Robust approximation of compact sets with unions of ellipsoids. Application to data clustering.

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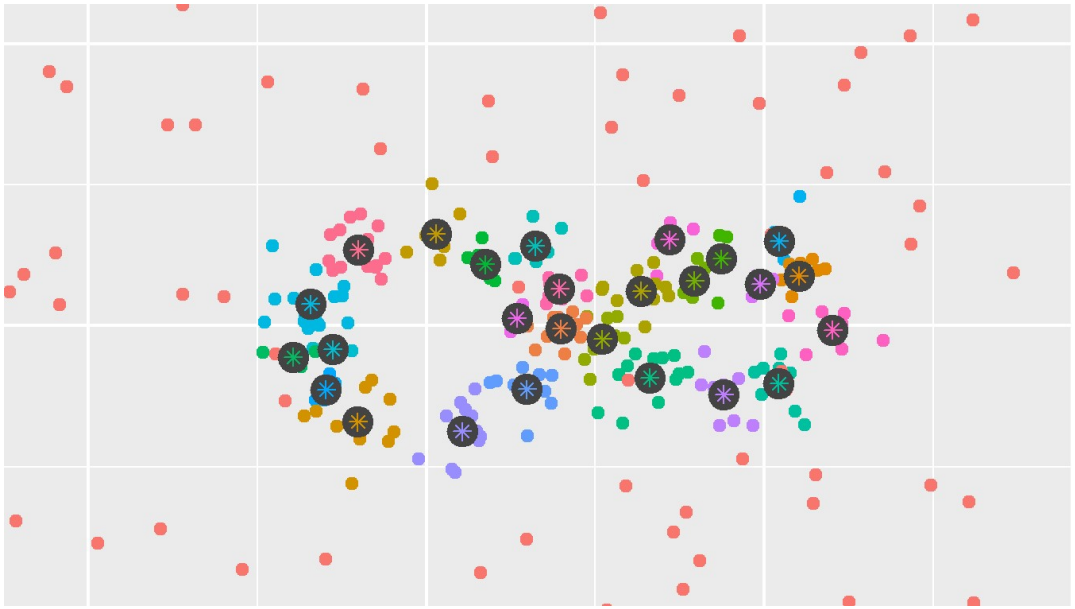
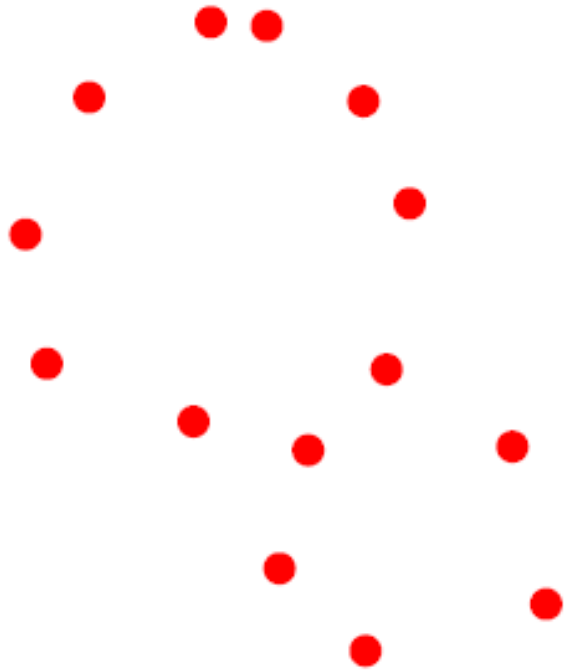
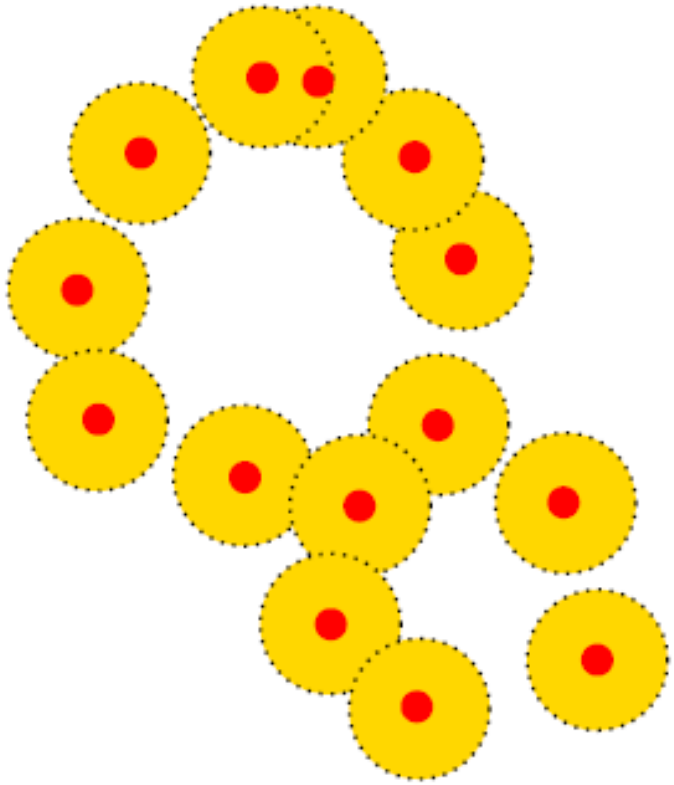
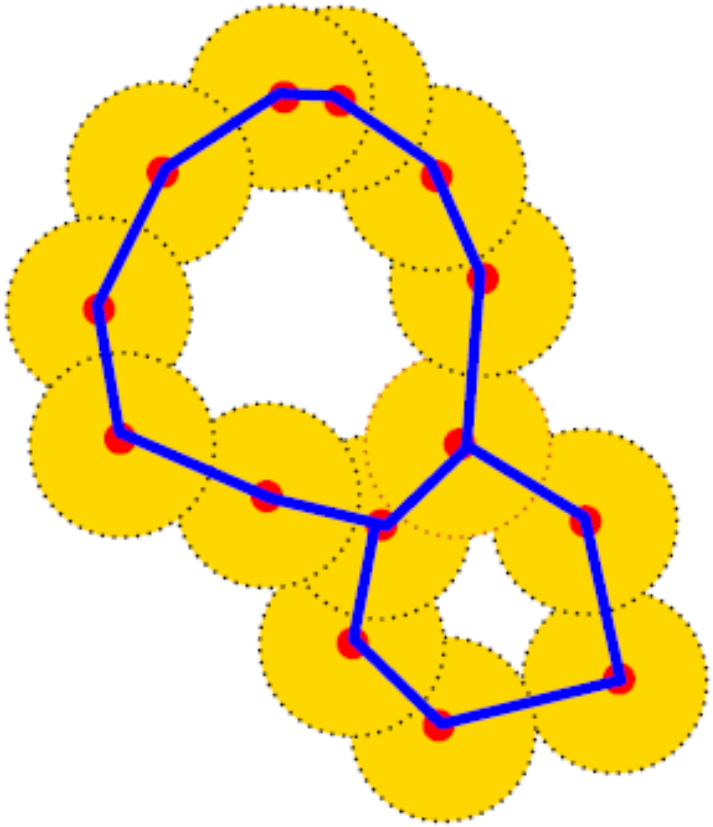
September, 23th 2022

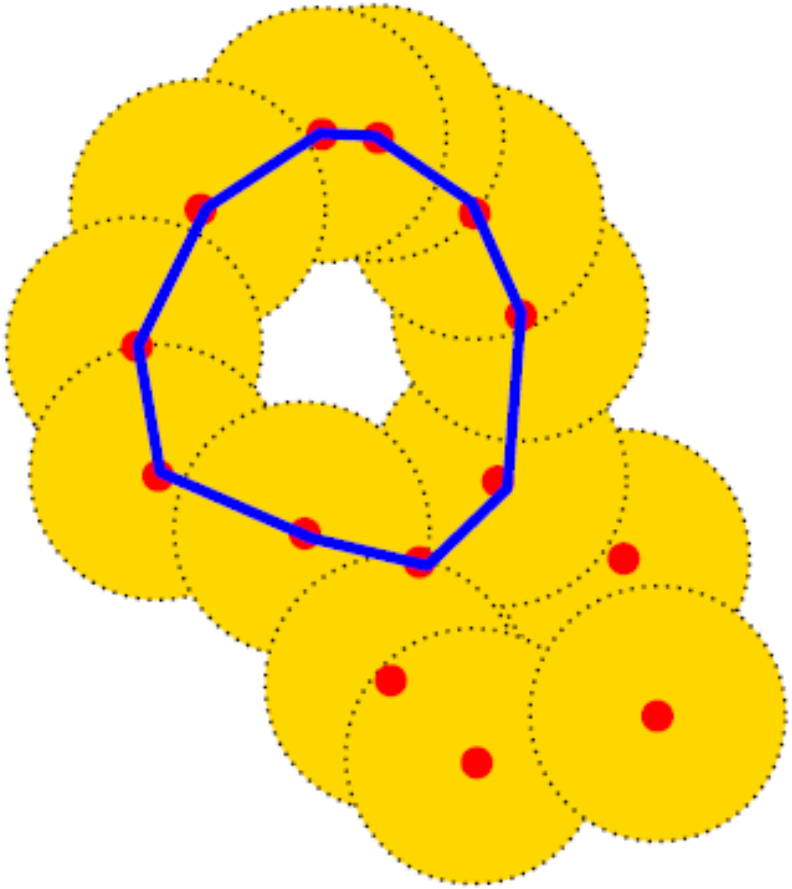
How to approximate a manifold with a set of k points, from a noisy sample ?

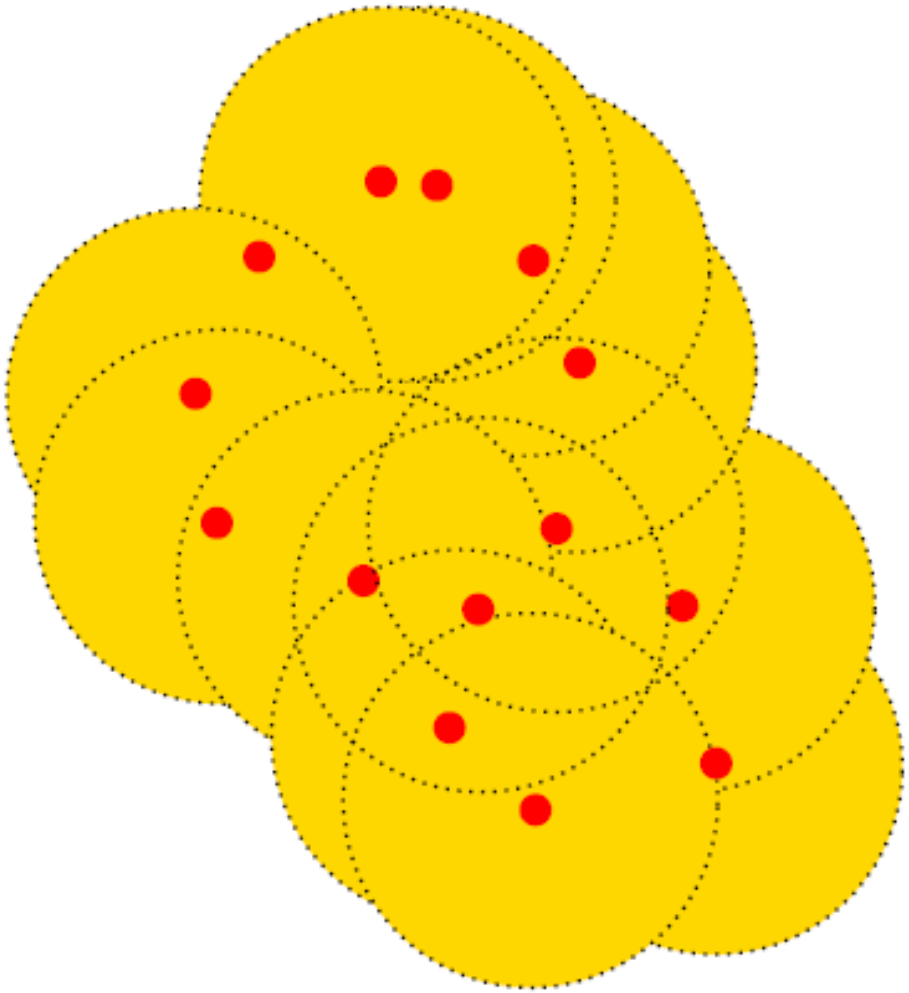












The k-means method

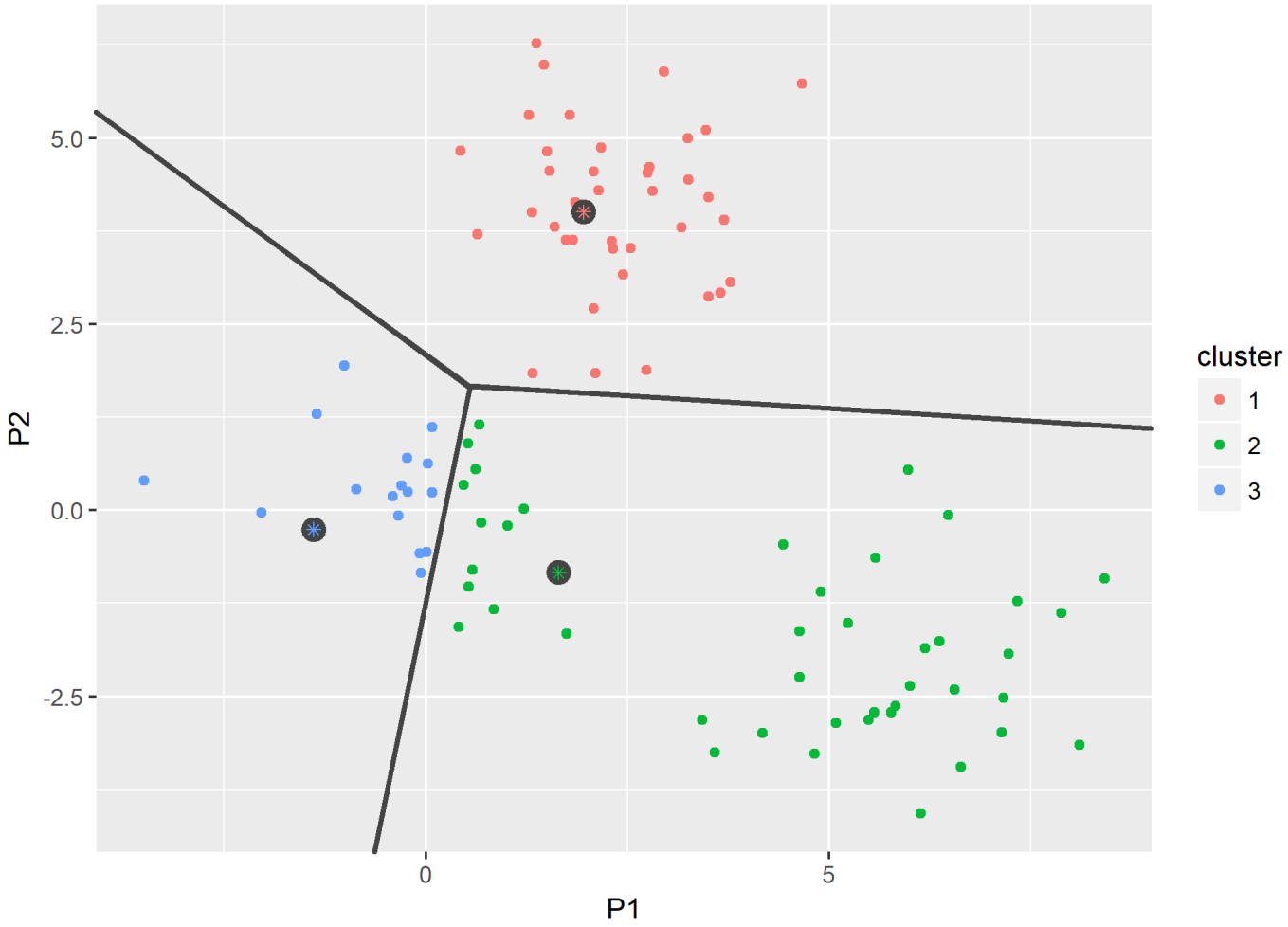
P distribution on $\mathbb{R}^d$
$\mathbf{c} = (c_1, c_2, \ldots, c_k) \in (\mathbb{R}^d)^k$ codebook

Definition

The optimal codebook $\mathbf{c}^*$ minimizes the k-means loss function

$$R : \mathbf{c} \mapsto P \min_{i=1..k} \|\cdot - c_i\|^2.$$

FIGURE – Lloyd's algorithm method



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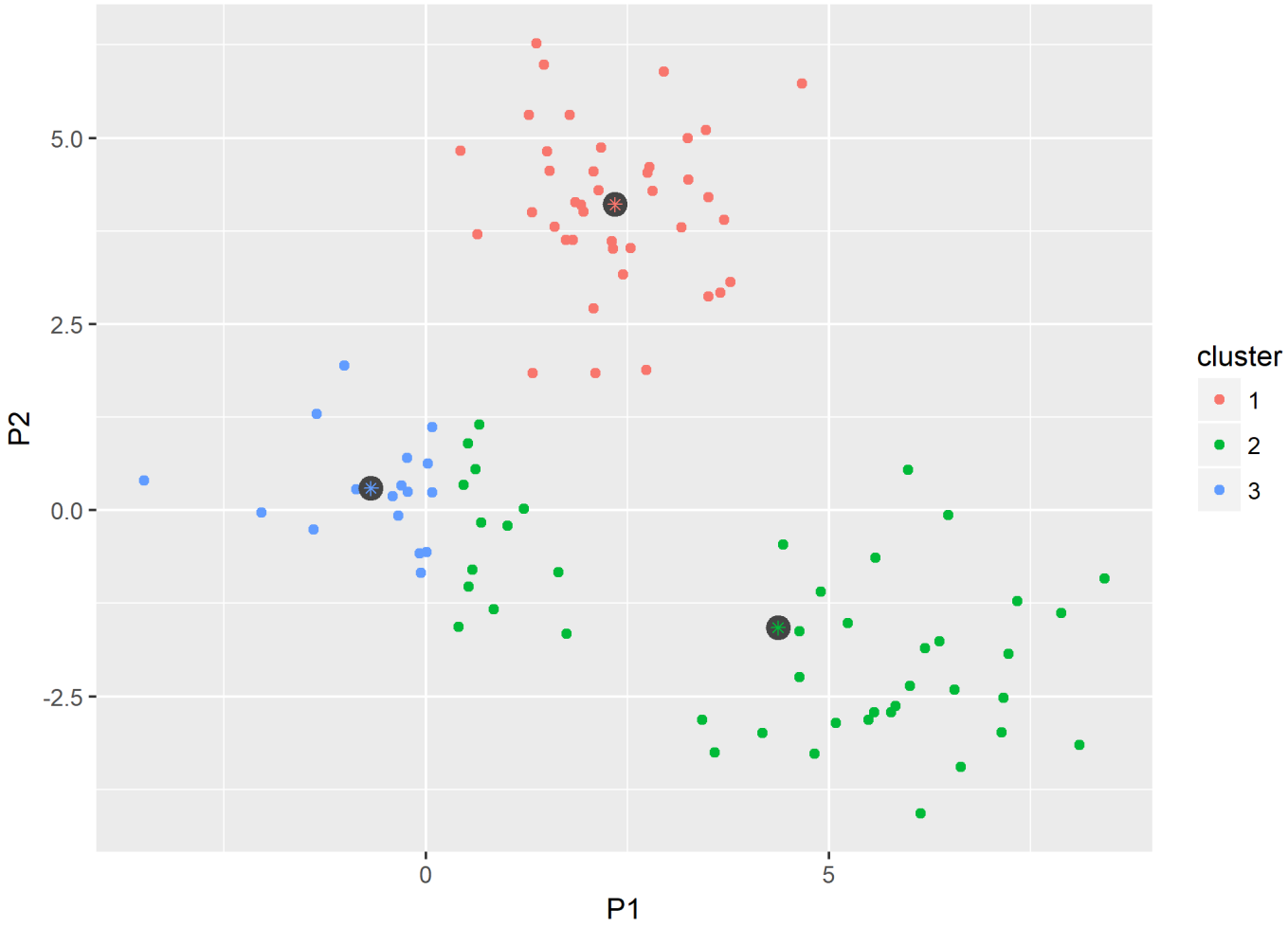

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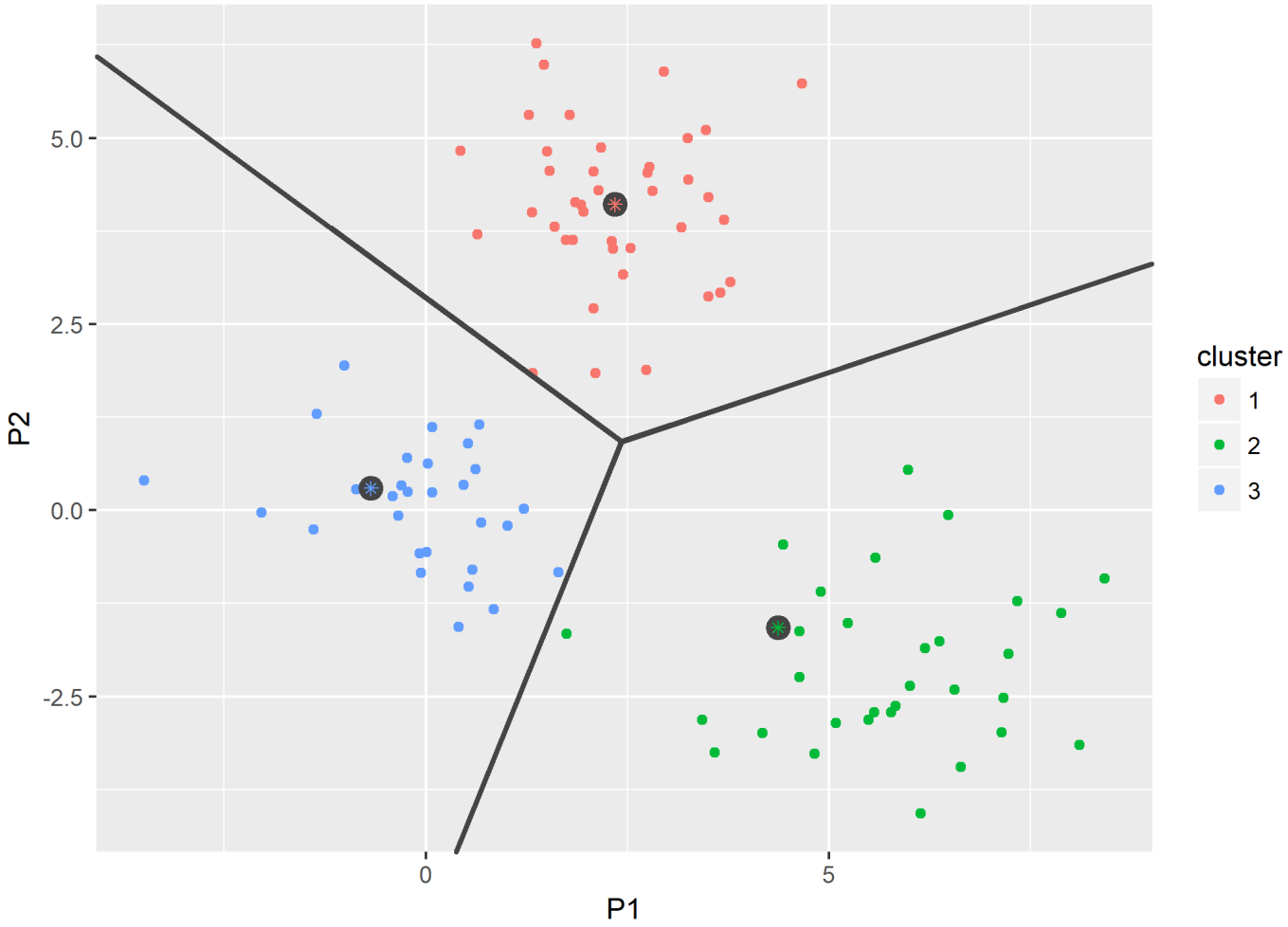

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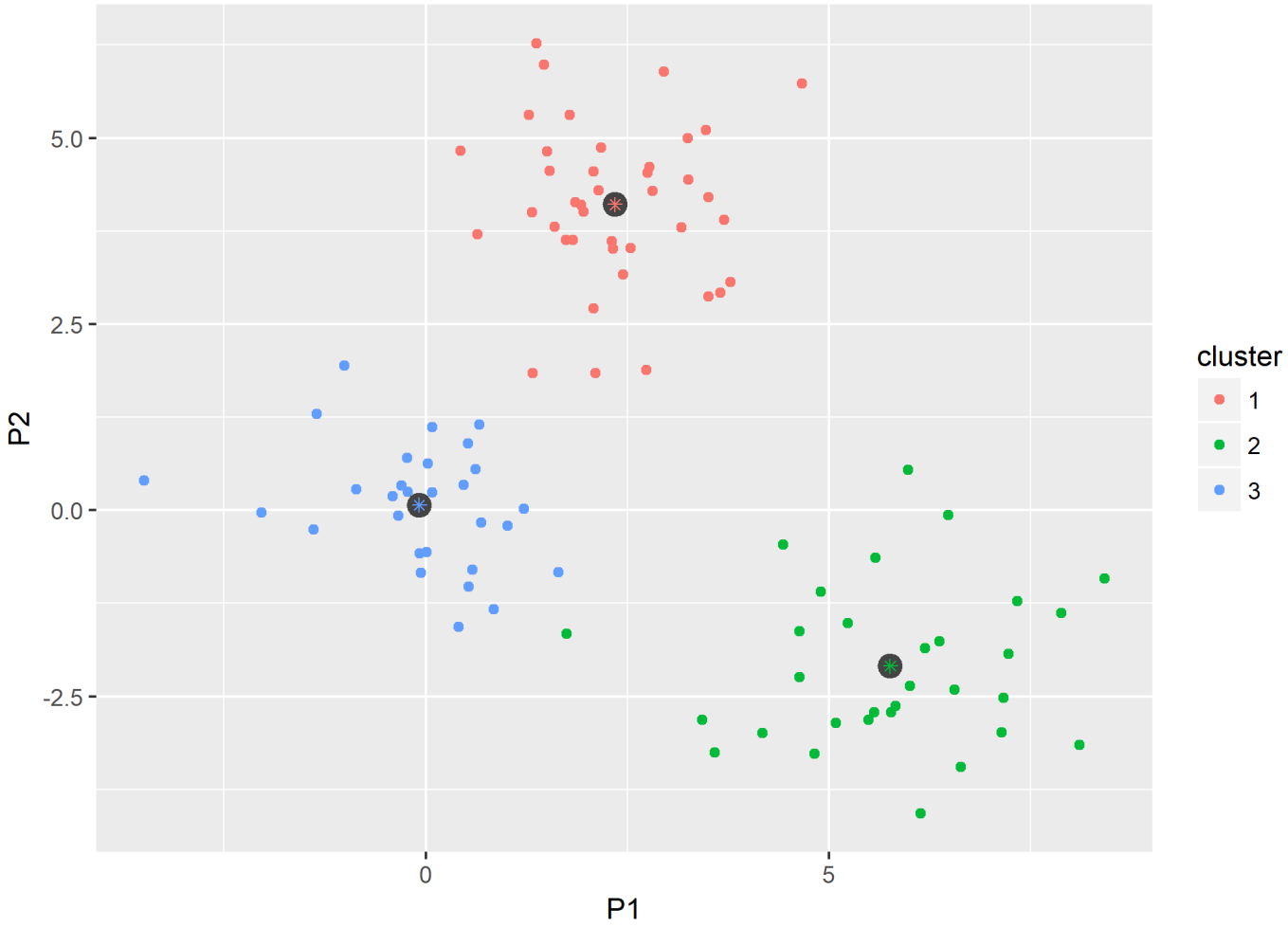

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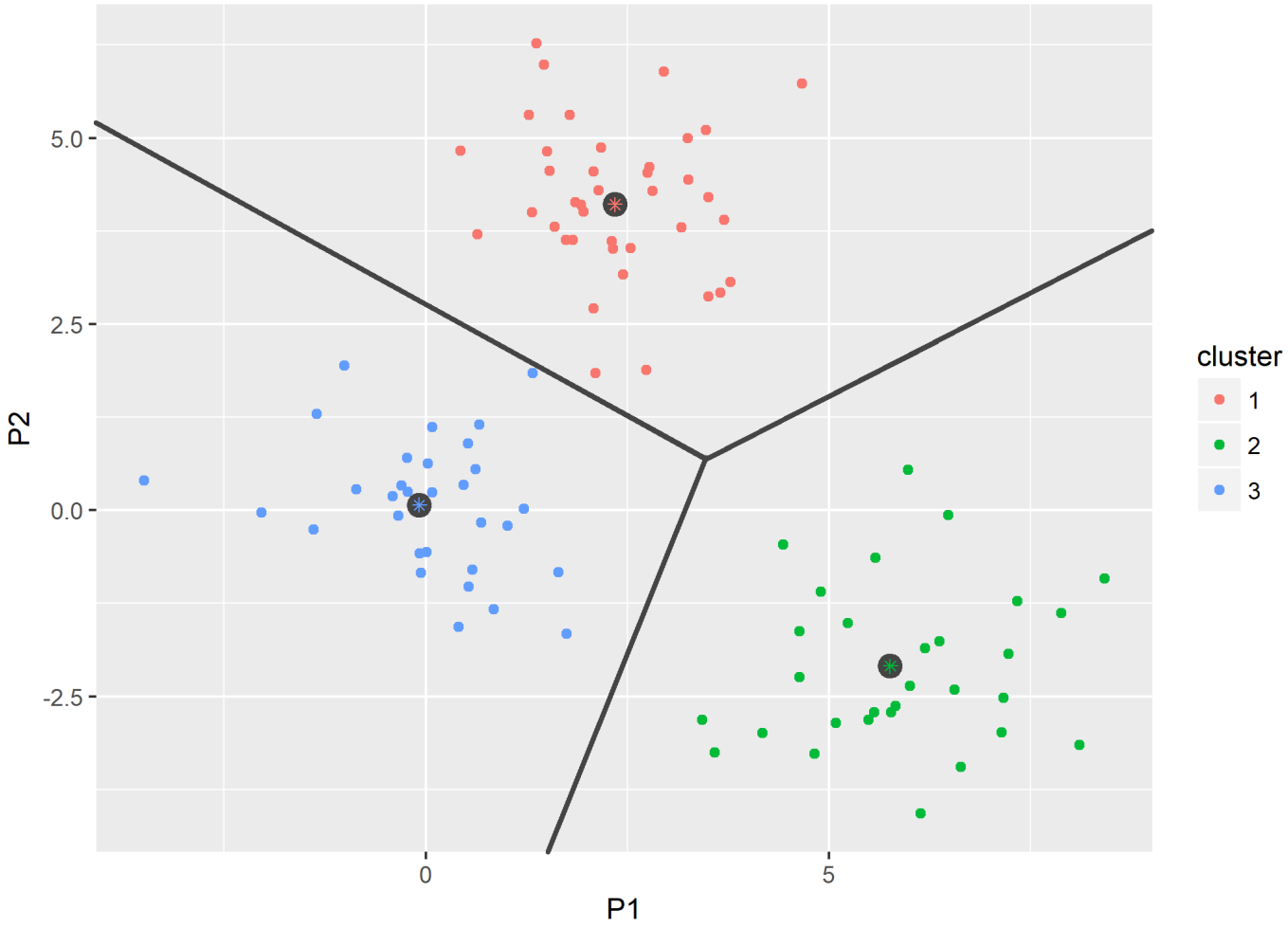
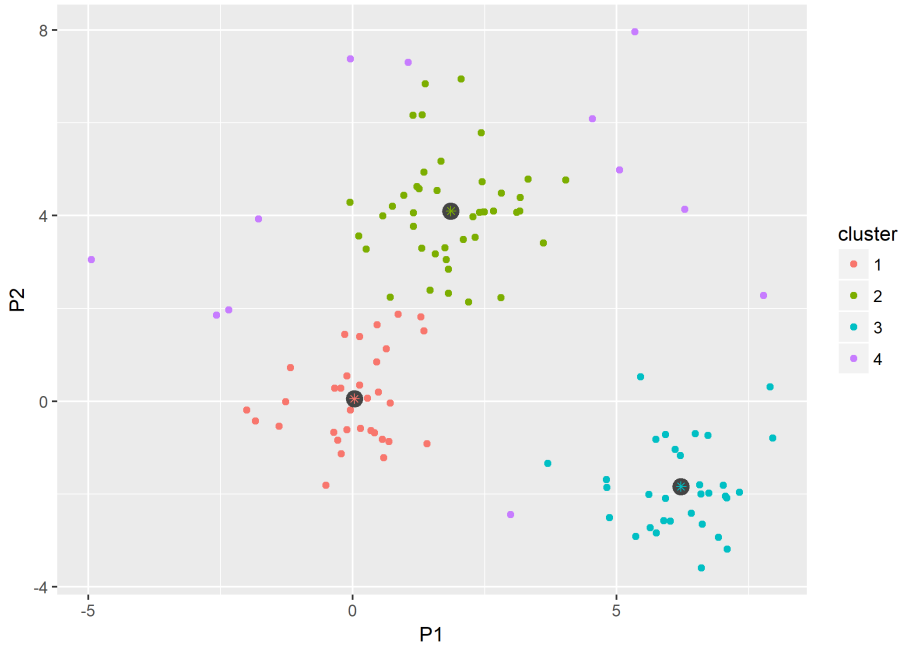


Definition

The optimal trimmed codebook $\mathbf{c}_h^*$ minimizes the trimmed k-means loss function

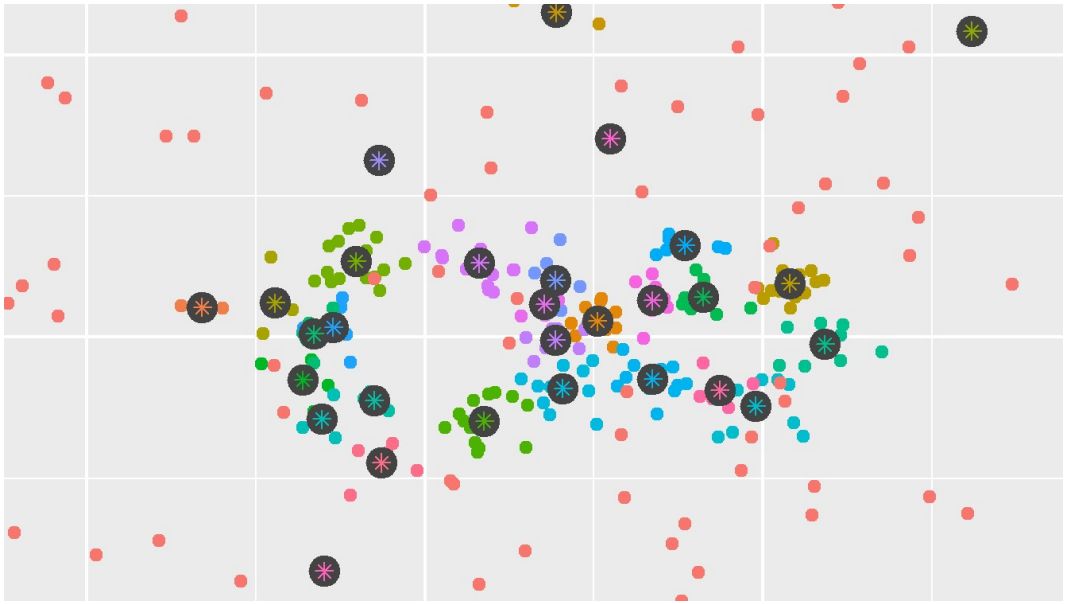
$$R_h : \mathbf{c} \mapsto \inf_{\tilde{P},\, h\tilde{P} \leq P} \tilde{P} \min_{i=1..k} \|\cdot - c_i\|^2.$$

FIGURE – Trimmed k-means

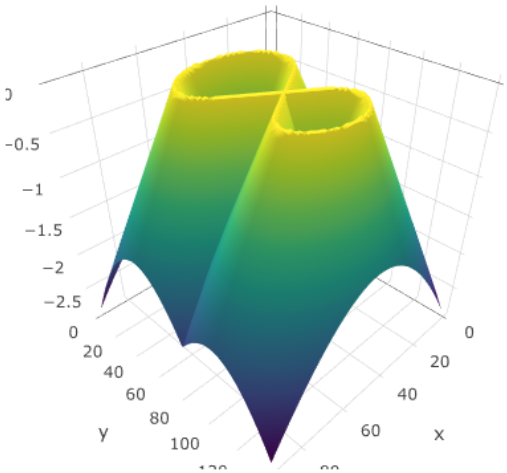


(Trimmed) k-means for the distance-approximation problem ?

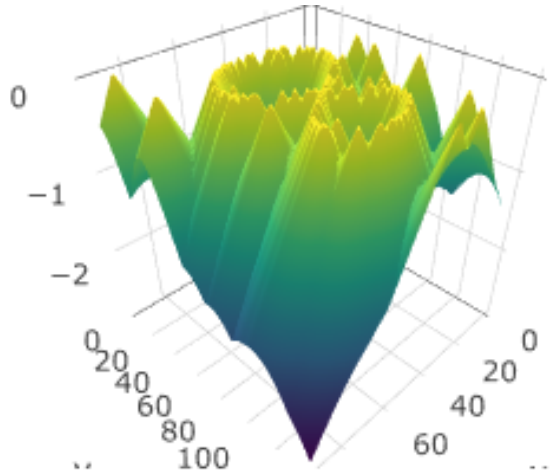
Trimmed k-means :



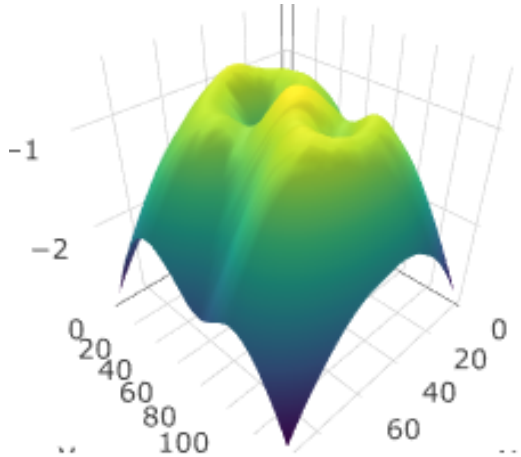
$\Rightarrow$ Not working...



Distance to the compact

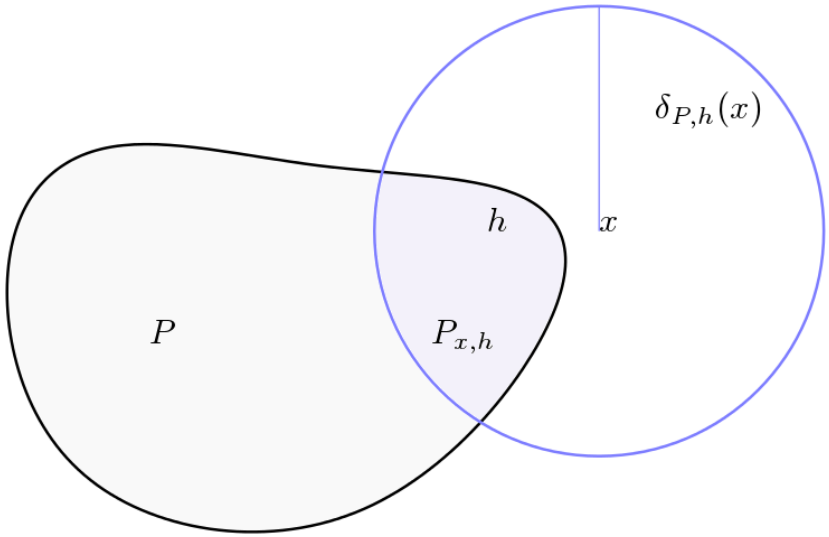


Distance to the sample



Distance to the empirical measure

Distance-to-measure (DTM)



$$\begin{aligned} \mathrm{d}^2_{P,h}(x) &= P_{x,h}\|\cdot - x\|^2 \\ &= \inf_{t\in\mathbb{R}^d} P_{t,h}\|\cdot - x\|^2 \\ &= \|m(P_{x,h}) - x\|^2 + v(P_{x,h}) \\ &= \inf_{t\in\mathbb{R}^d} \|m(P_{t,h}) - x\|^2 + v(P_{t,h}) \end{aligned}$$

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

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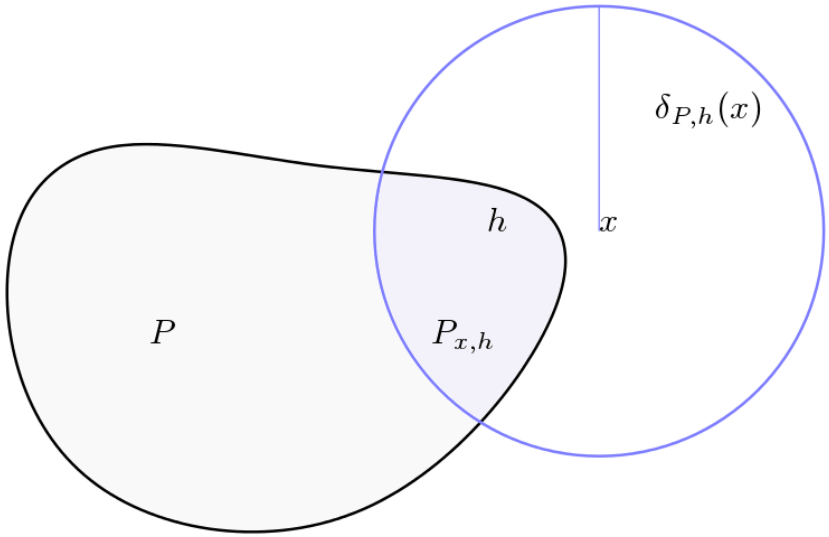

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Notation : Mean $m(P)$, Variance $v(P)$.

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

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

Definition

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

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

Approximation of the DTM with the empirical k-PDTM

$$P\left|\mathrm{d}^2_{Q_n,h,k}(\cdot)-\mathrm{d}^2_{P,h}(\cdot)\right| \leq P\left|\mathrm{d}^2_{Q_n,h,k}(\cdot)-\mathrm{d}^2_{Q,h,k}(\cdot)\right| + P\left|\mathrm{d}^2_{Q,h,k}(\cdot)-\mathrm{d}^2_{P,k}(\cdot)\right|$$

Wasserstein stability for the k-PDTM

Proposition

If $\mathrm{Supp}(P) \subset \mathrm{B}(0, K)$, *and* $Q\|.\| < \infty$,
then $P\left|\mathrm{d}^2_{Q,h,k}(.) - \mathrm{d}^2_{P,h}(.)\right|$ *is bounded from above by*

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

with $P\left(\mathrm{d}^2_{P,h,k}(.) - \mathrm{d}^2_{P,h}(.)\right)$ of order $k^{-\frac{2}{d'}}$ for a "d'-dimensional distribution".

Approximation of the k-PDTM from point clouds

$\mathrm{Supp}(P) = \mathcal{X} \subset \mathrm{B}(0, K)$
$X_i = Y_i + Z_i$, 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 (B. - Levrard 2020)

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

$$\left| P\mathrm{d}^2_{Q_n,h,k}(.) - \mathrm{d}^2_{Q,h,k}(.) \right| \leq C\sqrt{k\log(k)d}\,\frac{K^2((p+1)\log(n))^{\frac{3}{2}}}{h\sqrt{n}} + C\frac{K\sigma}{\sqrt{h}}.$$

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$\rightsquigarrow$ optimize in k the quantity

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

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

Algorithm 1 Approximation of the k-PDTM centers

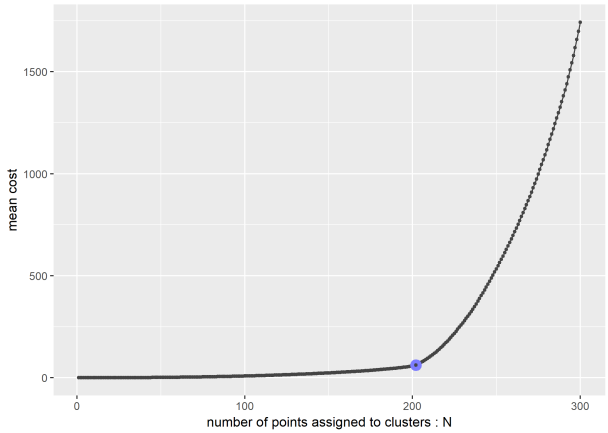
Input $\mathbb{X}_n$ a n-sample from P, q and k
Sample t_1, t_2,... t_k from $\mathbb{X}_n$ without replacement.
while the t_i's vary **do**
  for j in $1..n$ **do**
    Add X_j to some $\mathscr{C}(t_i)$ satisfying
    $\|X_j - m(t_i)\|^2 + v(t_i) \leq \|X_j - m(t_l)\|^2 + v(t_l)\, \forall l \neq i$
  end for
  for i in $1..k$ **do**
    $t_i = \frac{1}{|\mathscr{C}(t_i)|} \sum_{X \in \mathscr{C}(t_i)} X$
  end for
end while
Output $(t_1, t_2, \ldots, t_k)$.

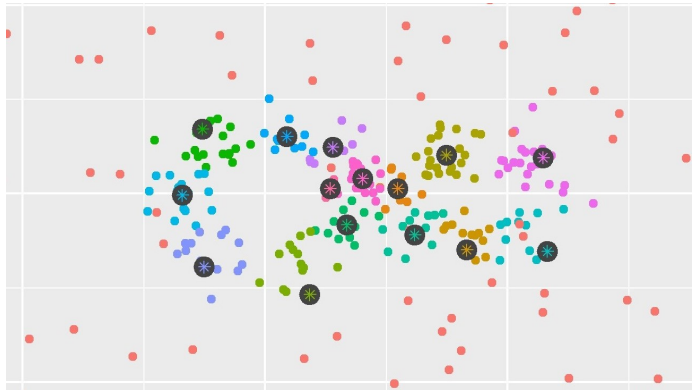
Let $h = \frac{q}{n}$, $q \in \mathbb{N}^*$. For $t \in \mathbb{R}^d$, $m(t) = \frac{1}{q} \sum_{i=1}^{q} X_i(t)$, $v(t) = \frac{1}{q} \sum_{i=1}^{q} \left(X_i(t) - m(t)\right)^2$ with $X_i(t)$ an i-th nearest neighbor of t and $\mathscr{C}(t)$ the weighted Voronoï cell of t.

B. - Levrard, 2020

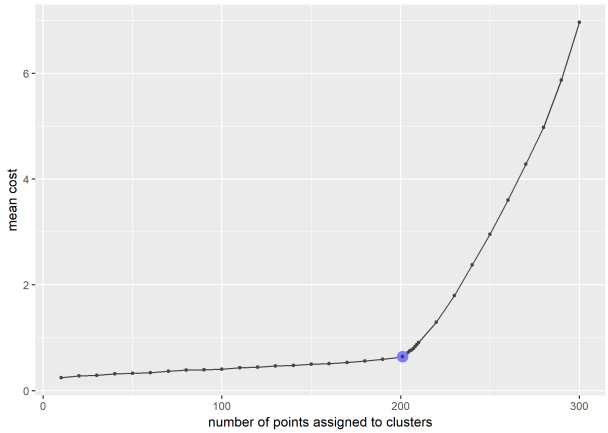
Convergence to a local minimum of $\mathbf{t} \mapsto P_n \min_{i=1..k} \|\cdot - m(P_{n\, t_i,h})\|^2 + v(P_{n\, t_i,h})$.

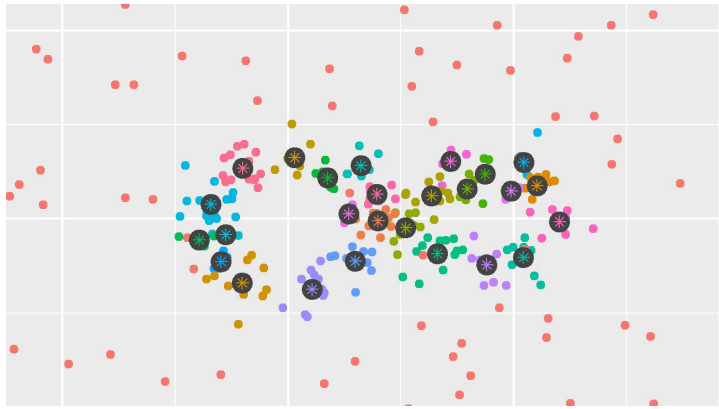
Numerical Illustrations





k-PDTM





Trimmed k-PDTM

Comparison to other methods

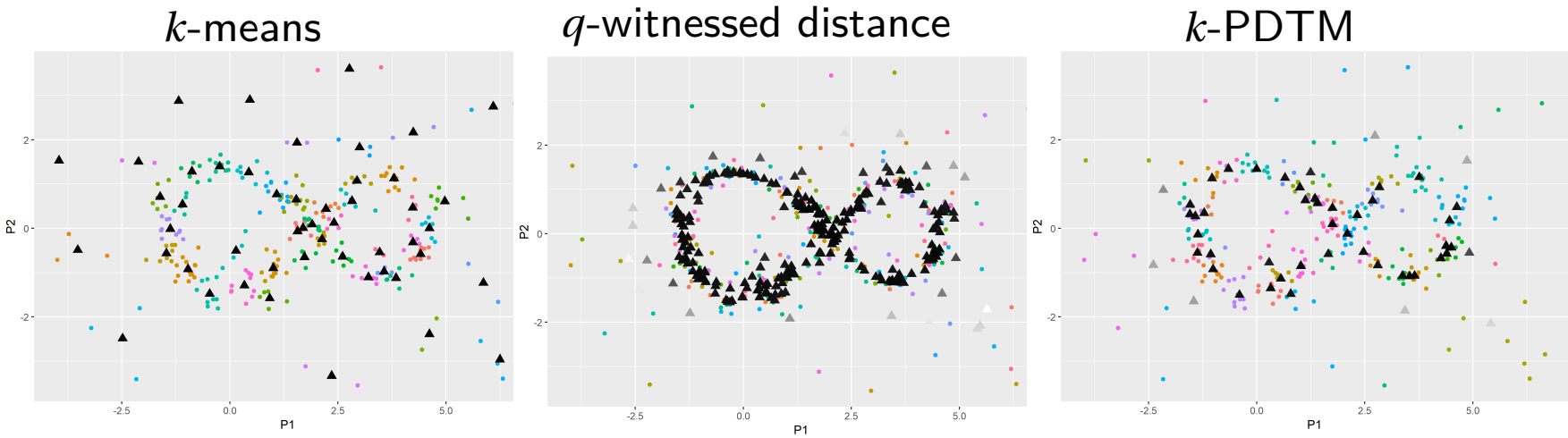


FIGURE – Comparison of the basic methods

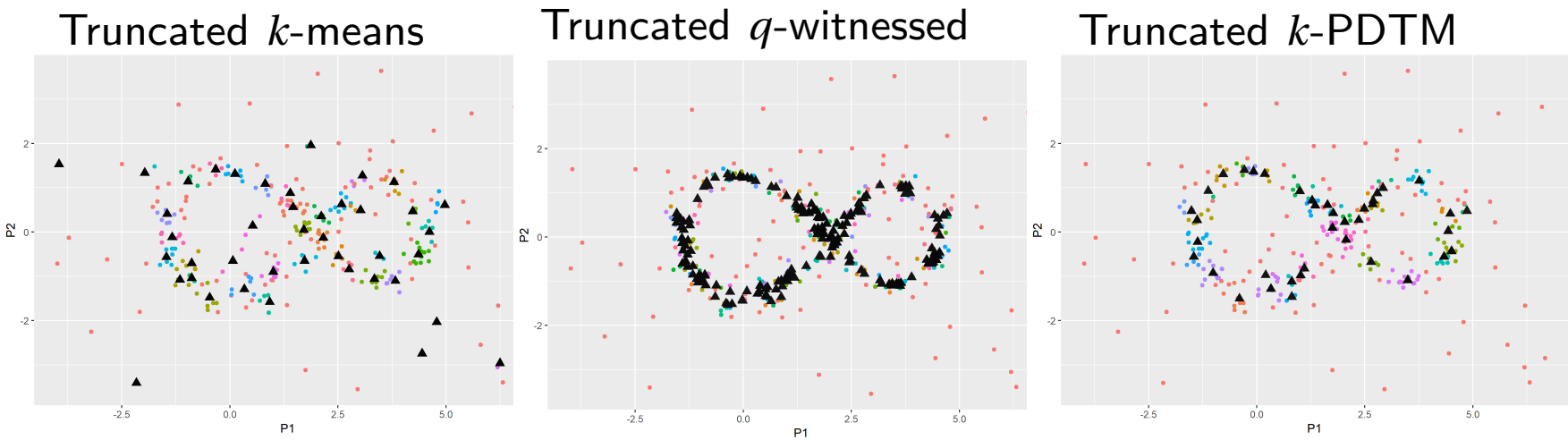
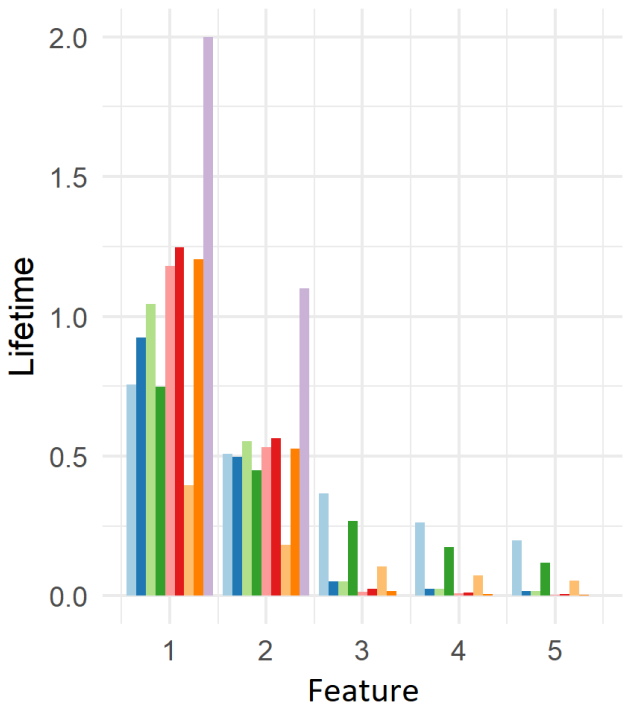
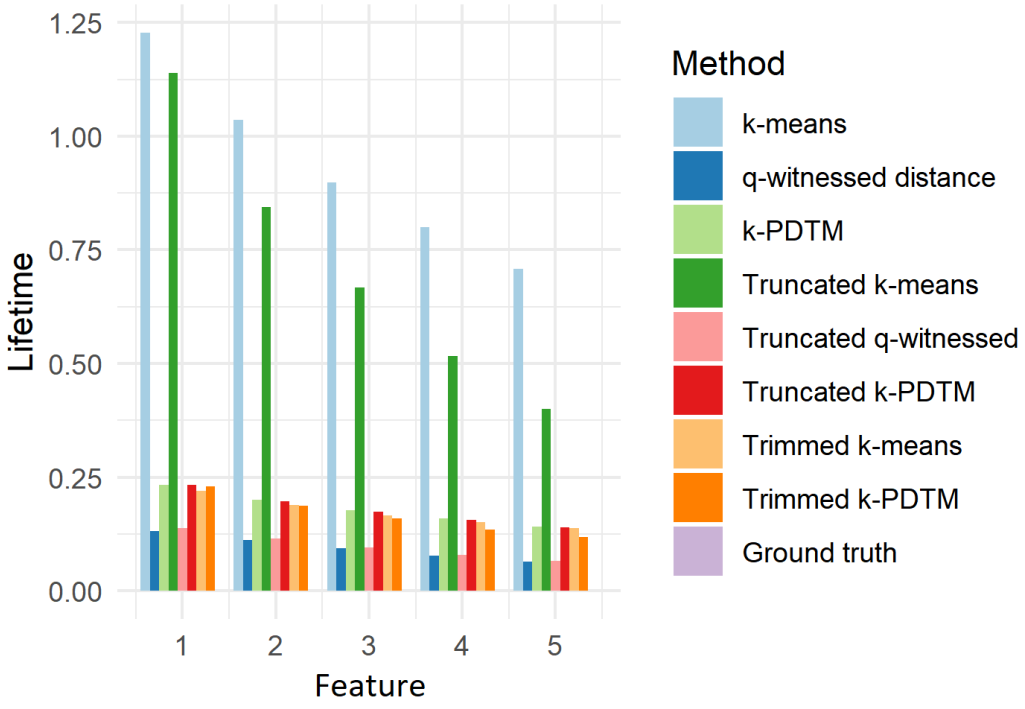


FIGURE – Comparison of the methods after thresholding

Features lifetimes comparison

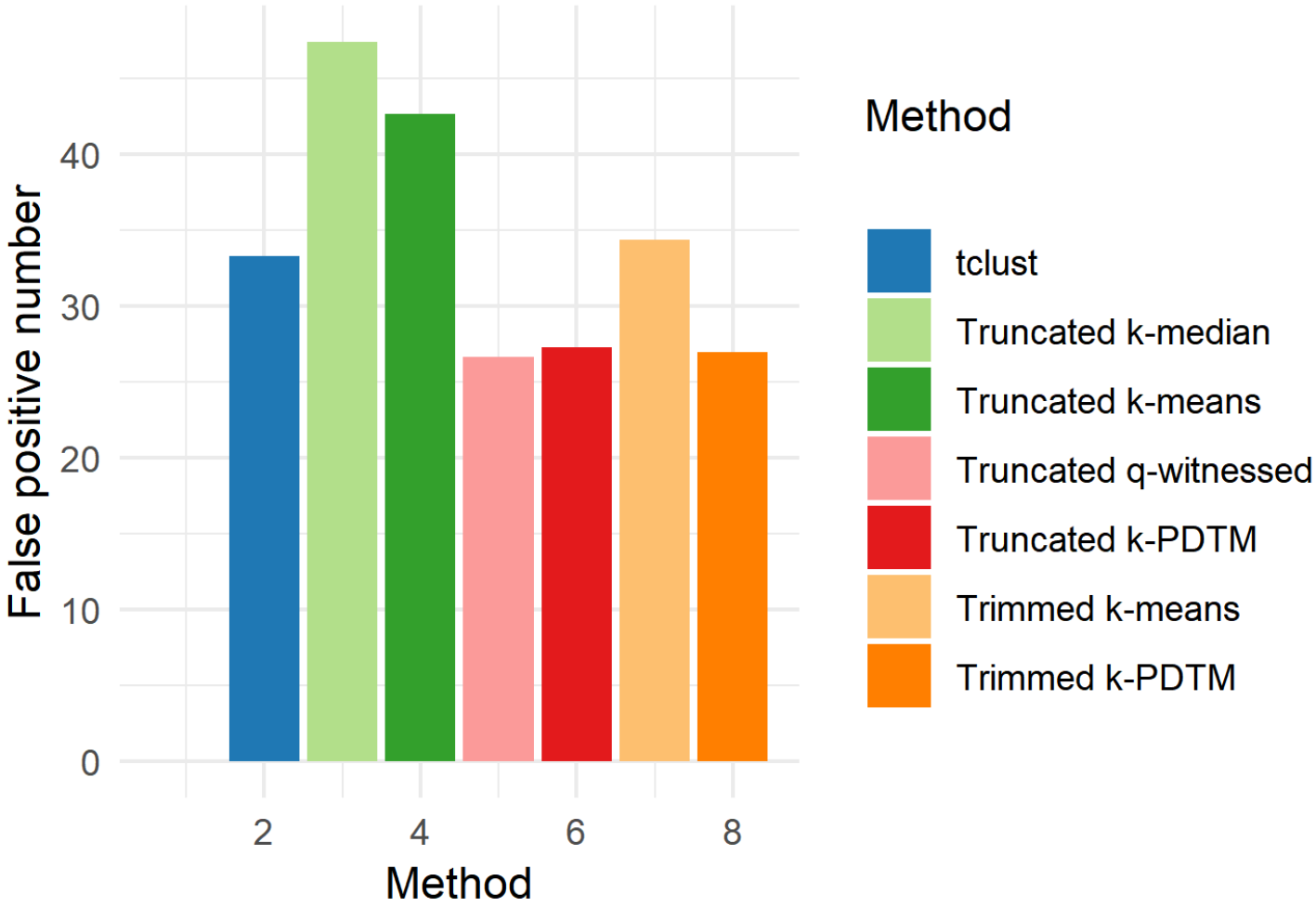


Holes

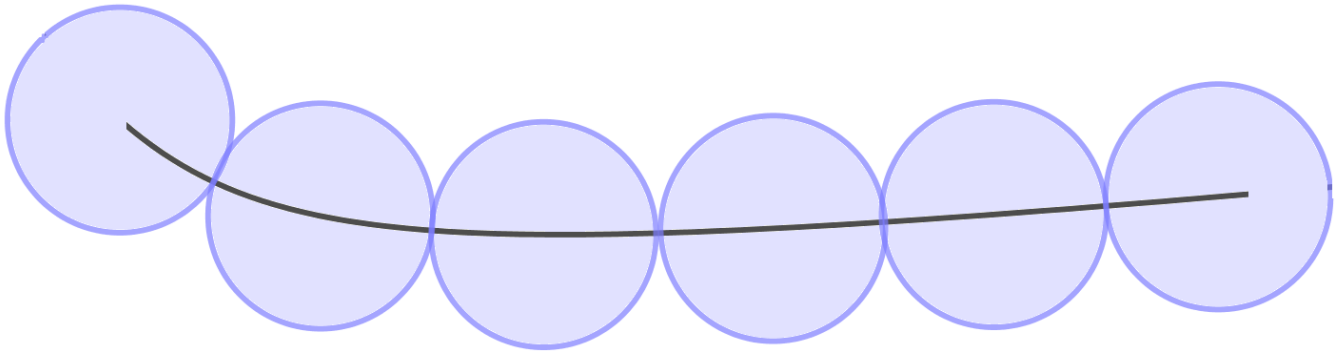


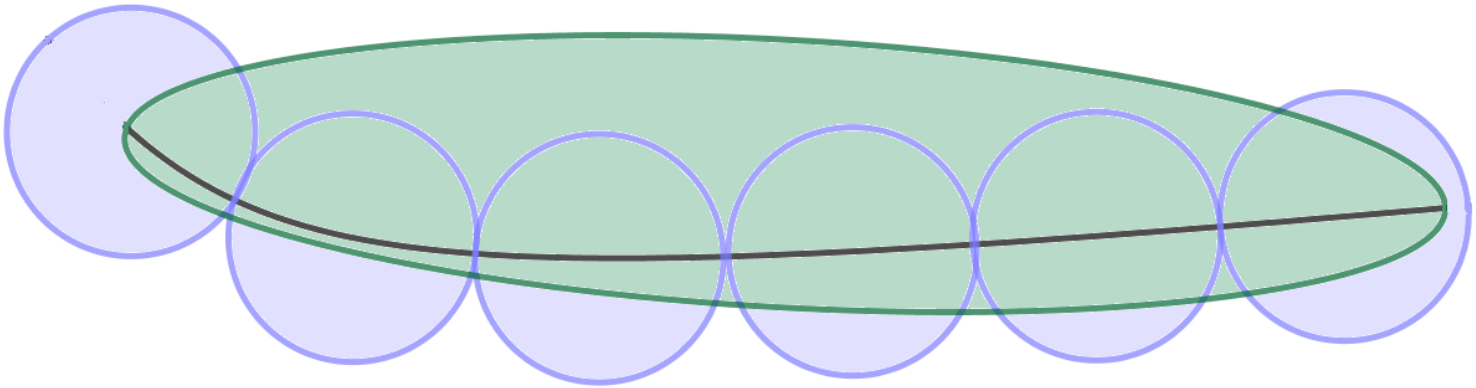
Connected components

Outliers detection



False positive number





How to approximate a manifold with a set of k ellipsoids, from a noisy sample ?

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By modifying the criterion, with Mahalanobis norms...

Squared Σ-Mahalanobis norm : $\|y\|^2_{\Sigma^{-1}} = y^T \Sigma^{-1} y$.

Definition

The optimal codebook $\boldsymbol{\theta}^* = (\theta_i^*)_{i=1..k} = ((t_i^*, \Sigma_i^*))_{i=1..k}$: a minimizer of

$$\boldsymbol{\theta} \mapsto P\left(\min_{i=1..k} \| \cdot - m_{\theta_i,h} \|^2_{\Sigma_i^{-1}} + v^{\Sigma_i}_{\theta_i,h} + \log(\det(\Sigma_i)) \right),$$

with $m_{\theta_i,h}$ the expectation of $P_{\theta_i,h}$ and $v^{\Sigma_i}_{\theta_i,h}$ its variance (for $\| \cdot \|_{\Sigma_i^{-1}}$).

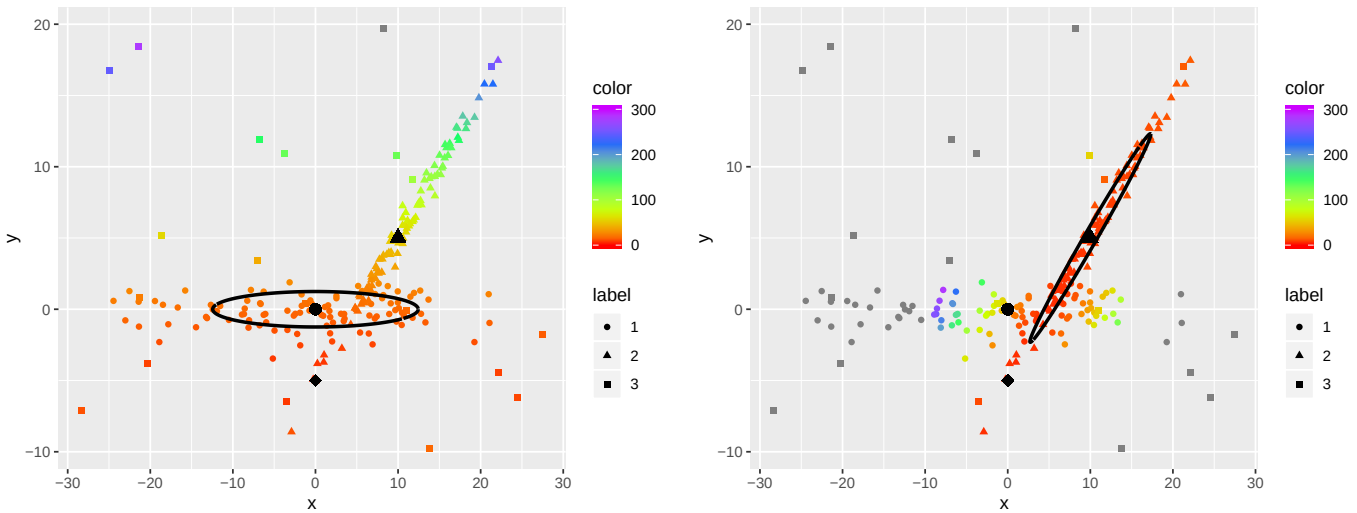


FIGURE – Illustration of the assignment phase

Algorithm 2 Approximation of the k-PLM centers

Input $\mathbb{X}_n$ a n-sample from P, $q = hn$ and k
Sample t_1, t_2,... t_k from $\mathbb{X}_n$ without replacement. Set $\Sigma_i = I_d$ for i in $1..k$.
while the $\theta_i = (t_i, \Sigma_i)$s vary **do**
    Set $\mathscr{C}(\theta_i) = \{\}$ for i in $1..k$.
    for j in $1..n$ **do**
        Add X_j to some $\mathscr{C}(\theta_i)$ satisfying
        $\|X_j - m(\theta_i)\|^2_{\Sigma_i^{-1}} + w(\theta_i) \leq \|X_j - m(\theta_l)\|^2_{\Sigma_l^{-1}} + w(\theta_l)\, \forall l \neq i$
    end for
    for i in $1..k$ **do**
        $t_i = \frac{1}{|\mathscr{C}(\theta_i)|} \sum_{X \in \mathscr{C}(\theta_i)} X$; $\Sigma_i = \Sigma(t_i, \Sigma_i, \mathscr{C}(\theta_i))$
        $\theta_i = (t_i, \Sigma_i)$
    end for
end while
Output $(\theta_1, \theta_2, \ldots, \theta_k)$.

For $\theta = (t, \Sigma)$, $m(\theta) = \frac{1}{q} \sum_{i=1}^{q} X_i(\theta)$, $w(\theta) = \frac{1}{q} \sum_{i=1}^{q} \|X_i(t) - m(\theta)\|^2_{\Sigma^{-1}} + \log(\det(\Sigma))$ with $X_i(\theta)$ an i-th $\|\cdot\|_\Sigma$-nearest neighbor of t and $\mathscr{C}(\theta)$ the cell of θ. Also, for $l, m = 1..d$, $\Sigma(t, \Sigma, \mathscr{C})_{l,m} = \frac{1}{|\mathscr{C}|} \sum_{X \in \mathscr{C}} P_{n,(t,\Sigma),h}(X_{(l)} - \cdot_{(l)})(X_{(m)} - \cdot_{(m)})$.

Optimum when $k = 1$:

f : density on $\mathbb{R}$
Σ : scatter matrix
$\mu \in \mathbb{R}^d$: location parameter
P on $\mathbb{R}^d$, with density :

$$f_{\mu,\Sigma,f} : x \mapsto \frac{C_{d,f}}{\sqrt{\det(\Sigma)}} f(\|x-\mu\|_{\Sigma^{-1}}).$$

Theorem (B. - Levrard - Michel, 2020)

If f is non-increasing, then, $t^* = \mu$ and $\Sigma^* = \left(1 + \frac{1}{h}\frac{M_{d+1}^{r_h}(f)}{M_{d+1}(f)}\right)\mathrm{Cov}(P)$.

$M_{d+1}^r(f) = \int_{u=0}^r u^{d+1} f(u)\mathrm{d}u$

$r_h \in \mathbb{R}_+$ such that $h = \frac{M_{d-1}^{r_h}(f)}{M_{d-1}(f)}$.

$$\mathscr{S}^*_{d,d',\sigma^2_{\min}} = \{\Sigma = PDP^T \mid PP^T = I_d,$$
$$D = \mathrm{diag}(\lambda_1, \dots, \lambda_{d'}, \sigma^2 \dots \sigma^2),$$
$$\lambda_1 \geq \dots \geq \lambda_{d'} \geq \sigma^2 \geq \sigma^2_{\min}\}.$$

P sub-Gaussian with variance V^2 : $\left(\forall r > V, P(\mathrm{B}(0,r)^c) \leq \exp\left(-\frac{r^2}{2V^2}\right)\right)$

$$R_h(\theta) = P\|\cdot - m_{\theta,h}\|^2_{\Sigma^{-1}} + v^{\Sigma}_{\theta,h} + \log(\det(\Sigma))$$

$\theta^*_{d'}$ (resp. $\hat{\theta}_{d'}$) an R_h-minimizer (resp. $\hat{R}_h$) in $\mathbb{R}^d \times \mathscr{S}^*_{d,d',\sigma^2_{\min}}$.

Theorem (B. - Levrard - Michel, 2020)

$$\mathbb{E}\left[R_h(\hat{\theta}_{d'}) - R_h(\theta^*_{d'})\right] \leq \frac{CV^2}{h\sigma^2_{\min}} \sqrt{\mathscr{D}_{d'}} \frac{\log n}{\sqrt{n}}$$

for some absolute constant $C > 0$, with

$$\mathscr{D}_{d'} = \max\left(d'\left(d - \frac{d'+1}{2}\right)\log(d'), (d'+1)\left(d+1-\frac{d'}{2}\right)\right).$$

$$\mathscr{C}^*_{d,d'} = \{\{x \mid \|x-c\|^2_{\Sigma^{-1}} \leq r\}, \Sigma \in \mathscr{S}^*_{d,d',0}, c \in \mathbb{R}^d, r > 0\}.$$

Lemma (B. - Levrard - Michel, 2020)

The Vapnik-Chervonenkis dimension of $\mathscr{C}^*_{d,d'}$ is bounded above by

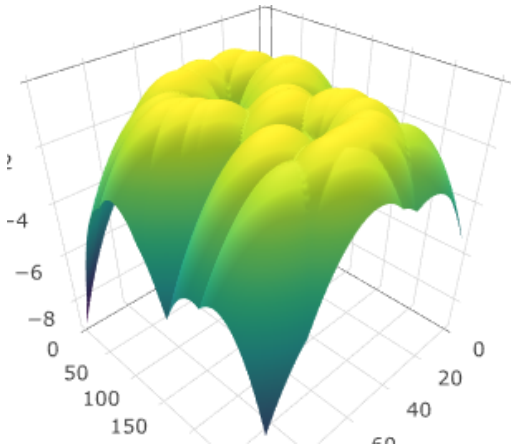
$$(12.416...)\left(d+1-\frac{d'}{2}\right)(d'+1).$$

(Dudley, 1979)

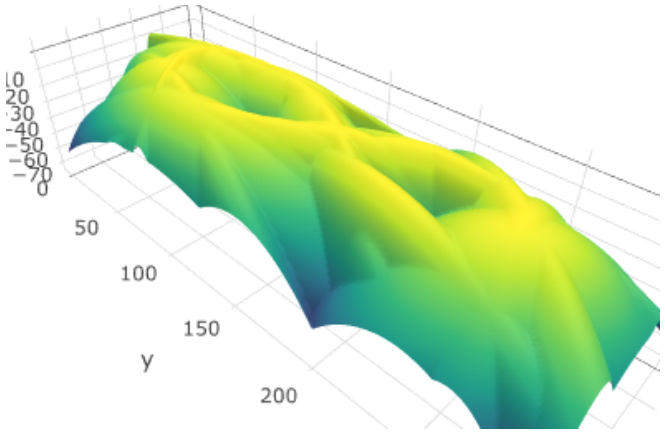
$$VC(\mathscr{C}^*_{d,0}) = d+2$$

(Akamaa, Irie, 2011)

$$VC(\mathscr{C}^*_{d,d}) = \frac{d^2+3d}{2}$$

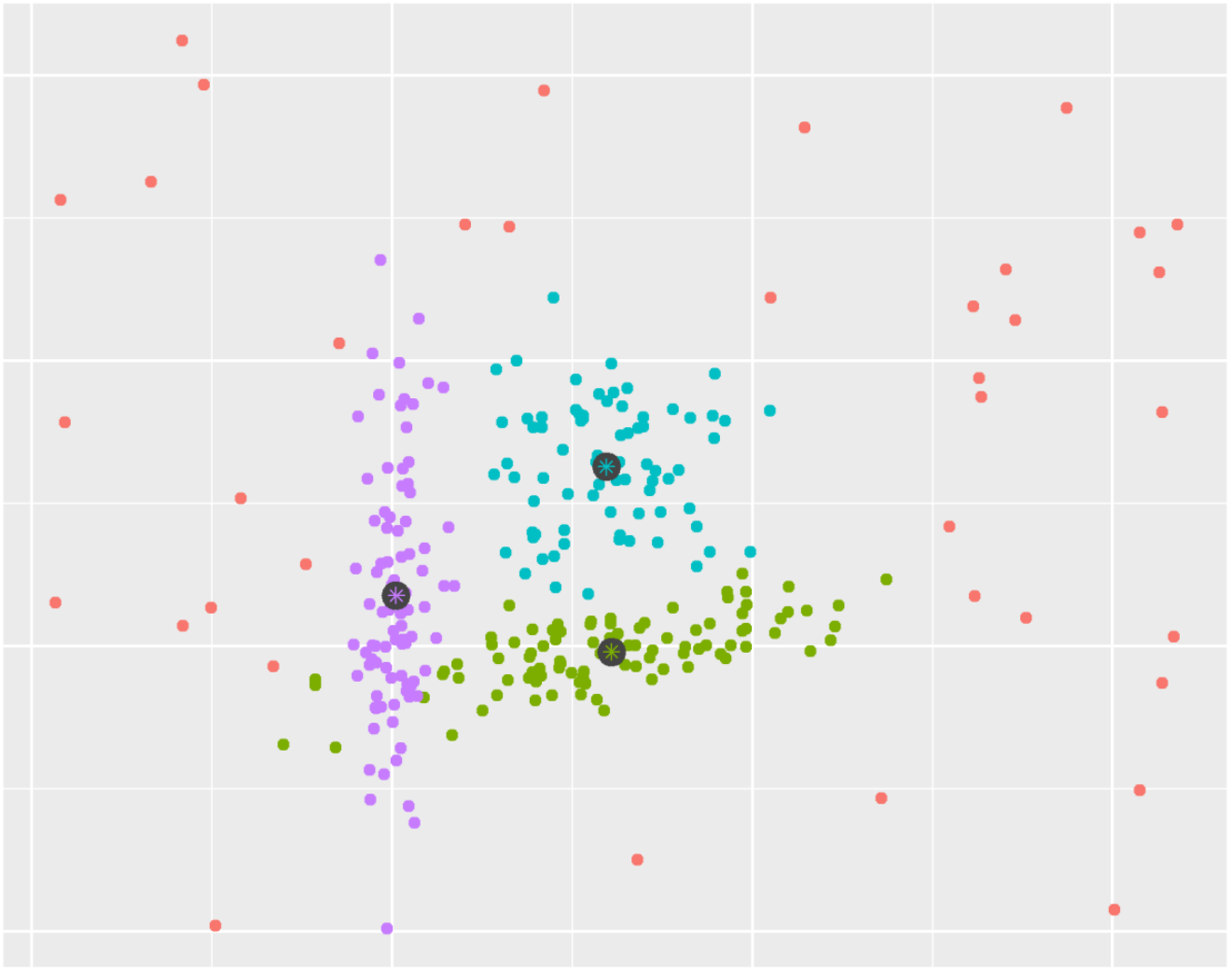


k-PDTM



k-PLM

Clustering with the k-PLM

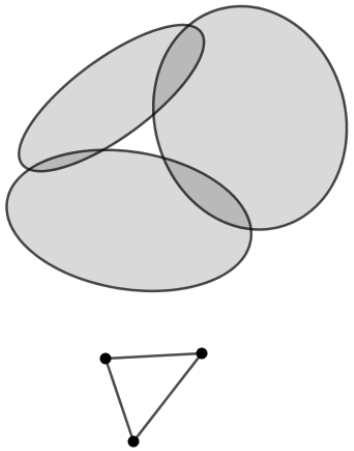


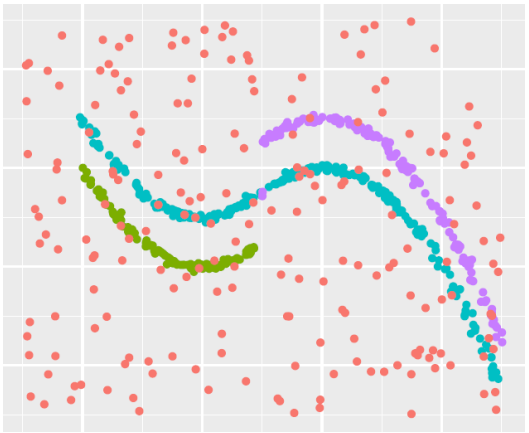
Clustering with unions of ellipsoids

We consider unions of ellipsoids indexed by $\alpha \in \mathbb{R}$:

$$\bigcup_{i=1..k} \{x \mid \|x - c_i\|^2_{\Sigma_i^{-1}} + \omega_i \leq \alpha\},$$

with $\omega_i \in \mathbb{R}$, $c_i \in \mathbb{R}^d$ and covariance matrices Σ_i.





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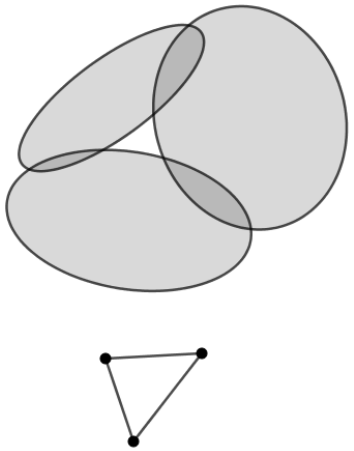

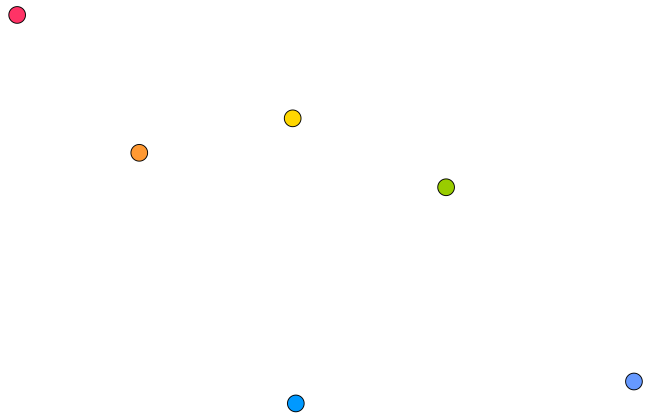

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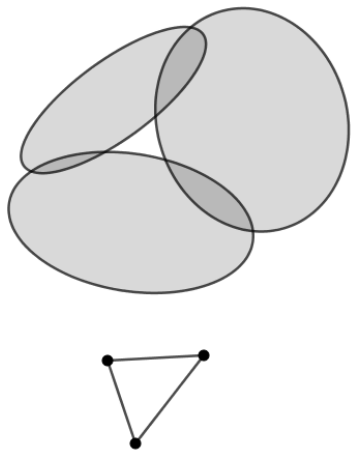

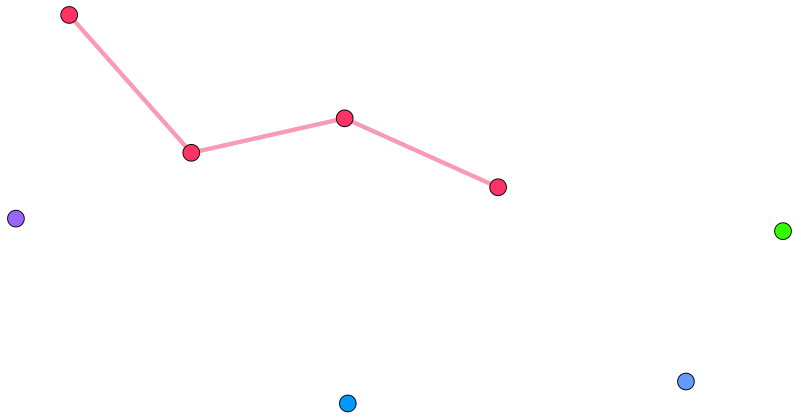

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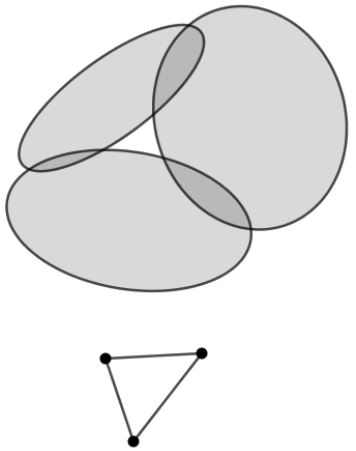

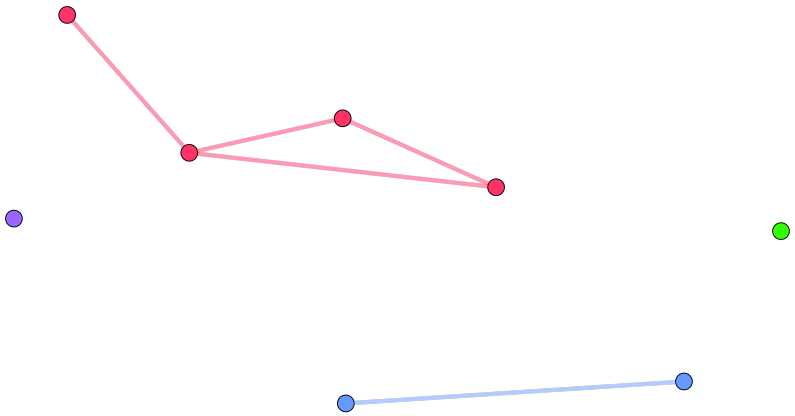

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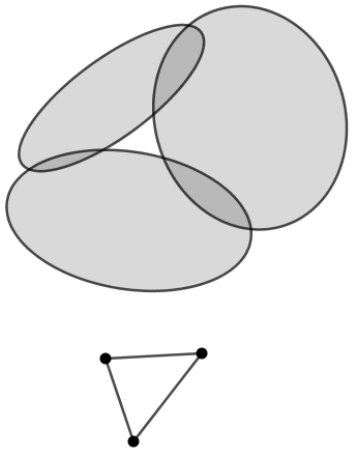

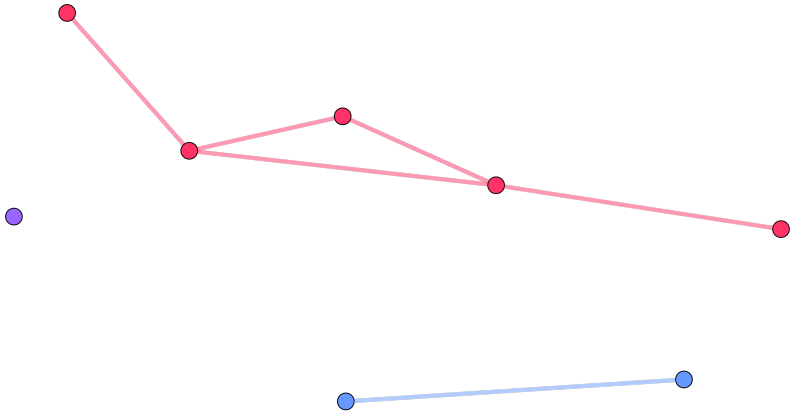

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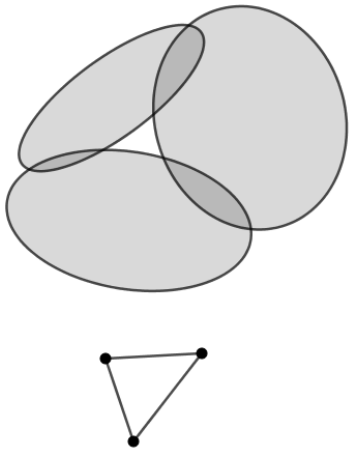

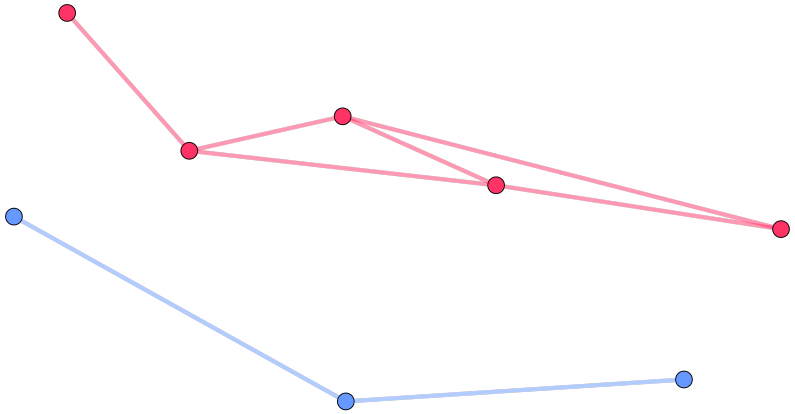

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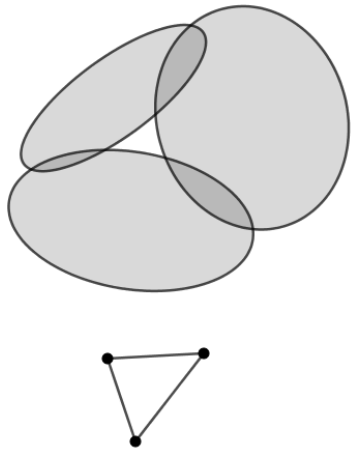

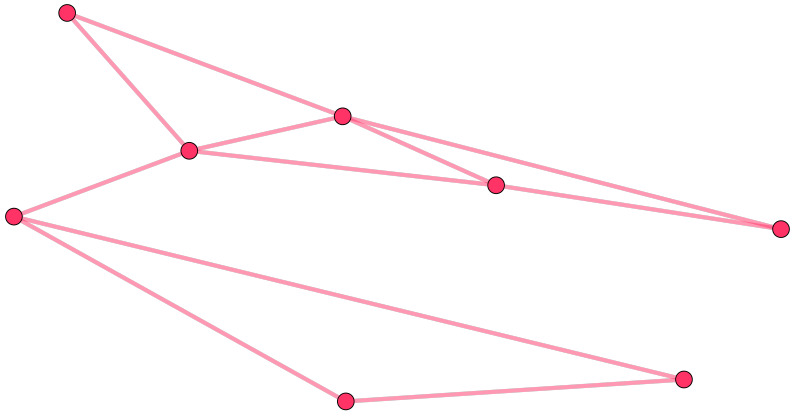

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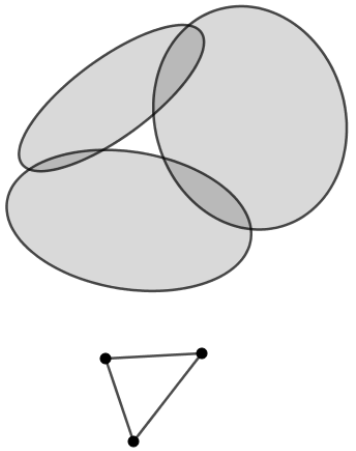

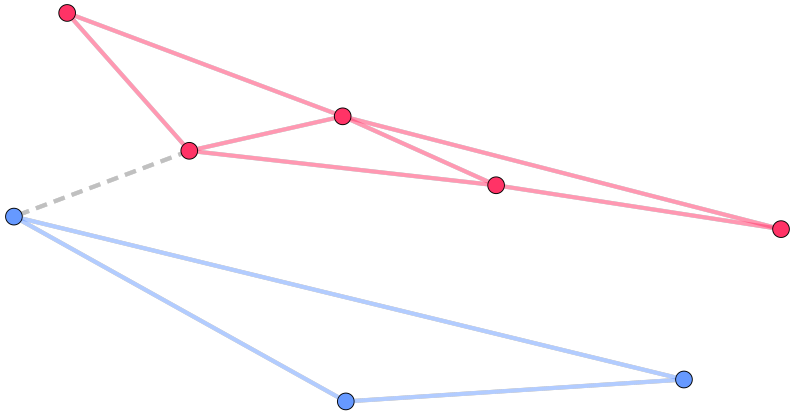

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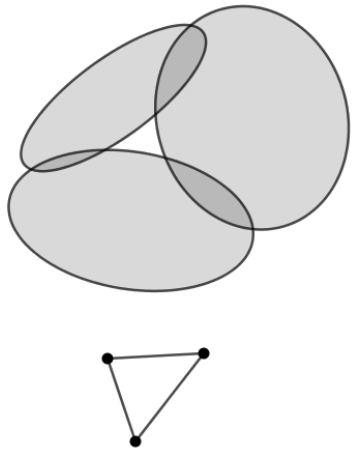
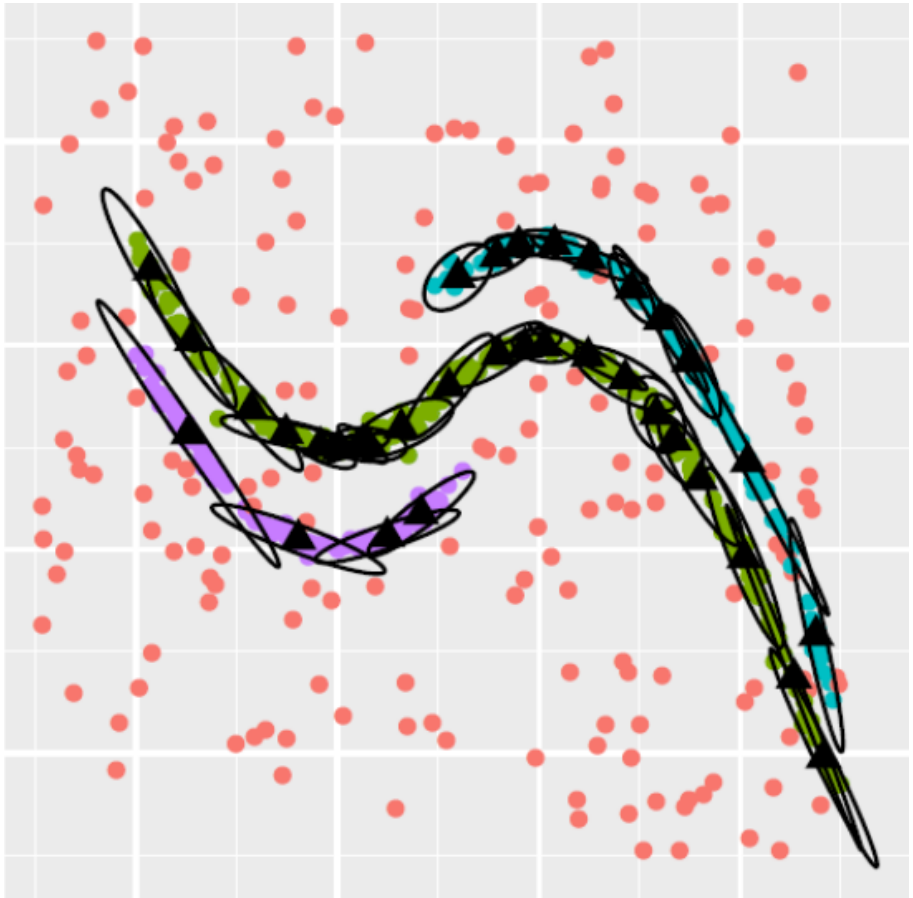




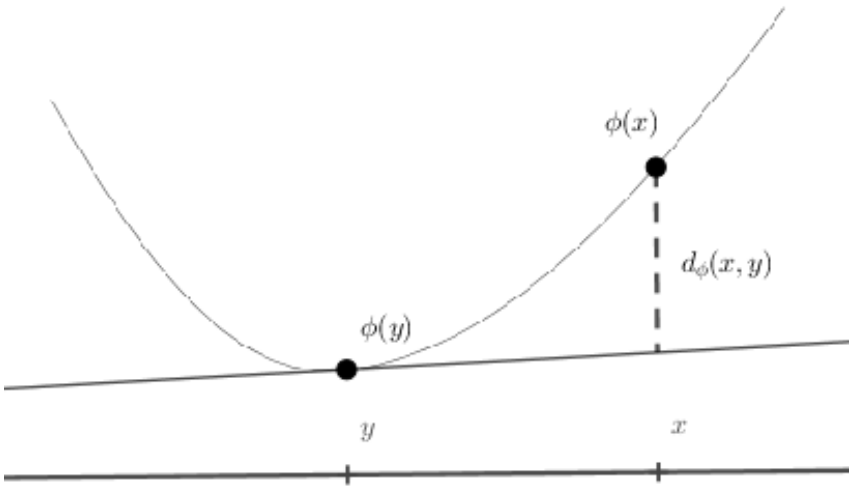
Partitionnement (B. 2020)

Bregman divergences definition

Definition

Let ϕ be a strictly convex $\mathscr{C}_1$ real-valued function, defined on a convex subset Ω of $\mathbb{R}^d$. The *Bregman divergence* associated with ϕ is the function d_ϕ defined on $\Omega \times \Omega$ by :

$$\forall x, y \in \Omega, \mathrm{d}_\phi(x, y) = \phi(x) - \phi(y) - \langle \nabla\phi(y), x - y \rangle.$$



Some examples

Example

1. **Squared Euclidean norm :** $\mathrm{d}_\phi(x,y) = \|x-y\|^2$
2. **Itakura-Saito distance :** $\mathrm{d}_\phi(x,y) = \frac{x}{y} - \ln\left(\frac{x}{y}\right) - 1$
3. **Kullback-Leibler divergence :** $\mathrm{d}_\phi(x,y) = \sum_{\ell=1}^{d} x_\ell \log_2 \frac{x_\ell}{y_\ell}$ (on the $d-1$-dimensional simplex of $\mathbb{R}^d$)
4. ...
5. **k-PDTM divergence (for absolutely continuous measures w.r.t. Lebesgue measure) :** $\mathrm{d}_\phi(x,y) = \|x - m(P_{y,h})\|^2 + v(P_{y,h})$ for the convex function $\phi : x \mapsto \|x\|^2 - \mathrm{d}^2_{P,h}(x)$.

Theorem (Well known)

- *For every* $x, y \in \Omega$, $\mathrm{d}_\phi(x, y) \geq 0$.
- *For every* $C \subset \mathcal{X} = \{x_1, x_2, \ldots, x_n\}$, *le barycenter* $\overline{x}_C = \frac{1}{|C|} \sum_{x \in C} x$ *minimises the function*

$$c \in \Omega \mapsto \frac{1}{|C|} \sum_{x \in C} \mathrm{d}_\phi(x, c).$$

- *For every* $c_1, c_2 \in \Omega$, *the intersection of the two Bregman-Voronoi cells*

$$\left\{x \in \Omega \mid \mathrm{d}_\phi(x, c_1) = \mathrm{d}_\phi(x, c_2)\right\}$$

is an hyperplane.

Consequently, the Lloyd's algorithm (and its trimmed version) applies to Bregman divergences. Moreover, the intersections of cells are affine subspaces.

Existence of optimal codebooks

Definition

We denote by R_h the criterion defined for every $\mathbf{c} = (c_1, c_2, \ldots, c_k) \in \Omega^k$ by :

$$R_h(\mathbf{c}) = \inf_{\tilde{P}, h\tilde{P} \leq P} \tilde{P} \min_{i=1..k} \mathrm{d}_\phi(\cdot, c_i).$$

Theorem (Brécheteau,Fischer,Levard 2021)

For every $0 < h < 1$, il $P\|\cdot\| < +\infty$, ϕ is $\mathscr{C}^2$ and strictly convex and $F_0 = \overline{\mathrm{Conv}(\mathrm{Supp}(P))} \subset \Omega^\circ$, that is, the closure of the convex hull of the support of P is a subset of the interior of Ω.
Then, the set $\mathrm{argmin}_{\mathbf{c} \in \Omega^{(k)}} R_h(\mathbf{c})$ is not empty.

We denote by $\mathbf{c}^*$ a minimizer of R_h, and $\hat{\mathbf{c}}_{n,h}$ a minimizer of the empirical criterion.

Convergence of codebooks

Theorem (Brécheteau, Fischer, Levrard 2021)

Assume that P is absolutely continuous with respect to the Lebesgue measure and satisfies $P\|\cdot\|^p < +\infty$ for some $p > 2$. Then, there exists $\mathbf{c}_h^*$ an optimal codebook such that

$$\lim_{n\to+\infty} R_{n,h}(\hat{\mathbf{c}}_{n,h}) = R_h(\mathbf{c}_h^*) \ a.e.$$

Moreover, up to extracting a subsequence, we have

$$\lim_{n\to+\infty} D(\hat{\mathbf{c}}_{n,h}, \mathbf{c}_h^*) = 0 \ a.e.,$$

where $D(\mathbf{c}, \mathbf{c}') = \min_{\sigma\in\Sigma_k} \max_{i\in[\![1,k]\!]} |c_i - c'_{\sigma(i)}|$ and Σ_k denotes the set of all permutations of $[\![1, k]\!]$.

Rates of convergence of codebooks

Theorem (Brécheteau, Fischer, Levrard 2021)

Assume that $P\|\cdot\|^p < \infty$ *where* $p > 2$. *Further, if* $R^*_{k,h}$ *denotes the optimal cost for* k *centers, assume that* $R^*_{k-1,h} - R^*_{k,h} > 0$.

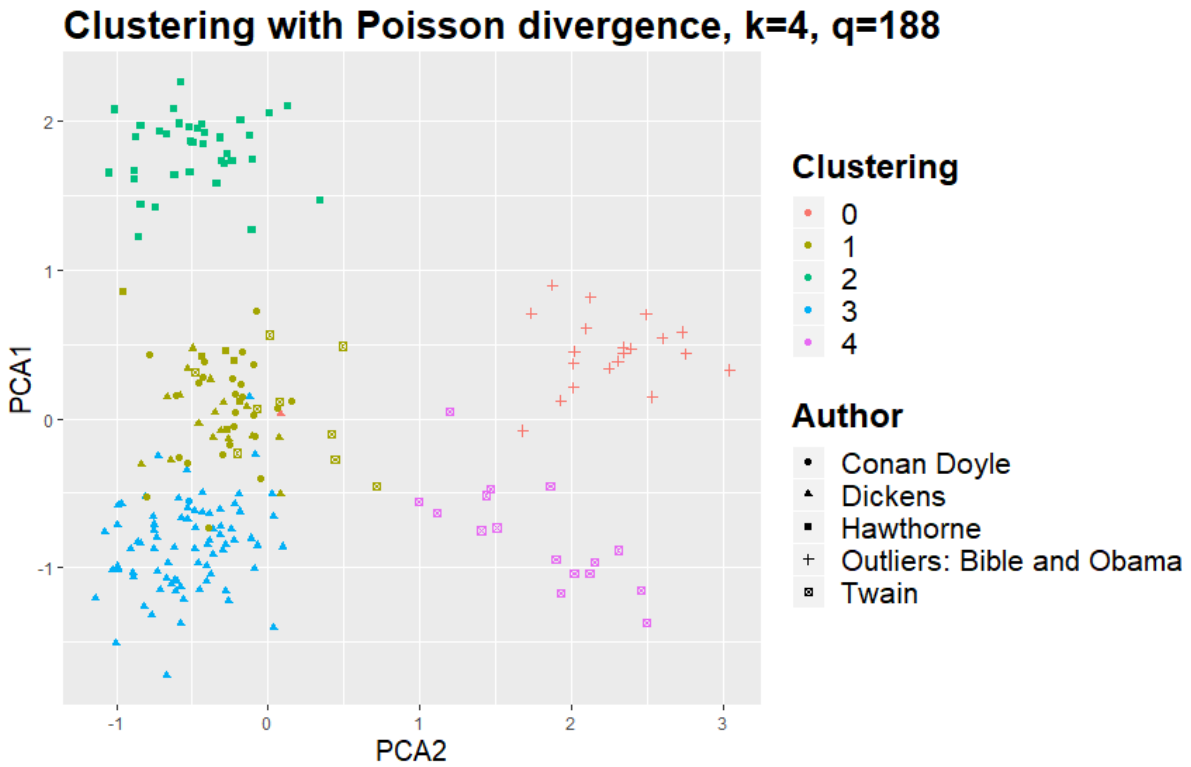
Then, for n *large enough, with probability larger than* $1 - n^{-\frac{p}{2}} - 2\exp(-x)$, *we have,*

$$R_h(\hat{\mathbf{c}}_{n,h}) - R_h(\mathbf{c}^*_h) \leq \frac{C_P}{\sqrt{n}}(1+\sqrt{x}).$$

Relation with other density functions

Some distributions which density or probability function p expresses as $p(x) = \exp(-\mathrm{d}_\phi(x,\mu)) \times f(x)$ for f a non-negative function, ϕ a $\mathscr{C}^1$ strictly convex function and μ the mean of the distribution.
$\Rightarrow$ Clustering with d_ϕ !

Example : Text clustering with the Bregman divergence $\mathrm{d}_\phi : (x,\mu) \mapsto x\ln\left(\frac{x}{\mu}\right) - (x-\mu)$ associated with the Poisson distribution with probability function $p : x \mapsto \frac{\mu^x}{x!}\exp(-\mu)$.



Thank you !