

Algorithme EM par les mélanges gaussiens

(X_i, Y) à valeurs dans $\mathbb{R}^d \times \{1, 2, \dots, K\}$

$$\begin{cases} \Pr[Y=j | X_i = x] = \pi_j > 0 & \sum_{j=1}^K \pi_j = 1 \\ X_i | Y=j \sim \text{NCP}(\mu_j, \Sigma_j) \end{cases}$$

$$Q_\theta = \{Q_\theta = \mathcal{L}(X, Y), \theta \in \Theta\}$$

$$\theta = (\pi_1, (\mu_1, \Sigma_1), \dots, (\mu_K, \Sigma_K))$$

$$\prod_{i=1}^n \prod_{j=1}^K \pi_j = 1 \quad \text{SOP}$$

Observations X_1, \dots, X_n iid de même loi que X .

$$S_n = \{S_n = \mathcal{L}(X), (X_i, Y) \sim Q_\theta\}$$

$$S_c = \{S_c = \mathcal{L}(Y|X), (X_i, Y) \sim Q_\theta\}$$

$$P_{\mu, \Sigma}(x) = \frac{1}{(2\pi)^{d/2} \sqrt{\det(\Sigma)}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}$$

$$g_\theta \text{ à peu près densité } g_\theta(x, y) = \pi_j P_{\mu_j, \Sigma_j}(x) \quad X_i, Y = y$$

$$m_\theta(x) = \sum_{y=1}^K g_\theta(x, y)$$

$$q_{\theta, x} : q_{\theta, x}(y) = \frac{g_\theta(x, y)}{m_\theta(x)}$$

▷ Expectation step

À l'itération t , $\hat{\theta}_t$

$Z_1^t, \dots, Z_n^t \sim \{(X_i, Z_i^t) / \hat{\theta}_t \dots (X_n, Z_n^t) / \hat{\theta}_t\}$ iid

$$Z_i^t / X_i^n \stackrel{\mathcal{D}}{=} Z_i^t / \hat{\theta}_t \sim \text{NCP}(\hat{\mu}_{\hat{\theta}_t}, \hat{\Sigma}_{\hat{\theta}_t})$$

$$\Pr[Z_i^t = j | X_i^n] = \frac{g_{\hat{\theta}_t}(x_{it})}{m_{\hat{\theta}_t}(x_i)} = p_{ij}^t$$

$$\text{Avec } F(\theta, \hat{\theta}_t) = E \left[\sum_{i=1}^n \log g_\theta(X_i, Z_i^t) | X_i^n \right]$$

$$= \sum_{i=1}^n \sum_{j=1}^K p_{ij}^t \log g_\theta(x_i, j)$$

avec $\log(g_\theta(x_{i,j})) = \log \pi_j^t - \frac{1}{2} (x_i - \mu_j)^T \Sigma_j^{-1} (x_i - \mu_j) - \frac{1}{2} \log(\det(\Sigma_j))$

$$\hat{\rho}_{ij}^t = \frac{\pi_j^t \rho_{ij, \hat{\Sigma}_j}(x_i)}{\sum_{\ell=1}^K \pi_\ell^t \rho_{i\ell, \hat{\Sigma}_\ell}(x_i)}$$

Maximisation step

$$\hat{\theta}_{t+1} \in \underset{\theta \in \Theta}{\operatorname{argmax}} F(\theta | \hat{\theta}_t)$$

$\rightarrow \alpha$
 $\rightarrow \mu$
 $\rightarrow \Sigma$

En dépos le cas, on obtient :

$$\begin{cases} \hat{\theta}_{t+1} = (\hat{\pi}^{t+1}, \hat{\mu}_j^{t+1}, \hat{\Sigma}_j^{t+1}) \\ \hat{\mu}_j^{t+1} = \frac{\sum_{i=1}^n \hat{\rho}_{ij}^t x_i}{\sum_{i=1}^n \hat{\rho}_{ij}^t} \\ \hat{\Sigma}_j^{t+1} = \frac{\sum_{i=1}^n \hat{\rho}_{ij}^t (x_i - \hat{\mu}_j^t)(x_i - \hat{\mu}_j^t)^T}{\sum_{i=1}^n \hat{\rho}_{ij}^t} \\ \hat{\pi}_j^{t+1} = \frac{1}{n} \sum_{i=1}^n \hat{\rho}_{ij}^t \end{cases}$$

$$\underset{\pi \in [0,1]^K}{\operatorname{maximize}} \sum_{j=1}^K \sum_{i=1}^n \hat{\rho}_{ij}^t \log(\pi_j) \quad \Leftrightarrow$$

$$\underset{\pi \in [0,1]^K}{\operatorname{minimize}} - \underbrace{\sum_{j=1}^K \frac{1}{n} \sum_{i=1}^n \hat{\rho}_{ij}^t \log \pi_j}_{\sum_j \left(\frac{1}{n} \sum_{i=1}^n \hat{\rho}_{ij}^t \right) \log \frac{\pi_j}{\hat{\rho}_{ij}^t}} + \sum_j \frac{1}{m} \sum_i \hat{\rho}_{ij}^t \log \left(\frac{\pi_j}{\sum_{j'=1}^K \hat{\rho}_{ij'}^t} \right)$$

$$\underset{\pi \in [0,1]^K}{\operatorname{minimize}} D_{KL}(\pi \| \pi_t) \quad \Leftrightarrow$$

$$\text{On a } \pi_j \in [0,1] \text{ et } \sum_{j=1}^K \pi_j = 1$$

$$\text{D'où } \hat{\pi}^{t+1} = \pi$$

EN CPC) au soft k-means

Itiner

$$\hat{\rho}_{ij}^t \approx \Pr(Y_i=j | X_i)$$

$$\frac{\mu_j}{\sum_j}$$

Cas général de l'EN

$$\left\{ \begin{array}{l} (X, Y) \sim Q_\theta = g_\theta(X, \alpha) \quad | X = (X_1, \dots, X_n) \\ X \sim M_\theta = \mu_\theta \cdot \nu \quad Y = (Y_1, \dots, Y_n) \\ Y | X \sim Q_{\theta, X} = g_{\theta, X} \cdot \nu \end{array} \right.$$

On cherche à un estimateur de θ , $f(\theta | \hat{\theta}) = \mathbb{E}[\log(g_\theta(X, Z)) | X]$
 $Z | X \sim Q_{\hat{\theta}, X}$.

Lemma

$$\hat{\theta}_Z = g_Z \cdot \nu \quad \text{et} \quad Z | X \sim Q_Z$$

$$\forall \theta \in \Theta, \log(\mu_\theta(x)) = \mathbb{E}[\log(g_\theta(X, Z)) | X] + D_{KL}(Q_x || Q_{\theta, X}) + H(Q)$$

$$D_{KL}(Q_x || Q_{\theta, X}) = \mathbb{E}\left[\log \frac{g_X(z)}{g_{\theta, X}(z)} | X\right] \quad \text{et} \quad H(Q_x) = \mathbb{E}[\log g_X(z) | X]$$

En particulier, $Q_x = Q_{\theta, X}$

$$\log \mu_\theta(x) = F(\theta | \theta') + D_{KL}(\theta' || \theta) + H(Q')$$

Preuve

Formule de Bayes, $g_\theta(x, z) = g_{\theta, X}(z) \mu_\theta(x)$

$$\log \mu_\theta(x) = \mathbb{E}[\log(\mu_\theta(x)) | X]$$

$$= \mathbb{E}[\log(g_\theta(x, z)) | X] - \mathbb{E}[\log(g_{\theta, X}(z)) | X] + \mathbb{E}[\log g_X(z) | X]$$

$$= \mathbb{E}[\log(g_\theta(x, z)) | X] - \underbrace{\mathbb{E}\left[\log \frac{g_X(z)}{g_{\theta, X}(z)} | X\right]}_{D_{KL}(Q_x || Q_{\theta, X})} - \underbrace{\mathbb{E}[\log g_X(z) | X]}_{H(Q_x)}$$

$$D_{KL}(Q_x || Q_{\theta, X})$$

□

Proposition

$P = p \cdot \nu$ et $Q = q \cdot \nu$. Alors : $0 \leq D_{KL}(P || Q) \in \overline{\mathbb{R}}$.

De plus, si $Q \ll P$:

$D_{KL}(P || Q) \Leftrightarrow p = q \quad p\text{-presque partout}$

Breve

$$D_{KL}(P \parallel Q) = E \left[\log \frac{p(z)}{q(z)} \right] \text{ avec } z \sim P$$

Si $P \ll Q$ alors $D_{KL} \rightarrow +\infty$

$$\begin{aligned} \text{Si } P \ll Q, D_{KL}(P \parallel Q) &= E \left[-\log \frac{q(z)}{p(z)} \right] \text{ car } p(z) > 0 \text{ ps} \\ &\geq -\underbrace{\log \left(E \left[\frac{q(z)}{p(z)} \right] \right)}_{\geq 0} \underbrace{\left(\frac{q(z)}{p(z)} \right)}_{1} \text{ par l'inégalité de Jensen.} \end{aligned}$$

Pour stricte concavité de la fonction $-\log$, on a :

$$D_{KL}(P \parallel Q) = 0 \text{ si } \frac{q(z)}{p(z)} = \text{cte ps}$$

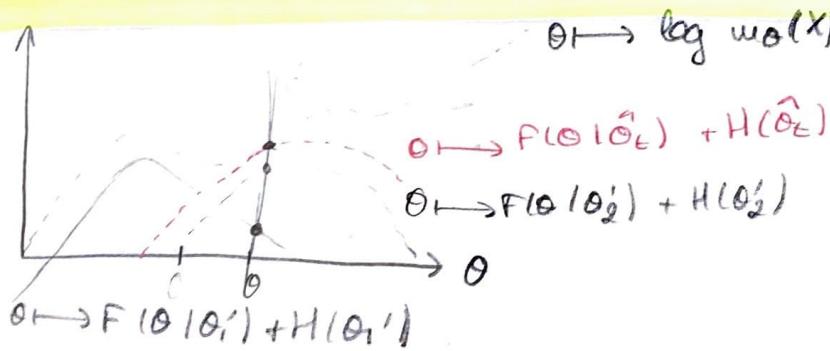
$$\text{ii } \frac{q}{p} = \text{cte } \frac{1}{P - ps} \text{ car } Q \ll P$$

Donc par intégration, $\int q = \text{cte}/p$ et $\text{cte} = 1$ et $p = q / (P - ps)$. \square

Proposition

$$\forall \theta, \theta^*, \log m_\theta(x) \geq F(\theta, \theta^*) + H(\theta^*)$$

$$\text{et } \log m_\theta(x) = F(\theta, \theta^*) + H(\theta^*) \text{ pour } \theta = \theta^*.$$



E step $\hat{\theta}_t^* \in \arg \max F(\hat{\theta}_t | \theta) + H(\theta)$.

$$\hat{\theta}_t' = \hat{\theta}_t$$

M step: $\hat{\theta}_{tm} \in \arg \max_{\theta} F(\theta | \hat{\theta}_t) + H(\hat{\theta}_t)$.

Theorème

$\hat{\theta}_t \in \arg \max_{\theta \in \Theta} f(\theta | \hat{\theta}_t)$, alors la suite $\log(w_t(x))$ est croissante

Preuve

$$\log(w_t(x)) = f(\hat{\theta}_t | \hat{\theta}_t) + H(\hat{\theta}_t)$$

$$\text{def max } \leftarrow F(\hat{\theta}_{t+1} | \hat{\theta}_t) + H(\hat{\theta}_t) \leq \log(w_{t+1}(x)).$$

II. Minimisation du coût l'inique.

Objectif: Partition $(G_1 \dots G_k)$ de \mathbb{R}^d tel que $(G_1 \dots G_k)$ minimise un risque empirique.

- coûts centrés (k-means)
- coût distribué (clustering spectral)

d: dissimilarité, $d(x, y) \geq 1$ pour $x \neq y$.

Pour $(G_1 \dots G_k)$ un partitionnement, $p(G) \in \arg \min_{P \in \mathcal{P}(\mathbb{R}^d)} E[d(X, p)] \mathbf{1}_{X \in G]$

Cœurs centrés

Quantification (cf Biou)

$$\mathbb{R}^d, q(x) = \sum_{j=1}^k p(G_j) \mathbf{1}_{x \in G_j}$$

$$D(G_1 \dots G_k) = E[d(X, q(x))]$$

$$\min_{(G_1 \dots G_k) \in \mathcal{P}(\mathbb{R}^d)} E[d(X, p(G))] \mathbf{1}_{X \in G} \quad D(G_1 \dots G_k)$$

② Coût des k-moyennes

$$d(x, y) = \|x - y\|_2$$

$$p(G_j) = \frac{1}{|\{x_i \in G_j\}|} E[X] \mathbf{1}_{X \in G_j}$$

Empiriquement: coût $D(G_1 \dots G_k) = \frac{1}{n} \sum_{j=1}^k \sum_{x \in G_j} \|x - \hat{G}_j\|^2$

$$\hat{G}_j = \bar{x}_j N(x_1, \dots, x_n)$$

$$p(\hat{G}_j) = \frac{1}{|\{x_i \in G_j\}|} \sum_{x \in G_j} X$$

② k-medoids

K-means interne

$$\mu(\hat{G}) = x_t \text{ avec } t \in \arg\min_{1 \leq t \leq n} \sum_{x \in \hat{G}} \|x - x_t\|_2^2$$

un point placé que la moyenne



③ k-medians

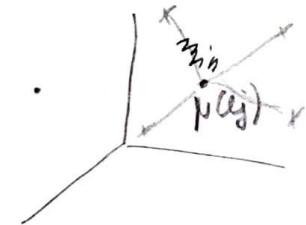
$$D(G, \dots, G) = \frac{1}{n} \sum \sum \|u\|_2^0$$

$$\mu(\hat{G}) \in \{x_1, \dots, x_n\}$$

Dispersion intra-classe

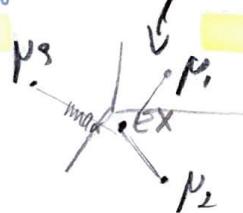
but des k-medians

$$D(G, \dots, G) = \mathbb{E} \left[\|x - \mu(\hat{G})\|_2^2 \mid x \in \hat{G} \right]$$



Propriétés

$$D(G, \dots, G) + \sum_{j=1}^k \mathbb{P}\{x \in G_j\} \mathbb{E}(x - \mu(G_j))^2 = \mathbb{E}\{x - \mathbb{E}[x]\|^2\}$$



Preuve

$$\mu(\hat{G}) = \frac{1}{\mathbb{P}\{x \in \hat{G}\}} \mathbb{E}[x \mid x \in \hat{G}]$$

TOOO ("c'est manquant")

$$D(G, \dots, G) = \frac{1}{n} \sum_{i=1}^n \|x_i - \mu(\hat{G})\|_2^2$$

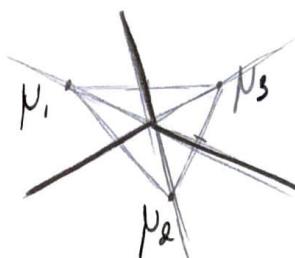
Algorithme

$$D(G \dots G_k) = \frac{1}{n} \sum_{j=1}^k \sum_{x \in G_j} \|x - \mu(G_j)\|^2$$

$$\min_{G_1 \dots G_k \in \mathcal{P}(\mathbb{R}^d)} D(G \dots G_k)$$

$$\min_{\substack{(G_1 \dots G_k) \in \mathcal{P}(\mathbb{R}^d) \\ (\mu_1 \dots \mu_k) \in \mathbb{R}^d}} \frac{1}{n} \sum \sum \|x - \mu_j\|^2$$

Algorithme des k-means



$\mu_1 \dots \mu_K$ initialisé

itérer : $(G^{t+1} \dots G_K^{t+1})$ = Partitionnement de Voronoi pour les centres $(\mu_1 \dots \mu_K)$

Maj de $\mu_1^{t+1} \dots \mu_K^{t+1}$ moyennes arithmétiques de chaque collecte $\hat{g}_j = g_j n / K$

$$G_t = \{x \in \mathbb{R}^d : \|x - \mu_k\| \leq \|x - \mu_l\|, \forall l \in [1, K] \}$$

$$G_{t+1} = \{x \in \mathbb{R}^d : \|x - \mu_{k+1}\| \leq \|x - \mu_k\| \quad \forall k \in [1, K] \} \quad \left(\bigcup_{k=1}^K G_k \right)$$

Proposition

$D(G^t \dots G_K^t) = \frac{1}{n} \sum_{j=1}^k \sum_{x \in G_j^t} \|x - \mu(G_j^t)\|^2$ est décroissante avec t .

Prouve

$$\begin{aligned} D(G^t \dots G_K^t) &= \frac{1}{n} \sum_{j=1}^k \sum_{x \in G_j^t} \|x - \mu(G_j^t)\|^2 \geq \frac{1}{n} \sum_{j=1}^k \sum_{x \in G_j^{t+1}} \|x - \mu_j^{t+1}\|^2 \\ &\stackrel{\text{Voronoi}}{\geq} \frac{1}{n} \sum_{j=1}^k \sum_{x \in G_j^{t+1}} \|x - \mu_j^{t+1}\|^2 = D(G^{t+1} \dots G_K^{t+1}) \end{aligned}$$

① $\forall x \in G^{t+1}, \|x - \mu_j^{t+1}\| \leq \|x - \mu_j^t\| \quad \forall j \in [1, K]$ vrai pour $x \in G^t$

② $\forall x \in \mathbb{R}^d, \sum_{j=1}^k \|x - \mu_j^t\|^2 \leq \sum_{j=1}^k \|x - \mu_j^t\|^2 \quad \forall x \in G^t$

$$\sum_{i=1}^n \sum \|x_i - \mu_j^t\|^2$$

$$\leq \sum_{i=1}^n \sum \|x_i - \mu_j\|^2$$

$$\textcircled{2} \quad p_j^{t+1} = \frac{1}{\text{card}(G^{t+1})} \sum_{i=1}^n \mathbb{1}_{X_i \in G^{t+1}} \in \underset{\mu \in \mathbb{R}^d}{\text{argmin}} \sum_{X_i \in G} \|x_i - \mu\|^2$$

Done $\sum_{j=1}^K \sum_{X_i \in G} \|x_i - p_j^{t+1}\|^2 \leq \sum_{j=1}^K \sum_{X_i \in G} \|x_i - p_j^t\|^2$

k-means

- ① Voronoi $\mathbb{1}_{X_i \in G}$
- ② Moy centroid

soft-k-means

- ① local $p_j^t \sim \mathbb{P}[Y=j | X_i]$ $\rightarrow \mathbb{P}_j$
- ② Ray p_j^t

$$\Leftrightarrow \begin{aligned} \sum_j p_j^t &= \sigma^2 b_i, \sigma^2 \rightarrow 0 \\ p_j^t &= \frac{1}{K} \end{aligned}$$

latts distancés

s: similitude, $s(x, y)$ grand si $x \sim y$

$$\hat{D}(z_1 \dots z_K) = \sum_{j=1}^K \sum_{\substack{x \in z_j \\ y \notin z_j}} s(x, y) \text{ minimiser}$$

W: matrice d'adjacence : $W_{ij} = s(x_i, x_j)$ s est symétrique
 W est symétrique

Partitionnement des indices $\{1 \dots n\}$, $(l_1 \dots l_K)$:

$$\hat{D}(z_1 \dots z_K) = \sum_{j=1}^K \sum_{\substack{i \in z_j \\ l \notin z_j}} W_{il}$$

Graph cut problem

$$s: \|x - y\|_2$$

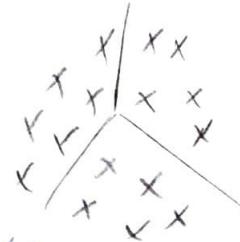
\hookrightarrow s: ϵ -neighborhood similarity :

$$s(x, y) = \begin{cases} 1 & \text{si } \|x - y\|_2 \leq \epsilon \\ 0 & \text{sinon} \end{cases}$$

$(l_1 \dots l_K)$ partition de $\{1 \dots n\}$ telle que :

$$\sum_{j=1}^K \sum_{\substack{i \in l_j \\ l \neq l_j}} W_{il} \downarrow \text{Graph cut.}$$

peu pertinent en pratique



$$x_i \cdot (w_{i1}, w_{i2})^\top$$

19/10/2021



Ratio cut:

$$\rightarrow D_n(Z) = \sum_{j=1}^n \frac{1}{|f_j|} \sum_{\substack{i \in f_j \\ G \notin f_j}} w_{i,j} \quad \text{avec } |f_j| = \text{card}(f_j)$$

Normalized cut

$$\rightarrow D_n(Z) = \sum_{j=1}^n \frac{1}{\text{vol}(f_j)} \sum_{\substack{i \in f_j \\ l \notin f_j}} w_{i,l} \quad \text{avec } \text{vol}(f_j) = \sum_{i \in f_j} d_i,$$

$d_i = \sum_{l=1}^n w_{i,l}$ (degré du i ème sommet)

Définition

Graphe $W \in \mathbb{R}^{n \times n}$ symétrique + la matrice des degrés $D = \begin{pmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & d_n \end{pmatrix}$.

Laplaciens du graphe : $L = D - W$.

Propriétés

(k_1, \dots, k_L) partition de $\{1, \dots, n\}$,

$$D_Z(Z) = \text{tr}(H^T L H) \quad \text{avec } H \in \mathbb{R}^{n \times k}, \quad h_{ij} = \frac{1}{\sqrt{|f_j|}} \sum_{i \in f_j}$$

De plus, $H^T H = I_K$.

Preuve

$\alpha H^T H = I_K$ calcul direct.

$$\alpha \text{tr}(H^T L H) = \text{tr}((L^{1/2} H)^T L^{1/2} H) = \sum_{j=1}^L \underbrace{(L^{1/2} h_j)^T (L^{1/2} h_j)}_{h_j^T L h_j}, \quad H = [h_1 | \dots | h_K]$$

$$\forall u \in \mathbb{R}^n, u^T L u = u^T D u - u^T W u = \sum_{i=1}^n d_i u_i^2 - \sum_{i,j} w_{ij} u_i u_j.$$

diagonale i,i

$$= \frac{1}{2} \left(\sum_i d_i u_i^2 + \sum_i d_i u_i^2 - 2 \sum_{i,j} w_{ij} u_i u_j \right) \quad \boxed{W \text{ symétrique}}$$

$$= \frac{1}{2} \left(\sum_{i,j} w_{ij} u_i^2 + \sum_f w_{ij} u_f^2 - 2 \sum_f \right) \quad \boxed{\text{?}}$$

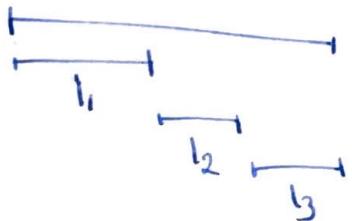
$$= \frac{1}{2} \left(\sum_i w_{ii} (u_i - u_f)^2 \right)$$

$$\text{Done } h_j^T L h_j = \frac{1}{2} \sum_{i \in \mathcal{Y}} w_i e \left[h_{ij} - \bar{h}_{j \mid \mathcal{Y}} \right]^2$$

$$\begin{aligned}
&= \frac{1}{\sqrt{|I_j|}} \sum_{i \in I_j} \frac{1}{\sqrt{|I_j|}} (w_i e - \bar{w}_{I_j \mid \mathcal{Y}}) w_i \\
&= \frac{1}{2} \sum_j \underbrace{\frac{1}{|I_j|} \sum_{\substack{i \in I_j \\ l \notin I_j}} (w_{i \mid l} - \bar{w}_{l \mid I_j}) w_{i \mid l}}_{= 1 \text{ si } i \in I_j \text{ et } l \notin I_j \\ i \notin I_j \text{ et } l \in I_j} \\
&= \frac{1}{2} \sum_j \frac{1}{|I_j|} \sum_{\substack{i \in I_j \\ l \notin I_j}} w_{i \mid l} = D_n(\mathcal{R})
\end{aligned}$$

example:

"one-hot-encoding"



$$H_n = \begin{pmatrix} 1/h_{11} \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1/h_{31} \end{pmatrix}$$

Ratio cut:

$$\left\{ \begin{array}{l} \text{minimise} \\ \mathcal{D} \in \mathcal{P}(\mathbb{R}, n) \end{array} \right. D_n(\mathcal{U})$$

$$\left\{ \begin{array}{l} \text{minimise} \\ H \in \mathbb{R}^{n \times k} \end{array} \right. \begin{array}{l} \tau(H^T L H) \\ H^T H = k \\ H_{ij} \in \{0, \frac{1}{\sqrt{|I_j|}}\} \end{array}$$

$$L = \sum_{i=1}^n d_i v_i v_i^T \text{ les propres de } L \text{ (réelle symétrique)}$$

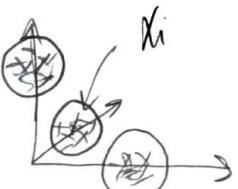
incarné!
→ retenir cette contrainte

$$\text{avec } d_1 \leq \dots \leq d_n$$

$$H = [v_1 | \dots | v_k] \quad | \quad x_i$$

$$x_i \quad \begin{matrix} & & 1/h_{ij} \\ \begin{matrix} & & \diagdown \\ & O & X & O \end{matrix} & \end{matrix}$$

$$x_i \rightarrow j \text{ tq } H_{ij} \neq 0 \quad j \in \arg \max_{1 \leq l \leq k} H_{il}$$



Algorithm: of notes de cours

k-moyennes

Algo itératif et simple
 ↳ solution approchée du pb exact

Normalized cut

$$D_n(Z) = \sum_{j=1}^k \frac{1}{\text{Vol}(Z_j)} \sum_{i \in j} w_{ij}$$

Propriétés

$$D_n(Z) = \text{tr}(H^T L H) \text{ avec } H_{ij} = \frac{1}{\sqrt{\text{Vol}(U_j)}} u_i e_j$$

$$H^T D H = I_k$$

Si D non inversible, un point du graphe est isolé

$$\begin{aligned} L_w &= D^{-1} L && \text{si } D \text{ est inversible} \\ &= \sum d_i v_i v_i^T, d_1 \leq \dots \leq d_n \end{aligned} \quad \left. \begin{array}{l} \\ \end{array} \right\} H = [v_1 | \dots | v_k]$$

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Cutting Spectral

Problème relaxé

↳ solution exacte

= solution approchée du problème original

mat avec 1 seule col \equiv quotient de Rayleigh

↳ cf Fisher généralisé et ss

D : matrice des degrés