

Optimal Transport Divergences induced by Scoring Functions

Silvana M. Pesenti, u. Toronto

joint with

Steven Vanduffel (Vrije Universiteit Brussel)

https://doi.org/10.48550/arXiv.2311.12183

Women in OT - April 17-19, 2024

Motivation - Why robustify?

Let $\rho \colon L^{\infty} \to \mathbb{R}$ be a risk measure. Of interest

$$\rho(X)$$

Motivation - Why robustify?

Let $\rho \colon L^{\infty} \to \mathbb{R}$ be a risk measure. Of interest

$$\rho(X)$$

- Distributional uncertainty missing / incomplete data
- Model uncertainty, e.g., $X = g(Z_1, \dots, Z_n)$
- Dependence uncertainty
- Distributional robust optimisation: "Best action in the worst case"
- Applications: robust decision making, portfolio management, hedging, partial identification, inequality measurement, ...

Worst-Case Risk Measures

Let $\rho\colon L^\infty\to\mathbb{R}$ be a risk measure. A distributional worst-case risk measure can be defined as

$$\sup_{X\in\mathcal{U}}\;\rho(X)\,,$$

for a suitable uncertainty set \mathcal{U} .

Worst-Case Risk Measures

Let $\rho\colon L^\infty\to\mathbb{R}$ be a risk measure. A distributional worst-case risk measure can be defined as

$$\sup_{X \in \mathcal{U}} \rho(X) \,,$$

for a suitable uncertainty set \mathcal{U} .

- ightarrow what are desirable properties of ${\cal U}$
- \rightarrow trade-off between too small and too large

Distributional robust risk measures

$$\sup_{G \in \mathcal{U}_{\varepsilon}} \rho(G)$$

Distributional robust risk measures

$$\sup_{G \in \mathcal{U}_{\varepsilon}} \rho(G)$$

Let F be a reference distribution

$$\mathcal{U}_{\varepsilon} := \Big\{ G \mid d_W(F, G)^2 \le \varepsilon \Big\},$$

where $d_W(G, F)$ denotes the Wasserstein distance of order 2, which for F, G, with finite second moment, has representation

$$d_W(F,G)^2 = \int_0^1 |F^{-1}(u) - G^{-1}(u)|^2 du.$$

Distributional robust risk measures

$$\sup_{G \in \mathcal{U}_{\varepsilon}} \rho(G)$$

Let F be a reference distribution

$$\mathcal{U}_{\varepsilon} := \Big\{ G \mid d_W(F, G)^2 \le \varepsilon \Big\},$$

where $d_W(G, F)$ denotes the Wasserstein distance of order 2, which for F, G, with finite second moment, has representation

$$d_W(F, G)^2 = \int_0^1 |F^{-1}(u) - G^{-1}(u)|^2 du.$$

! penalises losses and gains symmetrically

Let ho_{γ} be a concave distortion (coherent) risk measure

$$\int_0^1 \gamma(u) G^{-1}(u) du$$

Let ho_{γ} be a concave distortion (coherent) risk measure , then

$$\sup_{G \in \mathcal{U}_{\varepsilon}} \int_{0}^{1} \gamma(u) G^{-1}(u) \ du = \rho(F) + \sqrt{\varepsilon} \sqrt{\int_{0}^{1} \gamma(u)^{2} \ du}$$

and the worst-case quantile function is

$$F^{-1,*}(u) := F^{-1}(u) + \frac{\sqrt{\varepsilon}}{\sqrt{\int_0^1 \gamma(u)^2 \, du}} \, \gamma(u) \, .$$

Let ho_{γ} be a concave distortion (coherent) risk measure , then

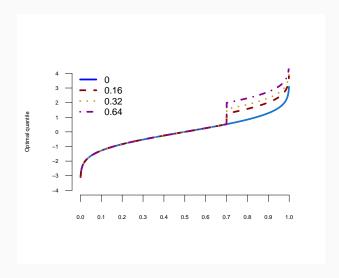
$$\sup_{G\in\mathcal{U}_\varepsilon}\,\int_0^1\gamma(u)\,G^{-1}(u)\;du=\rho(F)+\sqrt{\varepsilon}\;\sqrt{\int_0^1\gamma(u)^2\;du}$$

and the worst-case quantile function is

$$F^{-1,*}(u) := F^{-1}(u) + \frac{\sqrt{\varepsilon}}{\sqrt{\int_0^1 \gamma(u)^2 du}} \, \gamma(u) \,.$$

- ! robust risk measure: constant shift
- ! constant is independent of F

Worst-case Quantile Functions



Motivation

- Distances other than the *p*-Wasserstein distances
- Divergences that:
 - ▷ allow for comparison of distributions with differing support
 - ▷ are asymmetric, penalising different parts of the distribution

 - ▷ interpretation from a statistical and risk management

Motivation

- Distances other than the p-Wasserstein distances
- Divergences that:
 - ▷ allow for comparison of distributions with differing support
 - are asymmetric, penalising different parts of the distribution

 - ▷ interpretation from a statistical and risk management
- → connecting OT & risk measures & elicitability
- \rightarrow uncertainty sets induced by the risk to be assess

Monge-Kantorovich optimal transport problem

Definition 1

Let $c \colon \mathbb{R} \times \mathbb{R} \to \mathbb{R}_{\geq 0}$ be a cost function. Then the Monge-Kantorovich optimisation problem with respect to the cdfs F_1 and F_2 is given by

$$\inf_{\pi \in \Pi(F_1, F_2)} \left\{ \int_{\mathbb{R}^2} c(z_1, z_2) \, \pi(\mathrm{d}z_1, \mathrm{d}z_2) \right\}, \tag{1}$$

where $\Pi(F_1, F_2)$ denotes the set of all bivariate cdfs with marginal cdfs F_1 and F_2 , respectively.

Monge-Kantorovich optimal transport problem

Definition 1

Let $c \colon \mathbb{R} \times \mathbb{R} \to \mathbb{R}_{\geq 0}$ be a cost function. Then the Monge-Kantorovich optimisation problem with respect to the cdfs F_1 and F_2 is given by

$$\inf_{\pi \in \Pi(F_1, F_2)} \left\{ \int_{\mathbb{R}^2} c(z_1, z_2) \, \pi(\mathrm{d}z_1, \mathrm{d}z_2) \right\}, \tag{1}$$

where $\Pi(F_1, F_2)$ denotes the set of all bivariate cdfs with marginal cdfs F_1 and F_2 , respectively.

- $\rightarrow c(z_1, z_2) = |z_1 z_2|^p$ gives the *p*-Wasserstein distance.
- → Asymmetric cost functions? via scoring functions

Interlude - Scoring Functions

Scoring rules in statistics

- y_1, \ldots, y_N observations of r.v. $Y \sim F$
- ullet Aim: forecast functional $\mathit{T}(\mathit{F})$, e.g., mean, quantile, risk measure
- How to compare forecasts of models *A* & *B*:

(A)
$$z_1^{(A)},\ldots,z_N^{(A)}\in \mathsf{A}$$

(B)
$$z_1^{(B)},\ldots,z_N^{(B)}\in \mathsf{A}$$

Scoring rules in statistics

- y_1, \ldots, y_N observations of r.v. $Y \sim F$
- ullet Aim: forecast functional $\mathit{T}(\mathit{F})$, e.g., mean, quantile, risk measure
- How to compare forecasts of models *A* & *B*:
 - (A) $z_1^{(A)},\ldots,z_N^{(A)}\in \mathsf{A}$
 - (B) $z_1^{(B)}, \dots, z_N^{(B)} \in A$
- Use a loss/scoring function $S: A \times \mathbb{R} \to [0, \infty]$ and compare

$$L^{(A)} := \frac{1}{N} \sum_{i=1}^{N} S(z_i^{(A)}, y_i) \stackrel{?}{\leq} \frac{1}{N} \sum_{i=1}^{N} S(z_i^{(B)}, y_i) =: L^{(B)}.$$

Scoring rules in statistics

- y_1, \ldots, y_N observations of r.v. $Y \sim F$
- ullet Aim: forecast functional $\mathit{T}(\mathit{F})$, e.g., mean, quantile, risk measure
- How to compare forecasts of models A & B:

(A)
$$z_1^{(A)},\ldots,z_N^{(A)}\in \mathsf{A}$$

(B)
$$z_1^{(B)}, \dots, z_N^{(B)} \in A$$

• Use a loss/scoring function $S: A \times \mathbb{R} \to [0, \infty]$ and compare

$$L^{(A)} := \frac{1}{N} \sum_{i=1}^{N} S(z_i^{(A)}, y_i) \stackrel{?}{\leq} \frac{1}{N} \sum_{i=1}^{N} S(z_i^{(B)}, y_i) =: L^{(B)}.$$

 \rightarrow meaningful forecast comparison, model selection, regression, M-estimation, ...

Scoring Functions [Murphy & Daan, 1985, Engelberg et al., 2009]

- A scoring function is a measurable map $S \colon \mathsf{A} \times \mathbb{R} \to [0, \infty].$
- $T: \mathcal{M} \to A$ law-invariant functional of interest.
- \bullet $\,{\cal M}$ subset of probability measures on $\mathbb R$

Scoring Functions [Murphy & Daan, 1985, Engelberg et al., 2009]

- A scoring function is a measurable map $S: A \times \mathbb{R} \to [0, \infty]$.
- $T: \mathcal{M} \to A$ law-invariant functional of interest.
- \bullet $\,{\cal M}$ subset of probability measures on $\mathbb R$

For a functional $T: \mathcal{M} \to A$, we say

(i) S is consistent for T, if for all $F \in \mathcal{M}$ and for all $z \in A$

$$\int S(T(F), y) dF(y) \le \int S(z, y) dF(y).$$
 (2)

(ii) S is strictly consistent for T, if it is consistent for T and if (2) is strict for all $z \neq T(F)$.

Elicitability - Bayes act

T is elicitable on \mathcal{M} , if there exists a strictly \mathcal{M} -consistent scoring function for T. Moreover,

$$T(F) = \arg\min_{z \in \mathbb{R}} \int S(z, y) \, dF(y)$$
$$= \arg\min_{z \in \mathbb{R}} \mathbb{E}[S(z, Y)], \quad Y \sim F.$$

Elicitability – Bayes act

T is elicitable on \mathcal{M} , if there exists a strictly \mathcal{M} -consistent scoring function for T. Moreover,

$$T(F) = \arg \min_{z \in \mathbb{R}} \int S(z, y) \, dF(y)$$
$$= \arg \min_{z \in \mathbb{R}} \mathbb{E}[S(z, Y)], \quad Y \sim F.$$

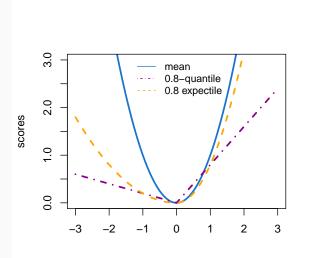
Example:

$$\mathbb{E}[Y] = \arg\min_{z \in \mathbb{R}} \ \mathbb{E}[(z - Y)^2]$$

T	S(z, y)
mean	$(x-y)^2$
median	x-y
VaR_{lpha}	$(\mathbb{1}_{\{y \le z\}} - \alpha)(z - y)$
variance	NO
Expected Shortfall (ES)	NO
(mean, variance)	YES!
$(\mathrm{VaR}_\alpha,\mathrm{ES}_\alpha)$	YES!

Scores for different functionals

S(0, y) as a function of realisations y



Proposition 1 (Elicitability of Mean - [Gneiting, 2011])

Under technical conditions, the class of (strictly) consistent scoring functions for the mean are

$$S_{\phi}(z,y) = B_{\phi}(y,z), \quad z, y \in \mathbb{R},$$
(3)

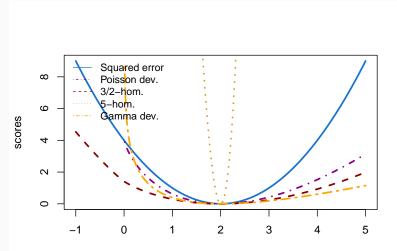
where B_ϕ is the Bregman divergence

$$B_{\phi}(x_1, x_2) := \phi(x_1) - \phi(x_2) - \phi'(x_2)(x_1 - x_2), \quad x_1, x_2 \in \mathbb{R},$$

and ϕ (strictly) convex.

Scores for the mean

S(2,y) as a function of realisations y



Monge-Kantorovich divergences with Scores

Let S be an \mathcal{M} -consistent score for T.

The Monge-Kantorovich (MK) divergence induced by S from the cdf $F_1 \in \mathcal{M}$ to the cdf $F_2 \in \mathcal{M}$ is

$$\mathscr{S}(F_1, F_2) := \inf_{\pi \in \Pi(F_1, F_2)} \left\{ \int_{\mathbb{R}^2} S(z_2, z_1) \, \pi(\mathrm{d}z_1, \mathrm{d}z_2) \right\}. \tag{4}$$

Monge-Kantorovich divergences with Scores

Let S be an \mathcal{M} -consistent score for T.

The Monge-Kantorovich (MK) divergence induced by S from the cdf $F_1 \in \mathcal{M}$ to the cdf $F_2 \in \mathcal{M}$ is

$$\mathscr{S}(F_1, F_2) := \inf_{\pi \in \Pi(F_1, F_2)} \left\{ \int_{\mathbb{R}^2} S(z_2, z_1) \, \pi(\mathrm{d}z_1, \mathrm{d}z_2) \right\}. \tag{4}$$

- \rightarrow non-negative; satisfies $\mathscr{S}(F,F)=0$
- $\rightarrow \mathscr{S}(F_1,F_2)=0$ need not imply $F_1=F_2$
- ightarrow depends on the choice of S
- \rightarrow What is the optimal coupling?

Bregman-Wasserstein divergence

Let *S* be a consistent score for the mean.

Then the MK divergence is the Bregman-Wasserstein divergence [Rankin & Wong, 2023]

$$\mathscr{B}_{\phi}(F_1, F_2) := \inf_{\pi \in \Pi(F_1, F_2)} \left\{ \int_{\mathbb{R}^2} B_{\phi}(z_1, z_2) \, \pi(\mathrm{d}z_1, \mathrm{d}z_2) \right\}, \tag{5}$$

reduces to 2-Wasserstein distance for $\phi(x) = x^2$.

Bregman-Wasserstein divergence

Let *S* be a consistent score for the mean.

Then the MK divergence is the Bregman-Wasserstein divergence [Rankin & Wong, 2023]

$$\mathscr{B}_{\phi}(F_1, F_2) := \inf_{\pi \in \Pi(F_1, F_2)} \left\{ \int_{\mathbb{R}^2} B_{\phi}(z_1, z_2) \, \pi(\mathrm{d}z_1, \mathrm{d}z_2) \right\}, \tag{5}$$

reduces to 2-Wasserstein distance for $\phi(x) = x^2$.

Theorem

The comonotonic coupling $(F_1^{-1}(U), F_2^{-1}(U))$, $U \sim U(0,1)$ is optimal, equivalently, the optimal transport map is $\alpha(x) = F_2^{-1}(F_1(x))$.

Bregman-Wasserstein divergence

Let S be a consistent score for the mean.

Then the MK divergence is the Bregman-Wasserstein divergence [Rankin & Wong, 2023]

$$\mathscr{B}_{\phi}(F_1, F_2) := \mathbb{E}\left[B_{\phi}\left(F_2^{-1}(U), F_1^{-1}(U)\right)\right]$$
 (5)

reduces to 2-Wasserstein distance for $\phi(x) = x^2$.

Theorem

The comonotonic coupling $(F_1^{-1}(U), F_2^{-1}(U))$, $U \sim U(0,1)$ is optimal, equivalently, the optimal transport map is $\alpha(x) = F_2^{-1}(F_1(x))$.

 \rightarrow For all choices of consistent scores for the mean.

(Generalised) Quantiles

Proposition 2 (Elicitability of Quantiles – [Gneiting, 2011])

Under technical conditions, the class of (strictly) consistent scores for the α -quantile are

$$S_g(z,y) = \left(\mathbb{1}_{\{y \le z\}} - \alpha\right) \left(g(z) - g(y)\right), \qquad z, y \in \mathbb{R},$$
 (6)

where g is a (strictly) increasing function.

(Generalised) Quantiles

Proposition 2 (Elicitability of Quantiles - [Gneiting, 2011])

Under technical conditions, the class of (strictly) consistent scores for the α -quantile are

$$S_g(z,y) = \left(\mathbb{1}_{\{y \le z\}} - \alpha\right) \left(g(z) - g(y)\right), \qquad z, y \in \mathbb{R},$$
 (6)

where g is a (strictly) increasing function.

Theorem 2

The optimal coupling of the MK divergence for any score \mathcal{S}_g is the comonotonic coupling.

(Generalised) Quantiles

Proposition 2 (Elicitability of Quantiles – [Gneiting, 2011])

Under technical conditions, the class of (strictly) consistent scores for the α -quantile are

$$S_g(z,y) = \left(\mathbb{1}_{\{y \le z\}} - \alpha\right) \left(g(z) - g(y)\right), \qquad z, y \in \mathbb{R},$$
 (6)

where g is a (strictly) increasing function.

Theorem 2

The optimal coupling of the MK divergence for any score S_g is the comonotonic coupling.

 \rightarrow Generalisable to Λ -quantiles

Expectiles – [Newey & Powell 1987]

$$e_{\alpha}(\,Y) := \underset{z \in \mathbb{R}}{\operatorname{argmin}} \;\; \alpha \; \mathbb{E}\big[\big(\,Y - z\big)_+^2 \big] + (1 - \alpha) \; \mathbb{E}\big[\big(\,Y - z\big)_-^2 \big]$$

OT divergences S. Pesenti 18

Expectiles – [Newey & Powell 1987]

$$e_{\alpha}(\mathit{Y}) := \underset{z \in \mathbb{R}}{\operatorname{argmin}} \ \alpha \ \mathbb{E}\big[\big(\mathit{Y}-\mathit{z}\big)_{+}^{2}\big] + (1-\alpha) \ \mathbb{E}\big[\big(\mathit{Y}-\mathit{z}\big)_{-}^{2}\big]$$

Proposition 3 (Elicitability of Expectiles – [Gneiting, 2011])

Under technical conditions, the class of (strictly) consistent scores for the α -expectile are

$$S(z,y) = \left| \mathbb{1}_{\{y \le z\}} - \alpha \right| B_{\phi}(y,z), \quad z, y \in \mathbb{R},$$
 (7)

where ϕ is (strictly) convex.

Expectiles – [Newey & Powell 1987]

$$e_{\alpha}(\mathit{Y}) := \underset{z \in \mathbb{R}}{\operatorname{argmin}} \ \alpha \ \mathbb{E}\big[\big(\mathit{Y}-\mathit{z}\big)_{+}^{2}\big] + (1-\alpha) \ \mathbb{E}\big[\big(\mathit{Y}-\mathit{z}\big)_{-}^{2}\big]$$

Proposition 3 (Elicitability of Expectiles – [Gneiting, 2011])

Under technical conditions, the class of (strictly) consistent scores for the α -expectile are

$$S(z,y) = \left| \mathbb{1}_{\{y \le z\}} - \alpha \right| B_{\phi}(y,z), \quad z, y \in \mathbb{R},$$
 (7)

where ϕ is (strictly) convex.

Theorem 3

The optimal coupling of the MK divergence for any scores in (7) is the comonotonic coupling.

Divergences where the comonotonic coupling is not optimal?

Proposition 4 (Osband's principle for OT)

- ullet \tilde{T} elicitable with (strictly) consistent score \tilde{S}
- ullet MK divergence of $ilde{S}$ is attained by the comonotonic coupling
- $T := g \circ \tilde{T}, \quad g \colon \mathbb{R} \to \mathbb{R}$ strictly monotone

Then T is elicitable with (strictly) consistent score

$$S(z,y) := \tilde{S}(g^{-1}(z),y)$$
. (8)

OT divergences S. Pesenti 19

Divergences where the comonotonic coupling is not optimal?

Proposition 4 (Osband's principle for OT)

- ullet \tilde{T} elicitable with (strictly) consistent score \tilde{S}
- ullet MK divergence of $ilde{S}$ is attained by the comonotonic coupling
- $T := g \circ \tilde{T}, \quad g \colon \mathbb{R} \to \mathbb{R}$ strictly monotone

Then T is elicitable with (strictly) consistent score

$$S(z,y) := \tilde{S}(g^{-1}(z),y)$$
. (8)

If g is increasing (decreasing), then the optimal coupling of the MK divergence of the score (8) is the comonotonic (antitonic) coupling.

OT divergences S. Pesenti 1

Divergences where the comonotonic coupling is not optimal?

Proposition 4 (Osband's principle for OT)

- ullet \tilde{T} elicitable with (strictly) consistent score \tilde{S}
- ullet MK divergence of $ilde{S}$ is attained by the comonotonic coupling
- $T := g \circ \tilde{T}, \quad g \colon \mathbb{R} \to \mathbb{R}$ strictly monotone

Then T is elicitable with (strictly) consistent score

$$S(z,y) := \tilde{S}(g^{-1}(z),y)$$
. (8)

If g is increasing (decreasing), then the optimal coupling of the MK divergence of the score (8) is the comonotonic (antitonic) coupling.

$$\rightarrow$$
 Example: $T(F) = \frac{1}{\tilde{T}(F)}$.

Law invariant risk measures

A risk measure ho is coherent, if for all r.v. X

- i) monotone: $\rho(X) \leq \rho(Y)$, if $X \leq Y$ a.s
- ii) translation invariant: $\rho(X+m) = \rho(X) + m$, for all $m \in \mathbb{R}$
- iii) positive homogeneous: $\rho(\lambda X) = \lambda \rho(X)$, $\lambda \ge 0$
- iv) subadditive: $\rho(X + Y) \le \rho(X) + \rho(Y)$.

Law invariant risk measures

A risk measure ho is coherent, if for all r.v. X

- i) monotone: $\rho(X) \leq \rho(Y)$, if $X \leq Y$ a.s
- ii) translation invariant: $\rho(X+m) = \rho(X) + m$, for all $m \in \mathbb{R}$
- iii) positive homogeneous: $\rho(\lambda X) = \lambda \rho(X)$, $\lambda \ge 0$
- iv) subadditive: $\rho(X + Y) \le \rho(X) + \rho(Y)$.

Theorem 4 (Coherent Risk Measures)

Let T be an elicitable coherent risk measure satisfying T(0)=0, and let S be any strictly consistent score for T. Then, the optimal coupling of the MK divergence induced by the score S is the comonotonic coupling.

Summary & Outlook

- Introduced asymmetric OT divergences & their optimal coupling
- Divergences that penalise different parts of the distribution asymmetrically
- Uncertainty set induced by the criterion to be optimised
- How to choose the MK divergence?
- How do uncertainty balls induced MK divergences look like?

Thank you!

References



Engelberg, J., Manski, C. F., & Williams, J. (2009).

Comparing the point predictions and subjective probability distributions of professional forecasters.

Journal of Business & Economic Statistics, 27(1), 30-41.



Gneiting, T. (2011).

Making and Evaluating Point Forecasts.

Journal of the American Statistical Association, 106(494), 746-762



Murphy, A. H. & Daan, H. (1985). Forecast Evaluation.

In A. H. Murphy & R. W. Katz (Eds.), Probability, Statistics and Decision Making in the Atmospheric Sciences (pp. 379-437). Westview Press. Boulder, Colorado.



Rankin, C. & Wong, T.-K. L. (2023). Bregman-wasserstein divergence: geometry and applications.

arXiv preprint arXiv:2302.05833.

Assumptions on scores

Assumption

Let S be an \mathcal{M} -consistent score for T and denote by $\delta_y,\ y\in\mathbb{R}$, point measures. Then it holds that

- $(i) \ S\big(T(\delta_y),y\big) < S(z,y) \ \text{for all} \ z \neq T(\delta_y) \ \text{and} \ y \in \mathbb{R} \text{, and}$
- $(\mathit{ii}) \ \mathit{S}\big(\mathit{T}(\delta_y), \mathit{y}\big) = 0 \ \text{for all} \ \mathit{y} \in \mathbb{R}.$
- (i) means strict consistency on Dirac measures
- (ii) normalisation.