Multivariate Optimal Transport

We have mentioned that, in dimension one

Theorem 4.6: Optimal map for continuous univariate distributions

The optimal Monge map $T^\star$ such that $T^\star_\# \mathbb{P}_{\mathtt{A}} = \mathbb{P}_{\mathtt{B}}$ is $T^\star = F_{\mathtt{B}}^{-1} \circ F_{\mathtt{A}}$.

- $T^\star$ is an increasing mapping.

Example Univariate Gaussian

$$x_{\mathtt{B}} = T^\star(x_{\mathtt{A}}) = \mu_{\mathtt{B}} + \sigma_{\mathtt{B}}\sigma_{\mathtt{A}}^{-1}(x_{\mathtt{A}} - \mu_{\mathtt{A}}).$$

Multivariate Optimal Transport

Theorem 4.7: Optimal map for continuous multivariate distributions, Brenier (1991)

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

Example Multidimensional Gaussian

$$\boldsymbol{x}_{\mathrm{B}} = \mathcal{T}^\star(\boldsymbol{x}_{\mathrm{A}}) = \boldsymbol{\mu}_{\mathrm{B}} + \boldsymbol{A}(\boldsymbol{x}_{\mathrm{A}} - \boldsymbol{\mu}_{\mathrm{A}}),$$

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

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

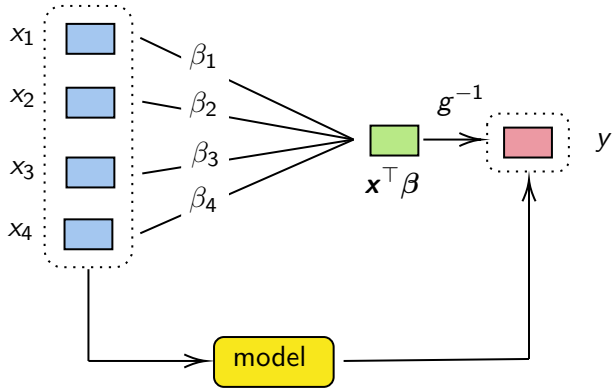
$$f_{\theta,\varphi}(y) = \exp\left(\frac{y\theta - b(\theta)}{\varphi} + c(y,\varphi)\right),$$

where θ is the canonical parameter, φ is a nuisance parameter, and $b : \mathbb{R} \to \mathbb{R}$ is some $\mathbb{R} \to \mathbb{R}$ function.

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

Generalized Linear Model

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



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

Generalized Linear Model

- We modeling, we want to solve problems such as

$$\begin{cases} \min\limits_{f \in \mathcal{F}} \{f(\boldsymbol{x})\} \\ \text{s.t. } f \in \mathcal{F}_0, \text{ where } \boldsymbol{x} \text{ is given.} \end{cases} \quad \text{or} \quad \begin{cases} \min\limits_{\boldsymbol{\theta} \in \mathbb{R}^k} \{f_{\boldsymbol{\theta}}(\boldsymbol{x})\} \\ \text{s.t. } \boldsymbol{\theta} \in \Theta, \text{ where } \boldsymbol{x} \text{ is given.} \end{cases}$$

- In optimisation, it is usually written the other way round,

$$\begin{cases} \min\limits_{\boldsymbol{x} \in \mathbb{R}^k} \{f(\boldsymbol{x})\} \\ \text{s.t. } \boldsymbol{x} \in \mathcal{E}, \text{ where } f \text{ is given.} \end{cases}$$

Generalized Linear Model

$$\begin{cases} \min_{\boldsymbol{x}\in\mathbb{R}^k} \{f(\boldsymbol{x})\} \\ \text{s.t. } \boldsymbol{x} \in \mathcal{E}, \text{ where } f \text{ is given.} \end{cases}$$

can be written

$$\min_{\boldsymbol{x}\in\mathbb{R}^k} \{f(\boldsymbol{x}) + \lambda p(\boldsymbol{x})\}$$

where $\lambda > 0$ is some penalty factor, and $p(\cdot)$ is some function. With

$$p(\boldsymbol{x}) = \begin{cases} 0 \text{ si } \boldsymbol{x} \in \mathcal{E} \\ +\infty \text{ si } \boldsymbol{x} \notin \mathcal{E} \end{cases}$$

the two problems are equivalent. Other p functions can be considered.

- p is said to be an exact penalty if the two problems are equivalent.

Generalized Linear Model

- E.g., if $\mathcal{E} = \mathbb{R}_+^k = \{\boldsymbol{x} : \boldsymbol{x} \geq \boldsymbol{0}\}$, we can consider

$$p(\boldsymbol{x}) = -\sum_{i=1}^{k} \log(x_i) \quad \text{(as suggested by Frisch (1955))}$$

Generalized Linear Model

- Consider problems

$$\min_{\boldsymbol{x}\in\mathbb{R}^k}\{f(\boldsymbol{x})\} \text{ under constraint } g(\boldsymbol{x})=\boldsymbol{0} \quad \text{or} \quad \min_{\boldsymbol{x}\in\mathbb{R}^k}\{f(\boldsymbol{x})\} \text{ under constraint } g(\boldsymbol{x})\leq\boldsymbol{0}$$

- Karush-Kuhn-Tucker condition is

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

where

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

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

Generalized Linear Model

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

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

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

Definition 4.41: Ridge Estimator (GLM)

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

Generalized Linear Model

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

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

Definition 4.43: LASSO Estimator (GLM)

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

Generalized Linear Model

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

- Elastic net

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

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)

Accuracy

Definition 4.44: ROC curve

The ROC curve is the parametric curve

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

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

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

where

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

Accuracy

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

Definition 4.45: AUC, area under the ROC curve

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

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

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

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

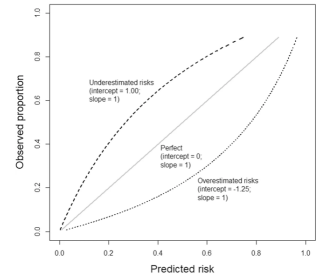
- "*Suppose that a forecaster sequentially assigns probabilities to events. He is* **well calibrated** *if, for example, of those events to which he assigns a probability 30 percent, the long-run proportion that actually occurs turns out to be 30 percent*," Dawid (1982).
- "*Out of all the times you 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)

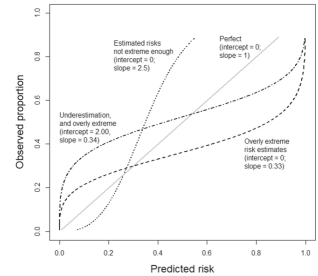
Calibration

- 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 Bier score, from Brier (1950) and Murphy (1973)
- Function plotted in psychological papers Keren (1991)

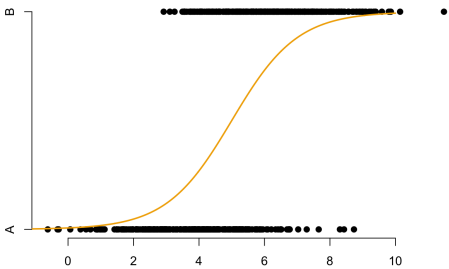


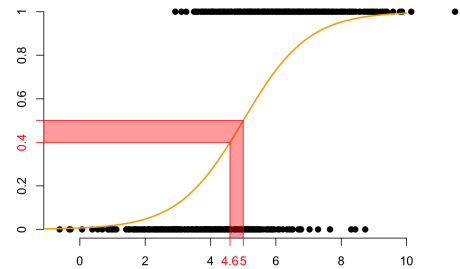


Calibration

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

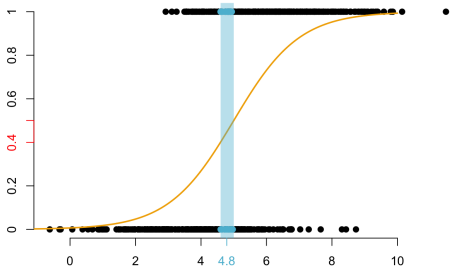
$\widehat{m}(x) = \dfrac{\exp(\widehat{\beta}_0 + \widehat{\beta}_1 x)}{1 + \exp(\widehat{\beta}_0 + \widehat{\beta}_1 x)}$ to estimate $\mathbb{P}[Y = \mathtt{B} | X = x]$ (logistic regression). Given $[p_-, p_+] \subset [0, 1]$ (here $[0.4, 0.5]$), set $\mathcal{I} = \{i : m(\boldsymbol{x}_i) \in [p_-,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

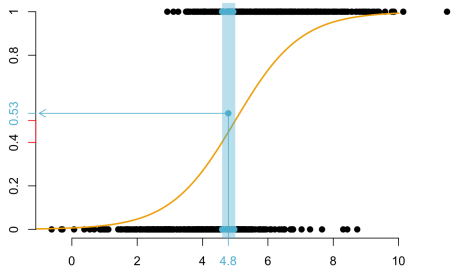




Calibration

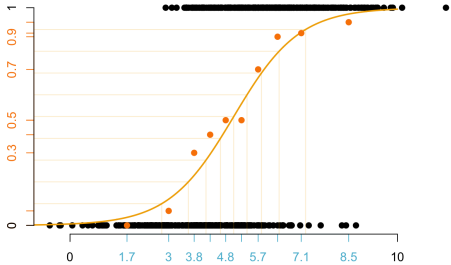
- Given $\mathcal{I} = \{i : m(\boldsymbol{x}_i) \in [p_-, p_+]\}$, set $\overline{y}_{\mathcal{I}} = \dfrac{1}{n_{\mathcal{I}}} \displaystyle\sum_{i \in \mathcal{I}} y_i$

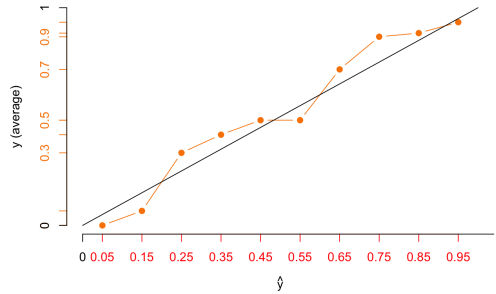




Calibration

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

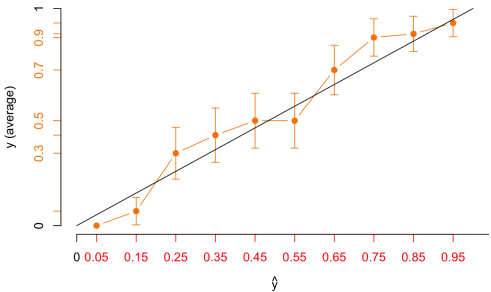


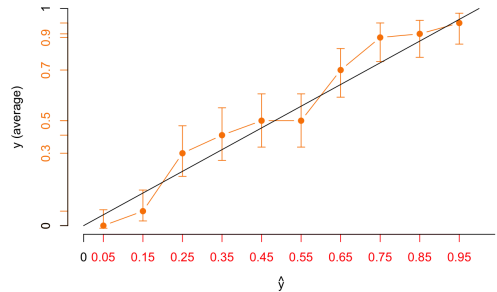


Calibration

- Asymptotic and Agresti and Coull (1998), $\tilde{n} = n + u_{1-\alpha/2}^2$ et $\tilde{p} = \frac{1}{\tilde{n}}\left(n\overline{x} + \frac{u_{1-\alpha/2}^2}{2}\right)$

$$\left[\widehat{p} \pm u_{1-\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}\right], \text{ and } \left[\tilde{p} \pm u_{1-\alpha/2}\sqrt{\frac{\tilde{p}(1-\tilde{p})}{\tilde{n}}}\right]$$

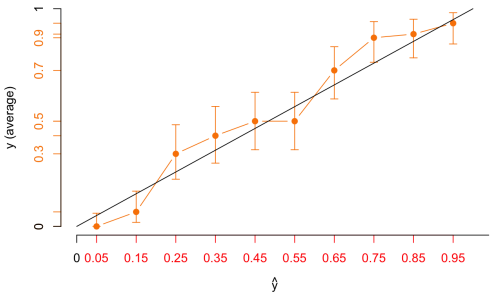


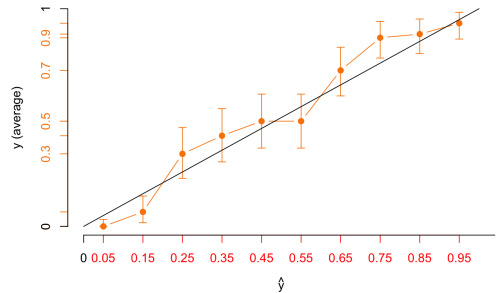


Calibration

- Exact, and Wilson (1927)

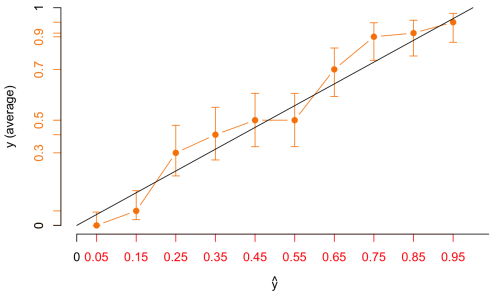
$$\left[\frac{1}{1+\frac{u^2_{1-\alpha/2}}{n}} \left(\hat{p} + \frac{u^2_{1-\alpha/2}}{2n} \right) \pm \frac{u_{1-\alpha/2}}{1+\frac{u^2_{1-\alpha/2}}{n}} \sqrt{\frac{\hat{p}(1-\hat{p})}{n} + \frac{u^2_{1-\alpha/2}}{4n^2}} \right]$$

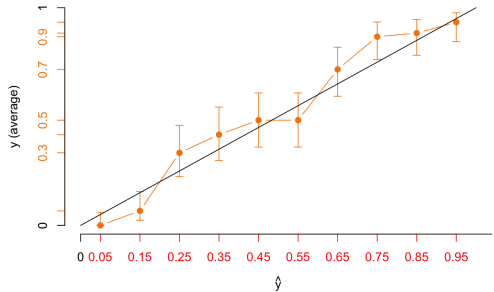




Calibration

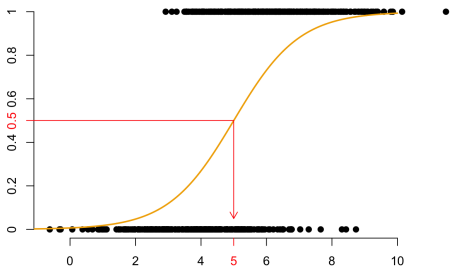
- Bayes and Probit (via `binom.confint` in `binom` package)

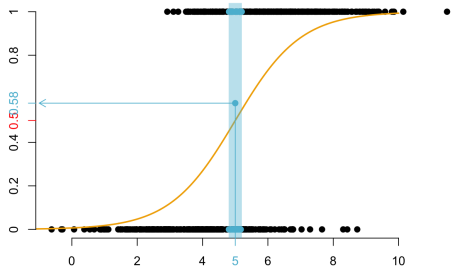




Calibration

- Given $p \in (0,1)$, consider $\mathcal{I}_p = \{i : \widehat{m}(\boldsymbol{x}_i) \in [p-h, p+h]\}$ for some $h > 0$, set $\overline{y}_p = \dfrac{1}{n_{\mathcal{I}_p}} \displaystyle\sum_{i \in \mathcal{I}_p} y_i$

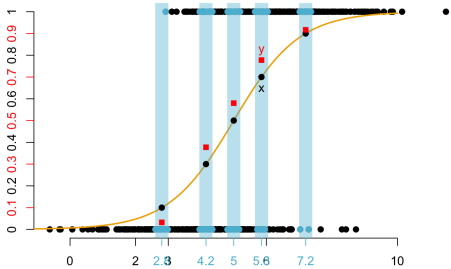


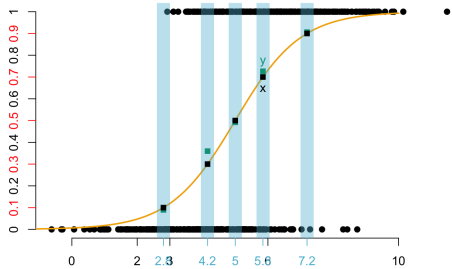


Calibration

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

One could also consider some kermel based average... $\overline{y}_p$

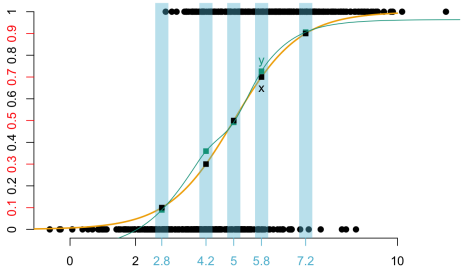


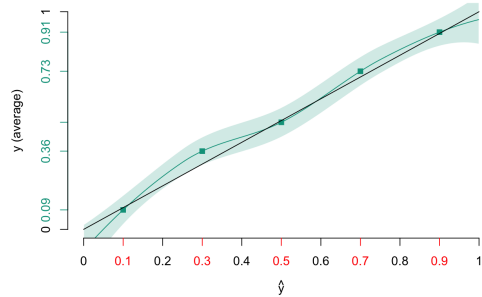


Calibration

- Compute $\overline{y}_p$ for various p, and plot $p \mapsto \overline{y}_p$, that is an estimate of $\mathbb{E}[Y|\widehat{m}(\boldsymbol{X}) = p]$.
- Add a confidence band around.

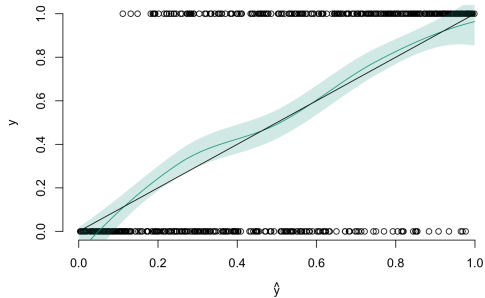
... but here, it works only because $\widehat{m}$ is smooth enough...

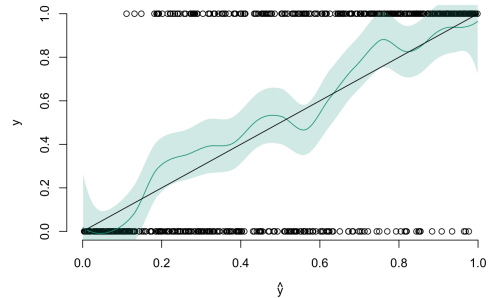




Calibration

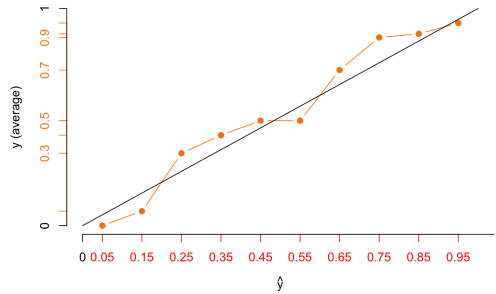
- More generally, consider the local regression of y_i's against $\widehat{y}_i = \widehat{m}(\boldsymbol{x}_i)$'s.





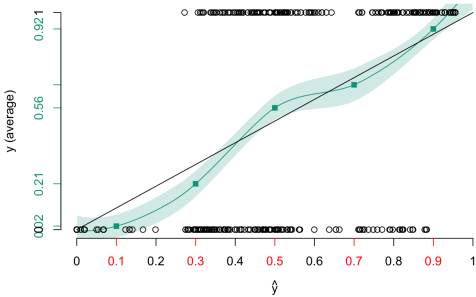
Calibration

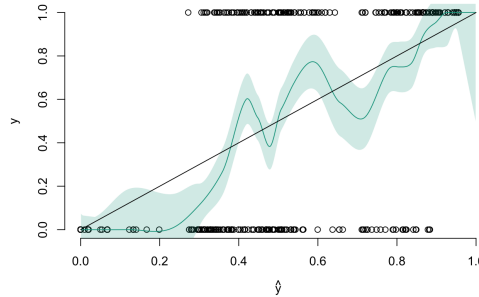
› Consider e.g., some random forest model for $\widehat{m}$, and then the calibration curve per decile,



Calibration

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





Calibration

Definition 4.48: Calibration plot

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

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

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

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

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

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 $\eta_i = \boldsymbol{x}_i^\top \boldsymbol{\beta} = \theta_i$)

$$\nabla \log \mathcal{L} = \boldsymbol{X}^\top(\boldsymbol{y} - \widehat{\boldsymbol{y}}) = \boldsymbol{0}$$

Proposition 4.33: Calibration of GLM

In the GLM framework with the canonical link function, $\widehat{m}(\boldsymbol{x}) = g_\star^{-1}(\boldsymbol{x}_i^\top \widehat{\boldsymbol{\beta}})$ is globally unbiased (on the training dataset), but possibly locally biased.

Calibration

- Otherwise

$$\nabla \log \mathcal{L} = \boldsymbol{X}^\top \boldsymbol{\Omega}(\boldsymbol{y} - \widehat{\boldsymbol{y}}) = \boldsymbol{0},$$

where $\boldsymbol{\Omega}$ is a diagonal matrix ($\boldsymbol{\Omega} = \boldsymbol{W}\boldsymbol{\Delta}$, where $\boldsymbol{W} = \text{diag}((V(\mu_i)g'(\mu_i)^2)^{-1})$ and $\boldsymbol{\Delta} = \text{diag}(g'(\mu_i))$, so that we recognize Fisher information - corresponding to the Hessian matrix (up to a negative sign) – $\boldsymbol{X}^\top \boldsymbol{W}\boldsymbol{X}$).

	training data					validation data				
	$\overline{y}$	GLM	CART	GAM	RF	$\overline{y}$	GLM	CART	GAM	RF
$\widehat{m}(\boldsymbol{x}, s)$	8.73	8.73	8.73	8.73	8.27	8.55	9.05	9.03	8.84	8.70
$\widehat{m}(\boldsymbol{x})$	8.73	8.73	8.73	8.73	8.29	8.55	9.05	9.03	8.84	8.73

Calibration

Definition 4.51: Brier score (binary classifier) Brier (1950)

Brier score is the mean squared error of probability estimate,

$$\text{BS} = \frac{1}{n}\sum_{i=1}^{n}\left(\widehat{m}(\boldsymbol{x}_i), y_i\right)^2$$

- Let g be the calibration function, $g(\widehat{m}(\boldsymbol{x})) \approx p(\boldsymbol{x})$.
- Platt scaling (from Platt et al. (1999)), $g(s) = [1 + e^{-(ws+b)}]^{-1}$.

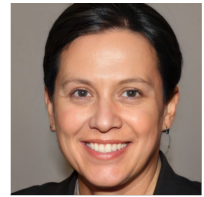
- "confidence" value given by `Picpurify`, using pictures generate by a GAN (a generative adversarial network, used in Hill and White (2020)).

Calibration

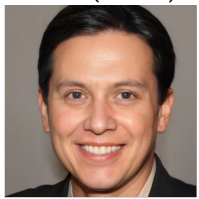
female (0.984)
male (0.016)

female (0.983)
male (0.017)

female (0.982)
male (0.018)

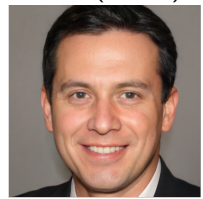


female (0.960)
male (0.040)



female (0.009)
male (0.991)

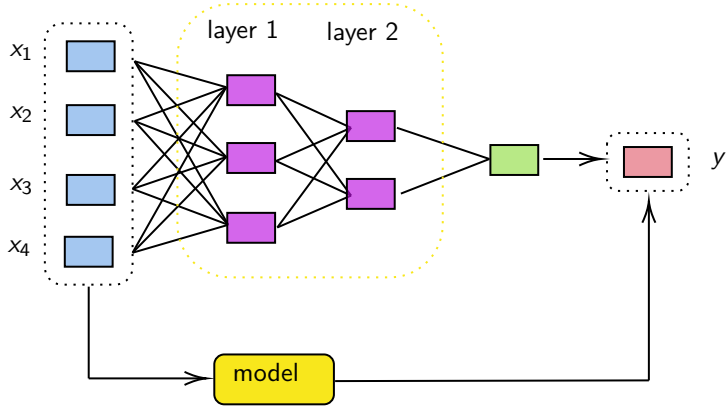
female (0.013)
male (0.987)



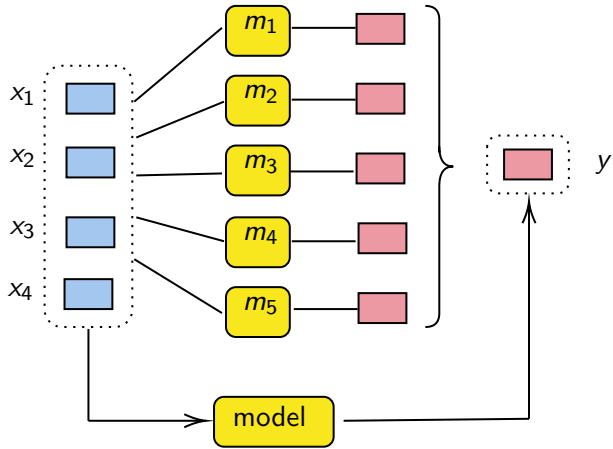
female (0.014)
male (0.986)

female (0.015)
male (0.985)

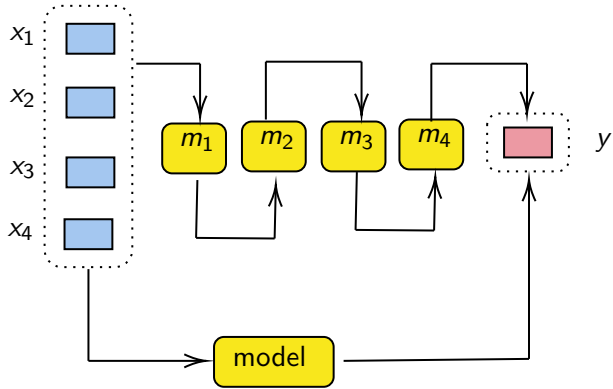
Standard modeling architecture



Standard modeling architecture



Standard modeling architecture

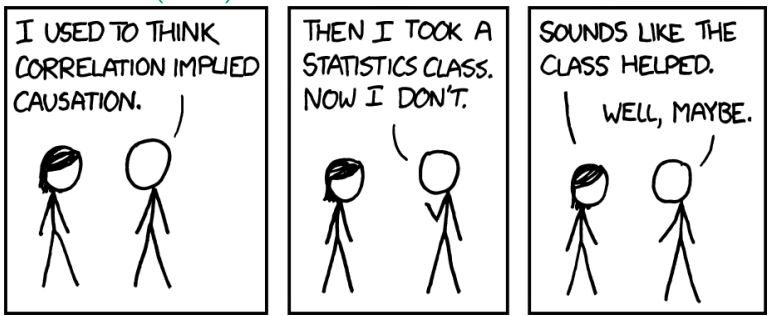


– Part 3 –

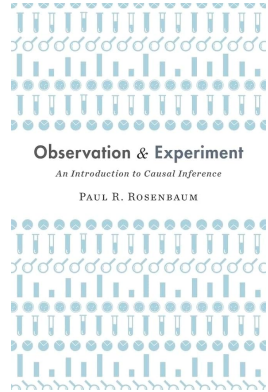
Data

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/



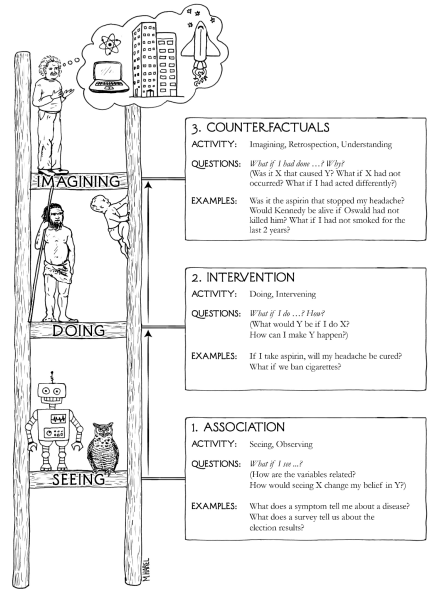
Data (the three rung ladder)

"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 $\varphi : \mathcal{X} \to \mathcal{Z}$ and $\psi : \mathcal{Z} \to \mathcal{Y}$ such that

$$\mathbb{P}[X = \psi(Z)] = \mathbb{P}[\varphi(X) = Z] = 1.$$

Proxy

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.

Independence

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 $\text{Cov}[X, Y] = 0$.

Independence

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 $\text{Cov}[X,Y] = \mathbb{E}\big[(X-\mathbb{E}[X])(Y-\mathbb{E}[Y])\big] = \mathbb{E}[XY]-\mathbb{E}[X]\mathbb{E}[Y]$.

Independence

Proposition 4.34: 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

$$r_{\min} = \frac{\text{Cov}[F_x^{-1}(U), F_y^{-1}(1-U)]}{\sqrt{\text{Var}[X] \cdot \text{Var}[Y]}} \text{ and } r_{\max} = \frac{\text{Cov}[F_x^{-1}(U), F_y^{-1}(U)]}{\sqrt{\text{Var}[X] \cdot \text{Var}[Y]}}$$

- 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).

Independence

Proposition 4.35

Consider two random variables X and Y. $X \perp\!\!\!\perp Y$ if and only if for any functions $\varphi : \mathbb{R} \to \mathbb{R}$ and $\psi : \mathbb{R} \to \mathbb{R}$ (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,

$$r^\star(X, Y) = \max_{\varphi,\psi} \{\text{Corr}[\varphi(X), \psi(Y)]\}.$$

Independence

- HGR because of Hirschfeld (1935), Gebelein (1941) and Rényi (1959) (also Sarmanov (1958a,b)).

$$r^\star(X,Y) = \max_{\varphi\in\mathcal{F}_x,\ \psi\in\mathcal{G}_y} \mathbb{E}[\varphi(X)\psi(Y)],$$

where

$$\begin{cases} \mathcal{F}_x = \{\varphi : \mathcal{X} \to \mathbb{R} : \mathbb{E}[\varphi(X)] = 0 \text{ and } \mathbb{E}[\varphi^2(X)] = 1\} \\ \mathcal{G}_y = \{\psi : \mathcal{Y} \to \mathbb{R} : \mathbb{E}[\psi(Y)] = 0 \text{ and } \mathbb{E}[\psi^2(Y)] = 1\} \end{cases}$$

- See either `ccaPP` or `acepack` package,

```
> ccaPP::maxCorProj(x = x, y = y, method = "pearson")
> corstar = acepack::ace(x = x, y = y)
> cor(corstar$tx, corstar$ty)
```

Proposition 4.36

Consider two random variables X and Y. $X \perp\!\!\!\perp Y$ if and only if $r^\star(X, Y) = 0$.

Proof: Given a random variable X, its characteristic function is $\phi_X(t) = \mathbb{E}[e^{itX}]$. Recall that

$$\begin{cases} \phi_X(t) = \phi_Y(t), \ \forall t \in \mathbb{R} \text{ if and only if } X \overset{\mathcal{L}}{=} Y \\ \phi_{X,Y}(s,t) = \mathbb{E}[e^{i(sX+tY)}] = \phi_X(s) \cdot \phi_Y(t), \ \forall s,t \in \mathbb{R} \text{ if and only if } X \perp\!\!\!\perp Y \end{cases}$$

If $r^\star(X, Y) = 0$, let $s, t \in \mathbb{R}$ and consider $\varphi(x) = \phi_X(x) = \mathbb{E}[e^{ixX}]$ and $\psi(y) = \phi_Y(y) = \mathbb{E}[e^{isY}]$, then $\text{Cov}[e^{isX}, e^{itY}] = \text{Cov}[X'_s, Y'_t] = 0$, i.e. $\mathbb{E}[X'_s Y'_t] = \mathbb{E}[X'_s]\mathbb{E}[Y'_t]$,

$$\underbrace{\mathbb{E}[e^{i(sX+tY)}]}_{\phi_{XY}(s,t)} = \underbrace{\mathbb{E}[e^{isX}] \cdot \mathbb{E}[e^{itY}]}_{\phi_X(s)\cdot\phi_Y(t)}, \ \forall s,t \in \mathbb{R} \text{ i.e. } X \perp\!\!\!\perp Y.$$

Independence

Proposition 4.37

Consider two random variables X and Y such that (X, Y) is a Gaussian vector. Then $r^\star(X, Y) = |\text{Corr[X,Y]}|$.

- See Lancaster (1957, 1958), and Gauss-Hermite decomposition

$$f(x,y) = \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left(-\frac{x^2 - 2\rho xy + y^2}{2\left[1-\rho^2\right]}\right) = \phi(x)\phi(y) \cdot \sum_{i=0}^{\infty} r^i H_i(x) H_i(y)$$

where H_i's are Hermite polynomial.

Independence

- Instead of

$$r^\star(X,Y) = \max_{\varphi\in\mathcal{F}_x,\ \psi\in\mathcal{G}_y} \mathbb{E}[\varphi(X)\psi(Y)],$$

where

$$\begin{cases} \mathcal{F}_x = \{\varphi : \mathcal{X} \to \mathbb{R} : \mathbb{E}[\varphi(X)] = 0 \text{ and } \mathbb{E}[\varphi^2(X)] = 1\} \\ \mathcal{G}_y = \{\psi : \mathcal{Y} \to \mathbb{R} : \mathbb{E}[\psi(Y)] = 0 \text{ and } \mathbb{E}[\psi^2(Y)] = 1\} \end{cases}$$

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 $\bar{\mathcal{G}}_y \subset \mathcal{G}_y$,

$$\bar{r}^\star(X,Y) = \max_{\varphi\in\bar{\mathcal{F}}_x,\psi\in\bar{\mathcal{G}}_y} \{\text{Corr}[\varphi(X),\psi(Y)]\}.$$

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 $\boldsymbol{X}$ and $\boldsymbol{Y}$, in $\mathbb{R}^{d_x}$ and $\mathbb{R}^{d_y}$, respectively. $\boldsymbol{X} \perp \boldsymbol{Y}$ if and only if for any $\boldsymbol{a} \in \mathbb{R}^{d_x}$ and $\boldsymbol{b} \in \mathbb{R}^{d_y}$

$$\text{Cov}[\boldsymbol{a}^\top \boldsymbol{X}, \boldsymbol{b}^\top \boldsymbol{Y}] = 0.$$

Definition 4.61: Independence

In a general context, consider two random vectors $\boldsymbol{X}$ and $\boldsymbol{Y}$. $\boldsymbol{X} \perp\!\!\!\perp \boldsymbol{Y}$ if and only if for any $\mathcal{A} \subset \mathbb{R}^{d_x}$ and $\mathcal{B} \subset \mathbb{R}^{d_y}$,

$$\mathbb{P}[\{\boldsymbol{X} \in \mathcal{A}\} \cap \{\boldsymbol{Y} \in \mathcal{B}\}] = \mathbb{P}[\{\boldsymbol{X} \in \mathcal{A}\}] \cdot \mathbb{P}[\{\boldsymbol{Y} \in \mathcal{B}\}].$$

Independence

Proposition 4.38: Independence

Consider two random vectors $\boldsymbol{X}$ and $\boldsymbol{Y}$. $\boldsymbol{X} \perp\!\!\!\perp \boldsymbol{Y}$ if and only if for any functions $\varphi : \mathbb{R}^{d_x} \to \mathbb{R}$ and $\psi : \mathbb{R}^{d_y} \to \mathbb{R}$ (such that the expected values below exist and are well-defined)

$$\mathbb{E}[\varphi(\boldsymbol{X})\psi(\boldsymbol{Y})] = \mathbb{E}[\varphi(\boldsymbol{X})] \cdot \mathbb{E}[\psi(\boldsymbol{Y})],$$

or equivalently

$$\text{Cov}[\varphi(\boldsymbol{X}), \psi(\boldsymbol{Y})] = 0.$$

Independence

Definition 4.62: Mutual Independence

Let $\boldsymbol{Y} = (Y_1, \cdots, Y_k)$ denote some random vector. All components of $\boldsymbol{Y}$ are (mutually) independent if for any $\mathcal{A}_1, \cdots, \mathcal{A}_k \subset \mathbb{R}$

$$\mathbb{P}\left[\{(Y_1, \cdots, Y_k) \in \bigcap_{i=1}^{k} \mathcal{A}_i\}\right] = \prod_{i=1}^{k} \mathbb{P}[\{Y_i \in \mathcal{A}_i\}].$$

Definition 4.63: Conditional Independence (dimension 2)

X and Y are independent conditionally on Z, denoted $X \perp\!\!\!\perp Y \mid Z$, if for any sets $\mathcal{A}, \mathcal{B}, \mathcal{C} \subset \mathbb{R}$,

$$\mathbb{P}[X \in \mathcal{A}, Y \in \mathcal{B} | Z \in \mathcal{C}] = \mathbb{P}[X \in \mathcal{A} | Z \in \mathcal{C}] \cdot \mathbb{P}[Y \in \mathcal{B} | Z \in \mathcal{C}].$$

Independence

Definition 4.64: Conditional Independence

In a general context, consider three random vectors $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{Z}$. $(\boldsymbol{X} \perp\!\!\!\perp \boldsymbol{Y})|\boldsymbol{Z}$ if and only if for any $\mathcal{A} \subset \mathbb{R}^{d_x}$, $\mathcal{B} \subset \mathbb{R}^{d_y}$ and $\mathcal{C} \subset \mathbb{R}^{d_z}$,

$$\mathbb{P}[\{\boldsymbol{X} \in \mathcal{A}\} \cap \{\boldsymbol{Y} \in \mathcal{B}\}|\boldsymbol{Z} \in \mathcal{C}] = \mathbb{P}[\{\boldsymbol{X} \in \mathcal{A}\}|\boldsymbol{Z} \in \mathcal{C}] \cdot \mathbb{P}[\{\boldsymbol{Y} \in \mathcal{B}\}|\boldsymbol{Z} \in \mathcal{C}].$$

Proposition 4.39

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 4.40: $X \perp Z,\ Y \perp Z \not\Longrightarrow \psi(X, Y) \perp Z$

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 $\psi : \mathbb{R}^2 \to \mathbb{R}$.

$$(X, Y, Z) = \begin{cases} (0,0,0) & \text{with probability } 1/4, \\ (0,1,1) & \text{with probability } 1/4, \\ (1,0,1) & \text{with probability } 1/4, \\ (1,1,0) & \text{with probability } 1/4. \end{cases}$$

Proposition 4.41

Consider a random vector $\boldsymbol{X}$ in $\mathbb{R}^k$, and a random variable Z.
$\boldsymbol{X} \perp Z$ does not imply that $\psi(\boldsymbol{X}) \perp Z$, for any $\psi : \mathbb{R}^k \to \mathbb{R}$.

Independence

Proposition 4.42

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 $\psi : \mathbb{R}^2 \to \mathbb{R}$.

Proposition 4.43

Consider a random vector $\boldsymbol{X}$ in $\mathbb{R}^k$, and a random variable Z.
$\boldsymbol{X} \perp\!\!\!\perp Z$ does not imply either that $\psi(\boldsymbol{X}) \perp Z$ **or** $\psi(\boldsymbol{X}) \perp\!\!\!\perp Z$, for any $\psi : \mathbb{R}^k \to \mathbb{R}$.

Causation

Definition 4.65: Common cause, Reichenbach (1956)

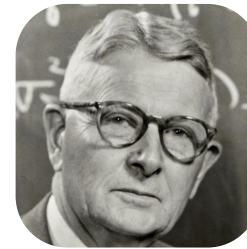
If X and Y are non-independent, $X \not\perp\!\!\!\perp Y$, then, either

$$\begin{cases} X \text{ causes } Y \\ Y \text{ causes } X \\ \text{there exists } Z \text{ such that } Z \text{ causes both } X \text{ and } Y. \end{cases}$$

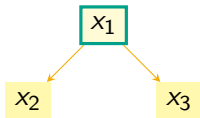
- See also Bollen and Pearl (2013)
- SCM, Goldberger (1972), Duncan (1975) or Bollen (1989)
- Bayesian network, Pearl (1985), Henrion (1988), Charniak (1991)
- Causal path diagrams and probabilistic DAGs, Spirtes et al. (1993)

Causation

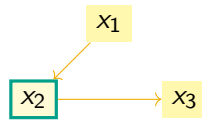
Sewall Wright (see Wright (1921, 1934)) use directed graphs to represent probabilistic cause and effect relationships among a set of variables, and developed path diagrams and path analysis



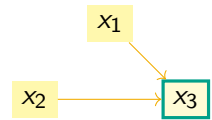
(a)
confounder



(b)
mediator



(c)
collider



Causation

Definition 4.66: Path

A path π 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 $\boldsymbol{x}_i$ is said to be d-separated with another set of nodes $\boldsymbol{x}_j$ by $\boldsymbol{x}_c$ whenever every path from any $x_i \in \boldsymbol{x}_i$ to any $x_j \in \boldsymbol{x}_j$ is blocked by $\boldsymbol{x}_c$. We will simply denote $\boldsymbol{x}_i \perp_{\mathcal{G}} \boldsymbol{x}_j \mid \boldsymbol{x}_c$.

Proposition 4.44

Two nodes x_i and x_j are d-separated by $\boldsymbol{x}_c$ if and only members of $\boldsymbol{x}_c$ 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 $\boldsymbol{x}$, the joint distribution of $\boldsymbol{X}$ satisfies the (global) Markov property with respect to $\mathcal{G}$ if, for any disjoints $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ and $\boldsymbol{x}_c$

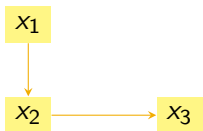
$$\boldsymbol{x}_1 \perp_{\mathcal{G}} \boldsymbol{x}_2 \mid \boldsymbol{x}_c \;\Rightarrow\; \boldsymbol{X}_1 \perp\!\!\!\perp \boldsymbol{X}_2 \mid \boldsymbol{X}_c.$$

Proposition 4.45: Probabilistic graphical model

If $\boldsymbol{X}$ satisfies the (global) Markov property with respect to $\mathcal{G}$

$$\mathbb{P}[x_1, \cdots, x_n] = \prod_{i=1}^{n} \mathbb{P}[x_i | \text{parents}(x_i)]$$

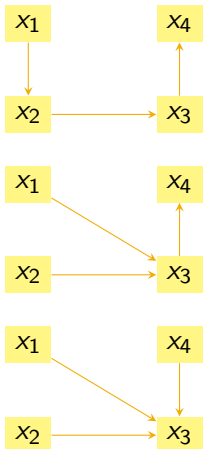
where parents(x_i) are nodes with edges directed towards x_i



› Path from x_1 to x_3 is blocked by x_2, i.e., $x_1 \perp_{\mathcal{G}} x_3 \mid x_2$, or $X_1 \perp\!\!\!\perp X_3 \mid X_2$. 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

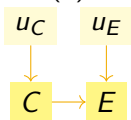
Definition 4.70: Structural Causal Models (SCM)

In a simple causal graph, with two nodes C (the cause) and E (the effect), the causal graph is $C \to E$, and the mathematical interpretation can be summarized in two assignments

$$\begin{cases} C = h_c(U_C) \\ E = h_e(C, U_E), \end{cases}$$

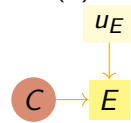
where U_C and U_E are two independent random variables, $U_C \perp\!\!\!\perp U_E$.

(a) observation



$$\begin{cases} C = h_c(U_C) \\ E = h_e(C, U_E) \end{cases}$$

(b) intervention



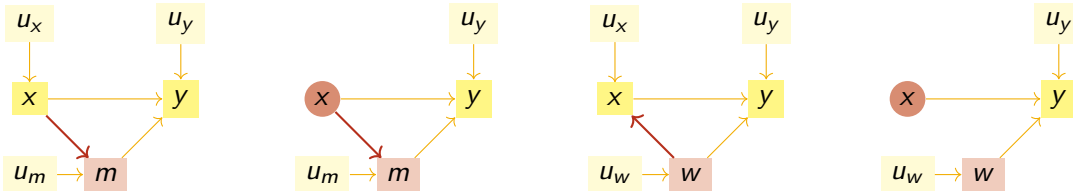
$$\begin{cases} C = c \quad (\text{or } \mathrm{do}(C = c)) \\ E_c^\star = h_e(c, U_E) \end{cases}$$

Intervention

(a) (b) (c) (d)

m mediator variable

w confounding variable



$$\begin{cases} \text{mediator}: & \mathbb{P}[Y_x^\star = 1] = \mathbb{P}[Y = 1|\text{do}(X = x)] = \mathbb{P}[Y = 1|X = x] \\ \text{confusion}: & \mathbb{P}[Y_x^\star = 1] = \mathbb{P}[Y = 1|\text{do}(X = x)] \neq \mathbb{P}[Y = 1|X = x]. \end{cases}$$

Intervention

› In fact, in the presence of a confounding factor, $\mathbb{P}[Y_x^\star = 1]$ 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, $\text{TE} = y^\star_{i,T\leftarrow 1} - y^\star_{i,T\leftarrow 0}$

$$\begin{cases} \text{observation} & : \ y^\star_{i,T\leftarrow 1} \text{ when } t_i = 1 \text{ is observed, and } \boldsymbol{x}_i \\ \text{counterfactual} & : \ y^\star_{i,T\leftarrow 0} \text{ when } t_i = 1 \text{ is observed, and } \boldsymbol{x}_i \end{cases}$$

- Here we want to observe counterfactuals $y^\star_{i,T\leftarrow t'}$ at the individual level.

	Gender	Name	Treatment	Outcome (Weight)				Height	⋯
			t_i	y_i	$y^\star_{i,T\leftarrow 0}$	$y^\star_{i,T\leftarrow 1}$	TE	x_i	⋯
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

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			t_i	y_i	$y^\star_{i,T\leftarrow 0}$	$y^\star_{i,T\leftarrow 1}$	TE	x_i	⋯
1	H	Alex	0	75	75	?	?	172	⋯
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Causal Inference and counterfactuals

Definition 4.71: Average Treatment Effect, Holland (1986)

Given a treatment T, the average treatment effect on outcome Y is

$$\tau = \text{ATE} = \mathbb{E}\big[Y^\star_{t\leftarrow 1} - Y^\star_{t\leftarrow 0}\big].$$

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 $\boldsymbol{X}$,is

$$\tau(\boldsymbol{x}) = \text{CATE}(\boldsymbol{x}) = \mathbb{E}\big[Y^\star_{t\leftarrow 1} - Y^\star_{t\leftarrow 0}\big|\boldsymbol{X} = \boldsymbol{x}\big].$$

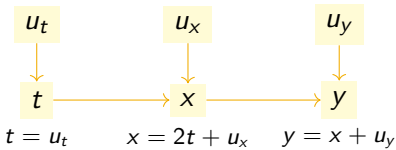
Definition 4.73: Individual Average Treatment Effect

Given a treatment T, the conditional average treatment effect on outcome Y, for individual i, given covariates $\boldsymbol{X}_i$, is

$$\text{IATE}(i) = \mathbb{E}\big[Y^\star_{i,t\leftarrow(1-t_i)} - Y^\star_{i,t\leftarrow t_i}\big].$$

Causal Inference and counterfactuals

- Pearl (2009) suggest to use a twin network representation of the counterfactual



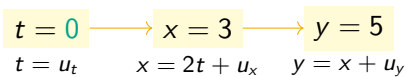
- Start with a simple structural causal model, e.g.,

$$\begin{cases} t = u_t \\ x = 2t + u_t \\ y = x + u_y \end{cases}$$

- Suppose we were able to estimate that model

Causal Inference and counterfactuals

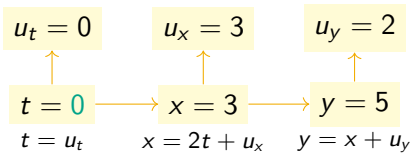
- Pearl (2009) suggest to use a twin network representation of the counterfactual



- Consider a single observation
- i.e. a triplet $(t_i, \boldsymbol{x}_i, y_i)$

Causal Inference and counterfactuals

- Pearl (2009) suggest to use a twin network representation of the counterfactual



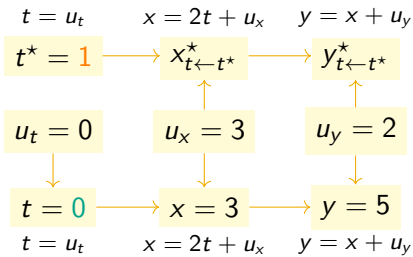
- Inverse the SCM

$$\begin{cases} u_t = t \\ u_t = x - 2t \\ u_y = y - x \end{cases}$$

- From that triplet $(t_i, \boldsymbol{x}_i, y_i)$
- Derive unobserved u's.

Causal Inference and counterfactuals

- Pearl (2009) suggest to use a twin network representation of the counterfactual

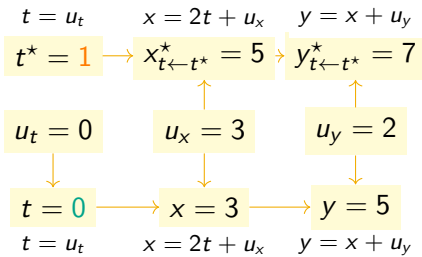


- Suppose that the same SCM holds in the counterfactual world

$$\begin{cases} t^\star \\ x^\star_{t\leftarrow t^\star} = 2t^\star + u_t \\ y^\star_{t\leftarrow t^\star} = x^\star_{t\leftarrow t^\star} + u_y \end{cases}$$

Causal Inference and counterfactuals

- Pearl (2009) suggest to use a twin network representation of the counterfactual

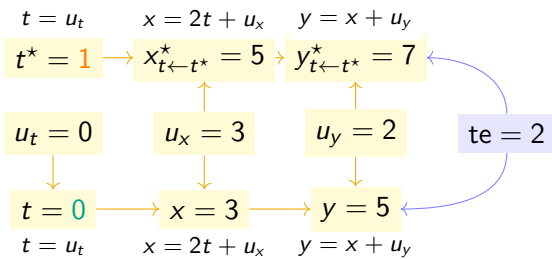


- Plugin u's obtained from $(t_i, \boldsymbol{x}_i, y_i)$

$$\begin{cases} t^\star \\ x^\star_{t\leftarrow t^\star} = 2t^\star + u_t \\ y^\star_{t\leftarrow t^\star} = x^\star_{t\leftarrow t^\star} + u_y \end{cases}$$

Causal Inference and counterfactuals

- Pearl (2009) suggest to use a twin network representation of the counterfactual

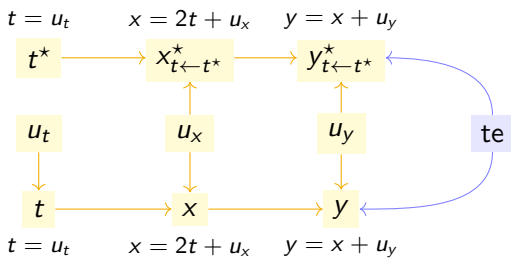


- We can compute the treatment effect

$$\text{te} = y - y^\star_{t\leftarrow t^\star}$$

Causal Inference and counterfactuals

- Pearl (2009) suggest to use a twin network representation of the counterfactual



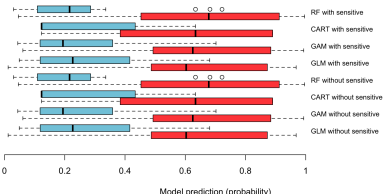
- Works well only if the SCM can be
- inverted (to derive the $\boldsymbol{u}$'s)

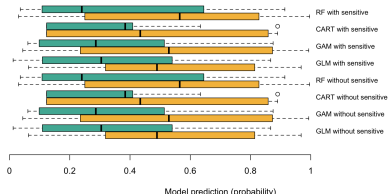
– Part 4 –

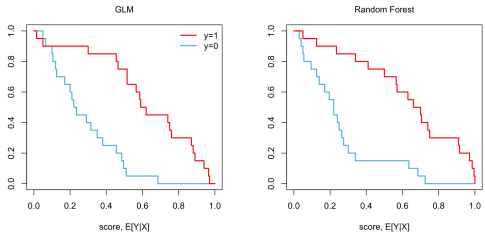
Group Fairness

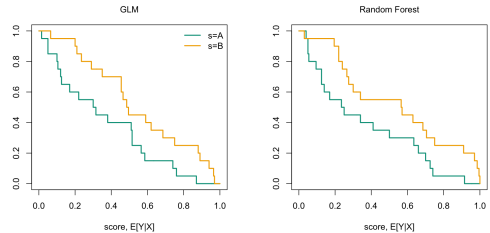
Group Fairness

- Back on `toydata2`, distributions of scores, $\widehat{m}(\boldsymbol{x}_i)$'s conditional on y_i and s_i









Group Fairness

Definition 5.1: 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 $m : \mathcal{X} \to \mathcal{Y}$.

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 5.2: Aware and unaware regression functions μ

The aware regression function is $\mu(\boldsymbol{x}, s) = \mathbb{E}[Y|\boldsymbol{X} = \boldsymbol{x}, S = s]$
and the unaware regression function is $\mu(\boldsymbol{x}) = \mathbb{E}[Y|\boldsymbol{X} = \boldsymbol{x}]$.

Historical Perspective: "Cultural Fairness" and "Statistical Discrimination"

Definition 5.3: Four definitions of cultural fairness, Darlington (1971)

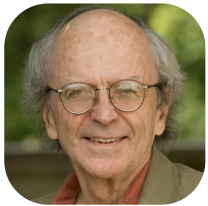
A test $(\widehat{y})$ is considered "culturally fair" if it fits the appropriate equation

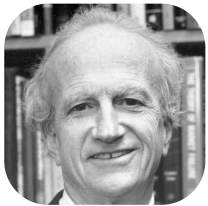
$$\begin{cases} \text{Cor}[S, \widehat{Y}] = \text{Cor}[S, Y]/\text{Cor}[Y, \widehat{Y}] \\ \text{Cor}[S, \widehat{Y}] = \text{Cor}[S, Y] \\ \text{Cor}[S, \widehat{Y}] = \text{Cor}[S, Y] \cdot \text{Cor}[Y, \widehat{Y}] \\ \text{Cor}[S, \widehat{Y}] = 0 \end{cases}$$

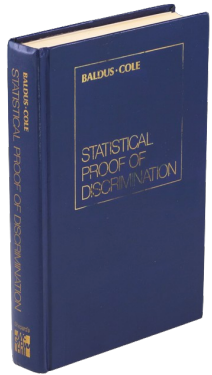
See also Thorndike (1971), Linn and Werts (1971), following Cleary (1968).

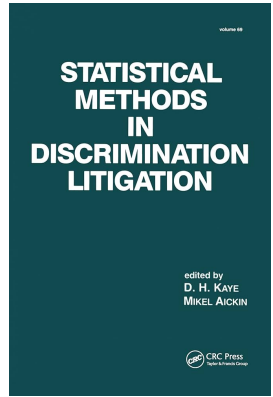
"Economics of Discrimination" and "Statistical Discrimination"

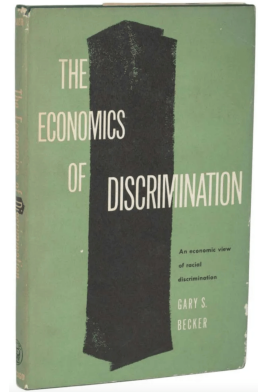
- See Becker (1957) or Baldus and Cole (1980), among (many) others.











Historical Perspective: Decomposition

$$\begin{cases} y_{A:i} = \boldsymbol{x}_{A:i}^\top \boldsymbol{\beta}_A + \varepsilon_{A:i} \quad \text{(group A)}, \ \overline{y}_A = \overline{\boldsymbol{x}}_A^\top \widehat{\boldsymbol{\beta}}_A \\ y_{B:i} = \boldsymbol{x}_{B:i}^\top \boldsymbol{\beta}_B + \varepsilon_{B:i} \quad \text{(group B)}, \ \overline{y}_B = \overline{\boldsymbol{x}}_B^\top \widehat{\boldsymbol{\beta}}_B. \end{cases}$$

- Using ordinary least squares estimates

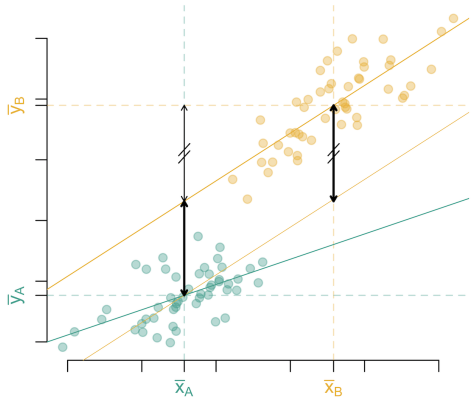
Definition 5.4: Kitagawa (1955), Oaxaca (1973), Blinder (1973)

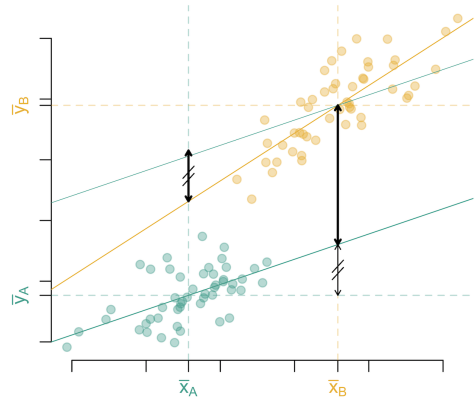
$$\overline{y}_A - \overline{y}_B = \underbrace{\left(\overline{\boldsymbol{x}}_A - \overline{\boldsymbol{x}}_B\right)^\top \widehat{\boldsymbol{\beta}}_B}_{\text{characteristics}} + \underbrace{\overline{\boldsymbol{x}}_A^\top \left(\widehat{\boldsymbol{\beta}}_A - \widehat{\boldsymbol{\beta}}_B\right)}_{\text{coefficients}}, \tag{5}$$

$$\overline{y}_A - \overline{y}_B = \underbrace{\left(\overline{\boldsymbol{x}}_A - \overline{\boldsymbol{x}}_B\right)^\top \widehat{\boldsymbol{\beta}}_A}_{\text{characteristics}} + \underbrace{\overline{\boldsymbol{x}}_B^\top \left(\widehat{\boldsymbol{\beta}}_A - \widehat{\boldsymbol{\beta}}_B\right)}_{\text{coefficients}}. \tag{6}$$

- Also Brown et al. (1980) and Conway and Roberts (1983).

Historical Perspective: Decomposition





$x_A(\widehat{\beta}_A - \widehat{\beta}_B)$ and $(\overline{x}_A - \overline{x}_B)\widehat{\beta}_B$ (as in Equation 5) on the left
$x_B(\widehat{\beta}_A - \widehat{\beta}_B)$ and $(\overline{x}_A - \overline{x}_B)\widehat{\beta}_A$ (as in Equation 6) on the right.

Independence and Demographic Parity

Definition 5.5: Independence, Barocas et al. (2017)

A model m satisfies the independence property if $m(\boldsymbol{Z}) \perp\!\!\!\perp S$, with respect to the distribution $\mathbb{P}$ of the triplet $(\boldsymbol{X}, S, Y)$.

by Solon Barocas, Moritz Hardt and Arvind Narayanan



› For classifiers, one might ask for independence $\widehat{Y} \perp\!\!\!\perp S$ (where $\widehat{y}$ is a class), as Darlington (1971).

Independence and Demographic Parity

Definition 5.6: Demographic Parity, Calders and Verwer (2010), Corbett-Davies et al. (2017)

A decision function $\widehat{y}$ – or a classifier m_t, taking values in $\{0,1\}$ – satisfies demographic parity, with respect to some sensitive attribute S if (equivalently)

$$\begin{cases} \mathbb{P}[\widehat{Y}=1|S=\mathtt{A}] = \mathbb{P}[\widehat{Y}=1|S=\mathtt{B}] = \mathbb{P}[\widehat{Y}=1] \\ \mathbb{E}[\widehat{Y}|S=\mathtt{A}] = \mathbb{E}[\widehat{Y}|S=\mathtt{B}] = \mathbb{E}[\widehat{Y}] \\ \mathbb{P}[m_t(\boldsymbol{Z})=1|S=\mathtt{A}] = \mathbb{P}[m_t(\boldsymbol{Z})=1|S=\mathtt{B}] = \mathbb{P}[m_t(\boldsymbol{Z})=1]. \end{cases}$$

by Toon Calders, Sicco Verwer, Sam Corbett-Davies, Emma Pierson, Sharad Goel, etc

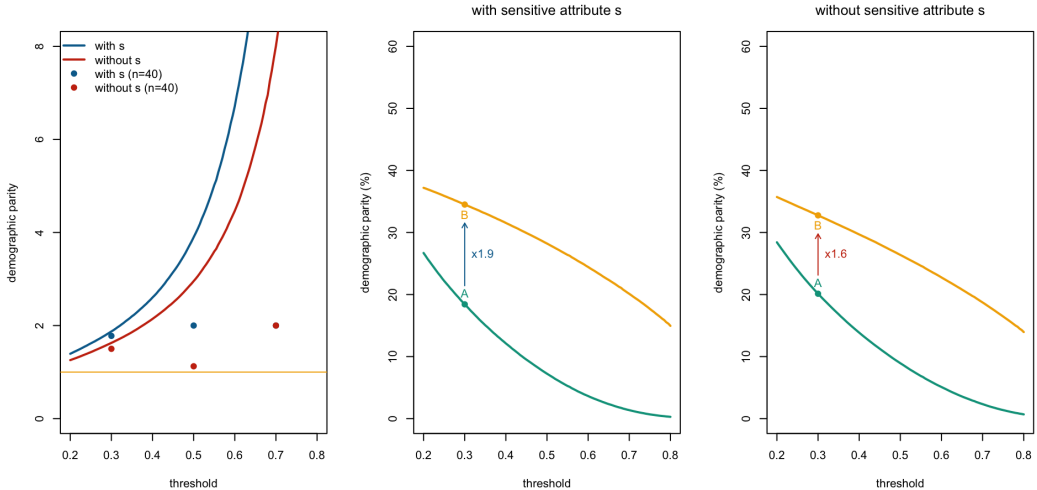
Independence and Demographic Parity

	unaware (without s)				aware (with s)			
	GLM	GAM	CART	RF	GLM	GAM	CART	RF
$n = 1000$, various t, ratio $\mathbb{P}[\widehat{Y} = 1 \vert S = \mathtt{B}]/\mathbb{P}[\widehat{Y} = 1 \vert S = \mathtt{A}]$								
$t = 30\%$	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`)

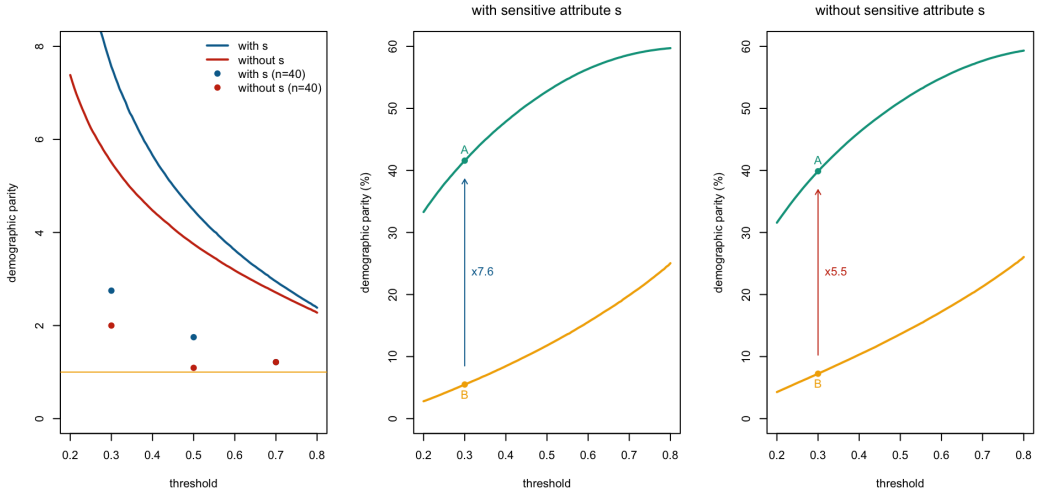
› On the left-hand side, evolution of the ratio ratio $\mathbb{P}[\widehat{Y} = 1 \vert S = \mathtt{B}]/\mathbb{P}[\widehat{Y} = 1 \vert S = \mathtt{A}]$. The horizontal line (at $y = 1$) corresponds to perfect demographic parity. In the middle $t \mapsto \mathbb{P}[m_t(\boldsymbol{X}) > t \vert S = \mathtt{B}]$ and $t \mapsto \mathbb{P}[m_t(\boldsymbol{X}) > t \vert S = \mathtt{A}]$ 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 $\mathbb{P}[\widehat{Y} = 1|S = \texttt{B}]/\mathbb{P}[\widehat{Y} = 1|S = \texttt{A}]$.

Independence and Demographic Parity



- On the left-hand side, evolution of the ratio ratio $\mathbb{P}[\widehat{Y} = 0|S = \mathtt{A}]/\mathbb{P}[\widehat{Y} = 0|S = \mathtt{B}]$

Independence and Demographic Parity

Definition 5.7: Weak Demographic Parity

A decision function $\widehat{y}$ satisfies weak demographic parity if

$$\mathbb{E}[\widehat{Y}|S = \texttt{A}] = \mathbb{E}[\widehat{Y}|S = \texttt{B}].$$

Definition 5.8: Strong Demographic Parity

A decision function $\widehat{y}$ satisfies demographic parity if $\widehat{Y} \perp\!\!\!\perp S$, i.e., for all A,

$$\mathbb{P}[\widehat{Y} \in \mathcal{A}|S = \texttt{A}] = \mathbb{P}[\widehat{Y} \in \mathcal{A}|S = \texttt{B}], \ \forall \mathcal{A} \subset \mathcal{Y}.$$

Independence and Demographic Parity

Proposition 5.1

A model m satisfies the strong demographic parity property if and only if

$$d_{\mathrm{TV}}(\mathbb{P}_{m|\mathtt{A}}, \mathbb{P}_{m|\mathtt{B}}) = d_{\mathrm{TV}}(\mathbb{P}_{\mathtt{A}}, \mathbb{P}_{\mathtt{B}}) = 0.$$

› $d_{\mathrm{TV}}(\mathbb{P}_{m|\mathtt{A}}, \mathbb{P}_{m|\mathtt{B}})$ 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 5.9: Conditional demographic parity, Corbett-Davies et al. (2017)

We will have a conditional demographic parity if (at choice) for all $\boldsymbol{x}$,

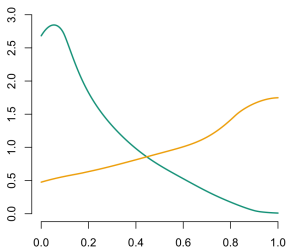
$$\begin{cases} \mathbb{P}[\widehat{Y}=1|\boldsymbol{X}_L=\boldsymbol{x},S=\mathtt{A}]=\mathbb{P}[\widehat{Y}=1|\boldsymbol{X}_L=\boldsymbol{x},S=\mathtt{B}],\ \forall y\in\{0,1\} \\ \mathbb{E}[\widehat{Y}|\boldsymbol{X}_L=\boldsymbol{x},S=\mathtt{A}]=\mathbb{E}[\widehat{Y}|\boldsymbol{X}_L=\boldsymbol{x},S=\mathtt{B}], \\ \mathbb{P}[\widehat{Y}\in\mathcal{A}|\boldsymbol{X}_L=\boldsymbol{x},S=\mathtt{A}]=\mathbb{P}[\widehat{Y}\in\mathcal{A}|\boldsymbol{X}_L=\boldsymbol{x},S=\mathtt{B}],\ \forall\mathcal{A}\subset\mathcal{Y}, \end{cases}$$

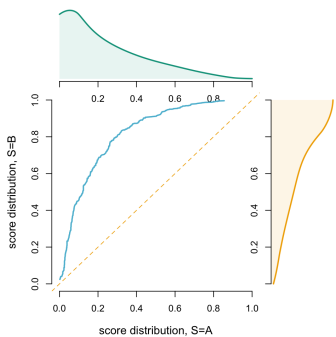
where L denotes a "legitimate" subset of unprotected covariates.

Independence and Demographic Parity

Proposition 5.2

A model m satisfies is strongly fair if and only if $W_2(\mathbb{P}_A, \mathbb{P}_B) = 0$.

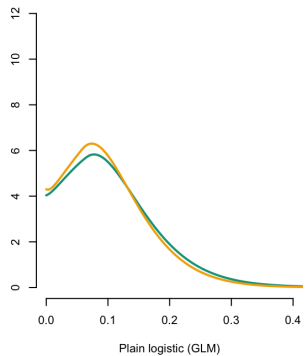


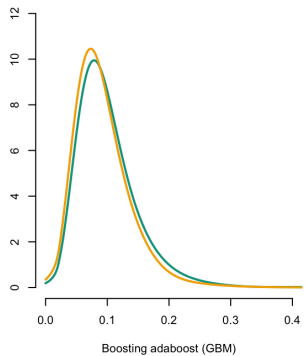


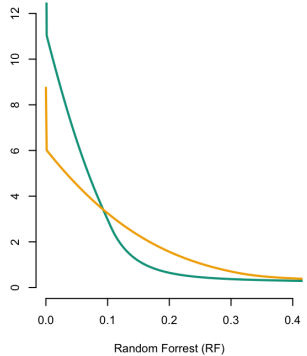

```
> model_glm = glm(y~x1
  +x2+x3, data=
  toydata2, family=
  binomial)
> pred_y_glm = predict
  (model_glm, type="
  response")
> sA = pred_y_glm[
  toydata2$sensitive
  =="A"]
> library(transport)
> wasserstein1d(sA,sB)
[1] 0.3860795
```

Independence and Demographic Parity

- On the `FrenchMotor` dataset, consider GLM, GBM and RF for claim occurence








```
> wasserstein1d(lA,lB)
[1] 0.007220468
```

```
> wasserstein1d(bA,bB)
[1] 0.008895917
```

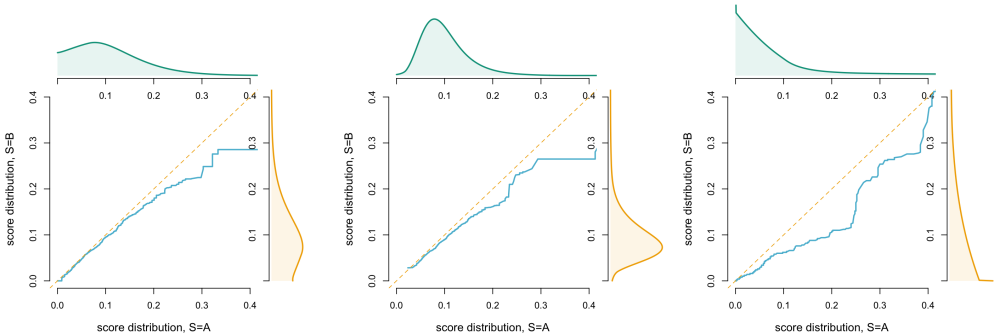
```
> wasserstein1d(fA,fB)
[1] 0.01001088
```

Independence and Demographic Parity

```
> wasserstein1d(lA,lB)
[1] 0.007220468
```

```
> wasserstein1d(bA,bB)
[1] 0.008895917
```

```
> wasserstein1d(fA,fB)
[1] 0.01001088
```



Independence and Demographic Parity

Definition 5.10: Unfairness, Denis et al. (2021); Chzhen and Schreuder (2022)

Given a model m, let $\mathbb{P}_m$ denote the distribution of $m(\boldsymbol{X}, S)$ and $\mathbb{P}_{m|s}$ denote the conditional distribution of $m(\boldsymbol{X}, S)$ given $S = s$, define

$$\begin{cases} \mathcal{U}_{\mathrm{TV}}(m) = \max\limits_{s\in\{\mathtt{A},\mathtt{B}\}} \left\{ d_{\mathrm{TV}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \text{ or } \sum\limits_{s\in\{\mathtt{A},\mathtt{B}\}} d_{\mathrm{TV}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \right. \\ \mathcal{U}_{\mathrm{KS}}(m) = \max\limits_{s\in\{\mathtt{A},\mathtt{B}\}} \left\{ d_{\mathrm{KS}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \right\} \text{ or } \sum\limits_{s\in\{\mathtt{A},\mathtt{B}\}} d_{\mathrm{KS}}(\mathbb{P}_m, \mathbb{P}_{m|s}) \\ \mathcal{U}_{\mathrm{W}_k}(m) = \max\limits_{s\in\{\mathtt{A},\mathtt{B}\}} \left\{ W_k(\mathbb{P}_m, \mathbb{P}_{m|s}) \right\} \text{ or } \sum\limits_{s\in\{\mathtt{A},\mathtt{B}\}} W_k(\mathbb{P}_m, \mathbb{P}_{m|s}) \end{cases}$$

› 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 5.3: Strong Demographic Parity

A model m is strongly fair if and only if $\mathcal{U}(m) = 0$.

Separation and Equalized Odds

Definition 5.11: Separation, Barocas et al. (2017)

A model $m : \mathcal{Z} \to \mathcal{Y}$ satisfies the separation property if $m(\boldsymbol{Z}) \perp\!\!\!\perp S \mid Y$, with respect to the distribution $\mathbb{P}$ of the triplet $(\boldsymbol{X}, S, Y)$.

by Solon Barocas, Moritz Hardt and Arvind Narayanan



Separation and Equalized Odds

Definition 5.12: True positive equality, (Weak) Equal Opportunity, Hardt et al. (2016)

A decision function $\widehat{y}$ – or a classifier $m_t(\cdot)$, taking values in $\{0,1\}$ – satisfies equal opportunity, with respect to some sensitive attribute S if

$$\begin{cases} \mathbb{P}[\widehat{Y}=1|S=\mathtt{A},Y=1]=\mathbb{P}[\widehat{Y}=1|S=\mathtt{B},Y=1]=\mathbb{P}[\widehat{Y}=1|Y=1] \\ \mathbb{P}[m_t(\boldsymbol{Z})=1|S=\mathtt{A},Y=1]=\mathbb{P}[m_t(\boldsymbol{Z})=1|S=\mathtt{B},Y=1]=\mathbb{P}[m_t(\boldsymbol{Z})=1|Y=1], \end{cases}$$

which corresponds to parity of true positives, in the two groups, $\{\mathtt{A},\mathtt{B}\}$.

Separation and Equalized Odds

Definition 5.13: Strong Equal Opportunity

A classifier $m(\cdot)$, taking values in $\{0, 1\}$, satisfies equal opportunity, with respect to some sensitive attribute S if

$$\mathbb{P}[m(\boldsymbol{X}, S) \in \mathcal{A} | S = \texttt{A}, Y = 1] = \mathbb{P}[m(\boldsymbol{X}, S) \in \mathcal{A} | S = \texttt{B}, Y = 1] = \mathbb{P}[m(\boldsymbol{X}, S) \in \mathcal{A} | Y = 1]$$

for all $\mathcal{A} \subset [0, 1]$.

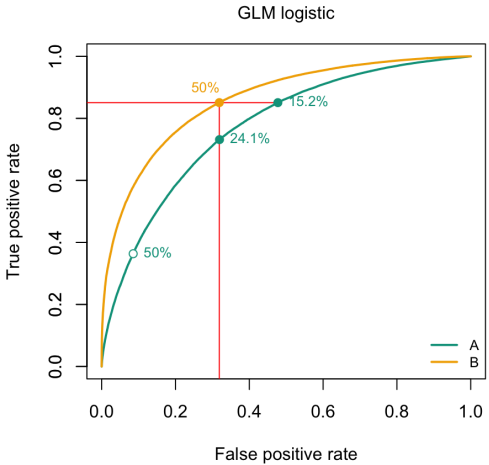
Separation and Equalized Odds

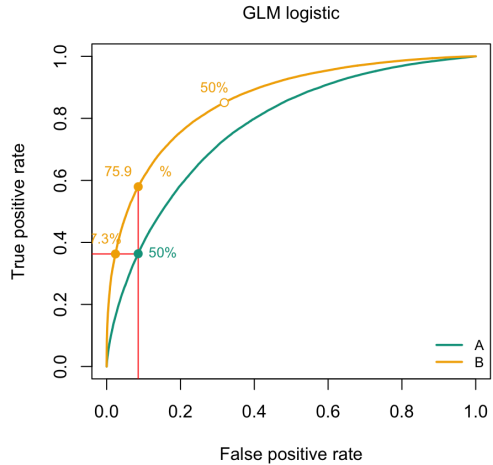
Definition 5.14: False positive equality, Hardt et al. (2016)

A decision function $\widehat{y}$ – or a classifier $m_t(\cdot)$, taking values in $\{0,1\}$ – satisfies parity of false positives, with respect to some sensitive attribute s, if

$$\begin{cases} \mathbb{P}[\widehat{Y}=1|S=\texttt{A},Y=0]=\mathbb{P}[\widehat{Y}=1|S=\texttt{B},Y=0]=\mathbb{P}[\widehat{Y}=1|Y=0] \\ \mathbb{P}[m_t(\boldsymbol{Z})=1|S=\texttt{A},Y=0]=\mathbb{P}[m_t(\boldsymbol{Z})=1|S=\texttt{B},Y=0]=\mathbb{P}[m_t(\boldsymbol{Z})=1|Y=0]. \end{cases}$$

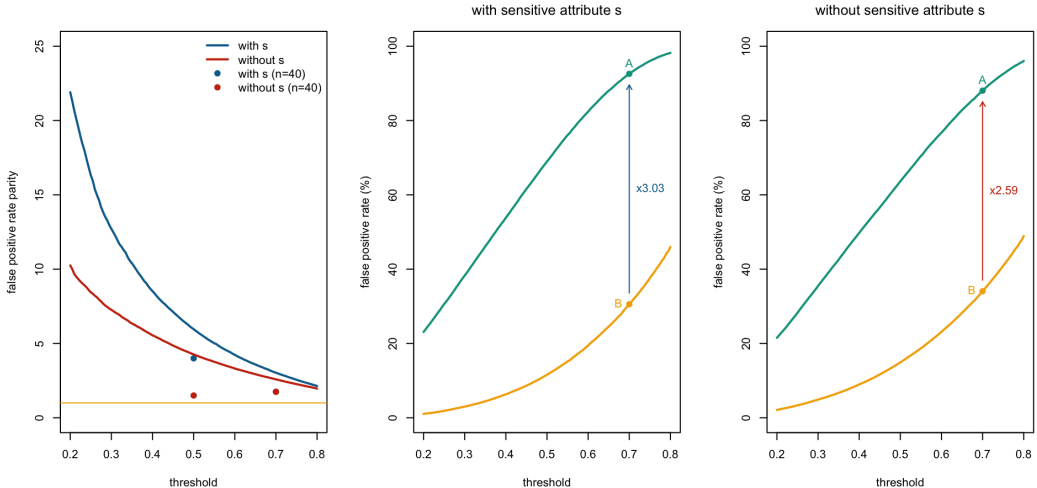
Separation and Equalized Odds





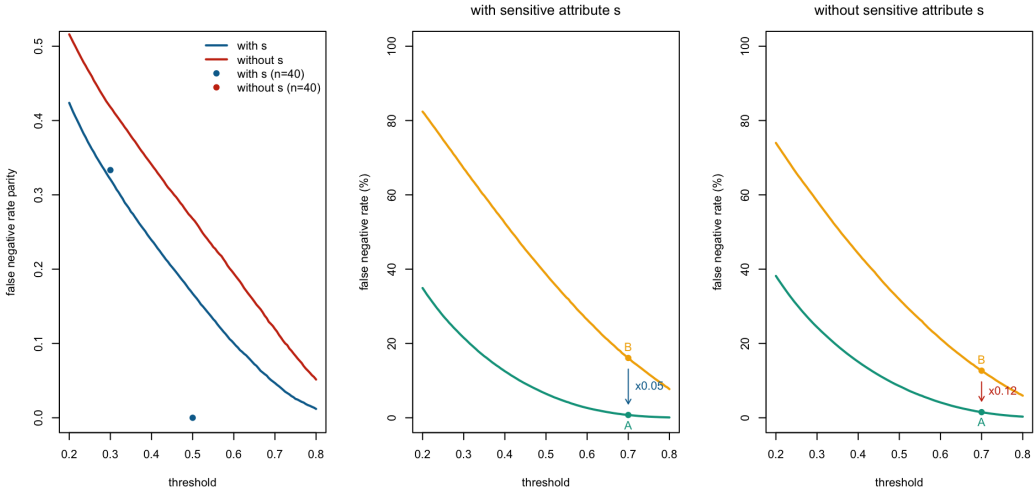
- ROC curves (TPR against FPR) for the logistic regression on `toydata2`.

Separation and Equalized Odds



- Evolution of the false positive rates, `fpr_parity` from `fairness`.

Separation and Equalized Odds



- Evolution of the false negative rates, `fnr_parity` from `fairness`.

Separation and Equalized Odds

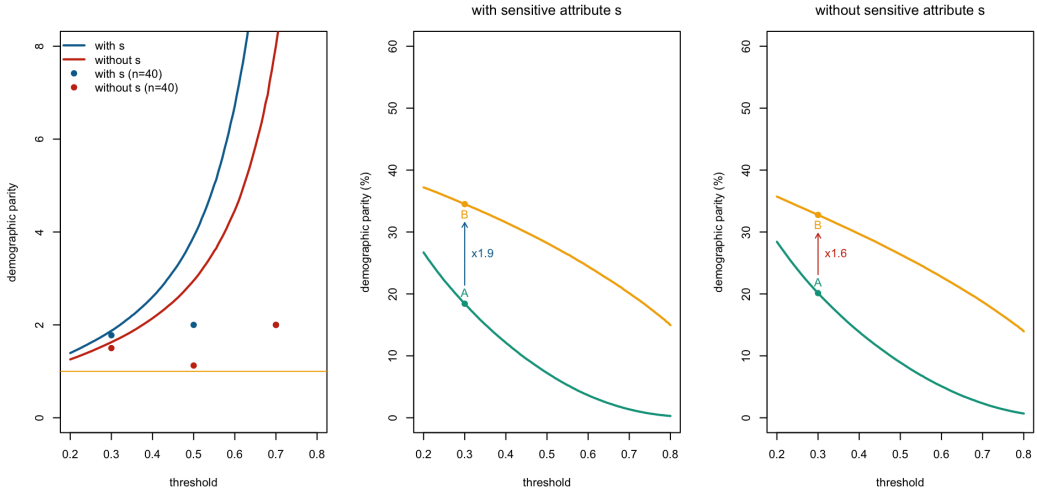
Definition 5.15: Equalized Odds, Hardt et al. (2016)

A decision function $\widehat{y}$ – or a classifier $m_t(\cdot)$ taking values in $\{0,1\}$ – satisfies equal odds constraint, with respect to some sensitive attribute S, if

$$\begin{cases} \mathbb{P}[\widehat{Y}=1|S=\texttt{A},Y=y]=\mathbb{P}[\widehat{Y}=1|S=\texttt{B},Y=y]=\mathbb{P}[\widehat{Y}=1|Y=y],\ \forall y\in\{0,1\} \\ \mathbb{P}[m_t(\boldsymbol{Z})=1|S=\texttt{A},Y=y]=\mathbb{P}[m_t(\boldsymbol{Z})=1|S=\texttt{B},Y=y],\ \forall y\in\{0,1\}, \end{cases},$$

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 ϕ (introduced in Yule (1912)), usually named "Matthews correlation coefficient"

Definition 5.16: ϕ-fairness, Chicco and Jurman (2020)

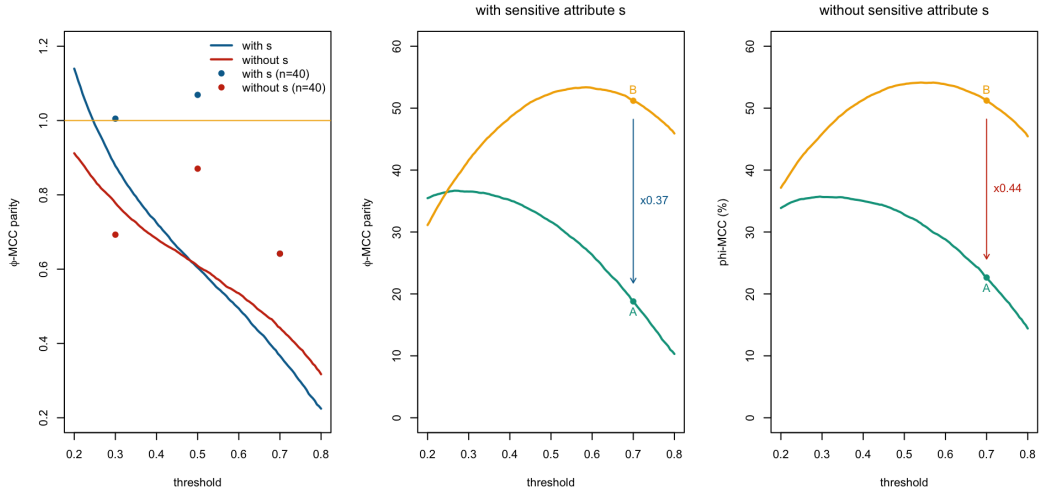
We will have ϕ-fairness if $\phi_{\mathtt{A}} = \phi_{\mathtt{B}}$, where ϕ_s denotes Matthews correlation coefficient for the s group,

$$\phi_s = \frac{\mathrm{TP}_s \cdot \mathrm{TN}_s - \mathrm{FP}_s \cdot \mathrm{FN}_s}{\sqrt{(\mathrm{TP}_s + \mathrm{FP}_s)(\mathrm{TP}_s + \mathrm{FN}_s) \cdot (\mathrm{TN}_s + \mathrm{FP}_s)(\mathrm{TN}_s + \mathrm{FN}_s)}}, \ s \in \{\mathtt{A}, \mathtt{B}\}.$$

› 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 considered later on.

Separation and Equalized Odds



- Evolution of the ϕ-fairness metric

Separation and Equalized Odds

Definition 5.17: Class Balance, Kleinberg et al. (2016)

We will have class balance in the weak sense if

$$\mathbb{E}[m(\boldsymbol{X})|Y=y,S=\texttt{A}]=\mathbb{E}[m(\boldsymbol{X})|Y=y,S=\texttt{B}],\ \forall y\in\{0,1\},$$

or in the strong sense if

$$\mathbb{P}[m(\boldsymbol{X})\in\mathcal{A}|Y=y,S=\texttt{A}]=\mathbb{P}[m(\boldsymbol{X})\in\mathcal{A}|Y=y,S=\texttt{B}],\ \forall\mathcal{A}\subset[0,1],\ \forall y\in\{0,1\}.$$

Separation and Equalized Odds

Definition 5.18: Similar Mistreatement, Zafar et al. (2019)

We will have similar mistreatment, or "*lack of disparate mistreatment*," if

$$\begin{cases} \mathbb{P}[\widehat{Y} = Y | S = \mathtt{A}] = \mathbb{P}[\widehat{Y} = Y | S = \mathtt{B}] = \mathbb{P}[\widehat{Y} = Y] \\ \mathbb{P}[m_t(\boldsymbol{X}) = Y | S = \mathtt{A}] = \mathbb{P}[m_t(\boldsymbol{X}) = Y | S = \mathtt{B}] = \mathbb{P}[m_t(\boldsymbol{X}) = Y]. \end{cases}$$

Definition 5.19: Equality of ROC curves, Vogel et al. (2021)

Let $\text{FRP}_s(t) = \mathbb{P}[m(\boldsymbol{X}) > t | Y = 0, S = s]$ and $\text{TPR}_s(t) = \mathbb{P}[m(\boldsymbol{X}) > t | Y = 1, S = s]$, where $s \in \{\mathtt{A}, \mathtt{B}\}$. Set $\Delta_{TPR}(t) = \text{TPR}_{\mathtt{B}} \circ \text{TPR}_{\mathtt{A}}^{-1}(t) - t$ et $\Delta_{FRP}(t) = \text{FPR}_{\mathtt{B}} \circ \text{FPR}_{\mathtt{A}}^{-1}(t) - t$. We will have fairness with respect to ROC curves if $\|\Delta_{TPR}\|_\infty = \|\Delta_{FPR}\|_\infty = 0$.

Separation and Equalized Odds

Definition 5.20: AUC Fairness, Borkan et al. (2019)

We will have AUC fairness if $\text{AUC}_A = \text{AUC}_B$, where 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 5.21: Sufficiency, Barocas et al. (2017)

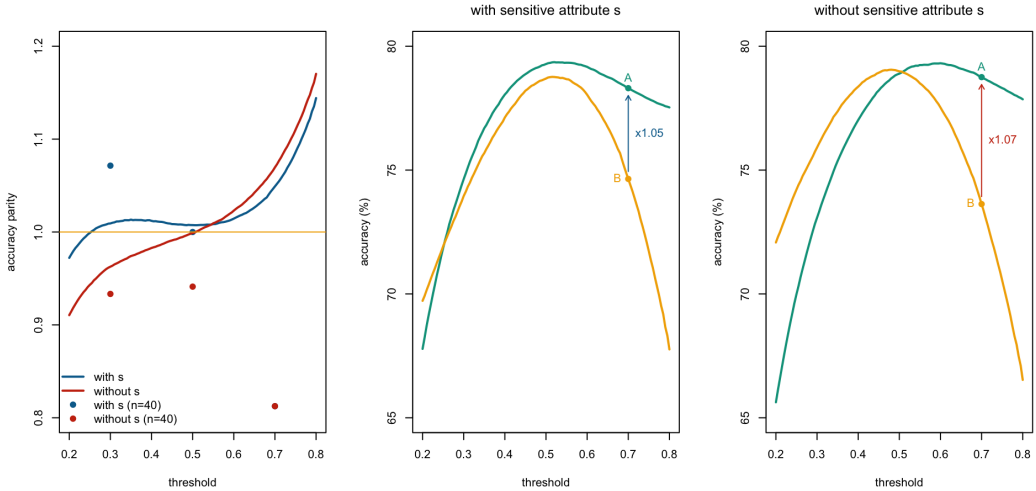
A model $m : \mathcal{Z} \to \mathcal{Y}$ satisfies the sufficiency property if $Y \perp\!\!\!\perp S \mid m(\boldsymbol{Z})$, with respect to the distribution $\mathbb{P}$ of the triplet $(\boldsymbol{X}, S, Y)$.

Definition 5.22: Calibration Parity, Accuracy Parity, Kleinberg et al. (2016), Zafar et al. (2019)

Calibration parity is met if

$$\mathbb{P}[Y = 1 | m(\boldsymbol{X}) = t, S = \texttt{A}] = \mathbb{P}[Y = 1 | m(\boldsymbol{X}) = t, S = \texttt{B}], \ \forall t \in [0, 1].$$

Sufficiency and Calibration



- Evolution of accuracy, in groups A and B.

Sufficiency and Calibration

Definition 5.23: Good Calibration, Kleinberg et al. (2017), Verma and Rubin (2018)

Fairness of good calibration is met if

$$\mathbb{P}[Y = 1 | m(\boldsymbol{X}) = t, S = \mathtt{A}] = \mathbb{P}[Y = 1 | m(\boldsymbol{X}) = t, S = \mathtt{B}] = t, \ \forall t \in [0, 1].$$

Definition 5.24: Non-Reconstruction of Protected Attribute, Kim (2017)

If we cannot tell from the result ($\boldsymbol{x}$, $m(\boldsymbol{x})$, y and $\widehat{y}$) whether the subject was a member of a protected group or not, we will talk about fairness by non-reconstruction of the protected attribute

$$\mathbb{P}[S = \mathtt{A} | \boldsymbol{X}, m(\boldsymbol{X}), \widehat{Y}, Y] = \mathbb{P}[S = \mathtt{B} | \boldsymbol{X}, m(\boldsymbol{X}), \widehat{Y}, Y].$$

Relaxation and Approximate Fairness

Definition 5.25: Disparate Impact, Feldman et al. (2015)

A decision function $\widehat{Y}$ has a disparate impact, for a given threshold τ, if,

$$\min\left\{\frac{\mathbb{P}[\widehat{Y}=1|S=\mathtt{A}]}{\mathbb{P}[\widehat{Y}=1|S=\mathtt{B}]}, \frac{\mathbb{P}[\widehat{Y}=1|S=\mathtt{B}]}{\mathbb{P}[\widehat{Y}=1|S=\mathtt{A}]}\right\} < \tau \text{ (usually 80\%)}.$$

› 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 5.10) unfairness as

$$\mathcal{U}_k(m) = \max_{s\in\{\texttt{A},\texttt{B}\}} \{W_k(\mathbb{P}_m, \mathbb{P}_{m|s})\},$$

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 5.26: ε-Approximate Fairness

Model m is ε-approximately fair if $\mathcal{U}_k(m) \leq \varepsilon \cdot \mathcal{U}_k(m^\star)$, where $m^\star$ is Bayes regressor, for some $\epsilon \geq 0$.

Three different concepts ?

$$\begin{cases} \text{Independence (Definition 5.5)}: & m(\boldsymbol{Z}) \perp\!\!\!\perp S \\ \text{Separation (Definition 5.11)}: & m(\boldsymbol{Z}) \perp\!\!\!\perp S \mid Y \\ \text{Sufficiency (Definition 5.21)}: & Y \perp\!\!\!\perp S \mid m(\boldsymbol{Z}) \end{cases}$$

- 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.

$$\begin{cases} \text{Independence (Definition 5.5)}: & m(\boldsymbol{Z}) \perp\!\!\!\perp S \\ \text{Separation (Definition 5.11)}: & m(\boldsymbol{Z}) \perp\!\!\!\perp S \mid Y \\ \text{Sufficiency (Definition 5.21)}: & Y \perp\!\!\!\perp S \mid m(\boldsymbol{Z}) \end{cases}$$

Proposition 5.4

Suppose that a model m satisfies the independence condition (5.5) and the sufficiency property (5.21), 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 , $S \perp\!\!\!\perp Y \mid m(\boldsymbol{Z})$, then, for $s \in \mathcal{S}$ and $\mathcal{A} \subset \mathcal{Y}$,

$$\mathbb{P}[S = s, Y \in \mathcal{A}] = \mathbb{E}\big[\mathbb{P}[S = s, Y \in \mathcal{A} | m(\boldsymbol{Z})]\big],$$

can be written

$$\mathbb{P}[S = s, Y \in \mathcal{A}] = \mathbb{E}\big[\mathbb{P}[S = s | m(\boldsymbol{Z})] \cdot \mathbb{P}[Y \in \mathcal{A} | m(\boldsymbol{Z})]\big].$$

And from the independence property (5.21), $m(\boldsymbol{Z}) \perp\!\!\!\perp S$, we can write the first component $\mathbb{P}[S = s | m(\boldsymbol{Z})] = \mathbb{P}[S = s]$, almost surely, and therefore

$$\mathbb{P}[S = s, Y \in \mathcal{A}] = \mathbb{E}\big[\mathbb{P}[S = s] \cdot \mathbb{P}[Y \in \mathcal{A} | m(\boldsymbol{Z})]\big] = \mathbb{P}[S = s] \cdot \mathbb{P}[Y \in \mathcal{A}],$$

for all $s \in \mathcal{S}$ and $\mathcal{A} \subset \mathcal{Y}$, corresponding to the independence between S and Y.

Impossibility theorems

Proposition 5.5

Consider a classifier m_t taking values in $\mathcal{Y} = \{0, 1\}$. Suppose that m_t satisfies the independence condition (5.5) and the separation property (5.11), with respect to a sensitive attribute s, then necessarily either $m_t(\boldsymbol{Z}) \perp\!\!\!\perp Y$ or $Y \perp\!\!\!\perp S$ (possibly both).

› Because m_t satisfies the independence condition (5.5), $m_t(\boldsymbol{Z}) \perp\!\!\!\perp S$, and the separation property (5.11), $m_t(\boldsymbol{Z}) \perp\!\!\!\perp S \mid Y$, them, for $\widehat{y} \in \mathcal{Y}$ and for $s \in \mathcal{S}$,

$$\mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}] = \mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y} | S = s] = \mathbb{E}[\mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y} | Y, S = s]],$$

that we can write

$$\mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}] = \sum_y \mathbb{P}\big[m_t(\boldsymbol{Z}) = \widehat{y} | Y = y, S = s\big] \cdot \mathbb{P}\big[Y = y | S = s\big],$$

Impossibility theorems

or

$$\mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}] = \sum_y \mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}|Y = y] \cdot \mathbb{P}[Y = y|S = s],$$

almost surely. Furthermore, we can also write

$$\mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}] = \sum_y \mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}|Y = y] \cdot \mathbb{P}[Y = y],$$

so that, if we combine the two expressions, we get

$$\sum_y \mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}|Y = y] \cdot \Big(\mathbb{P}[Y = y|S = s] - \mathbb{P}[Y = y]\Big) = 0,$$

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

$$\mathbb{P}[m_t(\boldsymbol{Z}) = \widehat{y}|Y = 1] \cdot \Big(\mathbb{P}[Y = 1|S = s] - \mathbb{P}[Y = 1]\Big)$$

Impossibility theorems

or

$$-\mathbb{P}\big[m_t(\boldsymbol{Z}) = \widehat{y}|Y=0\big] \cdot \Big(\mathbb{P}\big[Y=0|S=s\big] - \mathbb{P}\big[Y=0\big]\Big)$$

can be written

$$\mathbb{P}\big[m_t(\boldsymbol{Z}) = \widehat{y}|Y=0\big] \cdot \Big(\mathbb{P}\big[Y=1|S=s\big] - \mathbb{P}\big[Y=1\big]\Big).$$

Thus, either $\mathbb{P}\big[Y=1|S=s\big] - \mathbb{P}\big[Y=1\big]$ almost surely, or $\mathbb{P}\big[m_t(\boldsymbol{Z}) = \widehat{y}|Y=0\big] = \mathbb{P}\big[m_t(\boldsymbol{Z}) = \widehat{y}|Y=1\big]$ (or both).

- Of course, the previous proposition holds only when y is a binary variable.

Impossibility theorems

Proposition 5.6

Consider a classifier m_t taking values in $\mathcal{Y} = \{0, 1\}$. Suppose that m_t satisfies the sufficiency condition (5.21) and the separation property (5.11), with respect to a sensitive attribute s, then necessarily either $\mathbb{P}[m_t(\boldsymbol{Z}) = 1|Y = 1] = 0$ or $Y \perp\!\!\!\perp S$ or $m_t(\boldsymbol{Z}) \perp\!\!\!\perp Y$.

› Suppose that m_t satisfies the sufficiency condition (5.21) and the separation property (5.11), respectively $Y \perp\!\!\!\perp S \mid m_t(\boldsymbol{Z})$ and $m_t(\boldsymbol{Z}) \perp\!\!\!\perp S \mid Y$. For all $s \in \mathcal{S}$, we can write, using Bayes formula

$$\mathbb{P}[Y = 1|S = s, m_t(\boldsymbol{Z}) = 1] = \frac{\mathbb{P}[m_t(\boldsymbol{Z}) = 1|Y = 1, S = s] \cdot \mathbb{P}[Y = 1|S = s]}{\mathbb{P}[m_t(\boldsymbol{Z}) = 1|S = s]},$$

Impossibility theorems

i.e.,

$$\mathbb{P}[Y=1|S=s,m_t(\boldsymbol{Z})=1]=\frac{\mathbb{P}[m_t(\boldsymbol{Z})=1|Y=1]\cdot\mathbb{P}[Y=1|S=s]}{\sum_{y\in\{0,1\}}\mathbb{P}[m_t(\boldsymbol{Z})=1|Y=y]\cdot\mathbb{P}[Y=1|S=s]},$$

that should not depend on s (from the sufficiency property). So a similar property holds if $S=s'$. Observe further that $\mathbb{P}[m_t(\boldsymbol{Z})=1|Y=1]$ is the *true positive rate* (TPR) while $\mathbb{P}[m_t(\boldsymbol{Z})=1|Y=0]$ is the *false positive rate* (TPR). Let $p_s=\mathbb{P}[Y=1|S=s]$, so that

$$\mathbb{P}[Y=1|S=s,m_t(\boldsymbol{Z})=1]=\frac{\text{TPR}}{p_s\cdot\text{TPR}+(1-p_s)\cdot\text{FPR}}.$$

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 $\text{TPR} = \mathbb{P}[m_t(\boldsymbol{Z}) = 1|Y = 1] = 0$ as stated in the proposition), then

$$(p_s - p_{s'}) \cdot \text{TPR} = (p_s - p_{s'}) \cdot \text{FPR} \neq 0,$$

and therefore $m_t(\boldsymbol{Z}) \perp\!\!\!\perp Y$.

– Part 5 –

Individual Fairness

Individual Fairness

Definition 6.1: 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)

$$D_y(m(\boldsymbol{x}_i, s_i), m(\boldsymbol{x}_j, s_j)) \leq L \cdot D_x(\boldsymbol{x}_i, \boldsymbol{x}_j), \ \forall i, j = 1, \cdots, n,$$

for some $L < \infty$.

Individual Fairness

Definition 6.2: 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

$$\mathbb{E}_{(\boldsymbol{X},S)}\left[\limsup_{\boldsymbol{x}':D_x(\boldsymbol{X},\boldsymbol{x}')\to 0}\frac{D_y(m(\boldsymbol{X},S),m(\boldsymbol{x}',S))}{D_x(\boldsymbol{X},\boldsymbol{x}')}\right]\leq L<\infty.$$

Individual Fairness

Definition 6.3: Proxy Based Fairness, Kilbertus et al. (2017)

A decision making process $\widehat{y}$ exhibits no proxy discrimination with respect to sensitive attribute s if

$$\mathbb{E}\big[\widehat{Y}\big|\text{do}(S=\texttt{A})\big]=\mathbb{E}\big[\widehat{Y}\big|\text{do}(S=\texttt{B})\big].$$

Definition 6.4: Fairness on Average Treatment Effect, Kusner et al. (2017)

We achieve fairness on average treatment effect (counterfactual fairness on average)

$$\text{ATE}=\mathbb{E}\big[Y^\star_{S\leftarrow\texttt{A}}-Y^\star_{S\leftarrow\texttt{B}}\big]=0.$$

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 6.5: Counterfactual Fairness, Kusner et al. (2017)

We achieve counterfactual fairness for an individual with characteristics $\boldsymbol{x}$ if

$$\text{CATE}(\boldsymbol{x}) = \mathbb{E}\big[Y^{\star}_{S\leftarrow \text{A}} - Y^{\star}_{S\leftarrow \text{B}} \big| \boldsymbol{X} = \boldsymbol{x}\big] = 0.$$

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