

# MULTIVARIATE QUANTILES, OPTIMAL TRANSPORT

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**M**onge-Kantorovich quantiles are defined in an intuitive fashion through the optimal transportation from a reference distribution. My thesis is dedicated to their study, as they benefit from most of sought-after properties. The adaptivity of these concepts makes them attractive for building statistical tools, and has concentrated much attention in the recent years. My PhD partly belongs to this line of work, as we proposed multivariate definitions of superquantiles, expected shortfalls and related risk measures. In addition, we focused on the estimation of a regularized version of the Monge-Kantorovich quantile function, via a stochastic algorithm with almost-sure convergence guarantees.

## Ordering multivariate data

Consider a probability distribution  $\nu$  supported on  $\mathbb{R}^d$ . In the scalar case  $d = 1$ , the quantile function of  $\nu$  is nothing else than the generalized inverse  $F_\nu^{-1}$  of the cumulative distribution function  $F_\nu$ . This heavily relies on the left-to-right ranking of samples from  $\nu$ . However, in the multi-dimensional case  $d > 1$ , the lack of a canonical ordering precludes a consensual notion of quantiles, see [1, 2] and references therein. The key ingredient for a concept of quantiles is thus the ordering it provides for observations sampled from  $\nu$ .

Departing from what is known,  $F_\nu^{-1}$  appears to be the unique solution of the optimal transport (OT) problem between the uniform  $\mu = U([0, 1])$  and  $\nu$ . By stating this as a definition when  $d > 1$ , the authors of [1] generalized univariate quantiles to define the Monge-Kantorovich (MK) quantile function of  $\nu$  as

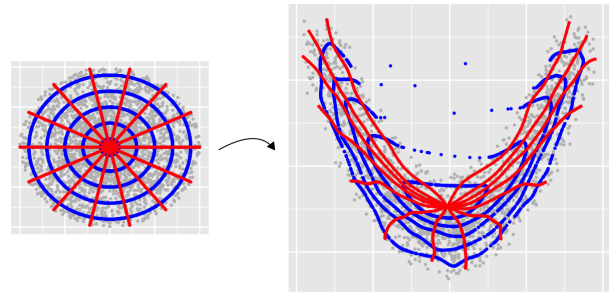
$$\mathbf{Q} = \operatorname{argmin}_{T: T_\# \mu = \nu} \mathbb{E}_{X \sim \mu} (\|X - T(X)\|^2),$$

where the push-forward constraint  $T_\# \mu = \nu$  means

$$\int_{\mathcal{X}} g d\nu = \int_{T^{-1}(\mathcal{X})} g \circ T d\mu.$$

A suitable choice of reference measure  $\mu$  is the one of the random vector  $R\Phi$ , where  $R$  and  $\Phi$  are independent and drawn uniformly from  $[0, 1]$  and the unit hypersphere  $\mathbb{S}^{d-1} = \{\varphi \in \mathbb{R}^d : \|\varphi\| = 1\}$ , respectively. With this choice, the unit balls  $\mathbb{B}(0, \alpha)$  have  $\mu$ -probability  $\alpha$ , and the regions  $\mathbf{Q}(\mathbb{B}(0, \alpha))$  are nested and have  $\nu$ -probability  $\alpha$ , and thus are appropriate candidates for quantile regions, [1, 2]. Descriptive plots in the spirit of multivariate boxplots are given in Figure 1.1 for a banana-shaped distribution  $\nu$ . The fact that the random vector  $\mathbf{Q}(U)$  follows  $\nu$  as soon as  $U$  is sampled from  $\mu$  is crucial. It allows to claim that  $\mathbf{Q}$  is able to capture all the available information. Roughly, in Figure 1.1, the same amount of mass is contained in the regions

delimited by two red curves, and the blue curves encapsulate quantile regions indexed by their probability contents.



**FIGURE 1.1** – For any distribution, on the right, a transported ordering from some reference measure, on the left.

## Statistical tools

In  $\mathbb{R}$ , the superquantiles and expected shortfalls complement the information given by the quantiles. By focusing on which univariate features we aim to extend, we defined in [3] the MK superquantile function

$$S(u) = \frac{1}{1 - \|u\|} \int_{\|u\|}^1 \mathbf{Q}(t \frac{u}{\|u\|}) dt,$$

and the MK expected shortfall function

$$E(u) = \frac{1}{\|u\|} \int_0^{\|u\|} \mathbf{Q}(t \frac{u}{\|u\|}) dt.$$

The counterpart of Figure 1.1 by using  $S$  and  $E$  instead of  $\mathbf{Q}$  induces the descriptive plots of Figure 1.2. These functions describe central and peripheral areas of point clouds, and they can be shown to characterize random vectors and their convergence in distribution, [3].

**Theorem.** Let  $\nu_1$  and  $\nu_2$  be probability distributions on  $\mathbb{R}^d$ , with respective MK superquantile and expected shortfall functions given by  $S_1, E_1$  and  $S_2, E_2$ . Then,

$$\nu_1 = \nu_2 \Leftrightarrow S_1 = S_2 \text{ } \mu\text{-a.e.} \Leftrightarrow E_1 = E_2 \text{ } \mu\text{-a.e.}$$

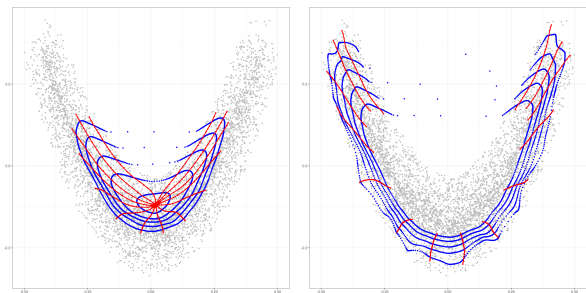


FIGURE 1.2 – Descriptive plots,  $E$  on the left,  $S$  on the right.

**Theorem.** Let  $\nu_n$  and  $\nu$  be such that their respective MK quantile functions  $\mathbf{Q}_n$  and  $\mathbf{Q}$  are continuous on  $\mathbb{B}(0, 1) \setminus \{0\}$ . Then the weak convergence of  $\nu_n$  towards  $\nu$  is equivalent to

$$\forall u \in \mathbb{B}(0, 1) \setminus \{0\}, \lim_{n \rightarrow +\infty} E_n(u) = E(u)$$

and, for any compact  $K \subset \mathbb{B}(0, 1) \setminus \{0\}$ ,

$$\lim_{n \rightarrow +\infty} \sup_{u \in K} \|E_n(u) - E(u)\| = 0.$$

Besides, if one assumes that, for every  $n \in \mathbb{N}$  and  $X_n$  drawn from  $\nu_n$ , there exists a random vector  $Z$  with  $\mathbb{E}[Z \ln(Z)] < +\infty$  such that  $\|X_n\| \leq Z$ , then the above weak convergence is also equivalent to

$$\forall u \in \mathbb{B}(0, 1) \setminus \{0\}, \lim_{n \rightarrow +\infty} S_n(u) = S(u).$$

Perhaps the most classical univariate application of these notions is the measurement of risk, with the fundamental risk measures given by the Value-at-Risk (VaR) and the Conditional-Value-at-Risk (CVaR). The risk framework considers a vector of losses  $X \in \mathbb{R}_+^d$  where each component is a positive measure. From our definitions, one can just select a point with maximal norm within a MK quantile contour (resp. superquantile) to get a multivariate VaR (resp. CVaR), see [3] for further detail. Such risk measurements summarize a given dataset to answer the following :

- With probability  $\alpha$ , what is the worst that can happen ?
- In case the worst happens, what shall we expect, in average ?

Using MK quantiles allows to take into account the multivariate probability for the assertion “with probability  $\alpha$ ”. These are illustrated in Figure 1.3, with different choices of reference measure that correspond to a center-outward or a left-to-right ordering for  $\nu$ .

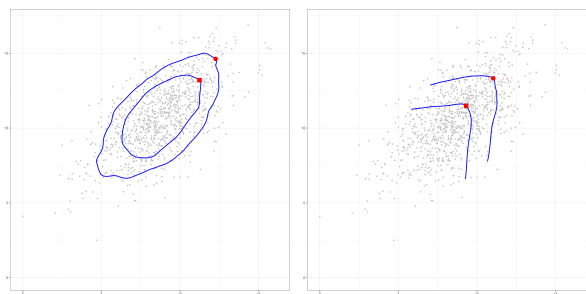


FIGURE 1.3 – VaR and CVaR, center-outward or left-to-right ordering.

## Estimation

In practice, the estimation of  $\mathbf{Q}$  amounts to solve an OT problem involving the empirical measure associated to samples  $Y_1, \dots, Y_n$  from  $\nu$ . Such problem yields a quantile function whose values are constrained to belong to the  $(Y_i)$ , unless one uses regularization in a second step. Interpolation is desirable as soon as the focus is on quantile contours and regions, or if it is required to compute out-of-sample estimates  $\mathbf{Q}(x)$ , for any  $x$ . The estimation of regularized MK quantiles is another direction of my thesis, in which we advocated the use of the entropic regularization of optimal transport, [4]. This results in the *entropic map*, that has the desirable feature of being the gradient of a convex function, even in practice, and that is rooted in the literature on computational optimal transport.

Therefore, the estimation procedure requires to solve the entropically regularized OT problem. Making use of the fact that one of the two distributions is held fixed, we were able to design a new algorithm tackling the continuous OT in the limit  $n \rightarrow +\infty$ , for  $n$  the size of the sample  $(Y_i)$ . The idea is to parametrize dual potentials in the Kantorovich formulation of OT by their Fourier coefficients, leading to a stochastic gradient descent in the Banach space of absolutely summable sequences. Using stochastic algorithms has two major consequences. On the practical side, it allows to avoid the storage of the cost matrix of size  $n^2$  between two samples of size  $n$ . On the theoretical side, one can use tools from stochastic optimization to obtain consistency results, as in [4] where we showed the almost sure convergence of the iterates of our algorithm.

## Directional data

The definition of Monge-Kantorovich quantile and distribution functions has recently been extended to non-euclidean data in [5]. Again, providing regularized estimators is highly desirable. To do so, we generalized the entropic map on the unit hypersphere  $\mathbb{S}^{d-1}$  and motivated its use in [6].

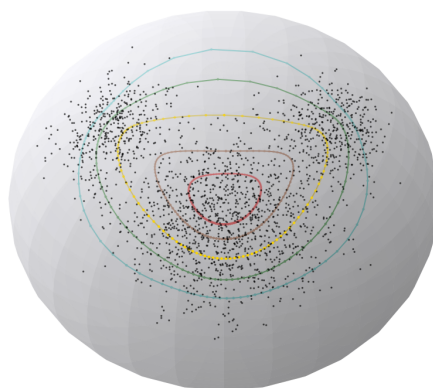


FIGURE 1.4 – MK quantile contours for spherical data.

On the computational side, we extended our computational approach by expanding dual potentials in the basis of spherical harmonics, the spherical analog of Fourier series. Our analysis also focused on the equivalent concept of statistical depth, with an investigation of its properties related to Liu-Zuo-Serfling axioms. We derived statistical tools based on these concepts, that emphasize the potential of entropic regularization for empirical spherical quantiles.

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