

Towards a robust vision of geometric inference

Claire Bréchet

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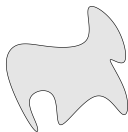
Under the supervision of
Pascal Massart (Université Paris-Sud 11) and Frédéric Chazal (Inria Saclay)

September 24, 2018

Geometric Inference : Recover geometric information from a point cloud sampled around some shape.



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Global setting :

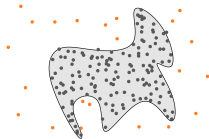
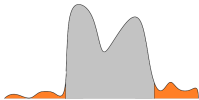
- (\mathcal{X}, δ) , metric space
- P , probability distribution supported on \mathcal{X}

That is, (\mathcal{X}, δ, P) is a **metric-measure space**.

- Q , probability distribution (close to P somehow)
- $\mathbb{X}_n = \{X_1, X_2, \dots, X_n\}$, n -sample from Q

Robustness :

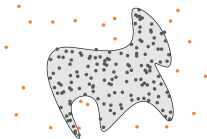
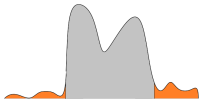
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Getting rid of a proportion $1-\eta$ of the probability (resp. of the data-points).

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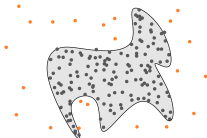
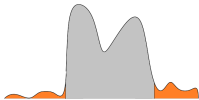


Getting rid of a proportion $1-\eta$ of the probability (resp. of the data-points).

$$t_{\eta}^* \in \arg \min_t \inf_{\eta \tilde{P} \leq P} \tilde{P}\gamma(t, \cdot)$$

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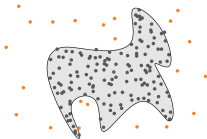
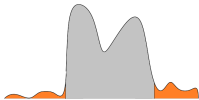
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P_η such that :

$$\inf_{\eta \tilde{P} \leq P} \tilde{P}\gamma(t_\eta^*, \cdot) = P_\eta\gamma(t_\eta^*, \cdot)$$

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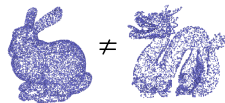
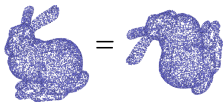
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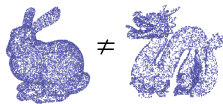
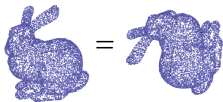
- 2 **Stability** (e.g. according to a Wasserstein metric W_p).
Small $W_p(P, Q) \rightsquigarrow$ Roughly the same geometric information in P and Q .



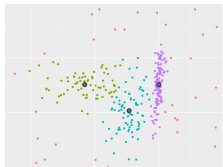
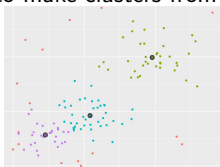
- How to compare two datasets?



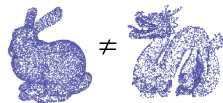
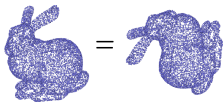
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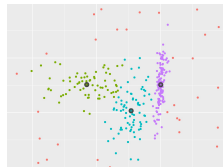
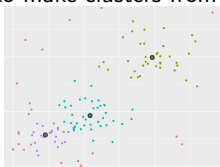
- How to make clusters from a dataset?



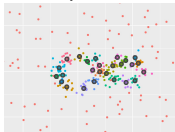
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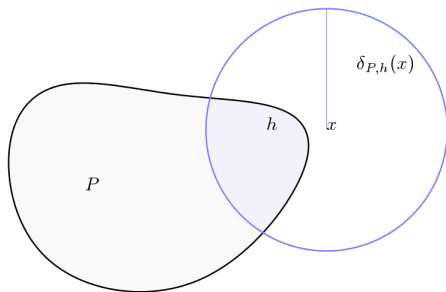
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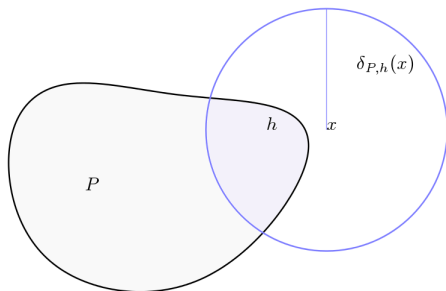
- How to infer the distance to a compact set, with a fixed budget ?



A multifunction tool : the distance-to-measure function



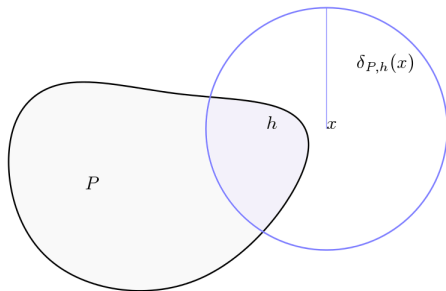
$$\delta_{P,h}(x) = \inf \{ r > 0 \mid P(\bar{B}(x, r)) > h \}$$



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The **distance-to-measure (DTM)** [Chazal, Cohen-Steiner, Mérigot 09'] is defined for all $x \in \mathcal{X}$ and $h \in [0, 1]$ by :

$$d_{P,h}(x) = \frac{1}{h} \int_0^h \delta_{P,l}(x) dl$$



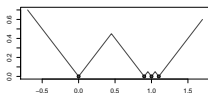
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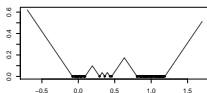
$$d_{P,h}^{(p)}(x) = \left(\frac{1}{h} \int_0^h \delta_{P,l}^{(p)}(x) dl \right)^{\frac{1}{p}}$$

- 1 When $h = 0$, $d_{P,0} = d_{\mathcal{X}}$.
- 2 $\left\| d_{P,h}^{(p)} - d_{Q,h}^{(p)} \right\|_{\infty} \leq h^{-\frac{1}{p}} W_p(P, Q)$ [Chazal, Cohen-Steiner, Mérigot 09'].

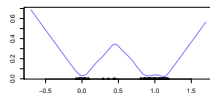
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Distance to \mathcal{X}



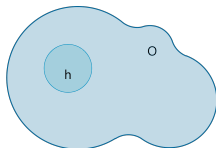
Distance to \mathbb{X}_n



DTM with $h = 0.2$

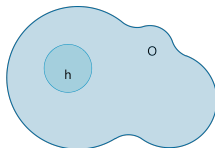
Theorem (Brécheteau)

P_O (uniform distribution on O) can be recovered from $d_{P_O, h}$ provided that h is small enough and O regular enough.



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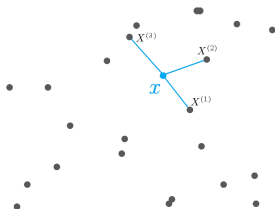
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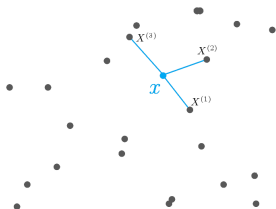
Theorem (Brécheteau)

P can be recovered from $(d_{P, h})_{h \in [0, 1]}$ provided that $(\mathcal{X}, \delta) = (\mathbb{R}^d, \|\cdot\|)$.

- 1 $\kappa = nh$
- 2 Empirical distribution $P_n = \sum_{i=1}^n \frac{1}{n} \delta_{X_i}$
- 3 $X^{(1)}, X^{(2)}, \dots, X^{(\kappa)}$: κ nearest neighbours of x in \mathbb{X}_n



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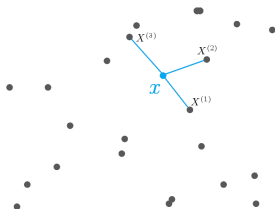


$$d_{P_n, h}(x) = \frac{1}{\kappa} \sum_{i=1}^{\kappa} \delta(X^{(i)}, x)$$

↪ Easy implementation of the DTM at a point x in practice!

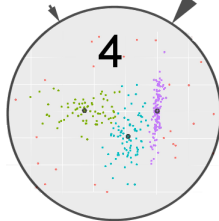
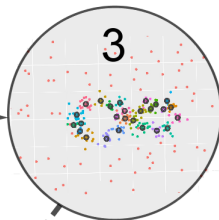
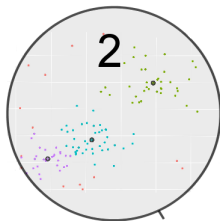
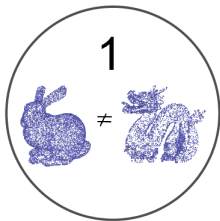
The DTM, an implementable tool

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$$d_{P_n, h}^{(p)}(x) = \left(\frac{1}{\kappa} \sum_{i=1}^{\kappa} \delta^p(X^{(i)}, x) \right)^{\frac{1}{p}}$$

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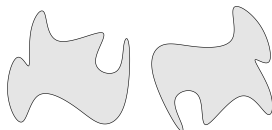


1) A statistical test of isomorphism between mm-spaces



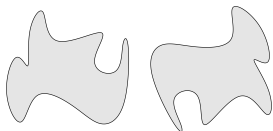
A statistical test of isomorphism between mm-spaces

Two mm-spaces (\mathcal{X}, δ, P) and $(\mathcal{Y}, \delta', P')$ are **isomorphic** [Gromov 81'] if :
 $\exists \phi: \mathcal{X} \mapsto \mathcal{Y}$ a one-to-one isometry, s.t. for all Borel set A , $P'(\phi(A)) = P(A)$.



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How to build a test of level $\alpha > 0$ to test the null hypothesis

H_0 : “ (\mathcal{X}, δ, P) and $(\mathcal{Y}, \delta', P')$ are isomorphic” ?

vs

H_1 : “ (\mathcal{X}, δ, P) and $(\mathcal{Y}, \delta', P')$ are not isomorphic” ?



(\mathcal{X}, δ, P)



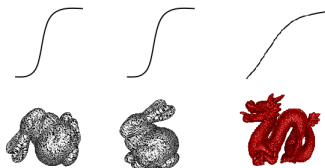
$(\mathcal{Y}, \delta', P')$

The **Gromov-Wasserstein distance** [Mémoli 10'] GW is a metric such that $GW((\mathcal{X}, \delta, P), (\mathcal{Y}, \delta', P')) = 0$ iff the mm-spaces are isomorphic.

⚠ Too high computational cost.

Definition

The **DTM-signature**, $d_{P,h}(P)$ is the distribution of $d_{P,h}(X)$ when $X \sim P$.



Theorem (Bréchet)

$$W_1(d_{P,h}(P), d_{P',h}(P')) \leq \frac{1}{h} GW(\mathcal{X}, \mathcal{Y})$$

Definition

Defined by $d_{P_N, h}(P_n)$ with P_N from (X_1, X_2, \dots, X_N) and P_n from (X_1, X_2, \dots, X_n) .

Statistic :

$$T = \sqrt{n}W_1(d_{P_N, h}(P_n), d_{P'_N, h}(P'_n))$$

Subsampling distribution :

$$\mathcal{L}^*(P) = \mathcal{L}^*(\sqrt{n}W_1(d_{P_N, h}(P_n^*), d_{P_N, h}(P_n^{*'})) | P_N)$$

Under hypothesis H_0 , $\mathcal{L}(T)$ is approximated with $\mathcal{L}^* = \frac{1}{2}\mathcal{L}^*(P) + \frac{1}{2}\mathcal{L}^*(P')$.

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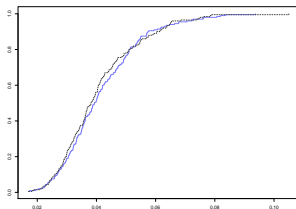
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Cdf of $\mathcal{L}(T)$ and $\mathcal{L}^*(P)$ (Bunny)

$N = 10000$, $n = 100$, $h = 0.1$

Test :

$$\phi_{N,n,h} = \mathbb{1}_{T \geq \hat{q}_{\alpha,N,n,h}}$$

with $\hat{q}_{\alpha,N,n,h}$, the α -quantile of \mathcal{L}^* .

Theorem (BréchetEAU)

If P is supported on compact subsets of \mathbb{R}^d ; $\mathcal{L}(\|\mathbb{G}_{P,h} - \mathbb{G}'_{P,h}\|_1)$ is atomless;

$n \sim N^{\frac{1}{\rho}}$;

- in the general case, if $\rho > \frac{\max\{d,2\}}{2}$,
- in the (a,b) -standard case, if $\rho > 1$,

then $\mathbb{P}_{(P,P)}(\phi_{N,n,h}) \rightarrow \alpha$, when $N \rightarrow \infty$.

$\mathbb{G}_{P,h}$ and $\mathbb{G}'_{P,h}$ independent Gaussian processes with covariance kernel

$\kappa(s,t) = F_{d_{P,h}(P)}(s) \left(1 - F_{d_{P,h}(P)}(t)\right)$ for $s \leq t$.

$n \sim N^{\frac{1}{\rho}}$ with $\rho > 1$

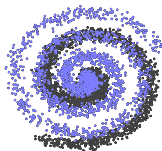
\mathcal{X}, \mathcal{Y} : compact subsets of \mathbb{R}^d .

Theorem (BréchetEAU)

There is $n_{P,P'}$ such that $\forall n \geq n_{P,P'}$,

$$\mathbb{P}_{(P,P')} (1 - \phi_{N,n,h}) \leq 4 \exp \left(- \frac{W_1^2(d_{P,h}(P), d_{P',h}(P'))}{3 \max\{\text{Diam}_{P'}^2, \text{Diam}_P^2\}} n \right)$$

$N = 2000$ points; $\alpha = 0.05$, $h = 0.05$, $n = 20$.

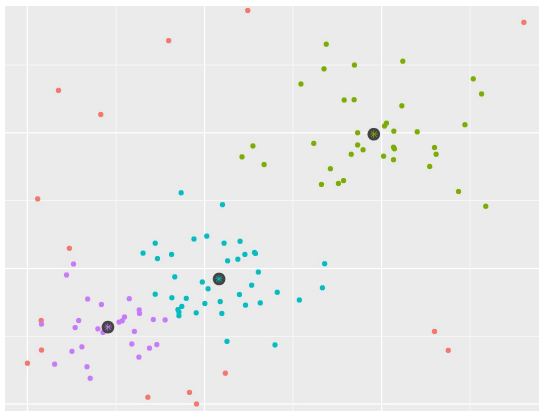


Comparison to the spiral with shape parameter 10 (grey).

spiral shape parameter	15	20	30	40	100
type I error DTM	0.050	0.049	0.051	0.044	0.051
type II error DTM	0.475	0.116	0.013	0.023	0.015
type II error KS	0.232	0.598	0.535	0.586	0.578

Type I and type II error approximations

2) Bregman trimmed clustering

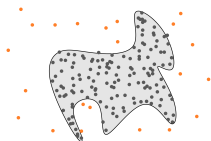
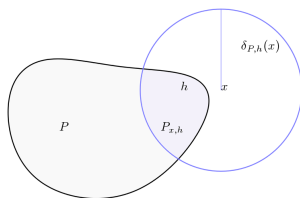


The DTM, a tool for trimming

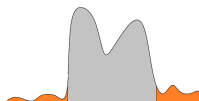
$P_{x,h}$: restriction of P to the ball of P -mass h

$$\begin{aligned}d_{P,h}^2(x) &= P_{x,h} \|\cdot - x\|^2 \\ &= \inf_{h\tilde{P} \leq P} \tilde{P}\gamma(x, \cdot)\end{aligned}$$

with $\gamma(x, \cdot) = \|\cdot - x\|^2$.



For the DTM :
 $1 - h \leftrightarrow 1 - \eta$



$$d_{P,\eta}^2 : x \mapsto \inf_{\eta\tilde{P} \leq P} \tilde{P}\|\cdot - x\|^2$$

Minimizer x^* : **Trimmed barycenter**

codebook $\mathbf{c} = (c_1, c_2, \dots, c_k)$

$$\gamma(\mathbf{c}, \cdot) = \min_{j \in 1..k} \|\cdot - c_j\|^2$$

$$\mathbf{B}(x, r) \leftrightarrow \bigcup_{i \in 1..k} \mathbf{B}(c_i, r).$$

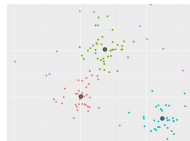
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$$B(x, r) \leftrightarrow \bigcup_{i \in 1..k} B(c_i, r).$$

$$d_{P, \eta}^2 : \mathbf{c} \mapsto \inf_{\tilde{P} \leq P} \tilde{P} \min_{j \in 1..k} \|\cdot - c_j\|^2$$

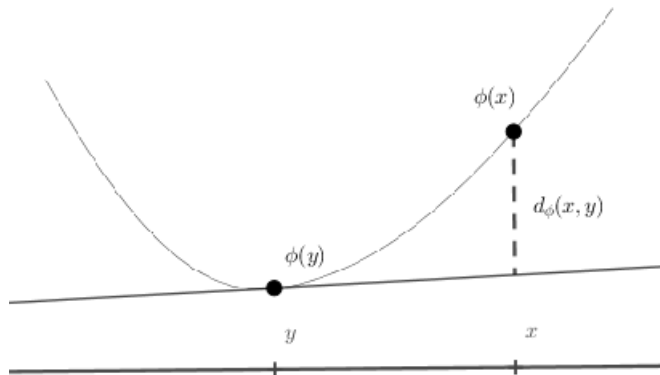
Minimizer \mathbf{c}^* : Optimal codebook for
Trimmed k -means [Cuesta et al. 97']



An example of trimmed clustering with a Bregman divergence

$\Omega \subset \mathbb{R}^d$ convex set, $\phi : \Omega \rightarrow \mathbb{R}$ strictly convex and \mathcal{C}^1 . Bregman divergence

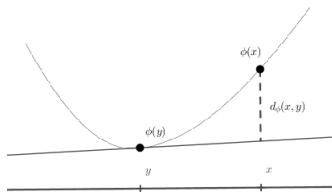
$$d_\phi : (x, y) \mapsto \phi(x) - \phi(y) - \langle \nabla_y \phi, x - y \rangle, \forall x, y \in \Omega$$



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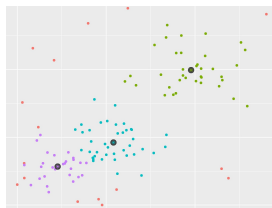


Poisson distribution :

$$\begin{aligned} -\log(p_\theta(x)) &= -\log\left(\frac{\theta^x}{x!} e^{-\theta}\right) \\ &= d_\phi(x, \theta) + C(x), \end{aligned}$$

for $\phi(x) = x \log(x) - x$,

and $d_\phi(x, c) = x \log\left(\frac{x}{c}\right) - (x - c)$.



Definition

Bregman h -trimmed variation given \mathbf{c} - or - Bregman-divergence-to-measure :

$$d_{\phi, P, \eta}^2(\mathbf{c}) = \inf_{\eta \tilde{P} \leq P} \tilde{P} \min_{j \in 1..k} d_{\phi}(\cdot, c_j)$$

Definition

A Bregman h -trimmed k -optimal codebook \mathbf{c}^* is any minimizer \mathbf{c} of the criterion $d_{\phi, P, \eta}(\mathbf{c})$.

Theorem (Bréchet, Fischer and Levrard)

Assume that ϕ is \mathcal{C}^2 and strictly convex and $F_0 = \overline{\text{Conv}(\text{Supp}(P))} \subset \overset{o}{\Omega}$.
Then, the minimum \mathbf{c}^* exists.

$\hat{\mathbf{c}}_n$: minimizer of $d_{\phi, P_n, \eta}$.

Theorem (BréchetEAU, Fischer and Levrard)

If P is continuous, $P\|\cdot\|^p < \infty$ for some $p > 2$, ϕ is \mathcal{C}_2 on Ω , $F_0 = \overline{\text{Conv}(\text{Supp}(P))} \subset \Omega^\circ$ and \mathbf{c}^* is the unique minimizer of $d_{\phi, P, \eta}$, then :

$$\lim_{n \rightarrow +\infty} \text{dist}(\hat{\mathbf{c}}_n, \mathbf{c}^*) = 0 \text{ a.e.}$$

and

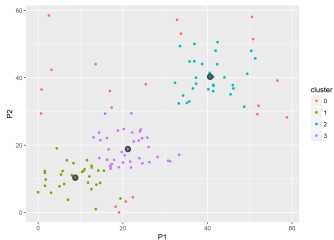
$$\lim_{n \rightarrow +\infty} d_{\phi, P, \eta}(\hat{\mathbf{c}}_n) = d_{\phi, P, \eta}(\mathbf{c}^*) \text{ a.e.}$$

This convergence holds at a parametric rate $\frac{1}{\sqrt{n}}$:

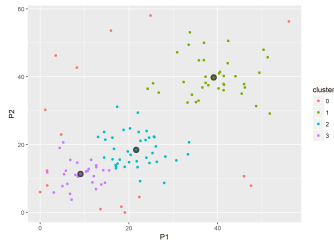
Theorem (BréchetEAU, Fischer and Levrard)

Assume that $P\|\cdot\|^p < \infty$. Then, for n large enough, with probability greater than $1 - n^{-\frac{p}{2}} - 2e^{-x}$, we have

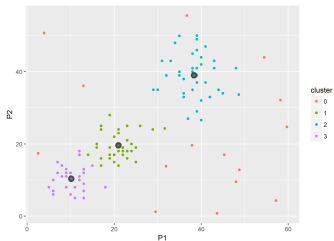
$$d_{\phi, P, \eta}(\hat{\mathbf{c}}_n) - d_{\phi, P, \eta}(\mathbf{c}^*) \leq \frac{C_P}{\eta\sqrt{n}}(1 + \sqrt{x}).$$



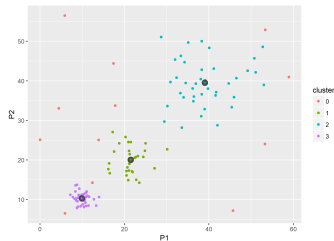
Gaussian mixture



Poisson mixture



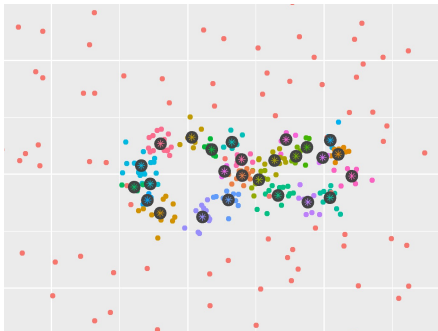
Binomial mixture



Gamma mixture

Clustering associated to the selected parameter η - dimension 2

3) Distance to a compact set inference, with a quantization point of view



Given P , Q or \mathbb{X}_n :

Find \mathbf{c} and $\boldsymbol{\omega}$ such that the k -power function

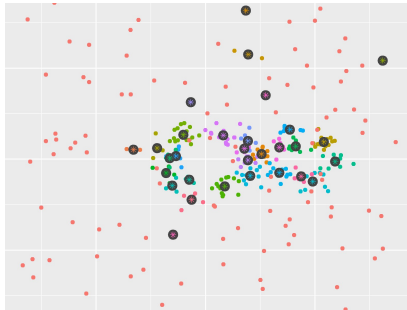
$$x \mapsto \min_{j \in 1..k} \|x - c_j\|^2 + \omega_j^2$$

is a good approximation of the square of the distance to \mathcal{X} ,

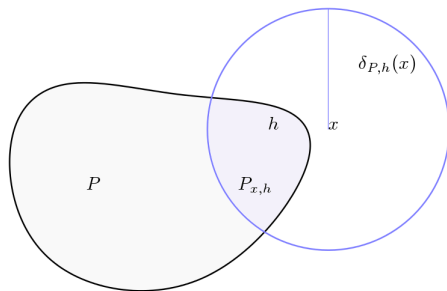
$$d_{\mathcal{X}}^2 : x \mapsto \min_{y \in \mathcal{X}} \|x - y\|^2$$

What about using (trimmed) k -means for quantization problem?

Trimmed k -means does not work...



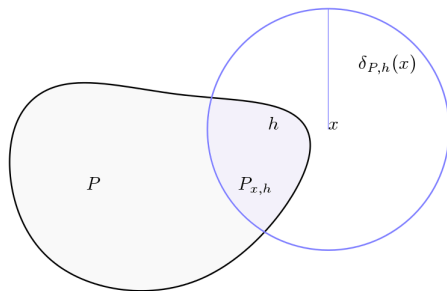
The DTM, an alternative definition as a power distance when $p = 2$ [Chazal, Cohen-Steiner, Mérigot 09']



$$\begin{aligned}d_{P,h}^2(x) &= P_{x,h} \|\cdot - x\|^2 \\ &= \inf_{h\tilde{P} \leq P} \tilde{P} \|\cdot - x\|^2 \\ &= \|m(P_{x,h}) - x\|^2 + v(P_{x,h}) \\ &= \inf_{h\tilde{P} \leq P} \|m(\tilde{P}) - x\|^2 + v(\tilde{P})\end{aligned}$$

Notation : Mean $m(P)$, Variance $v(P)$.

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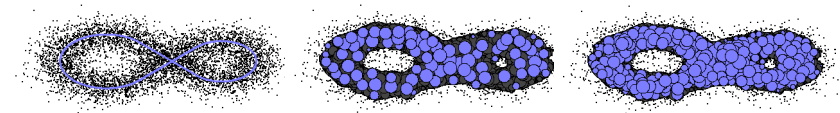


$$\begin{aligned}
 d_{P,h}^2(x) &= P_{x,h} \| \cdot - x \|^2 \\
 &= \inf_{\tilde{P} \leq P} \tilde{P} \| \cdot - x \|^2 \\
 &= \| m(P_{x,h}) - x \|^2 + v(P_{x,h}) \\
 &= \inf_{\tilde{P} \leq P} \| m(\tilde{P}) - x \|^2 + v(\tilde{P})
 \end{aligned}$$

Notation : Mean $m(P)$, Variance $v(P)$.

\rightsquigarrow Sublevel sets of the DTM : union of balls.

Approximation : κ -witnessed distance [Guibas Morozov Mérigot 11'] n balls



Set $\phi_{P,h}$ the function defined on \mathbb{R}^d by

$$\phi_{P,h} : x \mapsto \|x\|^2 - d_{P,h}^2(x). \quad (1)$$

[Chazal, Cohen-Steiner, Mérigot 09'] The map $\phi_{P,h}$ is convex.

The Bregman-divergence associate to $\phi_{P,h}$ satisfies for $x, t \in \mathbb{R}^d$:

$$d_{\phi_{P,h}}(x, t) = \|x - m(P_{t,h})\|^2 + v(P_{t,h}) - d_{P,h}^2(x)$$

$$\min_{j \in 1..k} d_{\phi_{P,h}}(x, t_j) = \left(\min_{j \in 1..k} \|x - m(P_{t,h})\|^2 + v(P_{t,h}) \right) - d_{P,h}^2(x)$$

\rightsquigarrow Bregman clustering with $d_{\phi_{P,h}}$!

Rq : Theory $1 - \eta = 0$ (For practice $1 - \eta \in [0, 1)$) !

$$\begin{aligned} \mathbf{t}^* &\in \arg \min_{\mathbf{t}} P \min_{j \in 1..k} d_{\phi_{P,h}}(\cdot, t_j) \\ &= \arg \min_{\mathbf{t}} P \min_{j \in 1..k} \|\cdot - m(P_{t_j, h})\|^2 + v(P_{t_j, h}) - d_{P,h}^2(\cdot) \end{aligned}$$

Definition

The k -power distance-to-measure (k -PDTM) $d_{P,h,k}$ is defined for $x \in \mathbb{R}^d$ by :

$$d_{P,h,k}^2(x) = \min_{j \in 1..k} \|x - m(P_{t_j^*, h})\|^2 + v(P_{t_j^*, h})$$

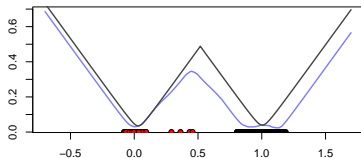
$$\omega(c) = \inf \left\{ \omega > 0 \mid \forall x \in \mathbb{R}^d, \|x - c\|^2 + \omega^2 \geq d_{P,h}^2(x) \right\}$$

Theorem (Bréchet and Levrard)

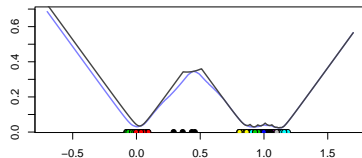
$$d_{P,h,k}^2(x) = \min_{j \in 1..k} \|x - c_j^*\|^2 + \omega^2(c_j^*)$$

for

$$\mathbf{c}^* \in \arg \min \left\{ P \min_{j \in 1..k} \|\cdot - c_j\|^2 + \omega^2(c_j) \right\}$$



k -PDTM, $k = 2$ centres



k -PDTM, $k = 10$ centres

Proposition

If $\text{Supp}(P) \subset B(0, K)$, and $Q \|\cdot\| < \infty$,

then $P \left| d_{Q,h,k}^2(\cdot) - d_{P,h}^2(\cdot) \right|$ is bounded from above by

$$3 \|d_{Q,h}^2 - d_{P,h}^2\|_{\infty, B(0,K)} + P \left(d_{P,h,k}^2(\cdot) - d_{P,h}^2(\cdot) \right) + 4W_1(P, Q) \sup_{s \in \mathbb{R}^d} \|m(P_s, h)\|$$

with $P \left(d_{P,h,k}^2(\cdot) - d_{P,h}^2(\cdot) \right)$ of order $k^{-\frac{2}{d'}}$ for a “ d' -dimensional distribution”.

$$\text{Supp}(P) = \mathcal{X} \subset B(0, K)$$

$X_i = Y_i + Z_i$, Y_i and Z_i all independent, $Y_i \sim P$, Z_i sub-Gaussian with variance $\sigma^2 \leq K^2$

$$Q_n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}.$$

Theorem (BréchetEAU and Levrard)

For every $p > 0$, with probability larger than $1 - 10n^{-p}$, we have

$$\left| Pd_{Q_n, h, k}^2(\cdot) - d_{Q, h, k}^2(\cdot) \right| \leq C\sqrt{kd} \frac{K^2((p+1)\log(n))^{\frac{3}{2}}}{h\sqrt{n}} + C \frac{K\sigma}{\sqrt{h}}.$$

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\rightsquigarrow optimize in k the quantity

$$\frac{C\sqrt{k}K^2((p+1)\log(n))^{\frac{3}{2}}}{h\sqrt{n}} + C_{P,h}k^{-\frac{2}{d}}.$$

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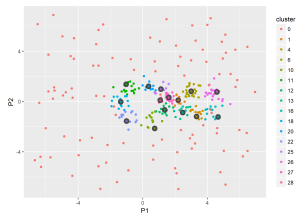
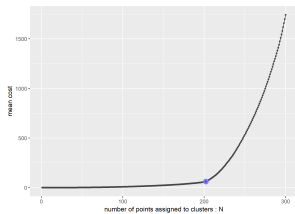
Optimal choice $k \sim n^{\frac{d'}{d'+4}}$.

Theorem (BréchetEAU and Levrard)

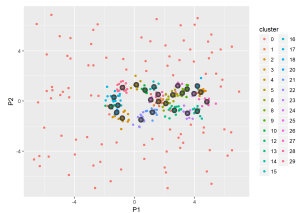
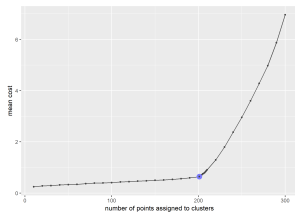
Assumption : $\forall x \in \mathcal{X}$, $P(B(x, r)) \geq C(P)r^{d'} \wedge 1$.

Set $\Delta_P^2 = Pd_{Q, h, k}^2(\cdot)$, then,

$$\sup_{x \in \mathbb{R}^d} |d_{Q, h, k}(x) - d_{\mathcal{X}}(x)| \leq C(P)^{-\frac{1}{d'+2}} \Delta_P^{\frac{2}{d'+2}} + 2\Delta_P + W_2(P, Q)h^{-\frac{1}{2}}.$$



k -PDTM ($\eta = 1$)



Trimmed k -PDTM ($\eta < 1$)

Method	New tool
Isomorphism Test Bregman clustering Quantization & $d_{\mathcal{X}}$ inference	DTM-signature $d_{P,h}(P)$ Bregman divergence-to-measure $\mathbf{c} \mapsto d_{\phi,P,\eta}(\mathbf{c})$ k -PDTM $x \mapsto d_{P,h,k}(x)$

Method	New tool
Isomorphism Test Bregman clustering Quantization & $d_{\mathcal{X}}$ inference	DTM-signature $d_{P,h}(P)$ Bregman divergence-to-measure $\mathbf{c} \mapsto d_{\phi,P,\eta}(\mathbf{c})$ k -PDTM $x \mapsto d_{P,h,k}(x)$

Future work :

Non asymptotic statistics for studying

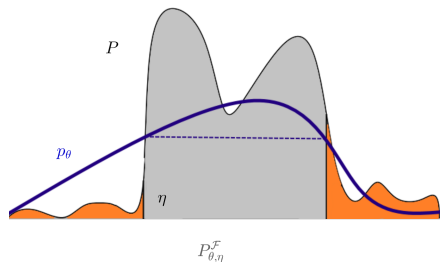
$$\hat{t}_{\eta} \in \arg \min_t \inf_{\eta \tilde{P}_n \leq P_n} \tilde{P}_n \gamma(t, \cdot)$$

Thank you !

$\mathcal{F} = \{P_\theta\}_\theta$; P_θ with density p_θ .

$\gamma(\theta, \cdot) = -\log(p_\theta(\cdot))$

$B(x, r) \leftrightarrow$ upper-level set of p_θ .



$$d_{P, \eta}^{\mathcal{F}} : \theta \mapsto \inf_{\tilde{P} \leq P} \tilde{P} - \log(p_\theta(\cdot))$$

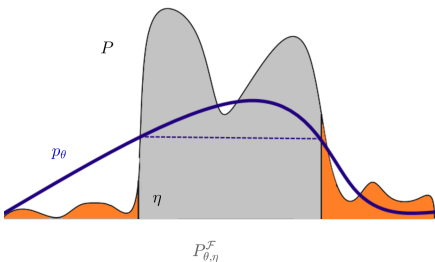
Minimizer θ^* : **Trimmed log-likelihood** maximizer

$\mathcal{F} = \{P_\theta\}_\theta$; P_θ with density p_θ .

$\theta = (\theta_1, \theta_2, \dots, \theta_k)$

$\gamma(\theta, \cdot) = \min_{j \in 1..k} -\log(p_{\theta_j}(\cdot))$

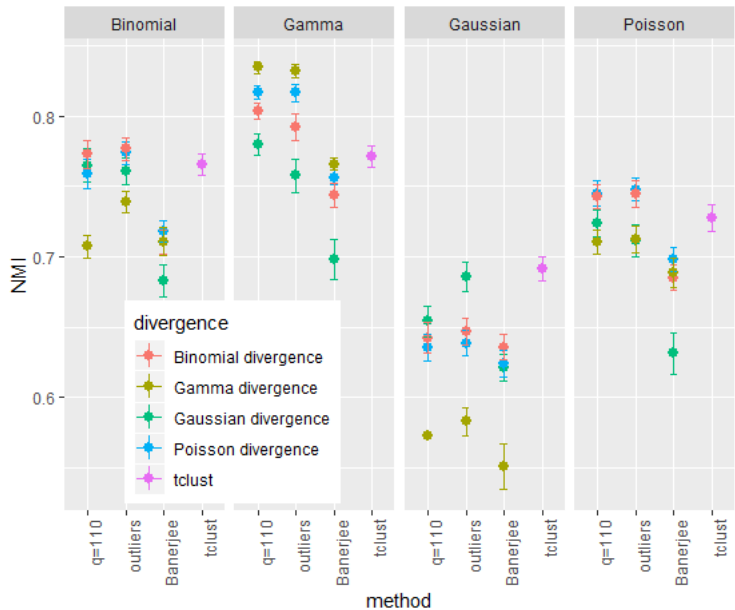
$B(x, r) \leftrightarrow$ union of upper-level set of the p_{θ_j} s.



$$d_{P, \eta}^{\mathcal{F}} : \theta \mapsto \inf_{\tilde{P} \leq P} \tilde{P} \min_{j \in 1..k} -\log(p_{\theta_j}(\cdot))$$

Minimizer θ^* : Optimal codebook for some trimmed clustering...

Experiments



Robust heteroscedastic Gaussian clustering

