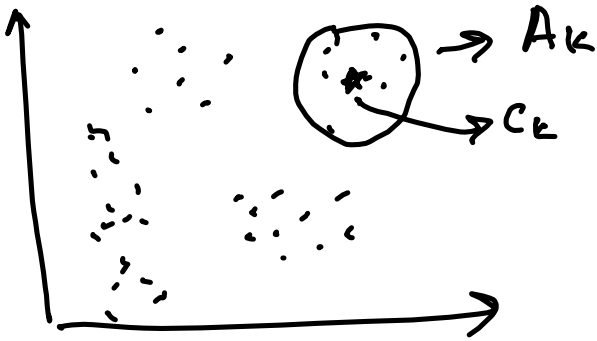
Кластеризация



k-means

$$Q = \sum_{k=1}^{K} \sum_{i: x_i \in A_k} \|x_i - c_k\|^2 \to \min_{c_1, \dots, c_K}$$

$$A_k = \{x_i \mid \rho(x_i, c_k) \le \rho(x_i, c_j) \quad \forall j \neq k\}$$

$i = 1, \dots, n$

$j = 1, \dots, K$

$$Q \to \min_{c_k}$$

$$\sum_{i: x_i \in A_k} \|x_i - c_k\|^2 \to \min_{c_k}$$

$$\|x_i - c_k\|^2 = (x_i^T - c_k^T)(x_i - c_k) =$$

$$= (x_i^T x_i - 2x_i^T c_k + c_k^T c_k)$$

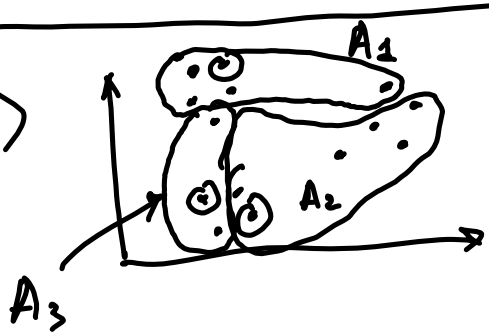
$$\nabla_{c_k} = -2x_i + 2c_k$$

$$\nabla_{c_k} \sum_{i:x_i \in A_k} \|x_i - c_k\|^2 = \sum_{i:x_i \in A_k} (-2x_i + 2c_k) = 0$$

$$-\sum_{i:x_i \in A_k} x_i + |A_k| \cdot c_k = 0$$

$$\boxed{c_k = \frac{1}{|A_k|} \cdot \sum_{i:x_i \in A_k} x_i}$$

1)



2) Пересчитываем центры.

Критерии останова:

1) Число набл. (доля), сменивших кластер.

2) $\| c_k^{old} - c_k^{new} \| < \varepsilon$

3) Изменение Q

$$\left| \frac{Q_{new} - Q_{old}}{Q_{old}} \right|$$

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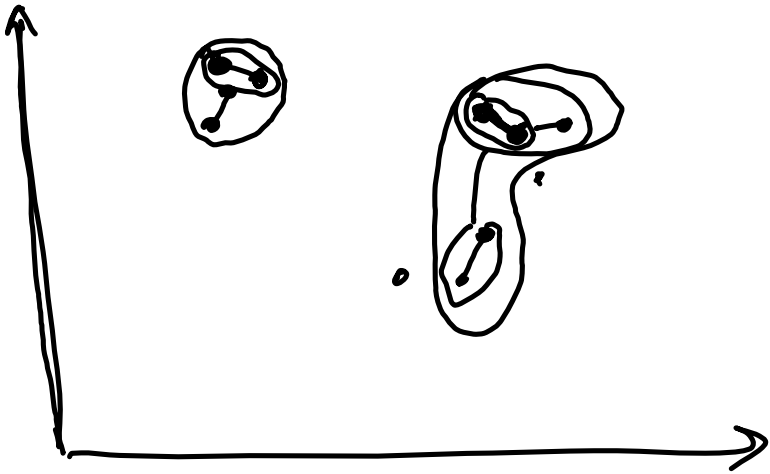
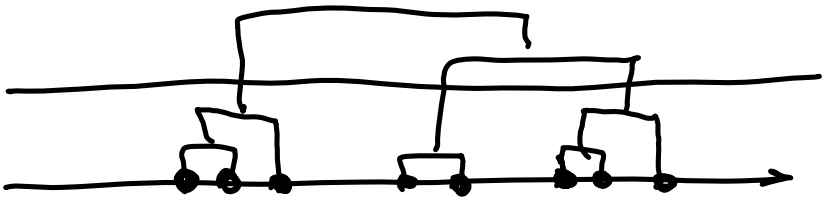
0) $\bar{p}_{внутр.}$, $\bar{p}_{межкл.}$

1) Индекс Дана = Dunn Index $= \frac{\bar{p}_{внутр.}}{\bar{p}_{межкл.}} \to \min$

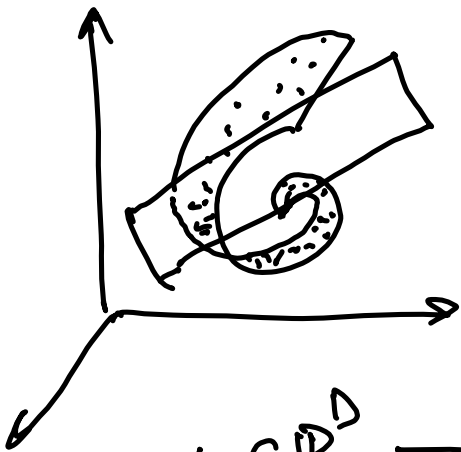
2) $Silouette_i = \frac{-(d(x_i, c_k) - d(x_i, c_{k+1}))}{d(x_i, c_{k+1})}$

$x_i : d(x_i, c_k) < d(x_i, c_{k+1})$





TSNE



$x_i \in \mathbb{R}^D \longrightarrow y_i \in \mathbb{R}^d$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\rho(x_i,x_j)-\rho(y_i,y_j)\right)^2 \to \min_{y_1,\dots,y_n}$$

~~MDS~~

$$\frac{\rho(x_i,x_j)}{\rho(x_i,x_k)} = \alpha \approx \frac{\rho(y_i,y_j)}{\rho(y_i,y_k)}$$

$$p_{j|i} = \frac{\exp\left(-\frac{\|x_i-x_j\|^2}{2\sigma^2}\right)}{\sum_{k\neq j}\exp\left(-\frac{\|x_i-x_k\|^2}{2\sigma^2}\right)}$$

$$p_{ij} = \frac{p_{i|j}+p_{j|i}}{2n}$$

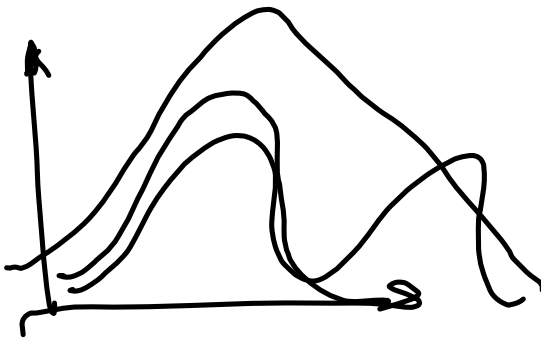
$$q_{ij} = \frac{q_{i|j}+q_{j|i}}{2n}$$

$$q_{j|i} = \frac{\left(1+\|y_i-y_j\|^2\right)^{-1}}{\sum_{k\neq j}\left(1+\|y_i-y_k\|^2\right)^{-1}}$$

$q_{ij} \approx p_{ij}$

$$KL(p \| q) = \int_{\mathbb{R}} p(x) \log \frac{p(x)}{q(x)} dx =$$

$$= E_p\left(\log \frac{p}{q}\right)$$



$$KL(N_1 \| N_2)$$

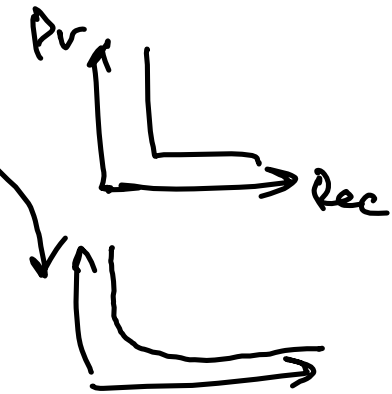
$$N_1 = N(a_1, b^2)$$

$$N_2 = N(a_2, b^2)$$

$$Q = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}} \to \min_{y_1, \dots, y_n}$$

Семинар:

1) $f_1 = \dfrac{2Pr \cdot Rec}{Pr + Rec}$



$\max(\min(Pr, Rec))$

2) AUC-ROC $= TPR(FPR)$

$$TPR = Rec = \frac{\sum_i [y_i = 1] \cdot [a_i = 1]}{\sum_i [y_i = 1]}$$

$$FPR = \frac{\sum_i [y_i = -1] \cdot [a_i = 1]}{\sum_i [y_i = -1]}$$

$$AUC\text{-}ROC = \frac{\sum_i \sum_j [y_i < y_j] \cdot [a_i < a_j]}{\sum_i \sum_j [y_i < y_j]} \quad \sum_i [y_i = -1] = n_+ \cdot n_-$$

3) $\mathbb{E}(AUC\text{-}ROC) = 0.5$

4)

$$\begin{cases} a_k^T \underset{D\times D}{\Sigma} a_k \to \max\limits_{a_k} \\ \|a_k\|^2 = 1 \end{cases}$$

$$\Sigma = \frac{1}{n}\sum_{i=1}^{n} x_i \cdot x_i^T \qquad x_i \in \mathbb{R}^D \qquad a_k \in \mathbb{R}^D$$

5) $x_i \in \mathbb{R}^D$, $A = \underset{D\times d}{\begin{bmatrix} | & & | \\ a_1 & \dots & a_d \\ | & & | \end{bmatrix}}$

$$\hat{x}_i = \underbrace{(A^T A)}_{I_d}{}^{-1} A^T x_i = A^T x_i$$

$\hat{x}_i \in \mathbb{R}^d$, A^T: $d\times D$, x_i: $D\times 1$