

Insurance, biases, discrimination & fairness

Arthur Charpentier

2024

– Part 2 –

Models

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 ℓ

A **loss function** ℓ 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

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

Definition 4.4: Minimax Estimator

An estimator is **minimax** if its maximal risk is minimal among all estimators. The minimax risk is, for a set \mathcal{P} of distributions,

$$R(\mathcal{P}) = \inf_{\hat{m} \in \mathcal{M}} \left\{ \sup_{(\mathbf{X}, Y) \sim \mathbb{P} \in \mathcal{P}} \{ \mathbb{E}_{\mathbb{P}} [\ell(\hat{m}(\mathbf{X}), Y)] \} \right\}.$$

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 4.5: 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 4.6: 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 μ consider a classifier based on \hat{m}

Definition 4.7: 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 4.8: 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 ℓ_2 is used

Definition 4.9: Quadratic loss, ℓ_2

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

- › Observe that

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

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 μ 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 ℓ_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 4.10: 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 Σ 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, $\|\vec{u}\| = 0 \iff \vec{u} = \vec{0}$

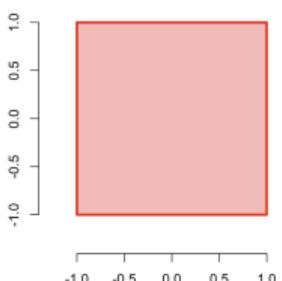
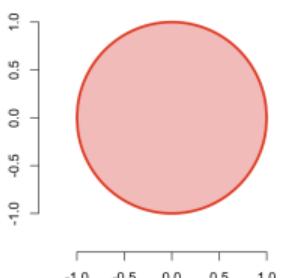
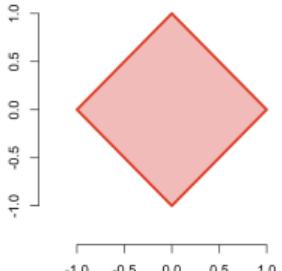
ℓ_1 norm: $\|\mathbf{x}\|_{\ell_1} = |x_1| + \cdots + |x_n|,$

ℓ_2 norm: $\|\mathbf{x}\|_{\ell_2} = \sqrt{x_1^2 + \cdots + x_n^2},$

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

ℓ_∞ 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 ℓ_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 4.11: Quantile loss, $\ell_{q,\alpha}$

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

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

- 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 4.12: 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*”



Illustration de Gustave Doré (1876)

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 4.13: 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 ψ 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 4.14: 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 4.15: 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 4.16: 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 4.17: 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 4.18: 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 4.19: 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 4.20: 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 ,

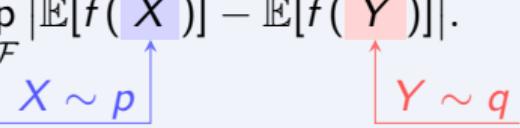
$$\mathbb{E}(\nabla_{\theta}D(\hat{p}_n, q_{\theta})) = \nabla_{\theta}D(p, q_{\theta}).$$

- › 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 4.21: 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

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


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 4.22: Projection, Bregman (1967), Bauschke et al. (1997)

Given a strictly convex function continuously differentiable ψ and the associated Bregman divergence D_ψ , 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_ψ , 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^ψ denote the orthogonal on K_i based on D_ψ ,

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

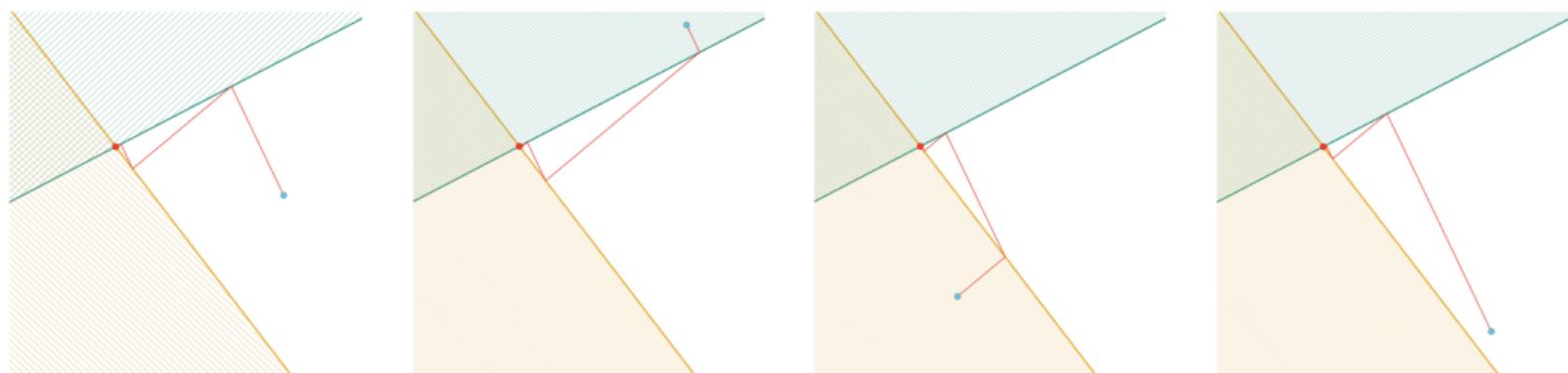
and consider the following iterative sequence of projections, until some $\mathbf{x}_j \in K$,

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

Distance Between Distributions

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

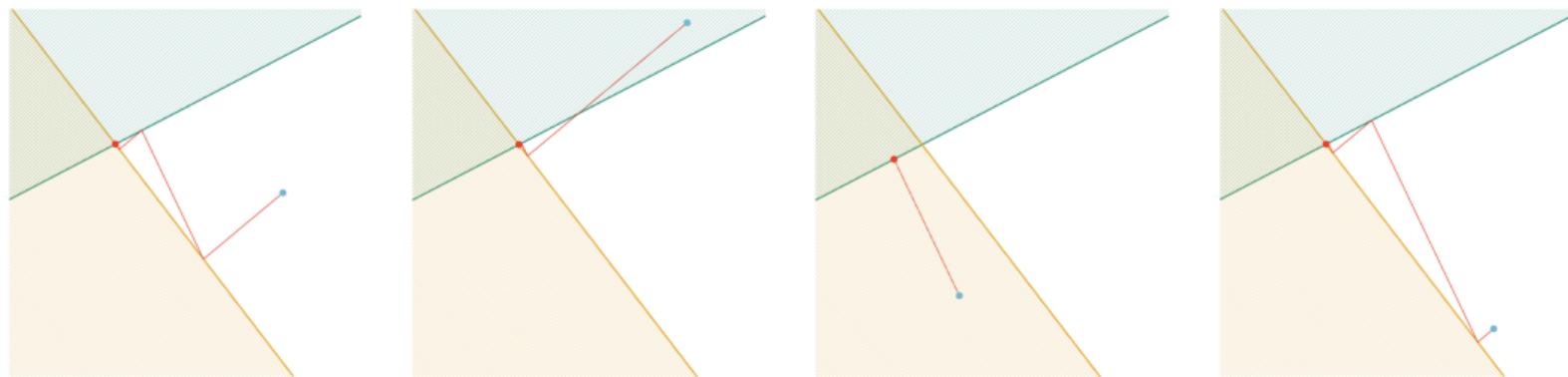
until some $x_j \in K$, see Boyle and Dykstra (1986) for the original idea



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 4.23: 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 distributions, 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

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

then use $B(a, b) = B(a, b) = \int_0^1 t^{a-1} (1-t)^{b-1} dt = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$.

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_ψ with $\psi(x) = \sum_{i=1}^n x_i^2$

Distance Between Distributions

Definition 4.24: Pearson/Neyman χ -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_ψ with $\psi_P(\mathbf{x}) = -2 \sum_{i=1} \sqrt{x_i}$ and $\psi_N(\mathbf{x}) = \sum_{i=1} x_i^{-1}$.
- › d_χ 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 4.25: 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 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 4.26: Kolmogorov-Smirnov, [Kolmogorov \(1933\)](#); ?

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 4.27: Entropy, Shannon (1948)

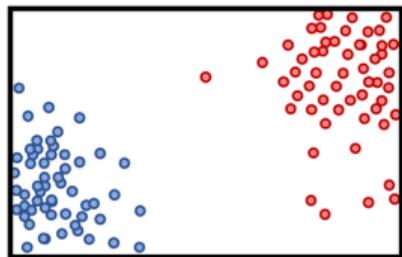
The entropy associated with distribution p is

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

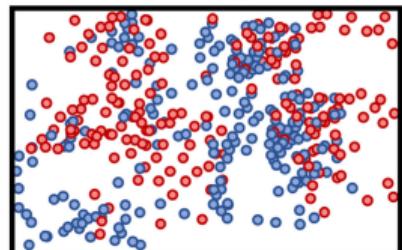
and define cross-entropy (of q relative to p) as

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

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



Low Entropy



High Entropy

Distance Between Distributions

Definition 4.28: 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

and

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

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_θ , 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 4.29: 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 4.30: 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 4.31: 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 ψ -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 α , $H_\alpha(X) = \frac{1}{1-\alpha} \log \left(\sum_i p(i)^\alpha \right)$, define

Definition 4.32: Rényi α -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 4.33: Cramér, Cramér (1928a,b) and Székely (2003)

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

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

- › 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

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

$\uparrow \quad \uparrow \quad \uparrow$
 k k' $X \sim p$ $Y \sim q$

\uparrow
 $k^{-1} + k'^{-1} = 1$

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

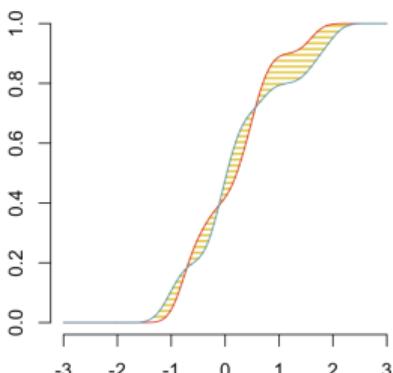
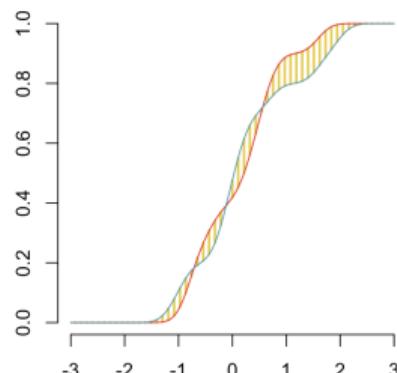
- › For example, if $k = 1$, $\|\nabla f\|_\infty \leq 1$ (corresponding to 1-Lipschitz functions).

Distance Between Distributions

Definition 4.34: Wasserstein, Wasserstein (1969)

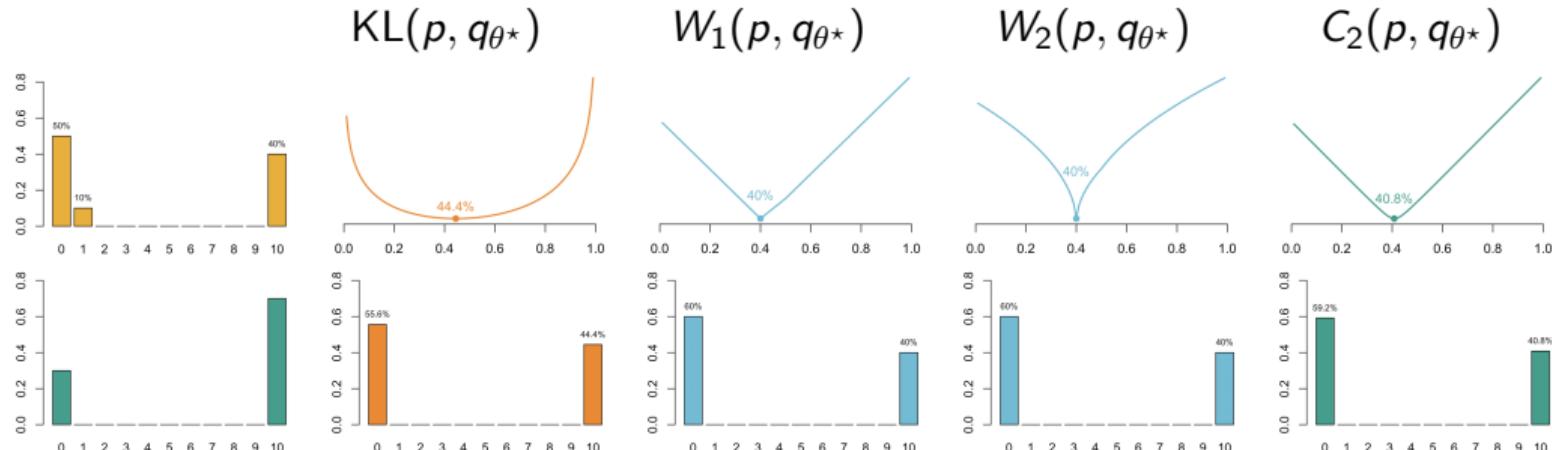
Consider two measures on p and q on \mathbb{R} . Then define **Wasserstein distance**

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



Distance Between Distributions

- › μ : multinomial distribution on $\{0, 1, 10\}$, with $p = (.5, .1, .4)$
- › ν_θ : binomial type distribution on $\{0, 10\}$, with $q_\theta = (1 - \theta, \theta)$
- › Let $\theta^* = \operatorname{argmin}\{d(p, q_\theta)\}$



Distance Between Distributions

Proposition 4.19

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 4.20

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 4.21

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 4.22: 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

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

≥ 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 \(1974\)](#),

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

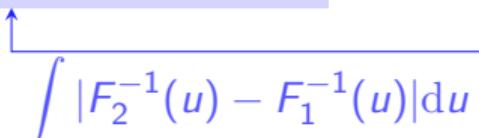
Distance Between Distributions

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

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

Example let $p_1 \leq p_2$

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

Proposition 4.23: 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 Γ define the covariance matrix of $(\mathbf{X}_1, \mathbf{X}_2)$,

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

Distance Between Distributions

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)

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

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.

Distance Between Distributions

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

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

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.

- Let us spend some time on the Wasserstein distance... and associated concepts.

Optimal transport

Definition 4.35: Wasserstein, Wasserstein (1969)

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

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

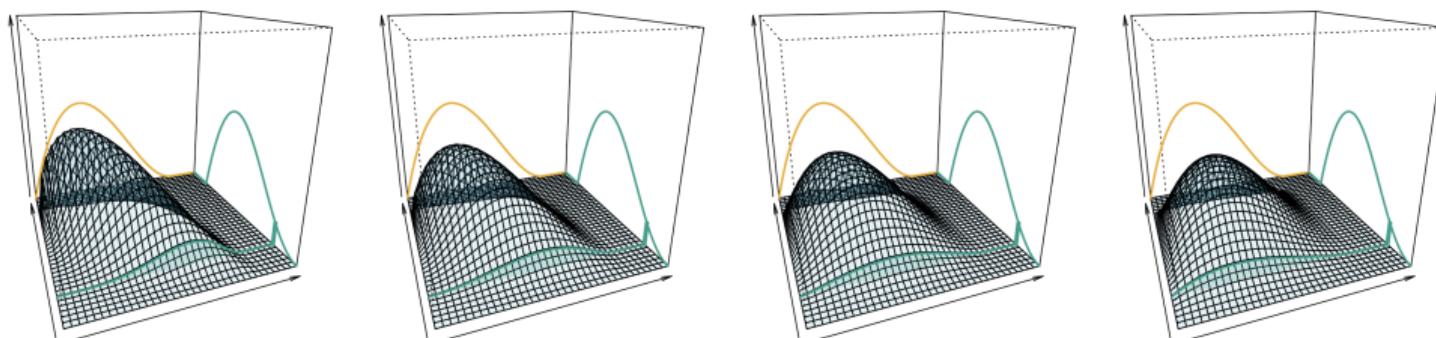
where $\Pi(p, q)$ is the set of all couplings of p and q .

- One can prove that $W_1(p, q) \leq W_k(p, q)$ for all $k \geq 1$. And because of Jensen's inequality, if $k \leq k'$,

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

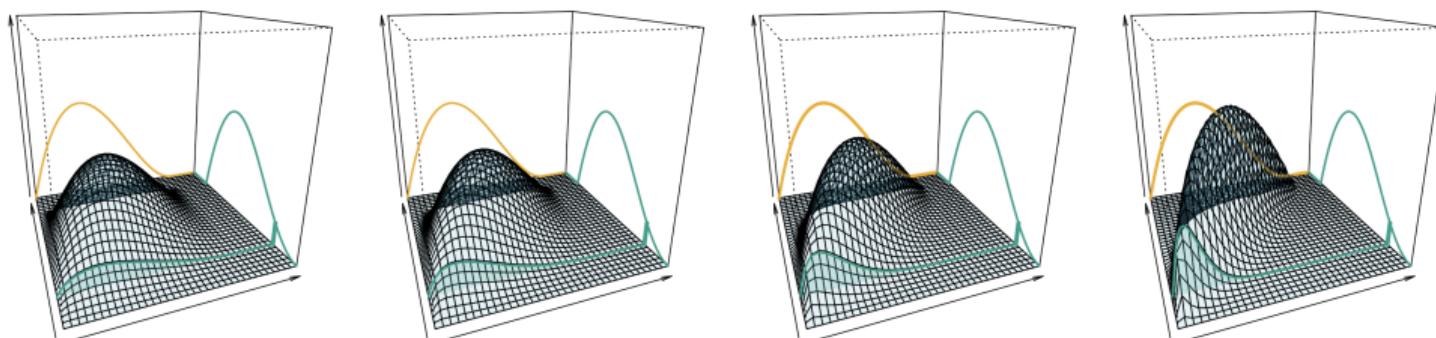
Optimal transport

- › Wasserstein/Monge-Kantorovich distance between probability measures \mathbb{P}_A and \mathbb{P}_B : how much (kinetic) energy does it require to move a mass from \mathbb{P}_A to \mathbb{P}_B ?
- › $\Pi(\mathbb{P}_A, \mathbb{P}_B)$ denotes the set of **joint probabilities** with “marginals” \mathbb{P}_A and \mathbb{P}_B



Optimal transport

- › Wasserstein/Monge-Kantorovich distance between probability measures \mathbb{P}_A and \mathbb{P}_B : how much (kinetic) energy does it require to move a mass from \mathbb{P}_A to \mathbb{P}_B ?
- › $\Pi(\mathbb{P}_A, \mathbb{P}_B)$ denotes the set of **joint probabilities** with “marginals” \mathbb{P}_A and \mathbb{P}_B



Optimal transport

- › If $\pi \in \Pi(\mathbb{P}_A, \mathbb{P}_B)$, for all \mathcal{A} and \mathcal{B} ,

$$P(\mathcal{A} \times \mathcal{Y}) = \mathbb{P}_A(\mathcal{A}) \text{ and } P(\mathcal{X} \times \mathcal{B}) = \mathbb{P}_B(\mathcal{B})$$

or, put differently, for all ψ and φ ,

$$\int_{\mathcal{X} \times \mathcal{Y}} (\psi(\mathbf{x}) + \varphi(\mathbf{y})) dP(\mathbf{x}, \mathbf{y}) = \int_{\mathcal{X}} \psi(\mathbf{x}) d\mathbb{P}_A(\mathbf{x}) + \int_{\mathcal{Y}} \varphi(\mathbf{y}) d\mathbb{P}_B(\mathbf{y}),$$

or equivalently

$$\sup_{\psi, \varphi} \left\{ \int_{\mathcal{X}} \psi(\mathbf{x}) d\mathbb{P}_A(\mathbf{x}) + \int_{\mathcal{Y}} \varphi(\mathbf{y}) d\mathbb{P}_B(\mathbf{y}) - \int_{\mathcal{X} \times \mathcal{Y}} (\psi(\mathbf{x}) + \varphi(\mathbf{y})) dP(\mathbf{x}, \mathbf{y}) \right\} = 0.$$

Wasserstein- k distance (with $k \geq 1$) is

$$W_k(\mathbb{P}_A, \mathbb{P}_B) = \left(\inf_{\pi \in \Pi(\mathbb{P}_A, \mathbb{P}_B)} \mathbb{E}_{\pi} [c(X, Y)^k] \right)^{1/k} \quad \text{where } (X, Y) \sim \pi.$$

Optimal transport

Definition 4.36: Kantorovich Problem

Kantorovich Problem is defined as

$$W_c(\mathbb{P}_A, \mathbb{P}_B) = \inf_{P \in \Pi(\mathbb{P}_A, \mathbb{P}_B)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) dP(x, y),$$

for cost function c (or loss function).



- › We can rewrite using a Lagrangian form

$$W_c(\mathbb{P}_A, \mathbb{P}_B) = \inf_P \left\{ \sup_{\psi, \varphi} \{L(P, \psi, \varphi)\} \right\},$$

where

$$L(P, \psi, \varphi) = \int_{\mathcal{X} \times \mathcal{Y}} (c(x, y) - (\psi(x) + \varphi(y))) dP(x, y) + \int_{\mathcal{X}} \psi(x) d\mathbb{P}_A(x) + \int_{\mathcal{Y}} \varphi(y) d\mathbb{P}_B(y).$$

Optimal transport

$$L(P, \psi, \varphi) = \int_{\mathcal{X} \times \mathcal{Y}} (c(\mathbf{x}, \mathbf{y}) - (\psi(\mathbf{x}) + \varphi(\mathbf{y}))) dP(\mathbf{x}, \mathbf{y}) + \int_{\mathcal{X}} \psi(\mathbf{x}) d\mathbb{P}_{\textcolor{teal}{A}}(\mathbf{x}) + \int_{\mathcal{Y}} \varphi(\mathbf{y}) d\mathbb{P}_{\textcolor{blue}{B}}(\mathbf{y}).$$

➤ The dual problem becomes

$$\sup_{\psi, \varphi} \left\{ \inf_P \{L(P, \psi, \varphi)\} \right\},$$

clearly

$$\inf_P \{L(P, \psi, \varphi)\} = \int_{\mathcal{X}} \psi(\mathbf{x}) d\mathbb{P}_{\textcolor{teal}{A}}(\mathbf{x}) + \int_{\mathcal{Y}} \varphi(\mathbf{y}) d\mathbb{P}_{\textcolor{blue}{B}}(\mathbf{y}) \text{ if } c(\mathbf{x}, \mathbf{y}) \geq \psi(\mathbf{x}) + \varphi(\mathbf{y}).$$

Optimal transport

Theorem 4.1: Minimax theorem, von Neumann (1928)

Let $\mathcal{X} \subset \mathbb{R}^n$ and $\mathcal{Y} \subset \mathbb{R}^m$ be compact convex sets. If $f : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$ is a continuous function that is concave-convex, i.e.

$$\begin{cases} f(\cdot, y) : \mathcal{X} \rightarrow \mathbb{R} \text{ is concave for fixed } y \\ f(x, \cdot) : \mathcal{Y} \rightarrow \mathbb{R} \text{ is convex for fixed } x, \end{cases}$$

Then we have that

$$\max_{x \in \mathcal{X}} \min_{y \in \mathcal{Y}} f(x, y) = \min_{y \in \mathcal{Y}} \max_{x \in \mathcal{X}} f(x, y).$$

- For example, $f(x, y) = x^\top A y$ for a finite matrix $A \in \mathbb{R}^{n \times m}$,

$$\max_{x \in \mathcal{X}} \min_{y \in \mathcal{Y}} x^\top A y = \min_{y \in \mathcal{Y}} \max_{x \in \mathcal{X}} x^\top A y.$$

Optimal transport

- Using a generalized minimax theorem, Parthasarathy (1970),

$$W_c(\mathbb{P}_A, \mathbb{P}_B) = \sup_{\psi, \varphi} \left\{ \int_{\mathcal{X}} \psi(x) d\mathbb{P}_A(x) + \int_{\mathcal{Y}} \varphi(y) d\mathbb{P}_B(y) \right\}, \text{ s.t. } c(x, y) \geq \psi(x) + \varphi(y),$$

the constraint can be rewritten

$$\psi(x) \leq \overbrace{\min_z \{c(x, z) - \varphi^c(z)\}}^{= \varphi^c(x)}$$

where φ^c is the c -transform of φ , and

$$W_c(\mathbb{P}_A, \mathbb{P}_B) = \sup_{\varphi} \left\{ \int_{\mathcal{X}} \varphi^c(x) d\mathbb{P}_A(x) + \int_{\mathcal{Y}} \phi(y) d\mathbb{P}_B(y) \right\}$$

called Kantorovich duality formula.

Optimal transport

Definition 4.37: Bures metric on positive-definite matrices, Bures (1969)

Bures distance between two positive-definite matrices,

$$d_B(\mathbf{A}, \mathbf{B}) = \sqrt{\text{tr}(\mathbf{A}) + \text{tr}(\mathbf{B}) - 2\text{tr}\left((\mathbf{A}^{\frac{1}{2}} \mathbf{B} \mathbf{A}^{\frac{1}{2}})^{\frac{1}{2}}\right)}$$

is a metric on the space of positive semidefinite matrices

- It is related to Hellinger distance if \mathbf{A} and \mathbf{B} are diagonal.

For two Gaussian distributions

$$W_2(\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1), \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2))^2 = \|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2\|_2^2 + d_B(\boldsymbol{\Sigma}_1, \boldsymbol{\Sigma}_2)^2.$$

Optimal transport and Monge mapping

Definition 4.38: 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 μ on \mathcal{X} . The **push-forward** of μ by T is the measure $\nu = T_{\#}\mu$ on \mathcal{Y} defined by

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

- By the change-of-variable formula

Proposition 4.24: 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 $T_{\#}\mu(B) = \mu(T^{-1}(B)) = \delta_{T(\mathbf{x})}$. 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 4.25: Existence of a map

If $\mathcal{X} = \mathcal{Y}$ is a compact subset of \mathbb{R}^k , if μ and ν are two measures, and if μ 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 μ and ν 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 4.39: Monge Problem

Monge problem

$$\inf_{T_{\#}\mathbb{P}_A = \mathbb{P}_B} \int_{\mathcal{X}} c(\mathbf{x}, T(\mathbf{x})) d\mathbb{P}_A(\mathbf{x}),$$

for cost function c .



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

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 μ is atomless,

Proposition 4.26: Monge/Kantorovich Problems

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

$\min\{\text{Monge problem, see Def. 4.39}\} = \min\{\text{Kantorovich problem, see Def. 4.36}\}.$

Optimal transport and Monge mapping

- › One can consider optimal transport for empirical measures, $\mathbb{P} = \sum_{i=1}^n \omega_i \delta_{\mathbf{x}_i}$.
- › 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

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

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

Optimal transport (discrete)

- 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

$$U(\mathbf{a}_A, \mathbf{a}_B) = \{M \in \mathbb{R}_+^{n_A \times n_B} : M\mathbf{1}_{n_B} = \mathbf{a}_0 \text{ and } M^\top \mathbf{1}_{n_A} = \mathbf{a}_1\}.$$

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, $C_{i,j} = d(x_i, y_j)^k$.

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

and “optimal transport”

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

Optimal transport (discrete)

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

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

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

- 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 γ -regularized optimal transport problem

$$P_\gamma^* = \underset{P \in U_{n_A, n_B}}{\operatorname{argmin}} \left\{ \langle P, C \rangle - \gamma \mathcal{E}(P) \right\} \quad (3)$$

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 4.2: 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

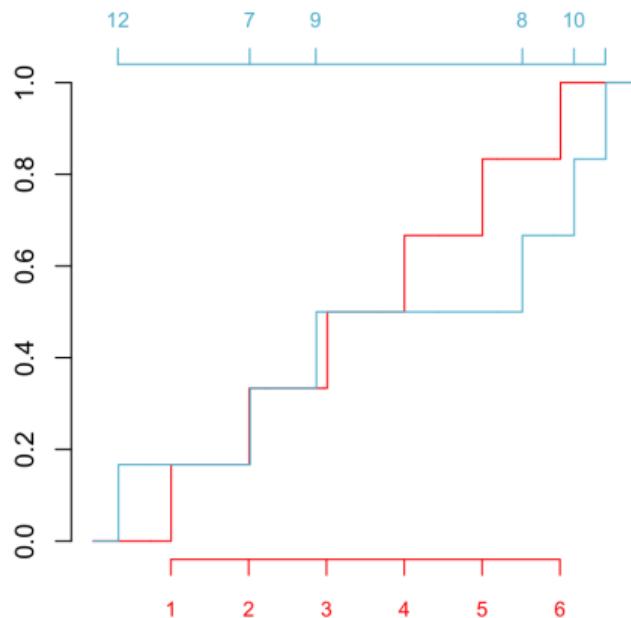
$$P_{\gamma}^* = \underset{P \in U_{\mathbf{a}_A, \mathbf{a}_B}}{\operatorname{argmin}} \left\{ \langle P, C \rangle + \gamma \cdot d_{\text{KL}}(P || \mathbf{a}_A \otimes \mathbf{a}_B) \right\} \quad (4)$$

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

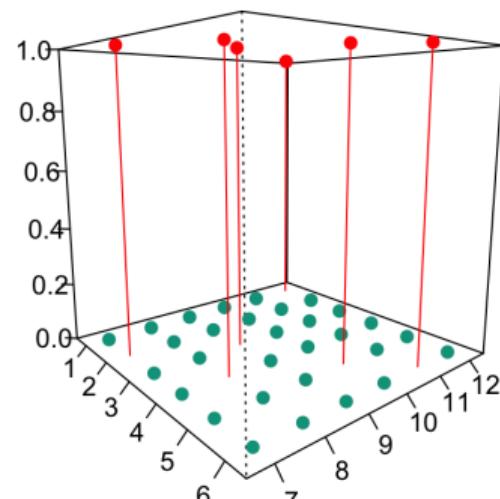
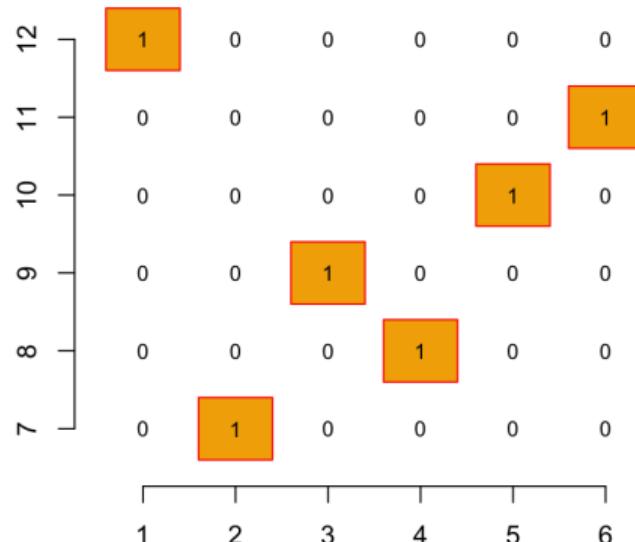
- The extension of Sinkhorn algorithm is the coordinate descent/ascent algorithm.

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
```

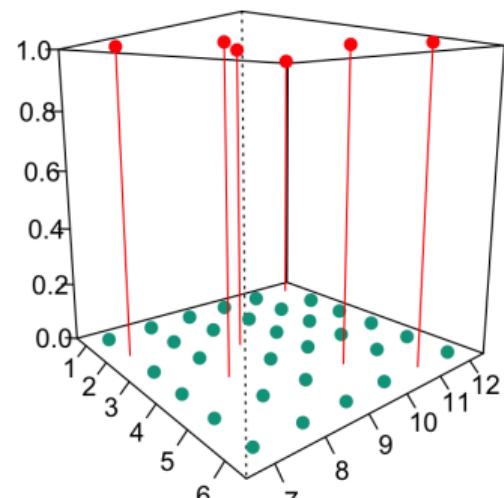
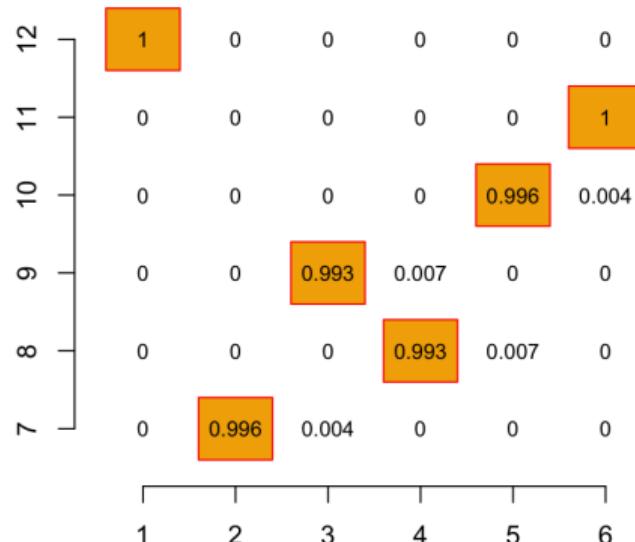


Optimal transport (discrete)



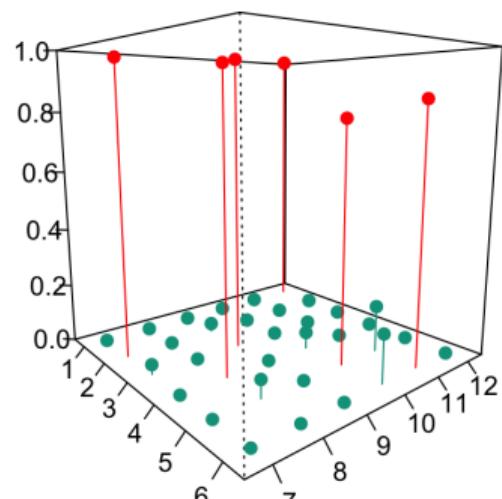
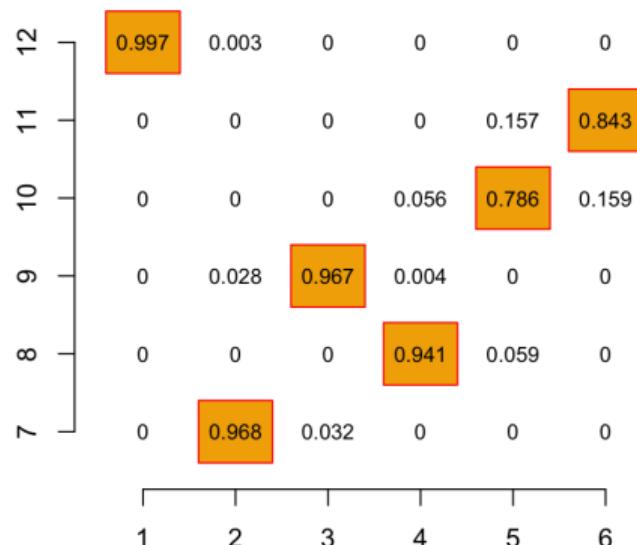
```
1 > Wxy = wasserstein(x,y[1:6])
2 > Wxy$plan
```

Optimal transport (discrete)



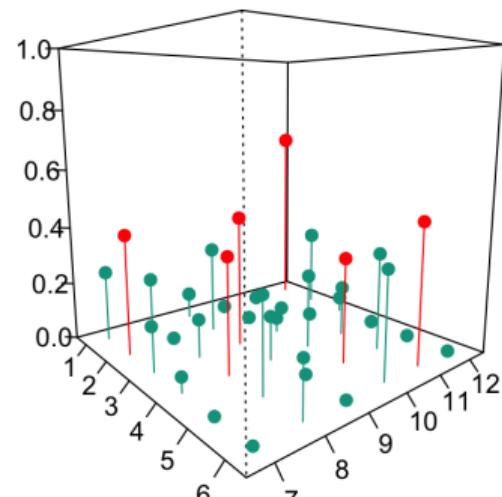
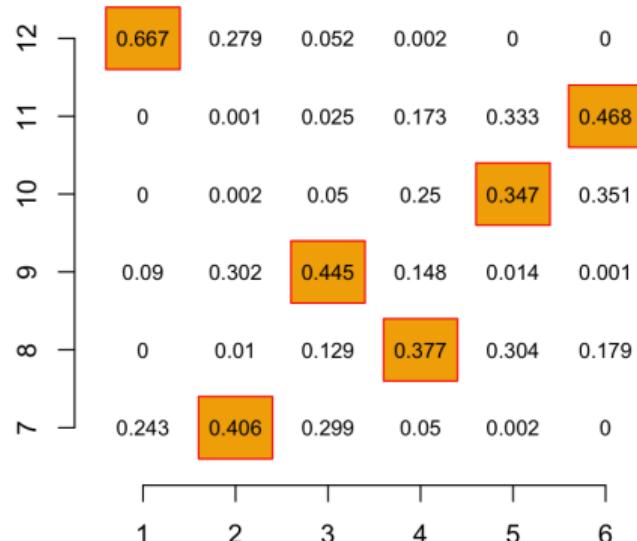
```
1 > Sxy = sinkhorn(x, y[1:6], p = 2, lambda = 0.001)
2 > Sxy$plan
```

Optimal transport (discrete)



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

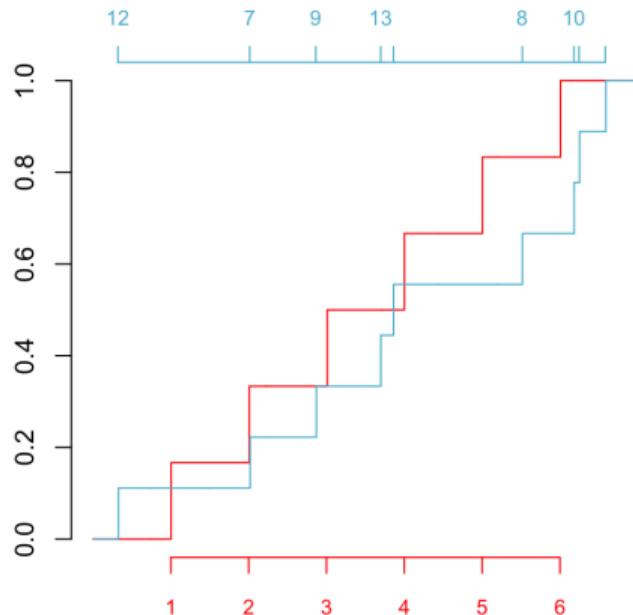
Optimal transport (discrete)



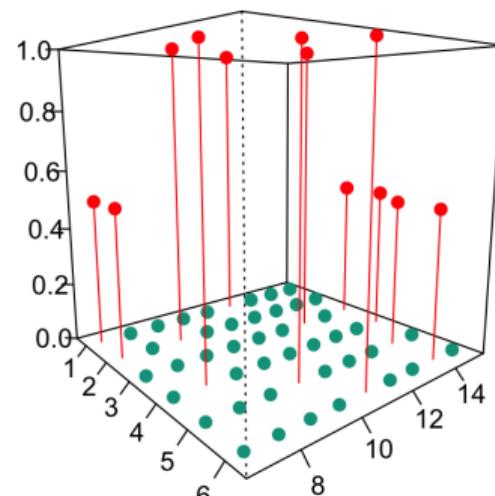
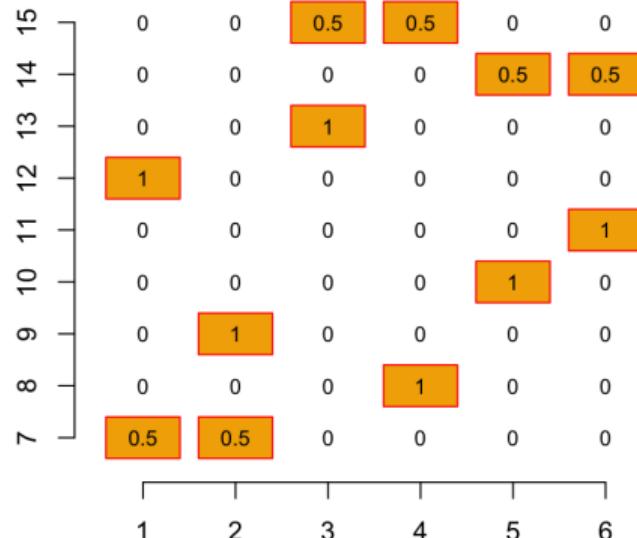
```
1 > Sxy = sinkhorn(x, y[1:6], p = 2, lambda = 0.05)
2 > Sxy$plan
```

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
```

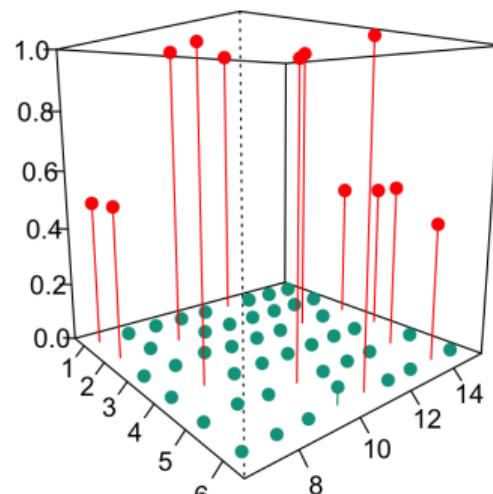
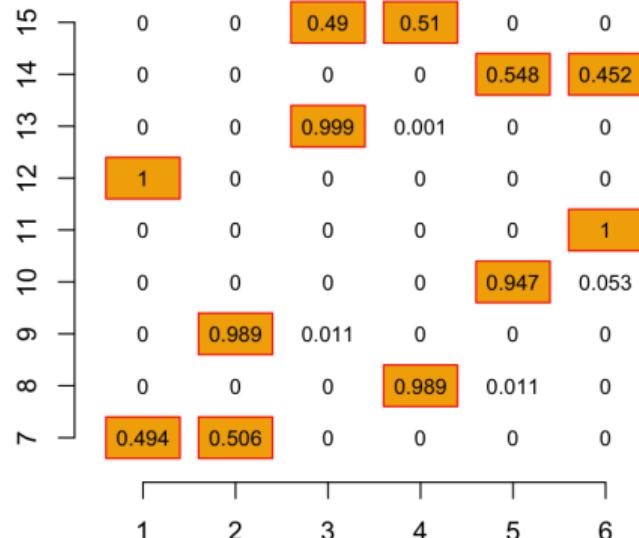


Optimal transport (discrete)



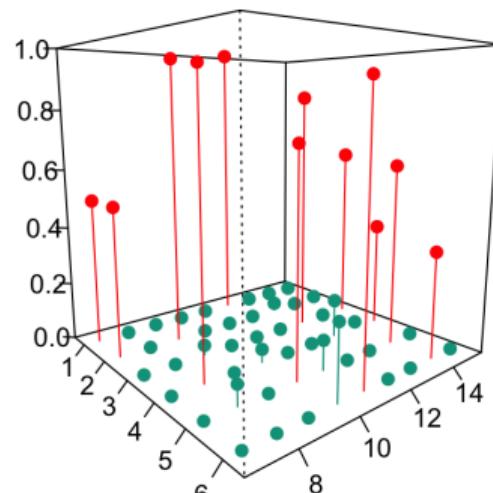
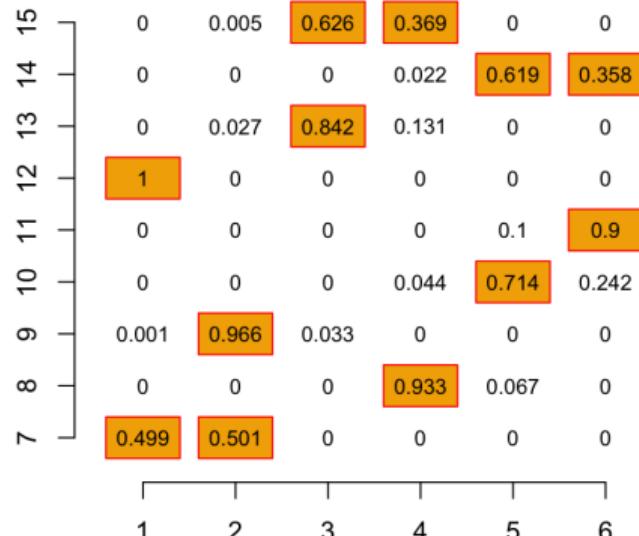
```
1 > Wxy = wasserstein(x,y)
2 > Wxy$plan
```

Optimal transport (discrete)



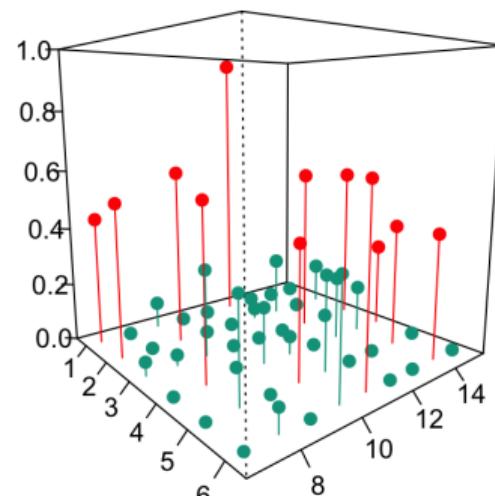
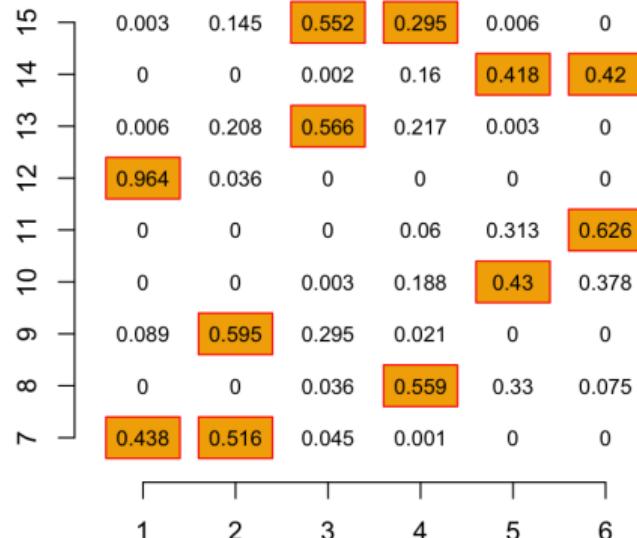
```
1 > Sxy = sinkhorn(x, y, p = 2, lambda = 0.001)
2 > Sxy$plan
```

Optimal transport (discrete)



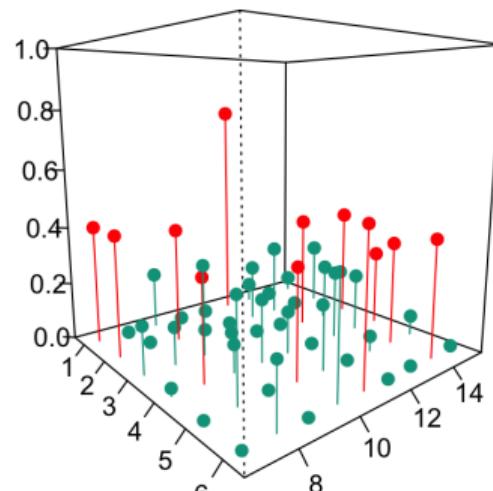
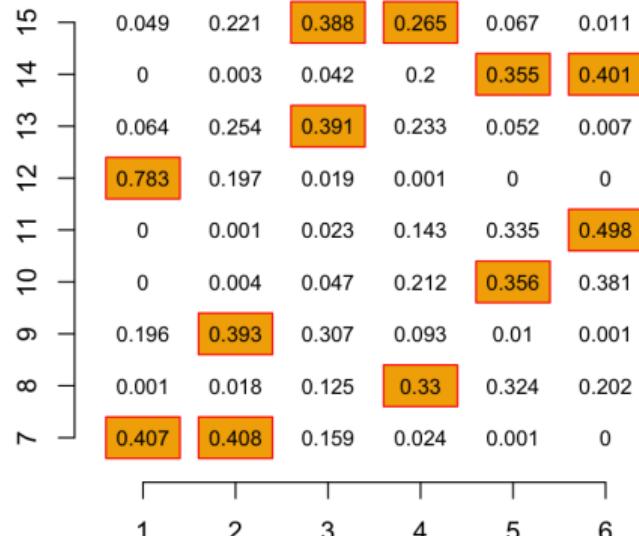
```
1 > Sxy = sinkhorn(x, y, p = 2, lambda = 0.005)
2 > Sxy$plan
```

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)

Univariate Optimal Transport

Proposition 4.27: 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, for every permutation σ of $\{1, 2, \dots, n\}$,

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

- This can be extended, from a product to more general function $\Phi(x_i, y_j)$.



Univariate Optimal Transport

Definition 4.40: 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, Φ is said to be submodular.

Univariate Optimal Transport

Proposition 4.28: 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 σ 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.

Univariate Optimal Transport

```
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
```

Univariate Optimal Transport

Theorem 4.3: 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 $k \geq 1$,

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

Theorem 4.4: Optimal transport for continuous univariate distributions

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

Univariate Optimal Transport

Theorem 4.5: 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

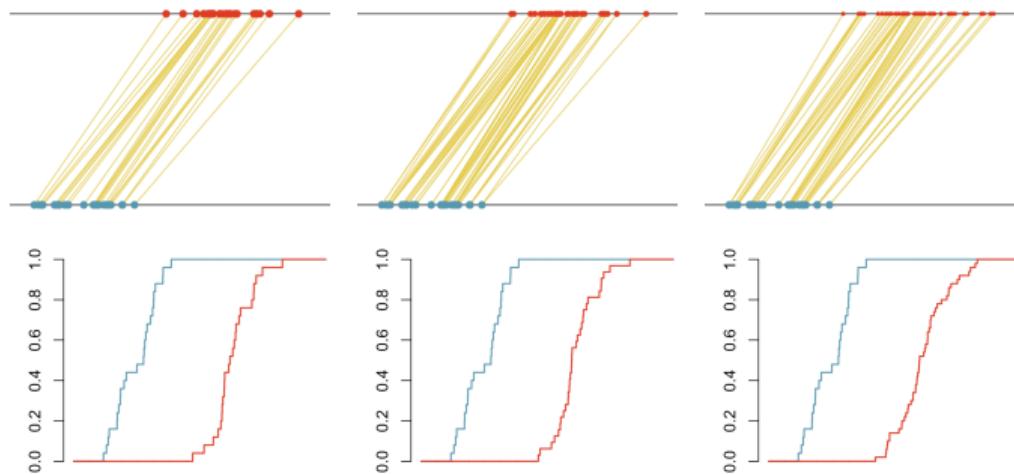
- ▶ π is optimal to Kantorovich problem (4.36)
 - ▶ π is the comonotone joint distribution with marginals \mathbb{P}_A and \mathbb{P}_B .
- ▶ If $c(x, y) = |x - y|$, the optimal transport solution might be non-unique.

Theorem 4.6: Optimal map for continuous univariate distributions

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

Univariate Optimal Transport

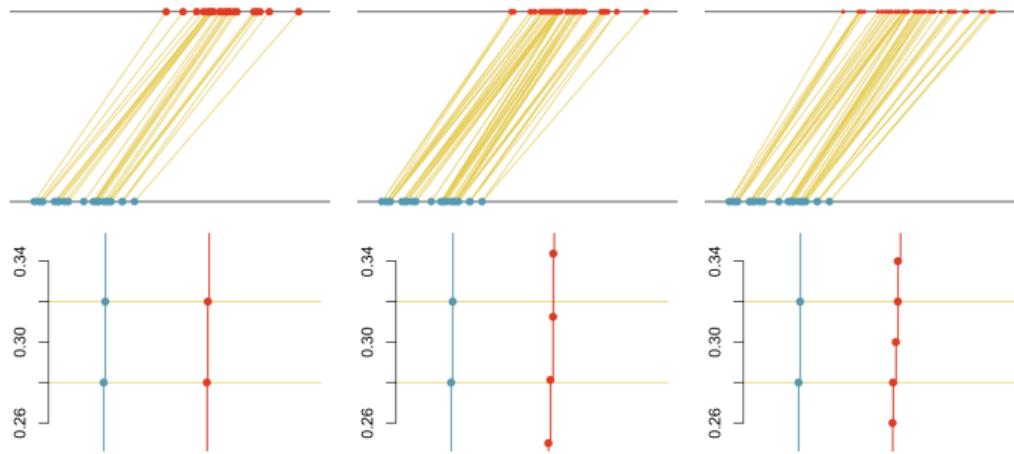
Consider $n_A = 25$ and $n_B = 25$ points in \mathbb{R} , $n_B = 32$ and $n_B = 50$



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

Univariate Optimal Transport

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

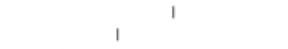


$$\hat{F}_{n_A}(x) = \frac{1}{n_A} \sum_{i=1}^{n_A} \mathbf{1}(x_i \leq x) \text{ and } \hat{F}_{n_B}(x) = \frac{1}{n_B} \sum_{i=1}^{n_B} \mathbf{1}(x_i \leq x)$$

Univariate Optimal Transport

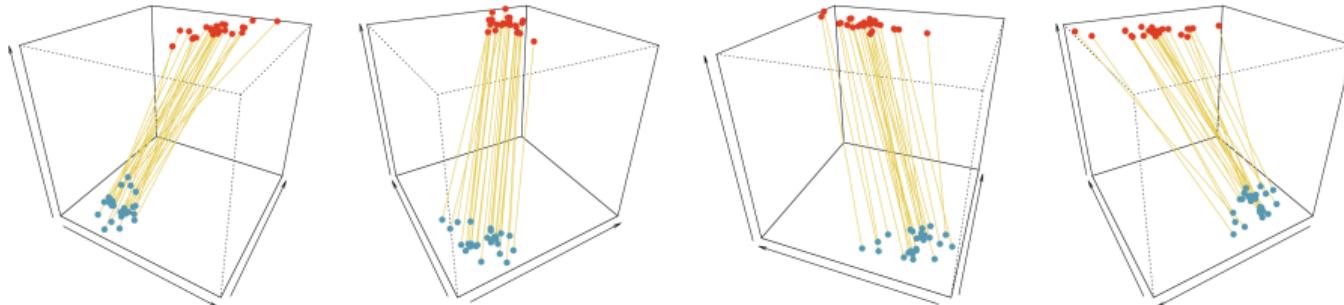
- In the univariate case, if $k = 1$,

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

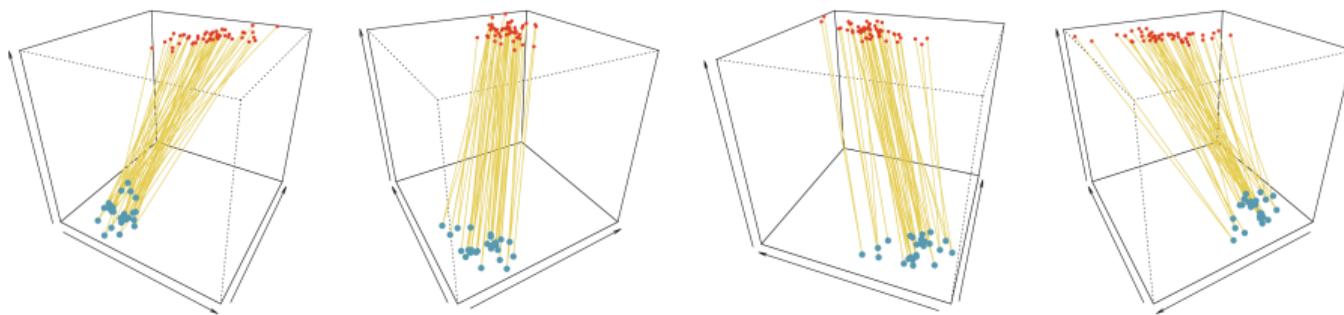


Multivariate Optimal Transport

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

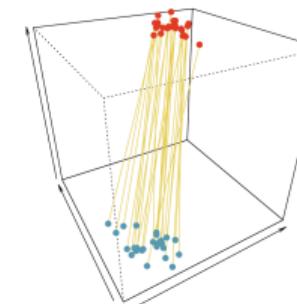
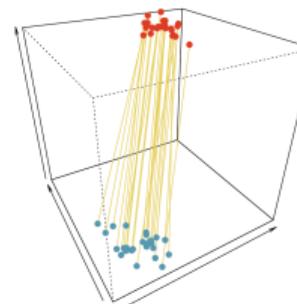
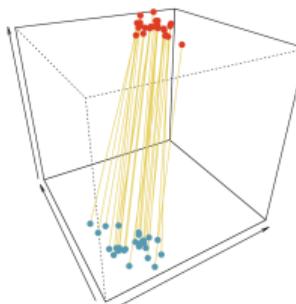
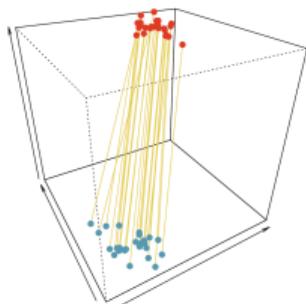


- Consider n and $2n$ points in \mathbb{R}^2

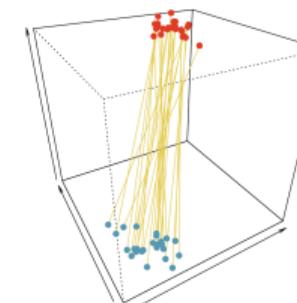
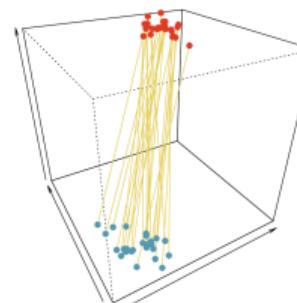
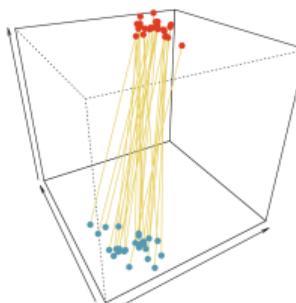
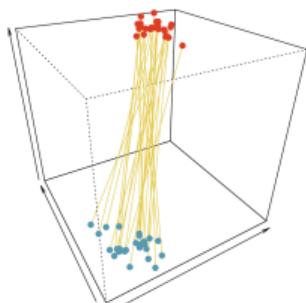


Multivariate Optimal Transport

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



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



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