ , its convex conjugate is

$$f^*(x^*) = \begin{cases} x^* \text{ on } [-1/2, 1/2], \\ +\infty \text{ else.} \end{cases}, \text{ and we obtain}$$

$$d_{\text{TV}}(p, q) = \sup_{|g| \leq 1/2} \mathbb{E}_p[g(X)] - \mathbb{E}_q[g(X)].$$

# Distance Between Distributions

- Extending Rényi entropy of order  $\alpha$ ,  $H_\alpha(X) = \frac{1}{1-\alpha} \log \left( \sum_i p(i)^\alpha \right)$ , define

## Definition 4.31: Rényi $\alpha$ -divergence, Rényi (1961)

Given  $\alpha \in (0, \infty)$ , define

$$D_\alpha(p\|q) = \frac{1}{\alpha-1} \log \left( \sum_i \frac{p(i)^\alpha}{q(i)^{\alpha-1}} \right)$$

and for absolutely continuous function

$$D_\alpha(p\|q) = \frac{1}{\alpha-1} \log \left( \int_{\mathbb{R}} \frac{p(x)^\alpha}{q(x)^{\alpha-1}} dx \right) \text{ or } \frac{1}{\alpha-1} \log \left( \int_{\mathbb{R}^k} \frac{p(\mathbf{x})^\alpha}{q(\mathbf{x})^{\alpha-1}} d\mathbf{x} \right).$$

# Distance Between Distributions

- Recall that

$$D_\alpha(p\|q) = \frac{1}{\alpha - 1} \log \left( \sum_i \frac{p(i)^\alpha}{q(i)^{\alpha-1}} \right) \text{ when } \alpha \in (0, \infty).$$

- One can define limiting cases,  $D_0(P\|Q) = -\log Q(\{i : p_i > 0\})$  and  $D_\infty(P\|Q) = \log \sup_i \frac{p_i}{q_i}$
- Observe also that  $D_1(p\|q) = D_{\text{KL}}(p\|q)$

# Distance Between Distributions

**Definition 4.32: Cramér, Cramér (1928a,b) and Székely (2003)**

Consider two measures on  $p$  and  $q$  on  $\mathbb{R}$ . Then define Cramér distance

$$C_k(p, q) = \left( \int_{-\infty}^{\infty} |F_p(x) - F_q(x)|^k dx \right)^{1/k}, \text{ for } k \geq 1$$

- ›  $C_2$  is named "energy-distance" in Székely (2003) and Rizzo and Székely (2016), and "continuous ranked probability score" in Gneiting et al. (2007).
- › It is an Integral Probability Metrics (IPM), since

$$C_k(p, q) = \sup_{\substack{f \in \mathcal{F}_{k'} \\ k^{-1} + k'^{-1} = 1}} |\mathbb{E}[f(X)] - \mathbb{E}[f(Y)]|.$$

$\uparrow \quad \uparrow \quad \uparrow$   
 $k^{-1} + k'^{-1} = 1$        $f \in \mathcal{F}_{k'}$        $X \sim p$        $Y \sim q$

where  $\mathcal{F}_{k'}$  is the set of absolutely continuous functions such that  $\|\nabla f\|_{k'} \leq 1$ .

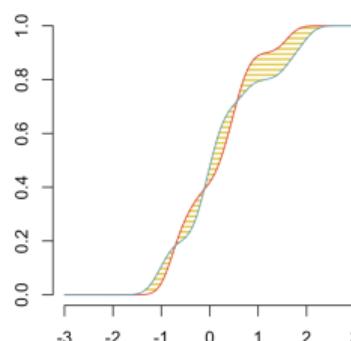
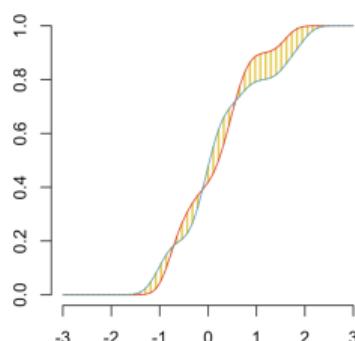
- › For example, if  $k = 1$ ,  $\|\nabla f\|_\infty \leq 1$  (corresponding to 1-Lipschitz functions).

# Distance Between Distributions

## Definition 4.33: Wasserstein, Wasserstein (1969)

Consider two measures on  $p$  and  $q$  on  $\mathbb{R}$ . Then define Wasserstein distance

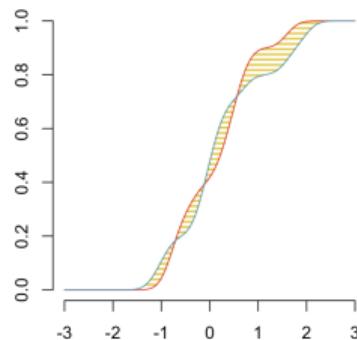
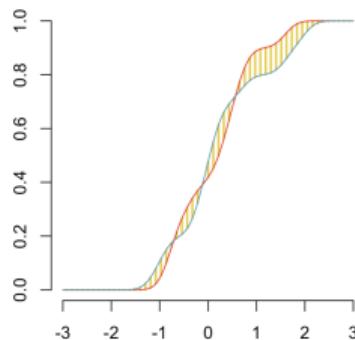
$$W_k(p, q) = \left( \int_0^1 |F_p^{-1}(u) - F_q^{-1}(u)|^k du \right)^{1/k}, \text{ for } k \geq 1$$



```
1 > c2 = function(x) (pnorm(x,0,1)-pnorm(x,1,2))^2
2 > w2 = function(u) (qnorm(u,0,1)-qnorm(u,1,2))^2
3 > sqrt(integrate(c2,-Inf,Inf)$value)
4 [1] 0.5167714
5 > sqrt(integrate(w2,0,1)$value)
6 [1] 1.414214
```

where  $F^{-1}$  denotes the generalized inverse of  $F$ ,  $F^{-1}(u) = \inf_{x \in \mathbb{R}} \{F(x) \geq u\}$ .

# Distance Between Distributions



```
> c1 = function(x) abs(pnorm(x,0,1) -  
+ pnorm(x,1,2))  
> w1 = function(x) abs(qnorm(x,0,1) -  
+ qnorm(x,1,2))  
> integrate(c1,-Inf,Inf)$value  
[1] 1.166631  
> integrate(w1,0,1)$value  
[1] 1.166636
```

## Proposition 4.19: $C_1$ and $W_1$

Consider two measures on  $p$  and  $q$  on  $\mathbb{R}$ .

$$W_1(p, q) = \int_0^1 |F_p^{-1}(u) - F_q^{-1}(u)| du = \int_{-\infty}^{\infty} |F_p(x) - F_q(x)| dx = C_1(p, q).$$

**Proof** See Prokhorov (1956), Dall'Aglio (1956) and Vallender (1974).

## Distance Between Distributions

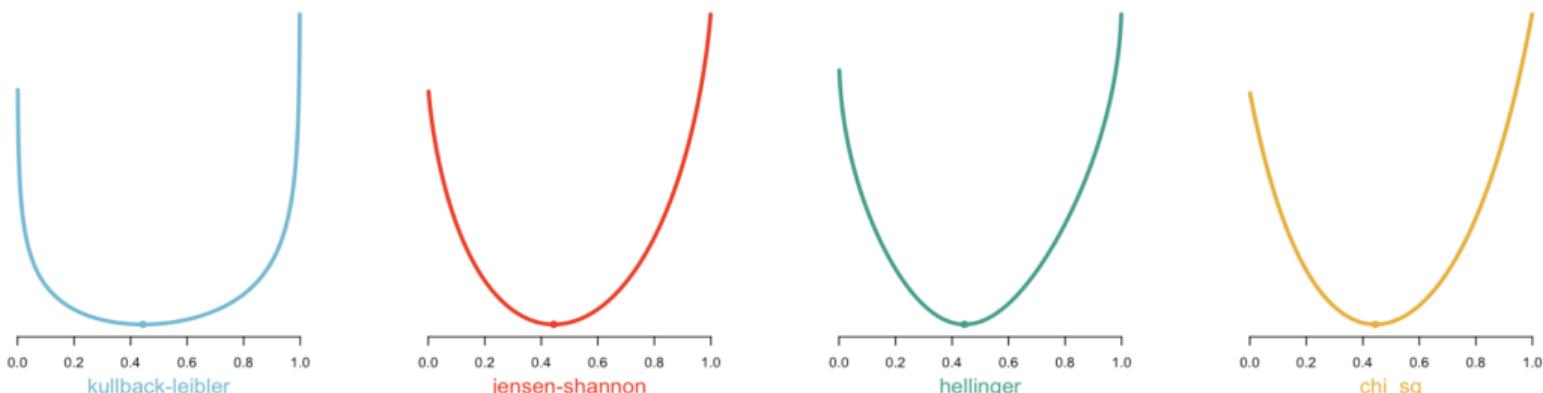
Instead of the geometric proof (see plot above), observe that

$$\begin{aligned}\int_0^1 |F_p^{-1}(u) - F_q^{-1}(u)| du &= \int_0^1 \int_{-\infty}^{\infty} g(u, x) dx du, \quad g(u, x) = 1 \text{ if } \begin{cases} x \in [F_p^{-1}(u), F_q^{-1}(u)] \\ x \in [F_q^{-1}(u), F_p^{-1}(u)] \end{cases} \\ &= \int_{-\infty}^{\infty} \int_0^1 h(u, x) du dx, \quad h(u, x) = 1 \text{ if } \begin{cases} u \in [F_p(x), F_q(x)] \\ u \in [F_q(x), F_p(x)] \end{cases} \\ &= \int_{-\infty}^{\infty} |F_p(x) - F_q(x)| dx\end{aligned}$$

(see Proposition 2.17 in [Santambrogio \(2015\)](#) for a proper justification)

# Distance Between Distributions

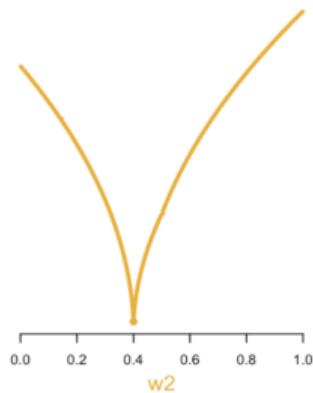
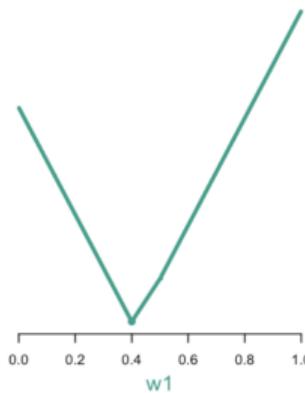
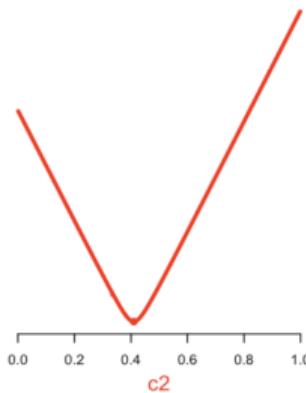
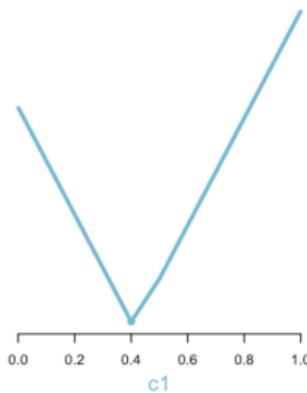
- ›  $\mu$ : multinomial distribution on  $\{0, 1, 10\}$ , with  $\mathbf{p} = (.5, .1, .4)$
- ›  $\nu_\theta$ : binomial type distribution on  $\{0, 10\}$ , with  $\mathbf{q}_\theta = (1 - \theta, \theta)$
- › Let  $\theta^* = \operatorname{argmin}\{d(p, q_\theta)\}$  or  $\theta^* = \operatorname{argmin}\{d(p \| q_\theta)\}$



- › with  $d_{KL}(p \| q_\theta)$ ,  $d_{JS}(p, q_\theta)$ ,  $d_H(p, q_\theta)$  and  $d_{H_{\chi^2}}(p \| q_\theta)$ .

# Distance Between Distributions

- $\mu$ : multinomial distribution on  $\{0, 1, 10\}$ , with  $\mathbf{p} = (.5, .1, .4)$
- $\nu_\theta$ : binomial type distribution on  $\{0, 10\}$ , with  $\mathbf{q}_\theta = (1 - \theta, \theta)$
- Let  $\theta^* = \operatorname{argmin}\{d(p, q_\theta)\}$



- with  $C_1(p, q_\theta)$ ,  $C_2(p, q_\theta)$ ,  $W_1(p, q_\theta)$  and  $W_2(p, q_\theta)$ .

# Distance Between Distributions

## Proposition 4.20

The Wasserstein metric is scale and sum invariant, but does not have unbiased sample gradients.

### Proof Bellemare et al. (2017b)

**Example** If  $x_i$  are drawn from a Bernoulli distribution

› Non-vanishing minimax bias:

$$\forall n, \exists p, q_\theta, |\mathbb{E}(\nabla_\theta W_k^k(\hat{p}_n, q_\theta)) - \nabla_\theta W_k^k(p, q_\theta)| \geq 2e^{-2}$$

› Wrong minimum: in general,

$$\hat{\theta}_n = \operatorname{argmin} \left\{ \mathbb{E}((W_k^k(\hat{p}_n, q_\theta))) \right\} \neq \operatorname{argmin} \left\{ W_k^k(\mathbb{P}, \mathbb{Q}_\theta) \right\} = \theta$$

# Distance Between Distributions

## Proposition 4.21

The Cramér metric is scale and sum invariant.

- ›  $C_k(X + Z, Y + Z) \leq C_k(X, Y)$  whenever  $Z \perp\!\!\!\perp X, Y$  and  $k \geq 1$ , and  
 $C_k(cX, cY) \leq |c|^{1/k} C_k(X, Y)$ .

## Proposition 4.22

$C_2$  has unbiased sample gradients (only  $k = 2$ ),

$$\mathbb{E}(\nabla_{\theta} C_2(\hat{p}_n, q_{\theta})) = \nabla_{\theta} C_2(p, q_{\theta}).$$

## Distance Between Distributions

- Consider first  $W_1$  (earth mover's distance), which was the only distance discussed in Wasserstein (1969). See also Vallender (1974) for an extensive review.
- $W_1$  is an IPM where  $\mathcal{F}$  the set of 1-Lipschitz functions, Kantorovich and Rubinstein (1958), i.e., if  $p$  and  $q$  have bounded support,

$$W_1(p, q) = \sup_{f \in \mathcal{F}} \left\{ \int_{-\infty}^{+\infty} f(x) d(p - q)(x) \right\},$$

$\mathcal{F}$  being the class of 1-Lipschitz functions

### Proposition 4.23: $W_1$ and First Order Dominance

Suppose that  $X_1 \preceq X_2$  (first order dominance,  $F_2^{-1}(u) \geq F_1^{-1}(u)$ ,  $\forall u \in (0, 1)$ ),

$$W_1(p_1, p_2) = \mathbb{E}[X_2] - \mathbb{E}[X_1].$$

# Distance Between Distributions

## Proof

$$W_1(p_1, p_2) = \int_0^1 |F_2^{-1}(u) - F_1^{-1}(u)| du$$

$\geq 0$

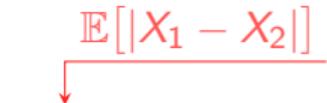
$\mathbb{E}[X_2]$        $\mathbb{E}[X_1]$



then (property discussed later)

$$W_1(p_1, p_2) = \inf_C \int \int |x_2 - x_1| dC(F_1(x_1), F_2(x_2)) = \inf_C \int \int |F_2^{-1}(v) - F_1^{-1}(u)| dC(u, v)$$

$\mathbb{E}[|X_1 - X_2|]$



As discussed in [Vallender \(1974\)](#),

$$\begin{aligned} \mathbb{E}[|X_1 - X_2|] &= \int [\mathbb{P}[X_1 < t, X_2 \geq t] + \mathbb{P}[X_1 \geq t, X_2 < t]] dt \\ &= \int [\mathbb{P}[X_1 < t] + \mathbb{P}[X_2 < t] - 2\mathbb{P}[X_1 < t, X_2 < t]] dt \end{aligned}$$

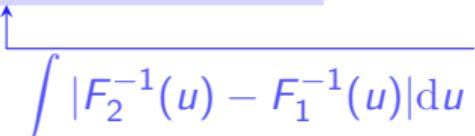
## Distance Between Distributions

$$\mathbb{E}[|X_1 - X_2|] = [F_1(t) + F_2(t) - 2C(F_1(t), F_2(t))] dt$$

From Fréchet-Hoeffding bounds,  $C(u, v) \leq M(u, v) = \min\{u, v\}$  and

$$F_1(t) + F_2(t) - 2C(F_1(t), F_2(t)) \geq F_1(t) + F_2(t) - 2M(F_1(t), F_2(t))$$

$$\mathbb{E}[|X_1 - X_2|] \geq \int \int |F_2^{-1}(v) - F_1^{-1}(u)| dM(u, v)$$



$$\int |F_2^{-1}(u) - F_1^{-1}(u)| du$$

**Example** let  $p_1 \leq p_2$

$$W_1(\mathcal{B}(p_1), \mathcal{B}(p_2)) = p_2 - p_1.$$

# Distance Between Distributions

- › We can also consider  $W_2$

## Proposition 4.24: $C_2$ and $W_2$

Consider two measures on  $p$  and  $q$  on  $\mathbb{R}$ .

$$W_2(p, q)^2 = \int_0^1 |F_p^{-1}(u) - F_q^{-1}(u)|^2 du \text{ while } C_2(p, q) = \int_{-\infty}^{\infty} |F_p(x) - F_q(x)|^2 dx.$$

# Distance Between Distributions

## Proposition 4.25: $W_2$ for Gaussian / Bernoulli distributions

Consider two Gaussian distributions, then

$$W_2(\mathcal{N}(\mu_1, \sigma_1^2), \mathcal{N}(\mu_2, \sigma_2^2))^2 = (\mu_1 - \mu_2)^2 + (\sigma_1 - \sigma_2)^2,$$

and for two Bernoulli distributions, if  $p_1 \leq p_2$

$$W_2(\mathcal{B}(p_1), \mathcal{B}(p_2)) = \sqrt{p_2 - p_1}.$$

## Distance Between Distributions

### Proposition 4.26: Representation for $W_2$

Consider two measures on  $p$  and  $q$  on  $\mathbb{R}$ .

$$W_2(p, q)^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (F_p(\min\{x, y\}) - F_q(\max\{x, y\}))_+ + (F_q(\min\{x, y\}) - F_p(\max\{x, y\}))_+ dx dy$$

or

$$W_2(p, q)^2 = 2 \int_{-\infty}^{\infty} \int_x^{\infty} [(F_p(x) - F_q(y))_+ + (F_q(x) - F_p(y))_+] dx dy$$

**Proof** Since  $W_2(p, q)^2 = \int_0^1 |F_p^{-1}(u) - F_q^{-1}(u)|^2 du$  observe that

$$F_p^{-1}(u) - F_q^{-1}(u) = F_p^{-1}(u) - F_p^{-1}(F_p(F_q^{-1}(u))) = F_p^{-1}(u) - F_p^{-1}(G(u)) \text{ where } G = F_p \circ F_q^{-1}.$$

## Distance Between Distributions

Since  $F_q$  is continuously differentiable, so that  $H = F'_p \circ F_p^{-1}$ , then

$$F_p^{-1}(u) - F_q^{-1}(u) = \int_{G(u)}^u \frac{dt}{H(t)}$$

and write

$$(F_p^{-1}(u) - F_q^{-1}(u))^2 = \int_{G(u)}^u \frac{dt}{H(t)} \frac{dv}{H(v)}$$

and depending on whether  $G(u) \leq u$  or  $u \leq G(u)$ , we can write

$$\begin{aligned} \int_0^1 (F_p^{-1}(u) - F_q^{-1}(u))^2 du &= \int_0^1 \int_0^1 (G^{-1}(\min\{t, v\}) - \max\{r, v\})_+ \\ &\quad + (\min\{t, v\} - G^{-1}(\max\{t, v\}))_+ dt dv. \end{aligned}$$

And finally, let  $t = F_p(x)$  and  $v = F_q(y)$ , so that  $G^{-1}(t) = F_q(x)$  and  $G^{-1}(v) = F_q(y)$ , and we get the desired expression.

# Distance Between Distributions

- › We can finally consider  $W_\infty$

## Proposition 4.27: $W_\infty$

Consider two measures on  $p$  and  $q$  on  $\mathbb{R}$ .

$$W_\infty(p, q) = \sup_{u \in (0,1)} |F_p^{-1}(u) - F_q^{-1}(u)|.$$

Furthermore,  $W_\infty(p, q)$  is the infimum over all  $h \geq 0$  such that

$$F_q(x - h) \leq F_p(x) \leq F_q(x + h), \text{ for all } x \in \mathbb{R}.$$

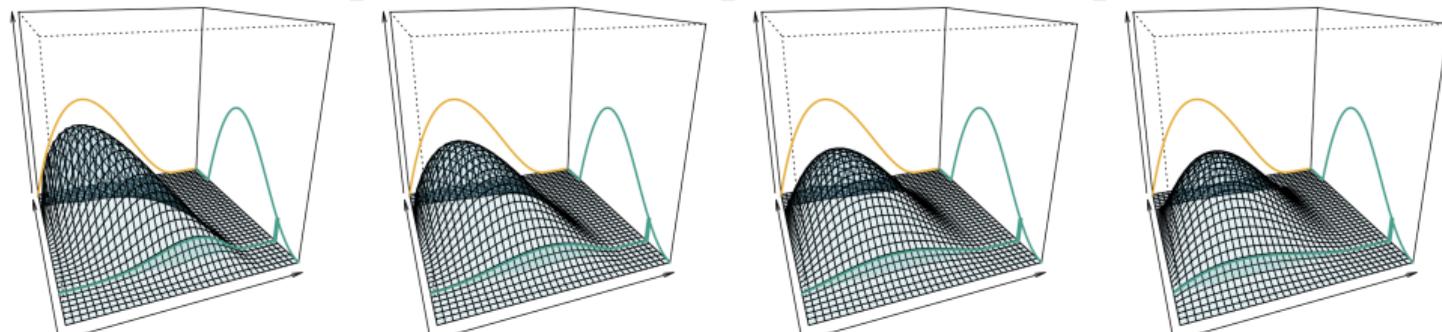
# Optimal transport and Wasserstein distance

## Definition 4.34: Wasserstein, Wasserstein (1969)

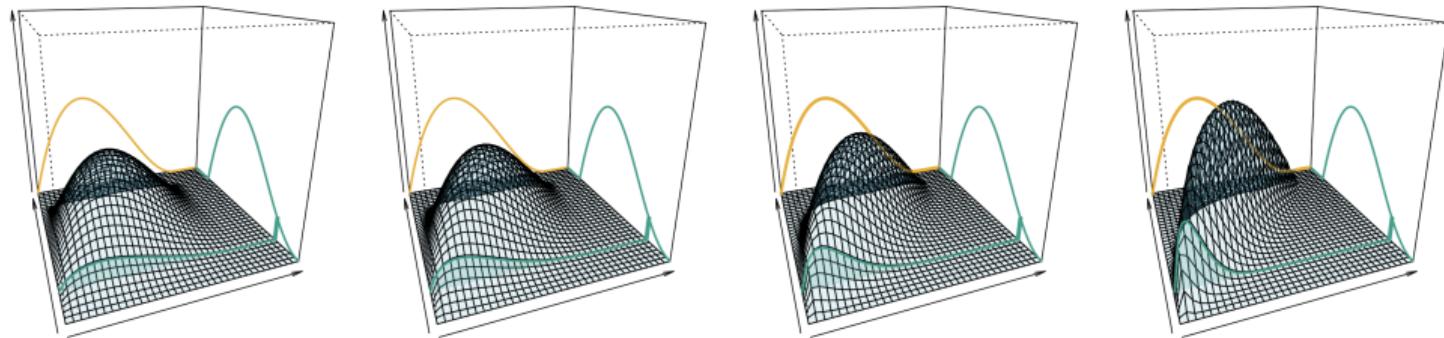
Consider two measures on  $p$  and  $q$  on  $\mathbb{R}^k$ , with a norm  $\|\cdot\|$  (on  $\mathbb{R}^k$ ). Then define

$$W_k(p, q) = \left( \inf_{\pi \in \Pi(p, q)} \int_{\mathbb{R}^k \times \mathbb{R}^k} \|x - y\|^k d\pi(x, y) \right)^{1/k},$$

where  $\Pi(p, q)$  is the set of all couplings of  $p$  and  $q$ .



# Optimal transport and Wasserstein distance



## Definition 4.35: Kantorovich Problem

Kantorovich Problem is defined as

$$W_c(p, q) = \inf_{\pi \in \Pi(p, q)} \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) d\pi(\mathbf{x}, \mathbf{y}),$$

for cost function  $c$  (or loss function).



# Optimal transport and Monge mapping

## Definition 4.36: Push-Forward and Transport Map

Given two metric spaces  $\mathcal{X}$  and  $\mathcal{Y}$ , a measurable map  $T : \mathcal{X} \rightarrow \mathcal{Y}$  and a measure  $\mu$  on  $\mathcal{X}$ . The **push-forward** of  $\mu$  by  $T$  is the measure  $\nu = T_{\#}\mu$  on  $\mathcal{Y}$  defined by

$$\forall \mathcal{B} \subset \mathcal{Y}, \quad T_{\#}\mu(\mathcal{B}) = \mu(T^{-1}(\mathcal{B})).$$

- By the change-of-variable formula

## Proposition 4.28: Push-Forward and Transport Map

For all measurable and bounded  $\varphi : \mathcal{Y} \rightarrow \mathbb{R}$ ,

$$\int_{\mathcal{Y}} \varphi(y) dT_{\#}\mu(y) = \int_{\mathcal{X}} \varphi(T(x)) d\mu(x).$$

# Optimal transport and Monge mapping

- › If  $\mathcal{Y}$  is a finite set  $\{\mathbf{y}_1, \dots, \mathbf{y}_n\}$ ,

$$T_{\#}\mu = \sum_{i=1}^n \mu(T^{-1}(\{\mathbf{y}_i\})) \cdot \delta_{\{\mathbf{y}_i\}}$$

- › If  $\mathcal{X}$  is a single atom,  $\{\mathbf{x}\}$ ,  $\mu = \delta_{\mathbf{x}}$  and  $T_{\#}\mu(\mathcal{B}) = \mu(T^{-1}(\mathcal{B})) = \delta_{T(\mathbf{x})}$ . If  $\text{Card}(\text{support}(\nu)) > 1$ , there is no transport map.
- › One solution is to allow mass to split, leading to Kantorovich's relaxation of Monge's problem

## Proposition 4.29: Existence of a map

If  $\mathcal{X} = \mathcal{Y}$  is a compact subset of  $\mathbb{R}^k$ , if  $\mu$  and  $\nu$  are two measures, and if  $\mu$  is atomless, then there exists  $T$  such that  $\nu = T_{\#}\mu$ .

see Santambrogio (2015).

# Optimal transport and Monge mapping

- › If  $\mathcal{X}$  and  $\mathcal{Y}$  are two sets of  $\mathbb{R}^k$ , and if measures  $\mu$  and  $\nu$  are absolutely continuous, with densities  $f$  and  $g$  (w.r.t. Lebesgue measure),

$$\int_{\mathcal{Y}} \varphi(\mathbf{y}) g(\mathbf{y}) d\mathbf{y} = \int_{\mathcal{X}} \varphi(T(\mathbf{x})) \cdot \underbrace{g(T(\mathbf{x})) \det \nabla T(\mathbf{x})}_{=f(\mathbf{x})} \cdot d\mathbf{x}.$$

## Definition 4.37: Monge Problem

Monge problem

$$\inf_{T \# \mu = \nu} \int_{\mathcal{X}} c(\mathbf{x}, T(\mathbf{x})) d\mathbb{P}_{\mathbf{A}}(\mathbf{x}),$$

for cost function  $c$ .



- › Note that the constraint and the objective function are non-convex.

# Optimal transport and Monge mapping

## Theorem 4.1: Optimal map for continuous univariate distributions

The optimal Monge map  $T^*$  for some strictly convex cost  $c$  such that  $T_\#^* \mathbb{P}_A = \mathbb{P}_B$  is  $T^* = F_B^{-1} \circ F_A$ .

- $T^*$  is an increasing mapping.

### Example Univariate Gaussian

$$x_B = T^*(x_A) = \mu_B + \sigma_B \sigma_A^{-1} (x_A - \mu_A).$$

# Optimal transport and Monge mapping

**Theorem 4.2: Optimal map for continuous multivariate distributions, Brenier (1991)**

With a quadratic cost, the optimal Monge map  $T^*$  is unique, and it is the gradient of a convex function,  $T^* = \nabla\varphi$ .

**Example** Multidimensional Gaussian

$$\mathbf{x}_B = T^*(\mathbf{x}_A) = \boldsymbol{\mu}_B + \mathbf{A}(\mathbf{x}_A - \boldsymbol{\mu}_A),$$

where  $\mathbf{A}$  is a symmetric positive matrix that satisfies  $\mathbf{A}\boldsymbol{\Sigma}_A\mathbf{A} = \boldsymbol{\Sigma}_B$ , which has a unique solution given by  $\mathbf{A} = \boldsymbol{\Sigma}_A^{-1/2} (\boldsymbol{\Sigma}_A^{1/2} \boldsymbol{\Sigma}_B \boldsymbol{\Sigma}_A^{1/2})^{1/2} \boldsymbol{\Sigma}_A^{-1/2}$ , where  $\mathbf{M}^{1/2}$  is the square root of the square (symmetric) positive matrix  $\mathbf{M}$  based on the Schur decomposition ( $\mathbf{M}^{1/2}$  is a positive symmetric matrix), as described in Higham (2008).

# Optimal transport and Monge mapping

Gangbo (1999) proved, when  $\mathcal{X} = \mathcal{Y}$  is a compact subset of  $\mathbb{R}$ , the infimum in Monge problem and the minimum in Kantorovich problem coincide, if  $\mu$  is atomless,

## Proposition 4.30: Monge/Kantorovich Problems

$\mathcal{X} = \mathcal{Y}$  is a compact subset of  $\mathbb{R}^k$  and if  $\mu$  is atomless,

$\min\{\text{Monge problem, see Def. 4.37}\} = \min\{\text{Kantorovich problem, see Def. 8.17}\}.$

## Optimal transport (discrete)

- One can consider optimal transport for empirical measures,  $\mathbb{P} = \sum_{i=1}^n \omega_i \delta_{x_i}$ .
- With uniform weights and  $n$  points for  $\mathbb{P}_A$  and  $\mathbb{P}_B$ ,  $W_k^k$  is the **optimal matching cost** (Hungarian algorithm, [Kuhn \(1955, 1956\)](#)), cast as a linear program

$$W_k(\mathbb{P}_A, \mathbb{P}_B) = \left( \min_{s \in \mathcal{S}_n} \frac{1}{n} \sum_{i=1}^n d(x_i, y_{s(i)})^k \right)^{1/k},$$

where  $\mathcal{S}_n$  is the set of permutations on  $\{1, 2, \dots, n\}$ .

## Optimal transport (discrete)

- Consider the set of  $n \times n$  doubly-stochastic matrices,

$$D_n = \{M \in \mathbb{R}_+^{n \times n} : M\mathbf{1}_n = \mathbf{1}_n \text{ and } M^\top \mathbf{1}_n = \mathbf{1}_n\},$$

and the subset of permutation matrices,

$$U_n = \{M \in \{0, 1\}^{n \times n} : M\mathbf{1}_n = \mathbf{1}_n \text{ and } M^\top \mathbf{1}_n = \mathbf{1}_n\}.$$

- Let  $C$  denote the cost matrix,  $C_{i,j} = d(x_i, y_j)^k$ , then

$$W_k(\mathbf{x}, \mathbf{y})^k = \underset{P \in U_n}{\operatorname{argmin}} \left\{ \langle P, C \rangle \right\}, \text{ where } \langle P, C \rangle = \sum_{i=1}^n \sum_{j=1}^n P_{i,j} C_{i,j} \quad (1)$$

and “optimal transport” permutation matrix

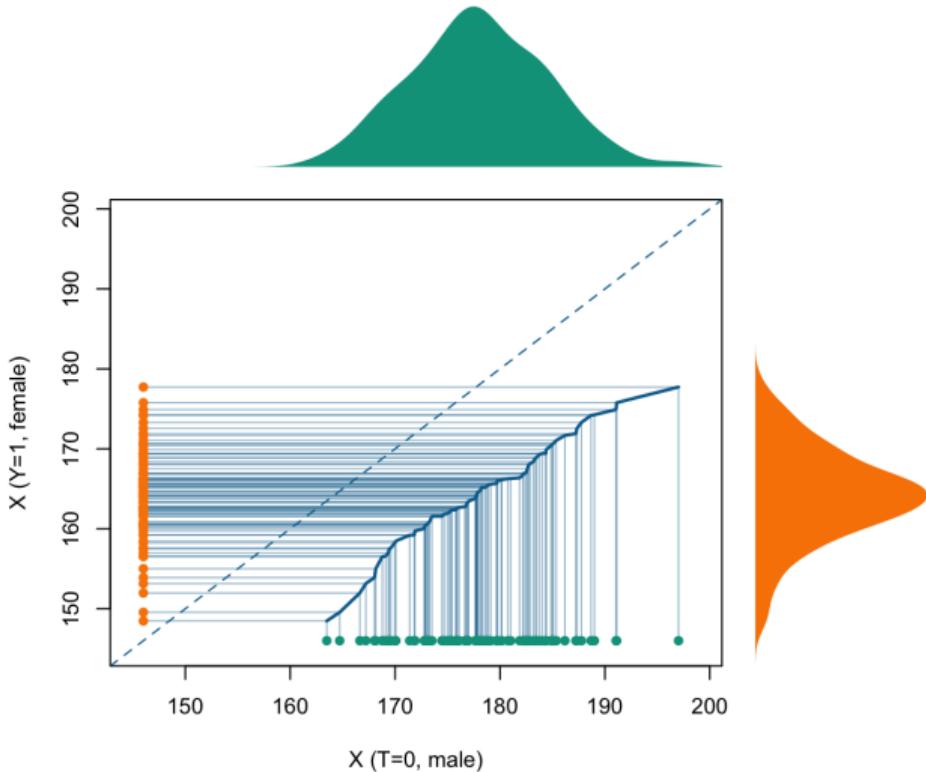
$$P^* \in \underset{P \in U_n}{\operatorname{argmin}} \left\{ \langle P, C \rangle \right\} \quad (2)$$

## Optimal transport (discrete)

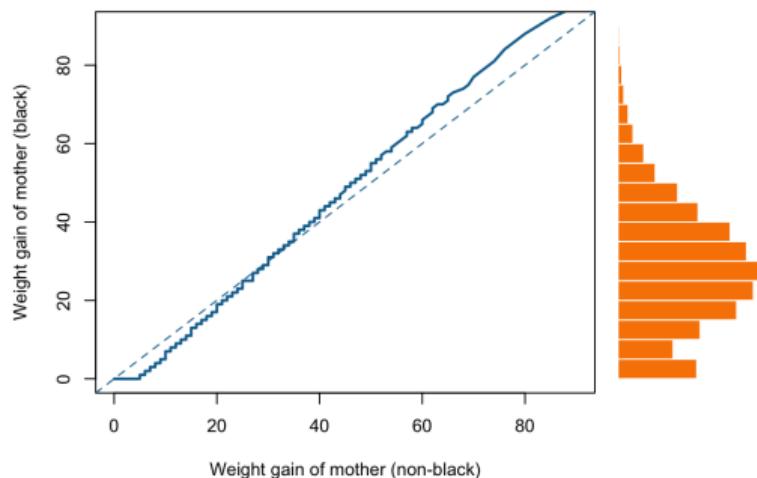
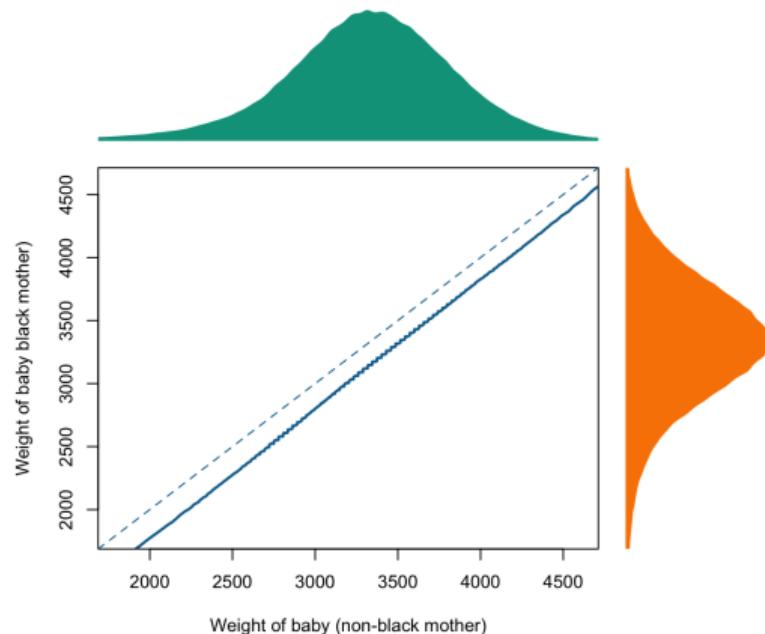
	7	8	9	10	11	12	
1	0.41	0.55	0.22	0.64	0.04	0.25	
2	0.28	0.24	0.73	0.22	0.64	0.80	
3	0.28	0.47	0.32	0.52	0.16	0.37	
4	0.28	0.62	0.81	0.25	0.64	0.85	
5	0.41	0.37	0.89	0.25	0.81	0.97	
6	0.66	0.76	0.21	0.89	0.22	0.14	
	7	8	9	10	11	12	
1	.	.	.	.	1	.	$1 \leftrightarrow 11$
2	.	1	.	.	.	.	$2 \leftrightarrow 8$
3	.	.	1	.	.	.	$3 \leftrightarrow 9$
4	1	.	.	.	.	.	$4 \leftrightarrow 7$
5	.	.	.	1	.	.	$5 \leftrightarrow 10$
6	.	.	.	.	.	1	$6 \leftrightarrow 12$

# Optimal transport (discrete)

- Consider two samples, with the height of **men** and **women** (both groups of size  $n$ ).
- On the following graph, we can visualize the optimal matching of individuals in the two groups.
- It is a **monotone mapping**.



# Optimal transport (discrete)



- Two groups, with **black** and **non-black** mothers, delivering babies (in the U.S.)
- $x_1 \leftrightarrow x_1$  (newborn weight) and  $x_2 \leftrightarrow x_2$  (weight gain of the mother)

# Optimal transport (discrete)

## Proposition 4.31: Hardy–Littlewood–Pólya inequality, [Hardy et al. \(1952\)](#)

Given  $x_1 \leq \dots \leq x_n$  and  $y_1 \leq \dots \leq y_n$   $n$  pairs of ordered real numbers, for every permutation  $\sigma$  of  $\{1, 2, \dots, n\}$ ,

$$\sum_{i=1}^n x_i y_{n+1-i} \leq \sum_{i=1}^n x_i y_{\sigma(i)} \leq \sum_{i=1}^n x_i y_i.$$

- various implications, e.g. bounds on the covariance, and the correlation, see Proposition 4.35.
- This can be extended to more general function  $\Phi(x_i, y_j)$ .



## Optimal transport (discrete)

### Definition 4.38: Supermodular, Topkis (1998)

Function  $\Phi : \mathbb{R}^k \times \mathbb{R}^k \rightarrow \mathbb{R}$  is **supermodular** if for any  $z, z' \in \mathbb{R}^k$ ,

$$\Phi(z \wedge z') + \Phi(z \vee z') \geq \Phi(z) + \Phi(z'),$$

where  $z \wedge z'$  and  $z \vee z'$  denote respectively the maximum and the minimum componentwise. If  $-\Phi$  is supermodular,  $\Phi$  is said to be submodular.

## Optimal transport (discrete)

### Proposition 4.32: Hardy–Littlewood–Pólya inequality, [Hardy et al. \(1952\)](#)

Given  $x_1 \leq \cdots \leq x_n$  and  $y_1 \leq \cdots \leq y_n$   $n$  pairs of ordered real numbers, and some supermodular function  $\Phi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ , for every permutation  $\sigma$  of  $\{1, 2, \dots, n\}$ ,

$$\sum_{i=1}^n \Phi(x_i, y_{n+1-i}) \leq \sum_{i=1}^n \Phi(x_i, y_{\sigma(i)}) \leq \sum_{i=1}^n \Phi(x_i, y_i),$$

while if  $\Phi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  is submodular,

$$\sum_{i=1}^n \Phi(x_i, y_i) \leq \sum_{i=1}^n \Phi(x_i, y_{\sigma(i)}) \leq \sum_{i=1}^n \Phi(x_i, y_{n+1-i}).$$

- » Functions  $\Phi(x, y) = \gamma(x - y)$  for some concave function  $\gamma : \mathbb{R} \rightarrow \mathbb{R}$ , such as  $\Phi(x, y) = -|x - y|^k$  with  $k \geq 1$ , are supermodular.

# Optimal transport (discrete)

```
1 > permutations = function(n){  
2 +   if(n==1){  
3 +     return(matrix(1))  
4 +   } else {  
5 +     sp = permutations(n-1)  
6 +     p = nrow(sp)  
7 +     A = matrix(nrow=n*p,ncol=n)  
8 +     for(i in 1:n){  
9 +       A[(i-1)*p+1:p,] =  
10 +         cbind(i,sp+(sp>=i))  
11 +     }  
12 +   return(A)  
13 + }  
14 + }
```

$$\Phi(x, y) = (x - y)^2, \text{ submodular function,}$$

› Consider  $x_1 \leq \dots \leq x_n$

```
1 > Phi = function(x,y) sum((x-y)^2)  
2 > set.seed(1)  
3 > x = sort(x)  
4 > y = y[1:6]  
5 > vect = permutations(6)  
6 > MY = matrix(vect, ncol=6)  
7 > MPhi = function(i) Phi(x, y[MY[i,]])  
8 > S = Vectorize(MPhi)(1:nrow(MY))  
9 > y[MY[which.min(S),]]  
10 [1] 0.046 0.288 0.409 0.788 0.883 0.940
```

## Optimal transport (discrete)

- In a very general setting (with  $n_A \neq n_B$ ), if  $\mathbf{a}_A \in \mathbb{R}_+^{n_A}$  and  $\mathbf{a}_B \in \mathbb{R}_+^{n_B}$  satisfy  $\mathbf{a}_A^\top \mathbf{1}_{n_A} = \mathbf{a}_B^\top \mathbf{1}_{n_B}$  (identical sums), define

$$U(\mathbf{a}_A, \mathbf{a}_B) = \{M \in \mathbb{R}_+^{n_A \times n_B} : M\mathbf{1}_{n_B} = \mathbf{a}_A \text{ and } M^\top \mathbf{1}_{n_A} = \mathbf{a}_B\}.$$

This set of matrices is a **convex transportation polytope** (see Brualdi (2006)).

- In our case, let  $U_{n_A, n_B}$  denote  $U\left(\mathbf{1}_{n_A}, \frac{n_A}{n_B} \mathbf{1}_{n_B}\right)$  ( $U_{n, n}$  is the set of permutation matrices associated with  $\mathcal{S}_n$ ). Let  $C$  denote the cost matrix,  $C_{i,j} = d(x_i, y_j)^k$ .

$$W_k(\mathbf{x}, \mathbf{y})^k = \underset{P \in U_{n_A, n_B}}{\operatorname{argmin}} \left\{ \langle P, C \rangle \right\}, \text{ where } \langle P, C \rangle = \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} P_{i,j} C_{i,j} \quad (3)$$

and “optimal transport”

$$P^* \in \underset{P \in U_{n_A, n_B}}{\operatorname{argmin}} \left\{ \langle P, C \rangle \right\} \quad (4)$$

## Optimal transport (discrete)

	7	8	9	10	11	12	13	14	15	16
1	0.41	0.55	0.22	0.64	0.04	0.25	0.24	0.77	0.74	0.55
2	0.28	0.24	0.73	0.22	0.64	0.80	0.76	0.76	0.12	0.10
3	0.28	0.47	0.32	0.52	0.16	0.37	0.27	0.68	0.63	0.45
4	0.28	0.62	0.81	0.25	0.64	0.85	0.58	0.32	0.51	0.48
5	0.41	0.37	0.89	0.25	0.81	0.97	0.91	0.81	0.05	0.25
6	0.66	0.76	0.21	0.89	0.22	0.14	0.33	0.96	0.99	0.79

	7	8	9	10	11	12	13	14	15	16
1	.	.	1/5	.	3/5	.	1/5	.	.	.
2	.	2/5	.	.	.	.	.	.	.	3/5
3	3/5	.	.	.	.	.	2/5	.	.	.
4	.	.	.	2/5	.	.	.	3/5	.	.
5	.	1/5	.	1/5	.	.	.	.	3/5	.
6	.	.	2/5	.	.	3/5	.	.	.	.

## Optimal transport (discrete)

- From Kantorovich (1942), one can use the dual linear programming problem

$$W_k(\mathbf{a}, \mathbf{b})^k = \begin{cases} \text{primal}(\mathbf{a}, \mathbf{b}, \mathbf{C}) = \min_{P \in U_{\mathbf{a}, \mathbf{b}}} \{\langle P, \mathbf{C} \rangle\} \\ \quad \text{or} \\ \text{dual}(\mathbf{a}, \mathbf{b}, \mathbf{C}) = \max_{(\mathbf{u}, \mathbf{v}) \in M_{\mathbf{C}}} \{\mathbf{u}^\top \mathbf{a} + \mathbf{v}^\top \mathbf{b}\} \end{cases}$$

where  $M_{\mathbf{C}} = \{(\mathbf{u}, \mathbf{v}) \in \mathbb{R}^{n_A + n_B} \mid u_i + v_j \leq C_{i,j}\}$ .

- If  $n_A \sim n_B \sim n$ ,  $O(n^3 \log(n))$  problem.

Set  $\psi_{\mathbf{b}}(\mathbf{a}, \mathbf{C}) = \max_{(\mathbf{u}, \mathbf{v}) \in M_{\mathbf{C}}} \{\mathbf{u}^\top \mathbf{a} + \mathbf{v}^\top \mathbf{b}\}$ ,  $\mathbf{a} \mapsto \psi_{\mathbf{b}}(\mathbf{a}, \mathbf{C})$  is a convex non-smooth map.

- The dual optimum  $\mathbf{u}^*$  is subgradient of  $\mathbf{a} \mapsto \psi_{\mathbf{b}}(\mathbf{a}, \mathbf{C})$ .
- If  $k = 2$  (Euclidean distance), convex quadratic problem.

## Optimal transport (discrete)

- Given  $P \in U_{n_A, n_B}$ , define the **entropy** as

$$\mathcal{E}(P) = - \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} P_{i,j} \log P_{i,j} \text{ or } \mathcal{E}'(P) = - \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} P_{i,j} [\log P_{i,j} - 1]$$

and consider the  $\gamma$ -regularized optimal transport problem

$$P_\gamma^* = \underset{P \in U_{n_A, n_B}}{\operatorname{argmin}} \left\{ \langle P, C \rangle - \gamma \mathcal{E}(P) \right\} \quad (5)$$

since the problem is strictly convex.

- The Lagrangian is here

$$\mathcal{L}(P, \lambda_A, \lambda_B) = \langle P, C \rangle - \gamma \mathcal{E}(P) - \langle \lambda_A, P \mathbf{1}_{n_B} - \mathbf{1}_{n_A} \rangle - \langle \lambda_B, P^\top \mathbf{1}_{n_A} - \mathbf{1}_{n_B} \rangle$$

## Optimal transport (discrete)

and the first order conditions are

$$C_{i,j} + \gamma \log(P_{i,j}) - \lambda_{A,i} - \lambda_{B,j} = 0,$$

i.e.

$$P_{i,j} = \exp[\lambda_{A,i} - C_{i,j} + \lambda_{B,j}] \text{ or } P = D_A \exp[-C] D_B$$

where  $D_A$  and  $D_B$  are diagonal matrices.

- This can be related to the [Doubly Stochastic Scaling Problem](#): let  $A$  be some  $n \times n$  matrix with positive coefficients, we want to find  $D_A$  and  $D_B$  two positive diagonal matrices ( $n \times n$ ) such that  $D_A A D_B$  is doubly stochastic (see [Parlett and Landis \(1982\)](#))
- More generally, this corresponds to the [Matrix Scaling Problem](#): Let  $A$  be some  $n_A \times n_B$  matrix with positive coefficients, we want to find  $D_A$  and  $D_B$  two positive diagonal matrices (respectively  $n_A \times n_A$  and  $n_B \times n_B$ ) such that  $D_A A D_B$  is in  $U(\mathbf{a}_A, \mathbf{a}_B)$ .

## Optimal transport (discrete)

### Theorem 4.3: Sinkhorn - Matrix Scaling, Sinkhorn (1962)

For any matrix  $\mathbf{A}$   $n \times m$  with positive entries, for any  $\mathbf{a}$  and  $\mathbf{b}$  in the simplex, there exist unique  $\mathbf{u} \in \mathbb{R}_+^n$  and  $\mathbf{v} \in \mathbb{R}_+^m$  such that

$$\text{diag}[\mathbf{u}] \mathbf{A} \text{diag}[\mathbf{v}] \in U_{\mathbf{a}, \mathbf{b}}.$$

- Sinkhorn and Knopp (1967) (extending Sinkhorn (1962, 1964, 1966)) suggested the following algorithm (updating alternatively  $D_A$  and  $D_B$ )

$$\begin{cases} D_A^{(t)} = \text{diag}(\mathbf{a}_A / (AD_B)^{(t-1)}) \\ D_B^{(t)} = \text{diag}(\mathbf{a}_B / (AD_A)^{(t)}) \end{cases}$$

(where the division here is element-wise).

## Optimal transport (discrete)

- An alternative way to write the entropic optimization problem is

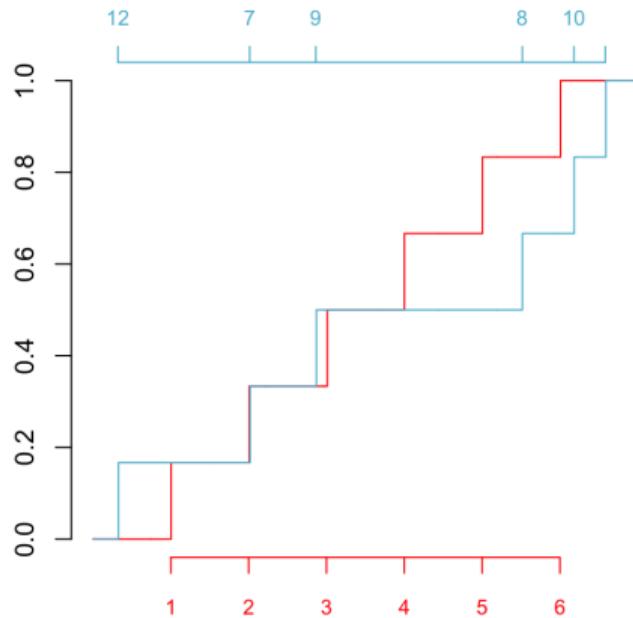
$$P_{\gamma}^* = \underset{P \in U_{\mathbf{a}_A, \mathbf{a}_B}}{\operatorname{argmin}} \left\{ \langle P, C \rangle + \gamma \cdot d_{\text{KL}}(P || \mathbf{a}_A \otimes \mathbf{a}_B) \right\} \quad (6)$$

Using mutual information here makes it easier to extend to the continuous case...

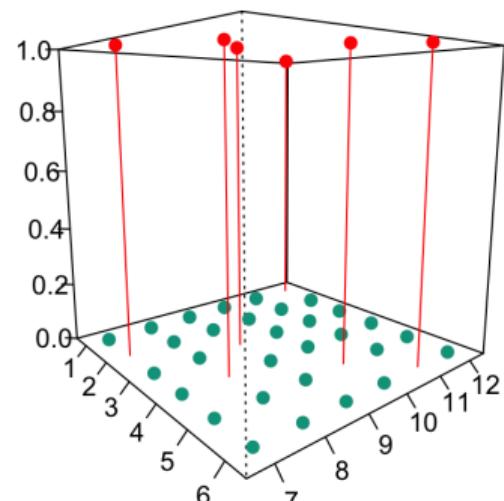
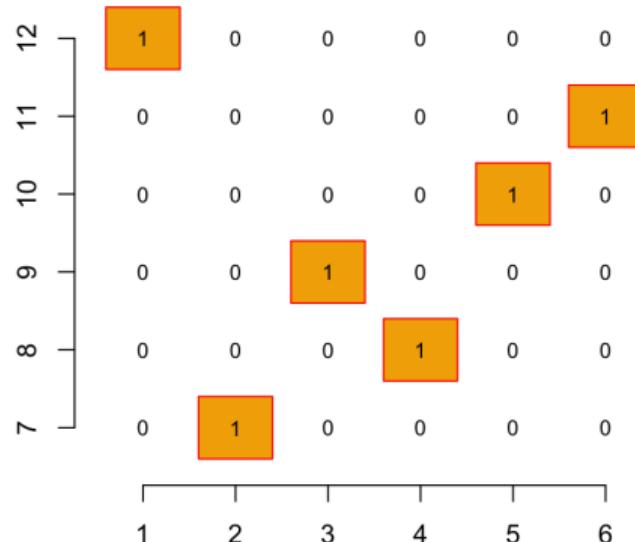
- The extension of Sinkhorn algorithm is the coordinate descent/ascent algorithm.

# Optimal transport (discrete)

```
1 > set.seed(123)
2 > x = (1:6)/7
3 > y = runif(9)
4 > x
5 [1] 0.14 0.29 0.43 0.57 0.71 0.86
6 > y[1:6]
7 [1] 0.29 0.79 0.41 0.88 0.94 0.05
8 > library(T4transport)
9 > Wxy = wasserstein(x,y[1:6])
10 > Wxy$plan
```

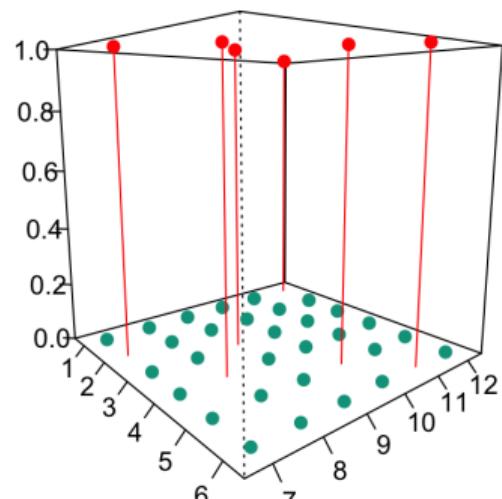
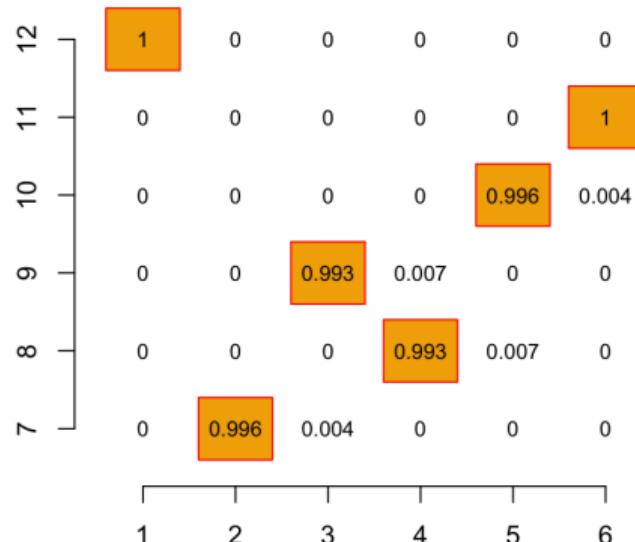


# Optimal transport (discrete)



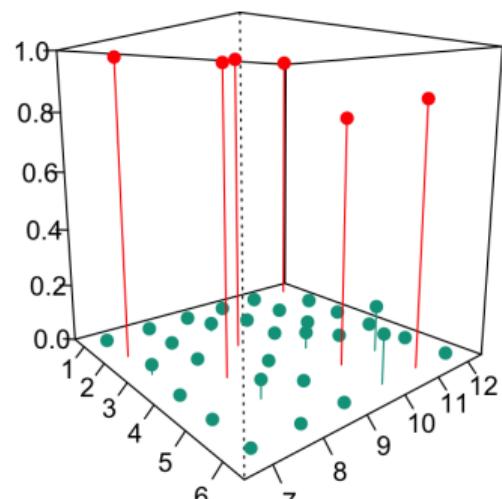
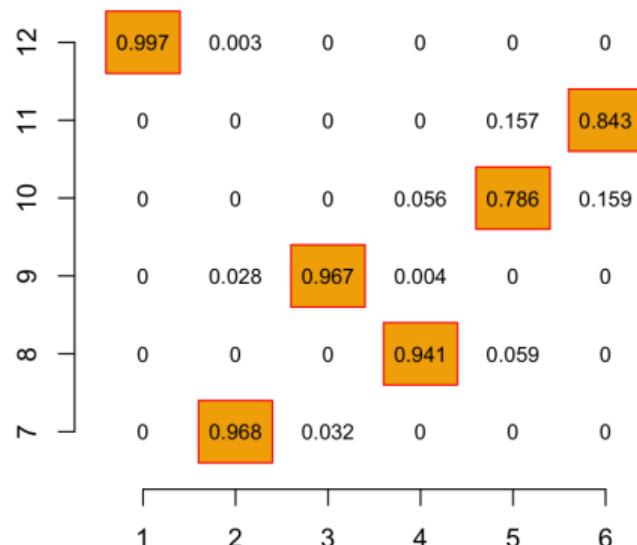
```
1 > Wxy = wasserstein(x,y[1:6])
2 > Wxy$plan
```

# Optimal transport (discrete)



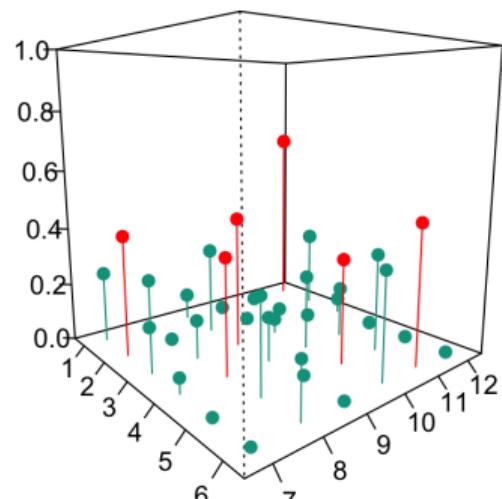
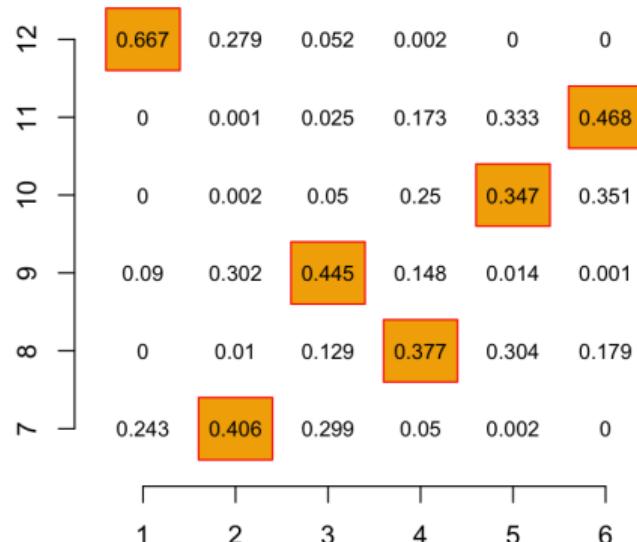
```
1 > Sxy = sinkhorn(x, y[1:6], p = 2, lambda = 0.001)
2 > Sxy$plan
```

# Optimal transport (discrete)



```
1 > Sxy = sinkhorn(x, y[1:6], p = 2, lambda = 0.005)
2 > Sxy$plan
```

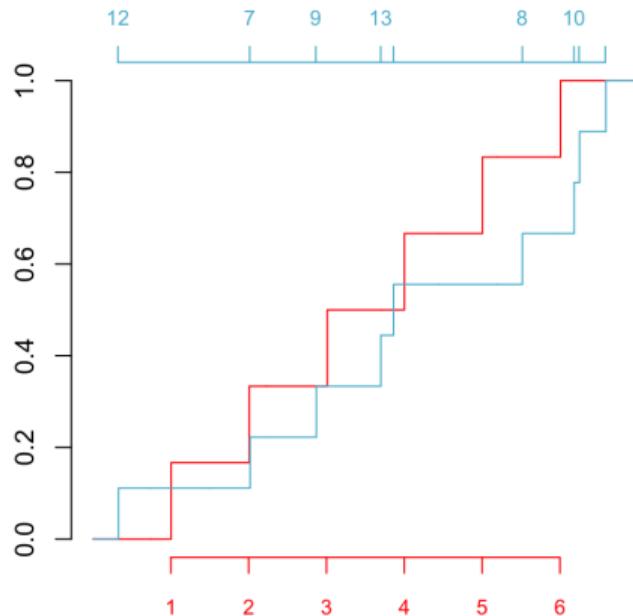
# Optimal transport (discrete)



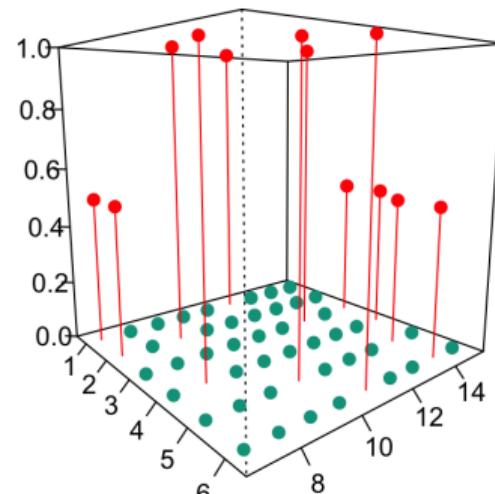
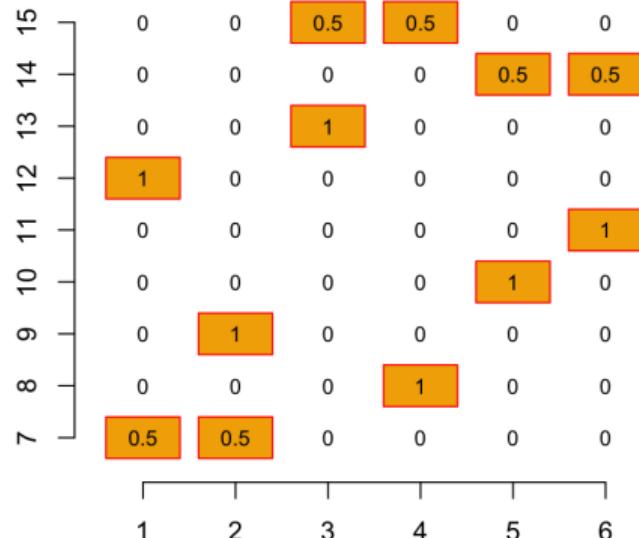
```
1 > Sxy = sinkhorn(x, y[1:6], p = 2, lambda = 0.05)
2 > Sxy$plan
```

# Optimal transport (discrete)

```
1 > y
2 [1] 0.29 0.79 0.41 0.88 0.94 0.05
3 [7] 0.53 0.89 0.55
4 > library(T4transport)
5 > Wxy = wasserstein(x,y)
6      [,1] [,2] [,3] [,4] [,5] [,6]
7 [1,] 0.5   0.5   0.0   0.0   0.0   0.0
8 [2,] 0.0   0.0   0.0   1.0   0.0   0.0
9 [3,] 0.0   1.0   0.0   0.0   0.0   0.0
10 [4,] 0.0   0.0   0.0   0.0   1.0   0.0
11 [5,] 0.0   0.0   0.0   0.0   0.0   1.0
12 [6,] 1.0   0.0   0.0   0.0   0.0   0.0
13 [7,] 0.0   0.0   1.0   0.0   0.0   0.0
14 [8,] 0.0   0.0   0.0   0.0   0.5   0.5
15 [9,] 0.0   0.0   0.5   0.5   0.0   0.0
```

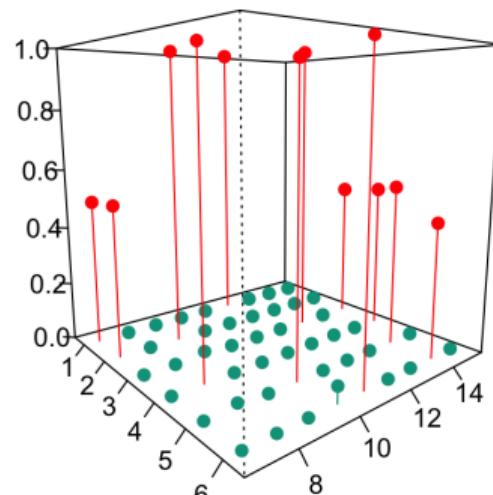
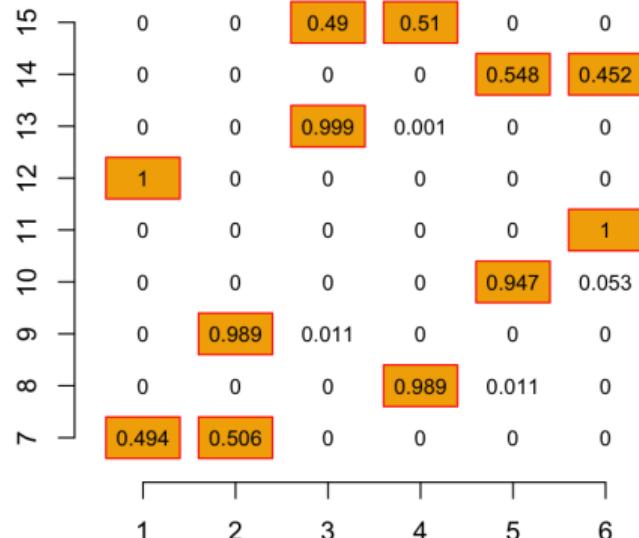


# Optimal transport (discrete)



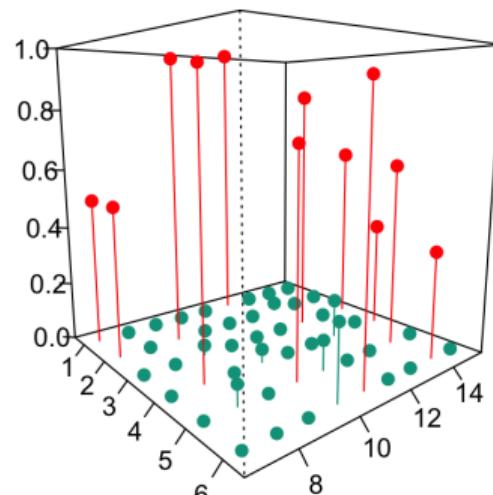
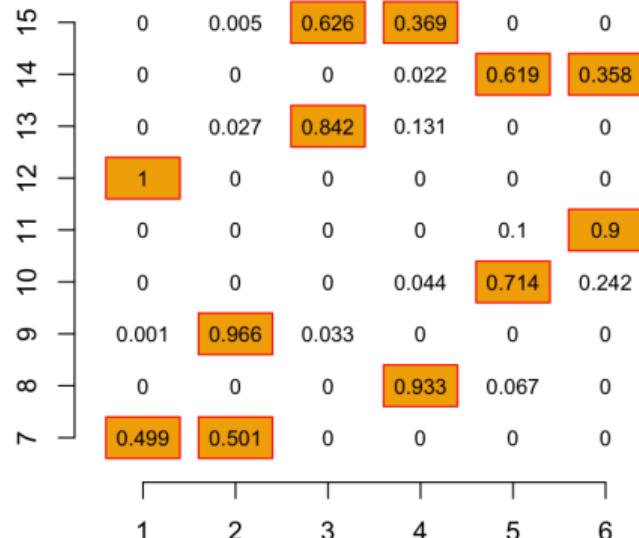
```
1 > Wxy = wasserstein(x,y)
2 > Wxy$plan
```

# Optimal transport (discrete)



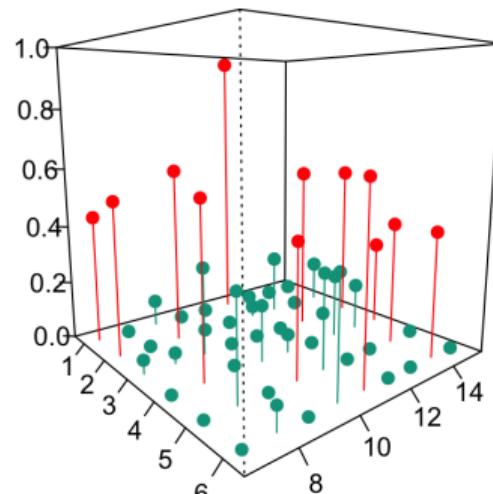
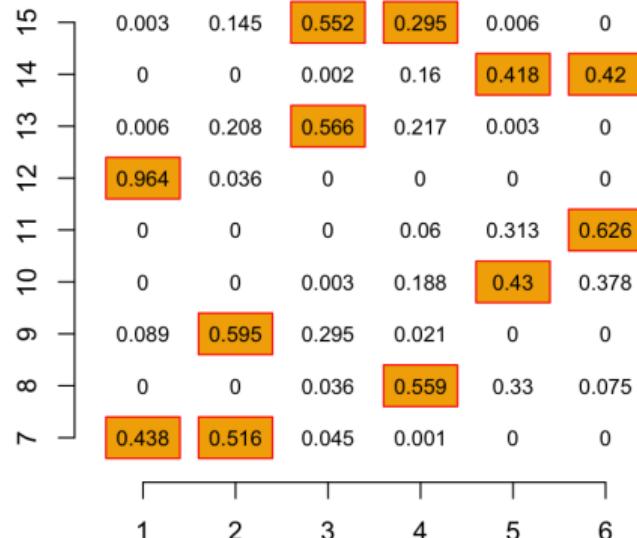
```
1 > Sxy = sinkhorn(x, y, p = 2, lambda = 0.001)
2 > Sxy$plan
```

# Optimal transport (discrete)



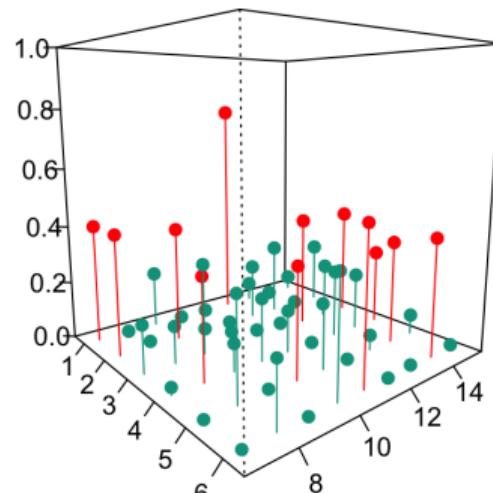
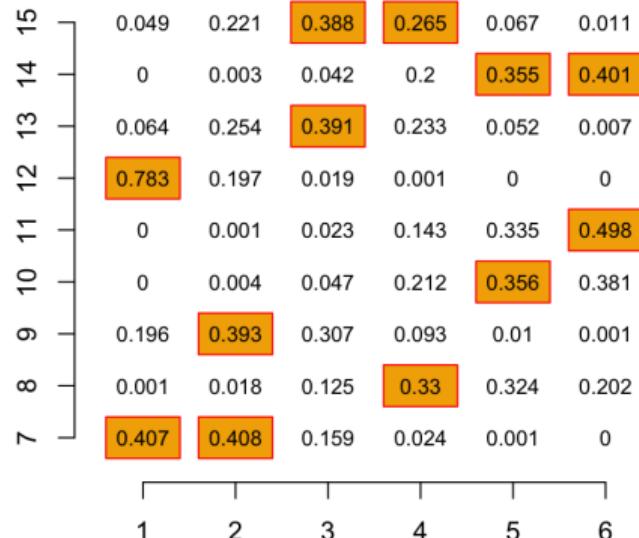
```
1 > Sxy = sinkhorn(x, y, p = 2, lambda = 0.005)
2 > Sxy$plan
```

# Optimal transport (discrete)



```
1 > Sxy = sinkhorn(x, y, p = 2, lambda = 0.02)
2 > Sxy$plan
```

# Optimal transport (discrete)



```
1 > Sxy = sinkhorn(x, y, p = 2, lambda = 0.05)
2 > Sxy$plan
```

# Optimal transport (discrete)

## Theorem 4.4: Optimal transport for discrete univariate distributions

Consider  $n$  points each group, on  $\mathbb{R}$ ,  $\{x_1, \dots, x_n\}$  and  $\{y_1, \dots, y_n\}$ , ordered in the senses that  $x_1 \leq x_2 \leq \dots \leq x_n$  and  $y_1 \leq y_2 \leq \dots \leq y_n$ , for any  $k \geq 1$ ,

$$W_k = \left( \frac{1}{n} \sum_{i=1}^n |x_i - y_i|^k \right)^{1/k}$$

## Theorem 4.5: Optimal transport for continuous univariate distributions

$$W_k = \left( \int_0^1 |F_x^{-1}(u) - F_y^{-1}(u)|^k du \right)^{1/k}$$

# Optimal transport (discrete)

## Theorem 4.6: Optimal transport for continuous univariate distributions

Let  $\mathbb{P}_A$  and  $\mathbb{P}_B$  be two probability measures on  $\mathbb{R}$ , and suppose that  $c(x, y) = h(x - y)$  for some strictly convex function  $h$ . Then there exists a unique  $\pi \in \Pi(\mathbb{P}_A, \mathbb{P}_B)$  such that

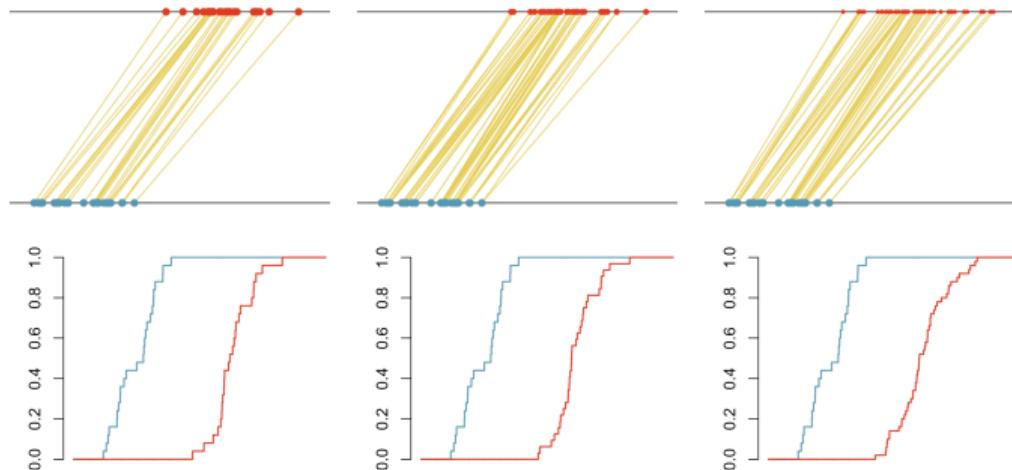
- ▶  $\pi$  is optimal to Kantorovich problem (8.17)
  - ▶  $\pi$  is the comonotone joint distribution with marginals  $\mathbb{P}_A$  and  $\mathbb{P}_B$ .
- If  $c(x, y) = |x - y|$ , the optimal transport solution might be non-unique.

## Theorem 4.7: Optimal map for continuous univariate distributions

The optimal Monge map  $T^*$  such that  $T_\#^*\mathbb{P}_A = \mathbb{P}_B$  is  $T^* = F_B^{-1} \circ F_A$ .

## Optimal transport (discrete)

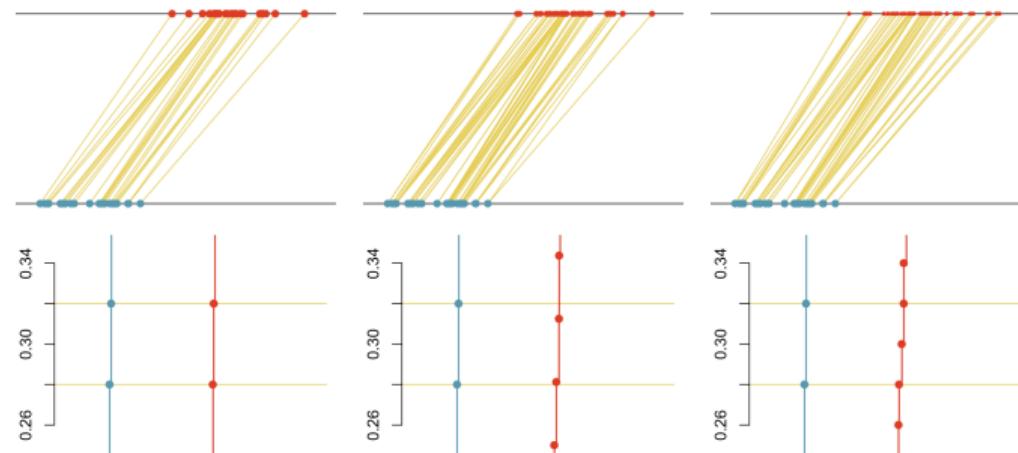
- Consider  $n_A = 25$  and  $n_B = 25$  points in  $\mathbb{R}$ ,  $n_B = 32$  and  $n_B = 50$



$$\hat{F}_{n_A}(x) = \frac{1}{n_A} \sum_{i=1}^{n_A} \mathbf{1}(x_i \leq x) \text{ and } \hat{F}_{n_B}(x) = \frac{1}{n_B} \sum_{i=1}^{n_B} \mathbf{1}(x_i \leq x)$$

## Optimal transport (discrete)

- Consider  $n_A = 25$  and  $n_B = 25$  points in  $\mathbb{R}$ ,  $n_B = 32$  and  $n_B = 50$

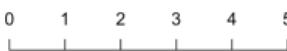


$$\hat{F}_{n_A}(x) = \frac{1}{n_A} \sum_{i=1}^{n_A} \mathbf{1}(x_i \leq x) \text{ and } \hat{F}_{n_B}(x) = \frac{1}{n_B} \sum_{i=1}^{n_B} \mathbf{1}(x_i \leq x)$$

# Optimal transport (discrete)

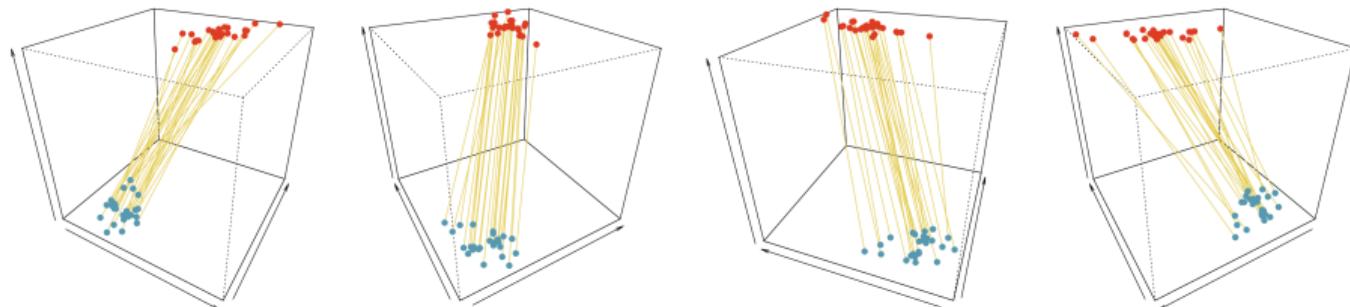
- In the univariate case, if  $k = 1$ ,

$$W_1 = \frac{1}{n} \sum_{i=1}^n |x_i - y_{\sigma(i)}|$$

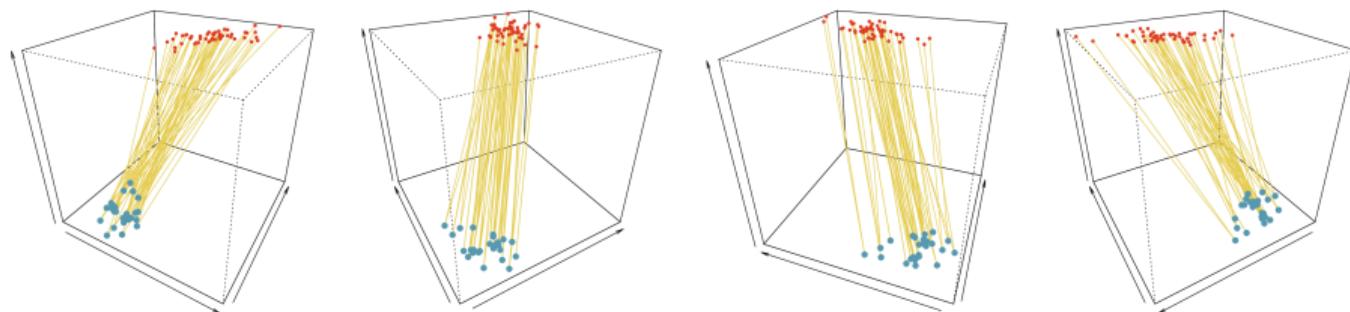


# Multivariate Optimal Transport

- Consider  $n$  and  $n$  points in  $\mathbb{R}^2$

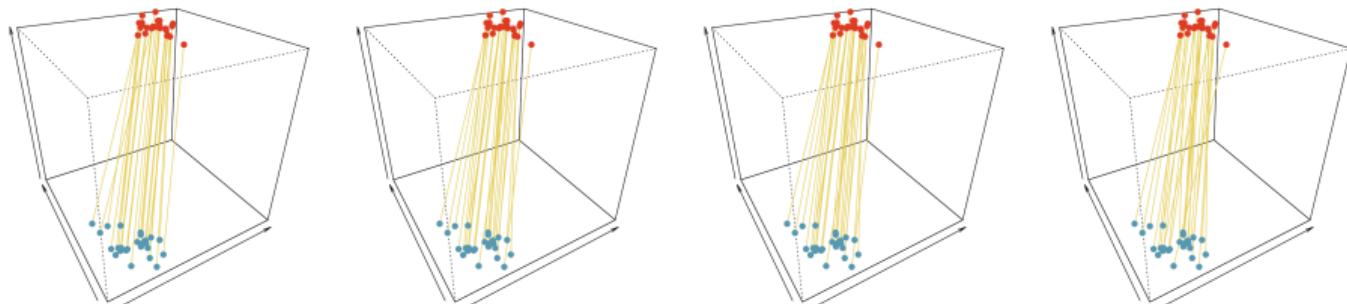


- Consider  $n$  and  $2n$  points in  $\mathbb{R}^2$

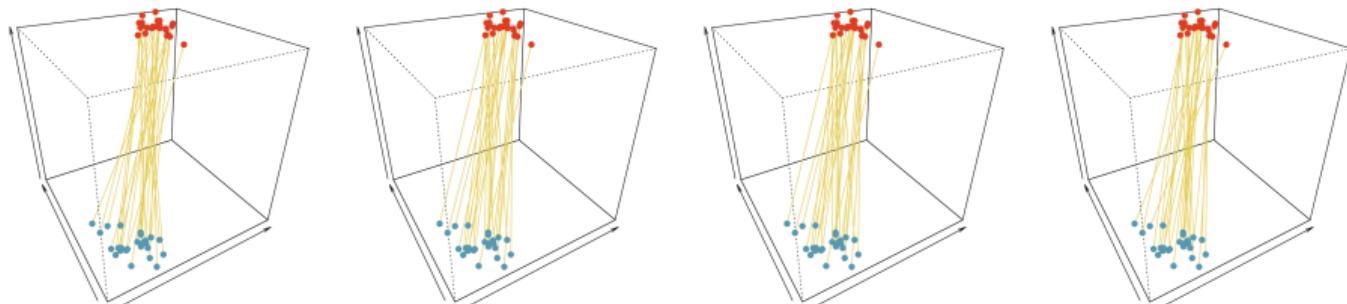


# Multivariate Optimal Transport

- Consider  $n$  and  $n$  points in  $\mathbb{R}^2$ , and  $k = 1, 2, 3, 4$ ,  $T_{\#}\mathbb{P}_A = \mathbb{P}_B$



- Consider  $n$  and  $n$  points in  $\mathbb{R}^2$ , and  $p = 1, 2, 3, 4$ ,  $T_{\#}\mathbb{P}_B = \mathbb{P}_A$



# Multivariate Optimal Transport

**Theorem 4.8: Optimal map for continuous multivariate distributions, Brenier (1991)**

With a quadratic cost, the optimal Monge map  $T^*$  is unique, and it is the gradient of a convex function,  $T^* = \nabla \varphi$ .

**Example** Multidimensional Gaussian

$$\mathbf{x}_B = T^*(\mathbf{x}_A) = \boldsymbol{\mu}_B + \mathbf{A}(\mathbf{x}_A - \boldsymbol{\mu}_A),$$

where  $\mathbf{A}$  is a symmetric positive matrix that satisfies  $\mathbf{A}\boldsymbol{\Sigma}_A\mathbf{A} = \boldsymbol{\Sigma}_B$ , which has a unique solution given by  $\mathbf{A} = \boldsymbol{\Sigma}_A^{-1/2} (\boldsymbol{\Sigma}_A^{1/2} \boldsymbol{\Sigma}_B \boldsymbol{\Sigma}_A^{1/2})^{1/2} \boldsymbol{\Sigma}_A^{-1/2}$ , where  $\mathbf{M}^{1/2}$  is the square root of the square (symmetric) positive matrix  $\mathbf{M}$  based on the Schur decomposition ( $\mathbf{M}^{1/2}$  is a positive symmetric matrix), as described in Higham (2008).

# Multivariate Optimal Transport

## Proposition 4.33: $W_2$ for Gaussian vectors

Consider two Gaussian distributions, then

$$W_2(\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1), \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2))^2 = \|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2\|_2^2 + \text{tr}(\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2 - 2(\boldsymbol{\Sigma}_1^{1/2}\boldsymbol{\Sigma}_2\boldsymbol{\Sigma}_1^{1/2})^{1/2})$$

**Proof:** Let  $\mathbf{X}_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$ ,  $\mathbf{X}_2 \sim \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$ , and  $\Gamma$  define the covariance matrix of  $(\mathbf{X}_1, \mathbf{X}_2)$ ,

$$\Gamma = \begin{pmatrix} \boldsymbol{\Sigma}_1 & C \\ C^\top & \boldsymbol{\Sigma}_2 \end{pmatrix}$$

where (generally),  $C$  is some  $n_1 \times n_2$  matrix. Recall that  $n_1 \times n_2$  matrices can have a pseudo-inverse, in the sense that (Penrose conditions)

$$\begin{cases} AA^{-}A = A \\ A^{-}AA^{-} = A^{-}, \end{cases} \quad \begin{cases} (AA^{-})^\top = AA^{-} \\ (A^{-}A)^\top = A^{-}A, \end{cases}$$

## Multivariate Optimal Transport

- Observe that  $\mathbb{E}(\|\mathbf{X}_1 - \mathbf{X}_2\|_{\ell_2}^2) = \text{tr}(\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2 - 2C)$ . Recall that  $C$  must satisfy the Schur complement constraint,  $\boldsymbol{\Sigma}_1 - C\boldsymbol{\Sigma}_2^{-1}C^\top \succeq 0$ , so that we want to solve

$$C^* = \operatorname{argmin}\{-2\text{tr}(C)\} \text{ s.t. } \boldsymbol{\Sigma}_1 - C\boldsymbol{\Sigma}_2^{-1}C^\top \succeq 0,$$

as studied in [Olkin and Pukelsheim \(1982\)](#), where  $\boldsymbol{\Sigma}_1$  and  $\boldsymbol{\Sigma}_2$  are positive ( $\succeq 0$ ) matrices.

Let  $\mathcal{G} = \{C, n_1 \times n_2 : \boldsymbol{\Sigma}_1 - C\boldsymbol{\Sigma}_2^{-1}C^\top \succeq 0\}$ ,  $\mathcal{S} = \{S : SS^\top \boldsymbol{\Sigma}_2 = \boldsymbol{\Sigma}_2\}$ , one can prove (standard duality and convexity arguments) that

$$\max_{C \in \mathcal{G}} \{2\text{tr}(C)\} = \max_{S \in \mathcal{S}} \{\text{tr}(\boldsymbol{\Sigma}_1 S + \boldsymbol{\Sigma}_2 S^\top)\} = 2\text{tr}(\boldsymbol{\Sigma}_2^{1/2} \boldsymbol{\Sigma}_1 \boldsymbol{\Sigma}_2^{1/2})$$

with respective (unique) solutions

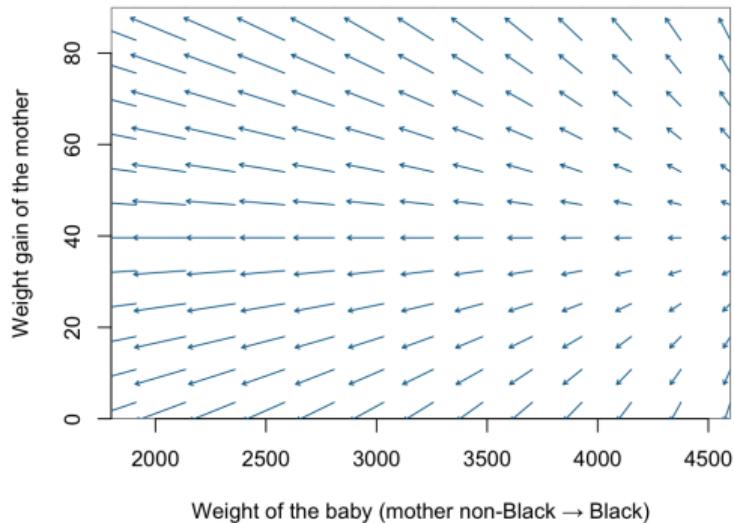
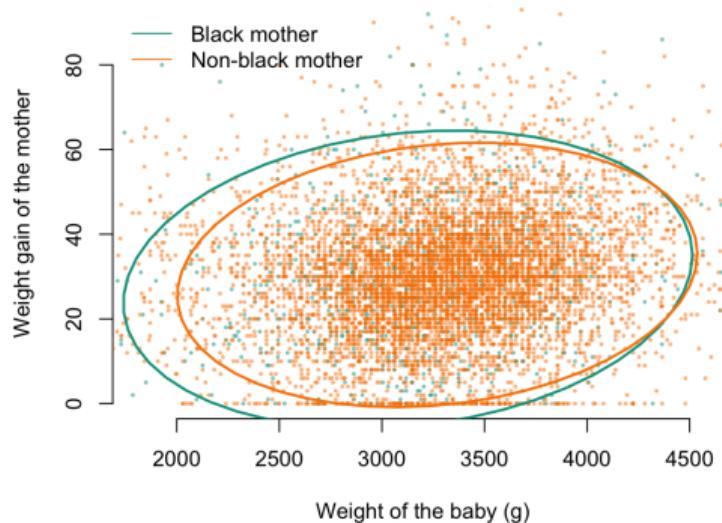
$$\begin{cases} C^* = \boldsymbol{\Sigma}_1 S^* \\ S^* = \boldsymbol{\Sigma}_2^{1/2} [(\boldsymbol{\Sigma}_2^{1/2} \boldsymbol{\Sigma}_1 \boldsymbol{\Sigma}_2^{1/2})^{1/2}] \boldsymbol{\Sigma}_2^{1/2} \end{cases}$$

# Multivariate Optimal Transport

- See Olkin and Pukelsheim (1982), Givens and Shortt (1984) and Knott and Smith (1984), or more recently Takatsu (2008) and Takatsu and Yokota (2012), with more geometric interpretations.
- To illustrate, consider the previous example, with newborn weight and weight gain of mothers, in the U.S., with Black and non-Black mothers, with here a joint mapping  $\mathbb{R}_2^+ \rightarrow \mathbb{R}_2^+$ .

# Multivariate Optimal Transport

$(x_1, x_2) \leftrightarrow (x_1, x_2)$  (newborn weight, weight gain of the mother)



– Part 3 –

# Models

# Generalized Linear Model

## Definition 4.39: Exponential family, McCullagh and Nelder (1989)

The distribution of  $Y$  is in the [exponential family](#) if its density (with respect to some appropriate measure) is

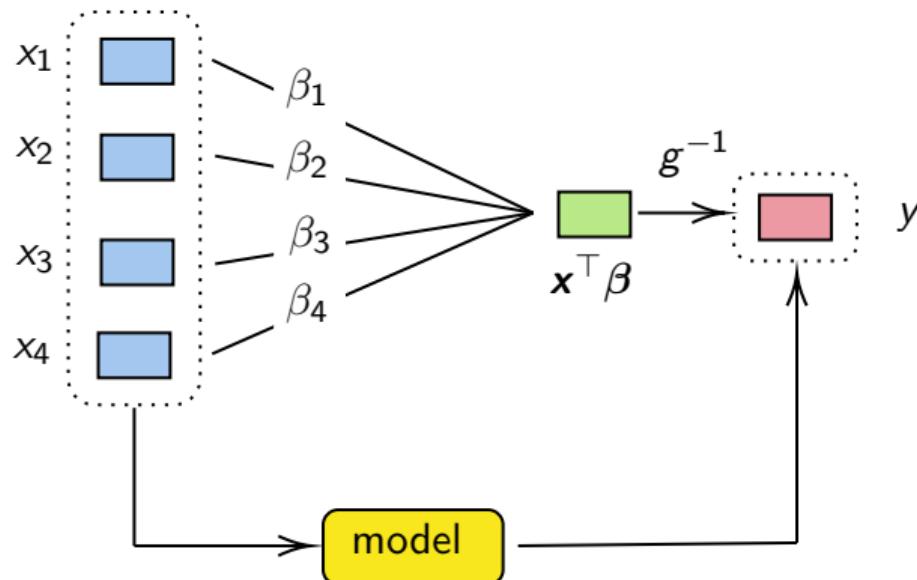
$$f_{\theta, \varphi}(y) = \exp \left( \frac{y\theta - b(\theta)}{\varphi} + c(y, \varphi) \right),$$

where  $\theta$  is the canonical parameter,  $\varphi$  is a nuisance parameter, and  $b : \mathbb{R} \rightarrow \mathbb{R}$  is some  $\mathbb{R} \rightarrow \mathbb{R}$  function.

- Such as the binomial, Poisson, Gaussian, gamma distributions, etc.
- Also compound Poisson / Tweedie (from [Tweedie \(1984\)](#)).

## Generalized Linear Model

- Given some dataset  $(y_i, \mathbf{x}_i)$ , suppose that  $\mu(\mathbf{x}) = g^{-1}(\mathbf{x}^\top \boldsymbol{\beta})$



- OLS,  $\mu(\mathbf{x}) = \mathbf{x}^\top \boldsymbol{\beta}$  and  $\hat{\boldsymbol{\beta}}^{\text{ols}} = \operatorname{argmin} \left\{ \sum_{i=1}^n (y_i - \mathbf{x}_i^\top \boldsymbol{\beta})^2 \right\} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ .

# Generalized Linear Model

- Consider problems

$$\min_{\mathbf{x} \in \mathbb{R}^k} \{f(\mathbf{x})\}$$

under constraint  $g(\mathbf{x}) = \mathbf{0}$

$$\min_{\mathbf{x} \in \mathbb{R}^k} \{f(\mathbf{x})\}$$

under constraint  $g(\mathbf{x}) \leq \mathbf{0}$

- Karush-Kuhn-Tucker condition is

$$\begin{cases} \nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}^*, \mathbf{z}^*) = \mathbf{0} \\ \nabla_{\mathbf{z}} \mathcal{L}(\mathbf{x}^*, \mathbf{z}^*) = \mathbf{0} \end{cases}$$

where

$$\mathcal{L}(\mathbf{x}, \mathbf{z}) = f(\mathbf{x}) + \mathbf{z}^\top g(\mathbf{x})$$

is the Lagrangian problem (parameter  $\mathbf{z}$  are multipliers)

freakonometrics

freakonometrics.hypotheses.org – Arthur Charpentier, 2024 (UQAM Course)

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# Generalized Linear Model

**Definition 4.40: Ridge Estimator (OLS), Hoerl and Kennard (1970)**

$$\hat{\beta}_\lambda^{\text{ridge}} = \underset{\beta \in \mathbb{R}^k}{\operatorname{argmin}} \left\{ \frac{1}{2} \sum_{i=1}^n (y_i - \mathbf{x}_i^\top \beta)^2 + \lambda \sum_{j=1}^k \beta_j^2 \right\}.$$

$$\hat{\beta}_\lambda^{\text{ridge}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

**Definition 4.41: Ridge Estimator (GLM)**

$$\hat{\beta}_\lambda^{\text{ridge}} = \underset{\beta \in \mathbb{R}^k}{\operatorname{argmin}} \left\{ - \sum_{i=1}^n \log f(y_i | \mu_i = g^{-1}(\mathbf{x}_i^\top \beta)) + \lambda \sum_{j=1}^k \beta_j^2 \right\}.$$

# Generalized Linear Model

**Definition 4.42:** LASSO Estimator (OLS), Tibshirani (1996)

$$\hat{\beta}_\lambda^{\text{lasso}} = \operatorname{argmin} \left\{ \frac{1}{2} \sum_{i=1}^n (y_i - \mathbf{x}_i^\top \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^k |\beta_j| \right\}.$$

**Definition 4.43:** LASSO Estimator (GLM)

$$\hat{\beta}_\lambda^{\text{lasso}} = \operatorname{argmin} \left\{ - \sum_{i=1}^n \log f(y_i | \mu_i = g^{-1}(\mathbf{x}_i^\top \boldsymbol{\beta})) + \lambda \sum_{j=1}^k |\beta_j| \right\}.$$

# Generalized Linear Model

```
1 > library(glmnet)
2 > fit_ridge = glmnet(x, y, alpha = 0)
3 > fit_lasso = glmnet(x, y, alpha = 1)
```

## ➤ Elastic net

$$\min \left\{ \frac{1}{2} \sum_{i=1}^n (y_i - \mathbf{x}_i^\top \boldsymbol{\beta})^2 + \lambda_1 \sum_{j=1}^k |\beta_j| + \frac{\lambda_2}{2} \sum_{j=1}^k \beta_j^2 \right\},$$

e.g.  $\lambda_1 = \alpha\lambda$  and  $\lambda_2 = (1 - \alpha)\lambda$  (two parameters — one for the global regularization, one for the trade-off between Ridge (Tikhonov) vs. Lasso)

to go further ➔ (for more details on penalization issues)

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## Definition 4.44: ROC curve

The ROC curve is the parametric curve

$$\{\mathbb{P}[m(\mathbf{X}) > t | Y = 0], \mathbb{P}[m(\mathbf{X}) > t | Y = 1]\} \text{ for } t \in [0, 1],$$

when the score  $m(\mathbf{X})$  and  $Y$  evolve in the same direction (a high score indicates a high risk).

$$C(t) = \text{TPR} \circ \text{FPR}^{-1}(t),$$

where

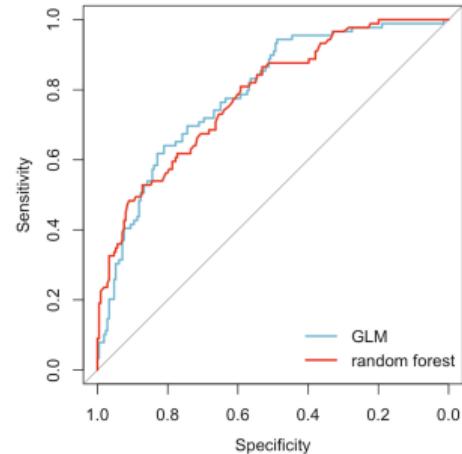
$$\begin{cases} \text{FPR}(t) = \mathbb{P}[m(\mathbf{X}) > t | Y = 0] = \mathbb{P}[m_0(\mathbf{X}) > t] \\ \text{TPR}(t) = \mathbb{P}[m(\mathbf{X}) > t | Y = 1] = \mathbb{P}[m_1(\mathbf{X}) > t]. \end{cases}$$

# Accuracy

```
1 > library(ROCR)
2 > pred = prediction(df$yhat, df$y)
3 > roc = performance(pred, "tpr", "fpr")
4 > plot(roc)
5 > auc = performance(pred, "auc")
```

see also

```
1 > library(pROC)
```

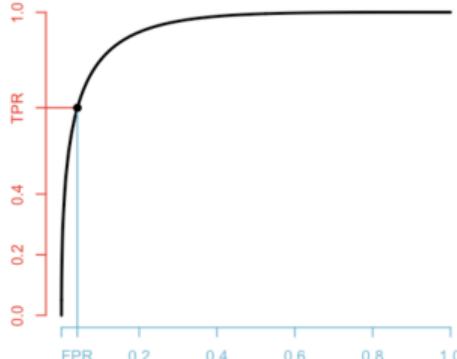
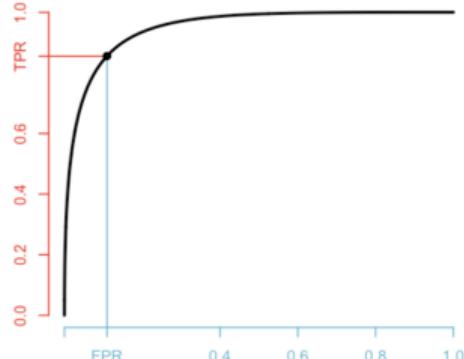
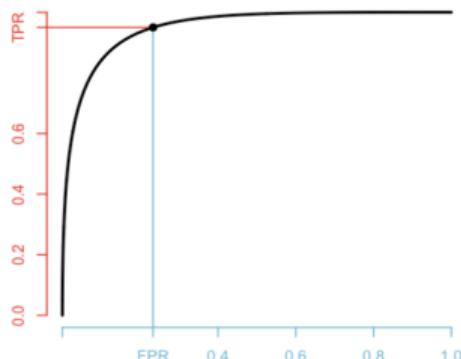
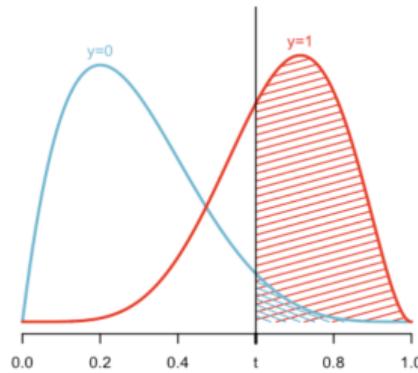
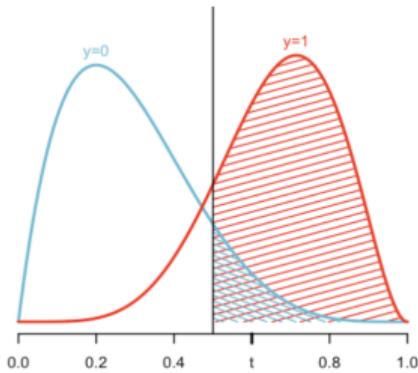
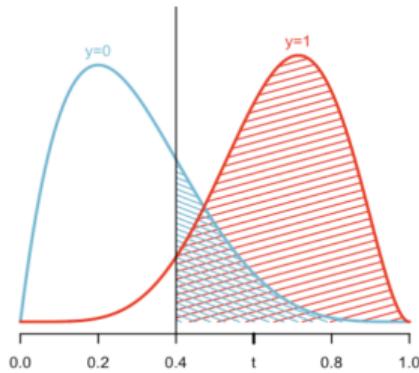


## Definition 4.45: AUC, area under the ROC curve

The area under the curve is defined as the area below the ROC curve,

$$\text{AUC} = \int_0^1 C(t)dt = \int_0^1 \text{TPR} \circ \text{FPR}^{-1}(t)dt.$$

# Accuracy



# Calibration

- Well-calibration was initially discussed in forecasting

**Definition 4.46: Well-calibrated (1), Van Calster et al. (2019), Krüger and Ziegel (2021)**

The forecast  $X$  of  $Y$  is a well-calibrated forecast of  $Y$  if  $\mathbb{E}(Y|X) = X$  almost surely, or  $\mathbb{E}[Y|X = x] = x$ , for all  $x$ .

- one can define “well-calibration” in prediction

**Definition 4.47: Well-calibrated (2), Zadrozny and Elkan (2002); Cohen and Goldszmidt (2004)**

The prediction  $m(\mathbf{X})$  of  $Y$  is a well-calibrated prediction if  $\mathbb{E}[Y|m(\mathbf{X}) = \hat{y}] = \hat{y}$ , for all  $\hat{y}$ .

# Calibration

**“Well calibrated classifiers** are probabilistic classifiers for which the output can be directly interpreted as a confidence level. For instance, a well calibrated (binary) classifier should classify the samples such that among the samples to which it gave a[predicted probability] value close to 0.8, approximately 80% actually belong to the positive class,” scikit learn: Probability calibration

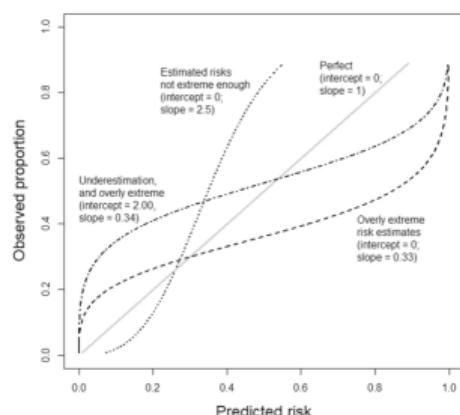
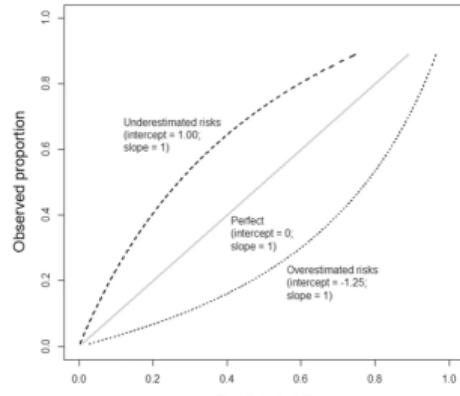
- “Suppose that a forecaster sequentially assigns probabilities to events. He is **well calibrated** if, for example, of those events to which he assigns a probability 30 percent, the long-run proportion that actually occurs turns out to be 30 percent,” Dawid (1982).
- “Out of all the times you said there was a 40 percent chance of rain, how often did rain actually occur? If, over the long run, it really did rain about 40 percent of the time, that means your forecasts were **well calibrated**,” Silver (2012),
- “we desire that the estimated class probabilities are reflective of the true underlying probability of the sample,” Kuhn and Johnson (2013)

## Calibration

- See Murphy and Epstein (1967), Roberts (1968), Gneiting and Raftery (2005) on ensemble methods for weather forecasting, or more generally Lichtenstein et al. (1977), Oakes (1985), Gneiting et al. (2007).

# Calibration

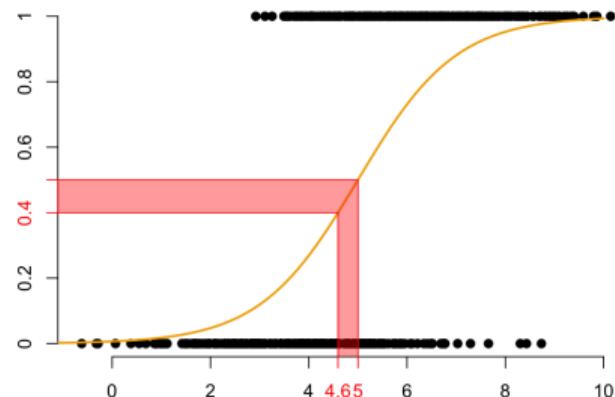
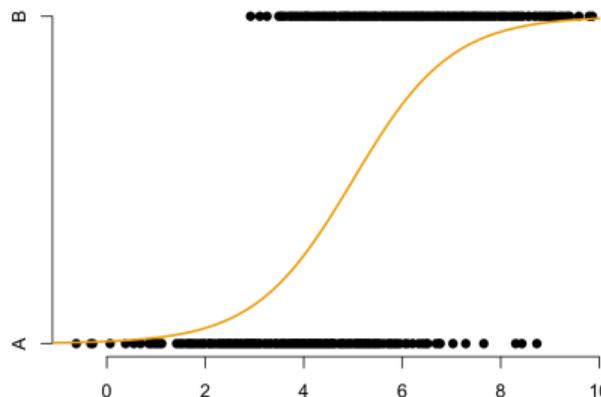
- As explained in Van Calster et al. (2019), "among patients with an estimated risk of 20%, we expect 20 in 100 to have or to develop the event",
  - ▶ If 40 out of 100 in this group are found to have the disease, the risk is **underestimated**
  - ▶ If we observe that in this group, 10 out of 100 have the disease, we have **overestimated** the risk.
- Hosmer-Lemeshow test, from Hosmer Jr et al. (2013) (logistic regression), and Brier score, from Brier (1950) and Murphy (1973)
- Function plotted in psychological papers Keren (1991)



## Calibration

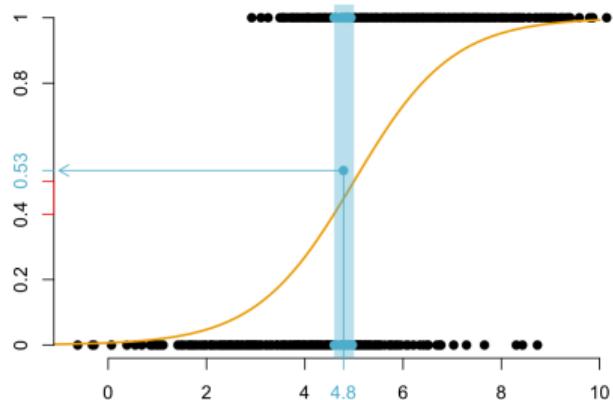
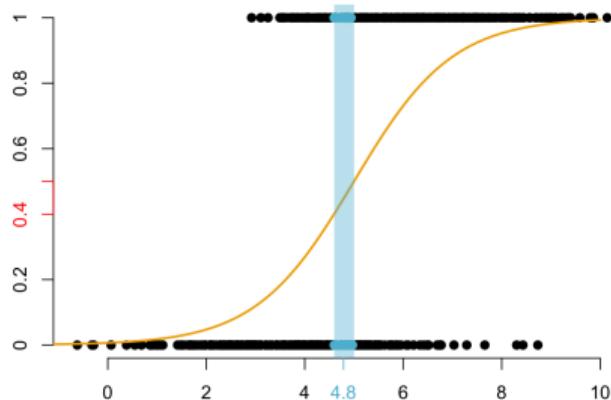
- Consider a dataset  $(x_i, y_i)$ ,  $y_i \in \{A, B\}$ , and consider model

$\hat{m}(x) = \frac{\exp(\hat{\beta}_0 + \hat{\beta}_1 x)}{1 + \exp(\hat{\beta}_0 + \hat{\beta}_1 x)}$  to estimate  $\mathbb{P}[Y = B|X = x]$  (logistic regression). Given  $[p_-, p_+] \subset [0, 1]$  (here  $[0.4, 0.5]$ ), set  $\mathcal{I} = \{i : m(x_i) \in [p_-, p_+]\}$ .



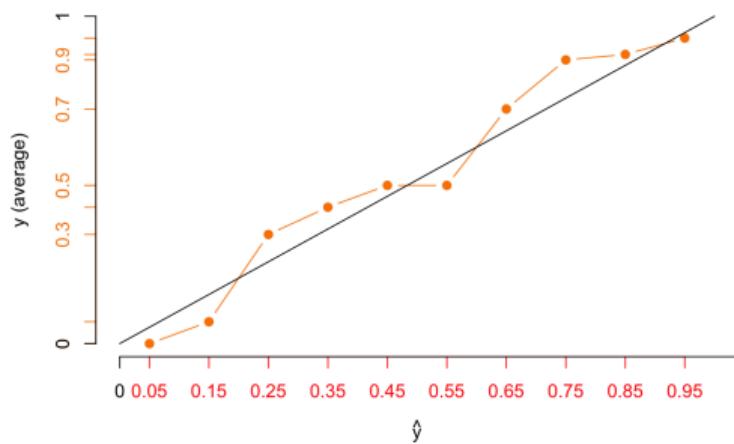
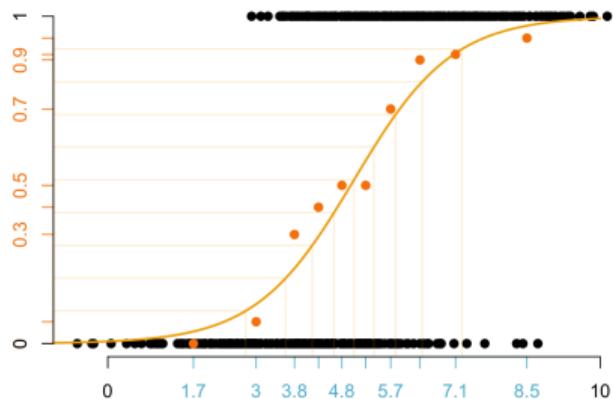
# Calibration

- Given  $\mathcal{I} = \{i : m(\mathbf{x}_i) \in [p_-, p_+]\}$ , set  $\bar{y}_{\mathcal{I}} = \frac{1}{n_{\mathcal{I}}} \sum_{i \in \mathcal{I}} y_i$



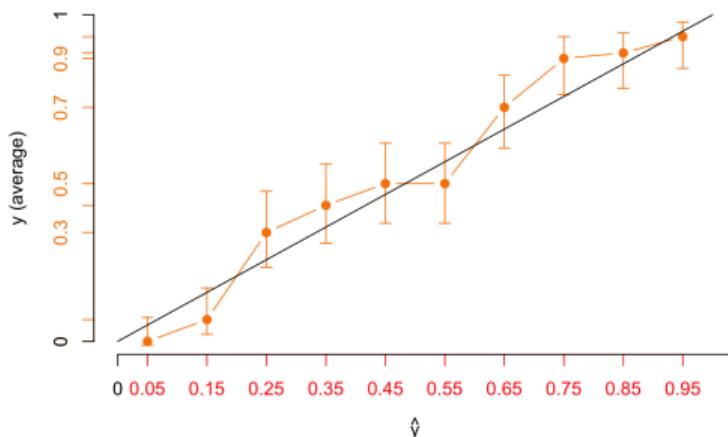
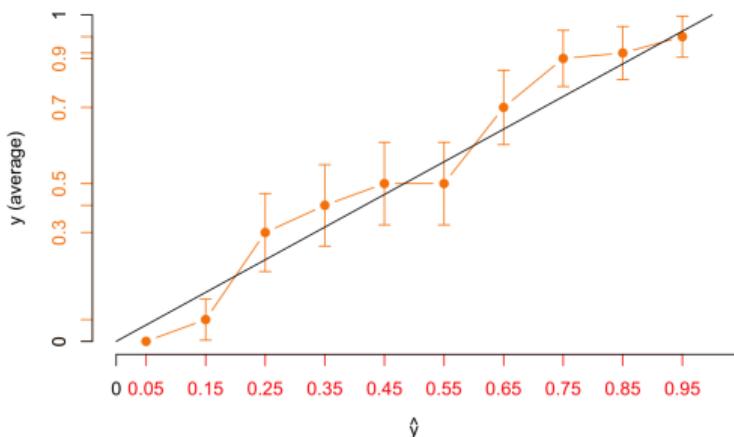
# Calibration

- Compute deciles  $\bar{y}_1, \dots, \bar{y}_{10}$  associated with  $[p_-, p_+]$  equal  $[0, 0.1], [0.1, 0.2], \dots, [0.9, 1]$ , with midpoints  $p_k$ . Then visualize  $\{(p_k, \bar{y}_k)\}$ , as in scikit-learn.



# Calibration

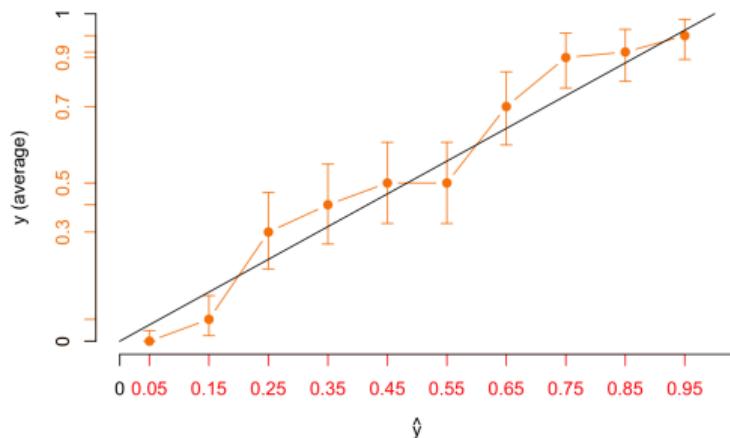
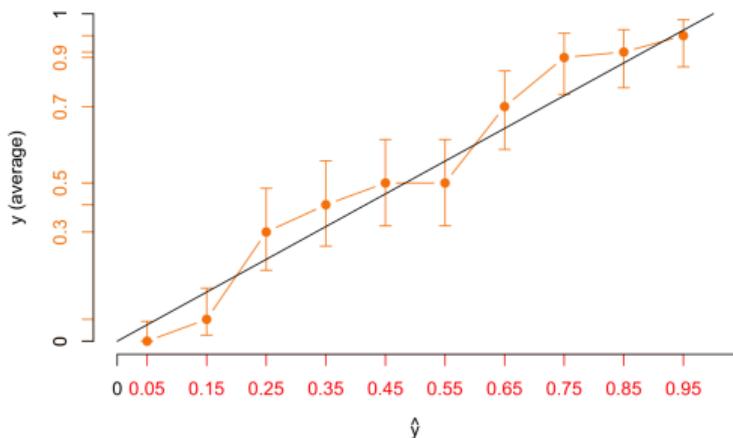
- Asymptotic and Agresti and Coull (1998),  $\tilde{n} = n + u_{1-\alpha/2}^2$  et  $\tilde{p} = \frac{1}{\tilde{n}} \left( n\bar{x} + \frac{u_{1-\alpha/2}^2}{2} \right)$   
$$\left[ \hat{p} \pm u_{1-\alpha/2} \sqrt{\frac{\hat{p}(1-\hat{p})}{n}} \right], \text{ and } \left[ \tilde{p} \pm u_{1-\alpha/2} \sqrt{\frac{\tilde{p}(1-\tilde{p})}{\tilde{n}}} \right]$$



# Calibration

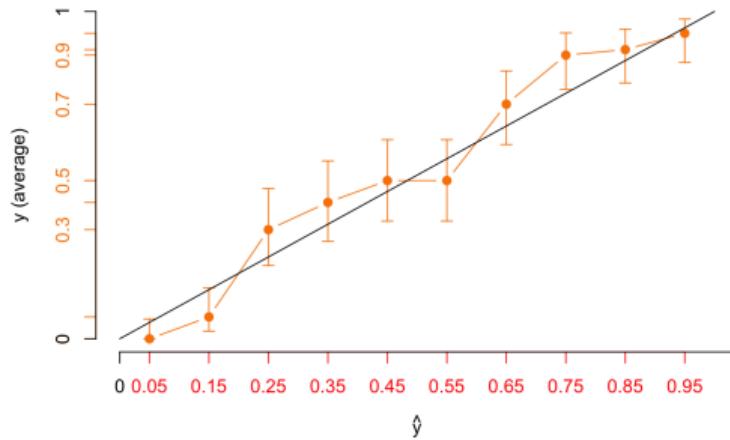
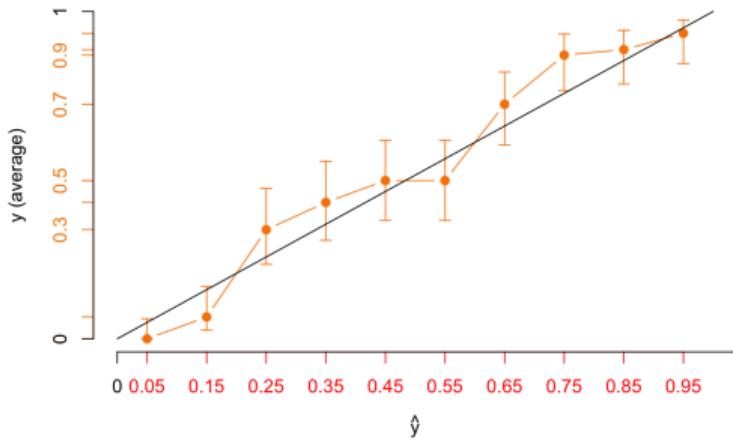
› Exact, and Wilson (1927)

$$\left[ \frac{1}{1 + \frac{u_{1-\alpha/2}^2}{n}} \left( \hat{p} + \frac{u_{1-\alpha/2}^2}{2n} \right) \pm \frac{u_{1-\alpha/2}}{1 + \frac{u_{1-\alpha/2}^2}{n}} \sqrt{\frac{\hat{p}(1 - \hat{p})}{n} + \frac{u_{1-\alpha/2}^2}{4n^2}} \right]$$



# Calibration

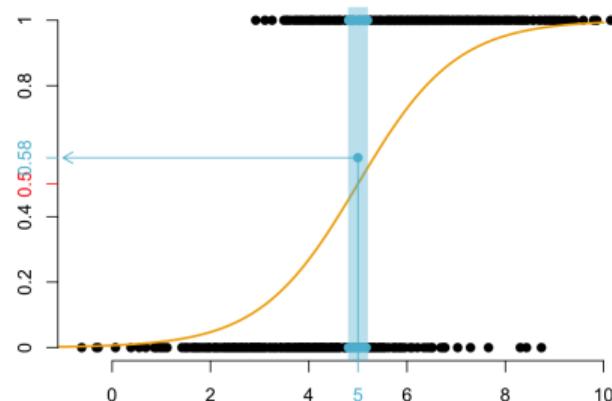
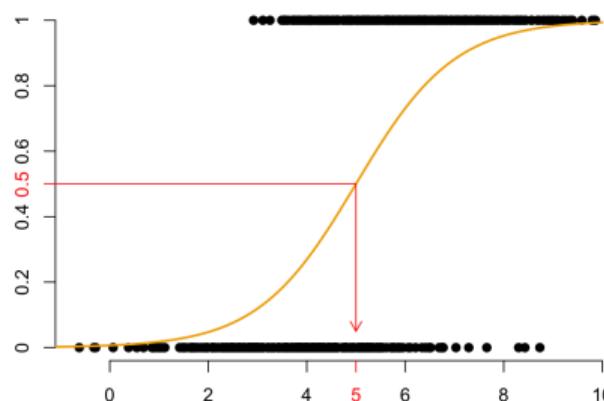
- Bayes and Probit (via `binom.confint` in `binom` package)



# Calibration

- Given  $p \in (0, 1)$ , consider  $\mathcal{I}_p = \{i : \hat{m}(\mathbf{x}_i) \in [p - h, p + h]\}$  for some  $h > 0$ , set

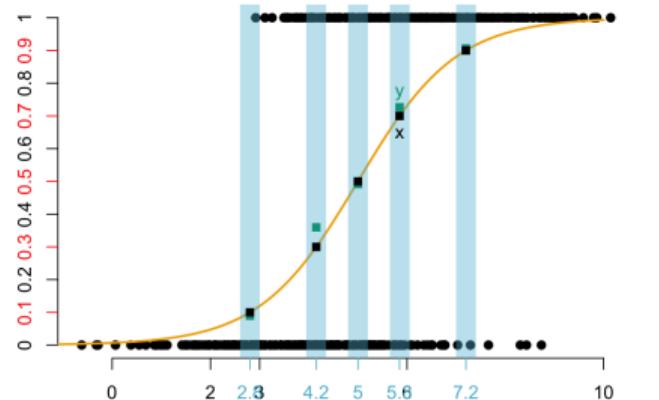
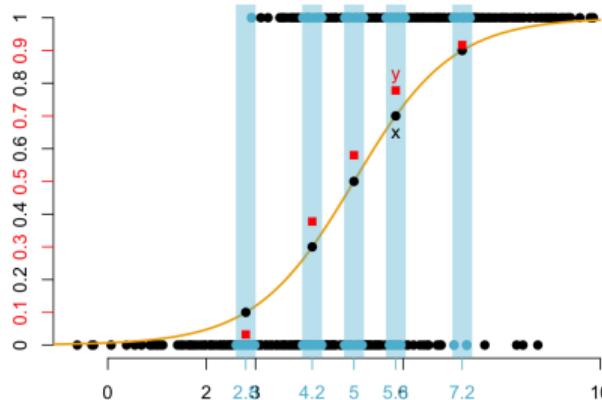
$$\bar{y}_p = \frac{1}{n_{\mathcal{I}_p}} \sum_{i \in \mathcal{I}_p} y_i$$



# Calibration

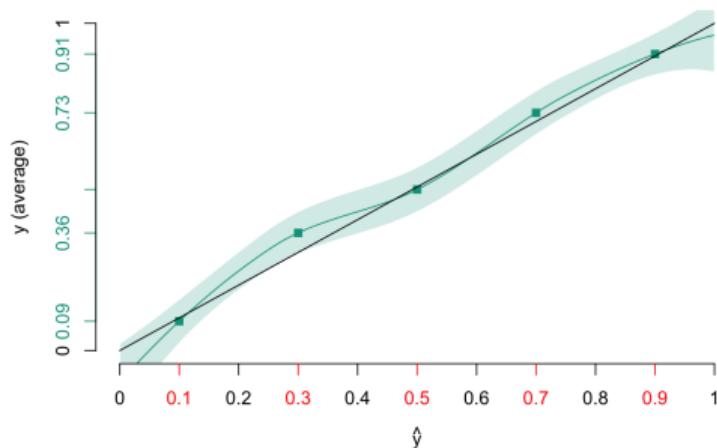
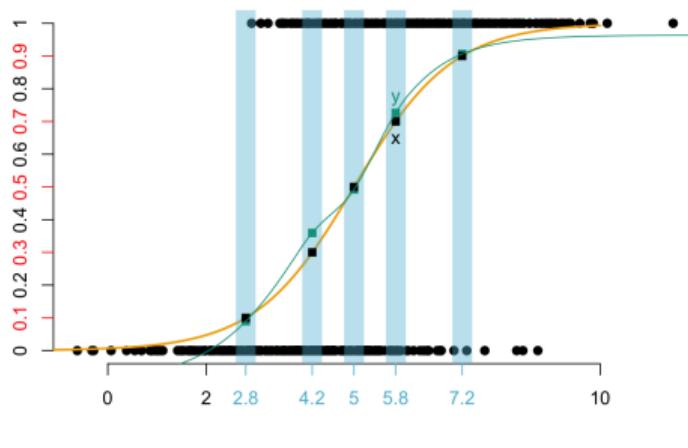
- Given  $p \in (0, 1)$ , compute  $\bar{y}_p = \frac{1}{n_{\mathcal{I}_p}} \sum_{i \in \mathcal{I}_p} y_i$  (for appropriate bandwidth  $h > 0$ )

One could also consider some kernel based average...  $\bar{y}_p$



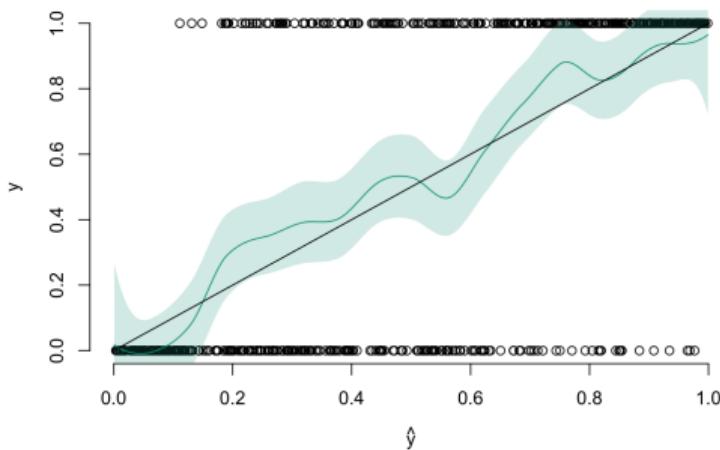
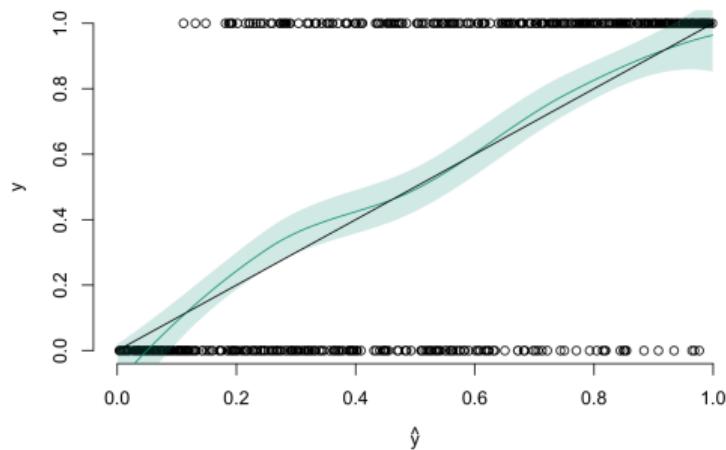
# Calibration

- › Compute  $\bar{y}_p$  for various  $p$ , and plot  $p \mapsto \bar{y}_p$ , that is an estimate of  $\mathbb{E}[Y|\hat{m}(\mathbf{X}) = p]$ .
- › Add a confidence band around.
- ... but here, it works only because  $\hat{m}$  is smooth enough...



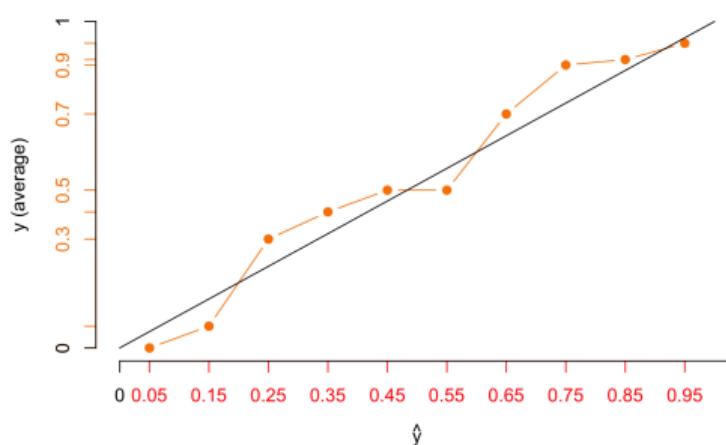
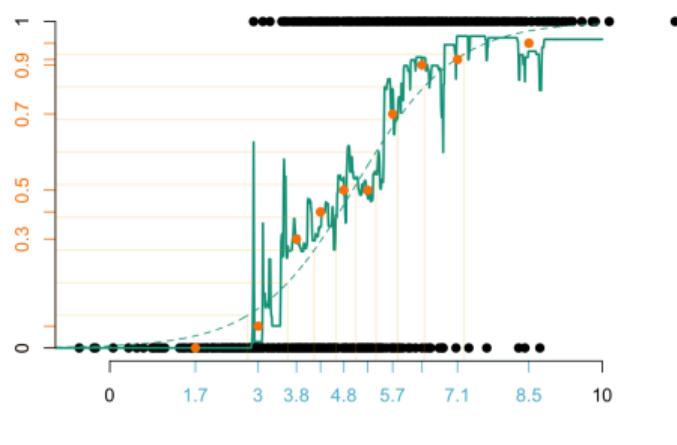
# Calibration

- More generally, consider the local regression of  $y_i$ 's against  $\hat{y}_i = \hat{m}(\mathbf{x}_i)$ 's.



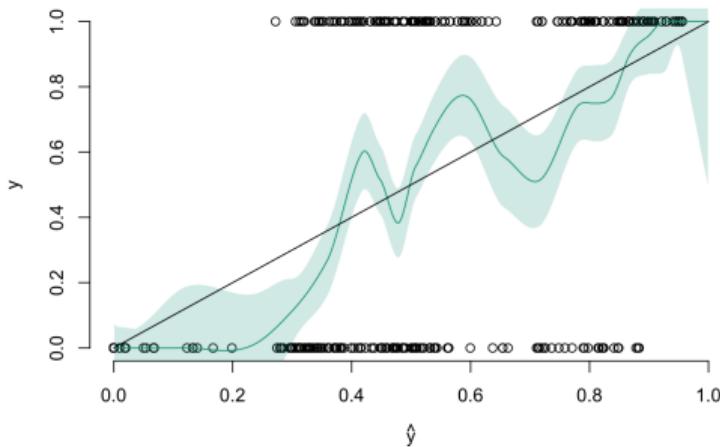
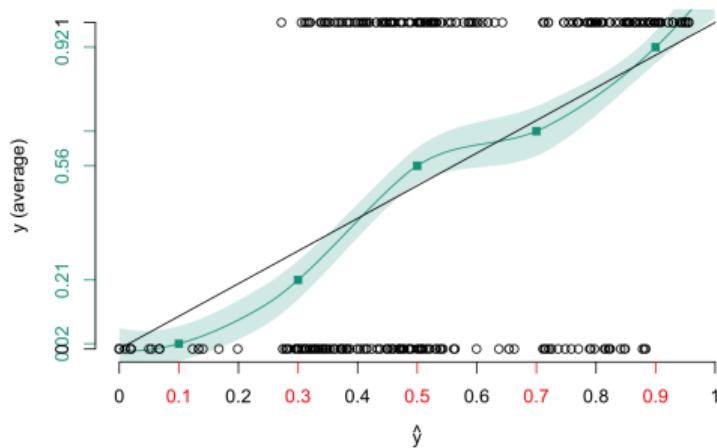
# Calibration

- Consider e.g., some random forest model for  $\hat{m}$ , and then the calibration curve per decile,



# Calibration

- Or, for our random forest model  $\hat{m}$ , some local regression approach



# Calibration

## Definition 4.48: Calibration plot

The calibration plot associated with model  $m$  is the function  $\hat{y} \mapsto \mathbb{E}(Y|m(\mathbf{X}) = \hat{y})$ . The empirical version is some local regression on  $\{y_i, m(\mathbf{x}_i)\}$ .

## Definition 4.49: Globally unbiased model $m$ , Denuit et al. (2021)

Model  $m$  is globally unbiased if  $\mathbb{E}[Y] = \mathbb{E}[m(\mathbf{X})]$ .

## Definition 4.50: Locally unbiased model $m$ , Denuit et al. (2021)

Model  $m$  is locally unbiased at  $\hat{y}$  if  $\mathbb{E}[Y|m(\mathbf{X}) = \hat{y}] = \hat{y}$ .

## Calibration

- › For GLM, remember that

$$f(y_i) = \exp\left(\frac{y_i\theta_i - b(\theta_i)}{\varphi} + c(y_i, \varphi)\right),$$

$$\frac{\partial \log \mathcal{L}_i}{\partial \beta_j} = \frac{\partial \log \mathcal{L}_i}{\partial \theta_i} \cdot \frac{\partial \theta_i}{\partial \mu_i} \cdot \frac{\partial \mu_i}{\partial \eta_i} \cdot \frac{\partial \eta_i}{\partial \beta_j} = \frac{\partial \log \mathcal{L}_i}{\partial \beta_j} = \frac{y_i - \mu_i}{\varphi} \cdot \frac{1}{V(\mu_i)} \cdot x_{i,j} \cdot \left(\frac{\partial \eta_i}{\partial \mu_i}\right)^{-1}$$

- › When  $g$  is the canonical link ( $g_\star = b'^{-1}$  or  $\eta_i = \mathbf{x}_i^\top \boldsymbol{\beta} = \theta_i$ )

$$\nabla \log \mathcal{L} = \mathbf{X}^\top (\mathbf{y} - \hat{\mathbf{y}}) = \mathbf{0}$$

### Proposition 4.34: Calibration of GLM

In the GLM framework with the canonical link function,  $\hat{m}(\mathbf{x}) = g_\star^{-1}(\mathbf{x}_i^\top \hat{\boldsymbol{\beta}})$  is globally unbiased (on the training dataset), but possibly locally biased.

# Calibration

- Otherwise

$$\nabla \log \mathcal{L} = \mathbf{X}^\top \boldsymbol{\Omega} (\mathbf{y} - \hat{\mathbf{y}}) = \mathbf{0},$$

where  $\boldsymbol{\Omega}$  is a diagonal matrix ( $\boldsymbol{\Omega} = \mathbf{W}\boldsymbol{\Delta}$ , where

$\mathbf{W} = \text{diag}((V(\mu_i)g'(\mu_i)^2)^{-1})$  and  $\boldsymbol{\Delta} = \text{diag}(g'(\mu_i))$ , so that we recognize Fisher information - corresponding to the Hessian matrix (up to a negative sign) –  $\mathbf{X}^\top \mathbf{W} \mathbf{X}$ ).

	training data					validation data				
	$\bar{y}$	GLM	CART	GAM	RF	$\bar{y}$	GLM	CART	GAM	RF
$\hat{m}(\mathbf{x}, s)$	8.73	8.73	8.73	8.73	8.27	8.55	9.05	9.03	8.84	8.70
$\hat{m}(\mathbf{x})$	8.73	8.73	8.73	8.73	8.29	8.55	9.05	9.03	8.84	8.73

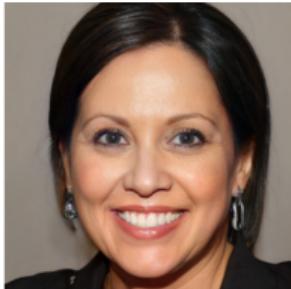
## Definition 4.51: Brier score (binary classifier) Brier (1950)

Brier score is the mean squared error of probability estimate,

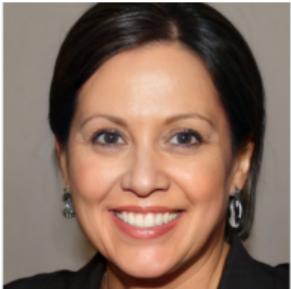
$$\text{BS} = \frac{1}{n} \sum_{i=1}^n (\hat{m}(\mathbf{x}_i), y_i)^2$$

- › Let  $g$  be the calibration function,  $g(\hat{m}(\mathbf{x})) \approx p(\mathbf{x})$ .
- › Platt scaling (from [Platt et al. \(1999\)](#)),  $g(s) = [1 + e^{-(ws+b)}]^{-1}$ .
- › “confidence” value given by [Picpurify](#), using pictures generate by a GAN (a generative adversarial network, used in [Hill and White \(2020\)](#)).

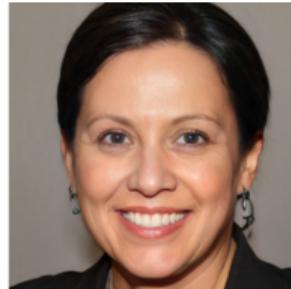
# Calibration



female (0.984)  
male (0.016)



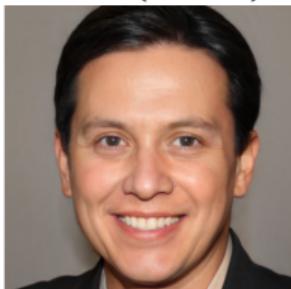
female (0.983)  
male (0.017)



female (0.982)  
male (0.018)



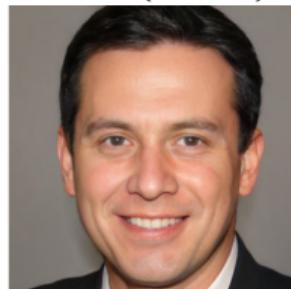
female (0.960)  
male (0.040)



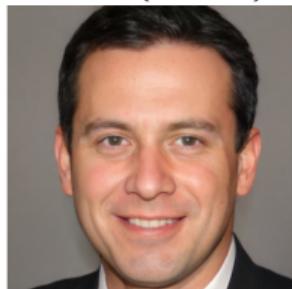
female (0.009)  
male (0.991)



female (0.013)  
male (0.987)

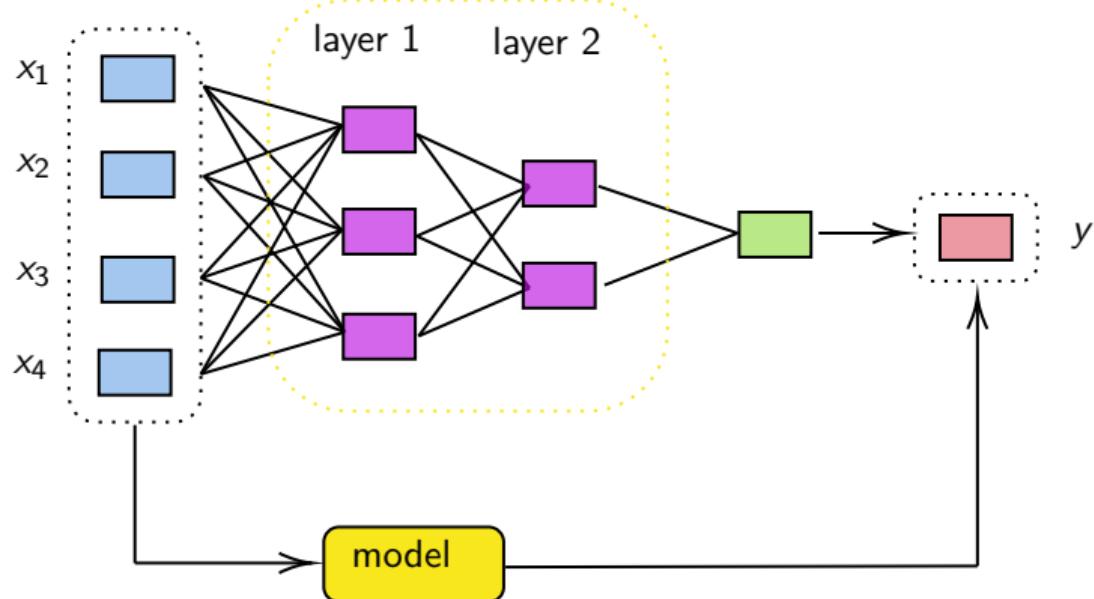


female (0.014)  
male (0.986)

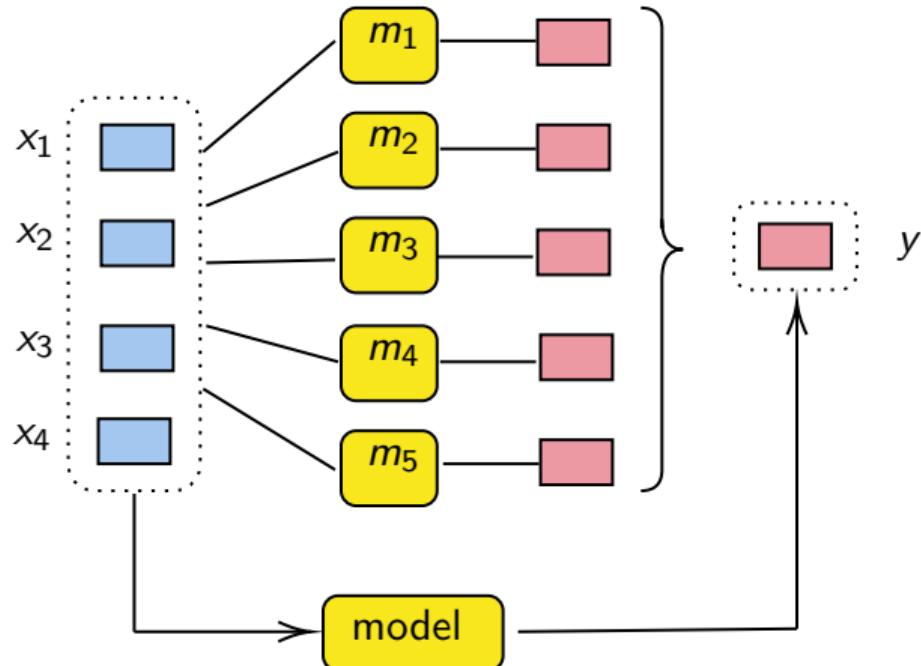


female (0.015)  
male (0.985)

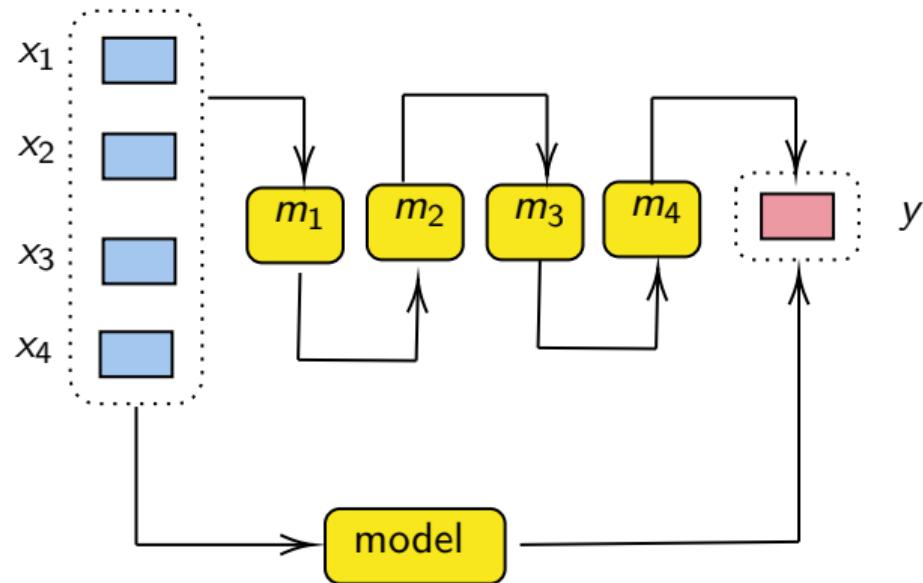
# Standard modeling architecture



# Standard modeling architecture



# Standard modeling architecture



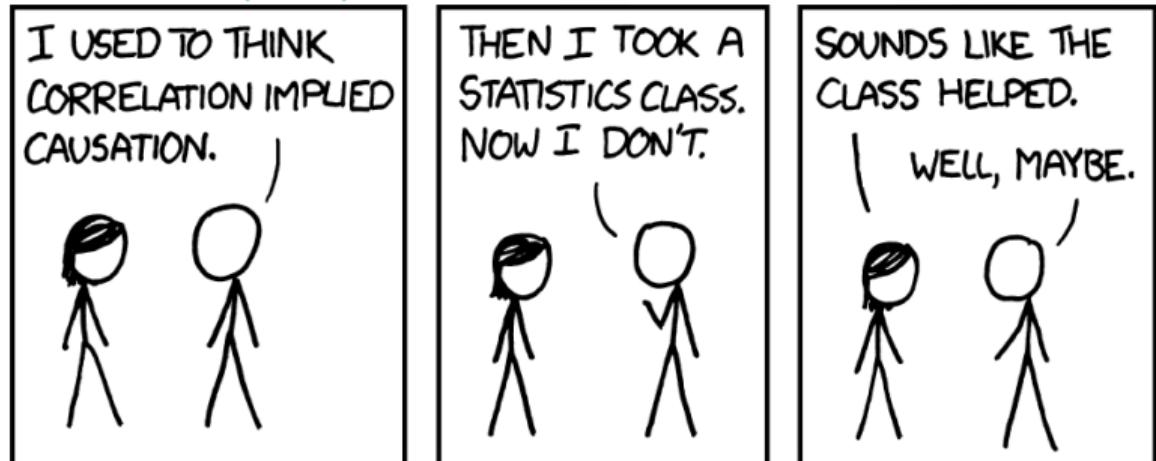
– Part 4 –

Data

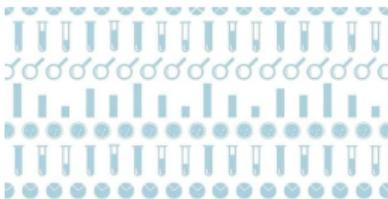
# Data (the two types)

*"It is often said, 'You cannot prove causality with statistics.' One of my professors, Frederick Mosteller, liked to counter, 'You can only prove causality with statistics.' (...) The title, 'Observation and Experiment,' marks the modern distinction between randomized experiments and observational studies."*

Rosenbaum (2018)



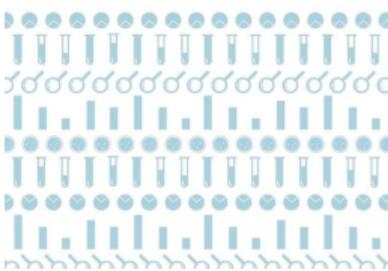
Correlation, Randall Munroe, 2009 <https://xkcd.com/552/>



## Observation & Experiment

*An Introduction to Causal Inference*

PAUL R. ROSENBAUM



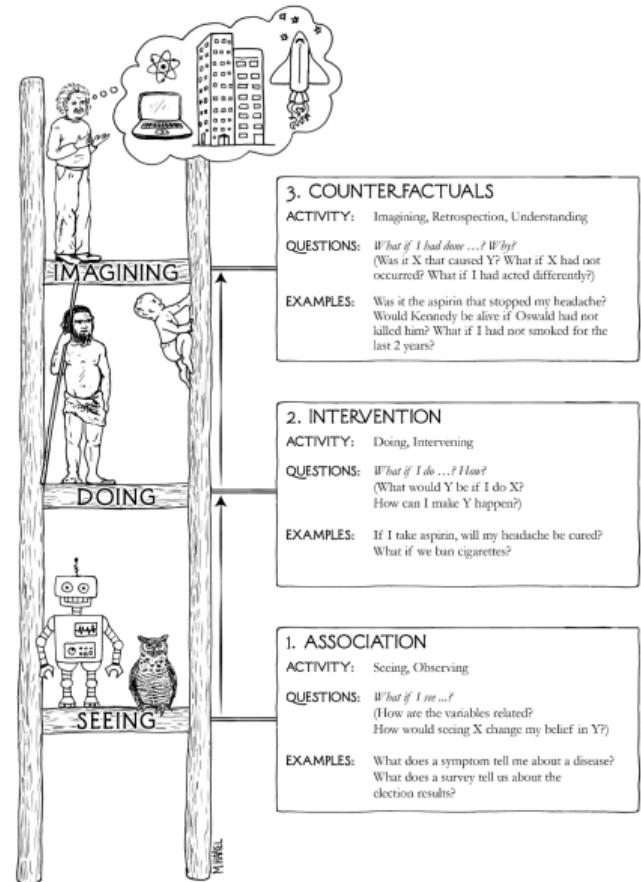
# Data (the three rung ladder)

“Ladder of causation” from Pearl et al. (2009)

- 3. Counterfactuals  
(Imagining, “*what if I had done...*”)
- 2. Intervention  
(Doing, “*what if I do...*”)
- 1. Association  
(Seeing, “*what if I see...*”)

Picture source: Pearl and Mackenzie (2018)

What would be the impact of a treatment  $T$  on a variable of interest  $Y$  ?



# Proxy

- “OK, let’s not use race, but should we use zip code, which of course is a proxy for race in our segregated society?,” O’Neil (2016).

## Definition 4.52: Proxy, Merriam-Webster (2022)

A **proxy** is a person authorized to act for another (from a contracted form of the Middle English word *procuracie* (from French “procuration”)).

## Definition 4.53: Perfect proxy, Datta et al. (2017)

A variable  $X$  is a perfect proxy for  $Z$  if there exist functions  $\varphi : \mathcal{X} \rightarrow \mathcal{Z}$  and  $\psi : \mathcal{Z} \rightarrow \mathcal{Y}$  such that

$$\mathbb{P}[X = \psi(Z)] = \mathbb{P}[\varphi(X) = Z] = 1.$$

## Definition 4.54: Comonotonicity, Hoeffding (1940); Fréchet (1951)

Variables  $X$  and  $Y$  are comonotonic if  $(X, Y) = (F_x^{-1}(U), F_y^{-1}(U))$  for some  $U \sim \mathcal{U}([0, 1])$ .

- See also Dhaene et al. (2002a,b) on comonotonic vectors.
- See also Prince and Schwarcz (2019), or Tschantz (2022) for discrimination by proxy.
- Range of possible situation between independence and perfect proxy.

## Definition 4.55: Independence (dimension 2)

$X$  and  $Y$  are independent, denoted  $X \perp\!\!\!\perp Y$ , if for any sets  $\mathcal{A}, \mathcal{B} \subset \mathbb{R}$ ,

$$\mathbb{P}[X \in \mathcal{A}, Y \in \mathcal{B}] = \mathbb{P}[X \in \mathcal{A}] \cdot \mathbb{P}[Y \in \mathcal{B}].$$

## Definition 4.56: Linear Independence (dimension 2)

Consider two random variables  $X$  and  $Y$ .  $X \perp Y$  if and only if  $\text{Cov}[X, Y] = 0$ .

## Definition 4.57: Correlation (dimension 2), Pearson (1895)

$X$  and  $Y$  are two random variables

$$\text{Corr}[X, Y] = \frac{\text{Cov}[X, Y]}{\sqrt{\text{Var}[X] \cdot \text{Var}[Y]}}.$$

where  $\text{Cov}[X, Y] = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$ .

## Proposition 4.35: Correlation bounds (dimension 2)

For any random variables  $X$  and  $Y$  (with finite variances),

$r_{\min} \leq \text{Corr}[X, Y] \leq r_{\max}$ , where

$$r_{\min} = \frac{\text{Cov}[F_x^{-1}(U), F_y^{-1}(1-U)]}{\sqrt{\text{Var}[X] \cdot \text{Var}[Y]}} \quad \text{and} \quad r_{\max} = \frac{\text{Cov}[F_x^{-1}(U), F_y^{-1}(U)]}{\sqrt{\text{Var}[X] \cdot \text{Var}[Y]}}$$

- Maximal correlation is obtained when  $X$  and  $Y$  are comonotonic (minimal correlation when  $X$  and  $-Y$  are comonotonic).
- Related to optimal transport, see also [Knott and Smith \(1984\)](#).

## Proposition 4.36

Consider two random variables  $X$  and  $Y$ .  $X \perp\!\!\!\perp Y$  if and only if for any functions  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$  and  $\psi : \mathbb{R} \rightarrow \mathbb{R}$  (such that the expected values below exist and are well-defined)  $\text{Cov}[\varphi(X), \psi(Y)] = 0$ , i.e.,

$$\mathbb{E}[\varphi(X) \cdot \psi(Y)] = \mathbb{E}[\varphi(X)] \cdot \mathbb{E}[\psi(Y)].$$

## Definition 4.58: Maximal Correlation, HGR

Consider two random variables  $X$  and  $Y$ ,

$$r^*(X, Y) = \max_{\varphi, \psi} \{ \text{Corr}[\varphi(X), \psi(Y)] \}.$$

# Independence

- HGR because of Hirschfeld (1935), Gebelein (1941) and Rényi (1959) (also Sarmanov (1958a,b)).

$$r^*(X, Y) = \max_{\varphi \in \mathcal{F}_x, \psi \in \mathcal{G}_y} \mathbb{E}[\varphi(X)\psi(Y)],$$

where

$$\begin{cases} \mathcal{F}_x = \{\varphi : \mathcal{X} \rightarrow \mathbb{R} : \mathbb{E}[\varphi(X)] = 0 \text{ and } \mathbb{E}[\varphi^2(X)] = 1\} \\ \mathcal{G}_y = \{\psi : \mathcal{Y} \rightarrow \mathbb{R} : \mathbb{E}[\psi(Y)] = 0 \text{ and } \mathbb{E}[\psi^2(Y)] = 1\} \end{cases}$$

- See either `ccaPP` or `acepack` package,

```
1 > ccaPP::maxCorProj(x = x, y = y, method = "pearson")
2 > corstar = acepack::ace(x = x, y = y)
3 > cor(corstar$tx, corstar$ty)
```

**Proposition 4.37**

Consider two random variables  $X$  and  $Y$ .  $X \perp\!\!\!\perp Y$  if and only if  $r^*(X, Y) = 0$ .

**Proof:** Given a random variable  $X$ , its characteristic function is  $\phi_X(t) = \mathbb{E}[e^{itX}]$ .

Recall that

$$\begin{cases} \phi_X(t) = \phi_Y(t), \forall t \in \mathbb{R} \text{ if and only if } X \stackrel{\mathcal{L}}{=} Y \\ \phi_{X,Y}(s,t) = \mathbb{E}[e^{i(sX+tY)}] = \phi_X(s) \cdot \phi_Y(t), \forall s, t \in \mathbb{R} \text{ if and only if } X \perp\!\!\!\perp Y \end{cases}$$

If  $r^*(X, Y) = 0$ , let  $s, t \in \mathbb{R}$  and consider  $\varphi(x) = \phi_X(x) = \mathbb{E}[e^{ixX}]$  and

$\psi(y) = \phi_Y(y) = \mathbb{E}[e^{iyY}]$ , then  $\text{Cov}[e^{isX}, e^{itY}] = \text{Cov}[X'_s, Y'_t] = 0$ , i.e.

$$\mathbb{E}[X'_s Y'_t] = \mathbb{E}[X'_s] \mathbb{E}[Y'_t],$$

$$\underbrace{\mathbb{E}[e^{i(sX+tY)}]}_{\phi_{X,Y}(s,t)} = \underbrace{\mathbb{E}[e^{isX}] \cdot \mathbb{E}[e^{itY}]}_{\phi_X(s) \cdot \phi_Y(t)}, \forall s, t \in \mathbb{R} \text{ i.e. } X \perp\!\!\!\perp Y.$$

## Proposition 4.38

Consider two random variables  $X$  and  $Y$  such that  $(X, Y)$  is a Gaussian vector. Then  $r^*(X, Y) = |\text{Corr}[X, Y]|$ .

- See [Lancaster \(1957, 1958\)](#), and Gauss-Hermite decomposition

$$f(x, y) = \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left(-\frac{x^2 - 2\rho xy + y^2}{2[1-\rho^2]}\right) = \phi(x)\phi(y) \cdot \sum_{i=0}^{\infty} r^i H_i(x)H_i(y)$$

where  $H_i$ 's are Hermite polynomial.

## Independence

- Instead of

$$r^*(X, Y) = \max_{\varphi \in \mathcal{F}_x, \psi \in \mathcal{G}_y} \mathbb{E}[\varphi(X)\psi(Y)],$$

where

$$\begin{cases} \mathcal{F}_x = \{\varphi : \mathcal{X} \rightarrow \mathbb{R} : \mathbb{E}[\varphi(X)] = 0 \text{ and } \mathbb{E}[\varphi^2(X)] = 1\} \\ \mathcal{G}_y = \{\psi : \mathcal{Y} \rightarrow \mathbb{R} : \mathbb{E}[\psi(Y)] = 0 \text{ and } \mathbb{E}[\psi^2(Y)] = 1\} \end{cases}$$

**Definition 4.59: Constrained Maximal Correlation, Bach and Jordan (2002), Gretton et al. (2005)**

Consider two random variables  $X$  and  $Y$ , as well as some Hilbert spaces  $\bar{\mathcal{F}}_x \subset \mathcal{F}_x$  and  $\bar{\mathcal{G}}_y \subset \mathcal{G}_y$ ,

$$\bar{r}^*(X, Y) = \max_{\varphi \in \bar{\mathcal{F}}_x, \psi \in \bar{\mathcal{G}}_y} \{\text{Corr}[\varphi(X), \psi(Y)]\}.$$

# Independence

- Kimeldorf and Sampson (1978) and Kimeldorf et al. (1982) suggested to consider for  $\bar{\mathcal{F}}_x$  and  $\bar{\mathcal{G}}_y$  as subsets of monotone functions.

$$\begin{cases} \bar{\mathcal{F}}_x = \{\varphi \in \mathcal{F}_x : \varphi \text{ monotone}\} \\ \bar{\mathcal{G}}_y = \{\psi \in \mathcal{G}_y : \psi \text{ monotone}\} \end{cases}$$

- See Mourier (1953), Hannan (1961), Jensen and Mayer (1977) and Lin (1987).

to go further ➔ (for more details on RKHS issues)

# Independence

## Definition 4.60: Linear Independence

In a general context, consider two random vectors  $\mathbf{X}$  and  $\mathbf{Y}$ , in  $\mathbb{R}^{d_x}$  and  $\mathbb{R}^{d_y}$ , respectively.  $\mathbf{X} \perp \mathbf{Y}$  if and only if for any  $\mathbf{a} \in \mathbb{R}^{d_x}$  and  $\mathbf{b} \in \mathbb{R}^{d_y}$

$$\text{Cov}[\mathbf{a}^\top \mathbf{X}, \mathbf{b}^\top \mathbf{Y}] = 0.$$

## Definition 4.61: Independence

In a general context, consider two random vectors  $\mathbf{X}$  and  $\mathbf{Y}$ .  $\mathbf{X} \perp\!\!\!\perp \mathbf{Y}$  if and only if for any  $\mathcal{A} \subset \mathbb{R}^{d_x}$  and  $\mathcal{B} \subset \mathbb{R}^{d_y}$ ,

$$\mathbb{P}[\{\mathbf{X} \in \mathcal{A}\} \cap \{\mathbf{Y} \in \mathcal{B}\}] = \mathbb{P}[\{\mathbf{X} \in \mathcal{A}\}] \cdot \mathbb{P}[\{\mathbf{Y} \in \mathcal{B}\}].$$

## Proposition 4.39: Independence

Consider two random vectors  $\mathbf{X}$  and  $\mathbf{Y}$ .  $\mathbf{X} \perp\!\!\!\perp \mathbf{Y}$  if and only if for any functions  $\varphi : \mathbb{R}^{d_x} \rightarrow \mathbb{R}$  and  $\psi : \mathbb{R}^{d_y} \rightarrow \mathbb{R}$  (such that the expected values below exist and are well-defined)

$$\mathbb{E}[\varphi(\mathbf{X})\psi(\mathbf{Y})] = \mathbb{E}[\varphi(\mathbf{X})] \cdot \mathbb{E}[\psi(\mathbf{Y})],$$

or equivalently

$$\text{Cov}[\varphi(\mathbf{X}), \psi(\mathbf{Y})] = 0.$$

# Independence

## Definition 4.62: Mutual Independence

Let  $\mathbf{Y} = (Y_1, \dots, Y_k)$  denote some random vector. All components of  $\mathbf{Y}$  are (mutually) independent if for any  $\mathcal{A}_1, \dots, \mathcal{A}_k \subset \mathbb{R}$

$$\mathbb{P}\left[\{(Y_1, \dots, Y_k) \in \bigcap_{i=1}^k \mathcal{A}_i\}\right] = \prod_{i=1}^k \mathbb{P}[\{Y_i \in \mathcal{A}_i\}].$$

## Definition 4.63: Conditional Independence (dimension 2)

$X$  and  $Y$  are independent conditionally on  $Z$ , denoted  $X \perp\!\!\!\perp Y | Z$ , if for any sets  $\mathcal{A}, \mathcal{B}, \mathcal{C} \subset \mathbb{R}$ ,

$$\mathbb{P}[X \in \mathcal{A}, Y \in \mathcal{B} | Z \in \mathcal{C}] = \mathbb{P}[X \in \mathcal{A} | Z \in \mathcal{C}] \cdot \mathbb{P}[Y \in \mathcal{B} | Z \in \mathcal{C}].$$

## Definition 4.64: Conditional Independence

In a general context, consider three random vectors  $\mathbf{X}$ ,  $\mathbf{Y}$  and  $\mathbf{Z}$ .  $(\mathbf{X} \perp\!\!\!\perp \mathbf{Y})|\mathbf{Z}$  if and only if for any  $\mathcal{A} \subset \mathbb{R}^{d_x}$ ,  $\mathcal{B} \subset \mathbb{R}^{d_y}$  and  $\mathcal{C} \subset \mathbb{R}^{d_z}$ ,

$$\mathbb{P}[\{\mathbf{X} \in \mathcal{A}\} \cap \{\mathbf{Y} \in \mathcal{B}\} | \mathbf{Z} \in \mathcal{C}] = \mathbb{P}[\{\mathbf{X} \in \mathcal{A}\} | \mathbf{Z} \in \mathcal{C}] \cdot \mathbb{P}[\{\mathbf{Y} \in \mathcal{B}\} | \mathbf{Z} \in \mathcal{C}].$$

## Proposition 4.40

Consider three random variables  $X$ ,  $Y$ , and  $Z$ . If  $X \perp Z$  and  $Y \perp Z$ , then  $aX + bY \perp Z$ , for any  $a, b \in \mathbb{R}$ .

# Independence

**Proposition 4.41:**  $X \perp Z, Y \perp Z \not\Rightarrow \psi(X, Y) \perp Z$

Consider three random variables  $X$ ,  $Y$ , and  $Z$ . If  $X \perp Z$  and  $Y \perp Z$ , it does not imply that  $\psi(X, Y) \perp Z$ , for any  $\psi : \mathbb{R}^2 \rightarrow \mathbb{R}$ .

$$(X, Y, Z) = \begin{cases} (0, 0, 0) & \text{with probability } 1/4, \\ (0, 1, 1) & \text{with probability } 1/4, \\ (1, 0, 1) & \text{with probability } 1/4, \\ (1, 1, 0) & \text{with probability } 1/4. \end{cases}$$

**Proposition 4.42**

Consider a random vector  $\mathbf{X}$  in  $\mathbb{R}^k$ , and a random variable  $Z$ .  
 $\mathbf{X} \perp Z$  does not imply that  $\psi(\mathbf{X}) \perp Z$ , for any  $\psi : \mathbb{R}^k \rightarrow \mathbb{R}$ .

## Proposition 4.43

Consider three random variables  $X$ ,  $Y$ , and  $Z$ . Even if  $X \perp\!\!\!\perp Z$  and  $Y \perp\!\!\!\perp Z$ , it does not imply either that  $\psi(X, Y) \perp Z$  or that  $\psi(X, Y) \perp\!\!\!\perp Z$ , for any  $\psi : \mathbb{R}^2 \rightarrow \mathbb{R}$ .

## Proposition 4.44

Consider a random vector  $\mathbf{X}$  in  $\mathbb{R}^k$ , and a random variable  $Z$ .

$\mathbf{X} \perp\!\!\!\perp Z$  does not imply either that  $\psi(\mathbf{X}) \perp Z$  **or**  $\psi(\mathbf{X}) \perp\!\!\!\perp Z$ , for any  $\psi : \mathbb{R}^k \rightarrow \mathbb{R}$ .

# Causation

## Definition 4.65: Common cause, Reichenbach (1956)

If  $X$  and  $Y$  are non-independent,  $X \not\perp\!\!\!\perp Y$ , then, either

$$\begin{cases} X \text{ causes } Y \\ Y \text{ causes } X \\ \text{there exists } Z \text{ such that } Z \text{ causes both } X \text{ and } Y. \end{cases}$$

- › See also Bollen and Pearl (2013)
- › SCM, Goldberger (1972), Duncan (1975) or Bollen (1989)
- › Bayesian network, Pearl (1985), Henrion (1988), Charniak (1991)
- › Causal path diagrams and probabilistic DAGs, Spirtes et al. (1993)

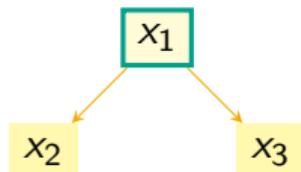


# Causation

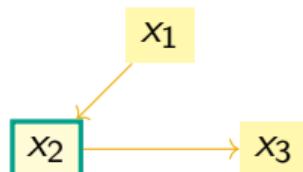
- Sewall Wright (see [Wright \(1921, 1934\)](#)) used directed graphs to represent probabilistic cause and effect relationships among a set of variables, and developed path diagrams and path analysis



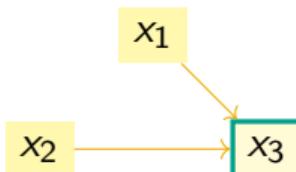
(a)  
confounder



(b)  
mediator



(c)  
collider



# Causation

## Definition 4.66: Path

A path  $\pi$  from a node  $x_i$  to another node  $x_j$  is a sequence of nodes and edges starting at  $x_i$  and ending at  $x_j$ .

## Definition 4.67: $d$ -separation

A set of nodes  $\mathbf{x}_i$  is said to be  $d$ -separated with another set of nodes  $\mathbf{x}_j$  by  $\mathbf{x}_c$  whenever every path from any  $x_i \in \mathbf{x}_i$  to any  $x_j \in \mathbf{x}_j$  is blocked by  $\mathbf{x}_c$ . We will simply denote  $\mathbf{x}_i \perp\!\!\!\perp_{\mathcal{G}} \mathbf{x}_j \mid \mathbf{x}_c$ .

## Proposition 4.45

Two nodes  $x_i$  and  $x_j$  are  $d$ -separated by  $\mathbf{x}_c$  if and only members of  $\mathbf{x}_c$  block all paths from  $x_i$  to  $x_j$ .

# Causation

- Chain rule : 
$$\begin{cases} \mathbb{P}[x_1, x_2, x_3, x_4] = \mathbb{P}[x_1] \times \mathbb{P}[x_2|x_1] \times \mathbb{P}[x_3|x_1, x_2] \times \mathbb{P}[x_4|x_1, x_2, x_3] \\ \mathbb{P}[x_1, x_2, x_3, x_4] = \mathbb{P}[x_4] \times \mathbb{P}[x_3|x_4] \times \mathbb{P}[x_2|x_3, x_4] \times \mathbb{P}[x_1|x_2, x_3, x_4] \end{cases}$$

## Definition 4.68: Directed acyclic graph, DAG (or causal graph)

A directed acyclic graph (DAG)  $\mathcal{G}$  is a directed graph with no directed cycles.

## Definition 4.69: Markov Property

Given a causal graph  $\mathcal{G}$  with nodes  $\mathbf{x}$ , the joint distribution of  $\mathbf{X}$  satisfies the (global) Markov property with respect to  $\mathcal{G}$  if, for any disjoints  $\mathbf{x}_1$ ,  $\mathbf{x}_2$  and  $\mathbf{x}_c$

$$\mathbf{x}_1 \perp_{\mathcal{G}} \mathbf{x}_2 \mid \mathbf{x}_c \Rightarrow \mathbf{X}_1 \perp\!\!\!\perp \mathbf{X}_2 \mid \mathbf{X}_c.$$

## Proposition 4.46: Probabilistic graphical model

If  $\mathbf{X}$  satisfies the (global) Markov property with respect to  $\mathcal{G}$

$$\mathbb{P}[x_1, \dots, x_n] = \prod_{i=1}^n \mathbb{P}[x_i | \text{parents}(x_i)]$$

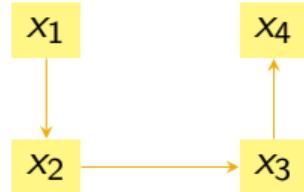
where  $\text{parents}(x_i)$  are nodes with edges directed towards  $x_i$



- Path from  $x_1$  to  $x_3$  is blocked by  $x_2$ , i.e.,  $x_1 \perp\!\!\!\perp x_3 | x_2$ , or  $X_1 \perp\!\!\!\perp X_3 | X_2$ . From the chain rule,

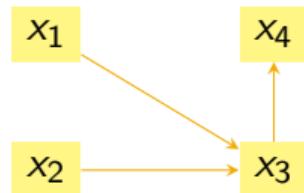
$$\mathbb{P}[x_1, x_2, x_3] = \mathbb{P}[x_1] \times \mathbb{P}[x_2 | x_1] \times \underbrace{\mathbb{P}[x_3 | x_2, x_1]}_{\mathbb{P}[x_3 | x_2]}$$

# Causation



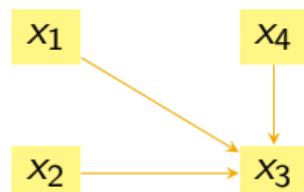
- From the chain rule, for the causal graph on the left (top),

$$\mathbb{P}[x_1, x_2, x_3, x_4] = \mathbb{P}[x_1] \times \mathbb{P}[x_2|x_1] \times \mathbb{P}[x_3|x_2] \times \mathbb{P}[x_4|x_3]$$



- From the chain rule, for the causal graph on the left (middle),

$$\mathbb{P}[x_1, x_2, x_3, x_4] = \mathbb{P}[x_1] \times \mathbb{P}[x_2] \times \mathbb{P}[x_3|x_1, x_2] \times \mathbb{P}[x_4|x_3]$$



- From the chain rule, for the causal graph on the left (bottom),

$$\mathbb{P}[x_1, x_2, x_3, x_4] = \mathbb{P}[x_1] \times \mathbb{P}[x_2] \times \mathbb{P}[x_3|x_1, x_2, x_4] \times \mathbb{P}[x_4]$$

# Intervention

- ›  $\mathbb{P}[Y \in \mathcal{A}|X = x]$  : how  $Y \in \mathcal{A}$  is likely to occur if  $X$  happened to be equal to  $x$
- › Therefore, it is an observational statement.
- ›  $P[Y \in \mathcal{A}|\text{do}(X = x)]$  : how  $Y \in \mathcal{A}$  is likely to occur if  $X$  is set to  $x$
- › It is here an intervention statement.
- › Using causal graphs, intervention  $\text{do}(X = x)$  means that all incoming edges to  $x$  are cut.
- › If  $P[Y \in \mathcal{A}|\text{do}(X = x)] \neq \mathbb{P}[Y \in \mathcal{A}|X = x]$ , it means that  $X$  and  $Y$  are confounded, see [Pearl \(2009\)](#).

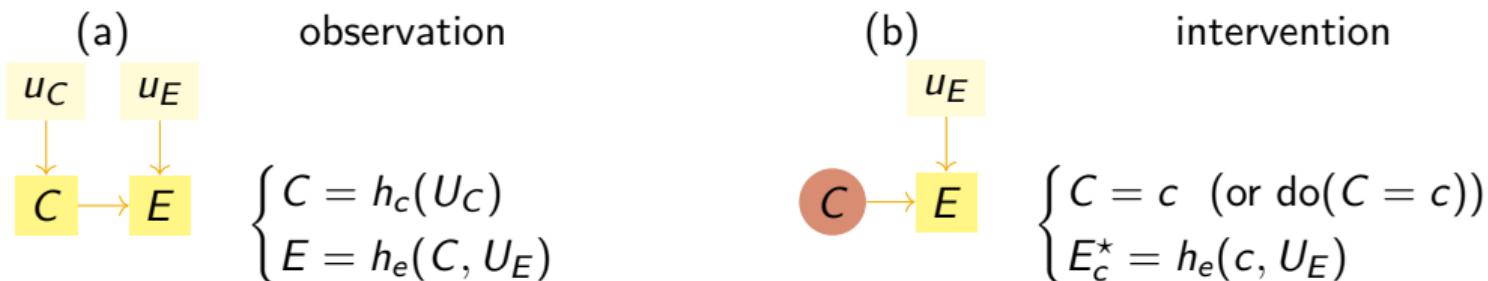
# Intervention

## Definition 4.70: Structural Causal Models (SCM)

In a simple causal graph, with two nodes  $C$  (the cause) and  $E$  (the effect), the causal graph is  $C \rightarrow E$ , and the mathematical interpretation can be summarized in two assignments

$$\begin{cases} C = h_c(U_C) \\ E = h_e(C, U_E), \end{cases}$$

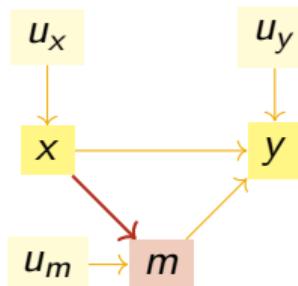
where  $U_C$  and  $U_E$  are two independent random variables,  $U_C \perp\!\!\!\perp U_E$ .



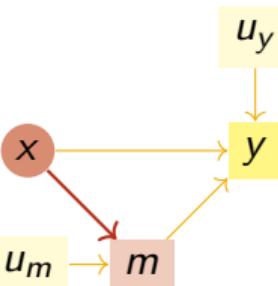
# Intervention

(a)

*m* mediator variable

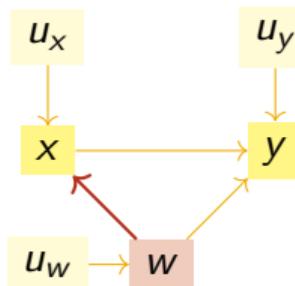


(b)

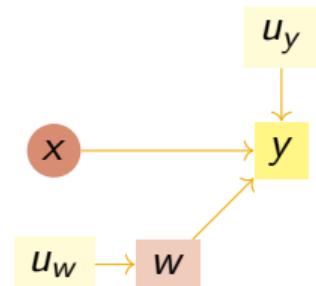


(c)

*w* confounding variable



(d)



$$\begin{cases} \text{mediator : } & \mathbb{P}[Y_x^* = 1] = \mathbb{P}[Y = 1|\text{do}(X = x)] = \mathbb{P}[Y = 1|X = x] \\ \text{confusion : } & \mathbb{P}[Y_x^* = 1] = \mathbb{P}[Y = 1|\text{do}(X = x)] \neq \mathbb{P}[Y = 1|X = x]. \end{cases}$$

# Intervention

- In fact, in the presence of a confounding factor,  $\mathbb{P}[Y_x^* = 1]$  which corresponds to  $\mathbb{P}[Y = 1|\text{do}(X = x)]$  should be written

$$\sum_w \mathbb{P}[Y = 1|W = w, X = x] \cdot \mathbb{P}[W = w] = \mathbb{E}(\mathbb{P}[Y = 1|W, X = x]).$$

## Causal Inference and counterfactuals

- Define potential outcomes to quantify the treatment effect,  $\text{TE} = y_{i,T \leftarrow 1}^* - y_{i,T \leftarrow 0}^*$

$\begin{cases} \text{observation} & : y_{i,T \leftarrow 1}^* \text{ when } t_i = 1 \text{ is observed, and } x_i \\ \text{counterfactual} & : y_{i,T \leftarrow 0}^* \text{ when } t_i = 1 \text{ is observed, and } x_i \end{cases}$

- Here we want to observe counterfactuals  $y_{i,T \leftarrow t'}^*$  at the individual level.

Gender	Name	Treatment $t_i$	Outcome (Weight)				Height $x_i$	...	
			$y_i$	$y_{i,T \leftarrow 0}^*$	$y_{i,T \leftarrow 1}^*$	TE			
1	H	Alex	0	75	75	64	11	172	...
2	F	Betty	1	52	67	52	15	161	...
3	F	Beatrix	1	57	71	57	14	163	...
4	H	Ahmad	0	78	78	61	17	183	...

- Different notations are used  $y(1)$  and  $y(0)$  in Imbens and Rubin (2015),  $y^1$  and  $y^0$  in Cunningham (2021), or  $y_{t=1}$  and  $y_{t=0}$  in Pearl and Mackenzie (2018).

# Causal Inference and counterfactuals

- Define potential outcomes to quantify the treatment effect,  $\text{TE} = y_{i,T \leftarrow 1}^* - y_{i,T \leftarrow 0}^*$

$\begin{cases} \text{observation} & : y_{i,T \leftarrow 1}^* \text{ when } t_i = 1 \text{ is observed, and } x_i \\ \text{counterfactual} & : y_{i,T \leftarrow 0}^* \text{ when } t_i = 1 \text{ is observed, and } x_i \end{cases}$

- Here we want to observe counterfactuals  $y_{i,T \leftarrow t'}^*$  at the individual level.

Gender	Name	Treatment $t_i$	Outcome (Weight)				Height $x_i$	...
			$y_i$	$y_{i,T \leftarrow 0}^*$	$y_{i,T \leftarrow 1}^*$	TE		
1	H	Alex	0	75	75	?	172	...
2	F	Betty	1	52	?	52	161	...
3	F	Beatrix	1	57	?	57	163	...
4	H	Ahmad	0	78	78	?	183	...

- Different notations are used  $y(1)$  and  $y(0)$  in Imbens and Rubin (2015),  $y^1$  and  $y^0$  in Cunningham (2021), or  $y_{t=1}$  and  $y_{t=0}$  in Pearl and Mackenzie (2018).

# Causal Inference and counterfactuals

## Definition 4.71: Average Treatment Effect, Holland (1986)

Given a treatment  $T$ , the average treatment effect on outcome  $Y$  is

$$\tau = \text{ATE} = \mathbb{E}[Y_{t \leftarrow 1}^* - Y_{t \leftarrow 0}^*].$$

## Definition 4.72: Conditional Average Treatment Effect, Wager and Athey (2018)

Given a treatment  $T$ , the conditional average treatment effect on outcome  $Y$ , given some covariates  $\mathbf{X}$ , is

$$\tau(\mathbf{x}) = \text{CATE}(\mathbf{x}) = \mathbb{E}[Y_{t \leftarrow 1}^* - Y_{t \leftarrow 0}^* | \mathbf{X} = \mathbf{x}].$$

## Definition 4.73: Individual Average Treatment Effect

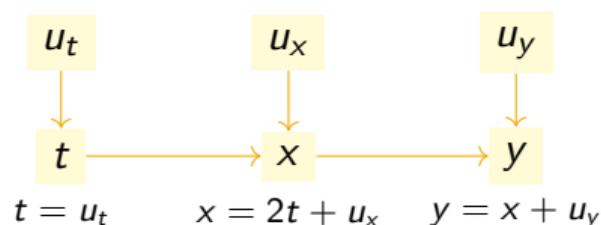
Given a treatment  $T$ , the conditional average treatment effect on outcome  $Y$ , for individual  $i$ , given covariates  $\mathbf{X}_i$ , is

$$\text{IATE}(i) = \mathbb{E}[Y_{i,t \leftarrow (1-t_i)}^* - Y_{i,t \leftarrow t_i}^*].$$

# Causal Inference and counterfactuals

› Pearl (2009) suggest to use a twin network representation of the counterfactual

› Start with a simple structural causal model, e.g.,

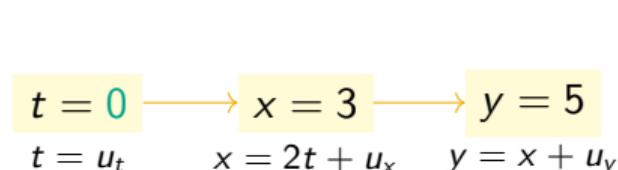


$$\begin{cases} t = u_t \\ x = 2t + u_x \\ y = x + u_y \end{cases}$$

› Suppose we were able to estimate that model

# Causal Inference and counterfactuals

- › Pearl (2009) suggest to use a twin network representation of the counterfactual

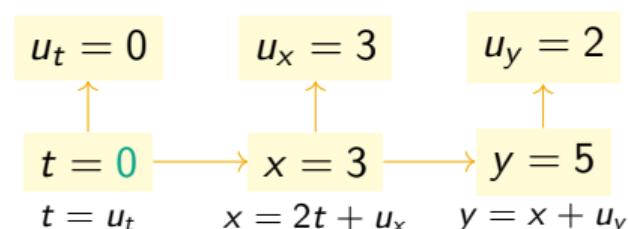


- › Consider a single observation
- › i.e. a triplet  $(t_i, \mathbf{x}_i, y_i)$

# Causal Inference and counterfactuals

› Pearl (2009) suggest to use a twin network representation of the counterfactual

› Inverse the SCM

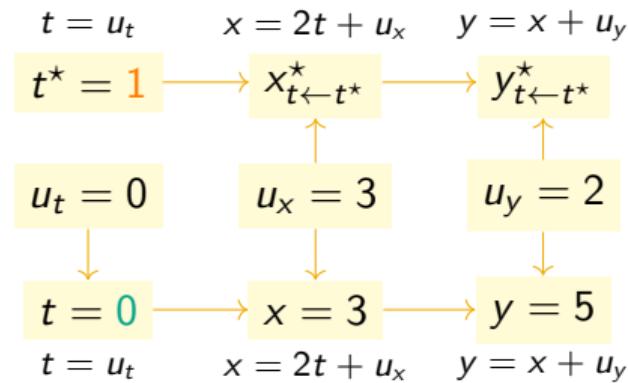


$$\begin{cases} u_t = t \\ u_t = x - 2t \\ u_y = y - x \end{cases}$$

- › From that triplet  $(t_i, x_i, y_i)$
- › Derive unobserved  $u$ 's.

# Causal Inference and counterfactuals

› Pearl (2009) suggest to use a twin network representation of the counterfactual

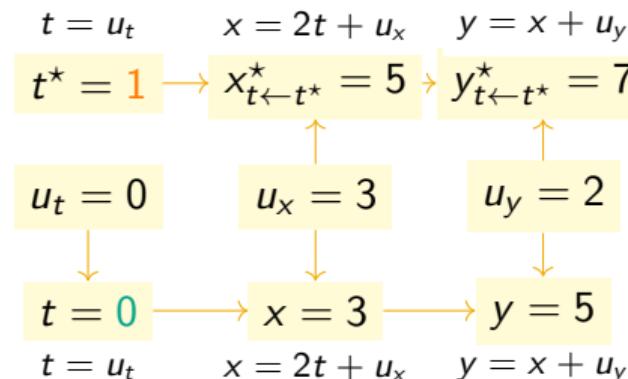


› Suppose that the same SCM holds in the counterfactual world

$$\begin{cases} t^* \\ x_{t \leftarrow t^*}^* = 2t^* + u_t \\ y_{t \leftarrow t^*}^* = x_{t \leftarrow t^*}^* + u_y \end{cases}$$

# Causal Inference and counterfactuals

› Pearl (2009) suggest to use a twin network representation of the counterfactual

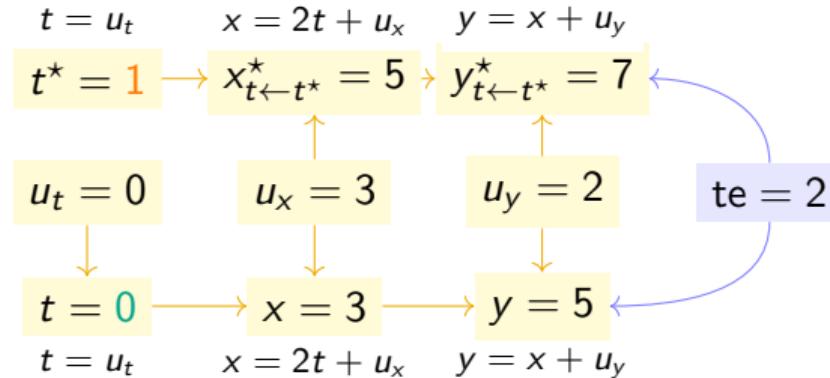


› Plugin  $u$ 's obtained from  $(t_i, \mathbf{x}_i, y_i)$

$$\begin{cases} t^* \\ x_{t \leftarrow t^*}^* = 2t^* + u_t \\ y_{t \leftarrow t^*}^* = x_{t \leftarrow t^*}^* + u_y \end{cases}$$

# Causal Inference and counterfactuals

- › Pearl (2009) suggest to use a twin network representation of the counterfactual



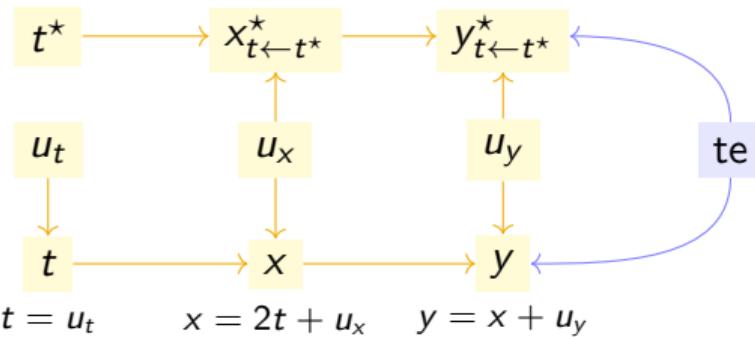
- › We can compute the treatment effect

$$te = y - y_{t \leftarrow t^*}^*$$

# Causal Inference and counterfactuals

- › Pearl (2009) suggest to use a twin network representation of the counterfactual

$$t = u_t \quad x = 2t + u_x \quad y = x + u_y$$



- › Works well only if the SCM can be inverted (to derive the  $u$ 's)

– Part 5 –

## Sensitive Variables and Proxies

## Context

- There exists a list of variables considered (by law) as sensitive (e.g., in Québec)

- ▶ race,
- ▶ color,
- ▶ sex,
- ▶ gender identity or expression,
- ▶ pregnancy,
- ▶ sexual orientation,
- ▶ civil status,
- ▶ age,
- ▶ religion,
- ▶ political convictions,
- ▶ language,
- ▶ ethnic or national origin,
- ▶ social condition,
- ▶ disability



# Explainability

- “On a collection of additional 60 images, the classifier predicts “Wolf” if there is snow (or light background at the bottom), and “Husky” otherwise, regardless of animal color, position, pose, etc.”, Ribeiro et al. (2016)



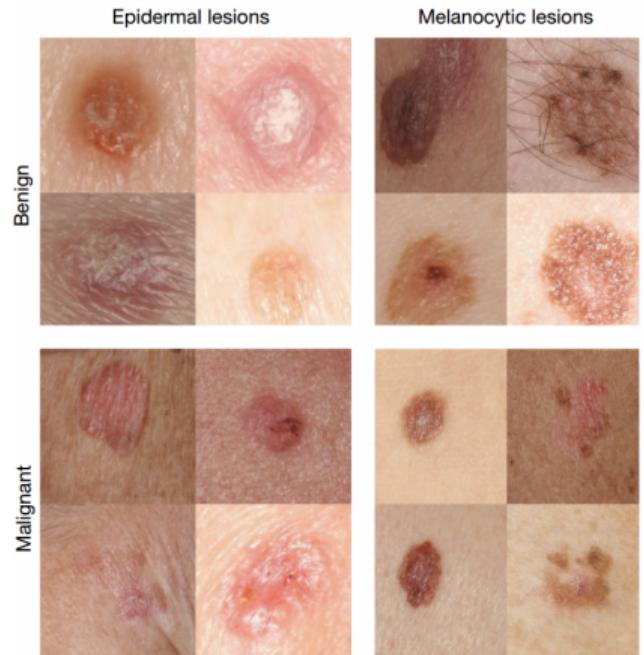
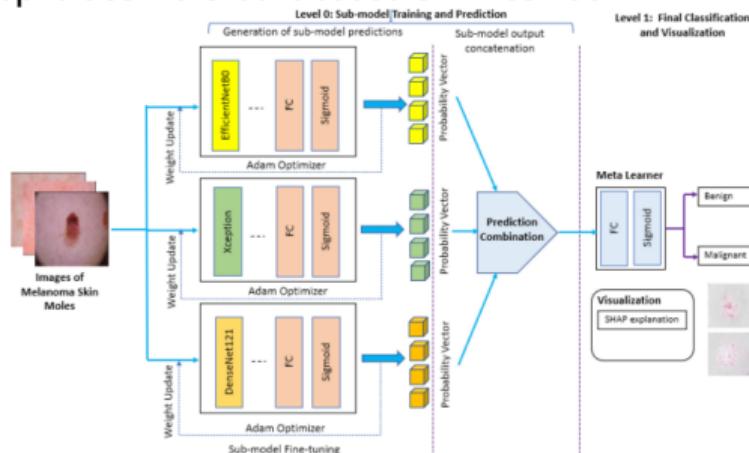
**Figure 11:** Raw data and explanation of a bad model’s prediction in the “Husky vs Wolf” task.

	Before	After
Trusted the bad model	10 out of 27	3 out of 27
Snow as a potential feature	12 out of 27	25 out of 27

**Table 2:** “Husky vs Wolf” experiment results.

# Explainability

Esteva et al. (2017) and Winkler et al. (2019) use deep-classifiers to detect skin cancer

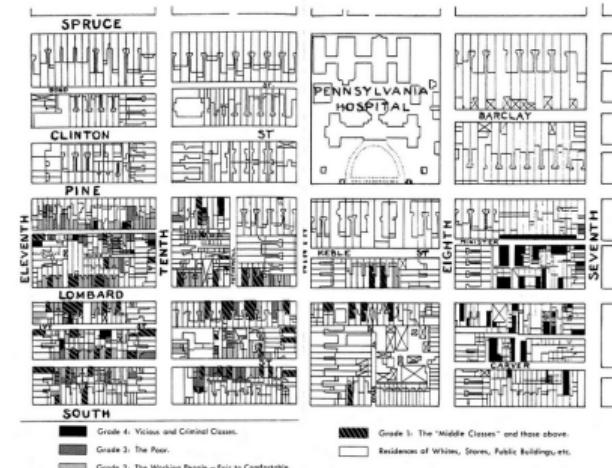
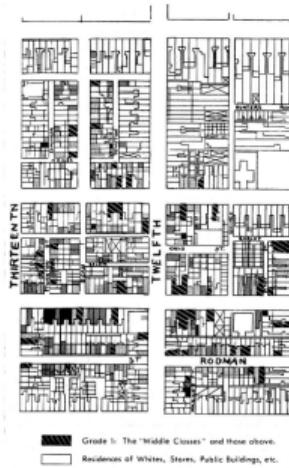
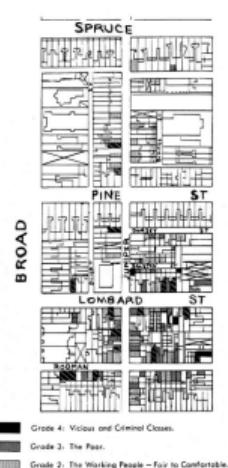


- “So in the set of biopsy images, if an image had a ruler in it, the algorithm was more likely to call a tumor malignant, because the presence of a ruler correlated with an increased likelihood a lesion was cancerous,” Patel (2017)

# Racial Discrimination

## Definition 5.1: Racism, Merriam-Webster (2022)

A belief that race is a fundamental determinant of human traits and capacities and that racial differences produce an inherent superiority of a particular race; *also* behavior or attitudes that reflect and foster this belief.

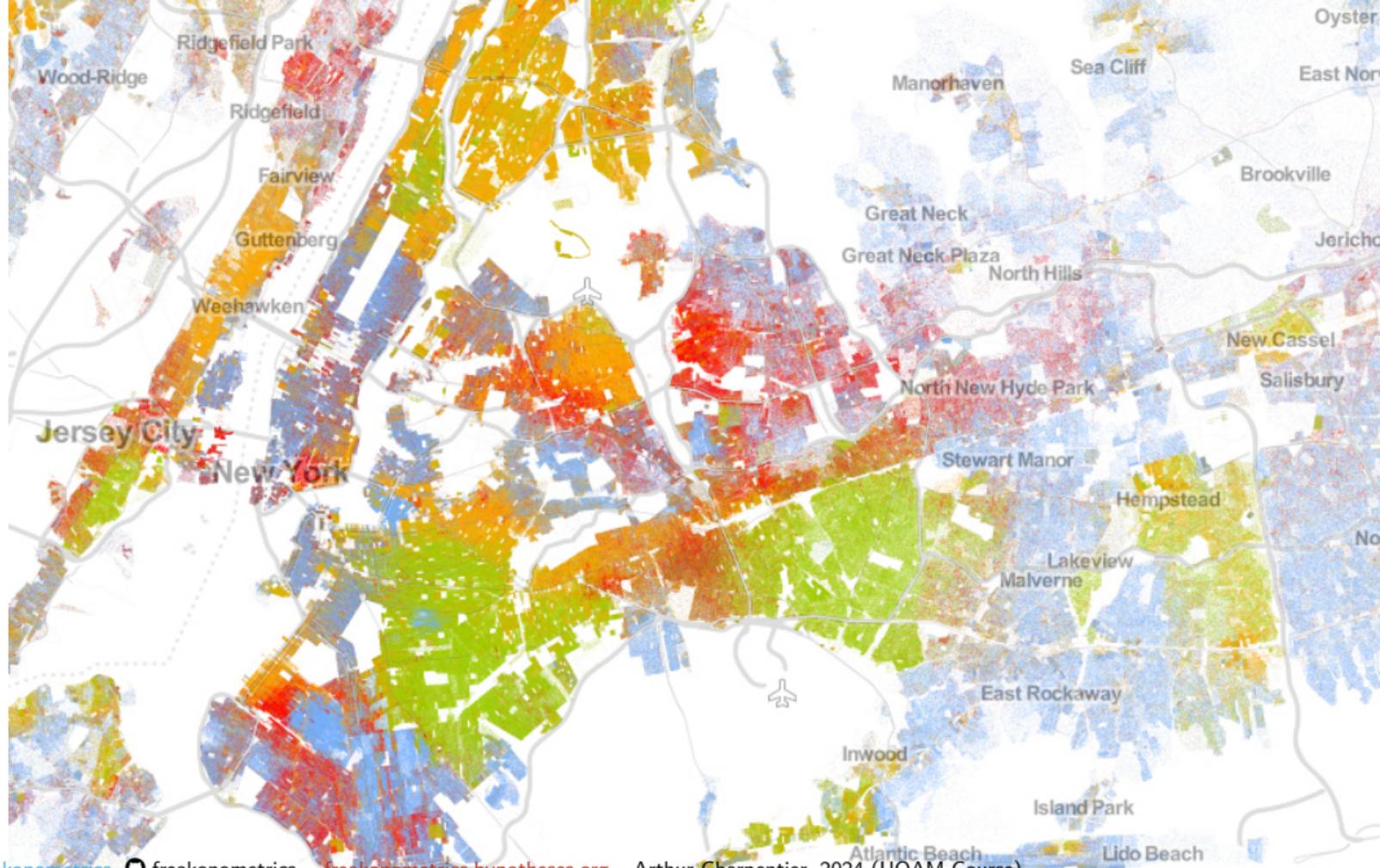


Du Bois (1899)

# Racial Discrimination

- Gannon (2016) “*race is a social construct*”
- In the U.S., “*an individual's response to the race question is based upon self-identification*”
  - ▶ White American, European American, or Middle Eastern American (59.3%)
  - ▶ “Hispanic or Latino Americans (18.9%)”
  - ▶ Black or African American (12.6%)
  - ▶ American Indian or Alaska Native (0.7%)
  - ▶ Asian American (5.9%)
  - ▶ Native Hawaiian or Other Pacific Islander (0.2%)
- See maps on <https://www.arcgis.com/apps/mapviewer/index.html>

U.S. Office of Personnel Management Guide to Personnel Data Standards			ETHNICITY AND RACE IDENTIFICATION (Please read the Privacy Act Statement and instructions before completing form.)		
Name (Last, First, Middle Initial)	Social Security Number	Birthday (Month and Year)			
Agency Use Only					
<b>Privacy Act Statement</b>					
Ethnicity and race information is requested under the authority of 42 U.S.C. Section 2000e-16 and in compliance with the Office of Management and Budget's 1997 Revisions to the Standards for the Classification of Federal Data on Race and Ethnicity. Providing this information is voluntary and has no impact on your employment status, but in the instance of missing information, your employing agency will attempt to identify your race and ethnicity by visual observation.					
This information is used as necessary to plan for equal employment opportunity throughout the Federal government. It is also used by the U. S. Office of Personnel Management or employing agency maintaining the records to locate individuals for personnel research or survey response and in the production of summary descriptive statistics and analytical studies in support of the function for which the records are collected and maintained, or for related workforce studies.					
Social Security Number (SSN) is requested under the authority of Executive Order 9397, which requires SSN be used for the purpose of uniform, orderly administration of personnel records. Providing this information is voluntary and failure to do so will have no effect on your employment status. If SSN is not provided, however, other agency sources may be used to obtain it.					
<b>Specific Instructions:</b> The two questions below are designed to identify your ethnicity and race. <b>Regardless of your answer to question 1, go to question 2.</b>					
<b>Question 1.</b> Are You Hispanic or Latino? (A person of Cuban, Mexican, Puerto Rican, South or Central American, or other Spanish culture or origin regardless of race.) <input type="checkbox"/> Yes <input type="checkbox"/> No					
<b>Question 2.</b> Please select the racial category or categories with which you most closely identify by placing an "X" in the appropriate box. Check as many as apply.					
RACIAL CATEGORY (Check as many as apply)	DEFINITION OF CATEGORY				
<input type="checkbox"/> American Indian or Alaska Native	A person having origins in any of the original peoples of North and South America (including Central America), and who maintains tribal affiliation or community attachment.				
<input type="checkbox"/> Asian	A person having origins in any of the original peoples of the Far East, Southeast Asia, or the Indian subcontinent including, for example, Cambodia, China, India, Japan, Korea, Malaysia, Pakistan, the Philippine Islands, Thailand, and Vietnam.				
<input type="checkbox"/> Black or African American	A person having origins in any of the black racial groups of Africa.				
<input type="checkbox"/> Native Hawaiian or Other Pacific Islander	A person having origins in any of the original peoples of Hawaii, Guam, Samoa, or other Pacific Islands.				
<input type="checkbox"/> White	A person having origins in any of the original peoples of Europe, the Middle East, or North Africa.				



# Racial Discrimination

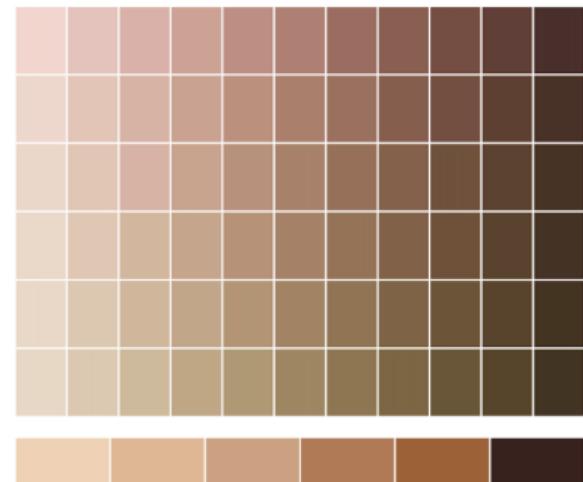
- By comparing skull anatomy and skin color, “*generis humani varietates quinae principes, species vero unica*” (one species, and five principle varieties of humankind), Blumenbach (1775)
  - ▶ the “*Caucasian*” (or white race, for Europeans, including Middle Easterners and South Asians in the same category),
  - ▶ the “*Mongolian*” (or yellow race, including all East Asians)
  - ▶ the “*Malayan*” (or brown race, including Southeast Asians and Pacific Islanders)
  - ▶ the “*Ethiopian*” (or black race, including all sub-Saharan Africans)
  - ▶ the “*American*” (or red race, including all Native Americans)

# Racial Discrimination

## Definition 5.2: Colourism, Merriam-Webster (2022)

Prejudice or discrimination especially within a racial or ethnic group favoring people with lighter skin over those with darker skin.

- Fitzpatrick Skin Scale (six levels), Telles (2014).



# Racial Discrimination

- In the context of insurance, several reference in the late XIX-th Century
- *“industrial insurers operated a high-volume business; so to simplify sales they charged the same nickel to everyone. The home office then calculated benefits according to actuarially defensible discrimination, by age initially and then by race. In November 1881, Metropolitan decided to mimic Prudential, allowing policies to be sold to African Americans once again, but with the understanding that black policyholders' survivors only received two-thirds of the standard benefit,”* Bouk (2015)
- 1884, Massachusetts state legislature passed the [Act to Prevent Discrimination by Life Insurance Companies Against People of Color](#)
- See Frederick L. Hoffman (1896) (discussed earlier)

# Racial Discrimination

- In auto insurance, Heller (2015) observed that African American neighbourhood pay 70% more, on average, for auto insurance premiums than other neighbourhoods.

Figure 6-1. Average Premium by Company and Percentage of African American Residents

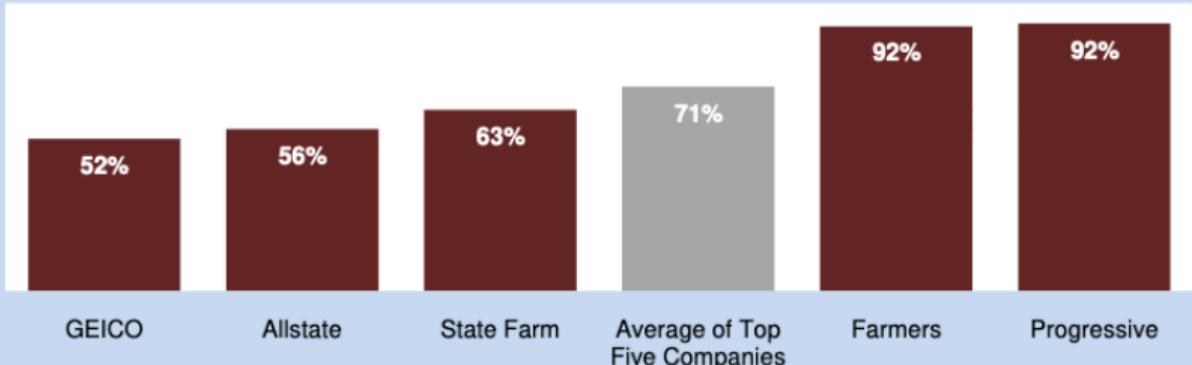
Company	<25% African American	25-49% African American	50-75% African American	≥75% African American	National Average	Percent Increase from <25% to ≥75% African American
Allstate	\$658	\$800	\$848	\$1,024	\$674	56%
Farmers	662	757	795	1,271	676	92%
GEICO	575	713	793	876	591	53%
Progressive	694	852	911	1,332	717	93%
State Farm	543	697	771	882	561	63%
<b>Top Five Companies</b>	<b>\$622</b>	<b>\$769</b>	<b>\$834</b>	<b>\$1,060</b>	<b>\$640</b>	<b>70%</b>

Source: CFA analysis of data provided by Quadrant Information Services, US Census

via <https://www.michiganautolaw.com/wp-content/uploads/2017/08/Consumer-Federation-of-America-High-Price-of-Mandatory-Auto-Insurance-in-Predominantly...>

# Racial Discrimination

Figure 6-2. Average Premium increase by Company in Predominantly African American Communities Compared with Predominantly White Communities



Source: CFA analysis of data provided by Quadrant Information Services, US Census

- The Property Casualty Insurers Association of America responded that “*insurance rates are color-blind and solely based on risk.*”

via <https://www.pciaa.net/pciwebsite/cms/content/viewpage?sitePageId=43349>

# Sex and Gender Discrimination

- See slides with life tables per gender (exist since 1720, see [Struyck \(1912\)](#))

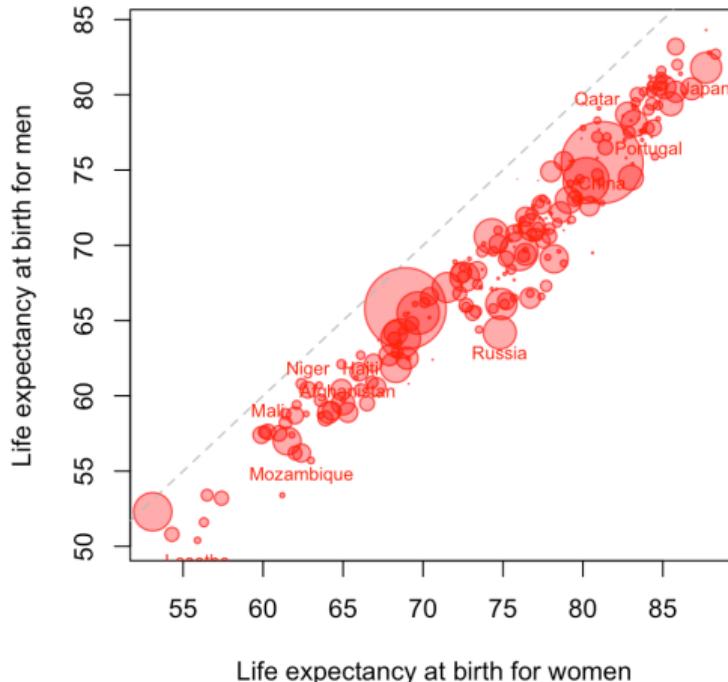
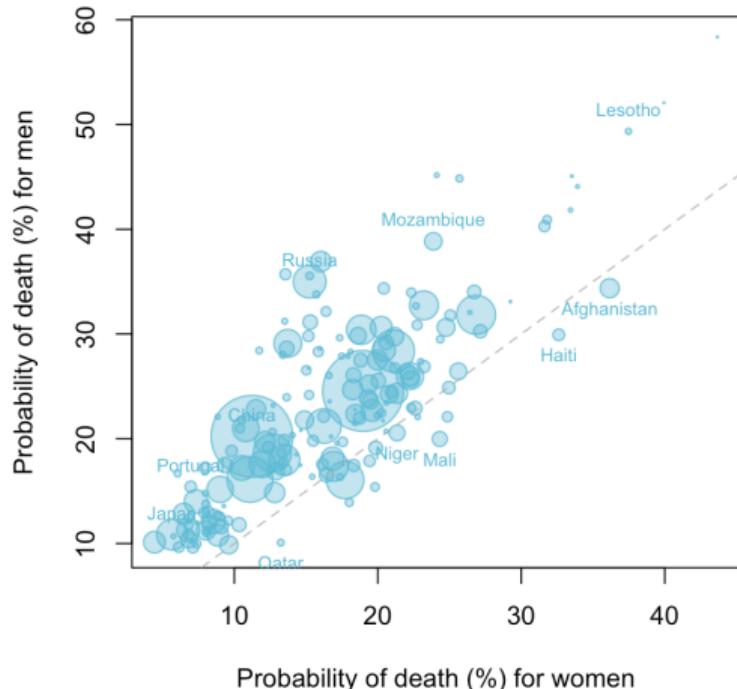
## Definition 5.3: Sexism, [Merriam-Webster \(2022\)](#)

Prejudice or discrimination based on sex especially, discrimination against women; *also* behavior, conditions, or attitudes that foster stereotypes of social roles based on sex.

- [Martin \(1977\)](#), [Hedges \(1977\)](#) and [Myers \(1977\)](#) in the U.S. In [Los Angeles, Department of Water and Power vs. Manhart](#), the Supreme Court considered a pension system in which female employees made higher contributions than males for the same monthly benefit because of longer life expectancy.
- See slides about the “Gender Directive” in Europe (and [Thiery and Van Schoubroeck \(2006\)](#)).

# Sex and Gender Discrimination

Probability of dying between 30 and 70 years old



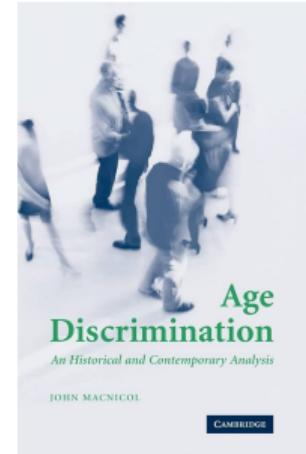
Data Ortiz-Ospina and Beltekian (2018).

# Age-based Discrimination

- › Age is not a club in which one enters at birth, and it will change with time, Macnicol (2006)
- › “*If you are not already part of a group disadvantaged by prejudice, just wait a couple of decades—you will be,*” Robbins (2015).

## Definition 5.4: Ageism, Merriam-Webster (2022)

Prejudice or discrimination against a particular age-group and especially the elderly.



- › COVID-19 Decision Support Tool used in England, in March 2020, provided by the NHS (National Health System).  
<https://www.nhsdghandbook.co.uk/wp-content/uploads/2020/04/COVID-Decision-Support-Tool.pdf>

# Age-based Discrimination

## COVID-19 DECISION SUPPORT TOOL



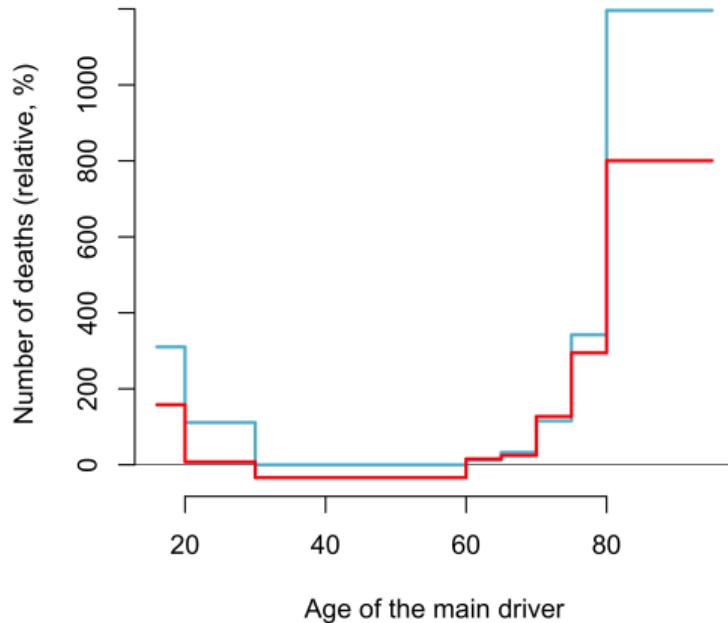
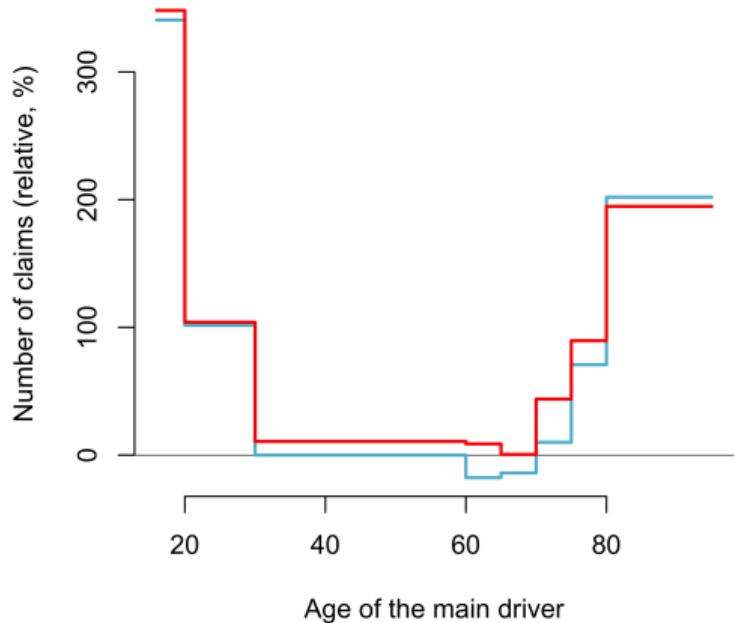
<b>1</b>	<b>2</b>	<b>3</b>	
<b>AGE</b>	<b>POINTS</b>	<b>CO-MORBIDITY</b>	
<50	0	In last 3 years, cardiac arrest from any cause	2
50-60	1	Chronic condition causing:	
61-65	2	• ≥3 hospital admissions in the last year	2
66-70	3	• ≥4 weeks continuous admission for current inpatients	2
71-75	4	Congestive heart failure with symptoms at rest or on minimal exertion	1
76-80	5	Chronic lung disease with symptoms at rest or on minimal exertion	1
>80	6	Hypertension	1
<b>TOTAL = SUM OF THE 3 DOMAINS ABOVE (-1 FOR FEMALE SEX)</b>			
<p><b>! There may be situations arising that are outside the scope of the framework that require special consideration, thus clinical discretion will continue to apply.</b></p> <p><b>Frailty scoring is used as a proxy for physiological frailty which leads to reduced chances of recovery in ICU, therefore where conditions pre-exist impact on physical activity but are stable and inappropriately affect the score, then that situation requires special consideration.</b></p>			

POINTS	TREATMENT	FAILURE OF FIRST LINE MANAGEMENT	NOTES	Deviations from ARDS guideline	Investigations	Support	Treatment
Group 1 ≤ 8	ICU-based care	Palliation or ECMO	Usual criteria for ECMO and <60 years	Step 1 ≤ 8	Tracheo-bronchial aspirate for respiratory viruses. Avoid CT & bronchoscopy unless indicated. H score screen blood tests, D-dimers, LSH & troponin (all days). Lung US to reduce X-ray usage	CPAP trial in ICU or with rapid access to intubation (for hours not days) <b>Avoid HFNO</b>	CAP antimicrobials Continue single agent prophylaxis in +ve pts Disease modifying agents as part of RCT
Group 2 ≥ 8	Ward-based care	Step 3	Consider trial of CPAP	Step 2 ≥ 8	Standard swabs	Ward-based CPAP	CAP antimicrobials Continue single agent prophylaxis in +ve pts
Group 3 Patients not normally for full active management or failed CPAP trial	Facemask oxygen	Palliation	Consider domiciliary care	Step 3 Patients not normally for full active management or failed CPAP trial	Standard swabs	Facemask oxygen	CAP antimicrobials Continue single agent prophylaxis in +ve pts

# Age-based Discrimination

- “*on the grounds of age do not constitute discrimination (...) if age is a determining factor in the assessment of risk for the service in question and this assessment is based on actuarial principles and relevant and reliable statistical data,*” of the European Union (2018)
- “*a society that relentlessly discriminates against people because of their age can still treat them equally throughout their lives. Everyone's turn [to be discriminated against] is coming,*” Gosseries (2014)
- Number of crashes (left) and number of fatalities (right), per million miles driven, for both males and females (males in blue and females in red), by driver age. The reference (0) are men aged 30-60 years. The number of accidents is three times higher (+200%) for those over 85, and the number of deaths more than ten times higher (+900%). (data source: Li et al. (2003))

# Age-based Discrimination

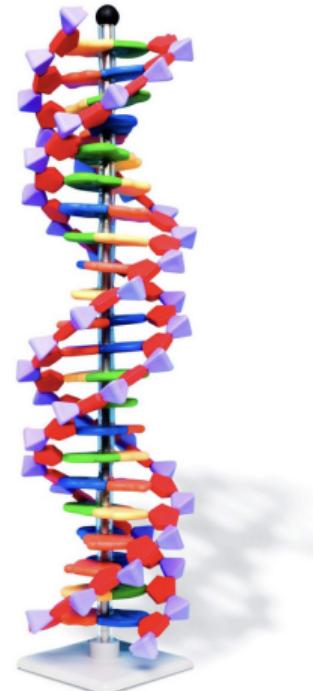


# Genetic or Social Identity

**Definition 5.5: Genetic discrimination, Ajunwa (2014, 2016)**

Genetic discrimination should be defined as when an individual is subjected to negative treatment, not as a result of the individual's physical manifestation of disease or disability, but solely because of the individual's genetic composition

- Related to “*genetic determinism*” (as defined in de Melo-Martín (2003) and Harden (2023)) or more recently “*genetic essentialism*” (as in Peters (2014)).



## Genetic or Social Identity

- According to [Rawls \(1999\)](#), the starting point for each person in society is the result of a social lottery (the political, social, and economic circumstances in which each person is born) and a natural lottery (the biological potentials with which each person is born)
- *“Those suffering from disease, a genetic defect, or disability on the basis of a natural lottery should not be penalized in insurance,”* [Wortham \(1986\)](#)
- Social identity refers to a person’s membership in a social group. The common groups that make up a person’s social identity are age, ability, ethnicity, race, gender, sexual orientation, socioeconomic status and religion, as discussed by [Tajfel \(1978\)](#) and [Tajfel et al. \(1986\)](#).

## Names, Text and Language

- › Icelandic surnames are different from most other naming systems in the modern Western world by being patronymic or occasionally matronymic, as mentioned in [Willson \(2009\)](#) and [Johannesson \(2013\)](#): they indicate the father (or mother) of the child and not the historic family lineage. Generally, with few exceptions, a person's last name indicates the first name of their father (patronymic) or in some cases mother (matronymic) in the genitive, followed by **-son** "(son)" or **-dóttir** ("daughter").
- › For instance, in 2017, Iceland's national Women's soccer team players were Agla Maria Albertsdóttir, Sigridur Gardarsdóttir, Ingibjorg Sigurdardóttir, Glodis Viggosdóttir, Dagny Brynjarsdóttir, Sara Bjork Gunnarsdóttir, Fanndis Fridriksdóttir, Hallbera Gisladóttir, Gudbjorg Gunnarsdóttir, Sif Atladóttir or Gunnhildur Jonsdóttir. In the national Men's soccer team, players were Hákon Rafn Valdimarsson, Patrik Gunnarsson, Höskuldur Gunnlaugsson, Július Magnússon, Viktor Örlygur Andrasen or Kristall Máni Ingason.
- › From [Gaddis \(2017\)](#), (data from [US Census \(2012\)](#))

## Names, Text and Language

Name	Rank	White (%)	Black (%)	Hispanic (%)
Washington	138	5.2%	89.9%	1.5%
Jefferson	594	18.7%	75.2%	1.6%
Booker	902	30.0%	65.6%	1.5%
Banks	278	41.3%	54.2%	1.5%
Jackson	18	41.9%	53.0%	1.5%
Becker	315	96.4%	0.5%	1.4%
Meyer	163	96.1%	0.5%	1.6%
Walsh	265	95.9%	1.0%	1.4%
Larsen	572	95.6%	0.4%	1.5%
Orozco	690	3.9%	0.1%	95.1%
Velazquez	789	4.0%	0.5%	94.9%
Gonzalez	23	4.8%	0.4%	94.0%
Hernandez	15	4.6%	0.4%	93.8%

# Names, Text and Language

- As discussed in [Riach and Rich \(1991\)](#) and [Rorive \(2009\)](#), a popular technique to test for discrimination (in a real life context) is to use “*practice testing*” or “*situation testing*”. This started probably in the 60's in the U.K., with [Daniel et al. \(1968\)](#)
- In France, Top 3 first names by sex and generations in France, according to the origin (Southern Europe or Maghreb) of grandparents, [Coulmont and Simon \(2019\)](#)

	immigrants	children	grandchildren
Southern Europe	José, Antonio, Manuel Maria, Marie, Ana	Jean, David, Alexandre Marie, Sandrine, Sandra	Thomas, Lucas, Enzo Laura, Léa, Camille
Maghreb	Mohamed, Ahmed, Rachid Fatima, Fatiha, Khaduja	Mohamed, Karim, Mehdi Sarah, Nadia, Myriam	Yanis, Nicolas, Mehdi Sarah, Ines, Lina

# Names, Text and Language

White	Black	Asian	Hispanic
Cost estimators	Postal service	Manicurists	Drywall installers
Farmers, ranchers	Nursing assistants	Medical scientists	Roofers
Construction	Security guards	Software developers	Carpet installers
Surveying	Probation officers	Computer engineers	Painters and paperhanglers
Heavy vehicle	Orderlies aides	Database administrators	Maids-housekeeping cleaners
Property appraisers	Bus drivers	Computer programmers	Construction laborers
Floral designers	Vocational nurses	Chemists	Cement masons
Electrical installers	Barbers	Pharmacists	Brickmasons
Logging workers	Shuttle drivers	Supervisors of personal care	Pipelayers
Brickmasons	Home health aides	Other physicians	Landscaping workers
Aircraft pilots	Social workers	Taxi drivers	Agricultural workers

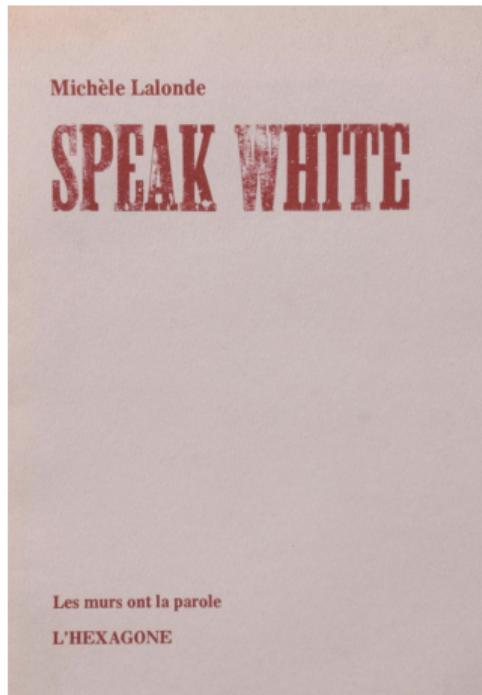
› <https://flowingdata.com/2024/01/31/occupation-and-race/>

# Names, Text and Language

- Jobs can also be related to gender (see <https://translate.google.com/>) in Turkish

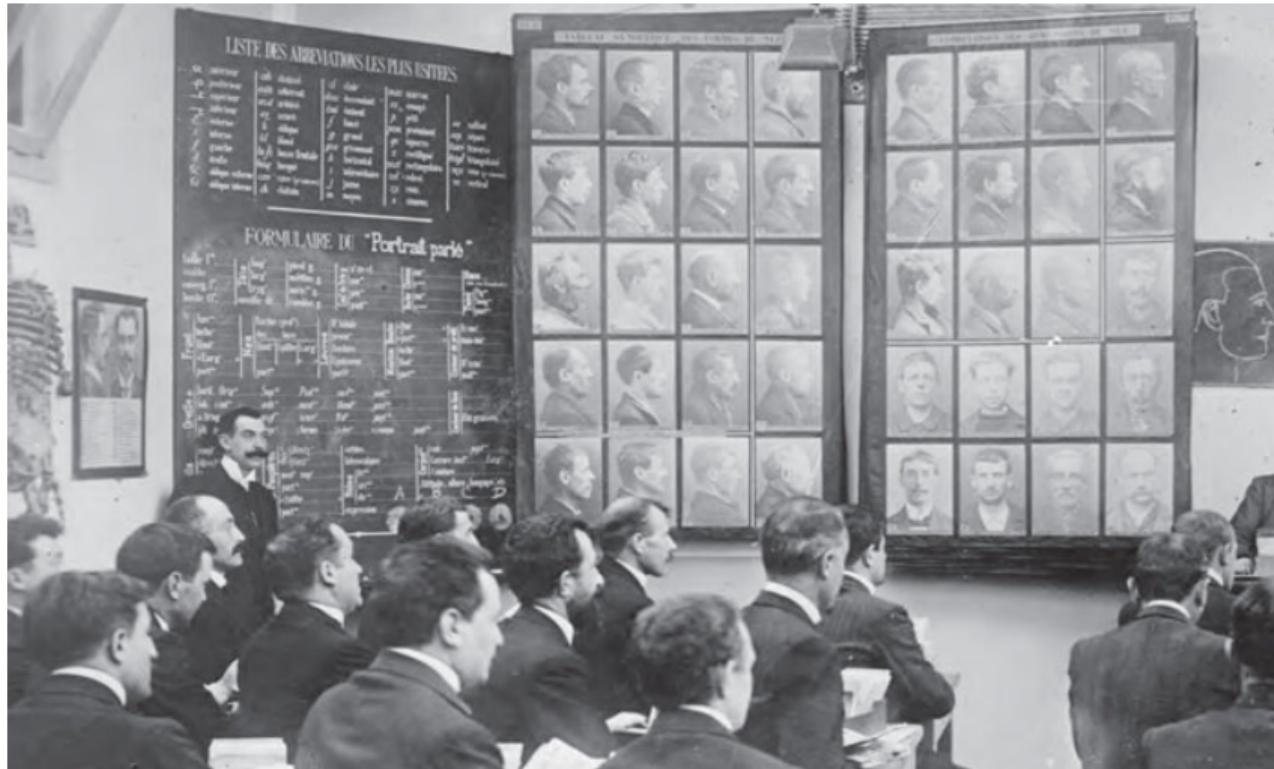
	2017	2023
o bir öğretmen	> she is a teacher	he is a teacher
o bir hemşire	> she is a nurse	she is a nurse
o bir doktor	> he is a doctor	she is a doctor
o bir Şarkıcı	> she is a singer	he is a singer
o bir sekreter	> she is a secretary	she is a secretary
o bir dişçi	> he is a dentist	he is a dentist
o bir çiçekçi	> she is a florist	she is a florist
o çalışan	> he is hard working	he is hard working
o tembel	> she is lazy	he is lazy
o güzel	> she is beautiful	she is beautiful
o çirkin	> he is ugly	he is ugly

# Names, Text and Language



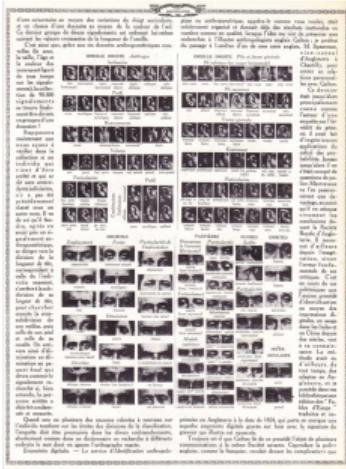
- “*Speak White* is the protest of white Negroes in America. Language here is the equivalent of colour for the American Negro. The French language is our black colour,” Michèle Lalonde, author of the 1968 poem “*Speak White*” (reported by [Dostie \(1974\)](#))
- “*phonostyle discrimination*,” Léon (1993), or of “*dias-tratic variation*,” with differences between usages by gender, age and social background (in the broad sense), in [Gadet \(2007\)](#).
- “*linguistic profiling*,” (identification of a person’s race from the sound of their voice), [Squires and Chadwick \(2006\)](#)

# Pictures



# Pictures

- More than a century ago, first **Lombroso (1876)**, and then **Bertillon and Chervin (1909)**, laid the foundations of phrenology and the “*born criminal*” theory, which assumes that physical characteristics are correlated with psychological traits and criminal inclinations (“*prima facie*”).



# Pictures

- › Faces generated by [Karras et al. \(2020\)](#). Gender and age were provided by `gender.toolpie`, `facelytics`, `picpurify` with a “confidence,” `cloud.google`, `howoldyoulook` and `facialage`



female, age: 38  
female (0.997)  
age: 34  
joy (74%)



female, age: 23  
female (0.989)  
age: 20  
joy (85%)



male, age: 37  
male (0.967)  
age: 27  
joy (81%)



male, age: 53  
male (0.985)  
age: 38  
joy (73%)

# Pictures

- › Faces generated by [Karras et al. \(2020\)](#). Gender and age were provided by [gender.toolpie](#), [facelytics](#), [picpurify](#) with a “confidence,” [cloud.google](#), [howolddoyoulook](#) and [facialage](#)



female, age: 30  
female (0.985)  
age: 28  
joy (82%)



male, age: 27  
male (0.983)  
age: 33  
joy (69%)



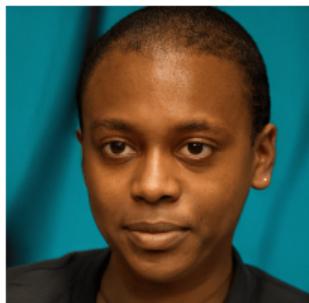
male, age: 43  
male (0.984)  
age: 38  
joy (78%)



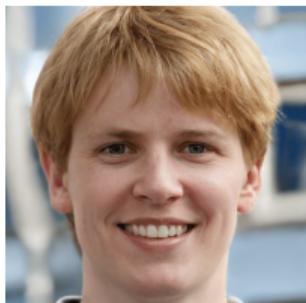
male, age: 37  
male (0.996)  
age: 38  
joy (56%)

# Pictures

- › Faces generated by [Karras et al. \(2020\)](#). Gender and age were provided by `gender.toolpie`, `facelytics`, `picpurify` with a “confidence,” `cloud.google`, `howoldyoulook` and `facialage`



male, age: 24  
male (0.944)  
age: 26  
joy (70%)



male, age: 33  
male (0.981)  
age: 32  
joy (81%)

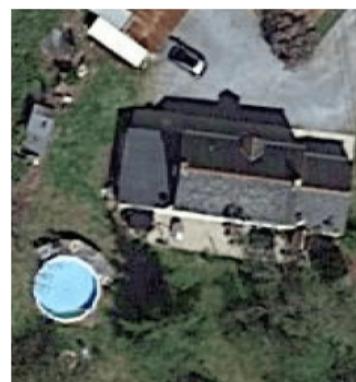
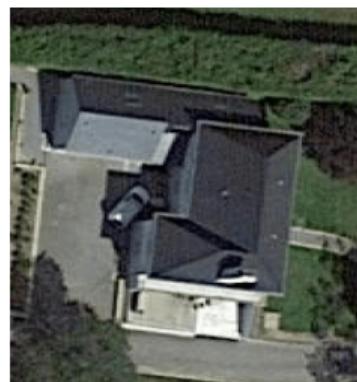


male, age: 34  
female (0.905)  
age: 34  
joy (82%)



male, age: 48  
male (0.989)  
age: 48  
joy (83%)

# Spatial Information



- “Geographic location is a well-established variable in many lines of insurance,” Bender et al. (2022).

# Spatial Information



- “Geographic information is crucial for estimating the future costs of an insurance contract,” Blier-Wong et al. (2021).

# Credit Scoring

- “*Credit scoring is one of the most successful applications of statistical and operations research modeling in finance and banking,*” Thomas et al. (2002).
- In the brief section “*how insurers determine your premium,*” in the National Association of Insurance Commissioners (2011, 2022) reports, it is explained that “*most insurers use the information in your credit report to calculate a credit-based insurance score. They do this because studies show a correlation between this score and the likelihood of filing a claim. Credit-based insurance scores are different from other credit scores.*”
- As shown in Dean and Nicholas (2018) and Dean et al. (2018), “*credit scores are increasingly used to understand health outcomes.*”

# Credit Scoring

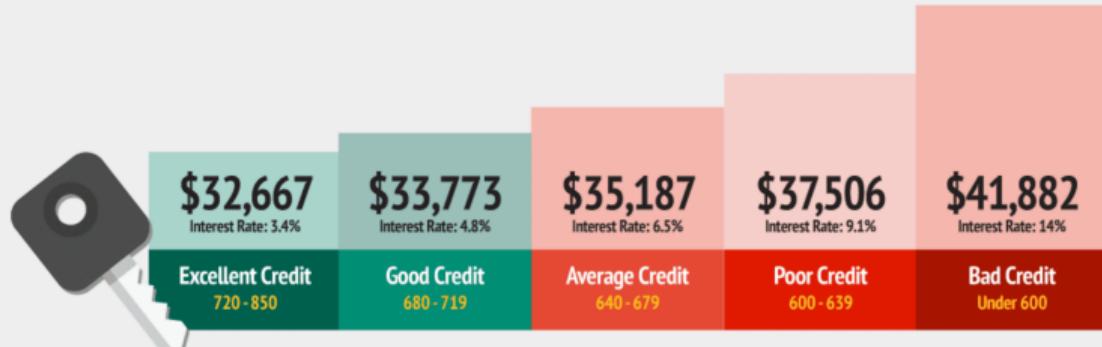
## Mortgage Rates

30-year Mortgage for \$150,000. Amount shown is principal and interest.



## Auto Loan Rates

60-month Auto Loan for \$30,000. Amount shown is principal and interest.



<https://www.incharge.org/debt-relief/credit-counseling/credit-score-and-credit-report/>

# Credit Scoring

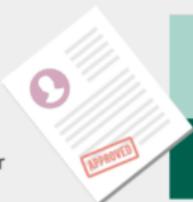
## Credit Card Rates

Average APR across all credit cards.  
Credit card rates will vary due to many different factors.



## Insurance Rates

30-year-old driver no tickets, no claims 4-door 2016 sedan driving 12,000 a year in city traffic.



<https://www.incharge.org/debt-relief/credit-counseling/credit-score-and-credit-report/>

# Networks

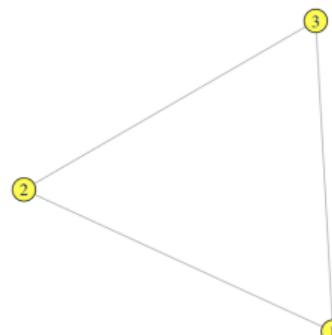
- “*Network and data analyses compound and reflect discrimination embedded within society,*” Bernstein (2007).
- “*You apply for a loan and your would-be lender somehow examines the credit ratings of your Facebook friends. If the average credit rating of these members is at least a minimum credit score, the lender continues to process the loan application. Otherwise, the loan application is rejected,*” Bhattacharya (2015)
- Homophily principle (in the sense of McPherson et al. (2001)), because as popular saying goes, “*birds of a feather flock together.*”
- “*Insurance companies can base premiums on all insured drivers in your household, including those not related by blood, such as roommates,*” National Association of Insurance Commissioners (2011, 2022)
- but there are a few things to bear in mind when using network data...

# Networks

## Definition 5.6: Network and Adjacency Matrix

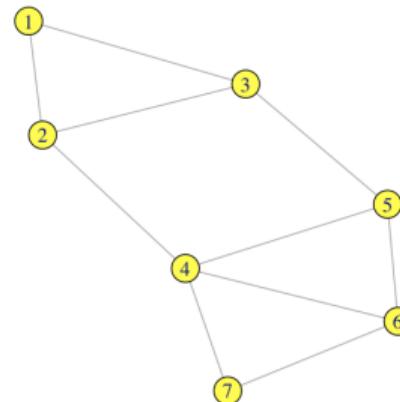
A **network** (or a **graph**) is a pair  $G = (V, E)$ , where  $V = \{1, \dots, n_V\}$  denote either **nodes**, or **vertices** and  $E \in \{0, 1\}^{n_V \times n_V}$  represents the **relationships**, through an adjacency matrix  $\mathbf{A}$ ,  $A_{i,j} = 1$  indicates a **link** - or **edge** - between  $i$  and  $j$ , or a collection of links  $\{e_1, \dots, e_{n_E}\}$ .

$$\begin{matrix} & 1 & 2 & 3 \\ \begin{matrix} 1 \\ 2 \\ 3 \end{matrix} & \left( \begin{matrix} . & 1 & 1 \\ 1 & . & 1 \\ 1 & 1 & . \end{matrix} \right) & = & \mathbf{A} \end{matrix}$$



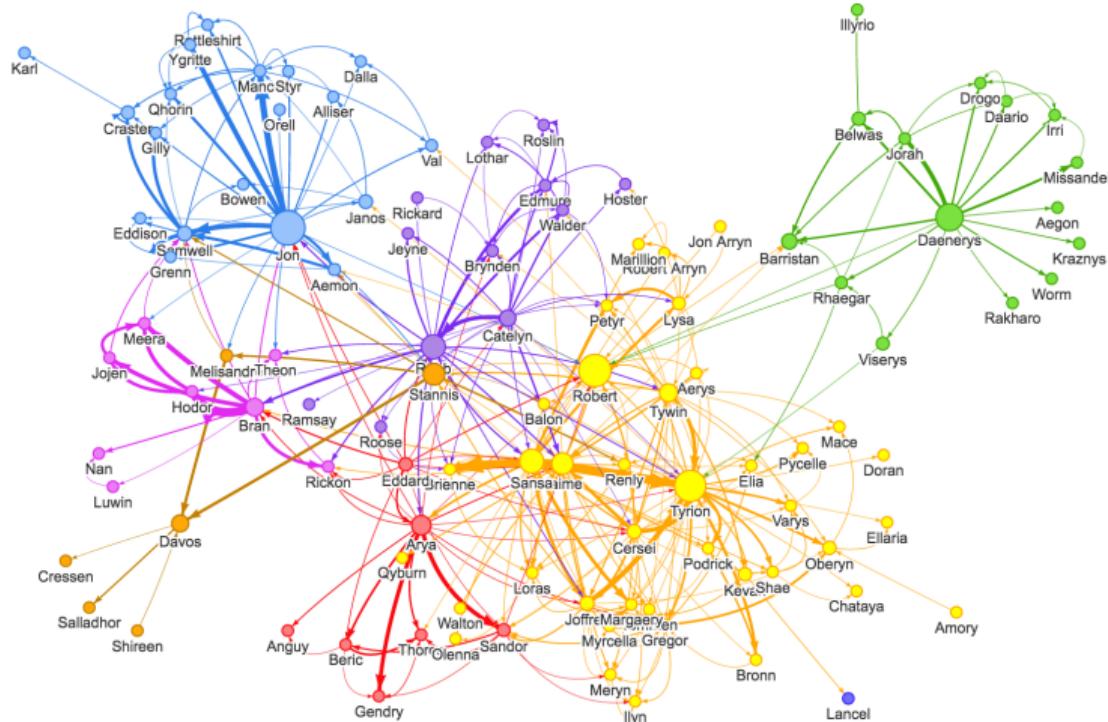
# Networks

$$\begin{matrix} & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{matrix} & \left( \begin{matrix} . & 1 & 1 & . & . & . & . \\ 1 & . & 1 & 1 & . & . & . \\ 1 & 1 & . & . & 1 & . & . \\ . & 1 & . & . & 1 & 1 & 1 \\ . & . & 1 & 1 & . & 1 & . \\ . & . & . & 1 & 1 & . & 1 \\ . & . & . & 1 & . & 1 & . \end{matrix} \right) = \mathbf{A} \end{matrix}$$

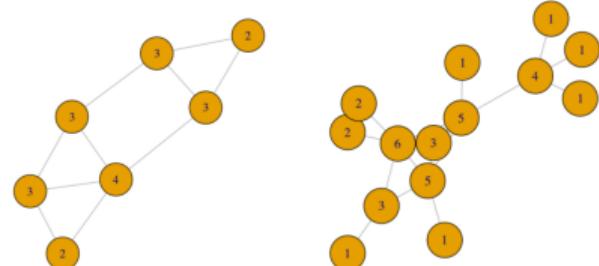


- There are no self-loops, i.e.  $A_{i,i} = 0$ .
- $A_{ij} = 1$  if and only if  $i$  and  $j$  are linked. The matrix is symmetric ( $A_{ij} = A_{ji}$ ), the network is undirected.

# Networks



$$\mathbf{A} = \begin{pmatrix} & & \\ \mathbf{A}_{\cdot,1} & \cdots & \mathbf{A}_{\cdot,n} \\ & & \end{pmatrix} = \begin{pmatrix} - & \mathbf{A}_{1,\cdot}^\top & - \\ \vdots & & \\ - & \mathbf{A}_{n,\cdot}^\top & - \end{pmatrix}$$



## Definition 5.7: Degrees

Row  $i$  contains list of vertices connected to vertice  $i$ .

$$d_i = \sum_{j=1}^n A_{i,j} = \mathbf{A}_{i,\cdot}^\top \mathbf{1}.$$

# Networks

- “on average your friends have more friends than you do.”

## Proposition 5.1: Friendship Paradox

The average number of friends of the collection of friends of individuals in a social network will be higher than the average number of friends of the collection of the individuals themselves. More formally

$$\frac{1}{n} \sum_{i=1}^n \left( \frac{1}{d_i} \sum_{j=1}^n A_{ij} d_j \right) \geq \frac{1}{n} \sum_{i=1}^n d_i.$$

Define differences  $\Delta_i$ 's between the average of its neighbours' degrees and its own degree, in the sense that

$$\Delta_i = \frac{1}{d_i} \sum_{j=1}^n A_{ij} d_j - d_i.$$

## Networks

Write the average as

$$\frac{1}{n} \sum_{i=1}^n \Delta_i = \frac{1}{n} \sum_{i=1}^n \left( \frac{1}{d_i} \sum_{j=1}^n A_{ij} d_j - d_i \right) = \frac{1}{n} \sum_{ij=1}^n \left( A_{ij} \frac{d_j}{d_i} - A_{ij} \right),$$

that yields

$$\frac{1}{n} \sum_{i=1}^n \Delta_i = \frac{1}{n} \sum_{ij=1}^n A_{ij} \left( \frac{d_j}{d_i} - 1 \right) \text{ but also } \frac{1}{n} \sum_{ij=1}^n A_{ij} \left( \frac{d_i}{d_j} - 1 \right),$$

by exchanging the summation indices, and because  $\mathbf{A}$  is a symmetric matrix. By adding the two, we can write

$$\frac{2}{n} \sum_{i=1}^n \Delta_i = \frac{1}{n} \sum_{ij} A_{ij} \left( \frac{d_j}{d_i} + \frac{d_i}{d_j} - 2 \right) = \frac{1}{2n} \sum_{ij} A_{ij} \left( \sqrt{\frac{d_j}{d_i}} - \sqrt{\frac{d_i}{d_j}} \right)^2 \geq 0.$$

(the exact equality holds only when  $d_i = d_j$  for all pairs of neighbors)

# Networks

- “*you apply for a loan and your would-be lender somehow examines the credit ratings of your Facebook friends. If the average credit rating of these members is at least a minimum credit score, the lender continues to process the loan application. Otherwise, the loan application is rejected,*” Bhattacharya (2015)
- “*il ne faut jamais juger les gens sur leurs fréquentations. Tenez, Judas, par exemple, il avait des amis irréprochables,*” Paul Verlaine
- For the generalized friendship paradox, which considers attributes other than degree, as in Cantwell et al. (2021), one can define an analogous quantity,  $\Delta_i^{(x)}$ , for some attribute  $x$  (such as the wealth) is defined as

$$\Delta_i^{(x)} = \frac{1}{d_i} \sum_j A_{ij} x_j - x_i,$$

## Networks

which measures the difference between the average of the attribute for node  $i$ 's neighbours and the value for  $i$  itself. When the average of this quantity over all nodes is positive one may say that the generalized friendship paradox holds. In contrast to the case of degree, this is not always true – the value of  $\Delta_i^{(x)}$  can be zero or negative – but we can write the average as

$$\frac{1}{n} \sum_i \Delta_i^{(x)} = \frac{1}{n} \sum_i \left( \frac{1}{d_i} \sum_j A_{ij} x_j - x_i \right) = \frac{1}{n} \sum_i \left( x_i \sum_j \frac{A_{ij}}{d_j} - x_i \right),$$

where the second line again follows from interchanging summation indices. Defining the new quantity

$$\delta_i = \sum_j \frac{A_{ij}}{d_j},$$

and noting that

$$\frac{1}{n} \sum_i \delta_i = \frac{1}{n} \sum_{ij} \frac{A_{ij}}{d_j} = \frac{1}{n} \sum_j \frac{1}{d_j} \sum_i A_{ij} = 1,$$

# Networks

we can then write

$$\frac{1}{n} \sum_i \Delta_i^{(x)} = \frac{1}{n} \sum_i x_i \delta_i - \frac{1}{n} \sum_i x_i \frac{1}{n} \sum_i \delta_i = \text{Cov}(\mathbf{x}, \boldsymbol{\delta}).$$

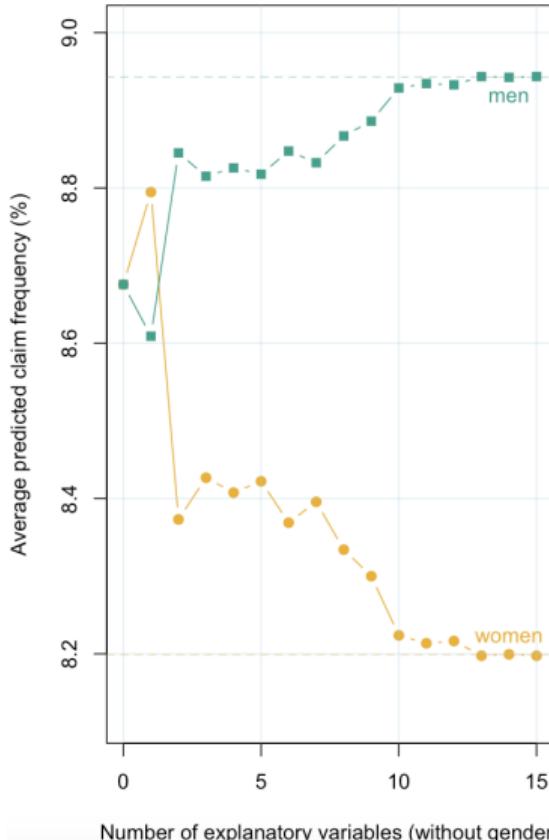
Thus, we will have a generalized friendship paradox in the sense defined here if (and only if)  $\mathbf{x}$  and  $\boldsymbol{\delta}$  are positively correlated. But this is not always the case

$$\left. \begin{array}{l} \text{Cov}(\mathbf{d}, \boldsymbol{\delta}) \geq 0 \\ \text{Cov}(\mathbf{x}, \boldsymbol{\delta}) \geq 0 \end{array} \right\} \not\Rightarrow \text{Cov}(\mathbf{d}, \mathbf{x}) \geq 0.$$

# On Proxy Discrimination

- On `frenchmotor` dataset, average claim frequencies are 8.94% (men) 8.20% (women).
- Consider some logistic regression to estimate annual claim frequency, on  $k$  explanatory variables **excluding gender**.

	men	women
$k = 0$	8.68%	8.68%
$k = 2$	8.85%	8.37%
$k = 8$	8.87%	8.33%
$k = 15$	8.94%	8.20%
empirical	8.94%	8.20%

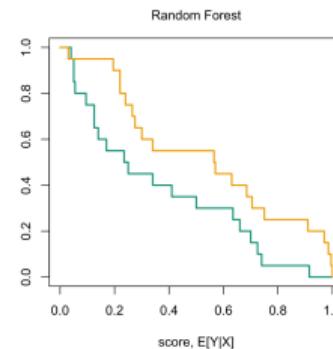
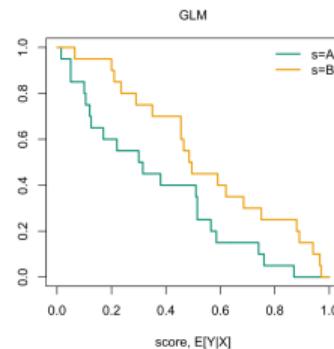
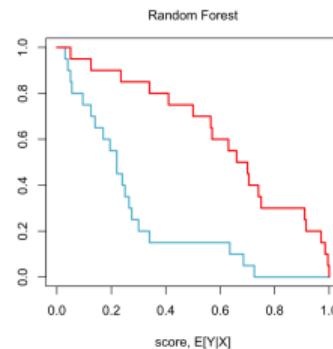
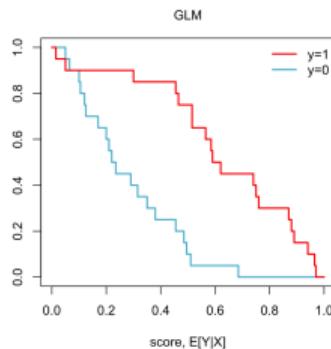
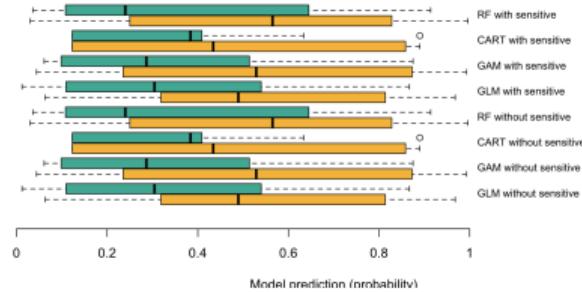
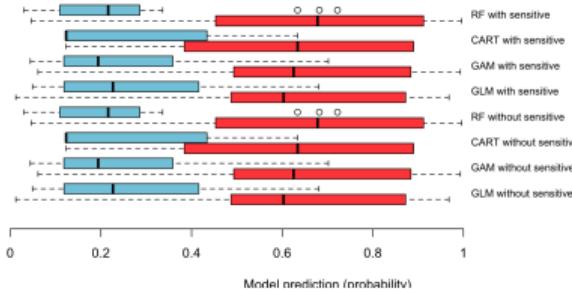


– Part 6 –

## Group Fairness

# Group Fairness

➤ Back on `toydata2`, distributions of scores,  $\hat{m}(\mathbf{x}_i)$ 's conditional on  $y_i$  and  $s_i$



## Definition 6.1: Fairness through unawareness, Dwork et al. (2012)

A model  $m$  satisfies the fairness through unawareness criteria, with respect to sensitive attribute  $s \in \mathcal{S}$  if  $m : \mathcal{X} \rightarrow \mathcal{Y}$ .

by Cynthia Dwork, Moritz Hardt, Toniann Pitassi, Omer Reingold and Richard Zemel,



# Group Fairness

- See introduction about the gender directive,

*“institutional messages of color blindness may therefore artificially depress formal reporting of racial injustice. Color-blind messages may thus appear to function effectively on the surface even as they allow explicit forms of bias to persist,”*  
Apfelbaum et al. (2010)

## Definition 6.2: Aware and unaware regression functions $\mu$

The aware regression function is  $\mu(\mathbf{x}, s) = \mathbb{E}[Y | \mathbf{X} = \mathbf{x}, S = s]$   
and the unaware regression function is  $\mu(\mathbf{x}) = \mathbb{E}[Y | \mathbf{X} = \mathbf{x}]$ .

# Historical Perspective: "Cultural Fairness" and "Statistical Discrimination"

## Definition 6.3: Four definitions of cultural fairness, Darlington (1971)

A test ( $\hat{y}$ ) is considered "culturally fair" if it fits the appropriate equation

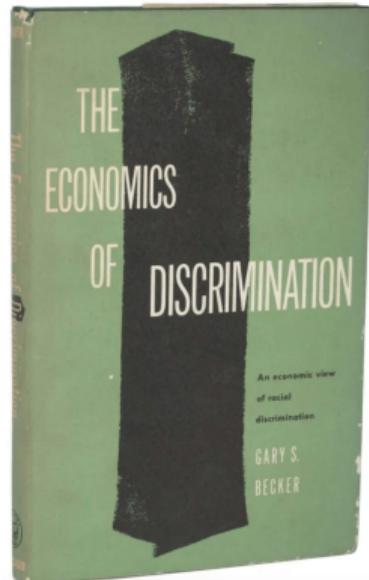
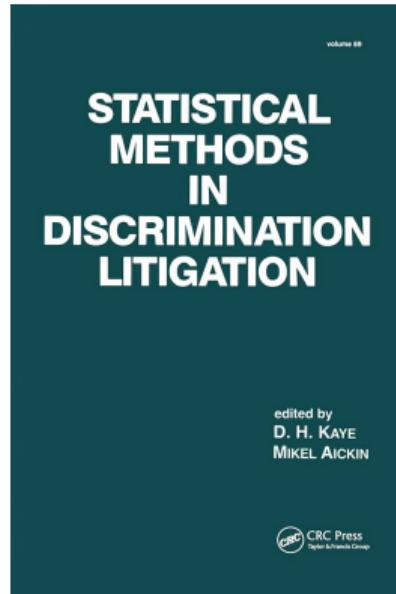
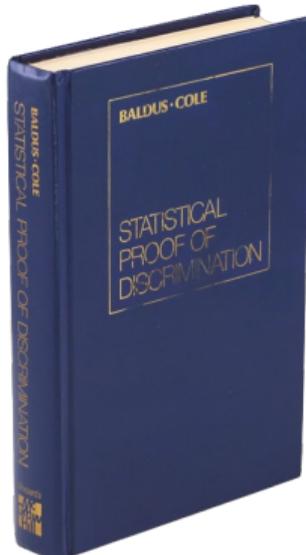
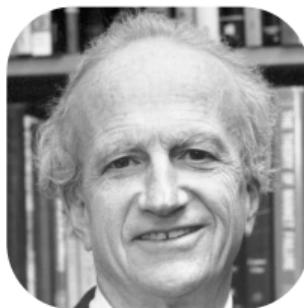
$$\left\{ \begin{array}{l} \text{Cor}[S, \hat{Y}] = \text{Cor}[S, Y]/\text{Cor}[Y, \hat{Y}] \\ \text{Cor}[S, \hat{Y}] = \text{Cor}[S, Y] \\ \text{Cor}[S, \hat{Y}] = \text{Cor}[S, Y] \cdot \text{Cor}[Y, \hat{Y}] \\ \text{Cor}[S, \hat{Y}] = 0 \end{array} \right.$$



See also Thorndike (1971), Linn and Werts (1971), following Cleary (1968).

# "Economics of Discrimination" and "Statistical Discrimination"

- See Becker (1957) or Baldus and Cole (1980), among (many) others.



# Historical Perspective: Decomposition

$$\begin{cases} y_{A:i} = \mathbf{x}_{A:i}^\top \boldsymbol{\beta}_A + \varepsilon_{A:i} & (\text{group A}), \quad \bar{y}_A = \bar{\mathbf{x}}_A^\top \hat{\boldsymbol{\beta}}_A \\ y_{B:i} = \mathbf{x}_{B:i}^\top \boldsymbol{\beta}_B + \varepsilon_{B:i} & (\text{group B}), \quad \bar{y}_B = \bar{\mathbf{x}}_B^\top \hat{\boldsymbol{\beta}}_B. \end{cases}$$

➤ Using ordinary least squares estimates

**Definition 6.4:** Kitagawa (1955), Oaxaca (1973), Blinder (1973)

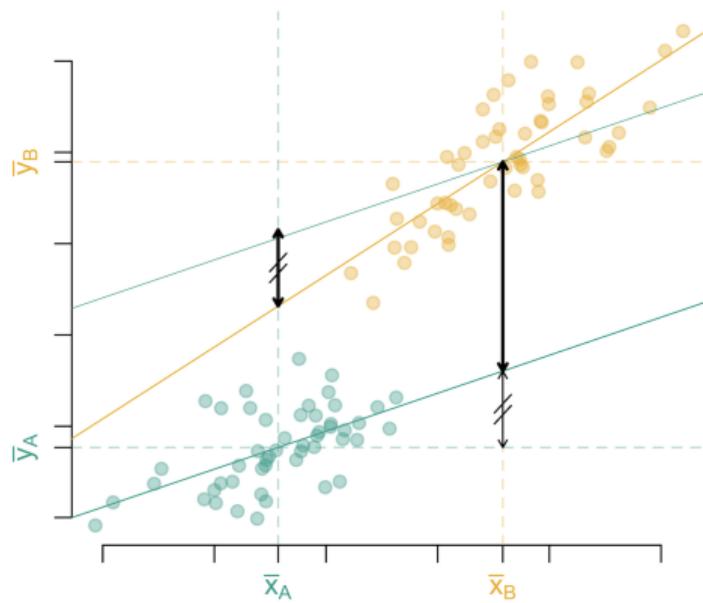
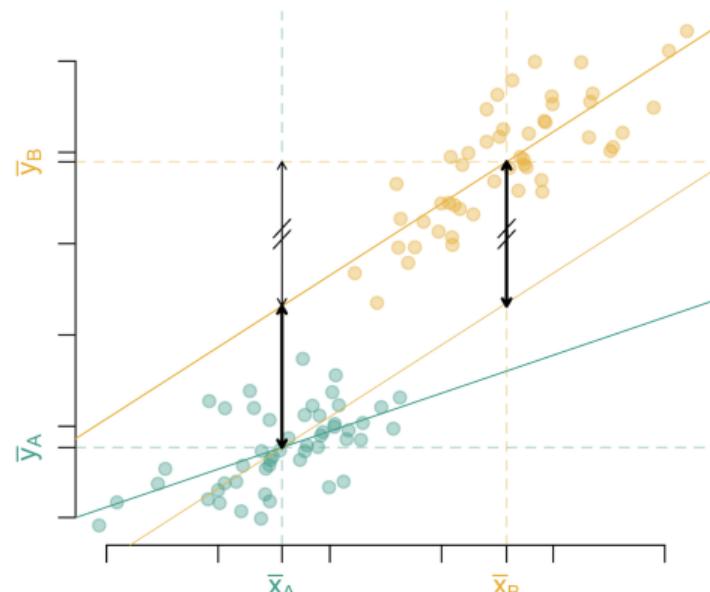
$$\bar{y}_A - \bar{y}_B = \underbrace{(\bar{\mathbf{x}}_A - \bar{\mathbf{x}}_B)^\top \hat{\boldsymbol{\beta}}_B}_{\text{characteristics}} + \underbrace{\bar{\mathbf{x}}_A^\top (\hat{\boldsymbol{\beta}}_A - \hat{\boldsymbol{\beta}}_B)}_{\text{coefficients}}, \quad (7)$$

$$\bar{y}_A - \bar{y}_B = \underbrace{(\bar{\mathbf{x}}_A - \bar{\mathbf{x}}_B)^\top \hat{\boldsymbol{\beta}}_A}_{\text{characteristics}} + \underbrace{\bar{\mathbf{x}}_B^\top (\hat{\boldsymbol{\beta}}_A - \hat{\boldsymbol{\beta}}_B)}_{\text{coefficients}}. \quad (8)$$



➤ Also Brown et al. (1980) and Conway and Roberts (1983).

# Historical Perspective: Decomposition



$x_A(\hat{\beta}_A - \hat{\beta}_B)$  and  $(\bar{x}_A - \bar{x}_B)\hat{\beta}_B$  (as in Equation 7) on the left

$x_B(\hat{\beta}_A - \hat{\beta}_B)$  and  $(\bar{x}_A - \bar{x}_B)\hat{\beta}_A$  (as in Equation 8) on the right.

# Independence and Demographic Parity

## Definition 6.5: Independence, Barocas et al. (2017)

A model  $m$  satisfies the independence property if  $m(\mathbf{Z}) \perp\!\!\!\perp S$ , with respect to the distribution  $\mathbb{P}$  of the triplet  $(\mathbf{X}, S, Y)$ .

by Solon Barocas, Moritz Hardt and Arvind Narayanan



- For classifiers, one might ask for independence  $\hat{Y} \perp\!\!\!\perp S$  (where  $\hat{y}$  is a class), as Darlington (1971).

# Independence and Demographic Parity

**Definition 6.6: Demographic Parity, Calders and Verwer (2010), Corbett-Davies et al. (2017)**

A decision function  $\hat{y}$  – or a classifier  $m_t$ , taking values in  $\{0, 1\}$  – satisfies demographic parity, with respect to some sensitive attribute  $S$  if (equivalently)

$$\begin{cases} \mathbb{P}[\hat{Y} = 1|S = A] = \mathbb{P}[\hat{Y} = 1|S = B] = \mathbb{P}[\hat{Y} = 1] \\ \mathbb{E}[\hat{Y}|S = A] = \mathbb{E}[\hat{Y}|S = B] = \mathbb{E}[\hat{Y}] \\ \mathbb{P}[m_t(\mathbf{Z}) = 1|S = A] = \mathbb{P}[m_t(\mathbf{Z}) = 1|S = B] = \mathbb{P}[m_t(\mathbf{Z}) = 1]. \end{cases}$$

by Toon Calders, Sicco Verwer, Sam Corbett-Davies, Emma Pierson, Sharad Goel, etc



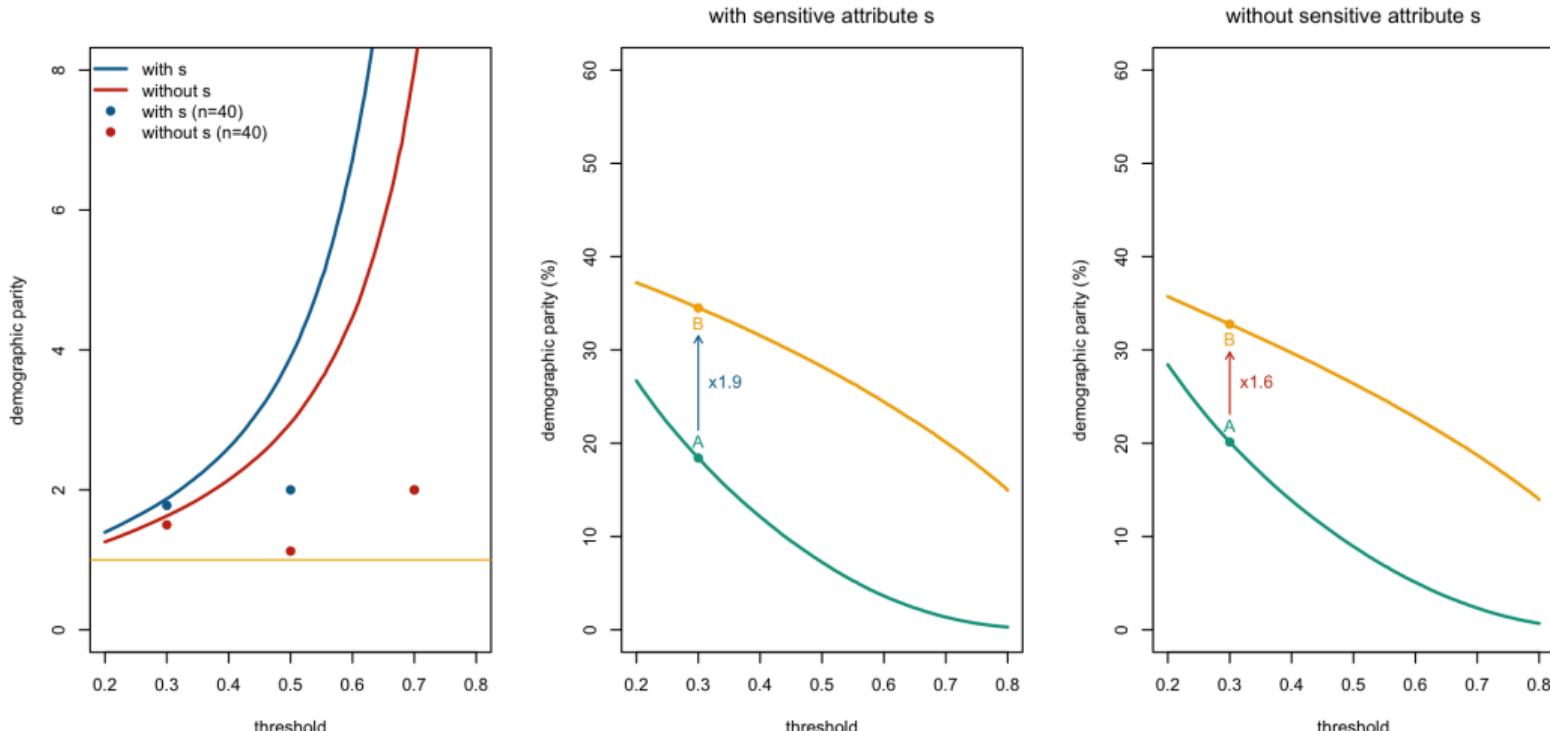
# Independence and Demographic Parity

	unaware (without $s$ )				aware (with $s$ )			
	GLM	GAM	CART	RF	GLM	GAM	CART	RF
$n = 1000$ , various $t$ , ratio $\mathbb{P}[\hat{Y} = 1 S = \text{B}]/\mathbb{P}[\hat{Y} = 1 S = \text{A}]$								
$t = 30\%$	1.652	1.519	1.235	1.559	1.918	1.714	1.235	1.798
$t = 50\%$	1.877	2.451	2.918	2.404	2.944	3.457	2.918	2.180
$t = 70\%$	6.033	8.711	26.000	4.621	7.917	19.333	26.000	4.578

(`dem_parity` from R package `fairness`)

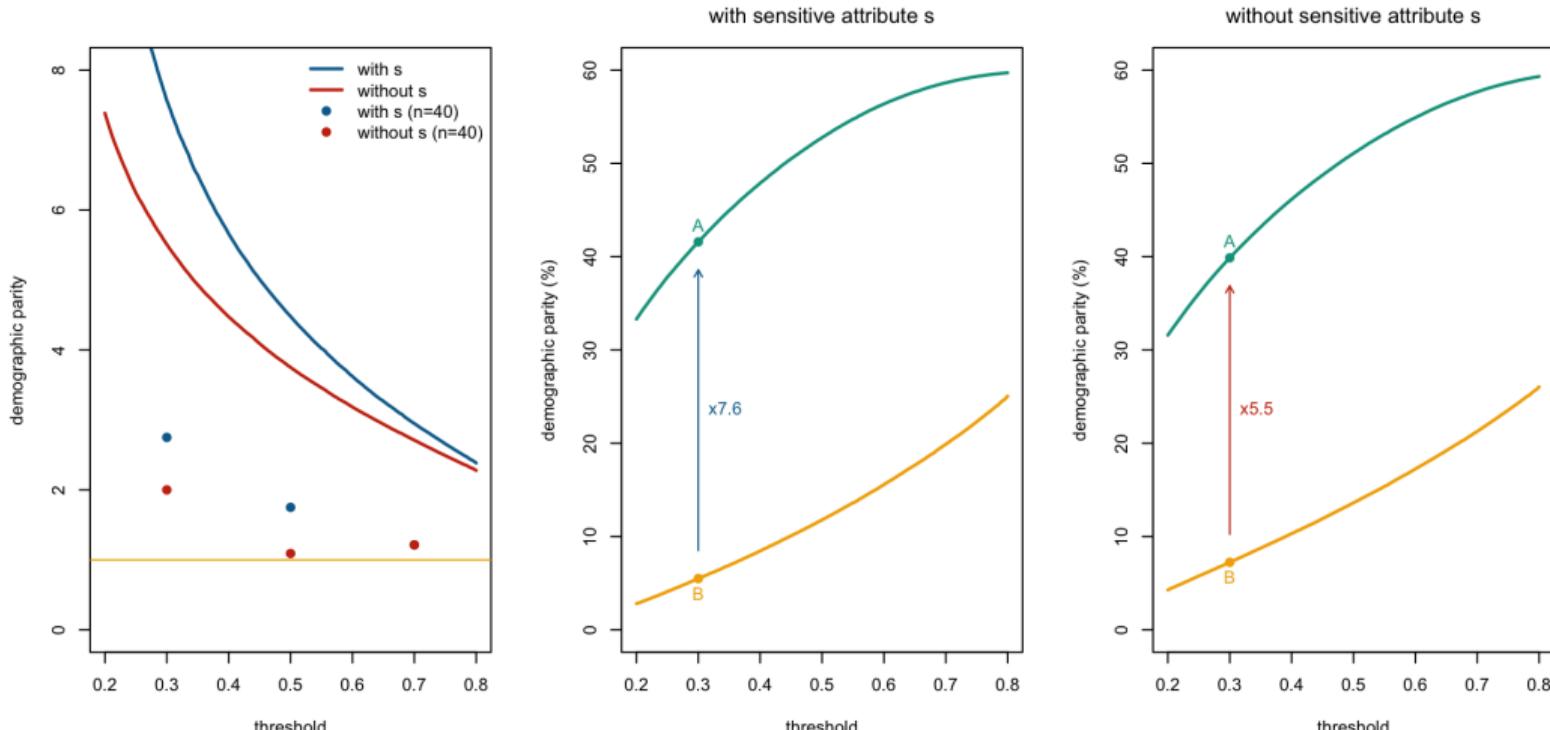
- On the left-hand side, evolution of the ratio ratio  $\mathbb{P}[\hat{Y} = 1|S = \text{B}]/\mathbb{P}[\hat{Y} = 1|S = \text{A}]$ . The horizontal line (at  $y = 1$ ) corresponds to perfect demographic parity. In the middle  $t \mapsto \mathbb{P}[m_t(\mathbf{X}) > t|S = \text{B}]$  and  $t \mapsto \mathbb{P}[m_t(\mathbf{X}) > t|S = \text{A}]$  on the model with  $s$ , and on the right-hand side without  $s$ .

# Independence and Demographic Parity



On the left-hand side, evolution of the ratio ratio  $\mathbb{P}[\hat{Y} = 1|S = \textcolor{orange}{B}]/\mathbb{P}[\hat{Y} = 1|S = \textcolor{teal}{A}]$ .

# Independence and Demographic Parity



- On the left-hand side, evolution of the ratio ratio  $\mathbb{P}[\hat{Y} = 0|S = \textcolor{teal}{A}]/\mathbb{P}[\hat{Y} = 0|S = \textcolor{orange}{B}]$

# Independence and Demographic Parity

## Definition 6.7: Weak Demographic Parity

A decision function  $\hat{y}$  satisfies weak demographic parity if

$$\mathbb{E}[\hat{Y}|S = \textcolor{teal}{A}] = \mathbb{E}[\hat{Y}|S = \textcolor{blue}{B}].$$

## Definition 6.8: Strong Demographic Parity

A decision function  $\hat{y}$  satisfies demographic parity if  $\hat{Y} \perp\!\!\!\perp S$ , i.e., for all  $A$ ,

$$\mathbb{P}[\hat{Y} \in \mathcal{A}|S = \textcolor{teal}{A}] = \mathbb{P}[\hat{Y} \in \mathcal{A}|S = \textcolor{blue}{B}], \quad \forall \mathcal{A} \subset \mathcal{Y}.$$

# Independence and Demographic Parity

## Proposition 6.1

A model  $m$  satisfies the strong demographic parity property if and only if

$$d_{\text{TV}}(\mathbb{P}_{m|\textcolor{teal}{A}}, \mathbb{P}_{m|\textcolor{blue}{B}}) = d_{\text{TV}}(\mathbb{P}_{\textcolor{teal}{A}}, \mathbb{P}_{\textcolor{blue}{B}}) = 0.$$

- $d_{\text{TV}}(\mathbb{P}_{m|\textcolor{teal}{A}}, \mathbb{P}_{m|\textcolor{blue}{B}})$  could be seen as a measure of “unfairness”, but for a non-binary sensitive attribute, a more general definition is necessary (see Denis et al. (2021)).

# Independence and Demographic Parity

**Definition 6.9: Conditional demographic parity, Corbett-Davies et al. (2017)**

We will have a conditional demographic parity if (at choice) for all  $\mathbf{x}$ ,

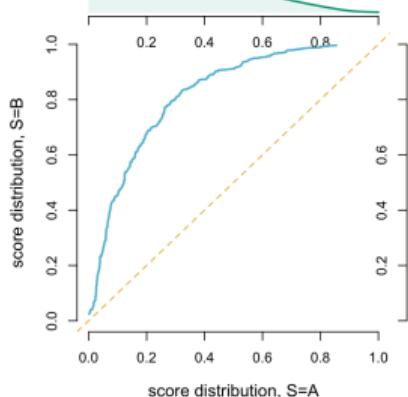
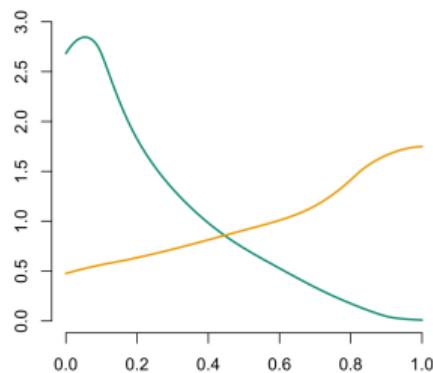
$$\begin{cases} \mathbb{P}[\hat{Y} = 1 | \mathbf{X}_L = \mathbf{x}, S = \textcolor{teal}{A}] = \mathbb{P}[\hat{Y} = 1 | \mathbf{X}_L = \mathbf{x}, S = \textcolor{blue}{B}], \forall y \in \{0, 1\} \\ \mathbb{E}[\hat{Y} | \mathbf{X}_L = \mathbf{x}, S = \textcolor{teal}{A}] = \mathbb{E}[\hat{Y} | \mathbf{X}_L = \mathbf{x}, S = \textcolor{blue}{B}], \\ \mathbb{P}[\hat{Y} \in \mathcal{A} | \mathbf{X}_L = \mathbf{x}, S = \textcolor{teal}{A}] = \mathbb{P}[\hat{Y} \in \mathcal{A} | \mathbf{X}_L = \mathbf{x}, S = \textcolor{blue}{B}], \forall \mathcal{A} \subset \mathcal{Y}, \end{cases}$$

where  $L$  denotes a “legitimate” subset of unprotected covariates.

# Independence and Demographic Parity

## Proposition 6.2

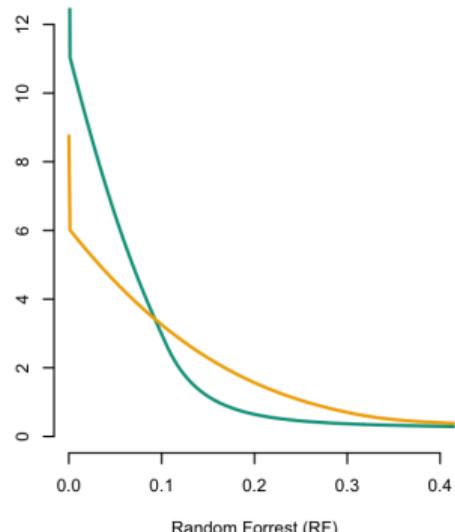
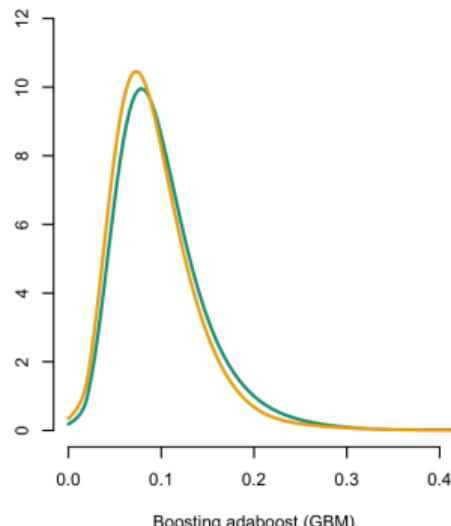
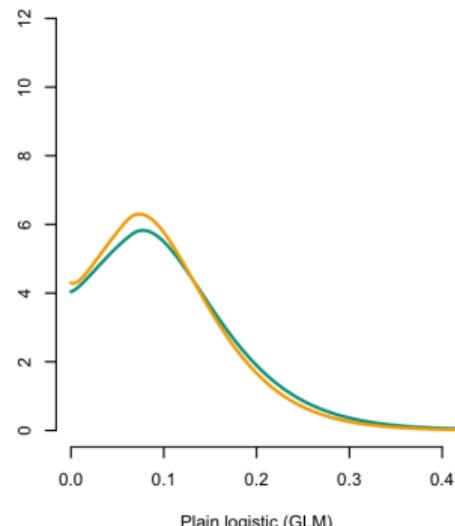
A model  $m$  satisfies is strongly fair if and only if  $W_2(\mathbb{P}_A, \mathbb{P}_B) = 0$ .



```
1 > model_glm = glm(y~x1  
+x2+x3, data=  
toydata2, family=  
binomial)  
2 > pred_y_glm = predict  
(model_glm, type="  
response")  
3 > sA = pred_y_glm[  
toydata2$sensitive  
=="A"]  
4 > library(transport)  
5 > wasserstein1d(sA,sB)  
6 [1] 0.3860795
```

# Independence and Demographic Parity

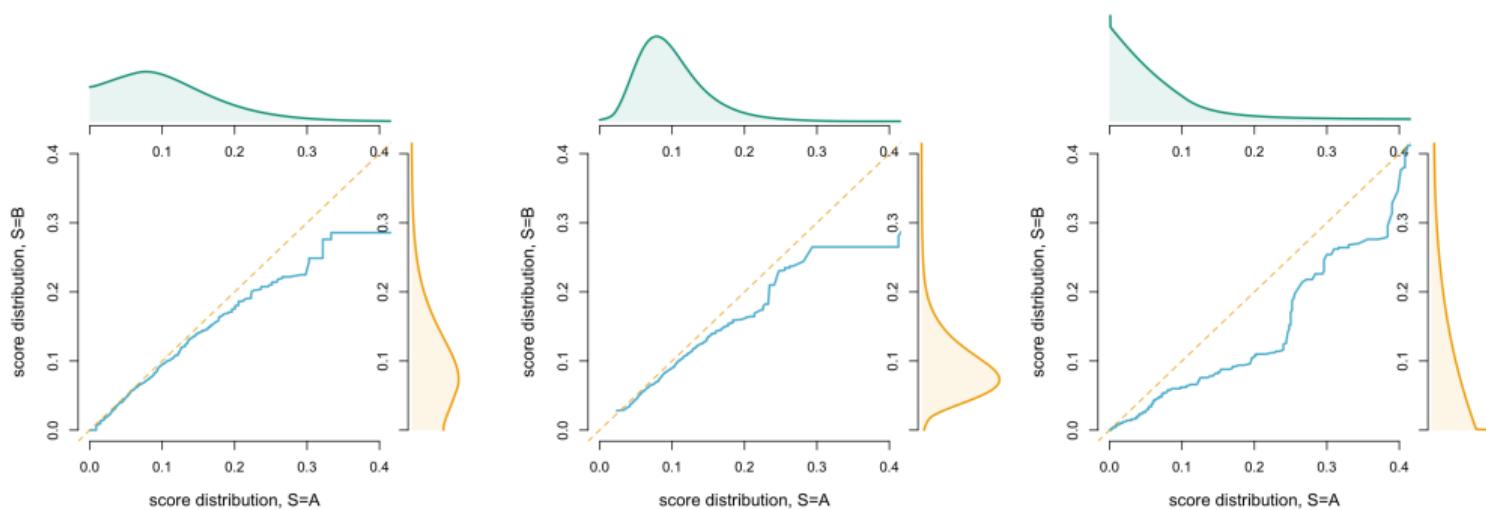
- On the **FrenchMotor** dataset, consider GLM, GBM and RF for claim occurence



```
1 > wasserstein1d(lA, lB) 1 > wasserstein1d(bA, bB) 1 > wasserstein1d(fA, fB)  
2 [1] 0.007220468          2 [1] 0.008895917          2 [1] 0.01001088
```

# Independence and Demographic Parity

```
1 > wasserstein1d(lA, lB) 1 > wasserstein1d(bA, bB) 1 > wasserstein1d(fA, fB)
2 [1] 0.007220468          2 [1] 0.008895917          2 [1] 0.01001088
```



# Independence and Demographic Parity

**Definition 6.10: Unfairness,** Denis et al. (2021); Chzhen and Schreuder (2022)

Given a model  $m$ , let  $\mathbb{P}_m$  denote the distribution of  $m(\mathbf{X}, S)$  and  $\mathbb{P}_{m|s}$  denote the conditional distribution of  $m(\mathbf{X}, S)$  given  $S = s$ , define

$$\begin{cases} \mathcal{U}_{\text{TV}}(m) = \max_{s \in \{\text{A,B}\}} \{ d_{\text{TV}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \text{ or } \sum_{s \in \{\text{A,B}\}} d_{\text{TV}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \} \\ \mathcal{U}_{\text{KS}}(m) = \max_{s \in \{\text{A,B}\}} \{ d_{\text{KS}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \} \text{ or } \sum_{s \in \{\text{A,B}\}} d_{\text{KS}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \\ \mathcal{U}_{W_k}(m) = \max_{s \in \{\text{A,B}\}} \{ W_k(\mathbb{P}_m, \mathbb{P}_{m|s}) \} \text{ or } \sum_{s \in \{\text{A,B}\}} W_k(\mathbb{P}_m, \mathbb{P}_{m|s}) \end{cases}$$

- In the original version, Chzhen and Schreuder (2022) suggested to use the one on the right.

# Independence and Demographic Parity

- Those measures characterize strong demographic parity,

## Proposition 6.3: Strong Demographic Parity

A model  $m$  is strongly fair if and only if  $\mathcal{U}(m) = 0$ .

# Separation and Equalized Odds

## Definition 6.11: Separation, Barocas et al. (2017)

A model  $m : \mathcal{Z} \rightarrow \mathcal{Y}$  satisfies the separation property if  $m(\mathcal{Z}) \perp\!\!\!\perp S | Y$ , with respect to the distribution  $\mathbb{P}$  of the triplet  $(X, S, Y)$ .

by Solon Barocas, Moritz Hardt and Arvind Narayanan



# Separation and Equalized Odds

**Definition 6.12: True positive equality, (Weak) Equal Opportunity, Hardt et al. (2016)**

A decision function  $\hat{y}$  – or a classifier  $m_t(\cdot)$ , taking values in  $\{0, 1\}$  – satisfies equal opportunity, with respect to some sensitive attribute  $S$  if

$$\begin{cases} \mathbb{P}[\hat{Y} = 1|S = \textcolor{teal}{A}, Y = 1] = \mathbb{P}[\hat{Y} = 1|S = \textcolor{blue}{B}, Y = 1] = \mathbb{P}[\hat{Y} = 1|Y = 1] \\ \mathbb{P}[m_t(\mathbf{Z}) = 1|S = \textcolor{teal}{A}, Y = 1] = \mathbb{P}[m_t(\mathbf{Z}) = 1|S = \textcolor{blue}{B}, Y = 1] = \mathbb{P}[m_t(\mathbf{Z}) = 1|Y = 1], \end{cases}$$

which corresponds to parity of true positives, in the two groups,  $\{\textcolor{teal}{A}, \textcolor{blue}{B}\}$ .

# Separation and Equalized Odds

## Definition 6.13: Strong Equal Opportunity

A classifier  $m(\cdot)$ , taking values in  $\{0, 1\}$ , satisfies equal opportunity, with respect to some sensitive attribute  $S$  if

$$\mathbb{P}[m(\mathbf{X}, S) \in \mathcal{A} | S = \textcolor{teal}{A}, Y = 1] = \mathbb{P}[m(\mathbf{X}, S) \in \mathcal{A} | S]$$

for all  $\mathcal{A} \subset [0, 1]$ .

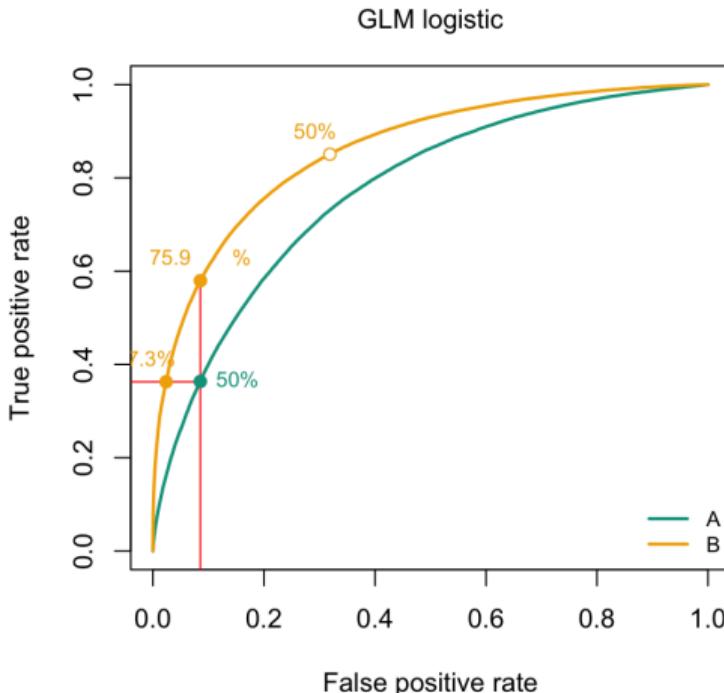
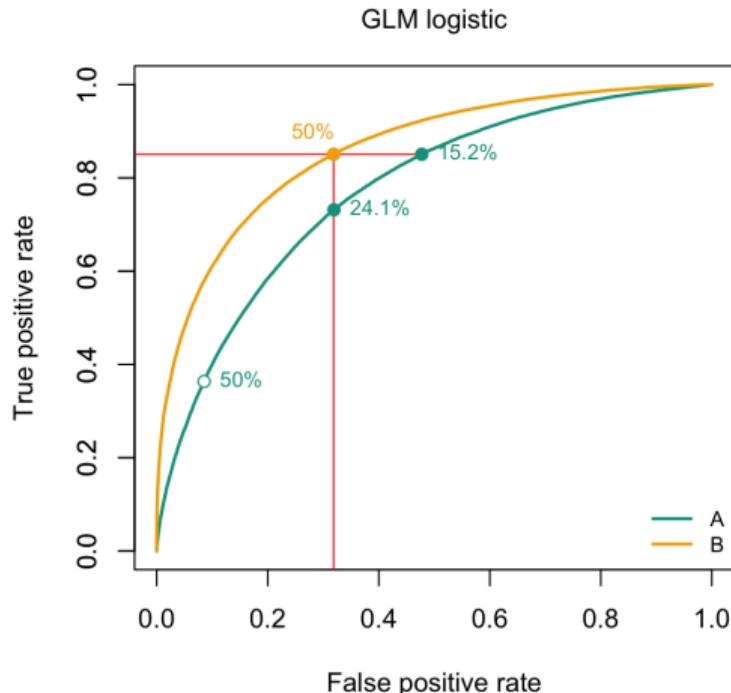
# Separation and Equalized Odds

## Definition 6.14: False positive equality, Hardt et al. (2016)

A decision function  $\hat{y}$  – or a classifier  $m_t(\cdot)$ , taking values in  $\{0, 1\}$  – satisfies parity of false positives, with respect to some sensitive attribute  $s$ , if

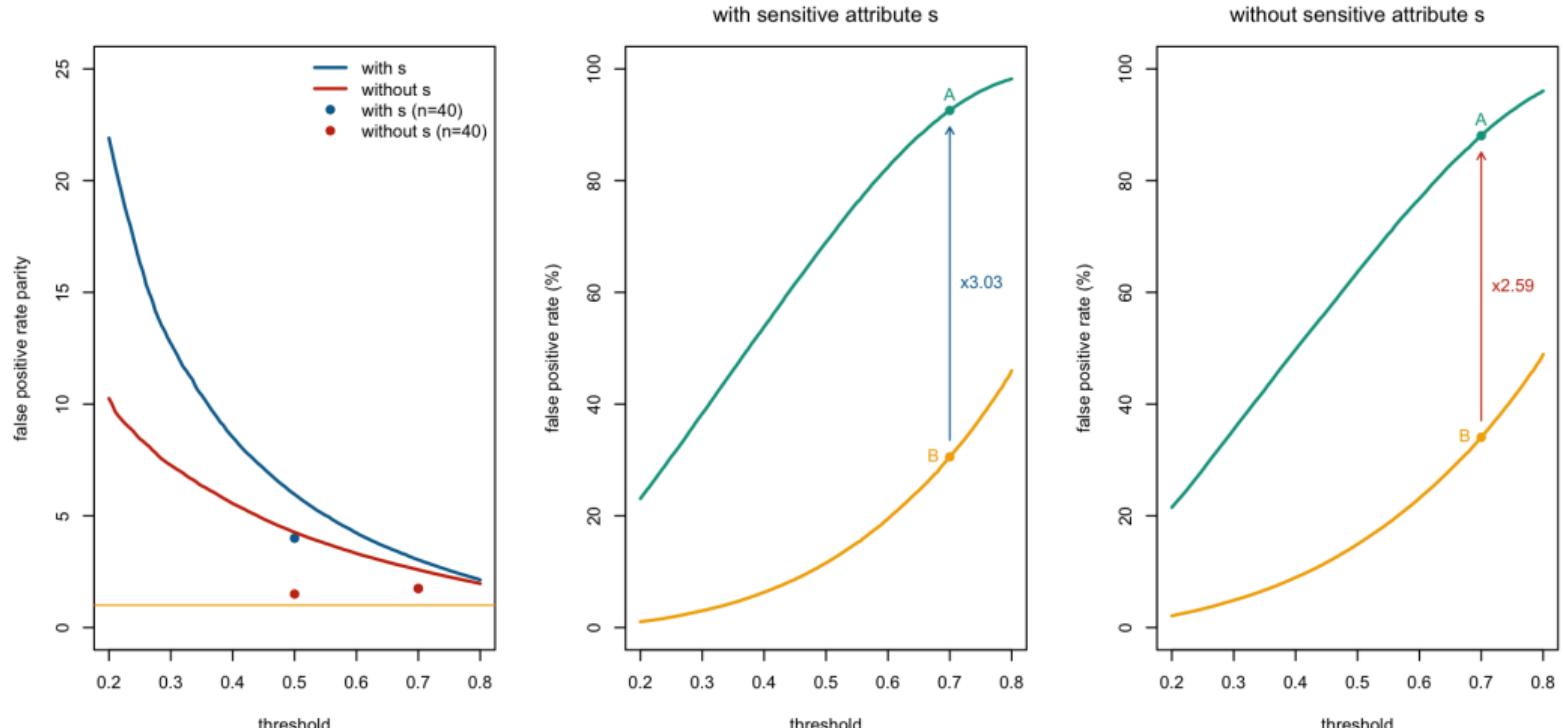
$$\begin{cases} \mathbb{P}[\hat{Y} = 1 | S = \textcolor{teal}{A}, Y = 0] = \mathbb{P}[\hat{Y} = 1 | S = \textcolor{blue}{B}, Y = 0] = \mathbb{P}[\hat{Y} = 1 | Y = 0] \\ \mathbb{P}[m_t(\mathbf{Z}) = 1 | S = \textcolor{teal}{A}, Y = 0] = \mathbb{P}[m_t(\mathbf{Z}) = 1 | S = \textcolor{blue}{B}, Y = 0] = \mathbb{P}[m_t(\mathbf{Z}) = 1 | Y = 0]. \end{cases}$$

# Separation and Equalized Odds



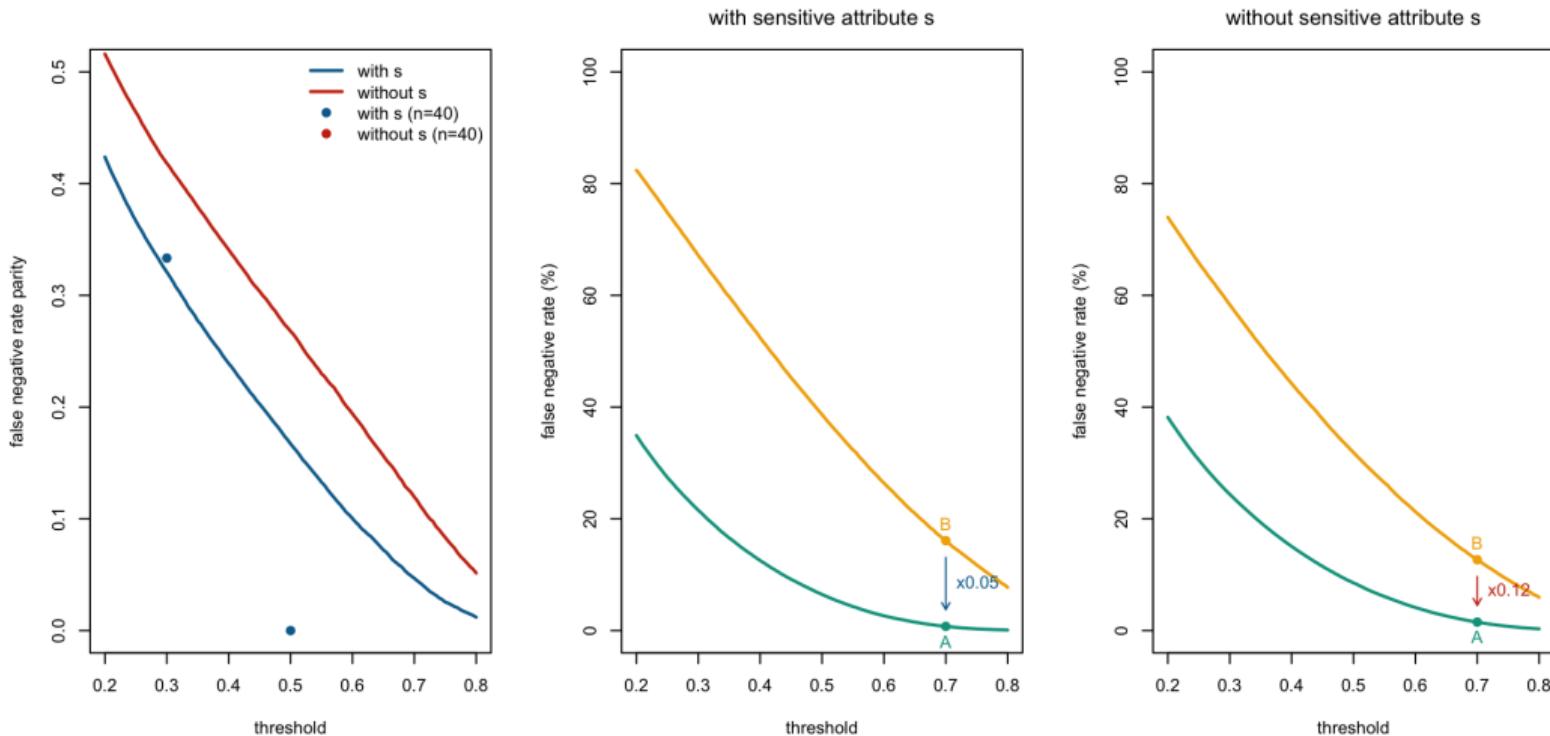
- ROC curves (TPR against FPR) for the logistic regression on `toydata2`.

# Separation and Equalized Odds



➤ Evolution of the false positive rates, **fpr<sub>parity</sub>** from **fairness**.

# Separation and Equalized Odds



➤ Evolution of the false negative rates, **fnr<sub>parity</sub>** from **fairness**.

# Separation and Equalized Odds

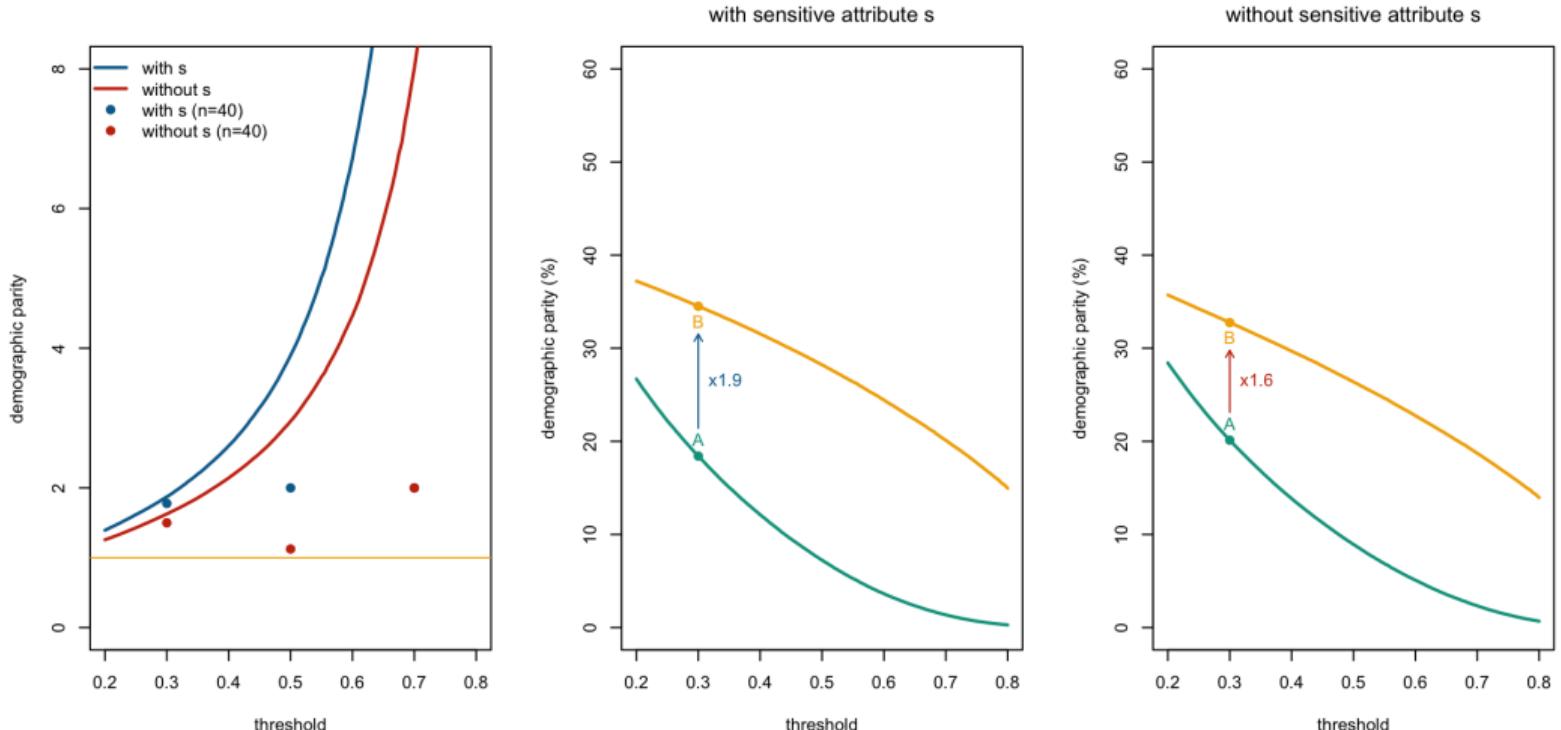
## Definition 6.15: Equalized Odds, Hardt et al. (2016)

A decision function  $\hat{y}$  – or a classifier  $m_t(\cdot)$  taking values in  $\{0, 1\}$  – satisfies equal odds constraint, with respect to some sensitive attribute  $S$ , if

$$\begin{cases} \mathbb{P}[\hat{Y} = 1 | S = \textcolor{teal}{A}, Y = y] = \mathbb{P}[\hat{Y} = 1 | S = \textcolor{blue}{B}, Y = y] = \mathbb{P}[\hat{Y} = 1 | Y = y], \quad \forall y \in \{0, 1\} \\ \mathbb{P}[m_t(\mathbf{Z}) = 1 | S = \textcolor{teal}{A}, Y = y] = \mathbb{P}[m_t(\mathbf{Z}) = 1 | S = \textcolor{blue}{B}, Y = y], \quad \forall y \in \{0, 1\}, \end{cases},$$

which corresponds to parity of true positive and false positive, in the two groups.

# Separation and Equalized Odds



## ➤ Evolution of the equalized odds metrics

# Separation and Equalized Odds

- One can also consider any kind of standard metrics on confusion matrices, such as  $\phi$  (introduced in [Yule \(1912\)](#)), usually named "Matthews correlation coefficient"

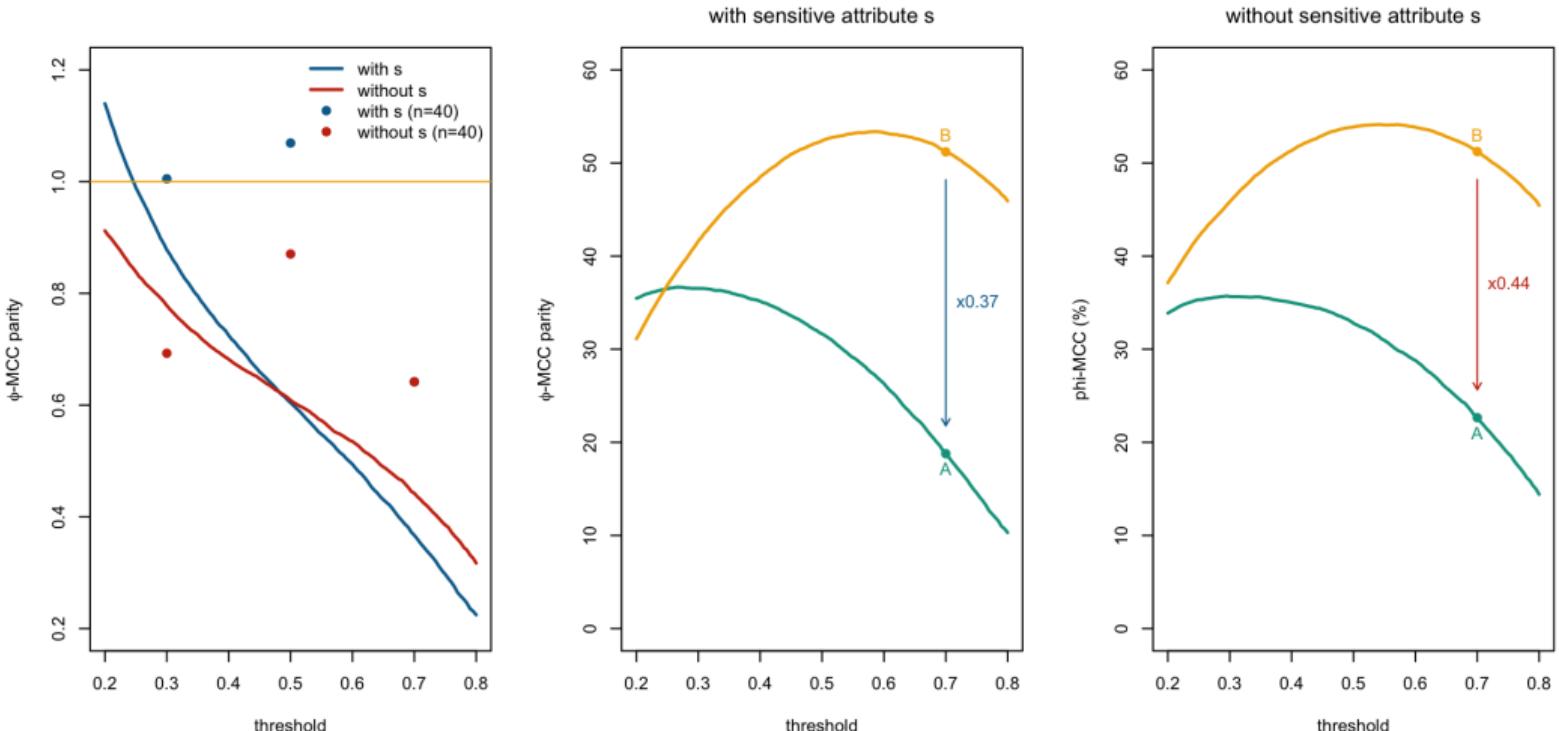
## Definition 6.16: $\phi$ -fairness, [Chicco and Jurman \(2020\)](#)

We will have  $\phi$ -fairness if  $\phi_A = \phi_B$ , where  $\phi_s$  denotes Matthews correlation coefficient for the  $s$  group,

$$\phi_s = \frac{TP_s \cdot TN_s - FP_s \cdot FN_s}{\sqrt{(TP_s + FP_s)(TP_s + FN_s) \cdot (TN_s + FP_s)(TN_s + FN_s)}}, \quad s \in \{A, B\}.$$

- but one could consider the  $F_1$ -score (as defined in [Van Rijsbergen \(1979\)](#)), Fowlkes–Mallows or Jaccard indices (in [Fowlkes and Mallows \(1983\)](#) or [Jaccard \(1901\)](#)).
- .. or AUC as we will consider later on.

# Separation and Equalized Odds



➤ Evolution of the  $\phi$ -fairness metric

# Separation and Equalized Odds

## Definition 6.17: Class Balance, Kleinberg et al. (2016)

We will have class balance in the weak sense if

$$\mathbb{E}[m(\mathbf{X})|Y = y, S = \textcolor{teal}{A}] = \mathbb{E}[m(\mathbf{X})|Y = y, S = \textcolor{blue}{B}], \forall y \in \{0, 1\},$$

or in the strong sense if

$$\mathbb{P}[m(\mathbf{X}) \in \mathcal{A}|Y = y, S = \textcolor{teal}{A}] = \mathbb{P}[m(\mathbf{X}) \in \mathcal{A}|Y = y, S = \textcolor{blue}{B}], \forall \mathcal{A} \subset [0, 1], \forall y \in \{0, 1\}.$$

# Separation and Equalized Odds

## Definition 6.18: Similar Mistreatment, Zafar et al. (2019)

We will have similar mistreatment, or “*lack of disparate mistreatment*,” if

$$\begin{cases} \mathbb{P}[\hat{Y} = Y | S = A] = \mathbb{P}[\hat{Y} = Y | S = B] = \mathbb{P}[\hat{Y} = Y] \\ \mathbb{P}[m_t(\mathbf{X}) = Y | S = A] = \mathbb{P}[m_t(\mathbf{X}) = Y | S = B] = \mathbb{P}[m_t(\mathbf{X}) = Y]. \end{cases}$$

## Definition 6.19: Equality of ROC curves, Vogel et al. (2021)

Let  $\text{FRP}_s(t) = \mathbb{P}[m(\mathbf{X}) > t | Y = 0, S = s]$  and  $\text{TPR}_s(t) = \mathbb{P}[m(\mathbf{X}) > t | Y = 1, S = s]$ , where  $s \in \{A, B\}$ . Set  $\Delta_{TPR}(t) = \text{TPR}_B \circ \text{TPR}_A^{-1}(t) - t$  et  $\Delta_{FPR}(t) = \text{FPR}_B \circ \text{FPR}_A^{-1}(t) - t$ . We will have fairness with respect to ROC curves if  $\|\Delta_{TPR}\|_\infty = \|\Delta_{FPR}\|_\infty = 0$ .

# Separation and Equalized Odds

## Definition 6.20: AUC Fairness, Borkan et al. (2019)

We will have AUC fairness if  $\text{AUC}_A = \text{AUC}_B$ , where  $\text{AUC}_s$  is the AUC associated with model  $m$  within the  $s$  group.

	unaware (without $s$ )				aware (with $s$ )			
	GLM	GAM	CART	RF	GLM	GAM	CART	RF
ratio of AUC	0.837	0.839	0.913	0.768	0.857	0.860	0.913	0.763

# Sufficiency and Calibration

- › Inspired by Cleary (1968), define

## Definition 6.21: Sufficiency, Barocas et al. (2017)

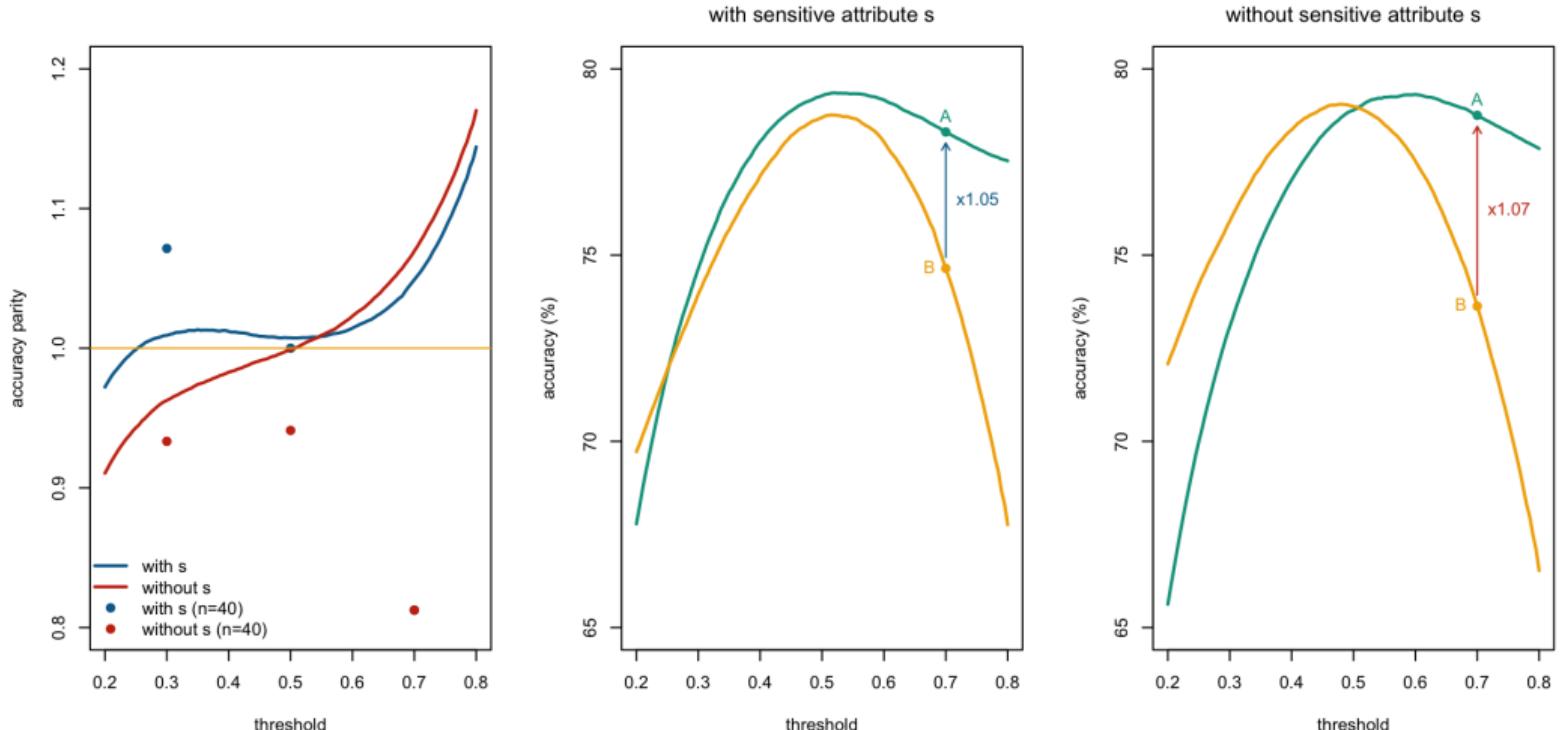
A model  $m : \mathcal{Z} \rightarrow \mathcal{Y}$  satisfies the sufficiency property if  $Y \perp\!\!\!\perp S | m(\mathcal{Z})$ , with respect to the distribution  $\mathbb{P}$  of the triplet  $(\mathbf{X}, S, Y)$ .

## Definition 6.22: Calibration Parity, Accuracy Parity, Kleinberg et al. (2016), Zafar et al. (2019)

Calibration parity is met if

$$\mathbb{P}[Y = 1 | m(\mathbf{X}) = t, S = \textcolor{teal}{A}] = \mathbb{P}[Y = 1 | m(\mathbf{X}) = t, S = \textcolor{blue}{B}], \forall t \in [0, 1].$$

# Sufficiency and Calibration



➤ Evolution of accuracy, in groups A and B.

## Sufficiency and Calibration

**Definition 6.23: Good Calibration**, Kleinberg et al. (2017), Verma and Rubin (2018)

Fairness of good calibration is met if

$$\mathbb{P}[Y = 1 | m(\mathbf{X}) = t, S = \textcolor{teal}{A}] = \mathbb{P}[Y = 1 | m(\mathbf{X}) = t, S = \textcolor{blue}{B}] = t, \forall t \in [0, 1].$$

**Definition 6.24: Non-Reconstruction of Protected Attribute**, Kim (2017)

If we cannot tell from the result ( $\mathbf{x}$ ,  $m(\mathbf{x})$ ,  $y$  and  $\hat{y}$ ) whether the subject was a member of a protected group or not, we will talk about fairness by non-reconstruction of the protected attribute

$$\mathbb{P}[S = \textcolor{teal}{A} | \mathbf{X}, m(\mathbf{X}), \hat{Y}, Y] = \mathbb{P}[S = \textcolor{blue}{B} | \mathbf{X}, m(\mathbf{X}), \hat{Y}, Y].$$

# Relaxation and Approximate Fairness

## Definition 6.25: Disparate Impact, [Feldman et al. \(2015\)](#)

A decision function  $\hat{Y}$  has a disparate impact, for a given threshold  $\tau$ , if,

$$\min \left\{ \frac{\mathbb{P}[\hat{Y} = 1 | S = A]}{\mathbb{P}[\hat{Y} = 1 | S = B]}, \frac{\mathbb{P}[\hat{Y} = 1 | S = B]}{\mathbb{P}[\hat{Y} = 1 | S = A]} \right\} < \tau \text{ (usually 80%).}$$

- › The [80% rule](#) was suggested by the "Technical Advisory Committee on Testing", from the State of California Fair Employment Practice Commission (FEPC) in 1971, or the 1978 "Uniform Guidelines on Employee Selection Procedures", a document used by the U.S. Equal Employment Opportunity Commission (EEOC), see [Biddle \(2017\)](#).

# Relaxation and Approximate Fairness

- › We have defined (Definition 6.10) unfairness as

$$\mathcal{U}_k(m) = \max_{s \in \{\textcolor{teal}{A}, \textcolor{blue}{B}\}} \{W_k(\mathbb{P}_m, \mathbb{P}_{m|s})\},$$

so that  $m$  is (strongly) fair if and only if  $\mathcal{U}_k(m) = 0$ .

- › Chzhen and Schreuder (2022) introduced the notion of Relative Improvement

## Definition 6.26: $\varepsilon$ -Approximate Fairness

Model  $m$  is  $\varepsilon$ -approximately fair if  $\mathcal{U}_k(m) \leq \varepsilon \cdot \mathcal{U}_k(m^*)$ , where  $m^*$  is Bayes regressor, for some  $\varepsilon \geq 0$ .

## Three different concepts ?

$$\begin{cases} \text{Independence (Definition 6.5)} : m(\mathbf{Z}) \perp\!\!\!\perp S \\ \text{Separation (Definition 6.11)} : m(\mathbf{Z}) \perp\!\!\!\perp S \mid Y \\ \text{Sufficiency (Definition 6.21)} : Y \perp\!\!\!\perp S \mid m(\mathbf{Z}) \end{cases}$$

- ▶ Independence assumes no differences among groups, regardless of accuracy
- ▶ Separation minimizes differences among groups by not trying to maximize accuracy
- ▶ Sufficiency maximizes accuracy by not trying to minimize differences among groups

See [Kleinberg et al. \(2016\)](#) or [Chouldechova \(2017\)](#).

## Impossibility theorems

- Unless very specific properties are assumed on  $\mathbb{P}$ , there is no prediction function  $m(\cdot)$  that can satisfy at the same time two fairness criteria.

$$\left\{ \begin{array}{l} \text{Independence (Definition 6.5)} : m(\mathbf{Z}) \perp\!\!\!\perp S \\ \text{Separation (Definition 6.11)} : m(\mathbf{Z}) \perp\!\!\!\perp S \mid Y \\ \text{Sufficiency (Definition 6.21)} : Y \perp\!\!\!\perp S \mid m(\mathbf{Z}) \end{array} \right.$$

### Proposition 6.4

Suppose that a model  $m$  satisfies the independence condition (6.5) and the sufficiency property (6.21), with respect to a sensitive attribute  $s$ , then necessarily,  $Y \perp\!\!\!\perp S$ .

- Therefore, unless the sensitive attribute  $s$  has no impact on the outcome  $y$ , there is no model  $m$  which satisfies independence and sufficiency simultaneously.

## Impossibility theorems

- From the sufficiency property ,  $S \perp\!\!\!\perp Y \mid m(\mathbf{Z})$ , then, for  $s \in \mathcal{S}$  and  $\mathcal{A} \subset \mathcal{Y}$ ,

$$\mathbb{P}[S = s, Y \in \mathcal{A}] = \mathbb{E}[\mathbb{P}[S = s, Y \in \mathcal{A} \mid m(\mathbf{Z})]],$$

can be written

$$\mathbb{P}[S = s, Y \in \mathcal{A}] = \mathbb{E}[\mathbb{P}[S = s \mid m(\mathbf{Z})] \cdot \mathbb{P}[Y \in \mathcal{A} \mid m(\mathbf{Z})]].$$

And from the independence property (6.21),  $m(\mathbf{Z}) \perp\!\!\!\perp S$ , we can write the first component  $\mathbb{P}[S = s \mid m(\mathbf{Z})] = \mathbb{P}[S = s]$ , almost surely, and therefore

$$\mathbb{P}[S = s, Y \in \mathcal{A}] = \mathbb{E}[\mathbb{P}[S = s] \cdot \mathbb{P}[Y \in \mathcal{A} \mid m(\mathbf{Z})]] = \mathbb{P}[S = s] \cdot \mathbb{P}[Y \in \mathcal{A}],$$

for all  $s \in \mathcal{S}$  and  $\mathcal{A} \subset \mathcal{Y}$ , corresponding to the independence between  $S$  and  $Y$ .

# Impossibility theorems

## Proposition 6.5

Consider a classifier  $m_t$  taking values in  $\mathcal{Y} = \{0, 1\}$ . Suppose that  $m_t$  satisfies the independence condition (6.5) and the separation property (6.11), with respect to a sensitive attribute  $s$ , then necessarily either  $m_t(\mathbf{Z}) \perp\!\!\!\perp Y$  or  $Y \perp\!\!\!\perp S$  (possibly both).

- Because  $m_t$  satisfies the independence condition (6.5),  $m_t(\mathbf{Z}) \perp\!\!\!\perp S$ , and the separation property (6.11),  $m_t(\mathbf{Z}) \perp\!\!\!\perp S \mid Y$ , then, for  $\hat{y} \in \mathcal{Y}$  and for  $s \in \mathcal{S}$ ,

$$\mathbb{P}[m_t(\mathbf{Z}) = \hat{y}] = \mathbb{P}[m_t(\mathbf{Z}) = \hat{y} \mid S = s] = \mathbb{E}[\mathbb{P}[m_t(\mathbf{Z}) = \hat{y} \mid Y, S = s]],$$

that we can write

$$\mathbb{P}[m_t(\mathbf{Z}) = \hat{y}] = \sum_y \mathbb{P}[m_t(\mathbf{Z}) = \hat{y} \mid Y = y, S = s] \cdot \mathbb{P}[Y = y \mid S = s],$$

## Impossibility theorems

or

$$\mathbb{P}[m_t(\mathbf{Z}) = \hat{y}] = \sum_y \mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = y] \cdot \mathbb{P}[Y = y | S = s],$$

almost surely. Furthermore, we can also write

$$\mathbb{P}[m_t(\mathbf{Z}) = \hat{y}] = \sum_y \mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = y] \cdot \mathbb{P}[Y = y],$$

so that, if we combine the two expressions, we get

$$\sum_y \mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = y] \cdot (\mathbb{P}[Y = y | S = s] - \mathbb{P}[Y = y]) = 0,$$

almost surely. And since we assumed that  $y$  was a binary variable,  $\mathbb{P}[Y = 0] = 1 - \mathbb{P}[Y = 1]$ , as well as  $\mathbb{P}[Y = 0 | S = s] = 1 - \mathbb{P}[Y = 1 | S = s]$ , and therefore

$$\mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = 1] \cdot (\mathbb{P}[Y = 1 | S = s] - \mathbb{P}[Y = 1])$$

# Impossibility theorems

or

$$-\mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = 0] \cdot (\mathbb{P}[Y = 0 | S = s] - \mathbb{P}[Y = 0])$$

can be written

$$\mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = 0] \cdot (\mathbb{P}[Y = 1 | S = s] - \mathbb{P}[Y = 1]).$$

Thus, either  $\mathbb{P}[Y = 1 | S = s] - \mathbb{P}[Y = 1]$  almost surely, or

$\mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = 0] = \mathbb{P}[m_t(\mathbf{Z}) = \hat{y} | Y = 1]$  (or both).

➤ Of course, the previous proposition holds only when  $y$  is a binary variable.

## Proposition 6.6

Consider a classifier  $m_t$  taking values in  $\mathcal{Y} = \{0, 1\}$ . Suppose that  $m_t$  satisfies the sufficiency condition (6.21) and the separation property (6.11), with respect to a sensitive attribute  $s$ , then necessarily either  $\mathbb{P}[m_t(\mathbf{Z}) = 1 | Y = 1] = 0$  or  $Y \perp\!\!\!\perp S$  or  $m_t(\mathbf{Z}) \perp\!\!\!\perp Y$ .

- Suppose that  $m_t$  satisfies the sufficiency condition (6.21) and the separation property (6.11), respectively  $Y \perp\!\!\!\perp S | m_t(\mathbf{Z})$  and  $m_t(\mathbf{Z}) \perp\!\!\!\perp S | Y$ . For all  $s \in \mathcal{S}$ , we can write, using Bayes formula

$$\mathbb{P}[Y = 1 | S = s, m_t(\mathbf{Z}) = 1] = \frac{\mathbb{P}[m_t(\mathbf{Z}) = 1 | Y = 1, S = s] \cdot \mathbb{P}[Y = 1 | S = s]}{\mathbb{P}[m_t(\mathbf{Z}) = 1 | S = s]},$$

# Impossibility theorems

i.e.,

$$\mathbb{P}[Y = 1|S = s, m_t(\mathbf{Z}) = 1] = \frac{\mathbb{P}[m_t(\mathbf{Z}) = 1|Y = 1] \cdot \mathbb{P}[Y = 1|S = s]}{\sum_{y \in \{0,1\}} \mathbb{P}[m_t(\mathbf{Z}) = 1|Y = y] \cdot \mathbb{P}[Y = 1|S = s]},$$

that should not depend on  $s$  (from the sufficiency property). So a similar property holds if  $S = s'$ . Observe further that  $\mathbb{P}[m_t(\mathbf{Z}) = 1|Y = 1]$  is the *true positive rate* (TPR) while  $\mathbb{P}[m_t(\mathbf{Z}) = 1|Y = 0]$  is the *false positive rate* (FPR). Let  $p_s = \mathbb{P}[Y = 1|S = s]$ , so that

$$\mathbb{P}[Y = 1|S = s, m_t(\mathbf{Z}) = 1] = \frac{\text{TPR}}{p_s \cdot \text{TPR} + (1 - p_s) \cdot \text{FPR}}.$$

## Impossibility theorems

- Suppose that  $Y$  and  $S$  are not independent (otherwise  $Y \perp\!\!\!\perp S$  as stated in the proposition), i.e., there are  $s$  and  $s'$  such that  $p_s = \mathbb{P}[Y = 1|S = s] \neq \mathbb{P}[Y = 1|S = s'] = p_{s'}$ . Hence,  $p_s \neq p_{s'}$ , but at the same time

$$\frac{\text{TPR}}{p_s \cdot \text{TPR} + (1 - p_s) \cdot \text{FPR}} = \frac{\text{TPR}}{p_{s'} \cdot \text{TPR} + (1 - p_{s'}) \cdot \text{FPR}}.$$

Supposes that  $\text{TPR} \neq 0$  (otherwise  $\text{TPR} = \mathbb{P}[m_t(\mathbf{Z}) = 1|Y = 1] = 0$  as stated in the proposition), then

$$(p_s - p_{s'}) \cdot \text{TPR} = (p_s - p_{s'}) \cdot \text{FPR} \neq 0,$$

and therefore  $m_t(\mathbf{Z}) \perp\!\!\!\perp Y$ .

# Group fairness, wrap-up

independence,  $\widehat{Y} \perp\!\!\!\perp S$ , (Definition 6.5)

<i>statistical parity</i>	Dwork et al. (2012)	$\mathbb{P}[\widehat{Y} = 1 S = s] = \text{cst}, \forall s$
<i>conditional statistical parity</i>	Corbett-Davies et al. (2017)	$\mathbb{P}[\widehat{Y} = 1 S = s, X = x] = \text{cst}_x, \forall s, y$

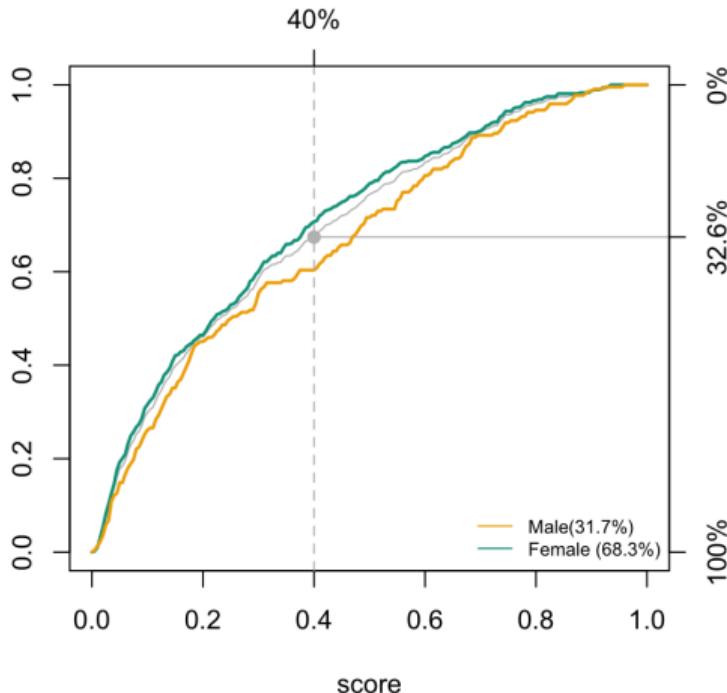
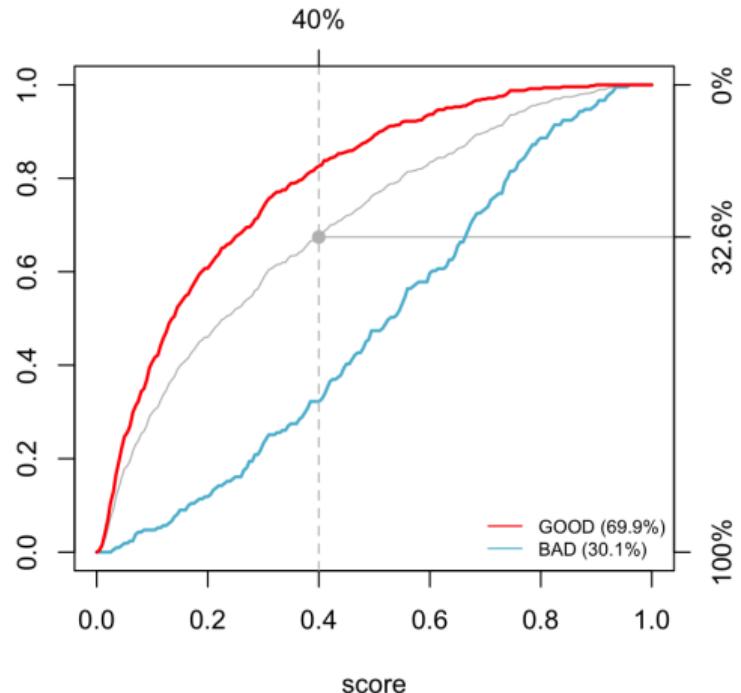
separation,  $\widehat{Y} \perp\!\!\!\perp S | Y$ , (Definition 6.11)

<i>equalized odds</i>	Hardt et al. (2016)	$\mathbb{P}[\widehat{Y} = 1 S = s, Y = y] = \text{cst}_y, \forall s, y$
<i>equalized opportunity</i>	Hardt et al. (2016)	$\mathbb{P}[\widehat{Y} = 1 S = s, Y = 1] = \text{cst}, \forall s$
<i>predictive equality</i>	Corbett-Davies et al. (2017)	$\mathbb{P}[\widehat{Y} = 1 S = s, Y = 0] = \text{cst}, \forall s$
<i>balance</i>	Kleinberg et al. (2016)	$\mathbb{E}[M S = s, Y = 1] = \text{cst}_y, \forall s, y$

sufficiency,  $Y \perp\!\!\!\perp S | \widehat{Y}$ , (Definition 6.21)

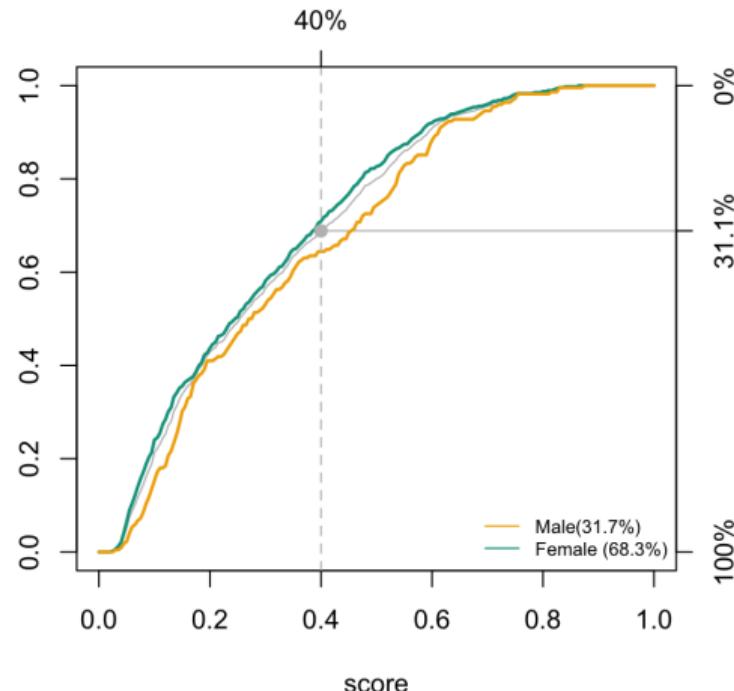
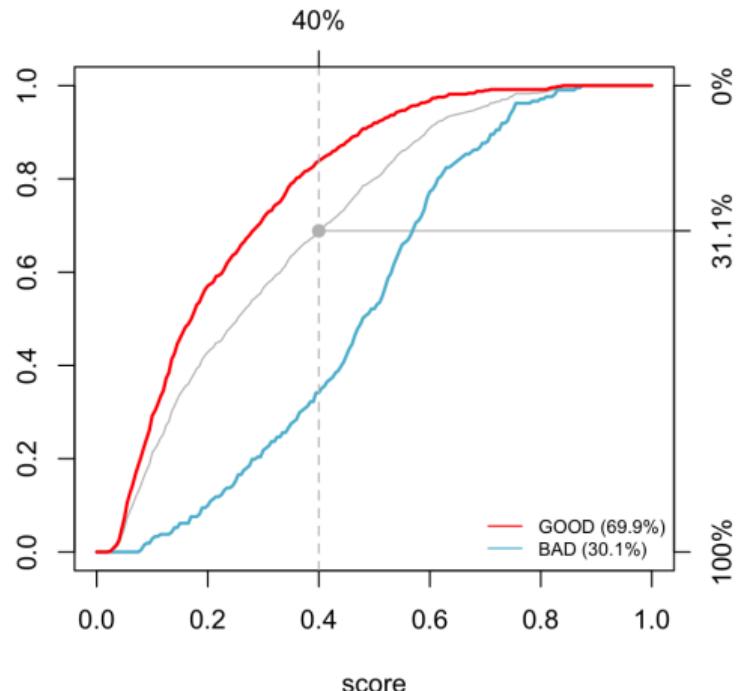
<i>disparate mistreatment</i>	Zafar et al. (2019)	$\mathbb{P}[Y = y S = s, \widehat{Y} = y] = \text{cst}_y, \forall s, y$
<i>predictive parity</i>	Chouldechova (2017)	$\mathbb{P}[Y = 1 S = s, \widehat{Y} = 1] = \text{cst}, \forall s$
<i>calibration</i>	Chouldechova (2017)	$\mathbb{P}[Y = 1 M = m, S = s] = \psi(m), \forall m, s$
<i>well-calibration</i>	Chouldechova (2017)	$\mathbb{P}[Y = 1 M = m, S = s] = m, \forall m, s$

## Numerical examples



Conditional distributions of scores on [GermanCredit](#), logistic regression.

## Numerical examples



Conditional distributions of scores on [GermanCredit](#), boosting model.

## Numerical examples

	with sensitive				without sensitive			
	GLM	tree	boosting	bagging	GLM	tree	boosting	bagging
$\mathbb{P}[m(\mathbf{X}) > t]$	51.7%	28.0%	54.7%	61.7%	50.7%	28.0%	56.0%	60.7%
Predictive Rate Parity	0.992	1.190	0.992	1.050	0.957	1.190	1.041	1.037
Demographic Parity	0.998	1.091	1.159	1.027	1.213	1.091	1.112	1.208
FNR Parity	1.398	0.740	1.078	1.124	1.075	0.740	1.064	0.970
Proportional Parity	0.922	1.008	1.071	0.949	1.121	1.008	1.027	1.116
Equalized odds	0.816	1.069	0.947	0.888	0.956	1.069	0.953	1.031
Accuracy Parity	0.843	1.181	0.912	0.904	0.896	1.181	0.943	0.966
FPR Parity	1.247	0.683	1.470	0.855	2.004	0.683	0.962	1.069
NPV Parity	0.676	1.141	0.763	0.772	0.735	1.141	0.799	0.823
Specificity Parity	0.941	1.439	0.930	1.028	0.851	1.439	1.007	0.990
ROC AUC Parity	0.928	1.162	0.997	1.108	0.926	1.162	1.004	1.090
MCC Parity	0.604	2.013	0.744	0.851	0.639	2.013	0.884	0.930

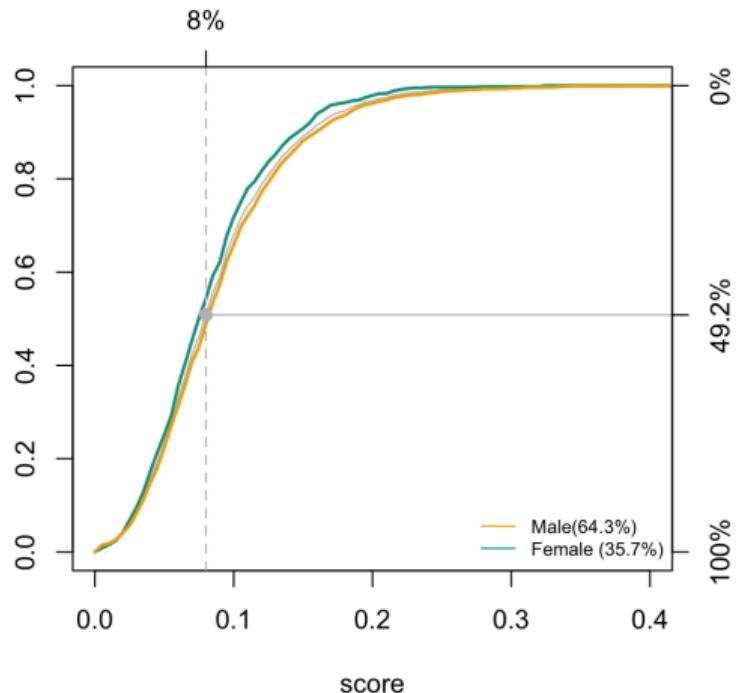
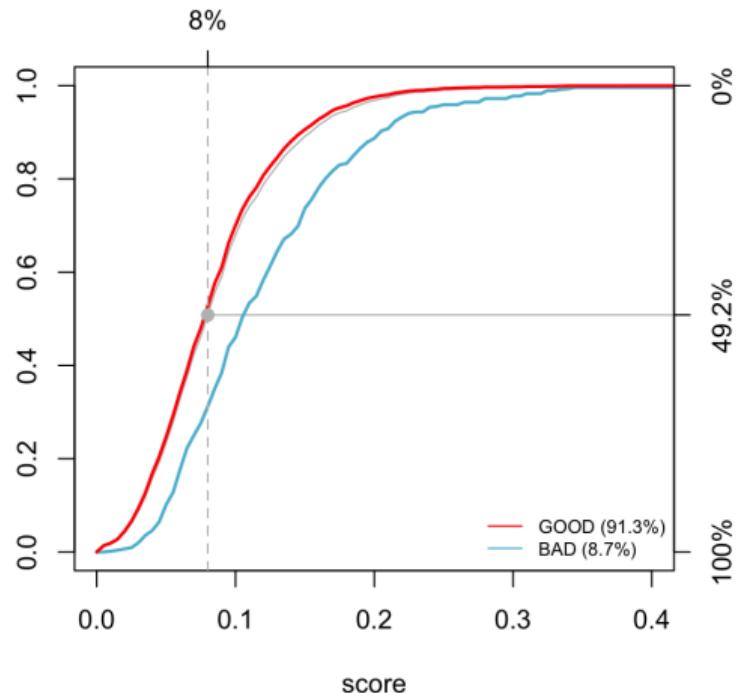
Fairness metrics on [GermanCredit](#), with threshold at 20%.

## Numerical examples

	with sensitive				without sensitive			
	GLM	tree	boosting	bagging	GLM	tree	boosting	bagging
$\mathbb{P}[m(\mathbf{X}) > t]$	30.3%	26.0%	27.7%	25.7%	30.7%	26.0%	28.0%	27.0%
Predictive Rate Parity	1.030	1.179	1.110	1.182	1.034	1.179	1.111	1.200
Demographic Parity	1.090	1.062	1.074	1.069	1.108	1.062	1.044	1.019
FNR Parity	1.533	0.851	1.110	0.781	1.342	0.851	1.322	0.962
Proportional Parity	1.007	0.981	0.992	0.987	1.024	0.981	0.964	0.942
Equalized odds	0.925	1.032	0.982	1.041	0.944	1.032	0.955	1.008
Accuracy Parity	0.949	1.154	1.054	1.164	0.963	1.154	1.038	1.159
FPR Parity	1.118	0.703	0.820	0.653	1.118	0.703	0.784	0.641
NPV Parity	0.738	1.080	0.890	1.108	0.766	1.080	0.848	1.082
Specificity Parity	0.935	1.470	1.169	1.480	0.935	1.470	1.203	1.652
ROC AUC Parity	0.928	1.162	0.997	1.108	0.926	1.162	1.004	1.090
MCC Parity	0.745	1.817	1.105	1.754	0.779	1.817	1.056	2.055

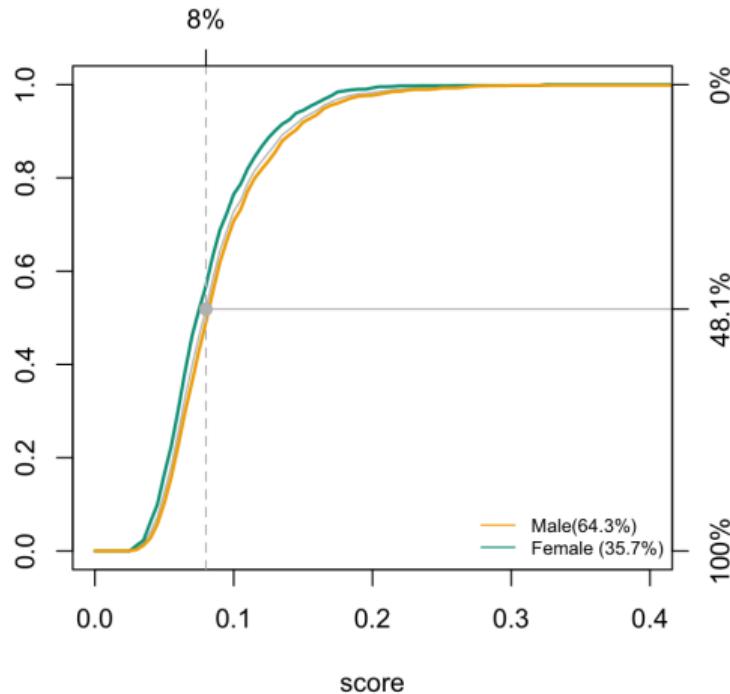
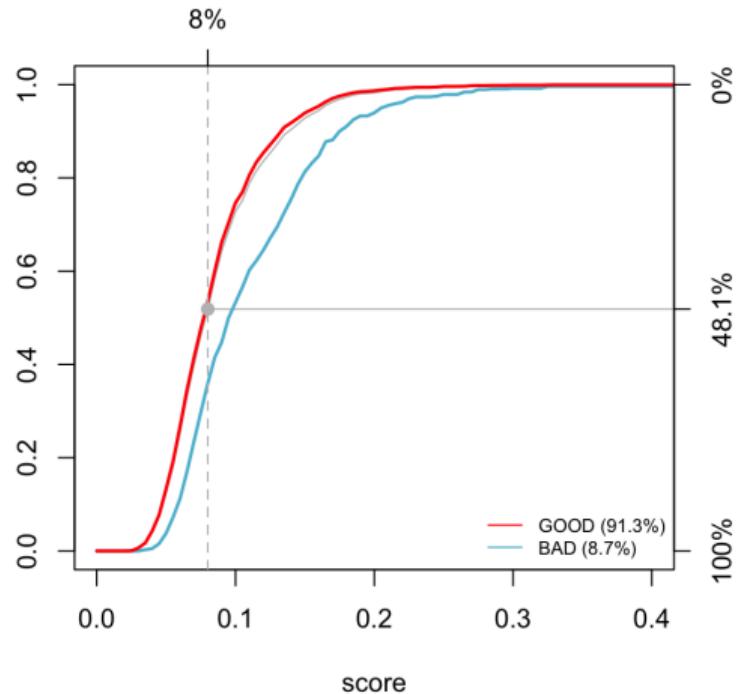
Fairness metrics on [GermanCredit](#), with threshold at 40%.

## Numerical examples



Conditional distributions of scores on [FrenchMotor](#), from the logistic regression.

## Numerical examples



Conditional distributions of scores on [FrenchMotor](#), from a boosting classification.

– Part 7 –

## Individual Fairness

## Definition 7.1: Similarity Fairness, Luong et al. (2011), Dwork et al. (2012)

Consider two metrics, one on  $\mathcal{Y} \times \mathcal{Y}$  (or for a classifier  $[0, 1]$  and not  $\{0, 1\}$ ) noted  $D_y$ , and one on  $\mathcal{X}$  noted  $D_x$ , such that we will have similarity fairness on a database of size  $n$  if we have the following property (called Lipschitz property)

$$D_y(m(\mathbf{x}_i, s_i), m(\mathbf{x}_j, s_j)) \leq L \cdot D_x(\mathbf{x}_i, \mathbf{x}_j), \quad \forall i, j = 1, \dots, n,$$

for some  $L < \infty$ .

## Definition 7.2: Local individual fairness, Petersen et al. (2021)

Consider two metrics, one on  $\mathcal{Y}$  ( $[0, 1]$  for a classifier and not  $\{0, 1\}$ ) noted  $D_y$ , and one on  $\mathcal{X}$  noted  $D_x$ , model  $m$  is locally individually fair if

$$\mathbb{E}_{(\mathbf{X}, S)} \left[ \limsup_{\mathbf{x}' : D_x(\mathbf{X}, \mathbf{x}') \rightarrow 0} \frac{D_y(m(\mathbf{X}, S), m(\mathbf{x}', S))}{D_x(\mathbf{X}, \mathbf{x}')} \right] \leq L < \infty.$$

# Individual Fairness

## Definition 7.3: Proxy Based Fairness, Kilbertus et al. (2017)

A decision making process  $\hat{y}$  exhibits no proxy discrimination with respect to sensitive attribute  $s$  if

$$\mathbb{E}[\hat{Y}|\text{do}(S = \textcolor{teal}{A})] = \mathbb{E}[\hat{Y}|\text{do}(S = \textcolor{blue}{B})].$$

## Definition 7.4: Fairness on Average Treatment Effect, Kusner et al. (2017)

We achieve fairness on average treatment effect (counterfactual fairness on average)

$$\text{ATE} = \mathbb{E}[Y_{S \leftarrow \textcolor{teal}{A}}^* - Y_{S \leftarrow \textcolor{blue}{B}}^*] = 0.$$

# Individual Fairness

- A decision satisfies counterfactual fairness if "*had the protected attributes (e.g., race) of the individual been different, other things being equal, the decision would have remained the same.*"

## Definition 7.5: Counterfactual Fairness, Kusner et al. (2017)

We achieve counterfactual fairness for an individual with characteristics  $\mathbf{x}$  if

$$\text{CATE}(\mathbf{x}) = \mathbb{E}[Y_{S \leftarrow \textcolor{teal}{A}}^* - Y_{S \leftarrow \textcolor{orange}{B}}^* | \mathbf{X} = \mathbf{x}] = 0.$$

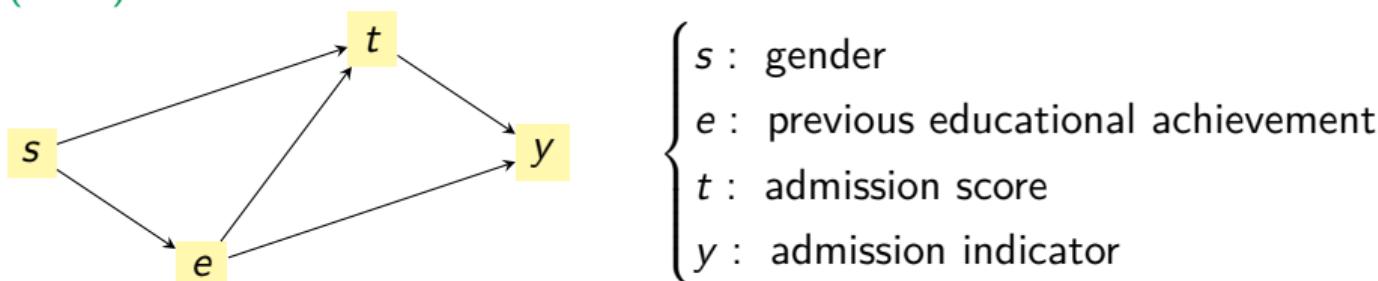
# Individual Fairness

## Definition 7.6: Path-Specific Counterfactual Effect, Wu et al. (2019)

Given a causal diagram, a factual condition (denoted  $\mathcal{F}$ ), and a path  $\pi$  some  $s$  to  $y$ , the  $\pi$ -effect of a change of  $s$  from  $B$  to  $A$  on  $y$  is

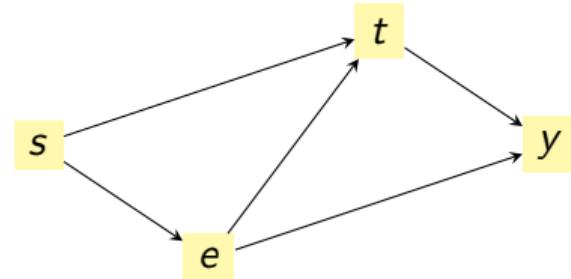
$$\text{PCE}_\pi(B \rightarrow A | \mathcal{F}) = \mathbb{E}[Y | \text{do}_\pi(S = A), \mathcal{F}] - \mathbb{E}[Y | S = B, \mathcal{F}].$$

- › A counterfactual value replaces the cause of interest, then propagates "downstream" the causal graph via the structural equations, *ceteris paribus*.
- › **fairadapt**, based on **twin network**, and "recursive substitution", Ma and Koenker (2006).



## Individual Fairness

- Following Ma and Koenker (2006), consider some structural model



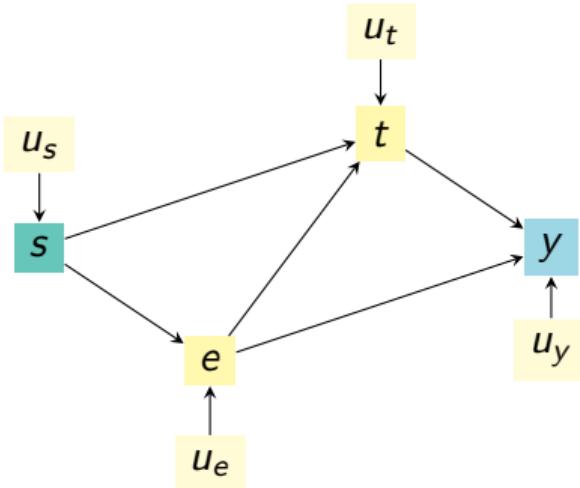
$$\begin{cases} s = U_s \\ e = h_e(s, U_e) \\ t = h_t(s, e, U_t) \\ y = h_y(e, t, U_y) \end{cases}$$

with  $U_s, U_e, U_t, U_y$  independent.

- Consider observation  $(s_i, e_i, t_i, y_i)$ .
- Can we get a counterfactual of that observation, where  $s_i = A$  ?
- Quantile regression (Koenker and Bassett Jr (1978), Koenker et al. (2017)), possibly quantile forest (Meinshausen and Ridgeway (2006)).

# Individual Fairness

# Individual Fairness

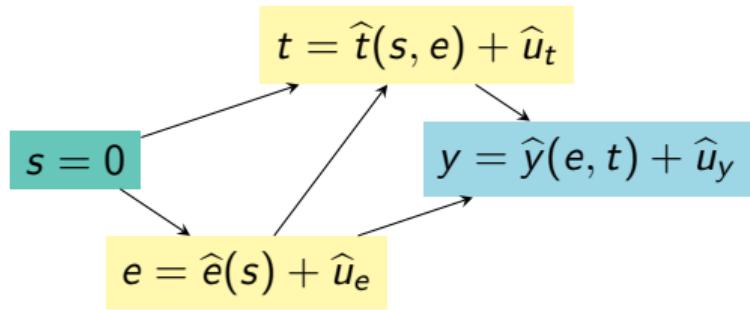


the DAG can be expressed as an additive SCM

$$\begin{cases} s = U_s \\ e = h_e(s) + U_e \\ t = h_t(s, e) + U_t \\ y = h_y(e, t) + U_y \end{cases}$$

with  $U_s, U_e, U_t, U_y$  independent.

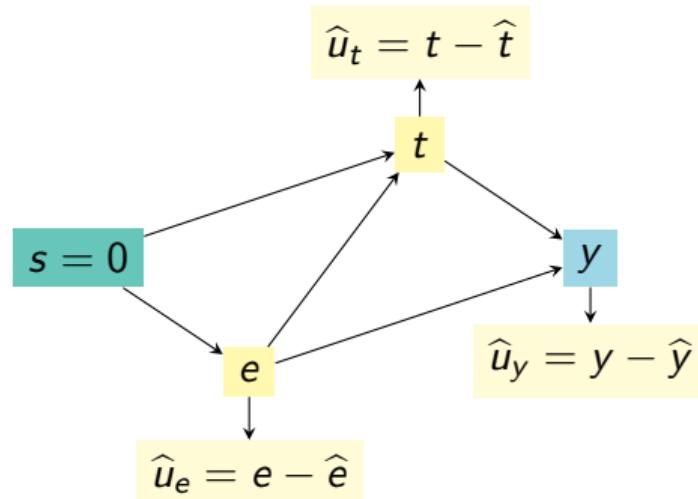
# Individual Fairness



Consider some individual in group  $s = 0$

$$\begin{cases} s = 0 \\ e = \hat{h}_e(s) + \hat{u}_e \\ t = \hat{h}_t(s, e) + \hat{u}_t \\ y = \hat{h}_y(e, t) + \hat{u}_y \end{cases}$$

# Individual Fairness



For that individuals, residuals are

$$\begin{cases} s = 0 \\ \hat{u}_e = e - \hat{h}_e(s) \\ \hat{u}_t = t - \hat{h}_t(s, e) \\ \hat{u}_y = y - \hat{h}_y(e, t) \end{cases}$$

To generate a counterfactual, suppose that residuals remain unchanged.

# Individual Fairness

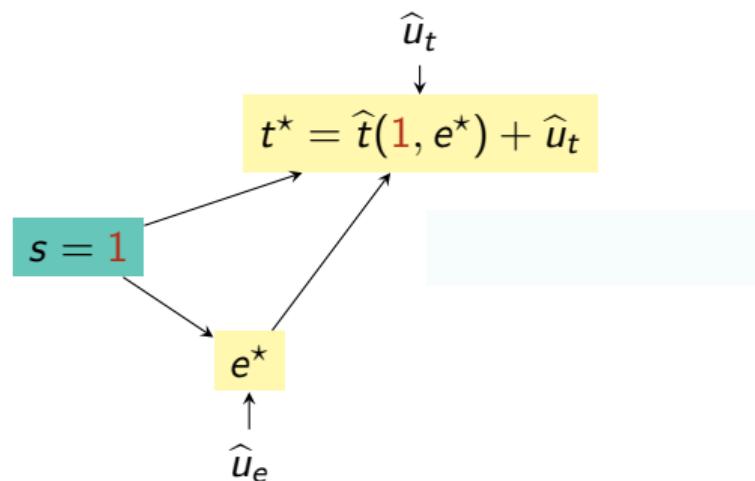
$s = 1$



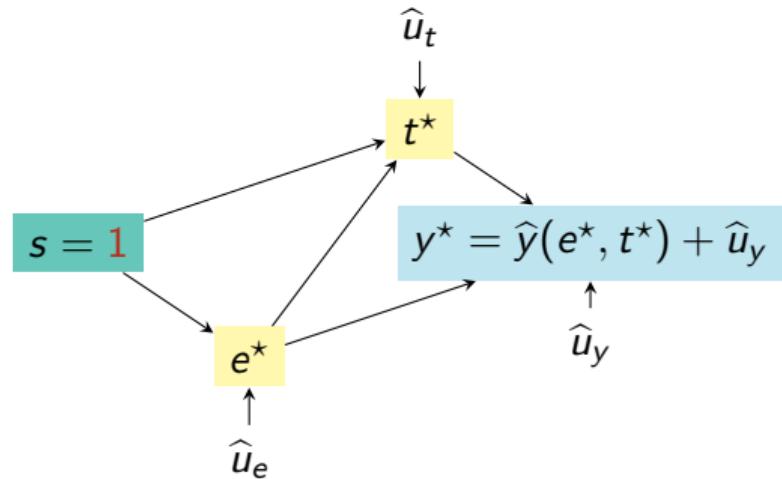
# Individual Fairness

$$s = 1$$
$$e^* = \hat{e}(s = 1) + \hat{u}_e$$
$$\uparrow$$
$$\hat{u}_e$$

# Individual Fairness



# Individual Fairness



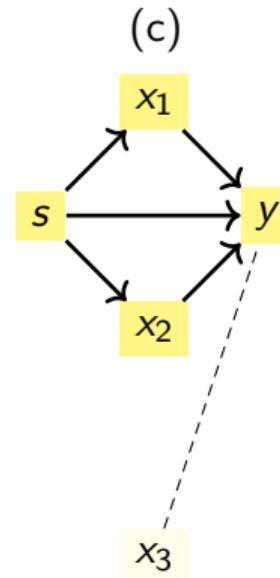
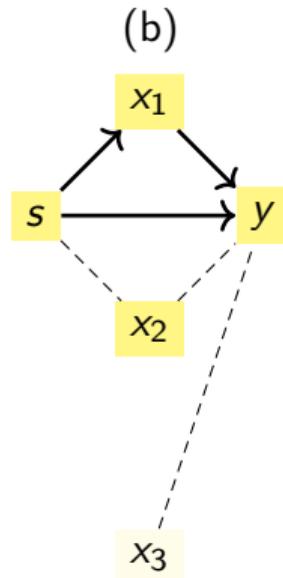
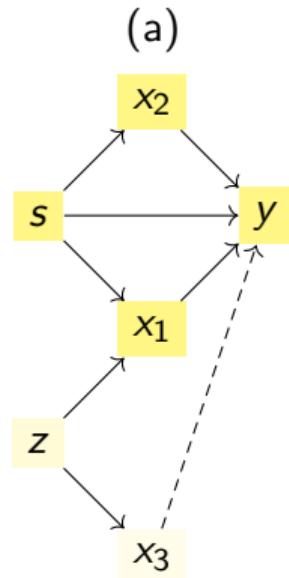
# Individual Fairness

# Individual Fairness

# Individual Fairness

Similarity Fairness ( <i>Lipschitz</i> )	Dwork et al. (2012)	$D_y(\hat{y}_i, \hat{y}_j) \leq D_x(\mathbf{x}_i, \mathbf{x}_j), \forall i, j$
Proxy Based Fairness,	Kilbertus et al. (2017)	$\mathbb{E}[Y do(S = A)] = \mathbb{E}[Y do(S = B)]$
Fairness on Average Treatment Effect	Kusner et al. (2017)	$\mathbb{E}[Y_{S \leftarrow A}^*] = \mathbb{E}[Y_{S \leftarrow B}^*]$
Counterfactual Fairness,	Kusner et al. (2017)	$\mathbb{E}[Y_{S \leftarrow A}^*   \mathbf{X} = \mathbf{x}] = \mathbb{E}[Y_{S \leftarrow B}^*   \mathbf{X} = \mathbf{x}]$
Path-Specific Effect	Avin et al. (2005)	$\mathbb{E}[Y do_\pi(S = A)] = \mathbb{E}[Y do_\pi(S = B)]$
Path-Specific Counterfactual Effect	Wu et al. (2019)	$\mathbb{E}[Y do_\pi(S = A), \mathcal{F}] = \mathbb{E}[Y do_\pi(S = B), \mathcal{F}]$
Mutatis Mutandis Counterfactual	Kusner et al. (2017)	$\mathbb{E}[Y_{S \leftarrow A}^*   \mathbf{X} = \mathcal{T}(\mathbf{x})] = \mathbb{E}[Y_{S \leftarrow B}^*   \mathbf{X} = \mathcal{T}(\mathbf{x})]$

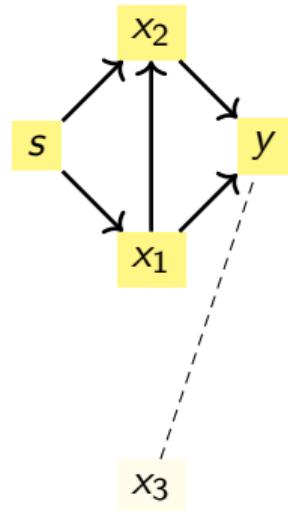
# Individual Fairness



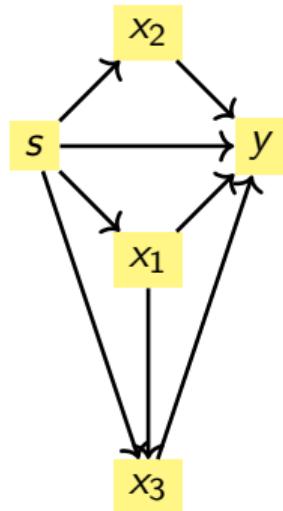
- (a) Causal graph used to generate variables in `toydata2`.
- (b) Causal graph, where  $s$  might cause  $y$ , either directly, or indirectly, through  $x_1$ .
- (c) Causal graph, where  $s$  might cause  $y$ , either directly or indirectly, via with two possible paths and two mediator variables,  $x_1$  and  $x_2$ .

## Individual Fairness

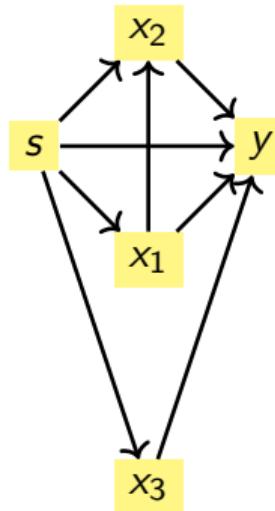
(d)



(e)



(f)



(d) Causal graph with no direct impact of  $s$  on  $y$ , but two mediators, and possibly,  $x_1$  might cause  $x_2$ .

(e) similar to (c) with an additional indirect connection from  $x_1$  to  $y$ , via mediator  $x_3$ .

(f) similar to (d) with an additional indirect connection from  $x_1$  to  $y$ , via mediator  $x_3$ .

# Individual Fairness

Original data

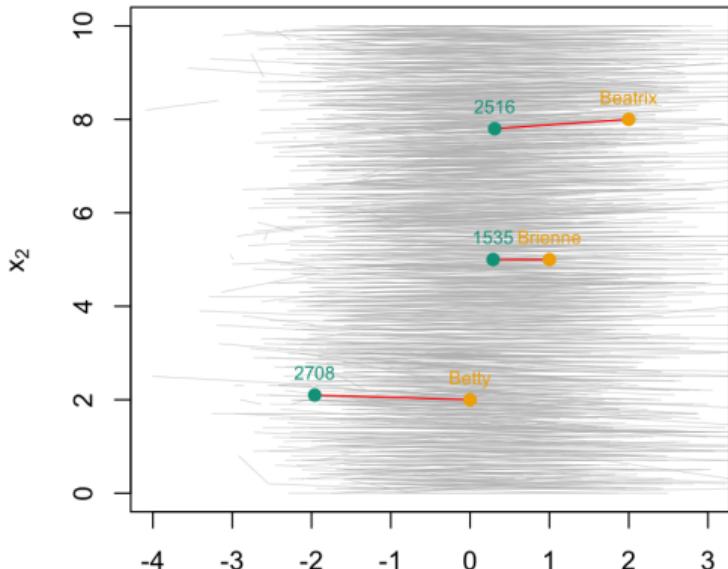
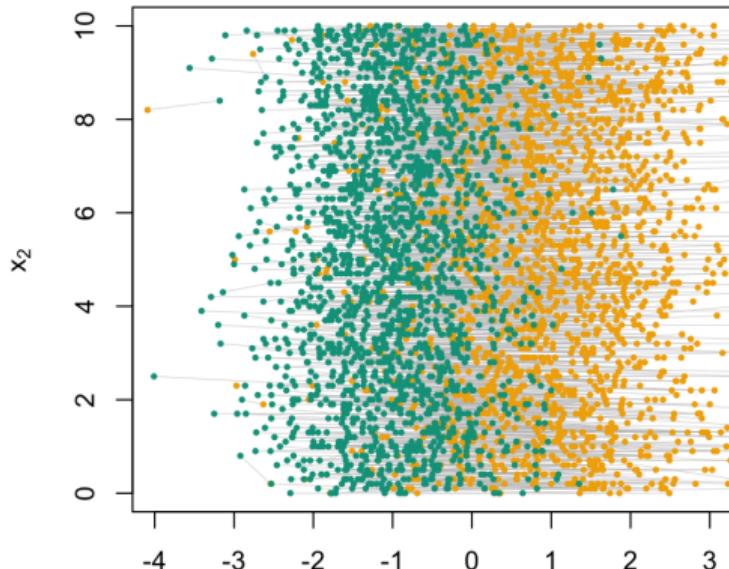
	$s$	$x_1$	$x_2$	$x_3$	$\hat{m}_{\text{glm}}(\mathbf{x})$	$\hat{m}_{\text{glm}}(\mathbf{x}, s)$	$\hat{m}_{\text{gam}}(\mathbf{x})$	$\hat{m}_{\text{gam}}(\mathbf{x}, s)$	$\hat{m}_{\text{rf}}(\mathbf{x})$	$\hat{m}_{\text{rf}}(\mathbf{x}, s)$
Betty	B	0	2	0	18.22%	24.06%	13.23%	17.63%	17.4%	29.6%
Brienne	B	1	5	1	67.19%	70.47%	66.18%	67.09%	63.60%	61.80%
Beatrix	B	2	8	2	94.95%	94.73%	97.53%	97.58%	96.60%	98.40%
Alex	A	0	2	0	18.22%	13.71%	13.23%	10.05%	17.40%	9.20%
Ahmad	A	1	5	1	67.19%	54.48%	66.18%	50.49%	63.60%	64.40%
Anthony	A	2	8	2	94.95%	90.02%	97.53%	90.51%	96.60%	68.20%

# Individual Fairness

## Counterfactual

$s$	$x_1$	$x_2$	$x_3$	$\hat{m}_{\text{glm}}(\mathbf{x})$	$\hat{m}_{\text{glm}}(\mathbf{x}, s)$	$\hat{m}_{\text{gam}}(\mathbf{x})$	$\hat{m}_{\text{gam}}(\mathbf{x}, s)$	$\hat{m}_{\text{rf}}(\mathbf{x})$	$\hat{m}_{\text{rf}}(\mathbf{x}, s)$
adjusted data, using marginal quantiles									
Betty	A	-1.68	2.1	-1.68	3.51%	3.58%	4.78%	4.85%	10.40%
Brienne	A	-0.98	5.1	-0.96	19.39%	17.65%	16.64%	16.13%	29.00%
Beatrix	A	-0.27	7.9	-0.26	59.83%	53.65%	51.89%	46.37%	53.60%
adjusted data, using optimal transport, (c)									
Betty	A	-1.96	2.1	-1.9	2.62%	2.82%	4.65%	4.81%	0.00%
Brienne	A	0.29	5	0.25	48.24%	38.92%	40.04%	32.14%	21.40%
Beatrix	A	0.31	7.8	0.21	72.83%	65.1%	67.5%	58.83%	20.80%
adjusted data, using Gaussian transport, (c)									
Betty	A	-1.58	2.15	-1.59	3.95%	3.96%	4.96%	4.99%	0.40%
Brienne	A	-0.98	4.96	-0.99	18.47%	16.84%	15.84%	15.40%	19.80%
Beatrix	A	-0.38	7.79	-0.38	55.71%	50.05%	47.86%	43.16%	51.80%

# Individual Fairness



Optimal matching, of individuals in group  $B$  to individuals in group  $A$ , on right, where points ● are Betty, Brienne and Beatrix, and • their counterfactual version in group  $A$ .

# Individual Fairness

## Counterfactual

$s$	$x_1$	$x_2$	$x_3$	$\hat{m}_{\text{glm}}(\mathbf{x})$	$\hat{m}_{\text{glm}}(\mathbf{x}, s)$	$\hat{m}_{\text{gam}}(\mathbf{x})$	$\hat{m}_{\text{gam}}(\mathbf{x}, s)$	$\hat{m}_{\text{rf}}(\mathbf{x})$	$\hat{m}_{\text{rf}}(\mathbf{x}, s)$
-----	-------	-------	-------	------------------------------------	---------------------------------------	------------------------------------	---------------------------------------	-----------------------------------	--------------------------------------

adjusted data, with fairAdapt, Figure (e)

Betty	A	-1.65	2	-1.32	3.63%	3.54%	4.72%	4.60%	14.60%	8.00%
Brienne	A	-0.97	4.55	-0.94	16.57%	14.96%	13.96%	13.51%	2.20%	5.20%
Beatrix	A	-0.33	7.72	-0.44	56.3%	50.71%	48.49%	43.74%	70.60%	74.80%

adjusted data, with fairAdapt, Figure (f)

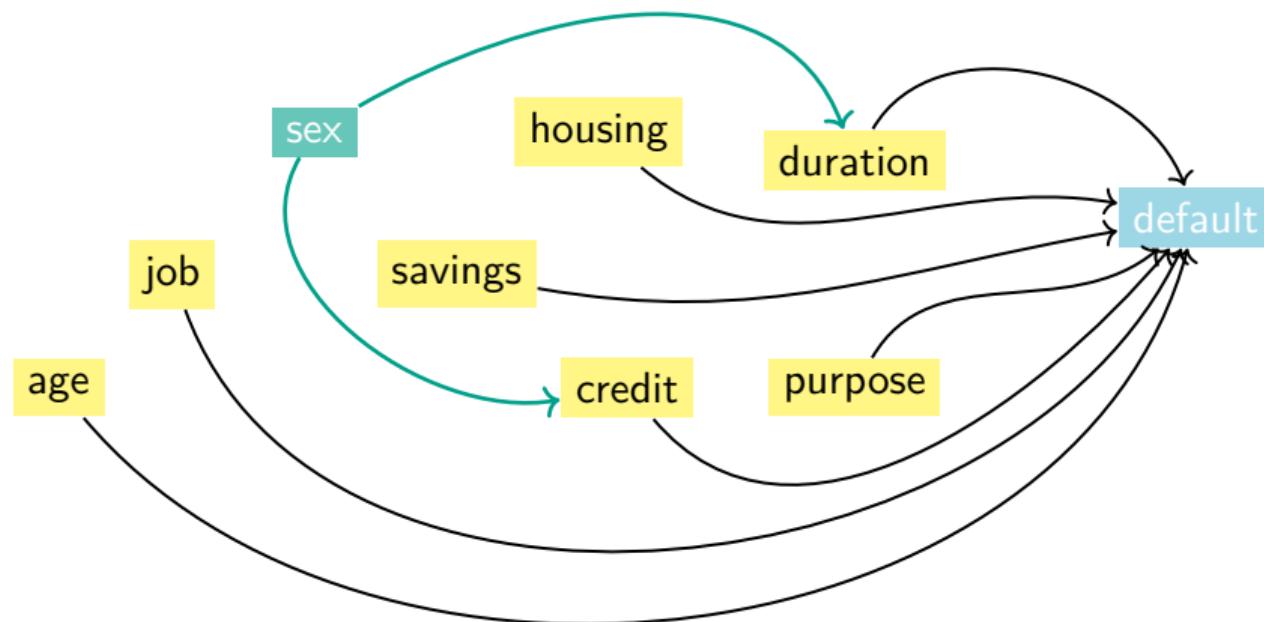
Betty	A	-1.75	2.28	-1.68	3.5%	3.6%	5.03%	5.13%	7.20%	7.00%
Brienne	A	-0.96	5.3	-0.96	20.9%	19.05%	17.91%	17.34%	5.80%	8.40%
Beatrix	A	-0.24	8.12	-0.34	62.31%	56.43%	54.8%	49.3%	45.60%	39.20%

# Numerical illustrations

Original data

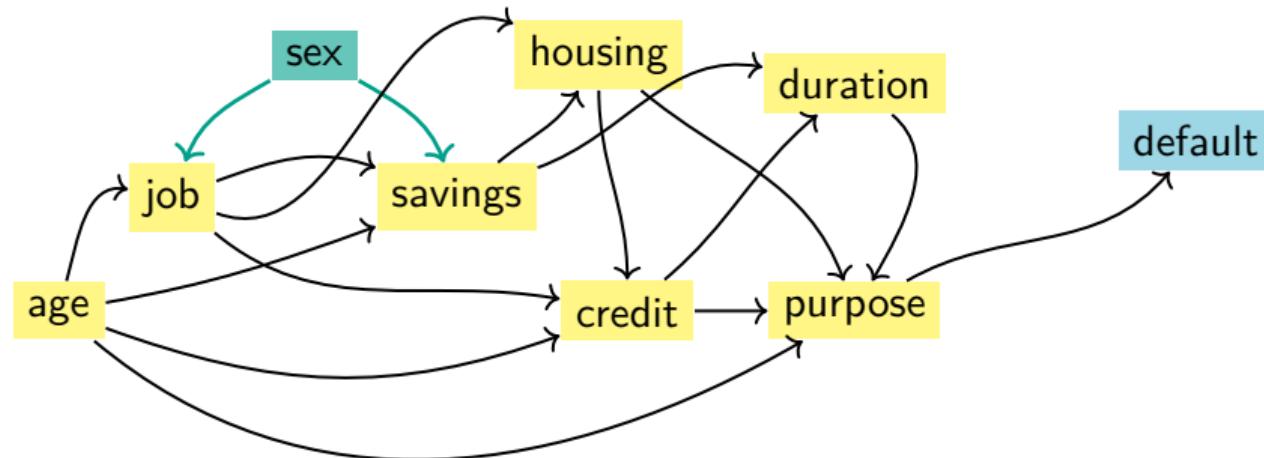
	$s$	$x_1$	$x_2$	$x_3$	$\hat{m}_{\text{glm}}(\mathbf{x})$	$\hat{m}_{\text{glm}}(\mathbf{x}, s)$	$\hat{m}_{\text{gam}}(\mathbf{x})$	$\hat{m}_{\text{gam}}(\mathbf{x}, s)$	$\hat{m}_{\text{rf}}(\mathbf{x})$	$\hat{m}_{\text{rf}}(\mathbf{x}, s)$
Betty	B	0	2	0	18.22%	24.06%	13.23%	17.63%	17.4%	29.6%
Brienne	B	1	5	1	67.19%	70.47%	66.18%	67.09%	63.60%	61.80%
Beatrix	B	2	8	2	94.95%	94.73%	97.53%	97.58%	96.60%	98.40%
Alex	A	0	2	0	18.22%	13.71%	13.23%	10.05%	17.40%	9.20%
Ahmad	A	1	5	1	67.19%	54.48%	66.18%	50.49%	63.60%	64.40%
Anthony	A	2	8	2	94.95%	90.02%	97.53%	90.51%	96.60%	68.20%

## Numerical illustrations



Simple causal graph on the [GermanCredit](#) dataset,

# Numerical illustrations



Causal graph on the [germancredit](#) dataset, from Watson et al. (2021)

# Numerical illustrations

	Alex	Ahmad	Anthony	Betty	Brienne	Beatrix
$s$ (gender)	M	M	M	F	F	F
$x_1$ Duration	12	18	30	12	18	30
$u = F_{1 s}(x_1)$	36%	57%	86%	34%	50%	79%
$\mathcal{T}(x_1) = F_{1 s=M}^{-1}(u)$	12	18	30	12	18	24
$x_2$ Credit	1262	2319	4720	1262	2319	4720
$u = F_{2 s}(x_2)$	25%	55%	82%	17%	45%	76%
$\mathcal{T}(x_2) = F_{2 s=M}^{-1}(u)$	1262	2319	4720	1074	1855	3854

# Numerical illustrations

On the [GermanCredit](#) dataset

Firstname	s	Firstname	s	Job	Savings	Housing		
Alex	M	Betty	F	highly qualified employee	100 DM	rent	radio	1
Ahmad	M	Brienne	F	skilled employee	100<...<500 DM	own	1	1
Anthony	M	Beatrix	F	unskilled - resident	no savings	for free	1	1

Original data

	s	Age	Duration	Credit	$\hat{m}_{\text{glm}}(x)$	$\hat{m}_{\text{glm}}(x, s)$	$\hat{m}_{\text{gbm}}(x)$	$\hat{m}_{\text{gbm}}(x, s)$	$\hat{m}_{\text{cart}}(x)$	$\hat{m}_{\text{cart}}(x, s)$
Betty	F	26	12	1262	39.69%	36.66%	42.30%	43.26%	31.75%	31.75%
Brienne	F	33	18	2320	24.30%	22.61%	23.88%	21.08%	21.31%	21.31%
Beatrix	F	45	30	4720	30.88%	30.08%	28.49%	30.42%	15.38%	15.38%
Alex	M	26	12	1262	39.69%	42.10%	42.30%	44.86%	31.75%	31.75%
Ahmad	M	33	18	2320	24.30%	26.84%	23.88%	22.18%	21.31%	21.31%
Anthony	M	45	30	4720	30.88%	35.08%	28.49%	31.82%	15.38%	15.38%

# Numerical illustrations

## Original data

	$s$	Age	Duration	Credit	$\hat{m}_{\text{glm}}(x)$	$\hat{m}_{\text{glm}}(x, s)$	$\hat{m}_{\text{gbm}}(x)$	$\hat{m}_{\text{gbm}}(x, s)$	$\hat{m}_{\text{cart}}(x)$	$\hat{m}_{\text{car}}$
Betty	M	26	12	1074	39.51%	41.90%	40.69%	44.86%	31.75%	31
Brienne	M	33	18	1855	23.95%	26.46%	23.88%	22.18%	21.31%	21
Beatrix	M	45	24	3854	24.91%	28.58%	20.55%	20.31%	21.31%	21

adjusted data, with fairAdapt, causal graph from Figure ??

Betty	M	26	12	1110	42.73%	45.18%	44.24%	46.64%	31.75%	31
Brienne	M	33	18	1787	23.90%	26.40%	23.88%	22.18%	21.31%	21
Beatrix	M	45	24	3990	25.01%	28.70%	22.17%	23.60%	21.31%	21

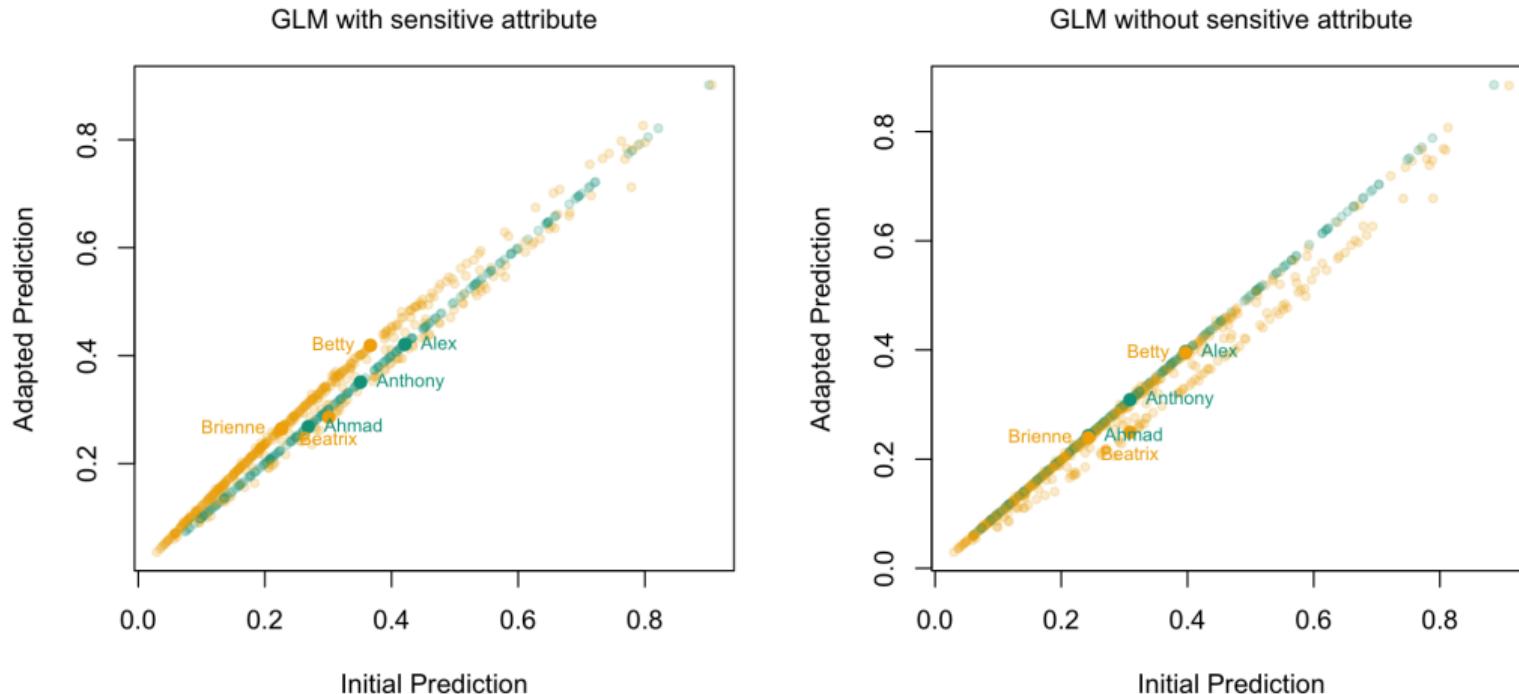
adjusted data, with fairAdapt, causal graph from Figure ??

Betty	M	26	18	1778	52.23%	54.03%	40.05%	46.81%	21.31%	21
Brienne	M	33	15	1864	32.25%	35.85%	31.60%	25.97%	21.31%	21
Beatrix	M	45	21	3599	39.70%	43.16%	28.36%	28.90%	21.31%	21

adjusted data, with fairAdapt, causal graph from Figure ??

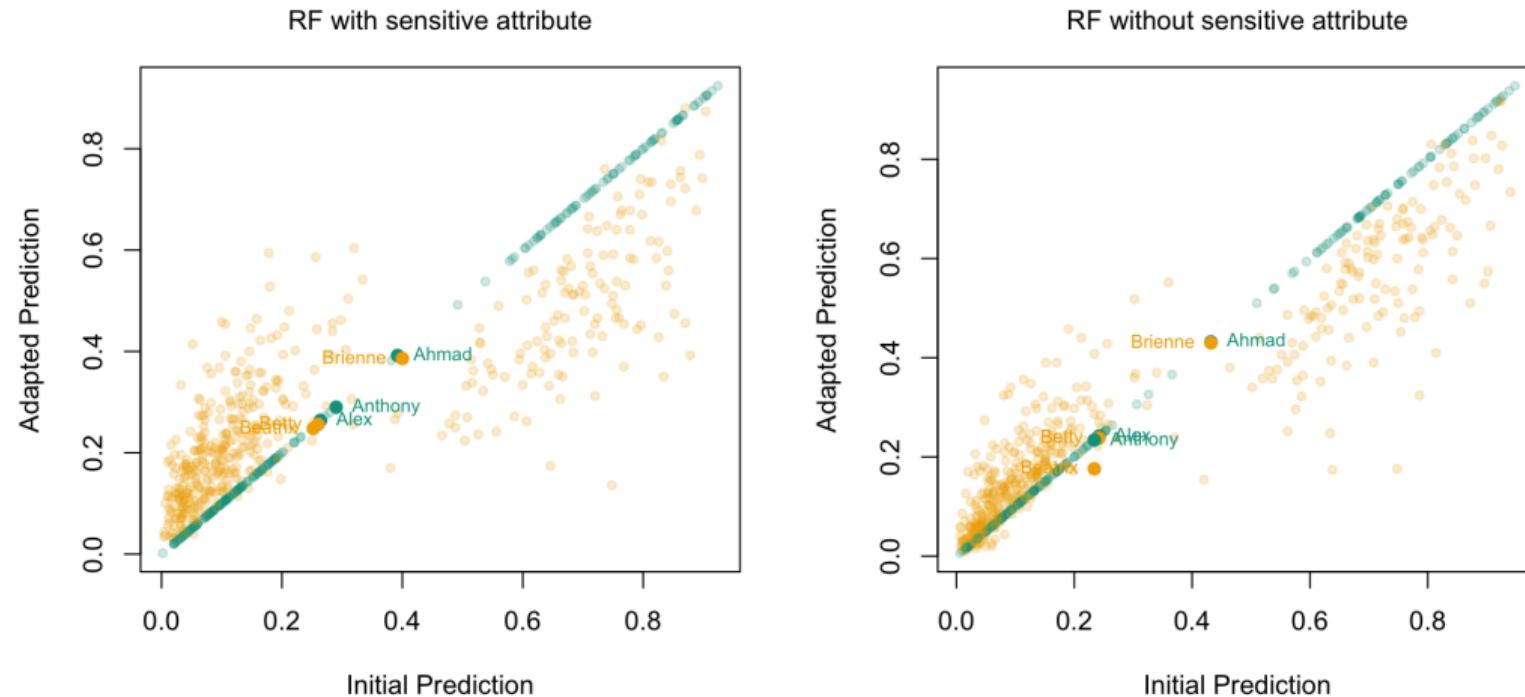
Betty	M	26	15	1882	49.05%	50.86%	35.32%	40.12%	21.31%	21
Brienne	M	33	18	1881	50.76%	53.49%	43.00%	38.77%	21.31%	21
Beatrix	M	45	24	3234	24.20%	26.23%	14.63%	16.84%	21.31%	21

# Numerical illustrations



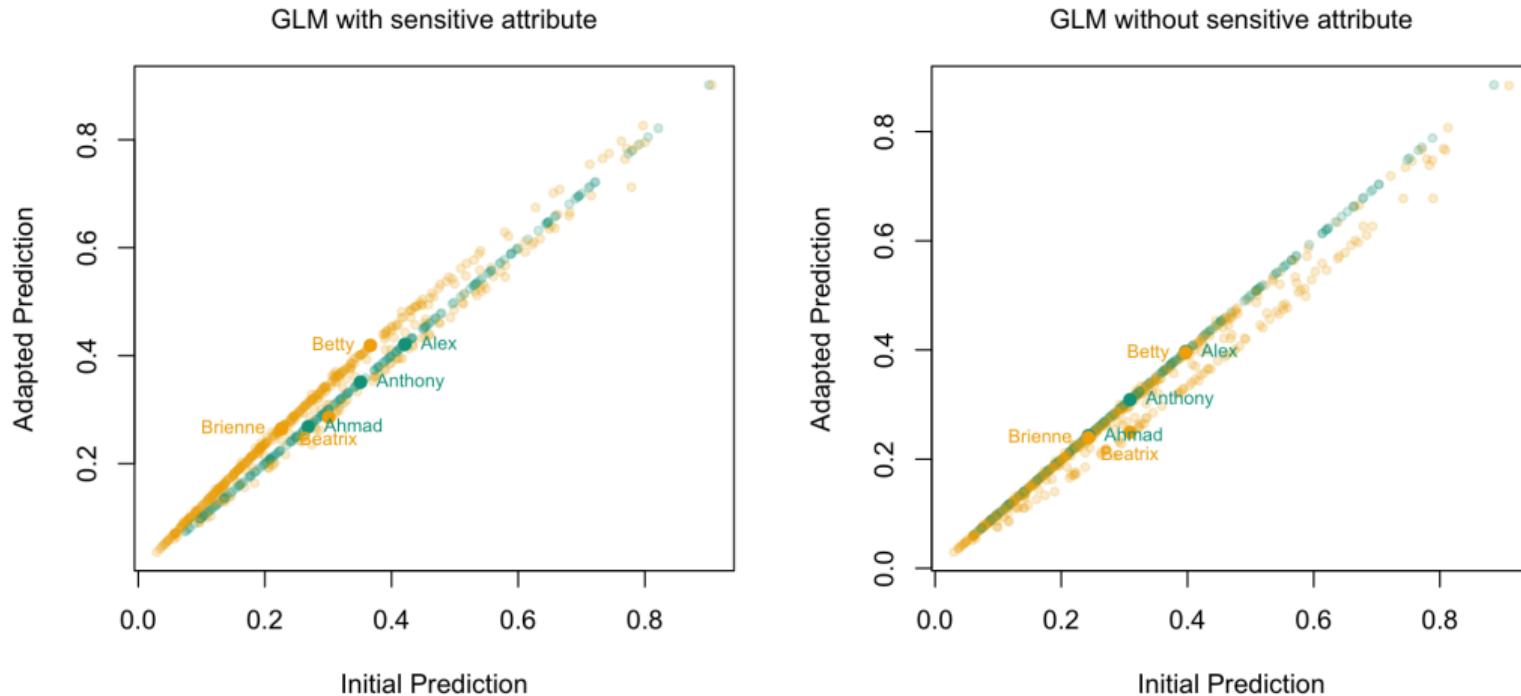
Scatterplot  $(m(\mathbf{x}_i), m(\mathcal{T}^*(\mathbf{x}_i)))$  for individuals in groups **M** and **F**.

# Numerical illustrations



Scatterplot  $(m(\mathbf{x}_i), m(\mathcal{T}^*(\mathbf{x}_i)))$  for individuals in groups **M** and **F**.

# Numerical illustrations



Scatterplot  $(m(\mathbf{x}_i), m(\mathcal{T}^*(\mathbf{x}_i)))$  for individuals in groups **M** and **F**.

– Part 8 –

## Mitigating Discrimination

# Achieving a Fair Prediction

- Mitigating discrimination is usually seen as paradoxical, because in order to avoid discrimination, we must create another discrimination. More precisely, Supreme Court Justice Harry Blackmun stated, in 1978, “*in order to get beyond racism, we must first take account of race. There is no other way. And in order to treat some persons equally, we must treat them differently,*” cited in [Knowlton \(1978\)](#), as mentioned in [Lippert-Rasmussen \(2020\)](#)).
- More formally, an argument in favor of affirmative action – called “*the present-oriented anti-discrimination argument*” – is simply that justice requires that we eliminate or at least mitigate (present) discrimination by the best morally permissible means of doing so, which corresponds to affirmative action. [Freeman \(2007\)](#) suggested a “*time-neutral anti-discrimination argument*,” in order to mitigate past, present, or future discrimination.



## Achieving a Fair Prediction

- But there are also arguments against affirmative action, corresponding to “*the reverse discrimination objection*,” as defined in [Goldman \(1979\)](#): some might consider that there is an absolute ethical constraint against unfair discrimination (including affirmative action). To quote another Supreme Court Justice, in 2007, John G. Roberts of the US Supreme Court submits: “*The way to stop discrimination on the basis of race is to stop discriminating on the basis of race*” ([Turner \(2015\)](#) and [Sabbagh \(2007\)](#)).



- The arguments against affirmative action are usually based on two theoretical moral claims, according to [Pojman \(1998\)](#). The first denies that groups have moral status (or at least meaningful status). According to this view, individuals are only responsible for the acts they perform as specific individuals and, as a corollary, we should only compensate individuals for the harms they have specifically suffered. The second asserts that a society should distribute its goods according to merit.

## Achieving a Fair Prediction

- › We have defined the risk of a model  $m \in \mathcal{M}$  as  $\mathcal{R}(m) = \mathbb{E}[\ell(Y, m(\mathbf{X}))]$ .
- › Define the classes of fair models,

$$\begin{cases} \mathcal{M}_{\text{DP}} = \{m \in \mathcal{M} \text{ s.t. } m(\mathbf{X}) \perp\!\!\!\perp S\} \\ \mathcal{M}_{\text{EO}} = \{m \in \mathcal{M} \text{ s.t. } m(\mathbf{X}) \perp\!\!\!\perp S \mid Y\} \end{cases}$$

- › Fairness is achieved by projection onto a fair subspace

$$\hat{m}_{\text{fair}} \in \operatorname{argmin}_{m \in \mathcal{M}_{\text{fair}}} \{\hat{\mathcal{R}}_n(m)\}$$

### Definition 8.1: Price of fairness

Given a risk  $\mathcal{R}$ , a class  $\mathcal{M}$  and the fair subclass  $\mathcal{M}_{\text{fair}}$ , the price of fairness

$$\mathcal{E}_{\text{fair}}(\mathcal{M}) = \min_{m \in \mathcal{M}_{\text{fair}}} \{\mathcal{R}(m)\} - \min_{m \in \mathcal{M}} \{\mathcal{R}(m)\}.$$

## Achieving a Fair Prediction

- Recall that Bayes estimator is the best model,

$$\mu(\mathbf{x}) = \mathbb{E}[Y|\mathbf{X} = \mathbf{x}] \text{ and set } \begin{cases} \mu_{\text{A}}(\mathbf{x}) = \mathbb{E}[Y|\mathbf{X} = \mathbf{x}, S = \text{A}] \\ \mu_{\text{B}}(\mathbf{x}) = \mathbb{E}[Y|\mathbf{X} = \mathbf{x}, S = \text{B}] \end{cases}$$

- From the definition of Wasserstein distance,

$$W_2(p, q) = \left( \inf_{\pi \in \Pi(p, q)} \int |x - y|^2 d\pi(x, y) \right)^{1/2}$$

Thus,

$$\mathbb{E}[|m(\mathbf{X}, S) - \mu_S(\mathbf{X})|^2 | S = s] \geq W_2(\mathbb{P}_m, \mathbb{P}_s)^2$$

# Achieving a Fair Prediction

## Proposition 8.1: Price of fairness and Wasserstein Barycenter

$$\mathcal{E}_{\text{fair}}(\mathcal{M}) = \min_{m \in \mathcal{M}_{\text{fair}}} \{\mathcal{R}(m)\} - \min_{m \in \mathcal{M}} \{\mathcal{R}(m)\} \geq \min_{g \in \mathcal{M}} \left\{ \mathbb{E} \left( W_2(\mathbb{P}_S, \mathbb{P}_{S,g})^2 \right) \right\}$$

where  $\mathbb{P}_S$  is the condition distribution of  $\mu(\mathbf{X}, S)$ , given  $S$ , and  $\mathbb{P}_{S,g}$  is the condition distribution of  $g(\mathbf{X}, S)$ , given  $S$ . Moreover, if  $\mathcal{M}_{\text{fair}} = \mathcal{M}_{\text{DP}}$ , and if  $\mathbb{P}_s$  is absolutely continuous (w.r.t. Lebesgue measure),

$$\mathcal{E}_{\text{DP}}(\mathcal{M}) = \min_{g \in \mathcal{M}} \left\{ \mathbb{E} \left( W_2(\mathbb{P}_S, \mathbb{P}_{S,g})^2 \right) \right\} = \min_{g \in \mathcal{M}} \left\{ \sum_s \mathbb{P}[S = s] \cdot W_2(\mathbb{P}_s, \mathbb{P}_{s,g})^2 \right\}$$

See Gouic et al. (2020).

- The minimum is reached at the **Wasserstein barycenter** of  $\mathbb{P}_S$ 's.

## Pre-Processing

- › Write the  $n \times k$  matrix  $\mathbf{S}$  as a collection of  $k$  vectors in  $\mathbb{R}^n$ ,  $\mathbf{S} = (\mathbf{s}_1 \ \cdots \ \mathbf{s}_k)$ , that will correspond to  $k$  sensitive attributes. The orthogonal projection on variables  $\{\mathbf{s}_1, \dots, \mathbf{s}_k\}$  is associated to matrix  $\Pi_S = \mathbf{S}(\mathbf{S}^\top \mathbf{S})^{-1} \mathbf{S}^\top$ , while the projection on the orthogonal of  $\mathbf{S}$  is  $\Pi_{S^\perp} = \mathbb{I} - \Pi_S$  (Gram-Schmidt orthogonalization,).
- › Let  $\tilde{\mathbf{S}}$  denote the collection of centered vectors (using matrix notations,  $\tilde{\mathbf{S}} = \mathbf{H}\mathbf{S}$  where  $\mathbf{H} = \mathbb{I} - (\mathbf{1}\mathbf{1}^\top)/n$ ).
- › Write the  $n \times p$  matrix  $\mathbf{X}$  as a collection of  $p$  vectors in  $\mathbb{R}^n$ ,  $\mathbf{X} = (\mathbf{x}_1 \ \cdots \ \mathbf{x}_p)$ . For any  $\mathbf{x}_j$ , define

$$\mathbf{x}_j^\perp = \Pi_{\tilde{\mathbf{S}}^\perp} \mathbf{x}_j = \mathbf{x}_j - \tilde{\mathbf{S}}(\tilde{\mathbf{S}}^\top \tilde{\mathbf{S}})^{-1} \tilde{\mathbf{S}}^\top \mathbf{x}_j.$$

One can easily prove that  $\mathbf{x}_j^\perp$  is then orthogonal to any  $\mathbf{s}$ , since

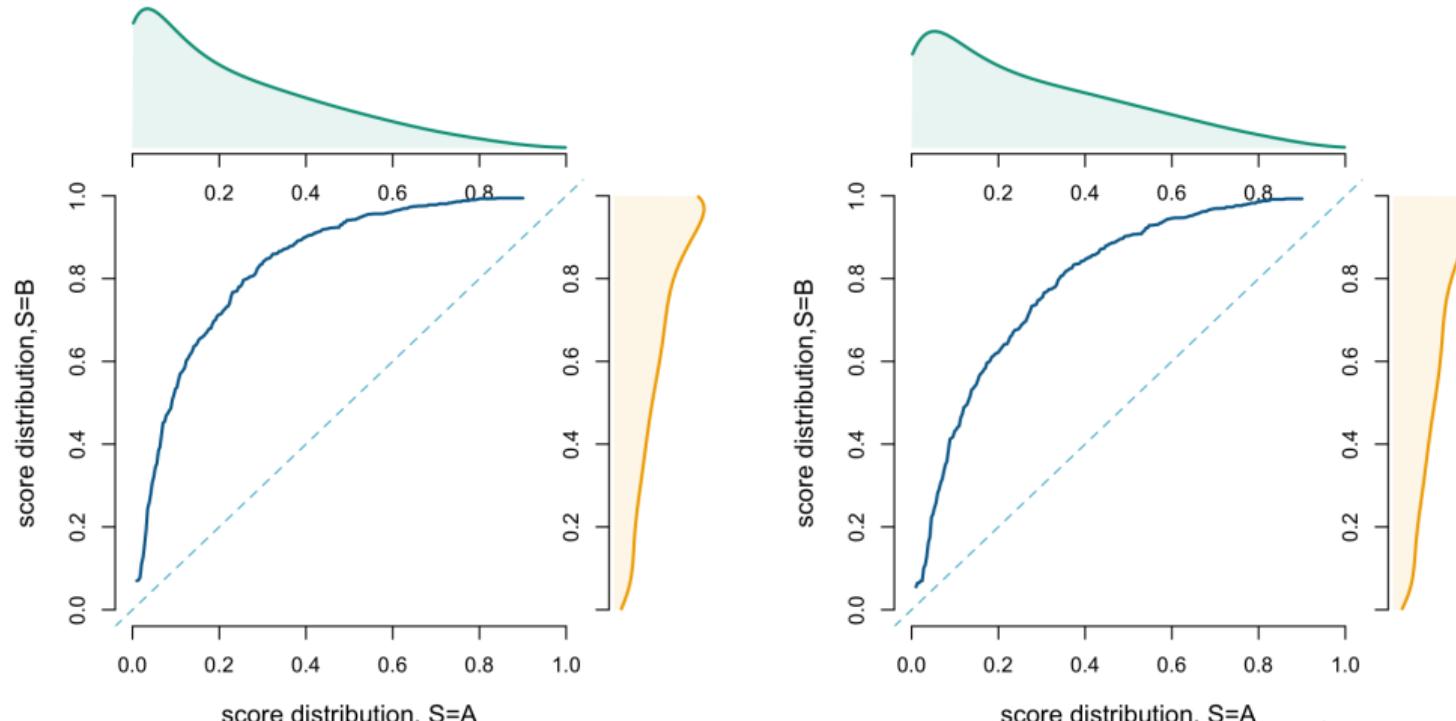
$$\text{Cov}(\mathbf{s}, \mathbf{x}_j^\perp) = \frac{1}{n} \mathbf{s}^\top \mathbf{H} \mathbf{x}_j^\perp = \frac{1}{n} \tilde{\mathbf{s}}^\top \Pi_{\tilde{\mathbf{S}}^\perp} \mathbf{x}_j = 0.$$

## Pre-Processing

- And similarly the centered version of  $\mathbf{x}_j^\perp$  is then also orthogonal to any  $\mathbf{s}$ . From an econometric perspective,  $\mathbf{x}_j^\perp$  can be seen as the residual of the regression of  $\mathbf{x}_j$  against  $\mathbf{s}$ 's, obtained from least square estimation

$$\mathbf{x}_j = \tilde{\mathbf{s}}^\top \hat{\boldsymbol{\beta}}_j + \mathbf{x}_j^\perp.$$

# Pre-Processing



Optimal transport between distributions of  $\hat{m}(\mathbf{x}_i, s_i)$ 's ( $x$ -axis) to  $\hat{m}^\perp(\mathbf{x}_i^\perp)$ 's ( $y$ -axis), for individuals in group **A** on the left-hand side, and in group **B** on the right-hand side.

## Pre-Processing

- › Consider the linear model  $\mathbf{y} = \mathbf{S}\alpha + \mathbf{X}^\perp\beta + \varepsilon$
- › Consider the fairness constraint

$$R_{\text{fair}}^2(\alpha, \beta) = \frac{\text{Var}[\mathbf{S}\alpha]}{\text{Var}[\mathbf{S}\alpha + \mathbf{X}^\perp\beta]} = \frac{\alpha^\top \text{Var}[\mathbf{S}]\alpha}{\alpha^\top \text{Var}[\mathbf{S}]\alpha + \beta^\top \text{Var}[\mathbf{X}^\perp]\beta}$$

- › Then solve

$$\min_{\alpha, \beta} \left\{ \mathbb{E}[\|\mathbf{y} - \mathbf{S}\alpha - \mathbf{X}^\perp\beta\|^2] \right\} \text{ s.t. } R_{\text{fair}}^2(\alpha, \beta) \leq r^2 (\in \mathbb{R}_+).$$

## Pre-Processing

- An alternative was considered in [Komiyama and Shimao \(2017\)](#), with a Ridge penalty

$$\min_{\alpha, \beta} \left\{ \mathbb{E}[\|\mathbf{y} - \mathbf{S}\alpha - \mathbf{X}^\perp\beta\|_{\ell_2}^2] + \lambda\|\alpha\|_{\ell_2}^2 \right\}$$

- The penalty is on  $\alpha$  only because (by construction) there is no discriminating information in  $\mathbf{X}^\perp$ . There is a closed form solution

$$\begin{pmatrix} (\mathbf{S}^\top \mathbf{S} + \lambda \mathbb{I})^{-1} \mathbf{S}^\top \mathbf{y} \\ (\mathbf{X}^{\perp\top} \mathbf{X}^\perp)^{-1} \mathbf{X}^\perp \mathbf{y} \end{pmatrix}$$

# In-Processing

- In a linear regression problem,  $\mathbf{y} = \mathbf{X}\beta + \epsilon$ . Zafar et al. (2017) suggested

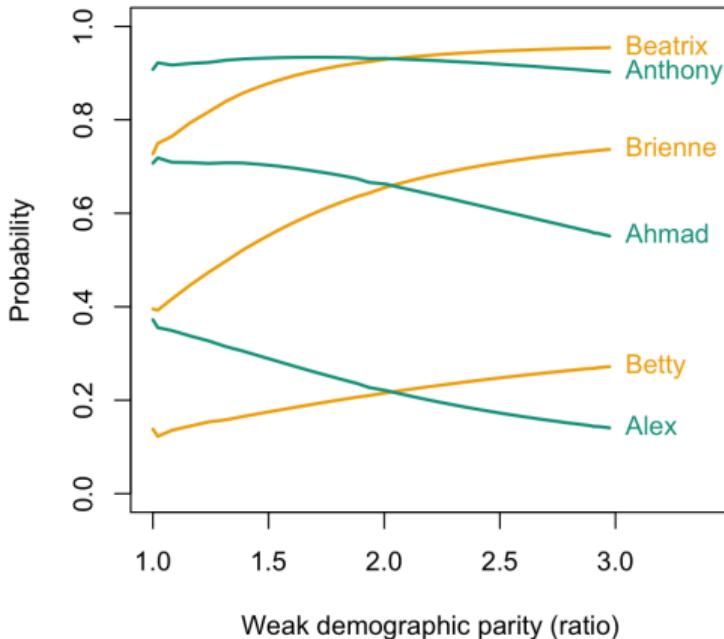
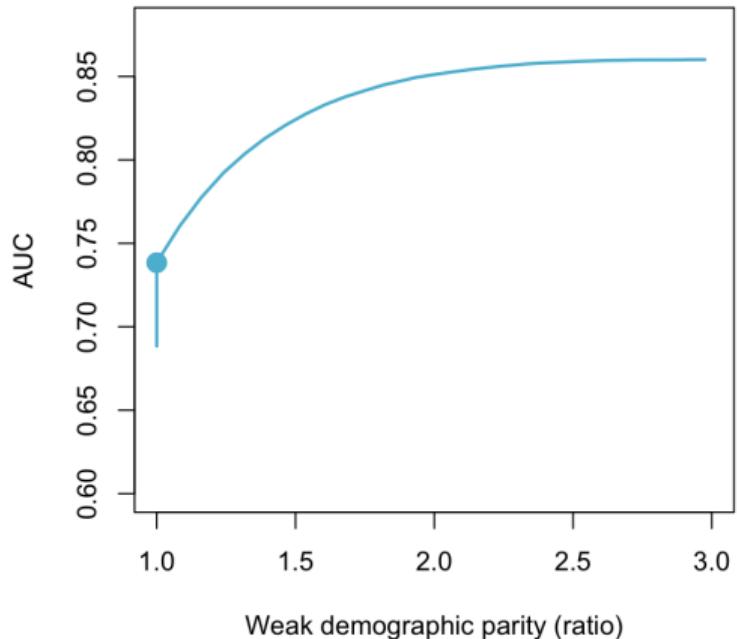
$$\hat{\beta}^* = \min_{\beta} \left\{ \mathbb{E}[\|\mathbf{y} - \mathbf{X}\beta\|^2] \right\} \text{ s.t. } |\text{Cov}[\mathbf{X}\beta, S]| \leq c \ (\in \mathbb{R}_+).$$

	$\hat{m}(\mathbf{x}, s)$ , aware					$\hat{m}(\mathbf{x})$ , unaware			
	← less fair		more fair →			← less fair		more fair →	
$\hat{\beta}_0$ (Intercept)	-2.55	-2.29	-1.97	-1.51	-1.03	-2.14	-1.98	-1.78	-1.63
$\hat{\beta}_1 (x_1)$	0.88	0.88	0.85	0.77	0.62	1.01	0.84	0.57	0.26
$\hat{\beta}_2 (x_2)$	0.37	0.37	0.35	0.32	0.25	0.37	0.35	0.31	0.24
$\hat{\beta}_3 (x_3)$	0.02	0.02	0.02	0.02	0.03	0.15	0.02	-0.15	-0.29
$\hat{\beta}_B (1_B)$	0.82	0.44	-0.03	-0.70	-1.31	-	-	-	-

# In-Processing

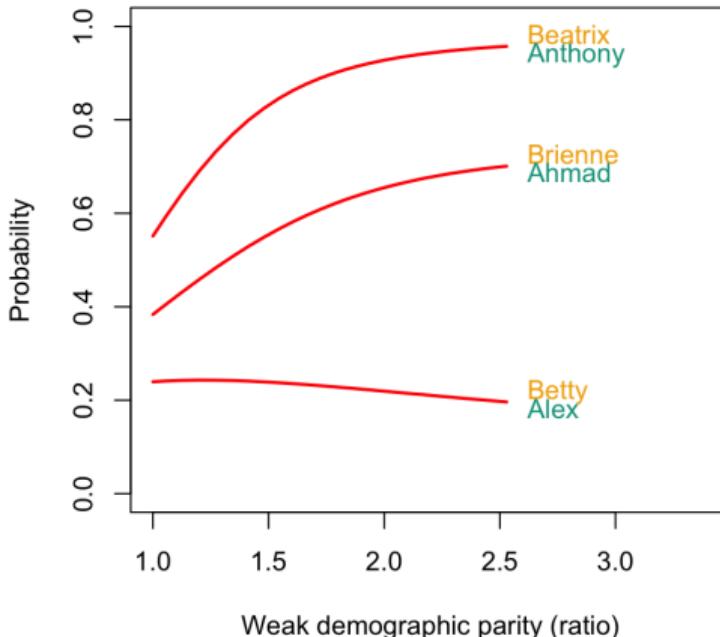
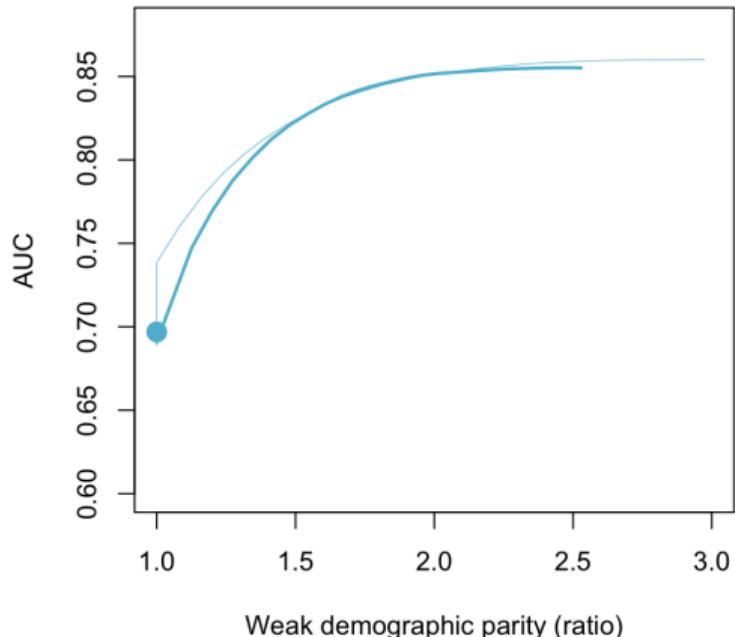
	$\hat{m}(x, s)$ , aware					$\hat{m}(x)$ , unaware			
	← less fair		more fair →			← less fair		more fair →	
Betty	0.27	0.25	0.22	0.17	0.14	0.20	0.22	0.24	0.24
Brienne	0.74	0.71	0.66	0.54	0.40	0.70	0.66	0.55	0.38
Beatrix	0.95	0.95	0.93	0.87	0.73	0.96	0.93	0.82	0.55
Alex	0.14	0.17	0.22	0.29	0.37	0.20	0.22	0.24	0.24
Ahmad	0.55	0.61	0.66	0.70	0.71	0.70	0.66	0.55	0.38
Anthony	0.90	0.92	0.93	0.93	0.91	0.96	0.93	0.82	0.55
$\mathbb{E}[\hat{m}(x_i, s_i)   S = A]$	0.23	0.26	0.31	0.36	0.42	0.25	0.30	0.37	0.41
$\mathbb{E}[\hat{m}(x_i, s_i)   S = B]$	0.67	0.65	0.61	0.53	0.42	0.64	0.61	0.54	0.41
(ratio)	$\times 2.97$	$\times 2.49$	$\times 2.01$	$\times 1.46$	$\times 1.00$	$\times 2.53$	$\times 2.02$	$\times 1.48$	$\times 1.00$
AUC	0.86	0.86	0.85	0.82	0.74	0.86	0.85	0.82	0.70

# In-Processing



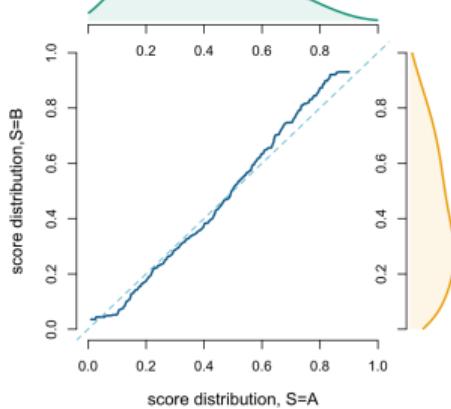
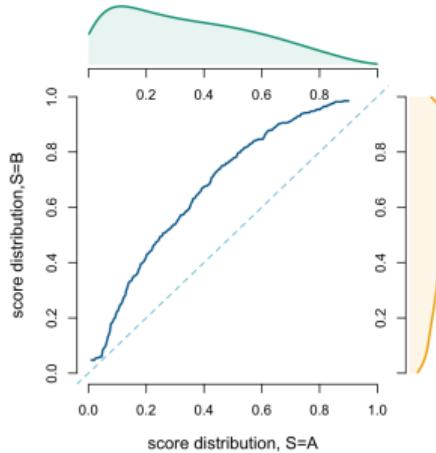
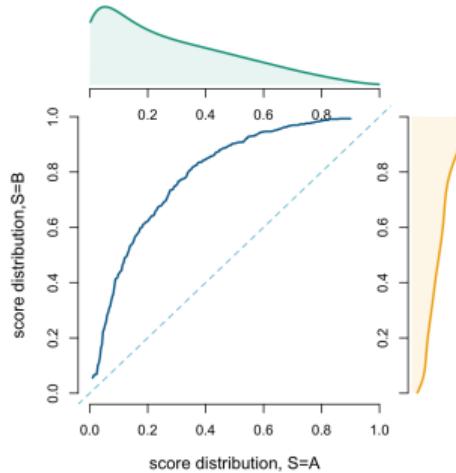
AUC of  $\hat{m}_{\beta_\lambda}$  and evolution of  $\hat{m}_{\beta_\lambda}(x_i, s_i)$  (with a logistic regression)

# In-Processing



AUC of  $\hat{m}_{\beta_\lambda}$  and evolution of  $\hat{m}_{\beta_\lambda}(x_i)$  (with a logistic regression)

# In-Processing



Optimal transport between distributions of  $\hat{m}_{\beta_\lambda}(\mathbf{x}_i, s_i)$ 's from individuals in group **A** and in **B**, for different values of  $\lambda$  (low value on the left-hand side and high value on the right-hand side), associated with a demographic parity penalty criteria

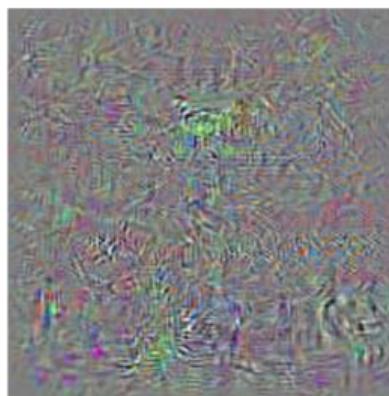
## In-Processing

- Adversarial learning has to do with robustness of learning algorithm, Szegedy et al. (2013) (“*are neural network stables?*”).
- “*Adversarial examples are inputs to machine learning models that an attacker has intentionally designed to cause the model to make a mistake*”, Bengio et al. (2017)



Schoolbus

+



Perturbation

=



Ostrich

## In-Processing

- › Adversarial learning deals with the problem that the distributions we obtain IRL are not the ones we train the model on... and we try to quantify what can go wrong
- › Popular in pictures (what happens if we rotate an object, add glasses to people, etc). Brittleness of ML algorithms...
- › Problem of data pollution (add outliers) and problems of adversarial examples.
- › Machine learning perspective

$$\min_{\theta} \{ \mathbb{E}_{(\mathbf{X}, Y) \sim \mathbb{P}} [\ell(m_{\theta}(\mathbf{X}), Y)] \}$$

- › Adversarial perspective

$$\max_{\varepsilon \in \mathcal{E}} \{ \mathbb{E}_{(\mathbf{X}, Y) \sim \mathbb{P}} [\ell(m_{\theta}(\mathbf{X} + \varepsilon), Y)] \}$$

leads to robust learning...

# In-Processing

$$\min_{\theta} \left\{ \max_{\varepsilon \in \mathcal{E}} \left\{ \mathbb{E}_{(\mathbf{X}, Y) \sim \mathbb{P}} [\ell(m_{\theta}(\mathbf{X} + \varepsilon), Y)] \right\} \right\}$$

↑  
training a robust classifier  
↓  
creating an adversarial example

- Approaches based on **robust optimization**, Ben-Tal et al. (2009), e.g., Danskin's Theorem, Danskin (1967),

$$\nabla_{\theta} \max_{\varepsilon \in \mathcal{E}} \{\ell(m_{\theta}(\mathbf{X} + \varepsilon), Y)\} = \nabla_{\theta} \ell(m_{\theta}(\mathbf{X} + \varepsilon^*), Y)$$

where  $\varepsilon^* = \operatorname{argmax}_{\varepsilon \in \mathcal{E}} \{\ell(m_{\theta}(\mathbf{X} + \varepsilon), Y)\}$ .

- Recall the **minimax** theorem from von Neumann (1928)

freakonometrics

freakonometrics.hypotheses.org – Arthur Charpentier, 2024 (UQAM Course)

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## Proposition 8.2: Nash equilibrium and Minimax

Let  $A$  be some  $m \times n$  real-valued matrix, there is a Nash equilibrium  $(\mathbf{x}_*, \mathbf{y}_*)$  associated with  $A$  if

$$\mathbf{y}_*^\top A \mathbf{x}_* = \max_{\mathbf{x} \in \mathcal{S}_m} \min_{\mathbf{y} \in \mathcal{S}_n} \{\mathbf{y}^\top A \mathbf{x}\} = \min_{\mathbf{y} \in \mathcal{S}_n} \max_{\mathbf{x} \in \mathcal{S}_m} \{\mathbf{y}^\top A \mathbf{x}\}.$$

## In-Processing

- Consider a **Minimax games**: given that the discriminator will try to do the best job it can, the generator is set to make the discriminator as wrong as possible

$$\min_{\theta_g} \max_{\theta_d} \{ \mathbb{E}_{\mathbf{X} \sim \mathbb{P}} [\log(m_{\theta_d}(\mathbf{x}))] + \mathbb{E}_{\mathbf{Z} \sim \mathbb{Q}} [\log(1 - m_{\theta_d}(G_{\theta_d}(\mathbf{z})))] \}$$

where  $\mathbf{X} \sim \mathbb{P}$  denotes data sampled from the training data, while  $\mathbf{Z} \sim \mathbb{Q}$  are sampled by the opponent

- See [Wadsworth et al. \(2018\)](#), [Xu et al. \(2021\)](#), [Lima et al. \(2022\)](#) for achieving fairness through adversarial learning

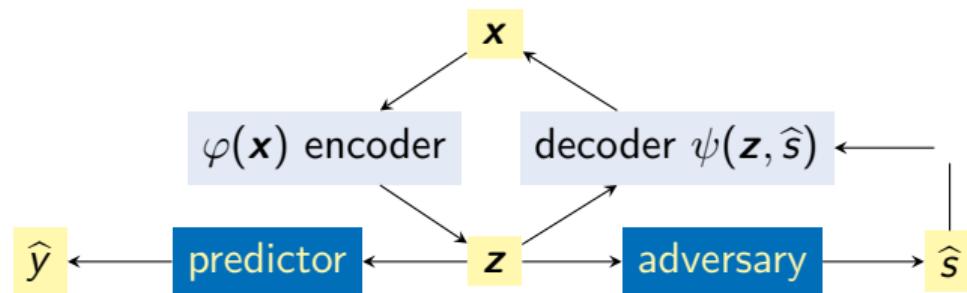
## In-Processing

- › FairGAN, Xu et al. (2018)

Pre-processing approach actually, with demographic parity (DP)

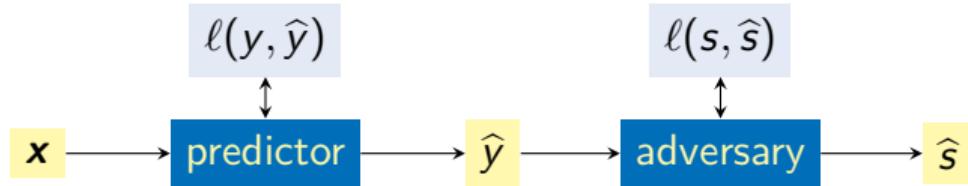
Other algorithms are in-processing approaches, with demographic parity (DP) and equalized odds (EO)

- › Learning adversarially fair and transferable representations, Madras et al. (2018)



- › Adversarially learning fair representations, Beutel et al. (2017)
- › Fair Adversarial Debiasing Approach, Zhang et al. (2018)

# In-Processing



Following [Zhang et al. \(2018\)](#)

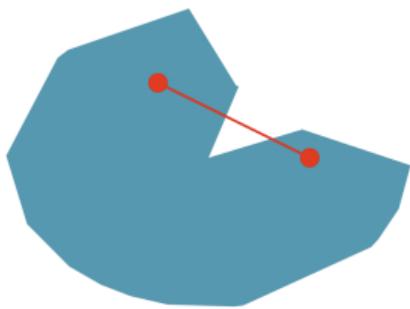
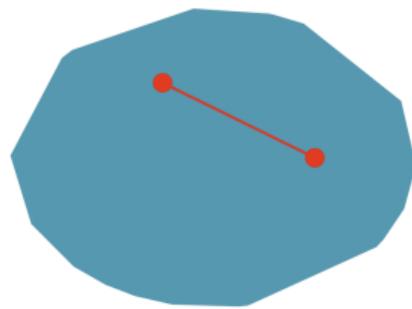
- › the predictor predicts  $y$  given  $x$ ,
- › the adversary tries to predict  $s$  based on the output of the predictor
- › the predictor targets to increase its prediction accuracy
- › and tries to increase the adversary's loss

## Barycenter

Several approaches can be considered to define means, averages, centroids, barycenters (etc.), as discussed in Fréchet (1948) and Grove and Karcher (1973),

- ▶ convex properties (from Möbius (1827) and Rockafellar (1970))
- ▶ axiomatization (from Nagumo (1930), Kolmogorov (1930) and Aczél (1948))
- ▶ optimization (from Hey (1814), Nathan (1952) and Agueh and Carlier (2011))

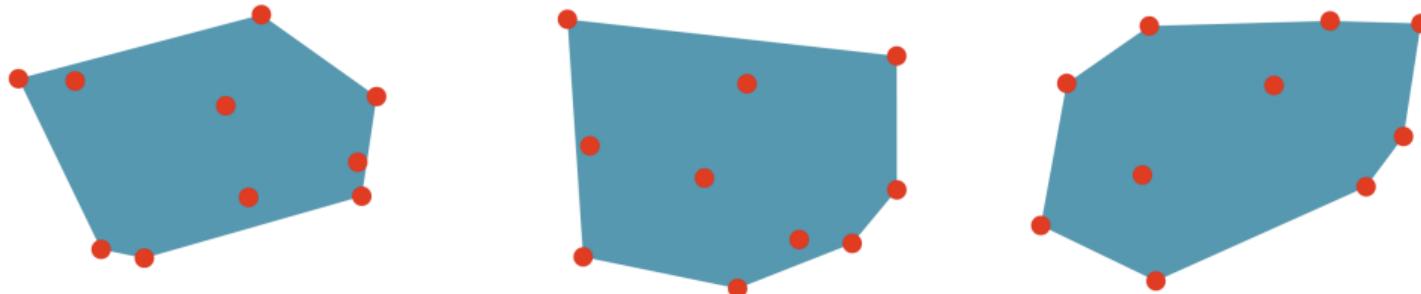
$C \subset \mathbb{R}^n$  is convex if  $\mathbf{x}, \mathbf{y} \in C \implies t\mathbf{x} + (1 - t)\mathbf{y} \in C$  for all  $t \in [0, 1]$



## Barycenter

Let  $\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathbb{R}^n$ , then a convex combination is any linear combination  $\omega_1 \mathbf{x}_1 + \dots + \omega_k \mathbf{x}_k$  with  $(\omega_1, \dots, \omega_k) \in \mathcal{S}_k \subset \mathbb{R}_+$ .

The convex hull of a set  $C$  is the set of all convex combinations of elements of  $C$ .



The geometric centroid of a convex object always lies in the object.

## Barycenter

Define the barycenter for two points, with equal weights as a function  $M : E \times E \rightarrow E$

- ▶ Reflexivity:  $M(\mathbf{x}, \mathbf{x}) = \mathbf{x}$ ,
- ▶ Symmetry:  $M(\mathbf{x}_1, \mathbf{x}_2) = M(\mathbf{x}_2, \mathbf{x}_1)$ ,
- ▶ Continuity:  $M(\cdot, \cdot)$  is continuous,
- ▶ Bisymmetry:  $M(M(\mathbf{x}_{11}, \mathbf{x}_{12}), M(\mathbf{x}_{21}, \mathbf{x}_{22})) = M(M(\mathbf{x}_{11}, \mathbf{x}_{21}), M(\mathbf{x}_{12}, \mathbf{x}_{22}))$

Then (see [Aczél \(1948\)](#)), there is  $f$  such that

$$M(\mathbf{x}_1, \mathbf{x}_2) = f^{-1} \left( \frac{1}{2} f(\mathbf{x}_1) + \frac{1}{2} f(\mathbf{x}_2) \right).$$

If  $E \subset \mathbb{R}^k$ , consider means on each coordinate axis independently.

➤ A natural extension is

$$B_f(\mathbf{x}, \boldsymbol{\omega}) = f^{-1} \left( \sum_{i=1}^n \omega_i f(x_i) \right).$$

## Barycenter

- For the optimisation approach, given a distance  $d$  on  $E$ , set

$$B_d(\mathbf{x}, \omega) = \operatorname{argmin}_{z \in E} \left\{ \sum_{i=1}^n \omega_i d(x_i, z) \right\}$$

- Consider some points  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\}$  in a metric space  $\mathbb{R}^2$
- The **mean** is

$$\bar{\mathbf{x}} = \frac{\mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_k}{k} = \frac{1}{k} \sum_{i=1}^k \mathbf{x}_i,$$

or equivalently

$$\bar{\mathbf{x}} = \operatorname{argmin}_{\mathbf{x}} \left\{ \frac{1}{k} \sum_{i=1}^k \|\mathbf{x} - \mathbf{x}_i\|_{\ell_2}^2 \right\}.$$

- But they can be defined using any distance/divergence/discrepancy

## Barycenter

- › Instead of points  $\{x_1, x_2, \dots, x_k\}$  in the metric space  $\mathbb{R}^2$ , we can consider some measures  $\{\mathbb{P}_1, \mathbb{P}_2, \dots, \mathbb{P}_k\}$ .
- › The **Euclidean mean** is

$$\overline{\mathbb{Q}} = \operatorname{argmin}_{\mathbb{Q}} \left\{ \frac{1}{k} \sum_{i=1}^k \Delta^2(\mathbb{Q}, \mathbb{P}_i) \right\},$$

where  $\Delta^2(\mathbb{Q}, \mathbb{P}_i) = \int_{\mathbb{R}^2} (d\mathbb{Q} - d\mathbb{P}_i)^2$ .

But any discrepancy function can be considered

- › One can consider Wasserstein discrepancy

## Barycenter

**Definition 8.2: Wasserstein  $W_2$  Barycenter, Aguech and Carlier (2011)**

$$\overline{\mathbb{Q}} = \operatorname{argmin}_{\mathbb{Q}} \left\{ \sum_{i=1}^k \omega_i W_2(\mathbb{Q}, \mathbb{P}_i)^2 \right\},$$

- › This can be seen as a multi-marginal optimal transport problem.
- › Recall that the “*push-forward*” measure is

$$\mathbb{P}_1(\mathcal{A}) = \mathcal{T}_{\#}\mathbb{P}_0(\mathcal{A}) = \mathbb{P}_0(\mathcal{T}^{-1}(\mathcal{A})), \quad \forall \mathcal{A} \subset \mathbb{R}.$$

An optimal transport  $\mathcal{T}^*$  (in Brenier's sense, from [Brenier \(1991\)](#), see [Villani \(2009\)](#) or [Galichon \(2016\)](#)) from  $\mathbb{P}_0$  towards  $\mathbb{P}_1$  will be solution of

$$\mathcal{T}^* \in \operatorname{arginf}_{\mathcal{T}: \mathcal{T}_{\#}\mathbb{P}_0 = \mathbb{P}_1} \left\{ \int_{\mathbb{R}^k} \ell(\mathbf{x}, \mathcal{T}(\mathbf{x})) d\mathbb{P}_0(\mathbf{x}) \right\},$$

## Barycenter

and for univariate distributions, the optimal transport  $\mathcal{T}^*$  is the monotone transformation.

$$\mathcal{T}^* : x_0 \mapsto x_1 = F_1^{-1} \circ F_0(x_0).$$

- Given a reference measure, say  $\mathbb{P}_1$ , it is possible to write the barycenter as the "*average push-forward*" transformation of  $\mathbb{P}_1$ : if  $\mathbb{P}_i = \mathcal{T}_\#^{1 \rightarrow i} \mathbb{P}_1$  (with the convention that  $\mathcal{T}_\#^{1 \rightarrow 1}$  is the identity),

**Proposition 8.3: Wasserstein  $W_2$  Barycenter,**

$$\overline{\mathbb{Q}} = \left( \sum_{i=1}^k \omega_i \mathcal{T}^{1 \rightarrow i} \right)_\# \mathbb{P}_1.$$

## Proposition 8.4: Wasserstein $W_2$ Barycenter,

$$\overline{\mathbb{Q}} = \left( \sum_{i=1}^k \omega_i \mathcal{T}^{1 \rightarrow i} \right)_{\#} \mathbb{P}_1.$$

- Computation of barycenters can be computationnaly difficult, [Altschuler and Boix-Adsera \(2021\)](#)
- For univariate distributions, there is a simple expression,  $\mathcal{T}^{1 \rightarrow i}$  is simply a rearrangement, defined as  $\mathcal{T}^{1 \rightarrow i} = F_i^{-1} \circ F_1$ , where  $F_i(t) = \mathbb{P}_i((-\infty, t])$  and  $F_i^{-1}$  is its generalized inverse

## Barycenter

### Proposition 8.5: Wasserstein $W_2$ Barycenter, univariate distributions

....  $\mathcal{T}^{1 \rightarrow i}$  is simply a rearrangement, defined as  $\mathcal{T}^{1 \rightarrow i} = F_i^{-1} \circ F_1$ , where  $F_i(t) = \mathbb{P}_i((-\infty, t])$  ...

$$\overline{\mathbb{Q}} = \left( \sum_{i=1}^n k\omega_i \mathcal{T}^{1 \rightarrow i} \right)_\# \mathbb{P}_1.$$

### Proposition 8.6: Wasserstein $W_2$ Barycenter, univariate distributions

Given two scores  $m(\mathbf{x}, s = \textcolor{teal}{A})$  and  $m(\mathbf{x}, s = \textcolor{blue}{B})$ , the “fair barycenter score” is

$$\begin{cases} m^*(\mathbf{x}, s = \textcolor{teal}{A}) = \mathbb{P}[S = \textcolor{teal}{A}] \cdot m(\mathbf{x}, s = \textcolor{teal}{A}) + \mathbb{P}[S = \textcolor{blue}{B}] \cdot F_{\textcolor{blue}{B}}^{-1} \circ F_{\textcolor{teal}{A}}(m(\mathbf{x}, s = \textcolor{teal}{A})) \\ m^*(\mathbf{x}, s = \textcolor{blue}{B}) = \mathbb{P}[S = \textcolor{teal}{A}] \cdot F_{\textcolor{teal}{A}}^{-1} \circ F_{\textcolor{blue}{B}}(m(\mathbf{x}, s = \textcolor{blue}{B})) + \mathbb{P}[S = \textcolor{teal}{B}] \cdot m(\mathbf{x}, s = \textcolor{blue}{B}). \end{cases}$$

## Barycenter

- › that is generally numerically intractable (computing one subgradient requires solving  $k$  optimal transports)
- › In the discrete case, if we consider a fixed grid (so that  $C$  can be computed once only)

$$\min_{\mathbf{a}} \left\{ \sum_{i=1}^k \min_{P_i \in U_{\mathbf{a}, \mathbf{b}_i}} \left\{ \langle P_i, C \rangle \right\} \right\},$$

- › We can write this as a large linear program
- $$\min_{\mathbf{Q}} \left\{ \min_{P_1, \dots, P_k, \mathbf{a}} \sum_{i=1}^k \left\{ \langle P_i, C \rangle \right\} \right\}, \text{ where } \begin{cases} P_1^\top \mathbf{1}_n = \mathbf{b}_1 \\ \vdots \\ P_k^\top \mathbf{1}_n = \mathbf{b}_k \\ P_1 \mathbf{1}_n = \dots = P_k \mathbf{1}_n = \mathbf{a} \end{cases}$$

- › In the Gaussian case, some linear algebra might help
- › A variance matrix  $\Sigma$  is a positive-semidefinite ( $\mathbf{a}^\top \Sigma \mathbf{a} \geq 0$  for all  $\mathbf{a} \in \mathbb{R}^n$ ) symmetric ( $\Sigma^\top = \Sigma$ ) matrix.

## Definition 8.3: Matrix Exponential

Consider some  $n \times n$  matrix  $\mathbf{X}$

$$\exp(\mathbf{X}) = \sum_{k=0}^{\infty} \frac{1}{k!} \mathbf{X}^k = \lim_{k \rightarrow \infty} \left( \mathbb{I} + \frac{1}{k} \mathbf{X} \right)^k$$

- › The matrix exponential of a real symmetric matrix is positive definite.

## Definition 8.4: Matrix Logarithm

Consider some  $n \times n$  matrix  $\mathbf{X}$  such that  $\|\mathbf{X} - \mathbb{I}\| < 1$

$$\log(\mathbf{X}) = \sum_{k=0}^{\infty} \frac{(-1)^{k+1}}{k} (\mathbf{X} - \mathbb{I})^k$$

- › As expected,  $\exp(\log(\mathbf{X})) = \mathbf{X}$ . In R, use `expm::expm` and `expm::logm`.
- › See Theorem 7.2.6 in [Horn and Johnson \(2012\)](#)

## Definition 8.5: Square root of a symmetric matrix

Let  $\mathbf{X}$  be a real positive semidefinite matrix, then there is exactly one positive semidefinite matrix  $\mathbf{Z}$  such that  $\mathbf{X} = \mathbf{Z}\mathbf{Z} = \mathbf{Z}^2$ ,

$$\mathbf{Z} = \mathbf{X}^{\frac{1}{2}} = \sum_{n=0}^{\infty} (-1)^n \binom{\frac{1}{2}}{n} (\mathbb{I} - \mathbf{X})^n.$$

- › From power series  $(1 - z)^{\frac{1}{2}} = \sum_{n=0}^{\infty} (-1)^n \binom{1/2}{n} z^n$ , if  $z = \mathbb{I} - \mathbf{X}$ .
- › In R, use `expm::sqrtm`.

$$\begin{pmatrix} 1 & 1.2 \\ 1.2 & 2 \end{pmatrix}^{\frac{1}{2}} = \begin{pmatrix} 0.8244771 & 0.5658953 \\ 0.5658953 & 1.2960565 \end{pmatrix}$$

## Barycenter

- › If  $\mathbb{P}_i$  is a Gaussian distribution  $\mathcal{N}(\mu_i, \Sigma_i)$ ,  $\bar{\mathbb{Q}} \sim \mathcal{N}(\mu, \Sigma)$  where  $\Sigma$  is some variance matrix (positive definite)

$$\mu = \sum_{i=1}^k \omega_i \mu_i \text{ and } \Sigma \text{ satisfies } \Sigma = \sum_{i=1}^k \omega_i (\Sigma^{1/2} \Sigma_i \Sigma^{1/2})^{1/2}$$

```
1 > library(T4transport)
2 > par_mean = rbind(mu1, mu2)
3 > par_vars = array(0,c(2,2,2))
4 > par_vars[,,1] = S1; par_vars[,,2] = S2
5 > gmean = gaussbarypd(par_mean, par_vars)
```

### Definition 8.6: Generalized Inverse, Rao and Mitra (1972)

Consider some  $m \times n$  matrix  $\mathbf{X}$ . Matrix  $n \times m$   $\mathbf{Y}$  is said to be a generalized inverse of  $\mathbf{X}$  if  $\mathbf{XYX} = \mathbf{X}$ . And  $\mathbf{Y}$  is denoted  $\mathbf{Y}^-$ .

# Barycenter

- From Shurbet et al. (1974), we can solve “quadratic matrix equations”

## Theorem 8.1: Matrix Equation $\mathbf{XAX} = \mathbf{B}$

- Equation  $\mathbf{XAX} = \mathbf{B}$  has a solution if and only if

$$\begin{cases} (\mathbf{AB})^{1/2} \text{ exists,} \\ \mathbf{AA}^{-1}(\mathbf{AB})^{\frac{1}{2}} = (\mathbf{AB})^{\frac{1}{2}}, \\ \mathbf{B}(\mathbf{AB})^{\frac{1}{2}} - (\mathbf{AB})^{\frac{1}{2}} = \mathbf{B}. \end{cases}$$

- If  $\mathbf{A}$  and  $\mathbf{B}$  are positive definite, the unique positive definite solution of  $\mathbf{XAX} = \mathbf{B}$  is

$$\mathbf{X} = \mathbf{A}^{-\frac{1}{2}} \left( \mathbf{A}^{\frac{1}{2}} \mathbf{B} \mathbf{A}^{\frac{1}{2}} \right)^{\frac{1}{2}} \mathbf{A}^{-\frac{1}{2}}.$$

## Theorem 8.2: Variance $\Sigma$

If  $k = 2$ ,  $\Sigma$  satisfies

$$\Sigma = \omega_1 (\Sigma^{1/2} \Sigma_1 \Sigma^{1/2})^{1/2} + \omega_2 (\Sigma^{1/2} \Sigma_2 \Sigma^{1/2})^{1/2}$$

and the explicit expression is

$$\Sigma = \omega_1^2 \Sigma_1 + \omega_2^2 \Sigma_2 + \omega_1 \omega_2 \left( \Sigma_1^{\frac{1}{2}} (\Sigma_1^{\frac{1}{2}} \Sigma_2 \Sigma_1^{\frac{1}{2}})^{\frac{1}{2}} \Sigma_1^{-\frac{1}{2}} + \Sigma_1^{-\frac{1}{2}} \Sigma_2 \Sigma_1^{\frac{1}{2}} )^{\frac{1}{2}} \Sigma_1^{\frac{1}{2}} \right)$$

## Proposition 8.7: Variance $\Sigma$

$\sum_{i=1}^k \omega_i \Sigma_i - \Sigma$  is a positive matrix.

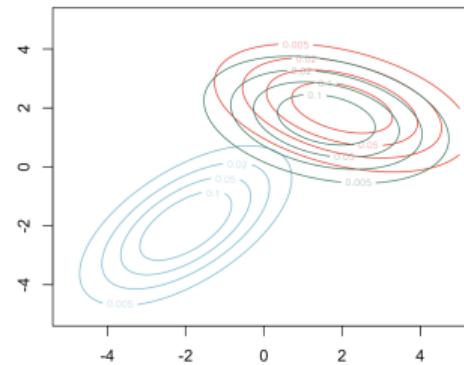
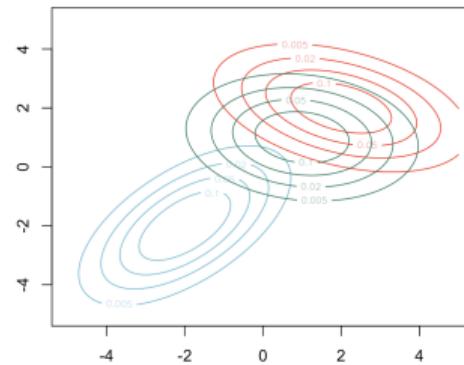
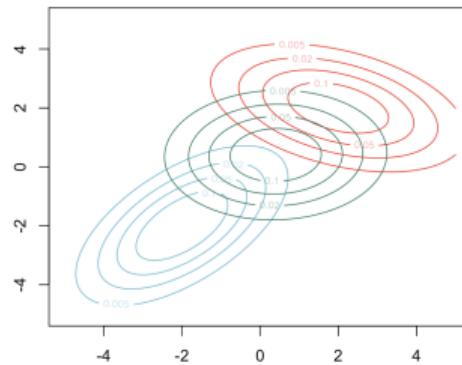
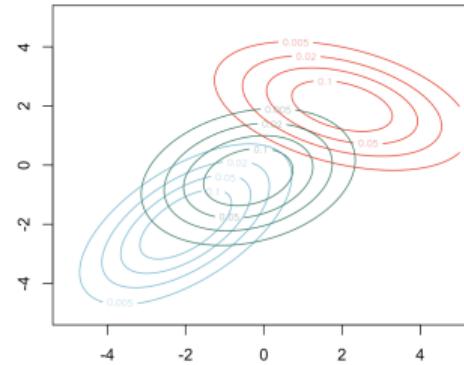
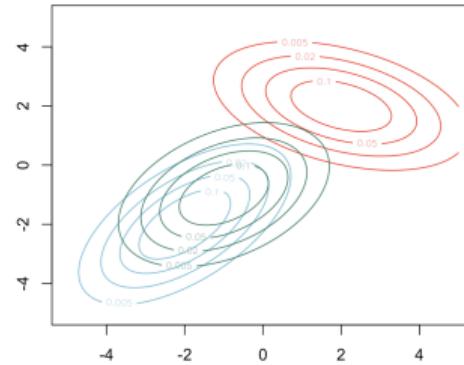
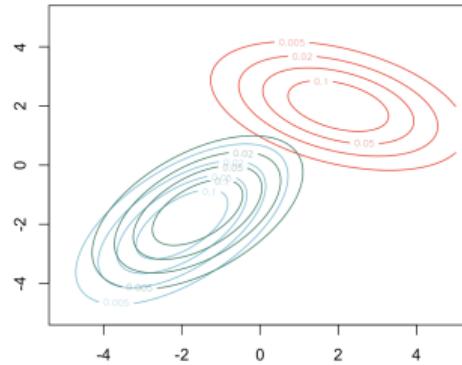
## Proposition 8.8: Variance $\Sigma$

$$\text{If } \boldsymbol{\Sigma}_i = \mathbf{P} \boldsymbol{\Delta}_i \mathbf{P}^\top, \text{ then } \boldsymbol{\Sigma} = \mathbf{P} \left( \sum_{i=1}^k \omega_i \boldsymbol{\Delta}_i^{\frac{1}{2}} \right)^2 \mathbf{P}^\top$$

Consider two Gaussian distributions,  $\mathcal{N}(\boldsymbol{\mu}_A, \boldsymbol{\Sigma}_A)$  and  $\mathcal{N}(\boldsymbol{\mu}_B, \boldsymbol{\Sigma}_B)$ , and weights  $\omega_A = t$  and  $\omega_B = 1 - t$ , with  $t \in [0, 1]$ .

# Barycenter

➤ Barycenter of two bivariate Gaussian distribution ( $t = 0.1, 0.25, 0.4, 0.6, 0.75, 0.9$ )



## Computational Issues

- › Barycenters and  $k$ -coupling
- › To simplify, suppose that  $\omega_1 = \dots = \omega_k$ , the uniform barycenter  $\overline{\mathbb{Q}}$  of  $(\mathbb{P}_i)$  is any solution of

$$\inf_{\mathbb{Q}} \left\{ \sum_{i=1}^k W_2(\mathbb{P}_i, \mathbb{Q})^2 \right\}$$

- › It is related to the  $k$ -coupling problem, defined in [Rüschendorf and Uckelmann \(2002\)](#), inspired by [Knott and Smith \(1994\)](#), who reduced 3-coupling to 2-coupling

$$\sup \left\{ \mathbb{E} \left[ \left\| \sum_{i=1}^k X_i \right\|^2 \right]; \text{ where } X_i \sim \mathbb{P}_i, \forall i \right\} \text{ and then } Y^* \sim \mathbb{Q}^*$$

as discussed in [Agueh and Carlier \(2011\)](#), under continuity assumptions.

## Computational Issues

If  $\bar{X} = \frac{1}{k} \sum_{i=1}^k X_i$ , recall that for all  $Y$ ,

$$\sum_{i=1}^k \|X_i - Y\|^2 \geq \sum_{i=1}^k \|X_i - \bar{X}\|^2$$

and we can write, if  $Z \sim \mathbb{Q}$ ,

$$\sum_{i=1}^k W_2(\mathbb{P}_i, \mathbb{Q})^2 = \sum_{i=1}^k \|X_i - Y\|^2 \geq \sum_{i=1}^k \|X_i - \bar{X}\|^2 \geq \sum_{i=1}^k W_2(\mathbb{P}_i, \bar{\mathbb{Q}})^2$$

and

$$\inf_{\mathbb{Q}} \left\{ \sum_{i=1}^k W_2(\mathbb{P}_i, \mathbb{Q})^2 \right\} = \inf \left\{ \sum_{i=1}^k \|X_i - \bar{X}\|^2; \text{ where } X_i \sim \mathbb{P}_i, \forall i \right\}$$

and simple arguments yield to the fact that this corresponds to an optimal  $k$ -coupling.

## Computational Issues

- ›  $\mathbf{X} = (X_1, \dots, X_k)$  is an optimal  $k$ -coupling if and only if the distribution of  $\bar{X}$  is a barycenter of  $\mathbb{P}_i$ 's.
- › Following Puccetti (2017), observe that an equivalent representation of  $k$  coupling is

$$\sup \left\{ \mathbb{E}[\psi(X_1, \dots, X_k)] \right\} \text{ where } \psi(x_1, \dots, x_k) = \sum_{i=1}^k \langle x_i, \sum_{j \neq i} x_j \rangle.$$

that can be solved using an iterative swapping algorithm (ISA), as in Puccetti et al. (2020)

- › Oberman and Ruan (2015) suggested multi-assignment problem

$$\max \left\{ \frac{1}{n} \sum_{j=1}^n \psi(\mathbf{x}_{1:\sigma_1(i)}, \dots, \mathbf{x}_{k:\sigma_k(i)}) \right\} \text{ where } \sigma_1, \dots, \sigma_k \text{ are permutations of } \{1, 2, \dots, n\}.$$

- › Usually this problem is a lower bound to the  $k$ -coupling problem, but they are equivalent in dimension  $k = 2$ .

# Computational Issues

- › Barycenters based on histograms, Cuturi and Doucet (2014), computed in `bary14C` and `histbary14C`, in package `T4transport`
- › Barycenters based on histograms, Benamou et al. (2015), computed in `bary15C` and `histbary15C`, in package `T4transport`
- › We can also compute barycenters of pictures

freakonometrics

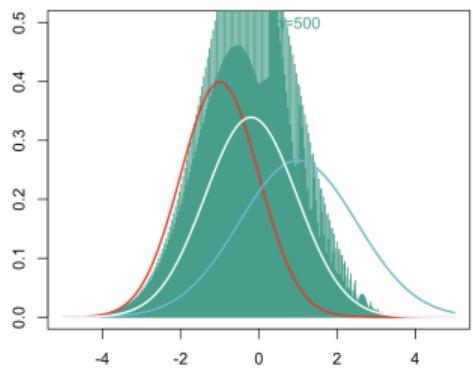
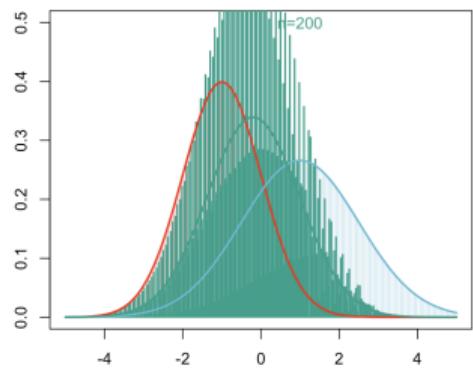
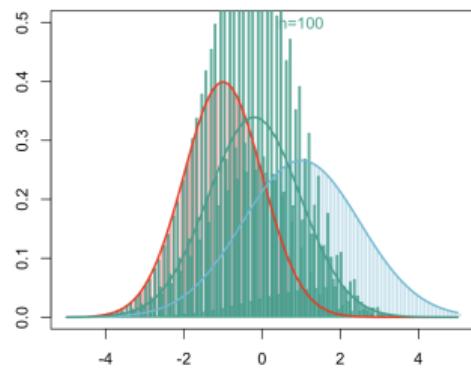
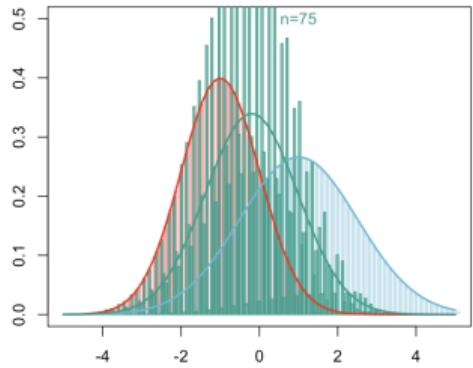
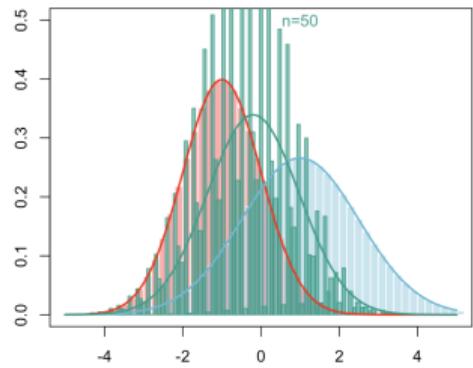
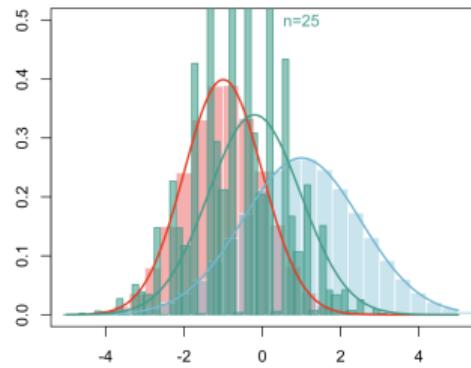
freakonometrics.hypotheses.org

– Arthur Charpentier, 2024 (UQAM Course)

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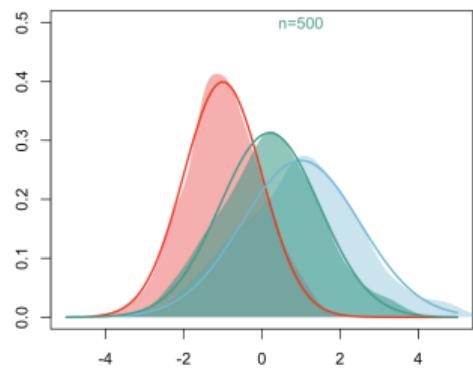
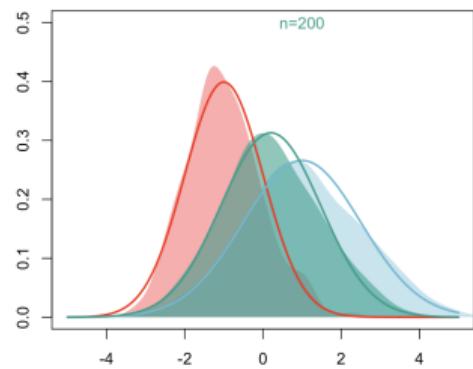
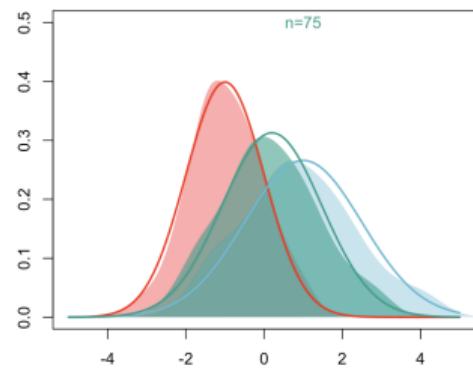
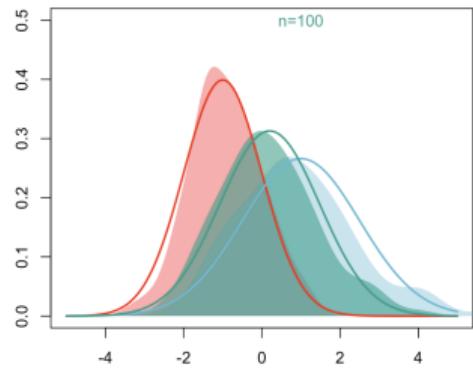
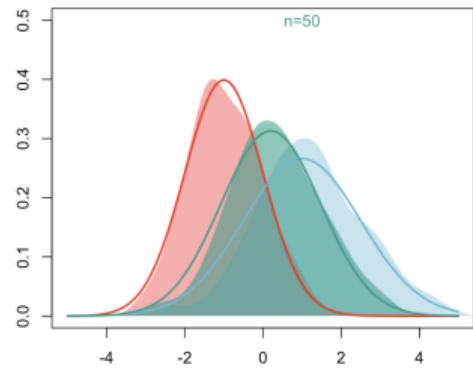
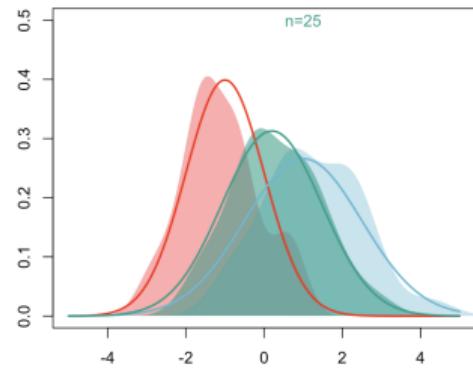
# Computational Issues

## › Numerical computation, Gaussian case



# Computational Issues

## › Numerical computation, Gaussian case (simulation and kernel density estimation)



## Barycenter of Several Pictures



## Barycenter of Several Pictures



## Barycenter of Several Pictures



- › A geodesic is a curve representing in some sense the shortest[a] path (arc) between two points in a surface, or more generally in a Riemannian manifold. It is the general extension of a segment.

## Definition 8.7: Constant Speed Geodesic

Consider some metric space,  $(E, d)$ . A constant speed geodesic between two points  $x_0, x_1 \in E$  is a continuous curve  $x : [0, 1] \rightarrow E$  such that for every  $s, t \in (0, 1)$ ,  $d(x_s, x_t) = |s - t|d(x_0, x_1)$ .

## Proposition 8.9

Consider  $\mu_0$  and  $\mu_1$  two measures on  $X \subset \mathbb{R}^k$ , compact and convex. Let  $\pi^* \in \Pi(\mu_0, \mu_1)$  be an optimal transport plan. Define

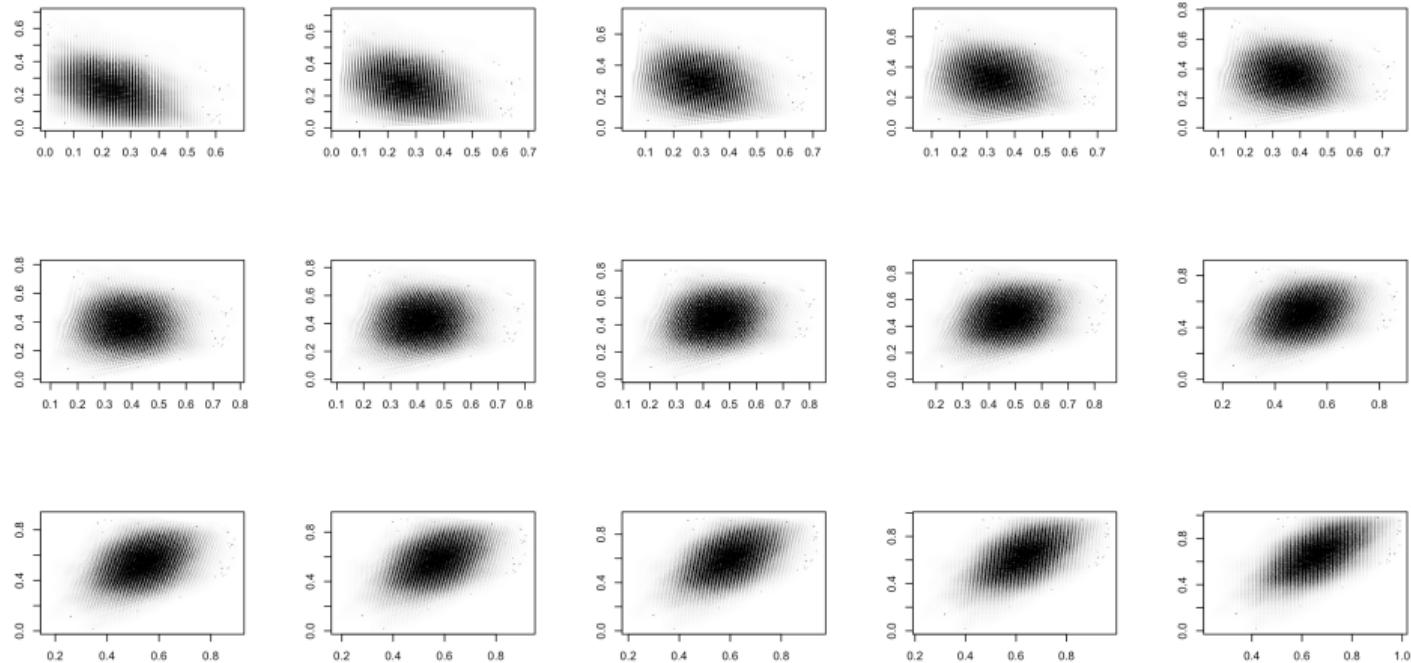
$$\mu_t = (\gamma_t)_\# \pi^*, \text{ where } \gamma_t(x, y) = (1 - t)x + ty, \quad t \in (0, 1).$$

$(\mu_t)$  is a constant speed geodesic between  $\mu_0$  and  $\mu_1$ .

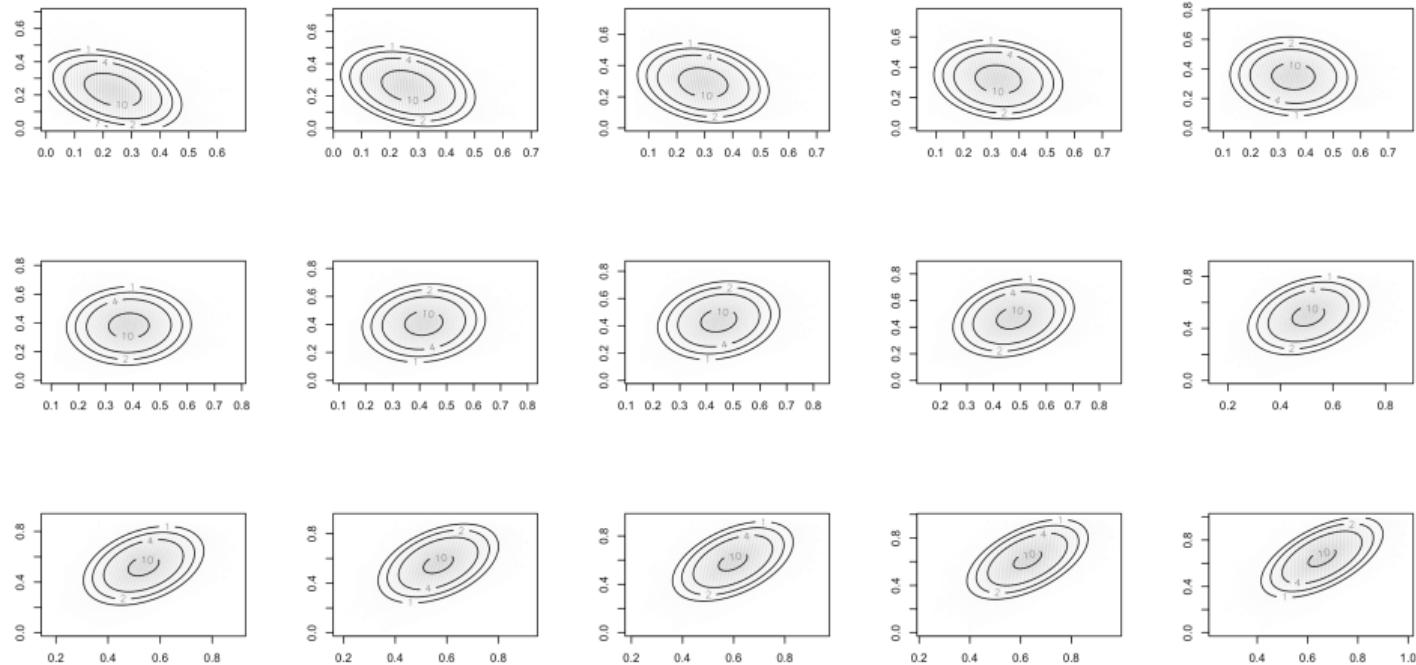
And if there exist an optimal transport map  $T^*$ ,

$$\mu_t = ((1 - t)\mathbf{I} + tT^*)_\# \mu_0, \text{ where } t \in (0, 1).$$

# Wasserstein Geodesic



# Wasserstein Geodesic

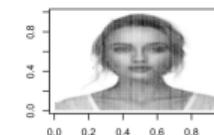
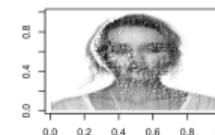
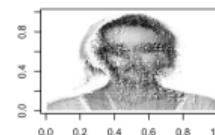
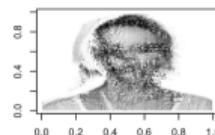
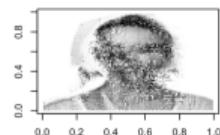
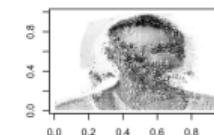
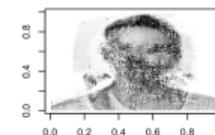
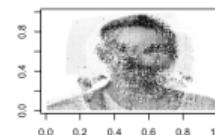
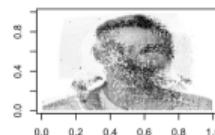
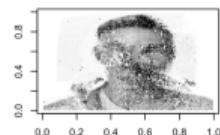
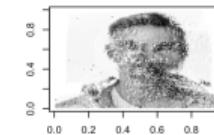
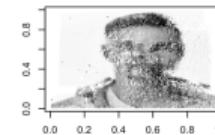
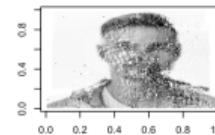
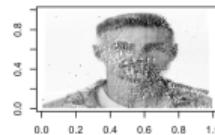
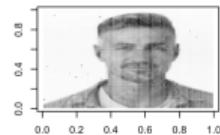


# Wasserstein Geodesic



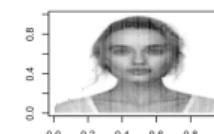
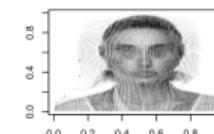
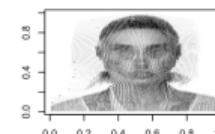
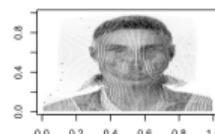
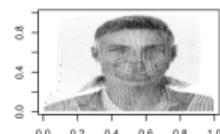
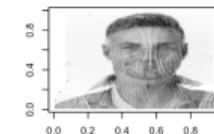
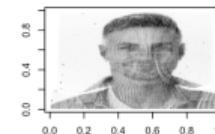
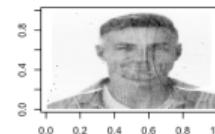
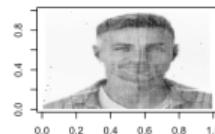
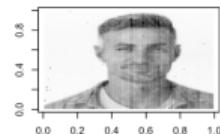
# Wasserstein Geodesic

with the  $\ell_1$  cost function



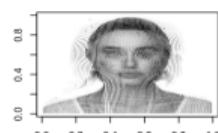
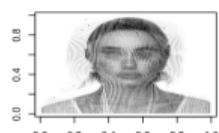
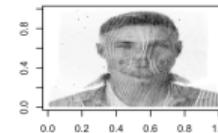
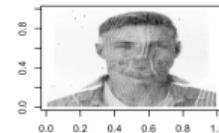
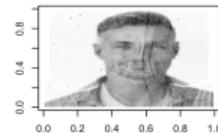
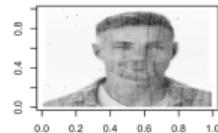
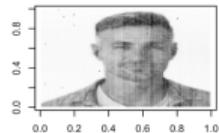
# Wasserstein Geodesic

with the  $\ell_2$  cost function

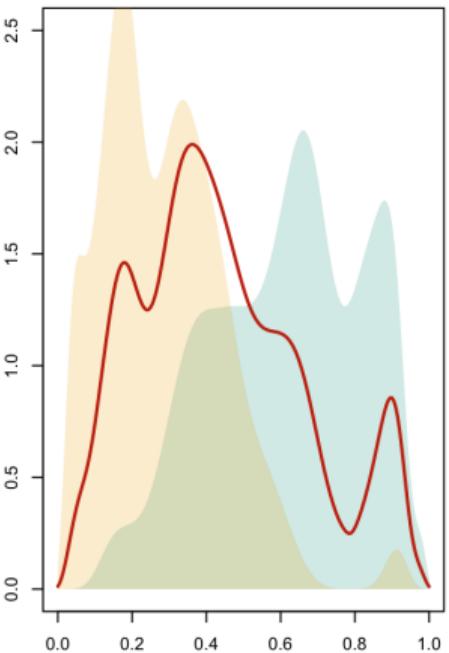
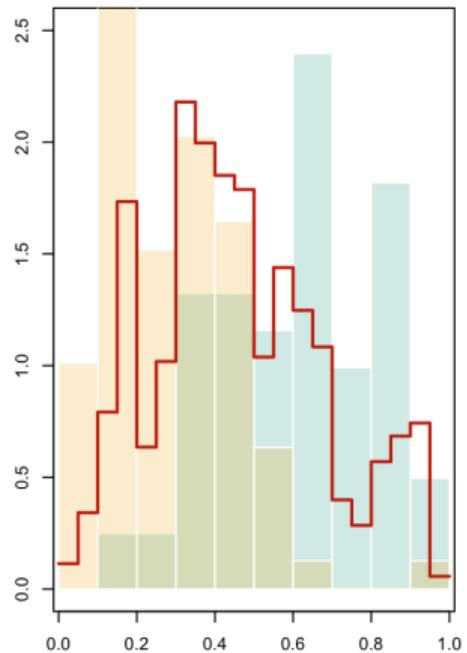
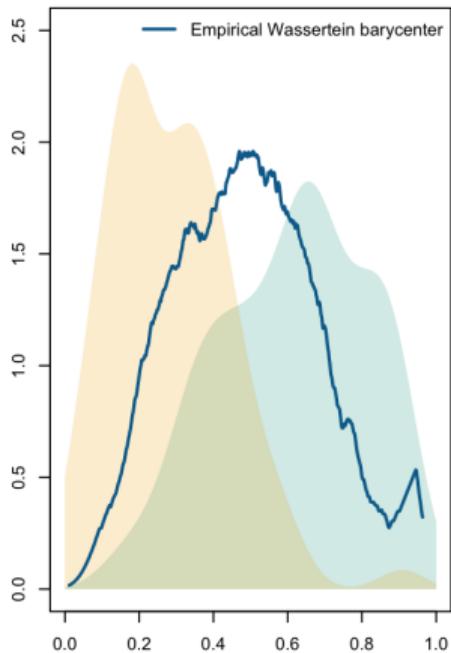


# Wasserstein Geodesic

with the  $\ell_3$  cost function



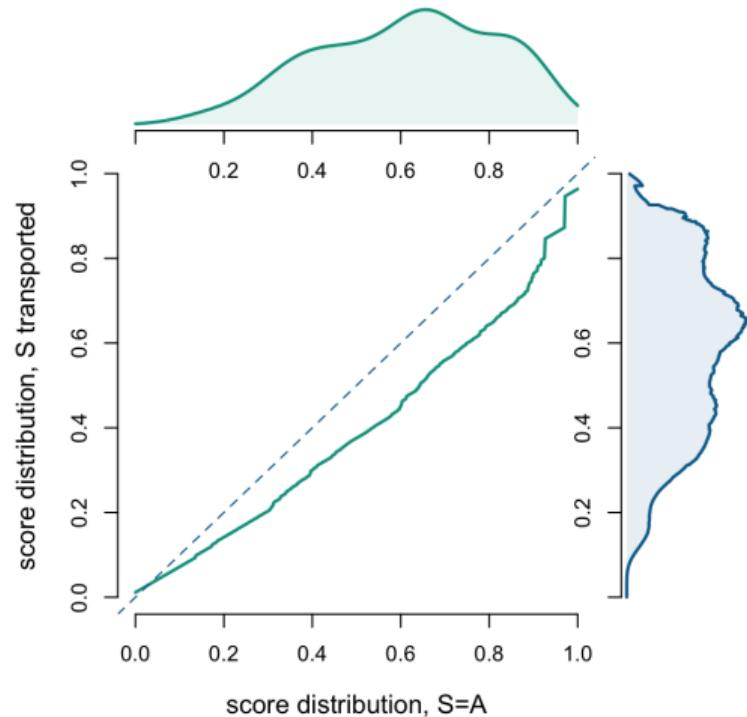
## Application to toydata1



## Application to toydata1

- Given scores  $m(\mathbf{x}, s = \text{A})$  and  $m(\mathbf{x}, s = \text{B})$ ,  
the “fair barycenter score” is

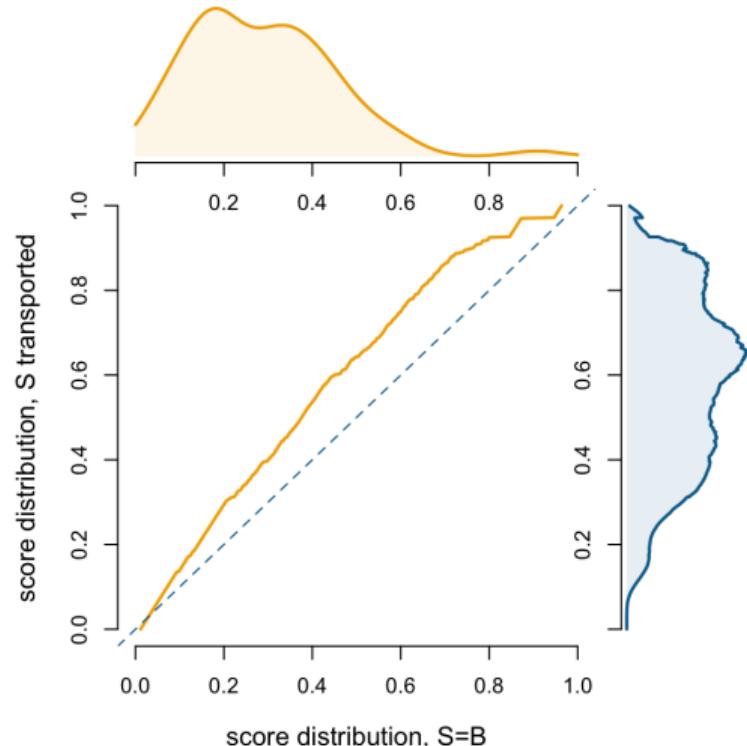
$$\begin{aligned} & m^*(\mathbf{x}, s = \text{A}) \\ &= \mathbb{P}[S = \text{A}] \cdot m(\mathbf{x}, s = \text{A}) \\ &+ \mathbb{P}[S = \text{B}] \cdot F_{\text{B}}^{-1} \circ F_{\text{A}}(m(\mathbf{x}, s = \text{A})) \end{aligned}$$



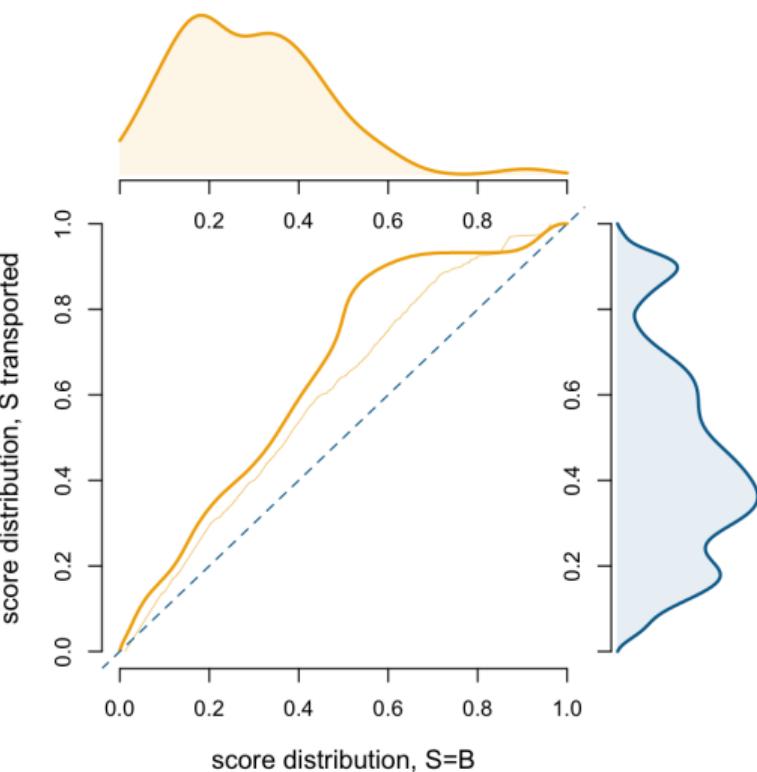
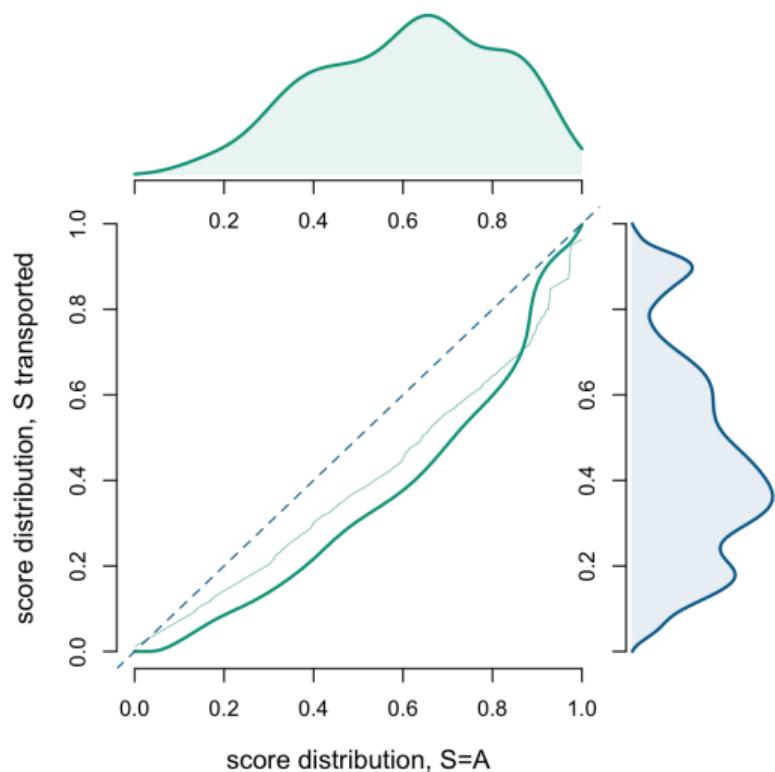
## Application to toydata1

- Given scores  $m(\mathbf{x}, s = \text{A})$  and  $m(\mathbf{x}, s = \text{B})$ ,  
the “fair barycenter score” is

$$\begin{aligned} & m^*(\mathbf{x}, s = \text{B}) \\ = & \mathbb{P}[S = \text{A}] \cdot F_{\text{A}}^{-1} \circ F_{\text{B}}(m(\mathbf{x}, s = \text{B})) \\ + & \mathbb{P}[S = \text{B}] \cdot m(\mathbf{x}, s = \text{B}) \end{aligned}$$



## Application to toydata1



## Application to toydata1

	$x$	$s$	$\bar{y}$	$\hat{m}(x, s)$	$\hat{m}(x)$	$\hat{m}_w^*(x)$	$\hat{m}_{jkl}^*(x)$
Alex	-1	A	0.475	0.250	0.219	0.154	0.094
Betty	-1	B	0.475	0.205	0.219	0.459	0.357
Ahmad	0	A	0.475	0.490	0.465	0.341	0.279
Brienne	0	B	0.475	0.426	0.465	0.719	0.692
Anthony	+1	A	0.475	0.734	0.730	0.571	0.521
Beatrix	+1	B	0.475	0.681	0.730	0.842	0.932

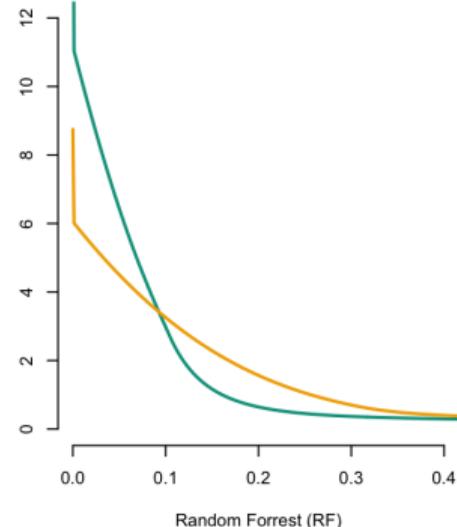
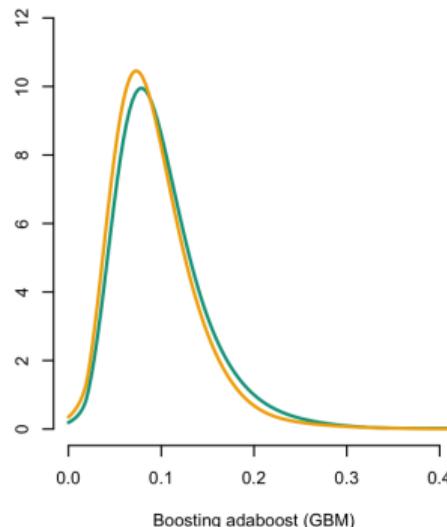
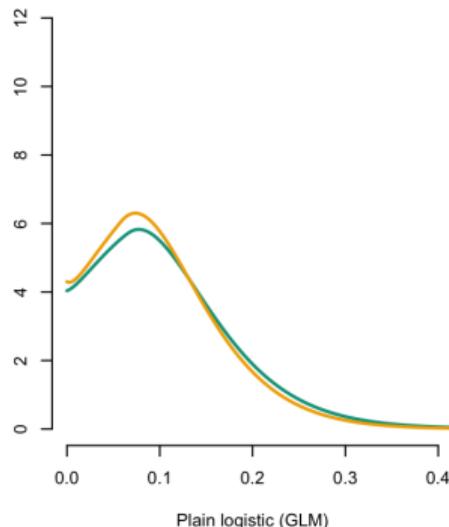
freakonometrics

freakonometrics.hypotheses.org – Arthur Charpentier, 2024 (UQAM Course)

496 / 653

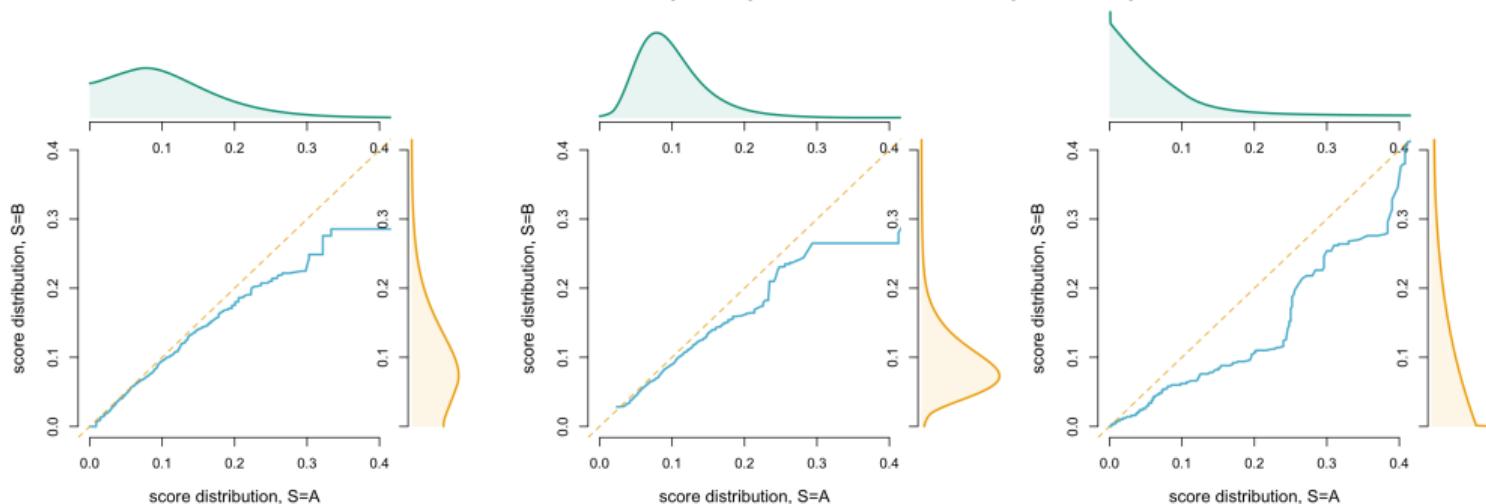
## Application to FrenchMotor

- › If the two models are balanced,  $m^*$  is also balanced.
- › Annual claim occurrence (motor insurance, Charpentier et al. (2023))
- › Three models (plain GLM, GBM, Random Forest)



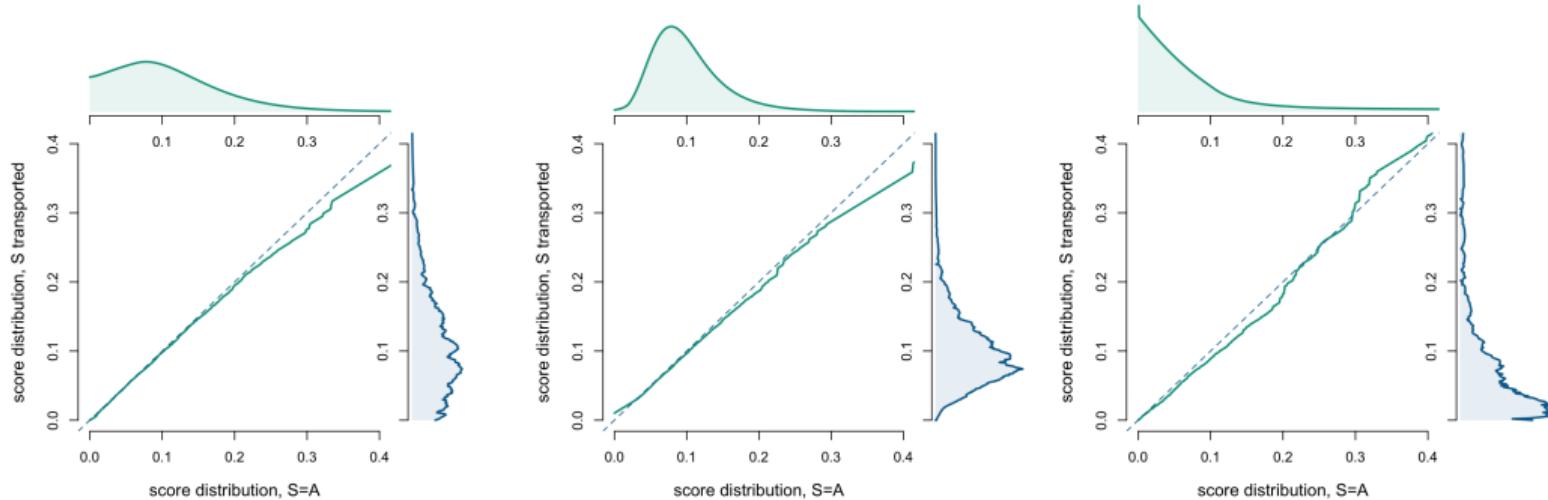
# Application to FrenchMotor

- › Predictions are different for men ( $= A$ ) and women ( $S = B$ )



- › since  $W_2 \neq 0$  consider post processing mitigation

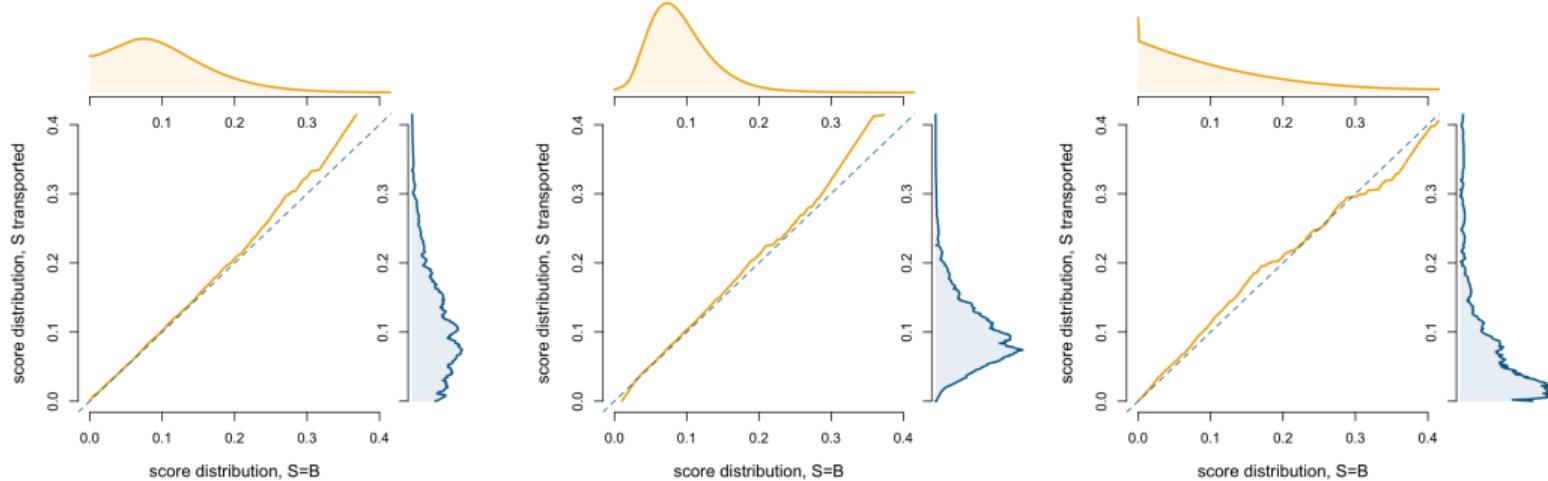
# Application to FrenchMotor



- Given scores  $m(\mathbf{x}, s = \text{A})$  and  $m(\mathbf{x}, s = \text{B})$ , the “fair barycenter score” is

$$m^*(\mathbf{x}, s = \text{A}) = \mathbb{P}[S = \text{A}] \cdot m(\mathbf{x}, s = \text{A}) + \mathbb{P}[S = \text{B}] \cdot F_{\text{B}}^{-1} \circ F_{\text{A}}(m(\mathbf{x}, s = \text{A}))$$

# Application to FrenchMotor

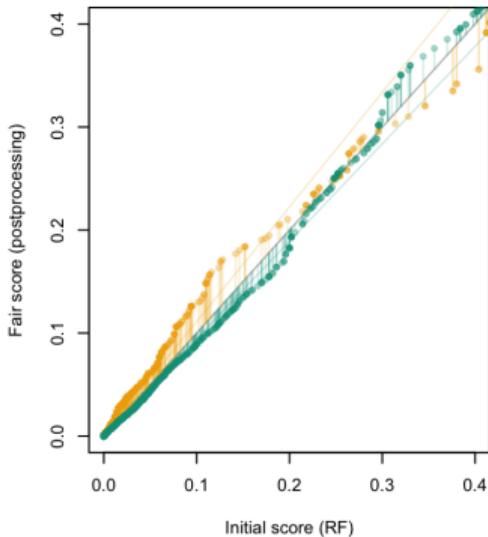
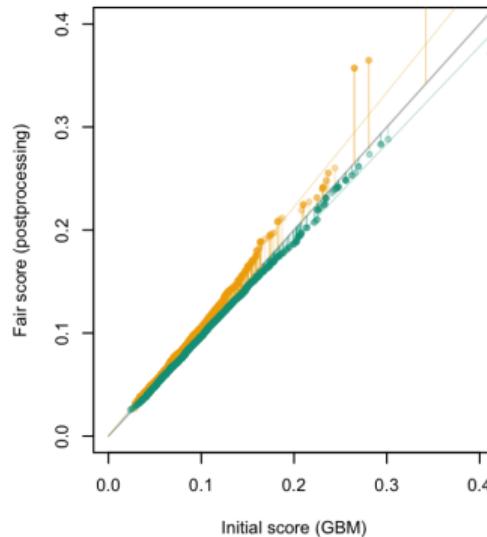
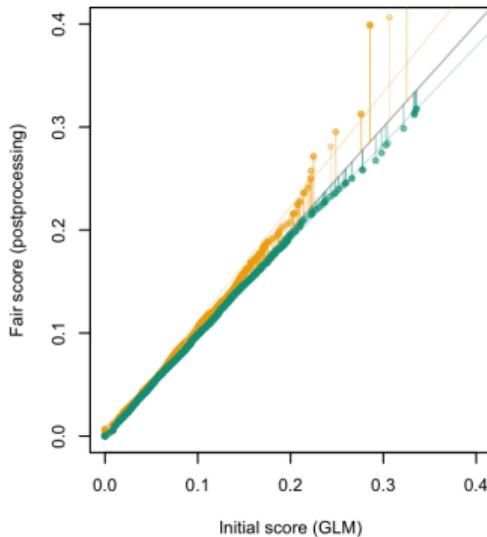


- Given scores  $m(\mathbf{x}, s = \text{A})$  and  $m(\mathbf{x}, s = \text{B})$ , the “fair barycenter score” is

$$m^*(\mathbf{x}, s = \text{B}) = \mathbb{P}[S = \text{A}] \cdot F_{\text{A}}^{-1} \circ F_{\text{B}}(m(\mathbf{x}, s = \text{B})) + \mathbb{P}[S = \text{B}] \cdot m(\mathbf{x}, s = \text{B})$$

# Application to FrenchMotor

- › We can plot  $\{(m(\mathbf{x}_i, \mathbf{A}), m^*(\mathbf{x}_i, \mathbf{A})\}$  and  $\{(m(\mathbf{x}_i, \mathbf{B}), m^*(\mathbf{x}_i, \mathbf{B})\}$



# Application to FrenchMotor

- › Numerical values, for initial occurrence probability of 5%, 10% and 20%, we have

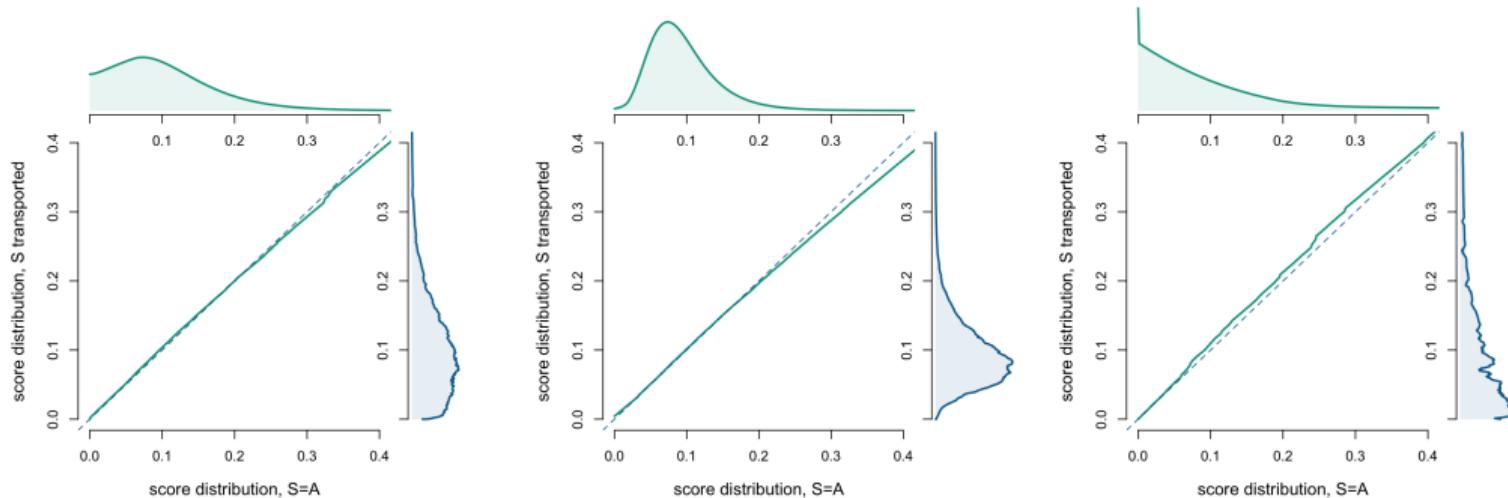
	A (men)				B (women)			
	$\times 0.94$	GLM	GBM	RF	$\times 1.11$	GLM	GBM	RF
$m(x) = 5\%$	4.73%	4.94%	4.80%	4.42%	5.56%	5.16%	5.25%	6.15%
$m(x) = 10\%$	9.46%	9.83%	9.66%	8.92%	11.12%	10.38%	10.49%	12.80%
$m(x) = 20\%$	18.91%	19.50%	18.68%	18.26%	22.25%	20.77%	21.63%	21.12%

# Application to FrenchMotor

We can do the same for discrimination against "old" drivers.

	A (younger < 65)				B (old > 65)			
	$\times 1.01$	GLM	GBM	RF	$\times 0.94$	GLM	GBM	RF
$m(\mathbf{x}) = 5\%$	5.05%	5.17%	5.10%	5.27%	4.71%	3.84%	3.84%	3.96%
$m(\mathbf{x}) = 10\%$	10.09%	10.37%	10.16%	11.00%	9.42%	7.81%	9.10%	6.88%
$m(\mathbf{x}) = 20\%$	20.19%	19.98%	19.65%	21.26%	18.85%	19.78%	23.79%	12.54%

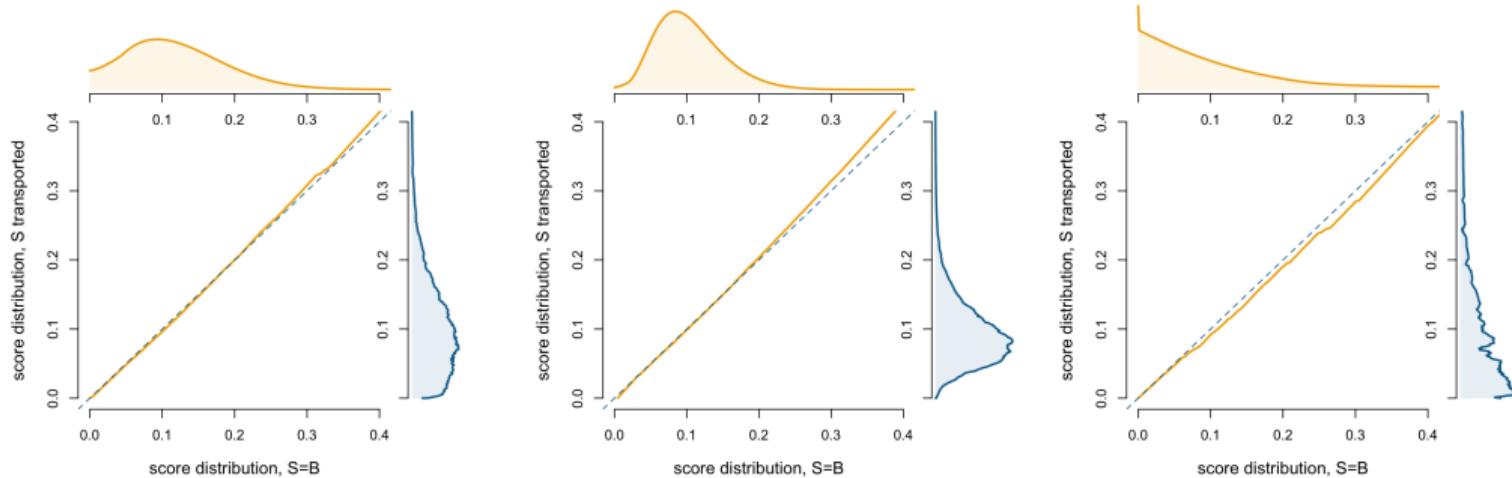
# Application to FrenchMotor



- Given scores  $m(\mathbf{x}, s = \text{A})$  and  $m(\mathbf{x}, s = \text{B})$ , the “fair barycenter score” is

$$m^*(\mathbf{x}, s = \text{A}) = \mathbb{P}[S = \text{A}] \cdot m(\mathbf{x}, s = \text{A}) + \mathbb{P}[S = \text{B}] \cdot F_{\text{B}}^{-1} \circ F_{\text{A}}(m(\mathbf{x}, s = \text{A}))$$

# Application to FrenchMotor

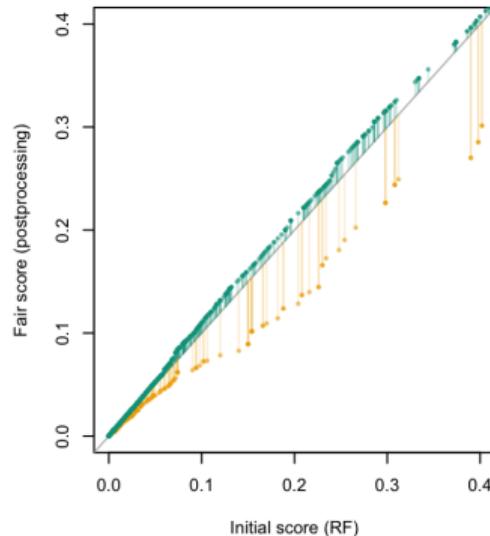
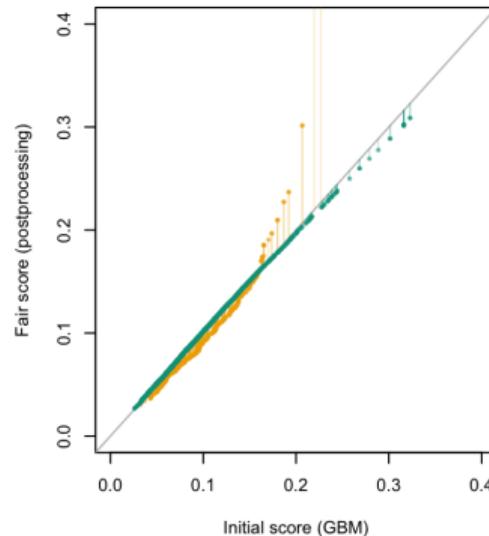
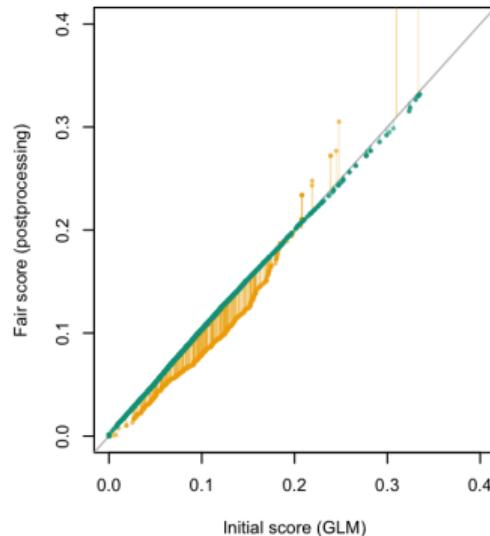


- Given scores  $m(\mathbf{x}, s = \text{A})$  and  $m(\mathbf{x}, s = \text{B})$ , the “fair barycenter score” is

$$m^*(\mathbf{x}, s = \text{B}) = \mathbb{P}[S = \text{A}] \cdot F_{\text{A}}^{-1} \circ F_{\text{B}}(m(\mathbf{x}, s = \text{B})) + \mathbb{P}[S = \text{B}] \cdot m(\mathbf{x}, s = \text{B})$$

# Application to FrenchMotor

- › We can plot  $\{(m(\mathbf{x}_i, \mathbf{A}), m^*(\mathbf{x}_i, \mathbf{A})\}$  and  $\{(m(\mathbf{x}_i, \mathbf{B}), m^*(\mathbf{x}_i, \mathbf{B})\}$



## What's next ?

- While algorithmic fairness may result in greater short-term benefits, studies indicate that common fairness criteria may not promote improvement over time, as claimed by Liu et al. (2018).
- For example, requiring a bank to give out loans to individuals who are less likely to repay them ultimately impoverishes the individuals who end up defaulting as a result. This is an issue that algorithmic fairness cannot address on its own.



– Appendix –

## Additional Results

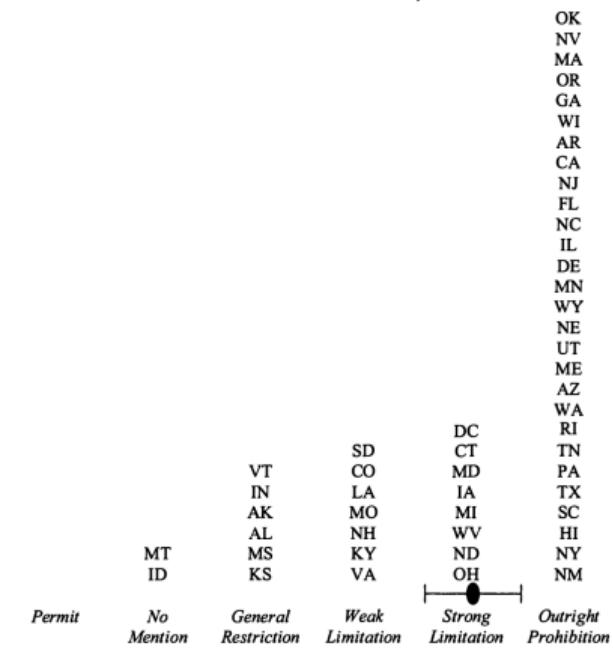
# Appendix: Sensitive attributes in insurance (in the U.S.)

⬅ to come back

From Avraham et al. (2013),

- **Expressly Permit (-1)** - The state has a statute expressly or impliedly permitting insurers to take the characteristic into account.
- **No Law on Point (0)** - The state laws are silent with respect to the particular characteristic.
- **General Restriction (1)** - The state has a statute that generally prohibits "unfair discrimination," either across all lines of insurance or in some lines of insurance, but that statute does not provide any explanation as to what constitutes unfair discrimination and does not single out any particular trait for limitation.

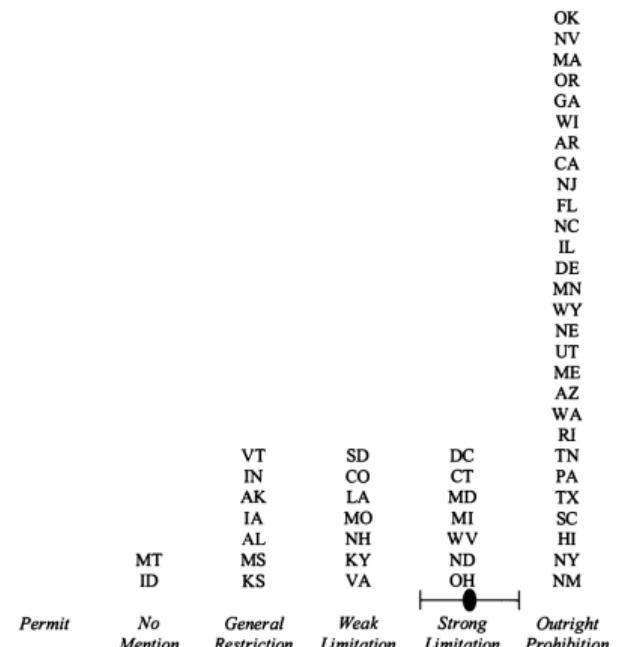
FIGURE 1a. Distribution of States' Scores for Race, in Auto Insurance



# Appendix: Sensitive attributes in insurance (in the U.S.)

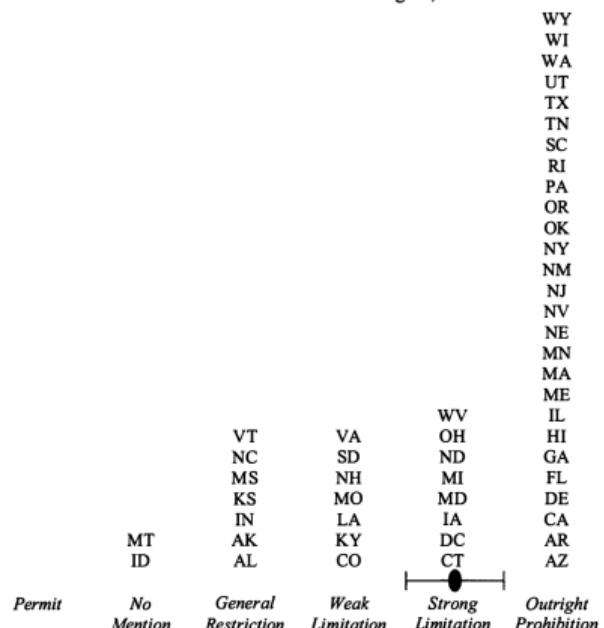
- › **Characteristic-Specific Weak Limitation (2)** - The state has a statute that limits the use of a particular characteristic in either issuance, renewal, or cancellation.
- › **Characteristic-Specific Strong Limitation (3)** - The state has a statute that prohibits the use of a particular characteristic when the policy is either issued, renewed, or cancelled, or the state has a statute that limits but does not completely prohibit the use of a particular characteristic in rate setting.
- › **Characteristic-Specific Prohibition (4)** - The state has a statute that expressly prohibits insurers from taking into account a specific characteristic in setting rates.

FIGURE 1b. Distribution of States' Scores for National Origin, in Auto Insurance



# Appendix: Sensitive attributes in insurance (in the U.S.)

FIGURE 1c. Distribution of States' Scores for Religion, in Auto Insurance

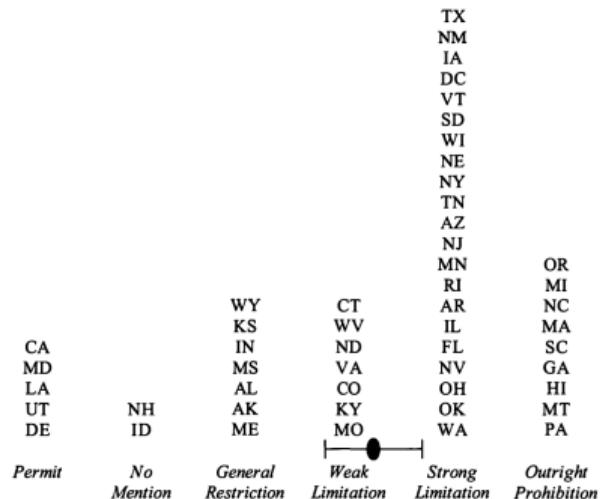


*"Race, national origin, and religion have a special place in this country's history; and, as discussed above, discrimination on the basis of these three characteristics has been subject to stricter scrutiny in American law than have other characteristics," Avraham et al. (2013)*

# Appendix: Sensitive attributes in insurance (in the U.S.)

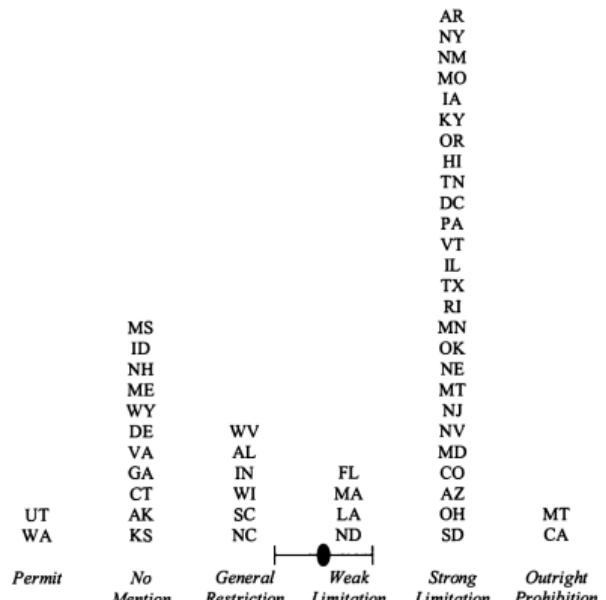
*"Gender-based discrimination in insurance has long been controversial. And differential treatment on the basis of gender is, of course, in many contexts widely considered unacceptable or illegal. Nevertheless, there does not seem to be the same level of agreement-as there is for race, religion, and national origin-that drawing gender-based distinctions is always wrong. Federal constitutional law treats gender as only a quasi-suspect classification; as a result, laws that discriminate on the basis of gender are subject to an intermediate level of scrutiny."* Avraham et al. (2013)

FIGURE 3a. Distribution of States' Scores for Gender, in Auto Insurance



# Appendix: Sensitive attributes in insurance (in the U.S.)

FIGURE 3c. Distribution of States' Scores for Gender, in Disability Insurance

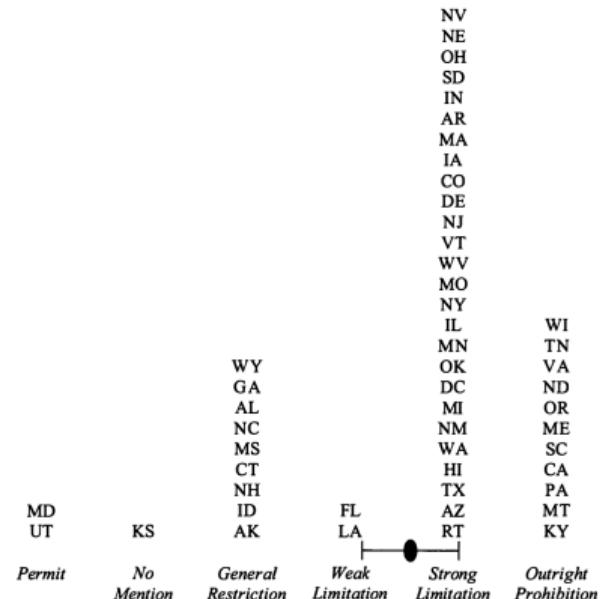


*"With respect to life insurance, we predict that the laws regulating gender discrimination will be on average relatively weak, since adverse selection in the life insurance market is especially problematic."* Avraham et al. (2013)

# Appendix: Sensitive attributes in insurance (in the U.S.)

FIGURE 3d. Distribution of States' Scores for Gender, in Property/Casualty Insurance

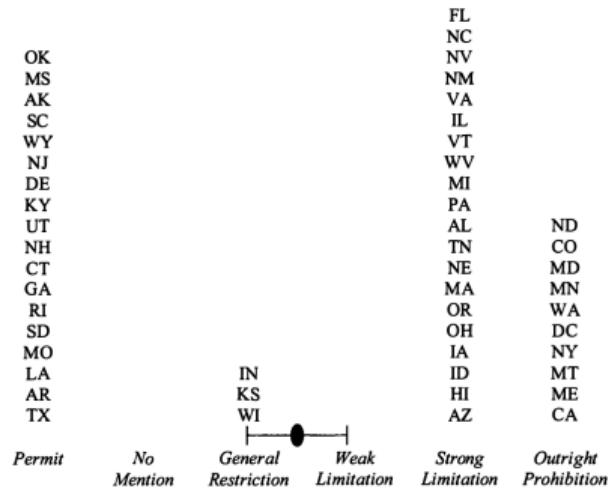
*"Regarding property/casualty insurance, as there seems to be no conceivable correlation between those risks and gender, we predict either states will cluster around no regulation, or, alternatively, states will cluster around forbidding the use of gender in property/casualty insurance on symbolic or expressive grounds."* Avraham et al. (2013)



# Appendix: Sensitive attributes in insurance (in the U.S.)

*"The gender discrimination will be more strictly regulated on average for health insurance (where gender-rated policies often result in higher premiums for women) than for auto insurance (where gender-rated policies result in higher premiums for men)."* Avraham et al. (2013)

FIGURE 3e. Distribution of States' Scores for Gender, in Health Insurance

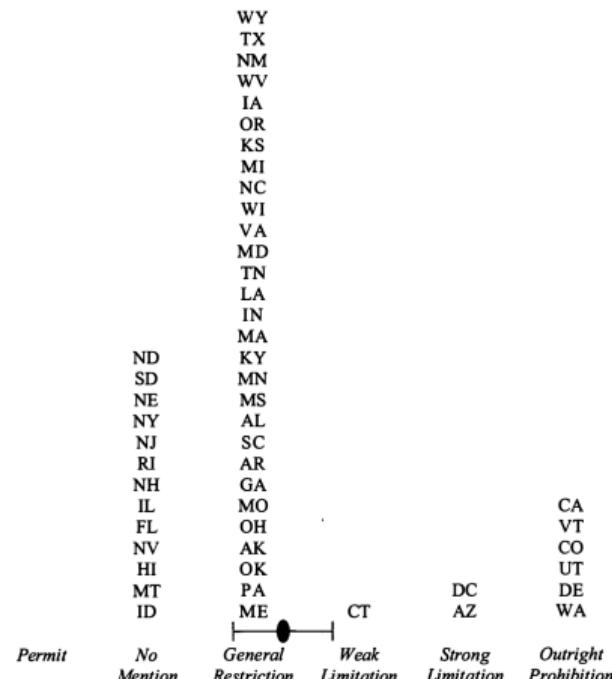


# Appendix: Sensitive attributes in insurance (in the U.S.)

FIGURE 4a. Distribution of States' Scores for Sexual Orientation, in Auto Insurance

*"Unlike with race, national origin, religion, and gender, legal classifications on the basis of an individual's sexual orientation have not clearly been identified by the Supreme Court as deserving special scrutiny. In addition, unlike race, national origin, and gender, there are no federal laws forbidding discrimination on the basis of sexual orientation in employment."*

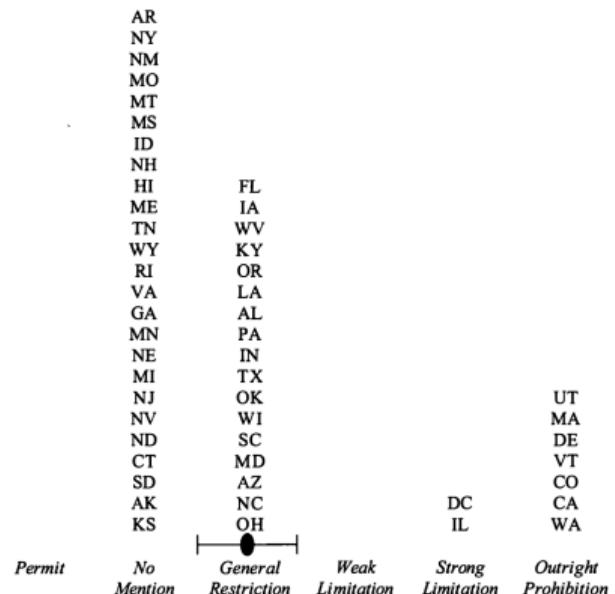
Avraham et al. (2013)



# Appendix: Sensitive attributes in insurance (in the U.S.)

FIGURE 4c. Distribution of States' Scores for Sexual Orientation, in Disability Insurance

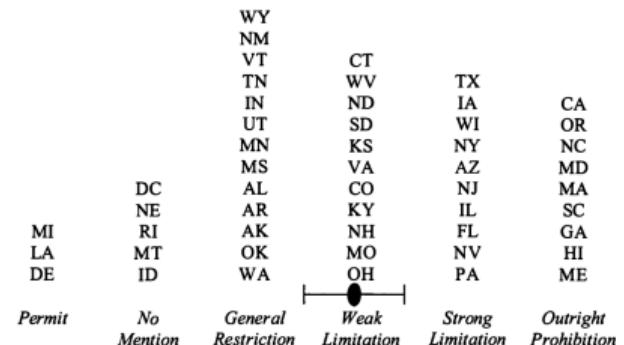
*"However, there are state laws that forbid discrimination on the basis of sexual orientation, and some lower courts have held that sexual orientation should be a suspect or quasi-suspect characterisation."* Avraham et al. (2013)



# Appendix: Sensitive attributes in insurance (in the U.S.)

*"We expect that age will have the lowest average regulatory score of all the risk characteristics we are studying. First, age is not a suspect classification, at least not by constitutional standards. Second, age tends to correlate causally with several important areas of risk (mortality, health, and perhaps disability risks), thereby increasing the perceived fairness of rating on that basis."* Avraham et al. (2013)

FIGURE 5a. Distribution of States' Scores for Age, in Auto Insurance

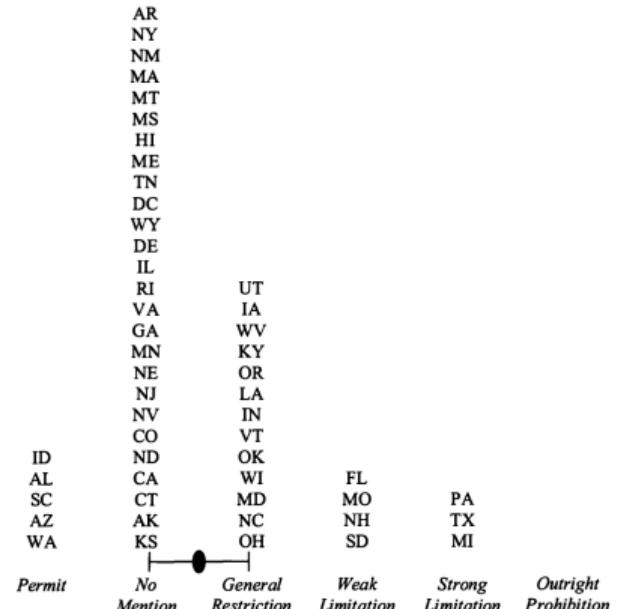


# Appendix: Sensitive attributes in insurance (in the U.S.)

FIGURE 5c. Distribution of States' Scores for Age, in Disability Insurance

*"Third, age can present serious adverse selection problems for insurers if they are forbidden from taking it into account, since individual insureds know their own age and the associated risks. Fourth, social solidarity arguments with respect to age are relatively weak, since individuals can spread risk over their lifetime through various income smoothing products."*

Avraham et al. (2013)



# Appendix: Sensitive attributes in insurance (in the U.S.)

Avraham et al. (2013) suggested to visualize the distribution of scores (Expressly Permit (-1) / No Law on Point (0) / General Restriction (1) / ... / Characteristic-Specific Prohibition (4))

FIGURE 6. Distribution of States' Scores for Age, by Line of Insurance

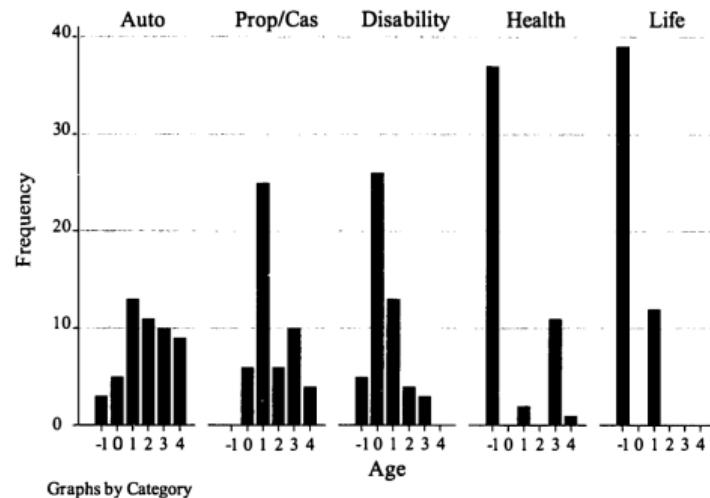
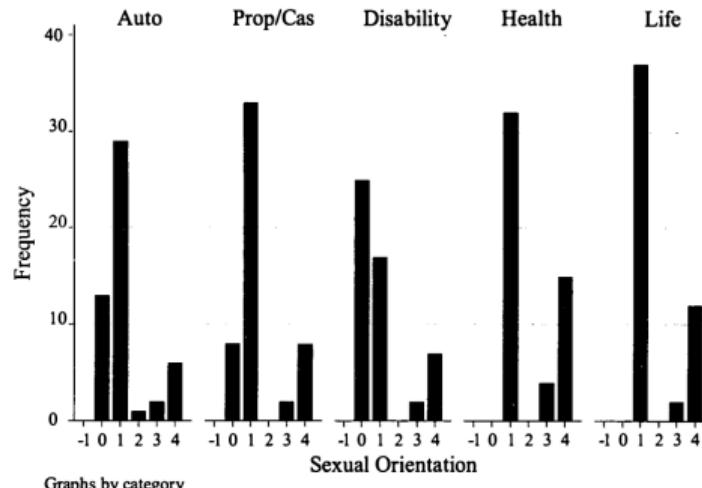


FIGURE 7. Distribution of States' Scores for Sexual Orientation, by Line of Insurance



# Appendix: Sensitive attributes in insurance (in the U.S.)

FIGURE 8. Distribution of States' Scores for Zip Code, by Line of Insurance

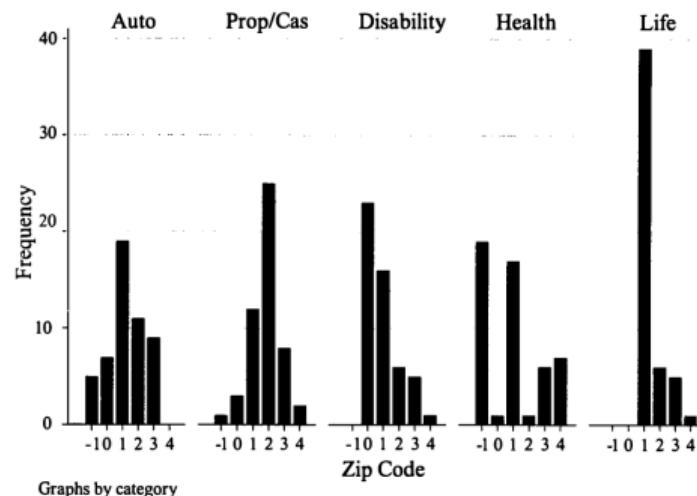
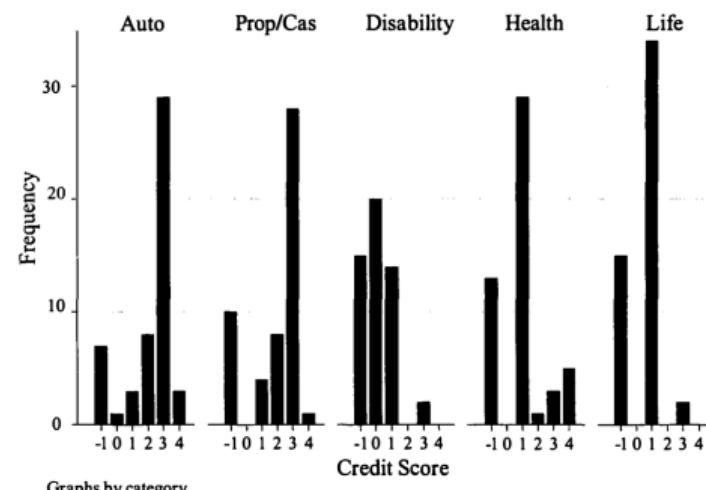


FIGURE 9. Distribution of States' Scores for Credit Score, by Line of Insurance



*"Credit score and zip code are not, by themselves, socially suspect characteristics. However, some commentators have argued that credit score and zip code are used by auto and home insurers as proxies for potentially socially suspect characteristics."*

## Appendix: $L^k$ and $L^2$

 to come back

**Note:** A Hilbert space is an abstract vector space possessing the structure of an inner product.

If  $\mathcal{H}$  is finite,  $\mathcal{H} = \{h_1, \dots, h_d\}$ ,  $\langle x, y \rangle_{\mathcal{H}}$  takes value  $K_{i,j}$  if  $x = h_i$  and  $y = h_j$ . Let  $\mathbf{K} = [K_{i,j}]$ .

$\mathbf{K}$  is a symmetric  $d \times d$  matrix,  $\mathbf{K} = \mathbf{V}\Lambda\mathbf{V}^\top$  for some orthogonal matrix  $\mathbf{V}$  where columns are eigenvectors, and  $\Lambda = \text{diag}[\lambda_i]$  (positive values). Let

$$\Phi(x) = (\sqrt{\lambda_1}V_{1,1}, \sqrt{\lambda_2}V_{2,1}, \dots, \sqrt{\lambda_d}V_{d,1}) \text{ if } x = h_i$$

Note that

$$K_{i,j} = [\mathbf{K}]_{i,j} = [\mathbf{V}\Lambda\mathbf{V}^\top]_{i,j} = \sum_{l=1}^d \lambda_l V_{i,l} V_{l,j} = \langle \Phi(h_i), \Phi(h_j) \rangle$$

## Appendix: $L^k$ and $L^2$

Matrix  $K$  defines an inner product, it is called a **kernel**. It is symmetric, associated with a positive semi-definite matrix.

Then  $K(u, u) \geq 0$  and  $K(u, v) \leq \sqrt{K(u, u) \cdot K(v, v)}$ .  
Let  $\Phi : u \mapsto K(\cdot, u)$ , then  $K(x, y) = \langle \Phi(x), \Phi(y) \rangle$

## Appendix: $L^k$ and $L^2$

### Proposition 8.10: $\ell_p$ norms for random variables

- ▶  $\|X\|_k \geq 0$ ,
- ▶  $\|X\|_k = 0$  if and only if  $X = 0$  (a.s., i.e.  $\mathbb{P}[X \neq 0] = 0$ ),
- ▶  $\|X + Y\|_k \leq \|X\|_k + \|Y\|_k$  (Minkowski inequality)

**Proof** for Minkowski inequality,  $(x, y) \mapsto g(x, y) = (x^{1/k} + y^{1/k})^k$  is concave, and from Jensen inequality, for positive variables  $U$  and  $V$  ( $\mathbb{R}_+^2$  is a convex set),

$$\mathbb{E}[(U^{1/k} + V^{1/k})^k] \leq ([\mathbb{E}(U)]^{1/k} + [\mathbb{E}(V)]^{1/k})^k$$

(then use  $U = |X|^k$  and  $V = |Y|^k$ )

## Appendix: $L^k$ and $L^2$

### Definition 8.8: $L^k$ (Lebesgue space)

For  $k \in [1, \infty)$ ,  $L^k = \{X \in \mathcal{V} : |X|^k < \infty\}$ .

### Proposition 8.11: Lyapunov inequality

If  $1 \leq j < k < \infty$ ,  $\|X\|_j \leq \|X\|_k$ , or  $L^k \subset L^j$ .

$d_k(X, Y) = \|X - Y\|_k = [\mathbb{E}(|X - Y|^k)]^{1/k}$  is a distance on  $\mathcal{V}$ .

## Appendix: $L^k$ and $L^2$

### Proposition 8.12: Inner product on $L^2$

$\langle X, Y \rangle = \mathbb{E}(XY)$  is an inner product on  $L^2$ ,

- ▶  $\langle X, Y \rangle = \langle Y, X \rangle$  (symmetric property),
- ▶  $\langle X, X \rangle \geq 0$  and  $\langle X, X \rangle = 0$  if and only if  $X = 0$  a.s. (positive property)
- ▶  $\langle aX, Y \rangle = a\langle X, Y \rangle$  (scaling property),
- ▶  $\langle X + Y, Z \rangle = \langle X, Z \rangle + \langle Y, Z \rangle$ , the additive property.

### Proposition 8.13: Hölder inequality

If  $1 \leq j < k < \infty$  with  $j^{-1} + k^{-1} = 1$ ,  $X \in L^j$  and  $Y \in L^k$ , then

$$\langle |X|, |Y| \rangle \leq \|X\|_j \cdot \|Y\|_k.$$

## Appendix: $L^k$ and $L^2$

Observe that  $\text{Cov}[X, Y] = \langle X - \mathbb{E}(X), Y - \mathbb{E}(Y) \rangle$ .

When  $j = k = 2$ , Hölder inequality is **Cauchy-Schwarz** inequality

$$\mathbb{E}(|X - \mathbb{E}(X)| \cdot |Y - \mathbb{E}(Y)|) \leq \sqrt{\mathbb{E}([X - \mathbb{E}(X)]^2)} \cdot \sqrt{\mathbb{E}([Y - \mathbb{E}(Y)]^2)}$$

Suppose that  $\mathcal{H}$  is a subspace of  $L^2$ . Let  $Y \in L^2$ , then the projection of  $Y$  onto  $\mathcal{H}$  (if it exists) is the vector  $X \in \mathcal{H}$  such that  $\langle X - Y, Z \rangle = 0, \forall Z \in \mathcal{H}$ . It will be denoted  $\mathbb{E}[Y|\mathcal{H}]$ .

## Appendix: $L^k$ and $L^2$

Let  $A = \mathbb{E}[Y|\mathcal{H}]$ ,  $B = Y - \mathbb{E}[Y|\mathcal{H}]$  and  $C = A + B = Y$ . Then, since  $\langle A, B \rangle = 0$ ,

$$\|A\|_2^2 + \|B\|_2^2 = \|C\|_2^2,$$

from Pythagorean theorem, or,

$$\mathbb{E}[\mathbb{E}(Y|\mathcal{H})^2] + \mathbb{E}[(Y - \mathbb{E}[Y|\mathcal{H}])^2] = \mathbb{E}[Y^2]$$

i.e., if we subtract  $\mathbb{E}(Y)^2$

$$\begin{aligned} & \mathbb{E}[\mathbb{E}(Y|\mathcal{H})^2] - \mathbb{E}(Y)^2 = -\mathbb{E}[\mathbb{E}(Y|\mathcal{H})]^2 \\ & \mathbb{E}[(Y - \mathbb{E}[Y|\mathcal{H}])^2] - \mathbb{E}(Y)^2 \\ & \quad \var(\mathbb{E}[Y|\mathcal{H}]) + \mathbb{E}[\var(Y|\mathcal{H})] = \var(Y) \\ & \quad = \var(Y - \mathbb{E}[Y|\mathcal{H}]) \end{aligned}$$

# Appendix: Optimisation Issues

 to come back

$f : \mathbb{R}^n \rightarrow \mathbb{R}$  is convex if  $\text{dom}(f)$  is convex and

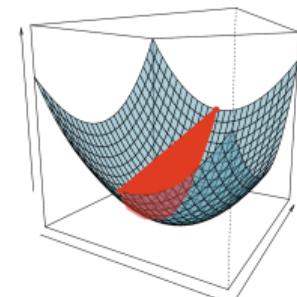
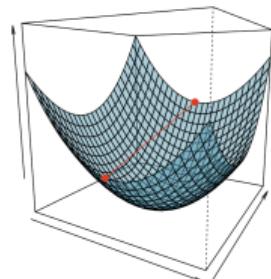
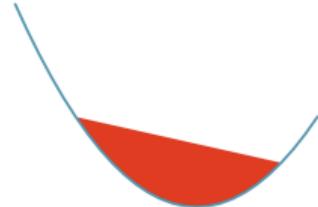
$$f(tx + (1 - t)y) \leq tf(x) + (1 - t)f(y)$$

for all  $x, y \in \text{dom}(f)$ .

## Proposition 8.14

If  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is differentiable, then  $f$  is convex if  $\text{dom}(f)$  is convex and for all  $x, y \in \text{dom}(f)$ ,

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x).$$



## Appendix: Optimisation Issues

If  $f$  is convex and non-differentiable, for all  $\mathbf{x}$ , there is  $\mathbf{g}$  such that

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{g}^\top (\mathbf{y} - \mathbf{x})$$

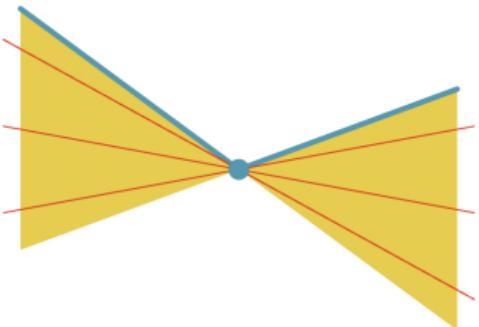
for all  $\mathbf{y} \in \text{dom}(f)$ .

$\mathbf{g}$  is called subgradient at point  $\mathbf{x}$ .

If  $f$  differentiable at  $\mathbf{x}$ ,  $\mathbf{g}$  is unique and  $\mathbf{g} = \nabla f(\mathbf{x})$

The set of subgradients of a convex function  $f$  is the subdifferential,

$$\partial f(\mathbf{x}) = \{\mathbf{g} \in \mathbb{R}^n : g \text{ is a subgradient at } \mathbf{x}\}$$



Note that  $\partial f(\mathbf{x})$  is a convex set, and if  $f$  is differentiable at point  $\mathbf{x}$ ,  $\partial f(\mathbf{x}) = \{\nabla f(\mathbf{x})\}$

## Appendix: Optimisation Issues

Consider the case of the median ( $\alpha = 1/2$ ). Given  $\{y_1, \dots, y_n\}$ , we want to solve

$$\min_{\mu} \left\{ \sum_{i=1}^n |y_i - \mu| \right\}$$

This problem is equivalent to

$$\min_{\mu, \mathbf{a}, \mathbf{b}} \left\{ \sum_{i=1}^n a_i + b_i \right\} \text{ s.t. } \begin{cases} a_i, b_i \geq 0 \\ y_i - \mu = a_i - b_i \end{cases}, \quad \forall i = 1, \dots, n$$

More generally, for a  $\alpha \in (0, 1)$ , solve

$$\min_{\mu, \mathbf{a}, \mathbf{b}} \left\{ \sum_{i=1}^n \tau a_i + (1 - \tau) b_i \right\} \text{ s.t. } \begin{cases} a_i, b_i \geq 0 \\ y_i - \mu = a_i - b_i \end{cases}, \quad \forall i = 1, \dots, n$$

## Appendix: Optimisation Issues

And for the quantile regression is

$$\min_{\gamma, \mathbf{a}, \mathbf{b}} \left\{ \sum_{i=1}^n \tau a_i + (1 - \tau) b_i \right\} \text{ s.t. } \begin{cases} a_i, b_i \geq 0 \\ y_i - \mathbf{x}_i^\top \gamma = a_i - b_i \end{cases}$$

Introduce **slack variables** to turn inequality constraints into equality constraints with positive unknowns : any inequality  $a_1 x_1 + \cdots + a_n x_n \leq c$  can be replaced by  $a_1 x_1 + \cdots + a_n x_n + u = c$  with  $u \geq 0$ .

A linear programming problem written in a **standard form** is

$$\text{Primal problem: } \min_{\mathbf{x} \in \mathbb{R}^n} \{ \mathbf{c}^\top \mathbf{x} \} \text{ s.t. } \begin{cases} A\mathbf{x} = \mathbf{b}, \\ \mathbf{x} \geq \mathbf{0}. \end{cases}$$

for some  $m \times n$   $A$  matrix,  $\mathbf{b} \in \mathbb{R}^m$  and  $\mathbf{c} \in \mathbb{R}^n$ , and

$$\text{Dual problem: } \max_{\mathbf{y} \in \mathbb{R}^m} \{ \mathbf{y}^\top \mathbf{b} \} \text{ s.t. } \mathbf{y}^\top A \leq \mathbf{c}^\top.$$

## Appendix: Optimisation Issues

The minimal cost and the maximal income coincide, i.e., the two problems are equivalent.

### Theorem 8.3: Strong duality theorem, Dantzig and Thapa (1997)

The primal problem has a nondegenerate solution  $\mathbf{x}^*$  if and only if the dual problem has a nondegenerate solution  $\mathbf{y}^*$ . And in this case  $\mathbf{y}^{*\top} \mathbf{b} = \mathbf{c}^\top \mathbf{x}^*$ .

In quantile regression,

$$\text{Primal problem: } \min_{\beta, \mathbf{u}, \mathbf{v}} \left\{ \tau \mathbf{1}^\top \mathbf{u} + (1 - \tau) \mathbf{1}^\top \mathbf{v} \right\} \text{ s.t. } \mathbf{y} = \mathbf{X}\beta + \mathbf{u} - \mathbf{v}, \text{ with } \mathbf{u}, \mathbf{v} \in \mathbb{R}_+^n$$

and

$$\text{Dual problem: } \max_{\mathbf{d}} \left\{ \mathbf{y}^\top \mathbf{d} \right\} \text{ s.t. } \mathbf{X}^\top \mathbf{d} = (1 - \tau) \mathbf{X}^\top \mathbf{1} \text{ with } \mathbf{d} \in [0, 1]^n$$

## Appendix: Optimisation Issues

For the median, Heuristically, the idea is to write  $y_i = \mu + \varepsilon_i$ , and then define  $a_i$ 's and  $b_i$ 's so that  $\varepsilon_i = a_i - b_i$  and  $|\varepsilon_i| = a_i + b_i$ , i.e.

$$\begin{cases} a_i = (\varepsilon_i)_+ = \max\{0, \varepsilon_i\} = |\varepsilon| \cdot \mathbf{1}_{\varepsilon_i > 0} \\ b_i = (-\varepsilon_i)_+ = \max\{0, -\varepsilon_i\} = |\varepsilon| \cdot \mathbf{1}_{\varepsilon_i < 0} \end{cases}$$

Thus, set  $\mathbf{z} = (\mu^+; \mu^-; \mathbf{a}, \mathbf{b})^\top \in \mathbb{R}_+^{2n+2}$ , and then write the constraint as  $\mathbf{A}\mathbf{z} = \mathbf{b}$  with  $\mathbf{b} = \mathbf{y}$  and  $\mathbf{A} = [\mathbf{1}_n; -\mathbf{1}_n; \mathbb{I}_n; -\mathbb{I}_n]$

For the objective function  $\mathbf{c} = (\mathbf{0}, \mathbf{1}_n, \mathbf{1}_n)^\top \in \mathbb{R}_+^{2n+2}$  and our program is

$$\min_{\mathbf{z}} \left\{ \mathbf{c}^\top \mathbf{z} \right\} \text{ s.t. } \mathbf{A}\mathbf{z} = \mathbf{b}, \mathbf{z} \geq \mathbf{0}.$$

```
1 > n = 101
2 > set.seed(1)
3 > y = rlnorm(n)
4 > median(y)
5 [1] 1.077415
6 > library(lpSolve)
```

```
1 > X = rep(1, n)
2 > A = cbind(X, -X, diag(n), -diag(n))
3 > b = y
4 > c = c(rep(0, 2), rep(1, n), rep(1, n))
5 > r = lp("min", c, A, rep("=", n), b)$solution
6 [1] 1.077415
```

## Appendix: Optimisation Issues

More generally, if the quantile of order  $\tau$  is a solution of  $\tau \in (0, 1)$ ,

$$\min_q \left\{ \sum_{i=1}^n \max\{\tau(y_i - \mu), (1 - \tau)(y_i - \mu)\} \right\}$$

The linear program is now

$$\min_{q^+, q^-, \mathbf{a}, \mathbf{b}} \left\{ \sum_{i=1}^n \tau a_i + (1 - \tau) b_i \right\}$$

with  $a_i, b_i, q^+, q^- \geq 0$  and  $y_i = q^+ - q^- + a_i - b_i, \forall i = 1, \dots, n$ .

```
1 > tau = .3
2 > quantile(y,tau)
3       30%
4 0.6741586
```

```
1 > c = c(rep(0,2), tau*rep(1,n), (1-tau)*rep(1,n))
2 > r = lp("min", c, A, rep("=",n), b)$solution
3 [1] 0.6741586
```

## Appendix: Optimisation Issues

In a regression, we use  $\mathbf{x}_i^\top \boldsymbol{\beta}$  instead of  $\mu$ . The linear program is

$$\min_{\boldsymbol{\beta}^+, \boldsymbol{\beta}^-, \mathbf{a}, \mathbf{b}} \left\{ \sum_{i=1}^n \tau a_i + (1 - \tau) b_i \right\}$$

with  $a_i, b_i \geq 0$  and  $y_i = \mathbf{x}^\top [\boldsymbol{\beta}^+ - \boldsymbol{\beta}^-] + a_i - b_i$ ,  $\forall i = 1, \dots, n$  and  $\beta_j^+, \beta_j^- \geq 0$   
 $\forall j = 0, \dots, k$ .

## Appendix: Optimisation Issues

Let  $\mathbf{Q}$  be a positive semidefinite matrix, the following problem corresponds to quadratic programming,

$$\begin{aligned} & \min_{\mathbf{x}} \left\{ \mathbf{c}^\top \mathbf{x} + \frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x} \right\} \\ & \text{subject to } \begin{cases} \mathbf{Dx} \geq \mathbf{d} \\ \mathbf{Ax} = \mathbf{b} \end{cases} \end{aligned}$$

More generally, consider a convex problem

$$\begin{aligned} & \min_{\mathbf{x} \in D} \{f(\mathbf{x})\} \\ & \text{subject to } \begin{cases} g_i(\mathbf{x}) \leq 0, \quad \forall i = 1, \dots, m \\ \mathbf{Ax} = \mathbf{b} \end{cases} \end{aligned}$$

for some convex function  $f, g_1, \dots, g_m$

## Definition 8.9: Dual vector space

Given a vector space  $E$ , its dual  $E^*$  is the set of all linear forms on  $E$ . Define  $\langle \cdot, \cdot \rangle : E^* \times E \rightarrow \mathbb{R}$  as  $\langle p, x \rangle = p(x)$ .

## Definition 8.10: Convex set

$C \subset E$  is a convex set if for all  $x, y \in C$ ,  $[x, y] = \{(1 - t)x + ty, t \in [0, 1]\} \subset C$ .

## Definition 8.11: Convex function

$f : E \rightarrow \mathbb{R}$  is a convex function if

$$f((1-t)x + ty) \leq (1-t)f(x) + tf(y), \quad \forall x, y \in E, \quad t \in [0, 1].$$

More generally (if  $f$  is not proper, i.e. taking values in  $[-\infty, +\infty]$ ),  $f$  is convex if its epigraph is convex, where  $\text{epi}(f) = \{(x, y) : y \geq f(x)\} \subset E \times \mathbb{R}$ .

## Proposition 8.15

Let  $f_i : E \rightarrow \mathbb{R}$  be convex functions, then  $f^+(x) = \sup\{f_i(x)\}$  is a convex function.

## Proposition 8.16

If  $f : E \rightarrow \mathbb{R}$  is convex, for every  $x_0 \in E$ , there exists an affine function  $\ell_{x_0}(x) = a_0x + y$  such that  $\ell_{x_0}(x_0) = f(x_0)$  and  $f$  lies above  $\ell_{x_0}$ .

**Proof:**

## Proposition 8.17: Hahn-Banach

A convex lower semi continuous (for every  $x_n \rightarrow x$ ,  $\lim f(x_n) \geq f(x)$ ) function  $f$  is equal to the supremum of affine functions.

# Convexity

**Proof:** Let  $\mathcal{L}$  denote the set of the affine functions from Proposition 8.16,  $\mathcal{L} = \{\ell_{x_0}, x_0 \in E\}$ . Then, for all  $x \in E$ ,

$$\begin{cases} \sup_{\ell \in \mathcal{L}} \{\ell(x)\} \geq \ell_x(x) = f(x) \text{ because } \ell_x \text{ passes through } (x, f(x)), \\ \sup_{\ell \in \mathcal{L}} \{\ell(x)\} \leq f(x) \text{ because all } \ell \text{ lies below } f \end{cases}$$

therefore  $f(x) = \sup_{\ell \in \mathcal{L}} \{\ell(x)\}$ .

## Definition 8.12: (Fenchel) convex conjugate

If  $f : E \rightarrow \mathbb{R}$  is a function, its convex conjugate  $f^* : E^* \rightarrow \mathbb{R}$  is defined as

$$f^*(p) = \sup_{x \in E} \langle p, x \rangle - f(x).$$

# Convexity

Let  $E$  denote some nonempty subset of  $\mathbb{R}^k$ , and define the indicator function of  $E$ ,

$$\mathbf{1}_E(\mathbf{x}) = \begin{cases} 0 & \text{if } \mathbf{x} \notin E \\ +\infty & \text{if } \mathbf{x} \in E \end{cases}$$

Then  $\mathbf{1}_E^*(\mathbf{s}) = \sup_{\mathbf{x} \in E} \{\mathbf{s}^\top \mathbf{x}\} = \sup_{\mathbf{x} \in E} \{\langle \mathbf{s}, \mathbf{x} \rangle\}$  which is the support function of  $E$ .

## Definition 8.13: Subgradient

If  $f : E \rightarrow \mathbb{R}$  is a convex function, the subgradient of  $f$  at point  $x \in E$  is the set of elements in  $E^*$  defined as

$$\partial f(x) = \{p \in E^* : f(y) \geq f(x) + \langle p, y - x \rangle \text{ for all } y \in E\}.$$

# Convexity

Therefore, with a little abuse of notations,

$$\langle \partial f(x) - \partial f(y), x - y \rangle \geq 0$$

## Proposition 8.18: Legendre-Fenchel identity

If  $f : E \rightarrow \mathbb{R}$  is a convex function,

$$p \in \partial f(x) \iff x \in \partial f^*(p) \iff f^*(p) + f(x) = \langle p, x \rangle.$$

If  $f : \mathbb{R}^k \rightarrow \mathbb{R}$  is convex, twice differentiable, then  $\nabla f^*(p) = [\nabla f]^{-1}(p)$ , or  $\nabla f^* \circ \nabla f$  and  $\nabla f \circ \nabla f^*$  are the identity (on  $E$  and  $E^*$  respectively).

Let  $X$  be a random variable with c.d.f.  $F_X$  and quantile function  $Q_X$ . The Fenchel-Legendre transform of

$$\Psi(x) = \mathbb{E}[(x - X)_+] = \int_{-\infty}^x z F_X(z) dz$$

# Convexity

is

$$\Psi^*(y) = \sup_{x \in \mathbb{R}} \{xy - \Psi(x)\} = \int_0^y Q_X(t) dt$$

on  $[0, 1]$ .

Indeed, from Fubini,

$$\Psi(x) = \int_{-\infty}^x z \mathbb{P}(X \leq z) dz = \int_{-\infty}^x z \mathbb{E}(\mathbf{1}_{X \leq z}) dz = \mathbb{E} \left( \int_{-\infty}^x z \mathbf{1}_{X \leq z} dz \right)$$

i.e.

$$\Psi(x) = \mathbb{E}([x - X]_+) = \int_0^1 [x - Q_X(t)]_+ dt$$

Observe that

$$\Psi^*(1) = \sup_{x \in \mathbb{R}} \{x - \Psi(x)\} = \lim_{x \uparrow \infty} \int_0^1 [x - (x - Q_X(t))_+] dt = \int_0^1 Q_X(t) dt$$

# Convexity

and  $\Psi^*(0) = 0$ . Now, the proof of the result when  $y \in (0, 1)$  can be obtained since

$$\frac{\partial xy - \Psi(x)}{\partial x} = y - F_X(x)$$

The optimum is then obtained when  $y = F_X(x)$ , or  $x = Q_Y(y)$ .

## Definition 8.14: Proximal Operator (Moreau-Yosida)

If  $f : E \rightarrow \mathbb{R}$  is a convex function, the proximal operator is defined as

$$\text{proximal}_{\epsilon,f}(x) = \underset{y}{\operatorname{argmin}} \left\{ f(y) + \frac{1}{2\epsilon} \|x - y\|^2 \right\} = (\text{Id} + \epsilon \partial f)^{-1} x$$

Note that  $\text{proximal}_{\epsilon,f}(x)$  is uniquely defined.

# Convex Optimization Problem

$$\min_{\mathbf{x}} \{f(\mathbf{x})\}$$

with  $f$  convex, and differentiable.

---

## Algorithm 1: Gradient Descent

---

- 1 initialization :  $\mathbf{x}^{(0)}$ ;
  - 2 **for**  $t=1,2,\dots$  **do**
  - 3    $\mathbf{x}^{(t)} \leftarrow \mathbf{x}^{(t-1)} - h_t \nabla f(\mathbf{x}^{(t-1)})$
- 

Heuristics: Taylor expansion

$$f(\mathbf{y}) \sim f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{1}{2h} \|\mathbf{y} - \mathbf{x}\|^2$$

Then one can prove that  $|f(\mathbf{x}^{(t)}) - f^*| \leq O(t^{-1})$ .

# Convex Optimization Problem

$$\min_{\mathbf{x}} \{f(\mathbf{x})\}$$

with  $f$  convex, and differentiable.

---

## Algorithm 2: Accelerated Gradient Descent (Nesterov)

---

- 1 initialization :  $\mathbf{x}^{(0)}, \mathbf{x}^{(-1)}$ ;
  - 2 **for**  $t=1,2,\dots$  **do**
  - 3    $\mathbf{y}^{(t-1)} \leftarrow \mathbf{x}^{(t-1)} + \frac{t-1}{t+2} (\mathbf{x}^{(t-1)} - \mathbf{x}^{(t-2)})$ ;
  - 4    $\mathbf{x}^{(t)} \leftarrow \mathbf{y}^{(t-1)} - h_t \nabla f(\mathbf{y}^{(t-1)})$ ;
- 

Then one can prove that  $|f(\mathbf{x}^{(t)}) - f^*| \leq O(t^{-2})$ .

# From Gradient Descent to Newton's Method

$$\min_{\mathbf{x}} \{f(\mathbf{x})\}$$

with  $f$  convex, twice differentiable.

---

### Algorithm 3: Newton's Method

---

- 1 initialization :  $\mathbf{x}^{(0)}$ ;
  - 2 **for**  $t=1,2,\dots$  **do**
  - 3     $\mathbf{H}_t \leftarrow \nabla^2 f(\mathbf{x}^{(t-1)})$ ;
  - 4     $\mathbf{x}^{(t)} \leftarrow \mathbf{x}^{(t-1)} - \mathbf{H}_t^{-1} \nabla f(\mathbf{x}^{(t-1)})$
- 

Use a better quadratic approximation in Taylor expansion –  $\frac{1}{h}\mathbb{I} \rightarrow H$ ,

$$f(\mathbf{y}) \sim f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{1}{2}(\mathbf{y} - \mathbf{x})^\top H(\mathbf{y} - \mathbf{x})$$

# Convex Optimization Problem

$$\min_{\mathbf{x}} \{f(\mathbf{x})\}$$

with  $f$  convex, but non-differentiable.

---

## Algorithm 4: Subgradient 'Descent'

---

- 1 initialization :  $\mathbf{x}^{(0)}$ ;
  - 2 **for**  $t=1,2,\dots$  **do**
  - 3    $\mathbf{g}^{(t-1)} \in \partial f(\mathbf{x}^{(t-1)})$ ;
  - 4    $\mathbf{x}^{(t)} \leftarrow \mathbf{x}^{(t-1)} - h_t \mathbf{g}^{(t-1)}$
- 

Note that it is not necessarily a descent, so pick

$$\mathbf{x}^* = \operatorname{argmin}\{f(\mathbf{x}^{(0)}), f(\mathbf{x}^{(1)}), f(\mathbf{x}^{(2)}), \dots\}$$

# Convex Optimization Problem

$$\min_{\mathbf{x}} \{f(\mathbf{x})\} \text{ or } \min_{\mathbf{x}} \{f_1(\mathbf{x}) + f_2(\mathbf{x})\}$$

with  $f_1$  and  $f_2$  convex, but  $f_2$  non-differentiable.

---

## Algorithm 5: Proximal Gradient 'Descent'

---

- 1 initialization :  $\mathbf{x}^{(0)}$ ;
  - 2 **for**  $t=1,2,\dots$  **do**
  - 3      $\gamma_h(x) = \frac{1}{h}(\mathbf{x} - \text{proximal}_{h,f_2}(\mathbf{x} - h\nabla f_1(\mathbf{x})))$ ;
  - 4      $\mathbf{x}^{(t)} \leftarrow \mathbf{x}^{(t-1)} - h_t \gamma_{h_{t-1}}(\mathbf{x}^{(t-1)}) = \text{proximal}_{h,f_2}(\mathbf{x}^{(t-1)} - h\nabla f_1(\mathbf{x}^{(t-1)}))$
- 

$\gamma_h$  is the "generalized gradient of  $f$ ".

The trick is that  $\text{proximal}_{h,f_2}(\cdot)$  usually has a closed form in most applications.

## Convex Optimization Problem

E.g. consider the LASSO objective,  $f(\beta) = \underbrace{\frac{1}{2} \|\mathbf{y} - \mathbf{X}\beta\|_2^2}_{=f_1(\beta)} + \underbrace{\lambda \|\beta\|_{\ell_1}}_{=f_2(\beta)}$ . The proximal

mapping is the soft-thresholding operator

$$\text{proximal}_h(\beta) = \operatorname{argmin}_{\mathbf{z}} \left\{ \frac{1}{2h} \|\beta - \mathbf{z}\|_2^2 + \lambda \|\mathbf{z}\|_{\ell_1} \right\} = S_{\lambda h}(\beta)$$

where

$$S_{\lambda h}(\beta_j) = \begin{cases} \beta_j - \lambda & \text{if } \beta_j > \lambda \\ \beta_j + \lambda & \text{if } \beta_j < -\lambda \\ 0 & \text{otherwise.} \end{cases}$$

Hence

$$\begin{cases} \nabla f_1(\beta) = -\mathbf{X}^\top (\mathbf{y} - \mathbf{X}\beta) \\ \gamma_h(\beta) = S_{\lambda h}(\beta + h \cdot \mathbf{X}^\top (\mathbf{y} - \mathbf{X}\beta)) \end{cases}$$

see Beck and Teboulle (2009), "iterative soft-thresholding algorithm".

# Convex Optimization Problem

$$\min_{\mathbf{x}} \{f(\mathbf{x})\} \text{ or } \min_{\mathbf{x}} \{f_1(\mathbf{x}) + f_2(\mathbf{x})\}$$

with  $f_1$  and  $f_2$  convex, but  $f_2$  non-differentiable.

---

## Algorithm 6: Accelerated Proximal Gradient 'Descent' (Nesterov)

---

- 1 initialization :  $\mathbf{x}^{(-1)}, \mathbf{x}^{(0)}$ ;
  - 2 **for**  $t=1,2,\dots$  **do**
  - 3      $\mathbf{y}^{(t-1)} \leftarrow \mathbf{x}^{(t-1)} + \frac{t-2}{t+1} [\mathbf{x}^{(t-1)} - \mathbf{x}^{(t-2)}]$ ;
  - 4      $\mathbf{x}^{(t)} \leftarrow \text{proximal}_{h,f_2}(\mathbf{y}^{(t-1)} - h_t \nabla f_2(\mathbf{y}^{(t-1)}))$
-

# Coordinate Descent

Let  $\{\vec{e}_1, \dots, \vec{e}_n\}$  denote the standard basis in  $\mathbb{R}^n$ ,

$$\vec{e}_i = (0, \dots, 0, 1, 0, \dots, 0) \in \mathbb{R}^n$$

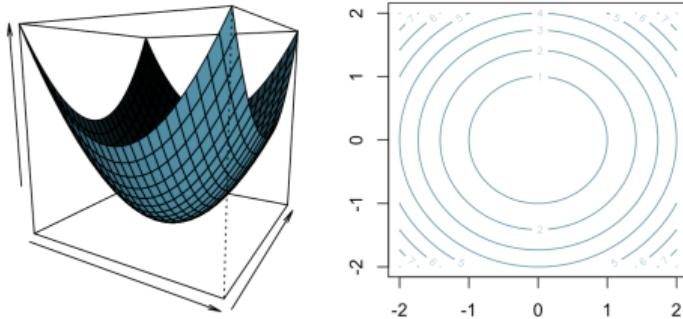
## Proposition 8.19

If  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is convex, differentiable,

$$f(\mathbf{x}) \leq f(\mathbf{x} + \delta \vec{e}_i), \quad \forall i \implies f(\mathbf{x}) = \min\{f\}$$

i.e. if we are at a point  $\mathbf{x}$  such that  $f(\mathbf{x})$  is minimized along each coordinate axis, then we have found a global minimizer.

# Coordinate Descent



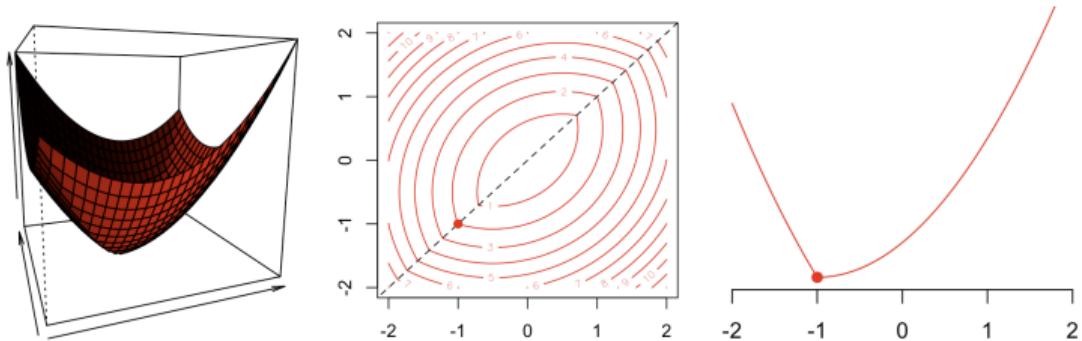
## Proposition 8.20

If  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is convex, but **not differentiable**,

$$f(\mathbf{x}) \leq f(\mathbf{x} + \delta \vec{\mathbf{e}}_i), \quad \forall i \Rightarrow f(\mathbf{x}) = \min\{f\}$$

i.e. if we are at a point  $\mathbf{x}$  such that  $f(\mathbf{x})$  is minimized along each coordinate axis, then we have **not** found a global minimizer.

# Coordinate Descent



## Proposition 8.21

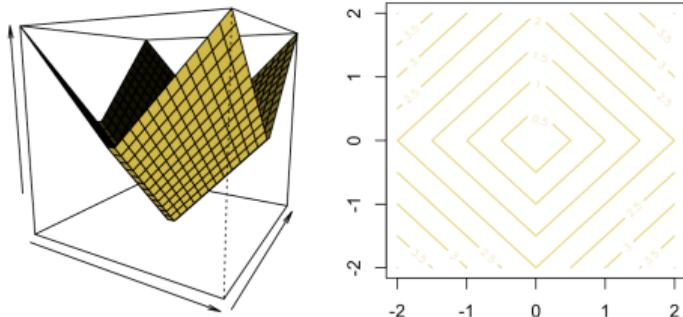
If  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  can be written

$$f(\mathbf{x}) = f_0(\mathbf{x}) + \underbrace{\sum_{i=1}^n f_i(x_i)}_{\text{separable}}, \quad \text{where } \begin{cases} f_0 \text{ convex and differentiable} \\ f_i \text{ convex and non-differentiable} \end{cases}$$

$$f(\mathbf{x}) \leq f(\mathbf{x} + \delta \vec{e}_i), \quad \forall i \implies f(\mathbf{x}) = \min\{f\}$$

i.e. if we are at a point  $\mathbf{x}$  such that  $f(\mathbf{x})$  is minimized along each coordinate axis, then we have found a global minimizer.

# Coordinate Descent



# Coordinate Descent

If we want to solve  $\min\{f(\mathbf{x})\}$  for some  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  such that

$$f(\mathbf{x}) = f_0(\mathbf{x}) + \underbrace{\sum_{i=1}^n f_i(x_i)}_{\text{separable}}, \quad \text{where } \begin{cases} f_0 \text{ convex and differentiable} \\ f_i \text{ convex and non-differentiable} \end{cases}$$

we can use a **coordinate descent algorithm**

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## Algorithm 7: Coordinate Descent

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- 1 initialization :  $\mathbf{x}^{(0)}$ ;
  - 2 **for**  $t=1,2,\dots$  **do**
  - 3   **for**  $j=1,2,\dots,n$  **do**
  - 4      $\mathbf{x}_j^{(t)} \leftarrow \operatorname{argmin}\{f(\mathbf{x}_1^{(t)}, \dots, \mathbf{x}_{j-1}^{(t)}, x_j, \mathbf{x}_{j+1}^{(t-1)}, \dots, \mathbf{x}_n^{(t-1)})\}$
-

## Gradient vs. Coordinate Descent

Consider the problem  $\min\{f(\beta)\}$  where  $f(\beta) = \frac{1}{2}\|\mathbf{y} - \mathbf{X}\beta\|^2$

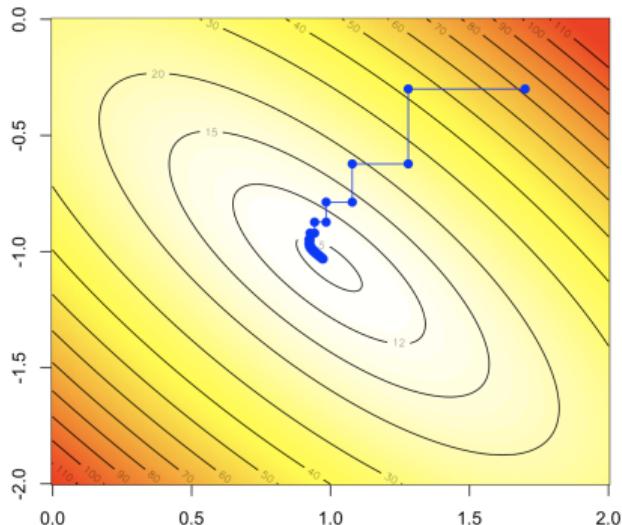
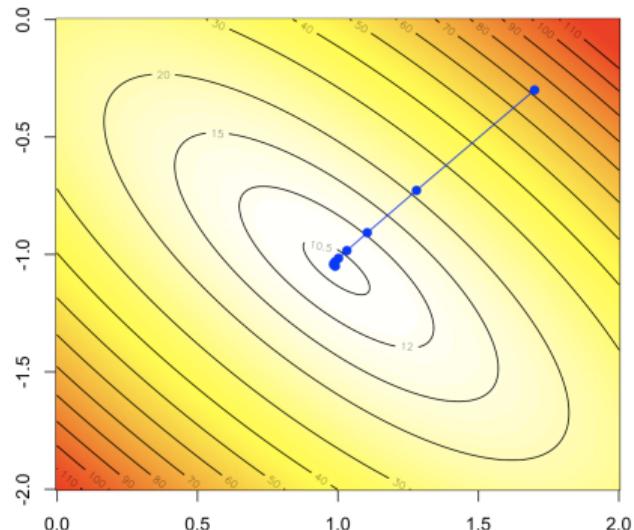
- ▶ Gradient descent,  $\beta \leftarrow \beta + h\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\beta)$
- ▶ Coordinate descent,  $\beta_j \leftarrow \beta_j + \frac{1}{\mathbf{X}_j^\top \mathbf{X}_j} \mathbf{X}_j^\top(\mathbf{y} - \mathbf{X}\beta)$

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# Gradient vs. Coordinate Descent



 to come back

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