

MULTIVARIATE TAIL QUANTILE CONTOURS  
based on  
OPTIMAL TRANSPORT



Cees DE VALK

Royal Netherlands  
Meteorological Institute

Johan SEGERS



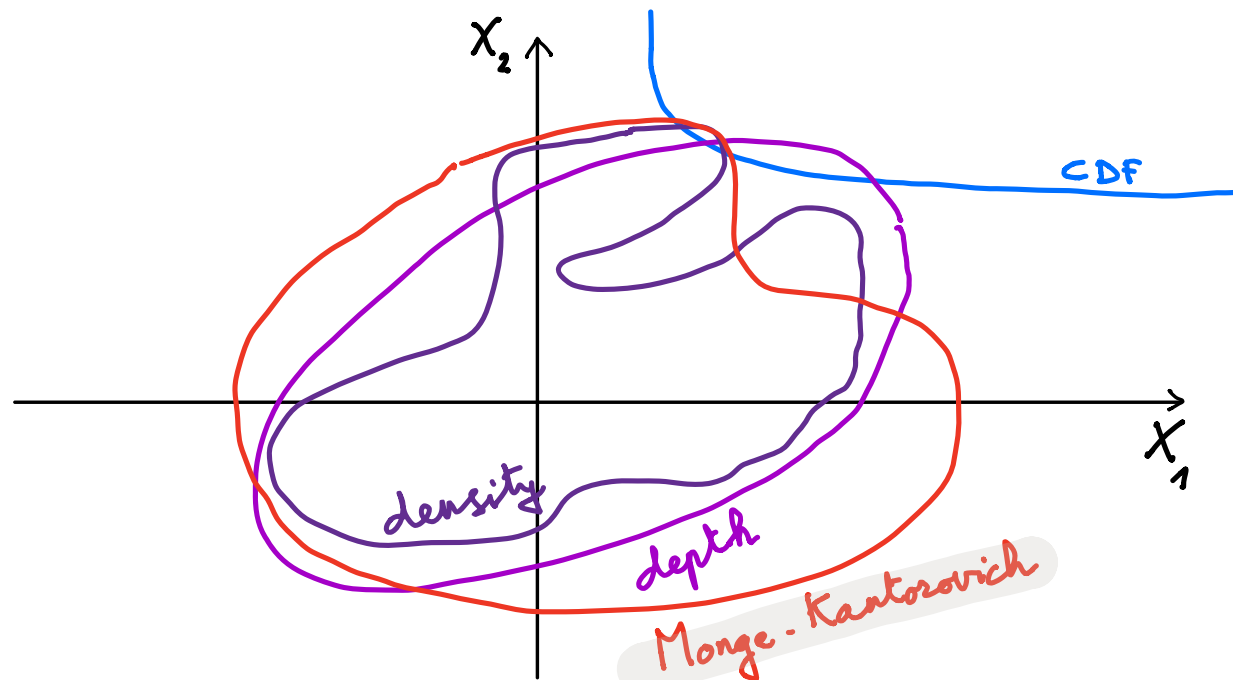
UCLouvain



Annual Meeting of the RBSS

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# QUANTILE CONTOURS

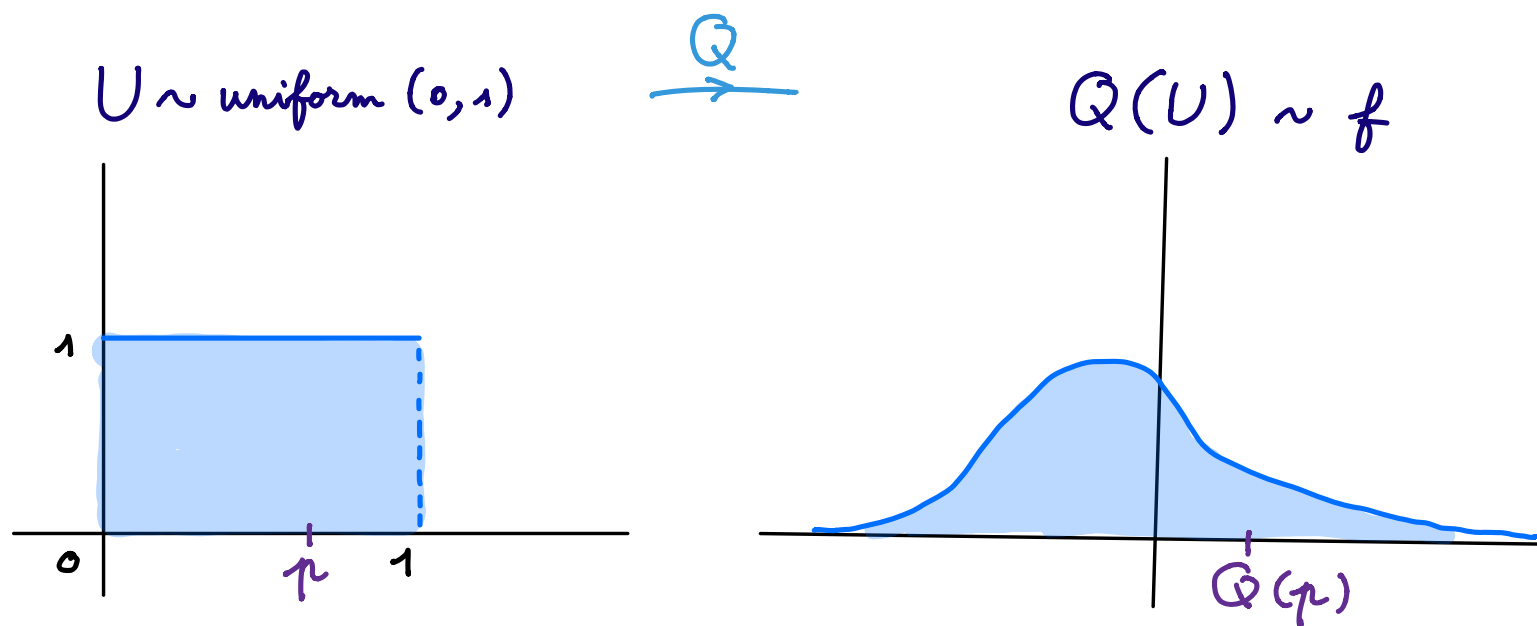


↳ Chernozhukov, Galichon,  
Hallin, Henry (AoS 2017)



MK Tail Quantile contours ?

# QUANTILE TRANSFORM



Among all  $T: \mathbb{R} \rightarrow \mathbb{R}$  such that  $T(U) \sim f$ :

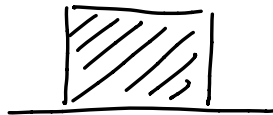
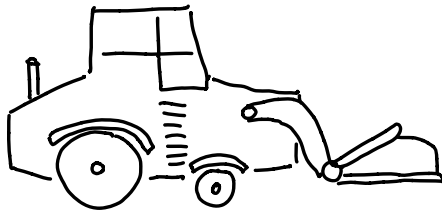
- $Q$  is the only monotone one
- $Q$  minimizes  $E[(U - T(U))^2]$   $\leadsto d \geq 2$  ?

# MONGE PROBLEM : OPTIMAL DETERMINISTIC COUPLING

$$\begin{array}{ccc} X \sim \mu & \xrightarrow{T} & T(X) = Y \sim \nu \\ \text{Reference} & & \text{Target} \end{array}$$

Among all  $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$  such that  $T(X) = Y$   
find the one that minimizes  $E[|X - T(X)|^2]$   
provided  $E|X|^2 < \infty$   
 $E|Y|^2 < \infty$

G. Monge (1776) "... déblais ... remblais "



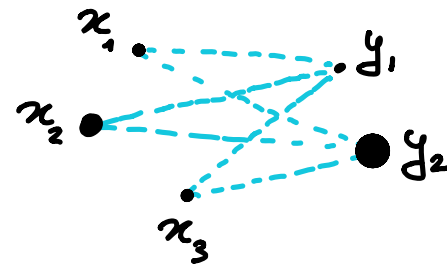
# KANTOROVICH : OPTIMAL RANDOM COUPLING

$$\begin{array}{l} X \sim \mu \\ Y \sim \nu \end{array} \quad \text{joint law } (X, Y) \sim \pi$$

Among all distributions  $\pi$  on  $\mathbb{R}^d \times \mathbb{R}^d$  with margins  $\mu$  and  $\nu$ , find the one that minimizes

$$\int |x - y|^2 d\pi(x, y) = E[|X - Y|^2]$$

- $Y = T(X)$  : MONGE
- finite 2<sup>nd</sup> moments
- minimum : WASSERSTEIN distance
- discrete case: linear program



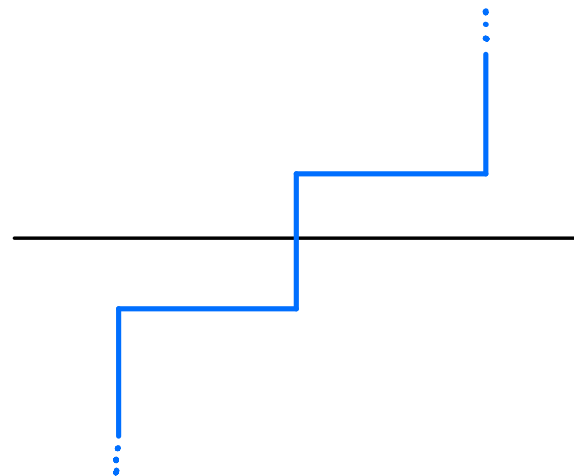
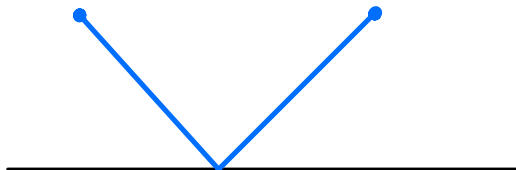
## SUBDIFFERENTIAL OF A CONVEX FUNCTION

$$\gamma : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$$

$$\partial\gamma : \mathbb{R}^d \rightrightarrows \mathbb{R}^d$$

$$\partial\gamma(x) =$$

$$\{y : \forall z, \gamma(z) \geq \gamma(x) + \langle y, z-x \rangle\}$$



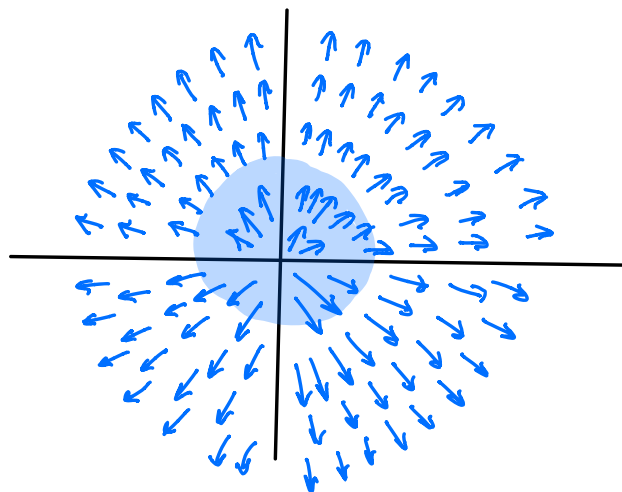
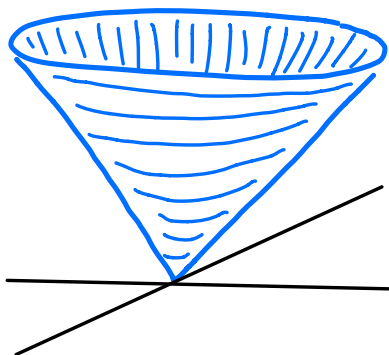
$$d = 1$$

## SUBDIFFERENTIAL OF A CONVEX FUNCTION

$$\psi: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$$

$$\partial\psi: \mathbb{R}^d \rightrightarrows \mathbb{R}^d$$

$$\begin{aligned} \partial\psi(x) = \\ \{y : \forall z, \psi(z) \geq \psi(x) + \langle y, z-x \rangle\} \end{aligned}$$



$$d=2$$

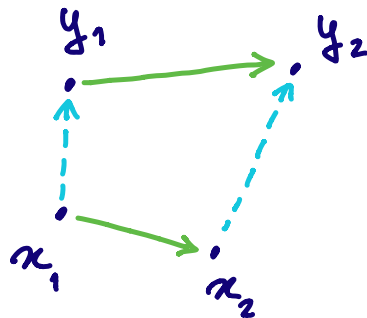
## MONOTONE MAPPINGS

$T : \mathbb{R}^d \Rightarrow \mathbb{R}^d$  is **monotone** if

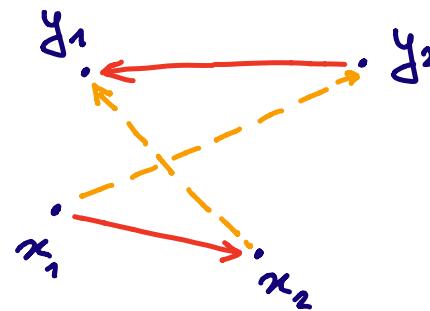
$$\forall y_1 \in T(x_1), y_2 \in T(x_2),$$

$$\langle y_2 - y_1, x_2 - x_1 \rangle \geq 0$$

*monotone :*



*not monotone :*



$$|x_1 - y_1|^2 + |x_2 - y_2|^2$$

$\leq$

$$|x_1 - y_2|^2 + |x_2 - y_1|^2$$

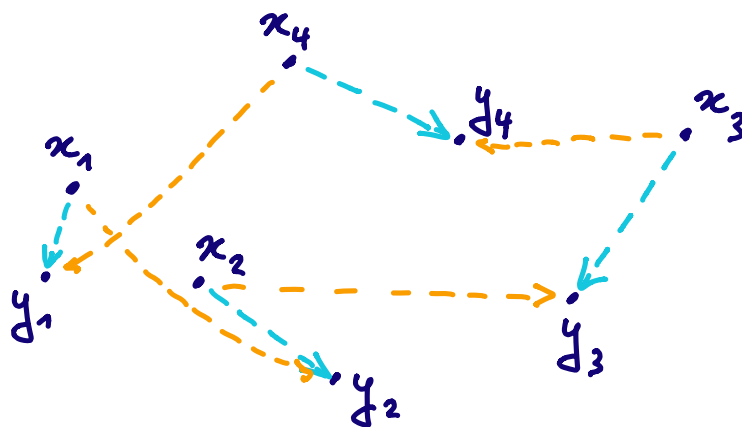


## CYCLICALLY MONOTONE MAPPINGS

$T : \mathbb{R}^d \rightrightarrows \mathbb{R}^d$  is cyclically monotone if

$\forall y_1 \in T(x_1), \dots, y_k \in T(x_k) :$

$$|x_1 - y_1|^2 + \dots + |x_k - y_k|^2 \leq |x_1 - y_2|^2 + \dots + |x_k - y_1|^2$$



• cyclically monotone  $\Rightarrow$  monotone

•  $d = 1 : \dots \Leftrightarrow \dots$

## ROCKAFELLER'S THEOREM

$T: \mathbb{R}^d \rightrightarrows \mathbb{R}^d$  is maximal cyclically monotone



$$T = \partial \psi$$

for some l.s.c. convex  $\psi: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$

$$\psi \neq +\infty$$



Rockafeller 1970  
"Convex Analysis"

## McCANN (1995)

$\mu, \nu$  distributions on  $\mathbb{R}^d$

- There exists a coupling  $\pi$  whose support is contained in the graph of  $\partial\psi$  for some l.s.c. convex  $\psi: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$
- If  $\mu$  vanishes on "small" sets, then  $\pi$  is the law of  $(X, \nabla\psi(X))$ ,  $X \sim \mu$

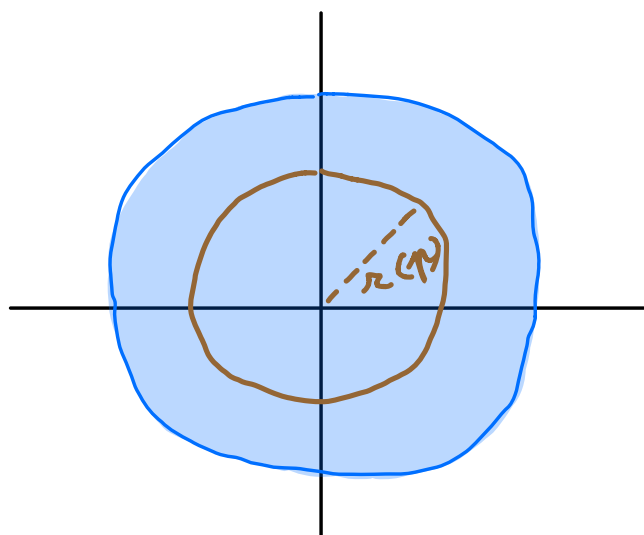
If finite 2<sup>nd</sup> moments,  $\pi$  and  $\nabla\psi$  solve M-k problem

BRENIER (1987) : smooth case

# M-K QUANTILE CONTOURS

Reference

$\mu$  : (some) uniform distribution  
on  $\{x \in \mathbb{R}^d : |x| \leq 1\}$

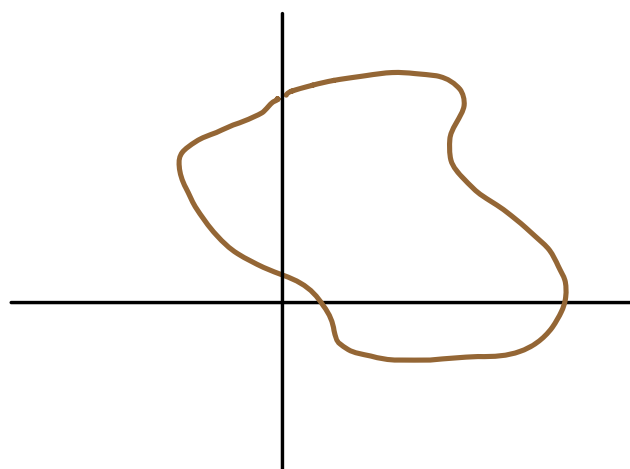


$$Q_{\mu}(p) = \{x : |x| = r(p)\}$$

Target

$$\nu = (\nabla \psi)_{\#} \mu$$

BRENIER/MCCANN



$$Q_{\nu}(p) = \bigcup_{|x|=r(p)} \partial \psi(x)$$

Chernozhukov, Galichon  
HALLIN, Henry (2017)

G. MONGE

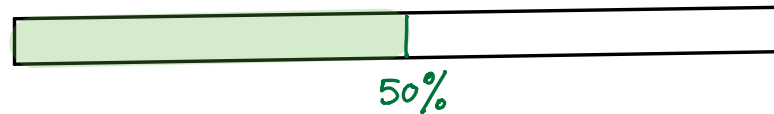
Quantiles

KANTOROVICH

Cyclic monotonicity

So far so good ...

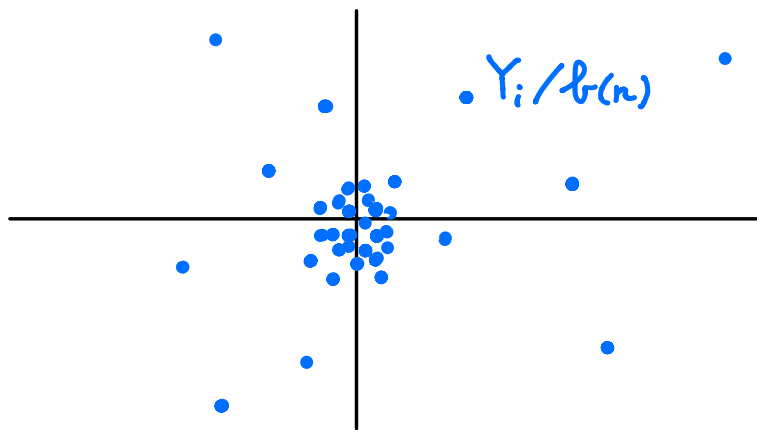
Now let's go into the tails!



## Zooming out on large observations

$$Y \sim \nu \text{ on } \mathbb{R}^d$$

$$\begin{aligned} Y_n(\cdot) &= \mathbb{E} \left[ \sum_{i=1}^n \mathbb{1} \left( \frac{1}{b(n)} Y_i \in \cdot \right) \right] \\ &= n \mathbb{P} \left[ \frac{1}{b(n)} Y \in \cdot \right] \quad \text{scaling } b(n) \rightarrow \infty \end{aligned}$$



Intensity measure of point process,  
total mass  $n \rightarrow \infty$

## REGULARLY VARYING DISTRIBUTIONS

$Y \in \mathbb{R}^d$  with law  $\nu$  is regularly varying if

$$\nu_n(\cdot) = n \mathbb{P}\left[\frac{1}{b(n)} Y \in \cdot\right] \xrightarrow{0} \bar{\nu}(\cdot)$$

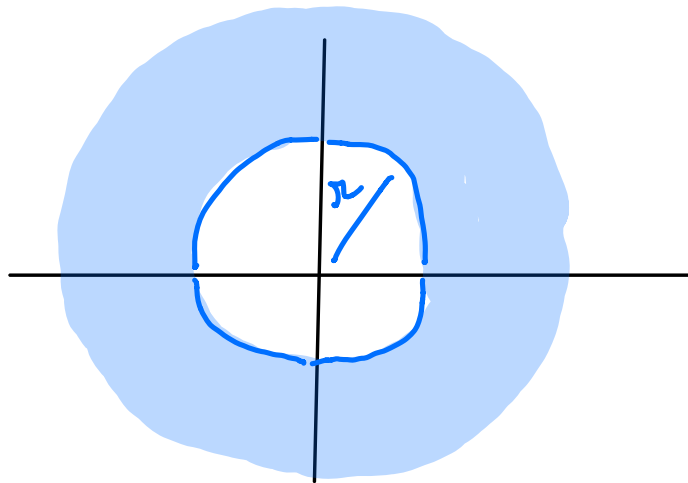
limit measure  $\bar{\nu}$  :

- infinite mass
- finite on sets bounded away from 0
- homogeneous:  $\exists \alpha > 0, \quad \nu(\lambda \cdot) = \lambda^{-\alpha} \nu(\cdot)$

S.I. Resnick  
(1987, 2007)

## RADIAL DISTRIBUTION

$$\bar{V}(\{y : |y| > r\}) = c \cdot r^{-\alpha}, \quad r > 0$$



Power law behaviour

2<sup>nd</sup> moment  $\infty$  if  $0 < \alpha < 2$



## CHOICE OF REFERENCE DISTRIBUTION

$\mu$  = spherically symmetric version of  $\nu$

= law of  $|Y| U$  with

$$Y \sim \nu$$

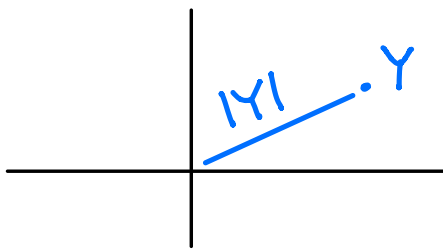
$$U \sim \text{uniform on } \{u : |u| = 1\}$$

$$Y \perp U$$

Radial distribution is preserved:

power law tail  
exponent  $-\alpha$

If  $X \sim \mu$  then  $|X| \stackrel{d}{=} |Y|$



## COUPLING REFERENCE & TARGET

Target  $Y \sim \nu$ , regularly varying

Reference  $X \sim \mu$ ,  $|X| \stackrel{d}{=} |Y|$   
spherically symmetric

McCANN (1995):  $\exists$  coupling  $(X, Y) \sim \pi$

$$\text{support}(\pi) \subset \text{graph}(\partial\psi) \subset \mathbb{R}^d \times \mathbb{R}^d$$

for some convex function  $\psi$  on  $\mathbb{R}^d$

$\mu$  need not be smooth:

not guaranteed that  $Y = \nabla\psi(X)$

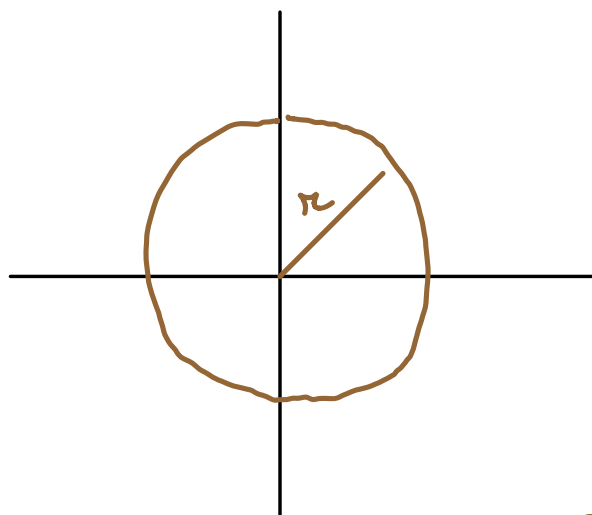
# QUANTILE CONTOURS

Reference

$$X \sim \mu$$

$$|X| \stackrel{d}{=} |Y|$$

$X$  spher. sym.



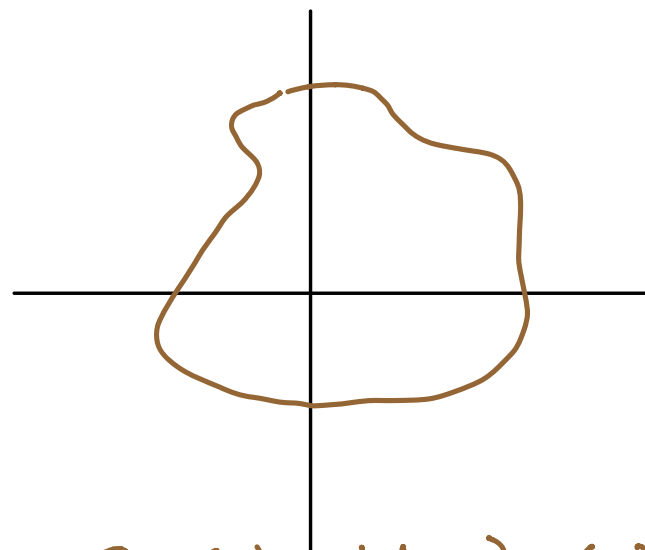
$$Q_X(r) = \{x : |x| = r\}$$

$$(X, Y) \sim \pi$$

$$\text{support}(\pi) \subset \{(x, y) : y \in \partial\psi(x)\}$$

Target

$$Y \sim \nu$$

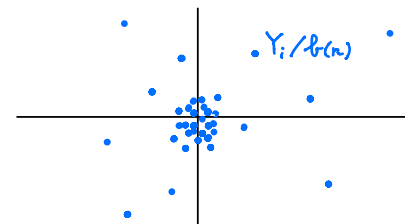


$$Q_Y(r) = \bigcup_{|x|=r} \partial\psi(x)$$

## REFERENCE LIMIT INTENSITY MEASURE

Recall regular variation :

$$n \mathbb{P} \left[ \frac{1}{b(n)} Y \in \cdot \right] \xrightarrow{o} \bar{\nu}(\cdot)$$



$\bar{\mu} :=$  spherically symmetric such that

$$\begin{aligned} \bar{\mu}(\{x : |x| > r\}) &= \bar{\nu}(\{y : |y| > r\}) \\ &= c \cdot r^{-\alpha}, \quad r > 0 \end{aligned}$$

infinite measures  $\Rightarrow$  McCANN theory does not apply!

## TAIL STABILITY

Recall:  $\text{suppat}(X, Y) = \text{graph}(\partial\psi)$

$$Q_Y(r) = \bigcup_{|x|=r} \partial\psi(x) \quad r \rightarrow \infty ?$$

$\exists!$  convex  $\bar{\psi}$  on  $\mathbb{R}^d$  with  $\bar{\psi}(0) = 0$  and

$$\bullet \quad \frac{1}{t} \partial\psi(t \cdot) \xrightarrow{g} \partial\bar{\psi}(\cdot), \quad t \rightarrow \infty$$

$\downarrow$   
graphical convergence  
implies local uniform convergence  
at  $x$  where  $\bar{\psi}$  is cont. diff.

$$\bullet \quad \bar{\psi}(\cdot) = \bar{\mu}(\{x : \nabla\bar{\psi}(x) \in \cdot\})$$

## THE LIMIT IS HOMOGENEOUS

$\bar{\Psi}$  and  $\partial \bar{\Psi}$  are homogeneous :

$$\bar{\Psi}(\lambda x) = \lambda^2 \bar{\Psi}(x)$$

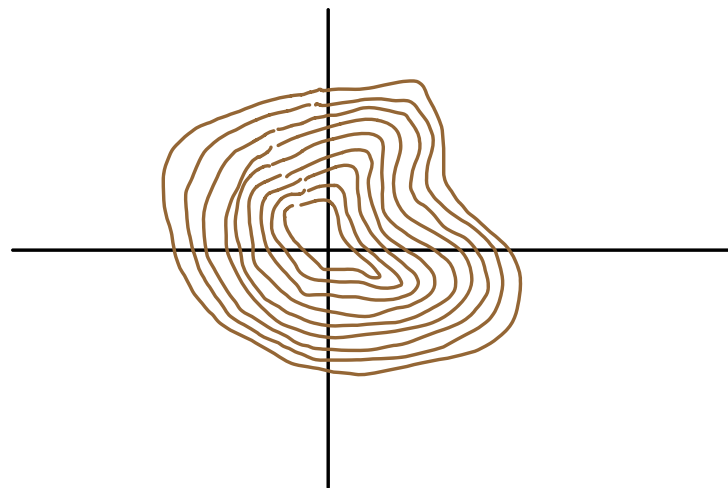
$$\partial \bar{\Psi}(\lambda x) = \lambda \partial \bar{\Psi}(x)$$

$$\lambda > 0 \\ x \in \mathbb{R}^d$$

Limit contours are homothetic :

$$Q_{\bar{\Psi}}(r) = r Q_{\bar{\Psi}}(1)$$

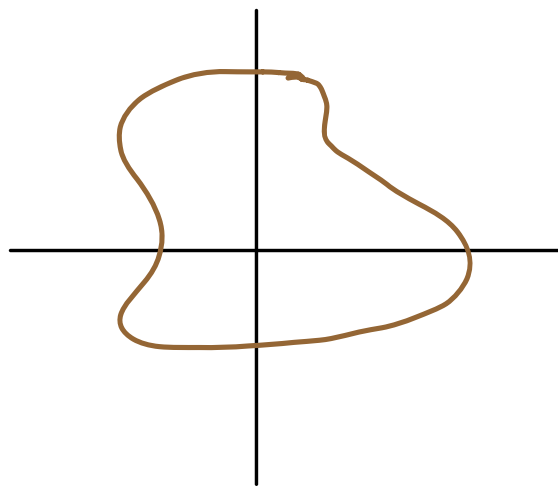
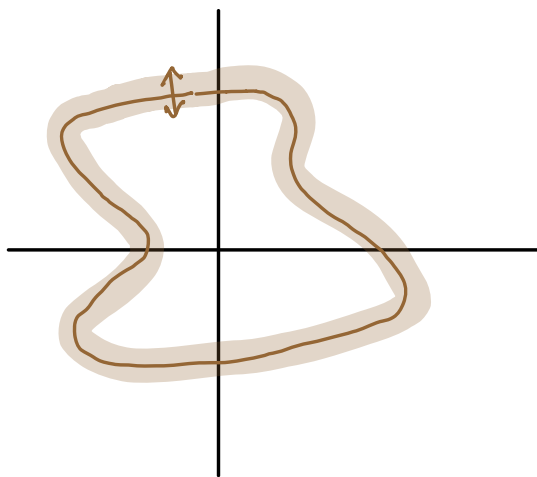
$$Q_{\bar{\Psi}}(1) = \bigcup_{|x|=1} \partial \bar{\Psi}(x)$$



## CONVERGENCE OF QUANTILE CONTOURS

For  $0 < a < b < +\infty$  :

$$\bigcup_{a \leq \lambda \leq b} \frac{1}{\lambda} Q_Y(\lambda) \xrightarrow[\lambda \rightarrow \infty]{\text{Hausdorff distance}} Q_{\bar{Y}}(1)$$



# Nonparametric tail quantile contour estimator

*Input:* points  $\mathbf{y}_1, \dots, \mathbf{y}_n$  in  $\mathbb{R}^d$

*Wanted:* estimator of  $Q_{\bar{\psi}}(1) = \lim_{r \rightarrow \infty} \bigcup_{|\mathbf{x}|=r} r^{-1} \partial\psi(\mathbf{x})$

## Algorithm:

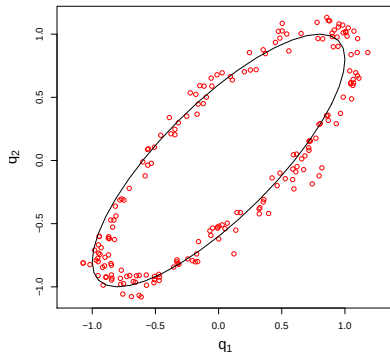
**Step 1** Find estimator  $\partial\hat{\psi}_n$  of optimal plan  $\partial\psi$  from  $\mu$  to  $\nu$ , with  $\mu$  spherically symmetric version of  $\nu$

**Step 2** Choose large  $r_n$  and put

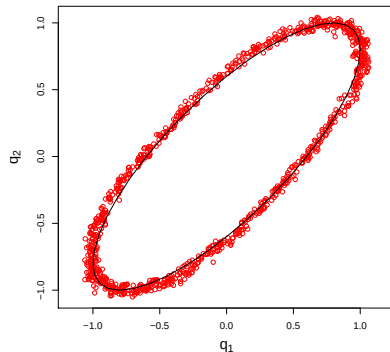
$$\hat{Q}_n := \left\{ \frac{1}{|\mathbf{x}|} \partial\hat{\psi}_n(\mathbf{x}) : |\mathbf{x}| > r_n \right\}$$



# Multivariate Student t distribution

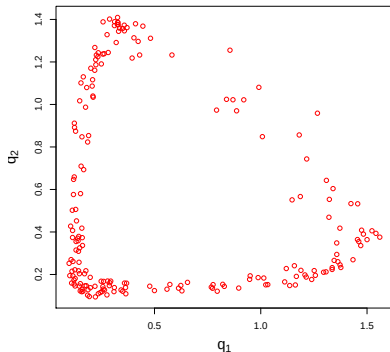


$n = 2000$   
 $k = 200$

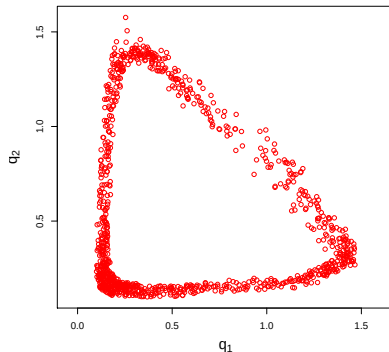


$n = 10000$   
 $k = 1000$

# Fréchet margins, independence copula

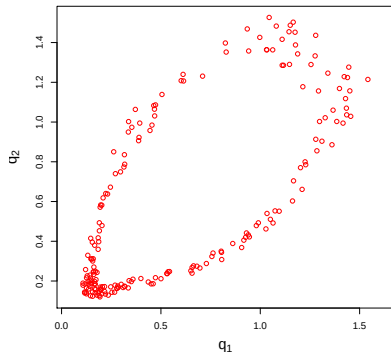


$n = 2000$   
 $k = 200$

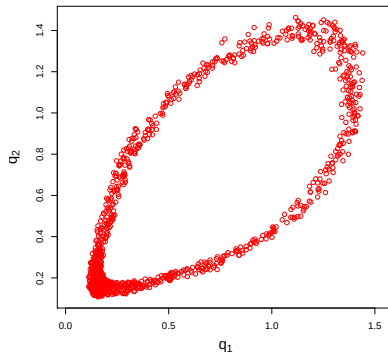


$n = 10000$   
 $k = 1000$

# Fréchet margins, Gumbel copula

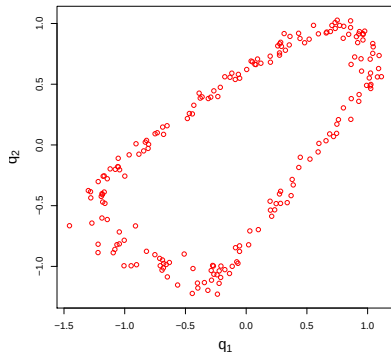


$n = 2000$   
 $k = 200$

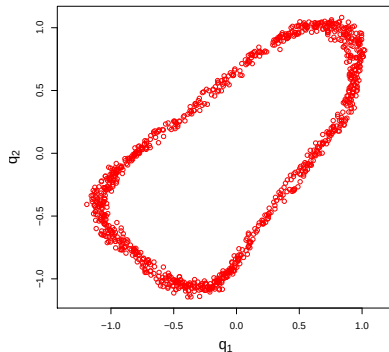


$n = 10000$   
 $k = 1000$

# Student t margins, Gumbel copula



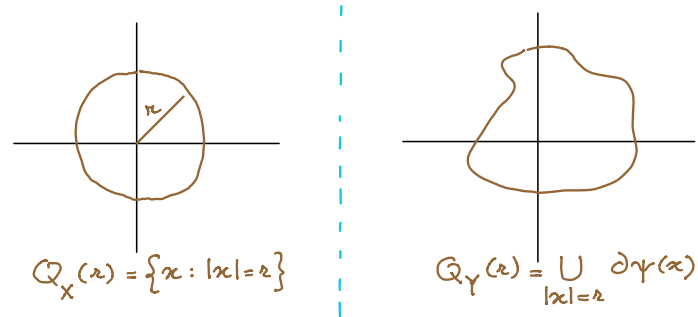
$n = 2000$   
 $k = 200$



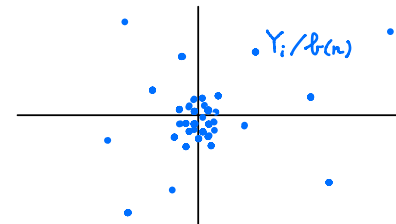
$n = 10000$   
 $k = 1000$

# TAIL QUANTILE CONTOURS

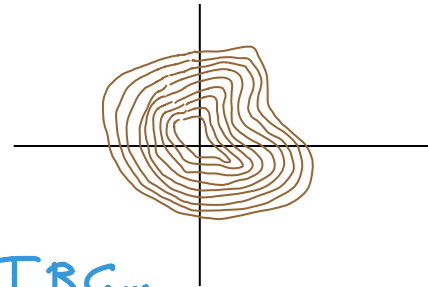
Quantile contours:  
transporting spheres  
via cyclically  
monotone mappings



Regular variation:  
zooming out, limiting  
intensity measure



tail quantile contours:  
homothetic to a single shape



Nonparametric estimation feasible: TBC...



# Bibliography I

- Bingham, N., C. Goldie, and J. Teugels (1987). *Regular variation*. Cambridge: Cambridge University Press.
- Brenier, Y. (1987). Décomposition polaire et réarrangement monotone des champs de vecteurs. *C. R. Acad. Sci. Paris Sér. I Math.* 305, 805–808.
- Chernozhukov, V., A. Galichon, M. Hallin, and M. Henry (2017). Monge–Kantorovich depth, quantiles, ranks and signs. *The Annals of Statistics* 45(1), 223–256.
- Cuesta-Albertos, J. and M. C. (1989). Notes on the Wasserstein metric in Hilbert spaces. *The Annals of Probability* 17, 1264–1276.
- Cuesta-Albertos, J., C. Matrán, and A. Tuero-Diaz (1997). Optimal transportation plans and convergence in distribution. *Journal of Multivariate Analysis* 60, 72–83.
- Fisher, R. and L. Tippett (1928). On the estimation of the frequency distributions of the largest or smallest member of a sample. *Proceedings of the Cambridge Philosophical Society* 24, 180–190.
- Gnedenko, B. (1943). *Annals of Mathematics* 44, 423–453.
- Hult, H. and F. Lindskog (2006). Regular variation for measures on metric spaces. *Publ. Inst. Math. (Beograd) (N.S.)* 80(94), 121–140.

## Bibliography II

- Karamata, J. (1930). Sur un mode de croissance régulière des fonctions. *Mathematica (Cluj)* 4, 38–53.
- McCann, R. J. (1995). Existence and uniqueness of monotone measure-preserving maps. *Duke Math. J.* 80(2), 309–323.
- Resnick, S. I. (1987). *Extreme values, regular variation, and point processes*. New York: Springer-Verlag.
- Resnick, S. I. (2007). *Heavy-tail phenomena. Probabilistic and statistical modeling*. New York: Springer.
- Rockafellar, R. and R. Wets (1998). *Variational Analysis*. New York: Springer.
- Rockafellar, R. T. (1970). *Convex Analysis*. Princeton: Princeton University Press.
- Rüschendorf, L. (1991). Fréchet bounds and their applications. In G. Dall’Aglio, S. Kotz, and G. Salinette (Eds.), *Advances in Probability Distributions with Given Marginals (Rome 1990)*, pp. 151–187. Dordrecht: Kluwer Academic Publishers.
- Schuhmacher, D., B. Bähre, C. Gottschlich, F. Heinemann, and B. Schmitzer (2017). *transport: Optimal Transport in Various Forms*. R package version 0.9-4.
- Villani, C. (2009). *Optimal Transport. Old and New*. Berlin: Springer-Verlag.