智能软件开发
方向基础

第八章 聚类(clustering)
--PART1. 聚类的引入与算法评价

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主要内容

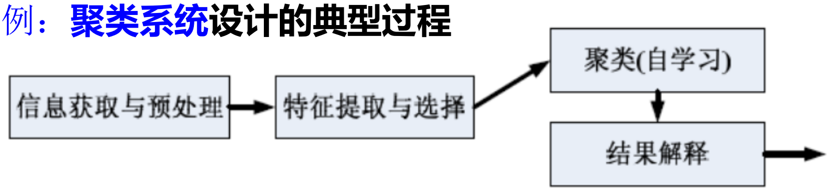
1. 聚类的引入

2. 聚类算法的评价

问题的引入

非监督式学习(密度函数估计、聚类、降维...)

例：**聚类系统设计的典型过程**



适用：

(1)大型数据挖掘：大量未标记数据训练分类器；
人工标记分组结果

(2)揭示观测数据的内在结构特性

(3)是分类或其它学习任务的前驱阶段
提取数据的基本特征，进一步用于分类...

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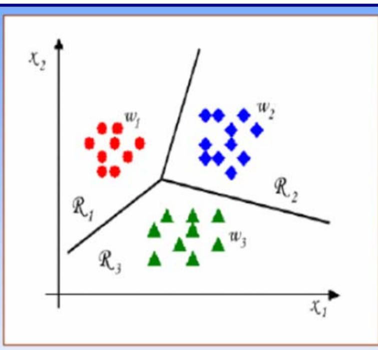
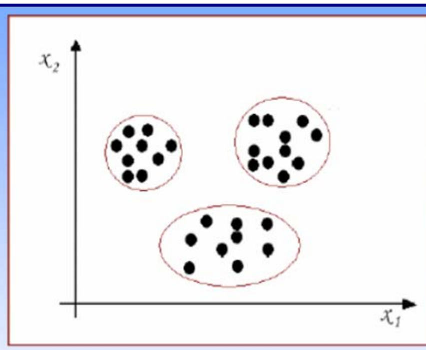
分类(Classification)与聚类(Clustering)



Given labeled training patterns, construct decision boundaries or partition the feature space



Given some patterns, discover the underlying structure (categories) in the data

什么是聚类(clustering)

To find a structure in a collection of unlabeled data.

- ***A loose definition of clustering could be "the process of organizing objects into groups whose members are similar in some way".***

- ***A cluster is therefore a collection of objects which are "similar" between them and are "dissimilar" to the objects belonging to other clusters.***

- ***High intra-class(cluster) similarity(簇内高相似)***
  Low inter-class(cluster) similarity(簇间低相似)

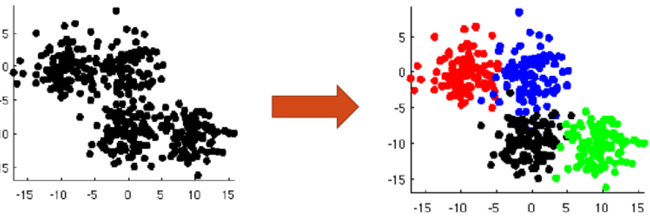
聚类问题的描述

输入： 无标签数据集 $\boldsymbol{D}=\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_N\}, \boldsymbol{x}_i=[x_{i1} \quad \cdots \quad x_{id}]^T \in R^d$

要生成的簇的数目 k

输出： k个互不相交的簇$\{\boldsymbol{C}_l \mid l=1,\dots,k\}$

$$\begin{cases} \boldsymbol{C}_i \bigcap_{i\neq j} \boldsymbol{C}_j = \Phi \\ \bigcup_{l=1}^{k} \boldsymbol{C}_l = \boldsymbol{D} \end{cases}$$



λ_j --样本$\boldsymbol{x}_j \in \boldsymbol{D}$的簇标记，$j\in\{1,2,\dots,k\}$

数据集$\boldsymbol{D}=\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_m\}$的标签集合$\boldsymbol{\lambda}=\{\lambda_1,\dots,\lambda_m\}$

聚类有很多典型应用，如：

- 相似功能的基因分组
- 相似政见的个体划分
- 相似主题的文档划分

…

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聚类任务的遵循步骤及有关问题

- 特征选择及样本描述
  选择什么样的特征？是否需要规范化预处理？
- 近邻测度
  如何度量样本之间的“相似”或“相异”
- 聚类准则
  依赖于专家对“可判别”的解释，聚类准则应以蕴涵于数据集内的类的类型为基础。
- 聚类算法
  选择特定的算法，用于揭示数据集的聚类结构
- 聚类性能评价、结果的解释

近邻测度与聚类准则

A. 向量(点)之间的测度

(1) Dissimilarity Metric

-- dist

$d: \boldsymbol{X} \times \boldsymbol{X} \to \Re$

对于$\forall \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in \boldsymbol{X}$, $dist(\bullet, \bullet)$须满足：

$$\begin{cases} \text{非负性：} \forall \boldsymbol{x}, \boldsymbol{y},\ dist(\boldsymbol{x}, \boldsymbol{y}) \geq 0 \\ \text{同一性：} dist(\boldsymbol{x}, \boldsymbol{y}) = 0 \text{当且仅当} \boldsymbol{x} = \boldsymbol{y} \\ \text{对称性：} dist(\boldsymbol{x}, \boldsymbol{y}) = dist(\boldsymbol{y}, \boldsymbol{x}) \\ \text{直递性：} dist(\boldsymbol{x}, \boldsymbol{y}) \leq dist(\boldsymbol{x}, \boldsymbol{z}) + dist(\boldsymbol{y}, \boldsymbol{z}) \end{cases}$$

(2) Similarity Metric -- s

$s: \boldsymbol{X} \times \boldsymbol{X} \to \Re$

对于$\forall \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in \boldsymbol{X}$, $s(\bullet)$须满足：

$$\begin{cases} \exists s_0 \quad -\infty < s(\boldsymbol{x}, \boldsymbol{y}) \leq s_0 < +\infty \qquad \forall \boldsymbol{x}, \boldsymbol{y} \\ \qquad\qquad s(\boldsymbol{x}, \boldsymbol{x}) = s_0 \\ s(\boldsymbol{x}, \boldsymbol{y}) = s(\boldsymbol{y}, \boldsymbol{x}) \\ s(\boldsymbol{x}, \boldsymbol{z}) s(\boldsymbol{y}, \boldsymbol{z}) \leq [s(\boldsymbol{x}, \boldsymbol{z}) + s(\boldsymbol{y}, \boldsymbol{z})] s(\boldsymbol{x}, \boldsymbol{y}) \end{cases}$$

例：向量之间的几种典型距离度量

有序属性之间的距离

对于$\forall \boldsymbol{x}, \boldsymbol{y} \in \boldsymbol{X} \subset \boldsymbol{R}^n \qquad \boldsymbol{x} = [x_1 \ \cdots \ x_n]^T \quad \boldsymbol{y} = [y_1 \ \cdots \ y_n]^T$

A. 闵可夫斯基距离 (*Minkowski distance*)

$$dist_{mk}(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_p = \left(\sum_{i=1}^{n} |x_i - y_i|^p \right)^{\frac{1}{p}}$$

加权闵可夫斯基距离 (*Weighted Minkowski distance*)

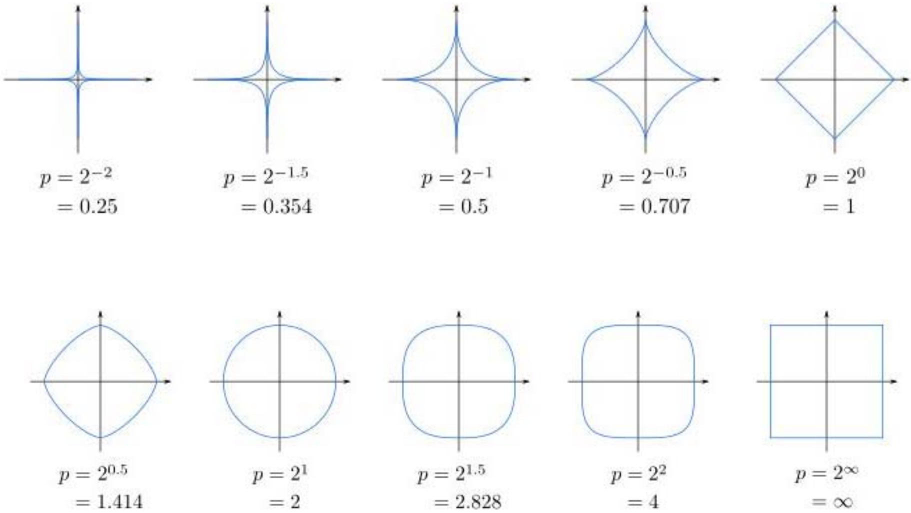
$$dist_{wmk}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \left(\sum_{u=1}^{n} w_u |x_{iu} - x_{ju}|^p \right)^{\frac{1}{p}}$$

$$w_u \geq 0, \qquad \sum_{u=1}^{n} w_u = 1$$

B. 曼哈顿距离 (*Manhattan distance*) $\quad dist_{man}(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_1 = \sum_{i=1}^{n} |x_i - y_i|$

例：不同p值下，平面坐标系内到原点的距离为1的点的轨迹

$$\{\boldsymbol{x} \mid \|\boldsymbol{x}\|_p = 1\}$$



对于$\forall \boldsymbol{x}, \boldsymbol{y} \in \boldsymbol{X} \subset \boldsymbol{R}^n \quad \boldsymbol{x} = [x_1 \ \cdots \ x_n]^T \ \ \boldsymbol{y} = [y_1 \ \cdots \ y_n]^T$

B. 曼哈顿距离(*Manhattan distance*)

$$dist_{man}(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_1 = \sum_{i=1}^{n} |x_i - y_i|$$

C. 欧式距离(*Eculidean distance*)

$$dist_{ed}(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_2 = \left(\sum_{i=1}^{n} |x_i - y_i|^2\right)^{\frac{1}{2}}$$

D. 切氏距离(*Chebyshev distance*)

$$dist_{che}(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_\infty = \max_{1 \le i \le n} |x_i - y_i|$$

E. 马氏距离(*Mahalanobis distance*)

$$d_{mah}(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{(\boldsymbol{x} - \boldsymbol{y})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{y})}$$

F. Camberra距离(*Lance* 距离,*Williams* 距离)

$$dist_{cam}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{n} \frac{|x_i - y_i|}{|x_i + y_i|} \qquad x_i, y_i \ge 0 且 x_i + y_i \ne 0$$

例：向量之间的几种典型距离度量

无序属性之间的距离

$m_{u,a}$ ——样本集内关于特征u取离散值a的样本数

$m_{u,a,i}$ ——样本集的第i簇中，特征u上取离散值为a的样本数

k ——样本集划分的聚类簇数目

[1]若描述样本的特征为d个离散特征，对于任意两个样本$\boldsymbol{x}_i, \boldsymbol{x}_j$

基于特征**VDM距离**，可以得到样本$\boldsymbol{x}_i, \boldsymbol{x}_j$之间距离：

$$\boldsymbol{MinkovDM}_p\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)=\left(\sum_{u=1}^{\mathrm{d}} \boldsymbol{VDM}_p\left(x_{iu}, x_{ju}\right)\right)^{\frac{1}{p}}$$

其中：特征u的两个离散值a,b之间的**VDM距离**$(Value\ \ Difference\ \ Metric)$

$$\boldsymbol{VDM}_p(a,b)=\sum_{i=1}^{k}\left|\frac{m_{u,a,i}}{m_{u,a}}-\frac{m_{u,b,i}}{m_{u,b}}\right|^p$$

[2]基于混合属性(d_c个有序属性以及$d-d_{\mathrm{c}}$个无序属性) 的样本之间距离

$$\boldsymbol{MinkovDM}_p\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)=\left(\sum_{u=1}^{d_c}\left|x_{iu}-x_{ju}\right|^p+\sum_{u=d_c+1}^{d} \boldsymbol{VDM}_p\left(x_{iu}, x_{ju}\right)\right)^{\frac{1}{p}}$$

例：向量之间的相似性度量

对于$\forall \boldsymbol{x}, \boldsymbol{y} \in \boldsymbol{X} \subset \boldsymbol{R}^n$ $\quad \boldsymbol{x} = [x_1 \ \cdots \ x_n]^T \quad \boldsymbol{y} = [y_1 \ \cdots \ y_n]^T$

A. 内积 $\quad s_{inner}(\boldsymbol{x}, \boldsymbol{y}) = \langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^T \boldsymbol{y} = \sum_{i=1}^{n} x_i y_i$

B. 余弦相似度 $\quad s_{\cos ine}(\boldsymbol{x}, \boldsymbol{y}) = \dfrac{\boldsymbol{x}^T \boldsymbol{y}}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|}$（**注意区分余弦距离**）

C. Pearson相关系数 $\quad r_{Pearson}(\boldsymbol{x}, \boldsymbol{y}) = \dfrac{(\boldsymbol{x} - \bar{x}\boldsymbol{1})^T (\boldsymbol{y} - \bar{y}\boldsymbol{1})}{\|\boldsymbol{x} - \bar{\boldsymbol{x}}\| \|\boldsymbol{y} - \bar{\boldsymbol{y}}\|}$

其中 $\quad \bar{x} = \dfrac{\sum_{i=1}^{n} x_i}{n} \quad \bar{y} = \dfrac{\sum_{i=1}^{n} y_i}{n}$

D. Tanimoto测度 $\quad s_T(\boldsymbol{x}, \boldsymbol{y}) = \dfrac{\boldsymbol{x}^T \boldsymbol{y}}{\|\boldsymbol{x}\|^2 + \|\boldsymbol{y}\|^2 - \boldsymbol{x}^T \boldsymbol{y}} = \dfrac{\boldsymbol{x}^T \boldsymbol{y}}{\|x - y\|^2 + \boldsymbol{x}^T \boldsymbol{y}}$

B. 样本与集合之间的测度

方式1.集合中所有样本对近邻测度$\wp(\boldsymbol{x}, \boldsymbol{C})$均有贡献。

设观测样本$\boldsymbol{x}, \boldsymbol{y}$之间近邻测度为$\wp(\boldsymbol{x}, \boldsymbol{y})$

则样本$\boldsymbol{x}$与聚类（或簇）C之间的近邻函数$\wp(\boldsymbol{x}, \boldsymbol{C})$，可以是：

最大近邻函数 $\quad \wp_{\max}^{ps}(\boldsymbol{x}, \boldsymbol{C}) = \max_{\boldsymbol{y} \in \boldsymbol{C}} \wp(\boldsymbol{x}, \boldsymbol{y})$

最小近邻函数 $\quad \wp_{\min}^{ps}(\boldsymbol{x}, \boldsymbol{C}) = \min_{\boldsymbol{y} \in \boldsymbol{C}} \wp(\boldsymbol{x}, \boldsymbol{y})$

平均近邻函数 $\quad \wp_{\text{avg}}^{ps}(\boldsymbol{x}, \boldsymbol{C}) = \dfrac{1}{n_C} \sum_{\boldsymbol{y} \in \boldsymbol{C}} \wp(\boldsymbol{x}, \boldsymbol{y}) \qquad n_C$为集合$C$的势

方式2.近邻性以样本x与集合C的表示之间的近邻性度量。

--集合的表示通常有点、超平面、超球面等.

C. 两集合之间的近邻函数

设两观测样本$\boldsymbol{x}, \boldsymbol{y}$之间近邻测度为$\mathscr{D}(\boldsymbol{x}, \boldsymbol{y})$

对于给定的两个向量集合$\boldsymbol{D}_i, \boldsymbol{D}_j$,近邻函数常见：

最大近邻函数 $\mathscr{D}_{\max}^{ss}\left(\boldsymbol{D}_i, \boldsymbol{D}_j\right)=\max\limits_{\boldsymbol{x}\in\boldsymbol{D}_i, \boldsymbol{y}\in\boldsymbol{D}_j} \mathscr{D}(\boldsymbol{x}, \boldsymbol{y})$

最小近邻函数 $\mathscr{D}_{\min}^{ss}\left(\boldsymbol{D}_i, \boldsymbol{D}_j\right)=\min\limits_{\boldsymbol{x}\in\boldsymbol{D}_i, \boldsymbol{y}\in\boldsymbol{D}_j} \mathscr{D}(\boldsymbol{x}, \boldsymbol{y})$

平均近邻函数 $\mathscr{D}_{avg}^{ss}\left(\boldsymbol{D}_i, \boldsymbol{D}_j\right)=\dfrac{1}{n_{D_i} n_{D_j}} \sum\limits_{\boldsymbol{x}\in\boldsymbol{D}_i} \sum\limits_{\boldsymbol{y}\in\boldsymbol{D}_j} \mathscr{D}(\boldsymbol{x}, \boldsymbol{y})$

其中$n_{D_i} n_{D_j}$为集合$\boldsymbol{D}_i, \boldsymbol{D}_j$的势

均值近邻函数 $\mathscr{D}_{mean}^{ss}\left(\boldsymbol{D}_i, \boldsymbol{D}_j\right)=\mathscr{D}\left(\boldsymbol{m}_{D_i}, \boldsymbol{m}_{D_j}\right)$

$\boldsymbol{m}_{D_i}, \boldsymbol{m}_{D_j}$是关于集合$\boldsymbol{D}_i, \boldsymbol{D}_j$的点描述，如均值点、中值等。

D. 聚类准则

- 类内距离准则
- 类间距离准则
- 基于类内、类间距离的准则函数
- 基于模式与类核的距离的准则函数

主要内容

1. 聚类的引入

2. 聚类算法的评价

评价的意义

(1)避免所发现的数据结构源自噪声干扰

(2)不同聚类算法的比较

(3)两个聚类集合(**two sets of clusters**)的比较

(4)两个聚类的比较

--> **聚类趋向：验证给定数据集是否具有聚类结构；发现数据中真实的结构**

评价的几个角度

- 明确给定数据集合中“聚类的趋势”
  如：区分给定数据集内是否存在非随机性“结构”

- “外部评价”--将聚类分析的结果与给定的结果(带有类别标签的专门数据)比较

- “内部评价”--评估聚类分析的结果是否与数据结构相符，而无需参考外部信息- 只借助数据本身

- 比较不同聚类算法的分析结果，以确定哪种聚类算法更好

- 确定正确的“聚类数目”

评价的几种类型(*types of validation measures*)

(1)外部评价(*external validation*)

需要关于研究对象相关领域的先验知识

如：一个预定义的划分

不足 强化了研究者的主观猜测；
会忽略某些与之前认识不符的现象；
导致错过发现新规律新模式的机会

(2)内部评价(*internal validation*)

基于数据本身内在的信息，量化分析

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外部评价的一些常见指标

Clustering metrics

See the Clustering performance evaluation section of the user guide for further details.

The `sklearn.metrics.cluster` submodule contains evaluation metrics for cluster analysis results. There are two forms of evaluation:

- supervised, which uses a ground truth class values for each sample.
- unsupervised, which does not and measures the 'quality' of the model itself.

`metrics.adjusted_mutual_info_score`(...[, ...])	Adjusted Mutual Information between two clusterings.
`metrics.adjusted_rand_score`(labels_true, ...)	Rand index adjusted for chance.
`metrics.calinski_harabasz_score`(X, labels)	Compute the Calinski and Harabasz score.
`metrics.davies_bouldin_score`(X, labels)	Compute the Davies-Bouldin score.
`metrics.completeness_score`(labels_true, ...)	Completeness metric of a cluster labeling given a ground truth.
`metrics.cluster.contingency_matrix`(...[, ...])	Build a contingency matrix describing the relationship between labels.
`metrics.cluster.pair_confusion_matrix`(...)	Pair confusion matrix arising from two clusterings.
`metrics.fowlkes_mallows_score`(labels_true, ...)	Measure the similarity of two clusterings of a set of points.
`metrics.homogeneity_completeness_v_measure`(...)	Compute the homogeneity and completeness and V-Measure scores at once.
`metrics.homogeneity_score`(labels_true, ...)	Homogeneity metric of a cluster labeling given a ground truth.
`metrics.mutual_info_score`(labels_true, ...)	Mutual Information between two clusterings.
`metrics.normalized_mutual_info_score`(...[, ...])	Normalized Mutual Information between two clusterings.
`metrics.rand_score`(labels_true, labels_pred)	Rand index.
`metrics.silhouette_score`(X, labels, *[, ...])	Compute the mean Silhouette Coefficient of all samples.
`metrics.silhouette_samples`(X, labels, *[, ...])	Compute the Silhouette Coefficient for each sample.
`metrics.v_measure_score`(labels_true, ...[, beta])	V-measure cluster labeling given a ground truth.

给定数据集$\boldsymbol{D}=\{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N\}, \boldsymbol{x}_i=[x_{i1} \quad \cdots \quad x_{id}]^T \in \boldsymbol{R}^d$

若 $\begin{cases} \text{由聚类算法给出的簇划分结果} & \boldsymbol{C}=\{\boldsymbol{C}_1,\ldots,\boldsymbol{C}_r\} \\ \text{参考模型给出的簇划分结果} & \boldsymbol{C}^*=\{\boldsymbol{C}_1^*,\ldots,\boldsymbol{C}_s^*\} \end{cases}$

数据集$\boldsymbol{D}$内各样本相应簇标记值集合 $\begin{cases} \boldsymbol{\lambda}=\{\lambda_1,\ldots,\lambda_N\} \\ \boldsymbol{\lambda}^*=\{\lambda_1^*,\ldots,\lambda_N^*\} \end{cases}$

数据集$\boldsymbol{D}$内样本两两配对，定义：

$$a=|\boldsymbol{SS}| \qquad \boldsymbol{SS}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i=\lambda_j, \lambda_i^*=\lambda_j^*, i<j\}$$

$$b=|\boldsymbol{SD}| \qquad \boldsymbol{SD}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i=\lambda_j, \lambda_i^*\neq\lambda_j^*, i<j\}$$

$$c=|\boldsymbol{DS}| \qquad \boldsymbol{DS}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i\neq\lambda_j, \lambda_i^*=\lambda_j^*, i<j\}$$

$$d=|\boldsymbol{DD}| \qquad \boldsymbol{DD}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i\neq\lambda_j, \lambda_i^*\neq\lambda_j^*, i<j\}$$

并且 $\begin{cases} \boldsymbol{A}=\boldsymbol{SS}\cup\boldsymbol{SD}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i=\lambda_j, i<j\} \\ \boldsymbol{B}=\boldsymbol{SS}\cup\boldsymbol{DS}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i^*=\lambda_j^*, i<j\} \end{cases}$ $\quad |\boldsymbol{A}\cap\boldsymbol{B}|=a, |\boldsymbol{A}\cup\boldsymbol{B}|=a+b+c$

$$d=|\boldsymbol{DD}|=C_N^2+\sum_{i=1}^{r}\sum_{j=1}^{s}C_{n_{ij}}^2-\sum_{i=1}^{r}C_{a_i}^2-\sum_{j=1}^{s}C_{b_j}^2 =\frac{1}{2}\left[N^2+\sum_{i=1}^{r}\sum_{j=1}^{s}n_{ij}^2-\sum_{i=1}^{r}a_i^2-\sum_{j=1}^{s}b_j^2\right]$$

$$a=|\boldsymbol{SS}|=\sum_{i=1}^{r}\sum_{j=1}^{s}C_{n_{ij}}^2 =\sum_{i=1}^{r}\sum_{j=1}^{s}\frac{1}{2}n_{ij}(n_{ij}-1)$$

$$b=|\boldsymbol{SD}|=\sum_{j=1}^{s}C_{b_j}^2-\sum_{i=1}^{r}\sum_{j=1}^{s}C_{n_{ij}}^2 =\frac{1}{2}\left[\sum_{j=1}^{s}b_j^2-\sum_{i=1}^{r}\sum_{j=1}^{s}n_{ij}^2\right]$$

$$c=|\boldsymbol{DS}|=\sum_{i=1}^{r}C_{a_i}^2-\sum_{i=1}^{r}\sum_{j=1}^{s}C_{n_{ij}}^2 =\frac{1}{2}\left[\sum_{i=1}^{r}a_i^2-\sum_{i=1}^{r}\sum_{j=1}^{s}n_{ij}^2\right]$$

$$\boxed{\begin{aligned} &a+b+c+d=C_N^2 \\ &a+d=\sum_{i=1}^{r}\sum_{j=1}^{s}n_{ij}^2+C_N^2-\frac{1}{2}\left[\sum_{i=1}^{r}a_i^2+\sum_{j=1}^{s}b_j^2\right] \\ &b+c=\frac{1}{2}\left[\sum_{i=1}^{r}a_i^2+\sum_{j=1}^{s}b_j^2\right]-\sum_{i=1}^{r}\sum_{j=1}^{s}n_{ij}^2 \end{aligned}}$$

$$\begin{cases} \boldsymbol{A}=\boldsymbol{SS}\cup\boldsymbol{SD}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i=\lambda_j, i<j\} \\ \boldsymbol{B}=\boldsymbol{SS}\cup\boldsymbol{DS}=\{(\boldsymbol{x}_i,\boldsymbol{x}_j) \mid \lambda_i^*=\lambda_j^*, i<j\} \\ |\boldsymbol{A}\cap\boldsymbol{B}|=a \\ |\boldsymbol{A}\cup\boldsymbol{B}|=a+b+c \end{cases}$$

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基于上述定义，给出用于聚类性能度量的常见**外部指标**

[1] ***Jaccard*** 系数（***Jaccard Coefficient***，简称 ***JC***，雅卡尔系数）

$$JC=\frac{|A\cap B|}{|A\cup B|}=\frac{a}{a+b+c}\in[0,1]$$

Jaccard 距离（***Jaccard Distance***，简称 ***JD***）　$JD=1-JC$

[2] ***FM*** 指数（***Fowlkes and Mallows Index***，简称 ***FMI***）

$$FMI=\sqrt{\frac{a}{a+b}\cdot\frac{a}{a+c}}\in[0,1]$$

*sklearn.metrics.**fowlkes_mallows_score**(labels_true, labels_pred, *, sparse=False)*

[3] ***Rand*** 指数（***Rand Index***，简称 ***RI***）

$$RI=\frac{a+d}{a+b+c+d}=\frac{2(a+d)}{N(N-1)}\in[0,1]$$

[4] 调整后的 ***Rand*** 指数（***Ajusted Rand Index***，简称 ***ARI***）

$X \backslash Y$	簇标签 Y_1	Y_2	$\ldots$	Y_s	Sums
真 X_1	n_{11}	n_{12}	$\ldots$	n_{1s}	a_1
实 X_2	n_{21}	n_{22}	$\ldots$	n_{2s}	a_2
标 $\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
签 X_r	n_{r1}	n_{r2}	$\ldots$	n_{rs}	a_r
Sums	b_1	b_2	$\ldots$	b_s	

为确保"在聚类结果随机产生的情况下，指标应该接近零"，引入调整兰德系数(Adjusted rand index)，以获取更高的区分度

列联表(contingency table)

n_{ij}----真实类别标签为i、簇标签为j的样本数目

总的样本数 $N=\sum_i\sum_j n_{ij}$

a_i———真实标签为i的样本数目，$a_i=\sum_j n_{ij}$

b_j———簇标签为j的样本数目，　$b_j=\sum_i n_{ij}$

$$ARI = \frac{RI - E[RI]}{max[RI] - E[RI]} = \frac{\sum_i \sum_j C_{n_{ij}}^2 - \frac{\sum_i C_{a_i}^2 \sum_j C_{b_j}^2}{C_N^2}}{\frac{1}{2}\left[\sum_i C_{a_i}^2 + \sum_j C_{b_j}^2\right] - \frac{\sum_i C_{a_i}^2 \sum_j C_{b_j}^2}{C_N^2}}$$

$$RI = \frac{\sum_i \sum_j C_{n_{ij}}^2}{C_N^2}$$

注意： $C_0^2 = C_1^2 = 1$

$$E[RI] = \left(\frac{\sum_i C_{a_i}^2}{C_N^2}\right)\left(\frac{\sum_j C_{b_j}^2}{C_N^2}\right)$$

$$E\left[\sum_i \sum_j C_{n_{ij}}^2\right] = \frac{\sum_i C_{a_i}^2 \sum_j C_{b_j}^2}{C_N^2}$$

$$max[RI] = \frac{1}{2}\left[\frac{\sum_i C_{a_i}^2 + \sum_j C_{b_j}^2}{C_N^2}\right]$$

		簇标签				
	$X \backslash Y$	Y_1	Y_2	$\dots$	Y_s	Sums
真	X_1	n_{11}	n_{12}	$\dots$	n_{1s}	a_1
实	X_2	n_{21}	n_{22}	$\dots$	n_{2s}	a_2
标	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
签	X_r	n_{r1}	n_{r2}	$\dots$	n_{rs}	a_r
	Sums	b_1	b_2	$\dots$	b_s	

sklearn.metrics.adjusted_rand_score(*labels_true*,*labels_pred*

[5]完整性(*Completeness*)

- 该指标最大值为1.
- 越接近1，越好。

$$Completeness = 1 - \frac{H(\lambda|C)}{H(\lambda)} = 1 - \frac{-\sum_i \frac{a_i}{N} \sum_j \frac{n_{ij}}{a_i} log\left(\frac{n_{ij}}{a_i}\right)}{-\sum_j \frac{b_j}{N} log\left(\frac{b_j}{N}\right)}$$

簇划分熵

以类别为条件的簇划分熵

		簇标签				
	$X \backslash Y$	Y_1	Y_2	$\dots$	Y_s	Sums
真	X_1	n_{11}	n_{12}	$\dots$	n_{1s}	a_1
实	X_2	n_{21}	n_{22}	$\dots$	n_{2s}	a_2
标	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
签	X_r	n_{r1}	n_{r2}	$\dots$	n_{rs}	a_r
	Sums	b_1	b_2	$\dots$	b_s	

对于一种聚类结果，如果来自同类的样本都聚为同一簇，就说这种聚类结果满足完整性。

*sklearn.metrics.**completeness_score**(labels_true, labels_pred)*

[6]同质性(***homogeneity***)

➢ 该指标最大值为1.
➢ 越接近1，越好。

$$Homogeneity = 1 - \frac{H(C|\lambda)}{H(C)} = 1 - \frac{-\sum_j \frac{b_j}{N}\sum_i \frac{n_{ij}}{b_j} log\left(\frac{n_{ij}}{b_j}\right)}{-\sum_i \frac{a_i}{N} log\left(\frac{a_i}{N}\right)}$$

类划分熵

以簇划分为条件的类划分熵

X \ Y	簇标签 Y_1	Y_2	$\ldots$	Y_s	Sums
真 X_1	n_{11}	n_{12}	$\ldots$	n_{1s}	a_1
实 X_2	n_{21}	n_{22}	$\ldots$	n_{2s}	a_2
标 $\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
签 X_r	n_{r1}	n_{r2}	$\ldots$	n_{rs}	a_r
Sums	b_1	b_2	$\ldots$	b_s	

对于一种聚类结果，如果聚为同一簇的样本都来自相同类，就说这种聚类结果满足**同质性**。

sklearn.metrics. homogeneity _score(labels_true, labels_pred)

[7]***V - Measure***

$$V = \frac{1}{\frac{\beta}{1+\beta} \times \frac{1}{completeness} + \frac{1}{1+\beta} \times \frac{1}{\mathrm{homogeneity}}} = \frac{(1+\beta) \times \mathrm{homogeneity} \times completeness}{\beta \times \mathrm{homogeneity} + completeness}$$

X \ Y	簇标签 Y_1	Y_2	$\ldots$	Y_s	Sums
真 X_1	n_{11}	n_{12}	$\ldots$	n_{1s}	a_1
实 X_2	n_{21}	n_{22}	$\ldots$	n_{2s}	a_2
标 $\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
签 X_r	n_{r1}	n_{r2}	$\ldots$	n_{rs}	a_r
Sums	b_1	b_2	$\ldots$	b_s	

➢ 是关于完整性、同质性的调和平均
➢ 该指标最大值为1.
➢ 越接近1，越好。

*sklearn.metrics.v_measure_score(labels_true, labels_pred, *, beta=1.0)*

[8]标准互信息($Normalized\ Mutual\ Infomation, NMI$)

用于衡量基于聚类的数据划分结果与类别分布的吻合程度。
由表可得两种信息熵:

➢ 类别分布的信息熵

$$H(C) = -\sum_{i=1}^{r} P_i log P_i$$
$$= -\sum_{i=1}^{r} \frac{a_i}{N} log\left(\frac{a_i}{N}\right)$$

➢ 簇分布的信息熵

$$H(J) = -\sum_{j=1}^{s} q_j log q_j$$
$$= -\sum_{j=1}^{s} \frac{b_j}{N} log\left(\frac{b_j}{N}\right)$$

X \ Y		簇标签 Y_1	Y_2	$\ldots$	Y_s	Sums
真	X_1	n_{11}	n_{12}	$\ldots$	n_{1s}	a_1
实	X_2	n_{21}	n_{22}	$\ldots$	n_{2s}	a_2
标	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
签	X_r	n_{r1}	n_{r2}	$\ldots$	n_{rs}	a_r
Sums		b_1	b_2	$\ldots$	b_s	

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类别分布与簇标签分布之间的互信息:

$$\mathrm{MI}(C,J) = -\sum_{i=1}^{r}\sum_{j=1}^{s} P(i,j) log\frac{P(i,j)}{p_i q_j}$$
$$= -\sum_{i=1}^{r}\sum_{j=1}^{s} \frac{n_{ij}}{N} log\frac{\frac{n_{ij}}{N}}{\frac{a_i}{N}\frac{b_j}{N}} = -\sum_{i=1}^{r}\sum_{j=1}^{s} \frac{n_{ij}}{N} log\frac{n_{ij}N}{b_j a_i}$$

➢ NMI取值区间[0,1]
➢ 该指标最大值为1.
➢ 越接近1，越好。

标准互信息:

$$\mathrm{NMI}(C,J) = \frac{\mathrm{MI}(C,J)}{\sqrt{H(C)H(J)}}$$

X \ Y		簇标签 Y_1	Y_2	$\ldots$	Y_s	Sums
真	X_1	n_{11}	n_{12}	$\ldots$	n_{1s}	a_1
实	X_2	n_{21}	n_{22}	$\ldots$	n_{2s}	a_2
标	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
签	X_r	n_{r1}	n_{r2}	$\ldots$	n_{rs}	a_r
Sums		b_1	b_2	$\ldots$	b_s	

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[9]调整后的互信息($\boldsymbol{Adjusted\ Mutual\ Infomation}, AMI$)

AMI取值位于区间[-1,1]，取值越大越好。

若 $\mathrm{NMI}(C,J)=\dfrac{\mathrm{MI}(C,J)}{\frac{H(C)+H(J)}{2}}$， 则 $\mathrm{AMI}=\dfrac{MI-E[MI]}{\frac{H(C)+H(J)}{2}-E[MI]}$

若 $\mathrm{NMI}(C,J)=\dfrac{\mathrm{MI}(C,J)}{\sqrt{H(C)H(J)}}$， 则 $\mathrm{AMI}=\dfrac{MI-E[MI]}{\sqrt{H(C)H(J)}-E[MI]}$

若 $\mathrm{NMI}(C,J)=\dfrac{\mathrm{MI}(C,J)}{\max\{H(C),H(J)\}}$， 则 $\mathrm{AMI}=\dfrac{MI-E[MI]}{\max\{H(C),H(J)\}-E[MI]}$

		簇标签				
	$X \diagdown Y$	Y_1	Y_2	$\dots$	Y_s	Sums
真实标签	X_1	n_{11}	n_{12}	$\dots$	n_{1s}	a_1
	X_2	n_{21}	n_{22}	$\dots$	n_{2s}	a_2
	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
	X_r	n_{r1}	n_{r2}	$\dots$	n_{rs}	a_r
	Sums	b_1	b_2	$\dots$	b_s	

$$E[MI(C,J)]=\sum_{i=1}^{r}\sum_{j=1}^{s}\left\{\sum_{n_{ij}=max\{0,a_i+b_j-N\}}^{min\{a_i,b_j\}}\frac{n_{ij}}{N}log\left(\frac{n_{ij}N}{b_ja_i}\right)P\left(\boldsymbol{Table}|a_i,b_j,n_{ij}\right)\right\}$$

$$=\sum_{i=1}^{r}\sum_{j=1}^{s}\left\{\sum_{n_{ij}=max\{0,a_i+b_j-N\}}^{min\{a_i,b_j\}}\frac{n_{ij}}{N}log\left(\frac{n_{ij}N}{b_ja_i}\right)\frac{a_i!b_j!(N-a_i)!(N-b_j)!}{N!n_{ij}!(a_i-n_{ij})!(b_j-n_{ij})!(N-a_i-b_j+n_{ij})!}\right\}$$

$$P\left(\boldsymbol{Table}|a_i,b_j,n_{ij}\right)$$

$$=\frac{C_N^{n_{ij}}C_{N-n_{ij}}^{b_j-n_{ij}}C_{N-n_{ij}}^{a_i-n_{ij}}}{C_N^{a_i}C_N^{b_j}}$$

$$=\frac{a_i!\,b_j!\,(N-a_i)!\,(N-b_j)!}{N!\,n_{ij}!\,(a_i-n_{ij})!\,(b_j-n_{ij})!\,(N-a_i-b_j+n_{ij})!}$$

		簇标签				
	$X \diagdown Y$	Y_1	Y_2	$\dots$	Y_s	Sums
真实标签	X_1	n_{11}	n_{12}	$\dots$	n_{1s}	a_1
	X_2	n_{21}	n_{22}	$\dots$	n_{2s}	a_2
	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
	X_r	n_{r1}	n_{r2}	$\dots$	n_{rs}	a_r
	Sums	b_1	b_2	$\dots$	b_s	

$$MI(C,J)\le min\{H(C),H(J)\}\le\sqrt{H(C)H(J)}\le\frac{H(C)+H(J)}{2}\le max\{H(C),H(J)\}\le H(C,J)$$

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内部评价的一些常见评价指标

Clustering metrics

See the Clustering performance evaluation section of the user guide for further details.

The `sklearn.metrics.cluster` submodule contains evaluation metrics for cluster analysis results. There are two forms of evaluation:

- supervised, which uses a ground truth class values for each sample.
- unsupervised, which does not and measures the 'quality' of the model itself.

`metrics.adjusted_mutual_info_score`(…[, …])	Adjusted Mutual Information between two clusterings.
`metrics.adjusted_rand_score`(labels_true, …)	Rand index adjusted for chance.
`metrics.calinski_harabasz_score`(X, labels)	Compute the Calinski and Harabasz score.
`metrics.davies_bouldin_score`(X, labels)	Compute the Davies-Bouldin score.
`metrics.completeness_score`(labels_true, …)	Completeness metric of a cluster labeling given a ground truth.
`metrics.cluster.contingency_matrix`(…[, …])	Build a contingency matrix describing the relationship between labels.
`metrics.cluster.pair_confusion_matrix`(…)	Pair confusion matrix arising from two clusterings.
`metrics.fowlkes_mallows_score`(labels_true, …)	Measure the similarity of two clusterings of a set of points.
`metrics.homogeneity_completeness_v_measure`(…)	Compute the homogeneity and completeness and V-Measure scores at once.
`metrics.homogeneity_score`(labels_true, …)	Homogeneity metric of a cluster labeling given a ground truth.
`metrics.mutual_info_score`(labels_true, …)	Mutual Information between two clusterings.
`metrics.normalized_mutual_info_score`(…[, …])	Normalized Mutual Information between two clusterings.
`metrics.rand_score`(labels_true, labels_pred)	Rand index.
`metrics.silhouette_score`(X, labels, *[, …])	Compute the mean Silhouette Coefficient of all samples.
`metrics.silhouette_samples`(X, labels, *[, …])	Compute the Silhouette Coefficient for each sample.
`metrics.v_measure_score`(labels_true, …[, beta])	V-measure cluster labeling given a ground truth.

给定数据集$D=\{x_1,\ldots,x_m\}, x_i=[x_{i1} \ \cdots \ x_{id}]^T \in R^d$

若由聚类给出的簇划分结果 $\mathcal{C}=\{C_1,\ldots,C_k\}$

并且 $\begin{cases} dist(\cdot,\cdot) \text{——两样本点之间距离} \\ \mu=\frac{1}{|C|}\sum_{x\in C} x \text{——任意簇} C\in\mathcal{C} \text{的中心点.} \end{cases}$

$\forall C\in\mathcal{C},$
簇C内样本间的平均距离

$$avg(C)=\frac{2}{|C|(|C|-1)}\sum_{1\le i<j\le|C|} dist(x_i,x_j)$$

簇C内样本间的最远距离

$$diam(C)=\max_{1\le i<j\le|C|} dist(x_i,x_j)$$

簇C_i,C_j样本间最近距离 $d_{\min}(C_i,C_j)=\min_{x_i\in C_i,x_j\in C_j} dist(x_i,x_j)$

簇C_i,C_j中心点之间距离 $d_{\text{cen}}(C_i,C_j)=dist(\mu_i,\mu_j)$

基于上述定义，给出用于聚类性能度量的常见**内部指标**

sklearn.metrics.davies_bouldin_score(X, labels)

[1] DBI ($Davies-Bouldin\ \ Index$, 戴维森-堡丁指数)

$$DBI=\frac{1}{k}\sum_{i=1}^{k}\max_{j\neq i}\left(\frac{avg(C_i)+avg(C_j)}{d_{\text{cen}}(C_i,C_j)}\right)$$

DBI值越小越好.

对于每个给定类别i，找到与其它类之间的最大比值

$$avg(C)=\frac{2}{|C|(|C|-1)}\sum_{1\le i<j\le|C|} dist(x_i,x_j)$$

$$d_{\text{cen}}(C_i,C_j)=dist(\mu_i,\mu_j)$$

$[2]$方差比$\begin{pmatrix} \textbf{Calinski and Harabasz score}, \\ \textbf{Variance Ratio Criterion} \end{pmatrix}$

$$\textbf{Variance Ratio Criterion} = \frac{\textbf{the within} - \textbf{cluster dispersion}}{\textbf{the between} - \textbf{cluster dispersion}}$$

$\textbf{Variance Ratio Criterion} \geq 0$，该值越小越好。

sklearn.metrics.calinski_harabasz_score(X, labels)

$[3]$ **Dunn**指数(**Dunn Index**, 简称**DI**)

$$\boldsymbol{DI} = \min_{1 \leq \boldsymbol{i} \leq \boldsymbol{k}} \left(\frac{\min_{j \neq i} \boldsymbol{d}_{\min}\left(\boldsymbol{C}_i, \boldsymbol{C}_j\right)}{\max_{1 \leq \boldsymbol{l} \leq \boldsymbol{k}} \boldsymbol{diam}\left(\boldsymbol{C}_l\right)} \right) \qquad \boldsymbol{DI} \in [0, \infty)$$

DI值越大越好.

minimal intercluster distance

maximal intracluster distance

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[4](平均)Silhouette宽度(average Silhouette width)

A. Silhouette值--样本x_i的Silhouette宽度--**基于样本**

sklearn.metrics.silhouette_samples(X, labels, *, metric='euclidean', **kwds)

$$S_i=\frac{b_i-a_i}{\max\{b_i,a_i\}}\qquad S_i\in[-1,1]$$

a_i--样本x_i与同类中其它样本的平均距离

b_i--样本x_i与其它与之最近"簇"的所有样本的平均距离

S_i值越接近1，表明样本x_i所在"簇"具有很好聚集性

S_i值越接近-1，表明样本x_i错分至其目前所在"簇"

该样本只是位于某两"簇"之间的某个地方

S_i=0，表明样本x_i也可以分至与其目前所在"簇"最近的那"簇"中

[4](平均)Silhouette宽度(average Silhouette width)

B.聚类C_k的平均Silhouette宽度 --**针对每簇**

$$S(C_k)=\frac{1}{N_k}\sum_{x_i\in C_k}S_i$$

$$\begin{cases}S(C_k)\in[-1,1]\\ C_k\in C\end{cases}$$

[4] (**平均**) *Silhouette*宽度 (*average* *Silhouette width*)

***C.Silhouette*宽度(剪影宽度，轮廓系数)**

--**整个数据集**所有样本平均***Silhouette***值

sklearn.metrics.silhouette_score()

$$Silhouette\text{宽度} = \frac{1}{|C|}\sum_{C_k \in C} S(C_k) = \frac{1}{N}\sum_{i=1}^{N} S_i$$

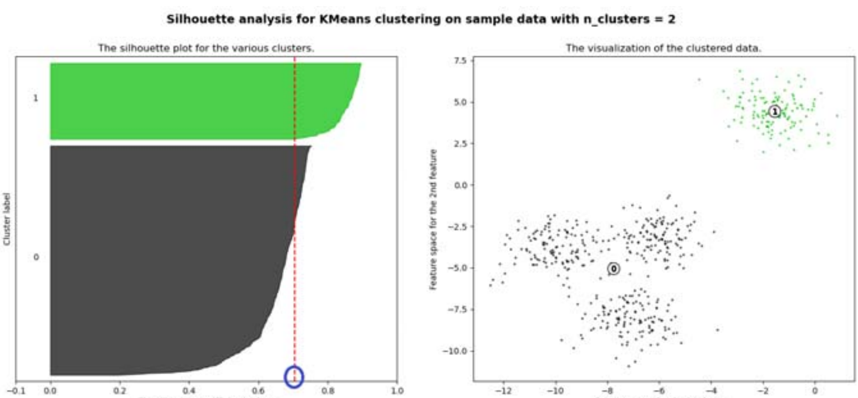
"***Silhouette*宽度**" 可用来：

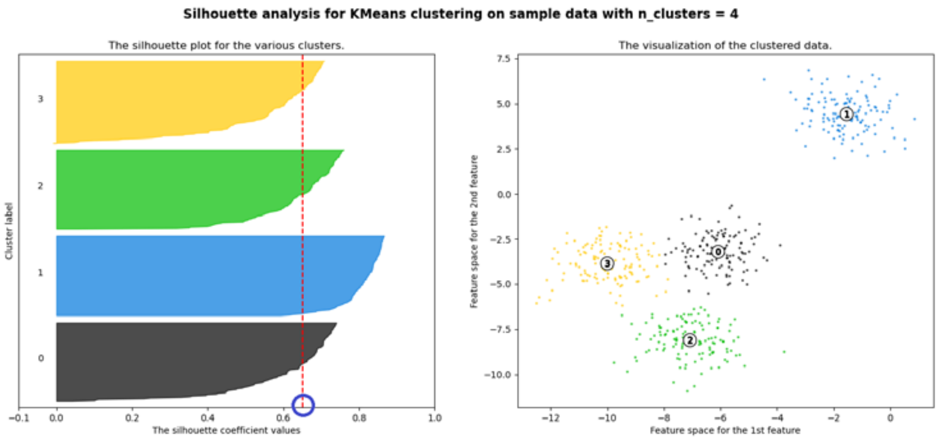
A--评价聚类的有效性，越接近于1越好

B--确定聚类数目的多少

例：利用平均剪影宽度辅助选择聚类数目

n_clusters = 2 The average silhouette_score =0.7049787496083262
n_clusters = 4 The average silhouette_score =0.6505186632729437
n_clusters = 6 The average silhouette_score =0.4504666294372765





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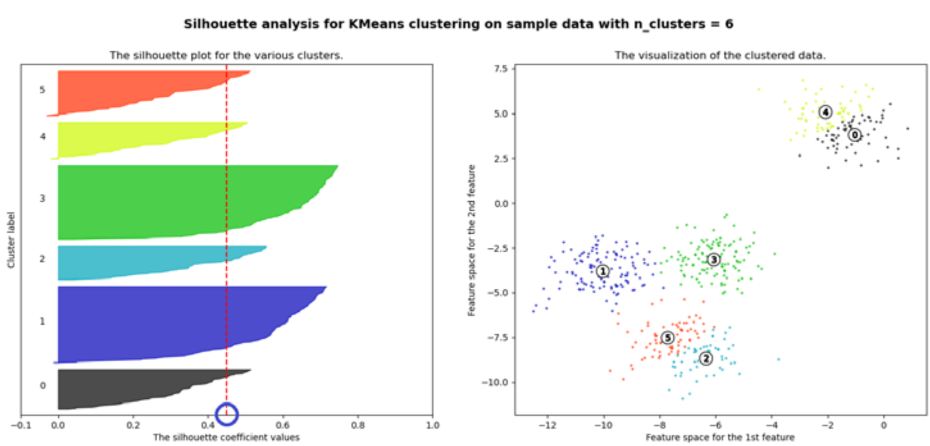

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