Reconocimiento de patrones

Clase 11: ISODATA





Para el día de hoy...

• ISODATA



ISODATA

- Determina los centros de los grupos de forma iterativa como la media de sus muestras
- Incorpora varias heurísticas
- El usuario debe tener una idea del número de grupos
 - La solución no excederá dos veces la estimación inicial
 - Ni será menos de la mitad

Esqueleto del algoritmo

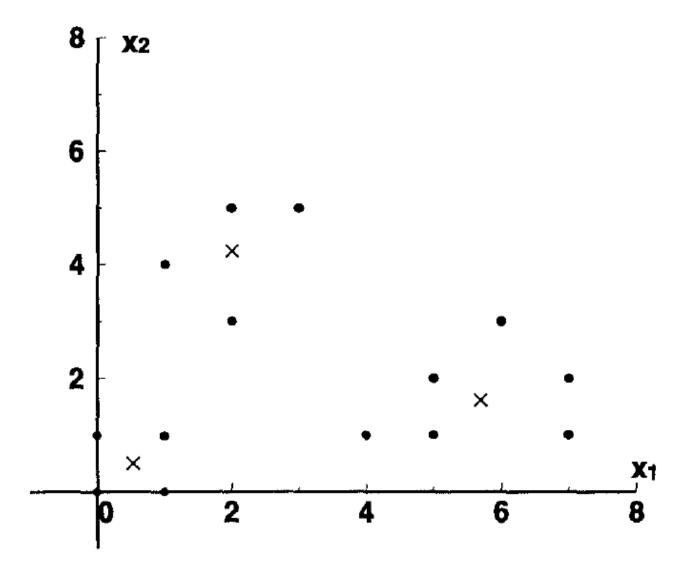
- Dados el número de grupos deseados, el mínimo de elementos por grupo, parámetros de agrupamiento, desviación estándar, grupos a agrupar e iteraciones
- Mientras no se cumpla el número de iteraciones
 - Distribuye las observaciones en los centros
 - Descarta los grupos con "pocas" muestras
 - Actualiza el centro de los grupos de acuerdo a la media
 - Calcula la distancia promedio de cada grupo y la distancia global
 - Si el número de grupos es menor a $\frac{k+1}{2}$ o impar menor a 2k intenta dividir un grupo
 - Detectar si se puede agrupar algún grupo

Ejemplo

• Considere las observaciones y centros dados en la figura

$$Y = \begin{cases} (0,0)^T, (1,0)^T, (1,1)^T, (0,1)^T, \\ (4,1)^T, (5,1)^T, (5,2)^T, (7,1)^T, \\ (7,2)^T, (6,3)^T, (2,3)^T, (1,4)^T, \\ (2,5)^T, (3,5)^T \end{cases}$$

- $Y = \{(0,0)^T, (4,1)^T, (7,2)^T, (2,3)^T, (3,5)^T\}$
- Los parámetros
 - c = 5
 - k = 3
 - $m_0 = 2$
 - $\sigma_0 = 1.5$
 - $\lambda = 0.5$
 - $d_0 = 2.5$
 - l = 2
 - N = 10



Ejemplo: inicialización

Considere las observaciones y centros dados en la figura

$$X = \begin{cases} (0,0)^T, (1,0)^T, (1,1)^T, (0,1)^T, \\ (4,1)^T, (5,1)^T, (5,2)^T, (7,1)^T, \\ (7,2)^T, (6,3)^T, (2,3)^T, (1,4)^T, \\ (2,5)^T, (3,5)^T \end{cases}$$

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 - *c* = 5
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Input:

n- the problem's dimension.

m- the number of the given samples.

 $X = \{x_i\}, 1 \le i \le m - \text{ the } m \text{ samples in } R^n$.

 $Y = \{y_i\}, Z = \{z_i\}, 1 \le i \le c -$ two identical sequences which contain the initial cluster centers.

k – the desired number of clusters.

 m_0 – minimum allowed size of a cluster.

 σ_0 – standard deviation threshold (for splitting).

 λ – splitting fraction: $0 < \lambda \le 1$.

 d_0 – lumping threshold.

 l- maximum number of pairs of clusters which may be lumped simultaneously.

ε – a given tolerance.

N – maximum number of iterations allowed.

S, L – vectors of size N. Initially

$$S(i) = L(i) = 2, 1 \le i \le N$$

After the i – th iteration, set S(i) = 0 or L(i) = 0 if splitting or lumping starts respectively. If splitting or lumping is

completed successfully, set S(i) = 1 or L(i) = 1 respectively.

NC – indicates a change in the set of cluster centers during the classification: Step 2 - Step 4.

Considere las observaciones y centros dados en la figura

$$Y = \begin{cases} (0,0)^T, (1,0)^T, (1,1)^T, (0,1)^T, \\ (4,1)^T, (5,1)^T, (5,2)^T, (7,1)^T, \\ (7,2)^T, (6,3)^T, (2,3)^T, (1,4)^T, \\ (2,5)^T, (3,5)^T \end{cases}$$

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Step 1. Set it = 0; S(i) = L(i) = 2, $1 \le i \le N$.

Considere las observaciones y centros dados en la figura

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Step 2. Set c'=c, $z_i=y_i$ $1 \le j \le c$ and NC=1.

Use the existing cluster centers and the minimum-distance principle to classify the samples, i.e.

$$x \in C_{j} \text{ iff } ||x - y_{j}|| \le ||x - y_{i}||, 1 \le i \le c, i \ne j$$
 (3.4.1)

for all $x \in X$, where C_j is the cluster centered at y_j with m_j samples $\{x_{l_n}\}_{i=1}^{m_j}$.

$$C_1$$
 C_2 C_3 C_4 C_5

$$(0,0)^T \quad (4,1)^T \quad (7,1)^T \quad (2,3)^T \quad (2,5)^T$$

$$(1,0)^T \quad (5,1)^T \quad (7,2)^T \quad (1,4)^T \quad (3,5)^T$$

$$(1,1)^T \quad (5,2)^T \quad (6,3)^T$$

$$(0,1)^T$$

• Considere las observaciones y centros dados en la figura

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 - k = 3
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Step 3. Each cluster center with fewer than m_0 samples is discarded. Its elements are distributed among the remaining clusters and we set $c \leftarrow c - 1$.

Considere las observaciones y centros dados en la figura

$$X = \begin{cases} (0,0)^T, (1,0)^T, (1,1)^T, (0,1)^T, \\ (4,1)^T, (5,1)^T, (5,2)^T, (7,1)^T, \\ (7,2)^T, (6,3)^T, (2,3)^T, (1,4)^T, \\ (2,5)^T, (3,5)^T \end{cases}$$

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Step 4. For $1 \le j \le c$ update the existing cluster centers by

$$\mathbf{y}_{j} \leftarrow \frac{1}{m_{j}} \sum_{i=1}^{m_{j}} \mathbf{x}_{l_{ij}} \tag{3.4.2}$$

If
$$c = c'$$
 and $\sum_{i=1}^{c} ||y_i - z_j|| < \varepsilon$ set $NC = 0$.

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$$\mathbf{y}_{j} \leftarrow \frac{1}{m_{j}} \sum_{i=1}^{m_{j}} \mathbf{x}_{l_{ij}}$$

$$\text{If } c = c' \text{ and } \sum_{i=1}^{c} \left\| \mathbf{y}_{j} - \mathbf{z}_{j} \right\| < \varepsilon \quad \text{set } NC = 0.$$

$$Y = \{(0.5, 0.5)^T, (4.667, 1.333)^T, (6.667, 2)^T, (1.5, 3.5)^T, (2.5, 5)^T\}$$

Considere las observaciones y centros dados en la figura

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Step 5. For $1 \le j \le c$ calculate the average distance of $x_{l_{ij}}$, $1 \le i \le m_j$ from y_i :

$$\overline{d}_{j} = \frac{1}{m_{j}} \sum_{i=1}^{m_{j}} \| \mathbf{x}_{l_{ij}} - \mathbf{y}_{j} \|$$
(3.4.3)

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(3.4.3)

$$\overline{d}_1 = 0.707, \overline{d}_2 = 0.654, \overline{d}_3 = 0.863, \overline{d}_4 = 0.707, \overline{d}_5 = 0.500$$

Considere las observaciones y centros dados en la figura

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Step 6. Calculate the global average distance \overline{d} of all the m samples from their respective cluster centers, i.e.

$$\vec{d} = \frac{1}{m} \sum_{j=1}^{c} m_j \vec{d}_j \tag{3.4.4}$$

This is the end of an iteration. Set $it \leftarrow it + 1$.

Considere las observaciones y centros dados en la figura

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$$\overline{d}_1 = 0.707, \overline{d}_2 = 0.654, \overline{d}_3 = 0.863, \overline{d}_4 = 0.707, \overline{d}_5 = 0.500$$

$$\overline{d} = (4\overline{d}_1 + 3\overline{d}_2 + 3\overline{d}_3 + 2\overline{d}_4 + 2\overline{d}_5)/14 = 0.700$$

Considere las observaciones y centros dados en la figura

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Step 7. If it = N go to Step 13. Otherwise

- (a) If $c \le \left\lceil \frac{k+1}{2} \right\rceil$ go to Step 8 (splitting a cluster).
- (b) If $\left[\frac{k+1}{2}\right] < c < 2k$ and it is odd, go to Step 8.
- (c) If $c \ge 2k$ go to Step 10 (lumping clusters).
- (d) If $\left[\frac{k+1}{2}\right] < c < 2k$ and it is even, go to Step 10.

Considere las observaciones y centros dados en la figura

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 - $m_0 = 2$
 - $\sigma_0 = 1.5$
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 - l = 2
 - N = 10

Step 8. Trying to split. Set S(it) = 0. For every cluster denote the cluster center and the cluster samples by

$$\mathbf{y}_{j} = (y_{j}^{(1)}, y_{j}^{(2)}, ..., y_{j}^{(n)})^{T}, 1 \le j \le c$$
 (3.4.5)

$$\mathbf{x}_{l_{kj}} = \left(x_{l_{kj}}^{(1)}, x_{l_{kj}}^{(2)}, \dots, x_{l_{kj}}^{(n)}\right)^{T}, \ 1 \le j \le c, \ 1 \le k \le m_{j}$$
(3.4.6)

respectively. Calculate the standard deviation vectors

$$\sigma_j = \left(\sigma_j^{(1)}, \sigma_j^{(2)}, \dots, \sigma_j^{(n)}\right)^T, \quad 1 \le j \le c$$
 (3.4.7)

where

$$\sigma_j^{(i)} = \left(\frac{\sum_{k=1}^{m_j} \left(x_{l_{i_l}}^{(i)} - y_j^{(i)}\right)^2}{m_j}\right)^{1/2}, \ 1 \le j \le c, \ 1 \le i \le n$$
(3.4.8)

Each $\sigma_j^{(i)}$ is the standard deviation of the j-th cluster population along the i-th coordinate. Denote $\sigma_j^{(i_0)} = \max \sigma_j^{(i)}$, $1 \le i \le n$ (clearly i_0 depends on j).

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- Los parámetros

•
$$c = 5$$

•
$$k = 3$$

•
$$m_0 = 2$$

•
$$\sigma_0 = 1.5$$

•
$$\lambda = 0.5$$

•
$$d_0 = 2.5$$

•
$$l = 2$$

•
$$N = 10$$

$$C_1$$
 C_2 C_3 C_4 C_5

$$C_1$$
 C_2 C_3 C_4 C_5

$$(0.0)^T$$
 $(4.1)^T$ $(7.1)^T$ $(2.2)^T$ (2.5)

$$(0,0)^{T}$$
 $(4,1)^{T}$ $(7,1)^{T}$ $(2,3)^{T}$ $(2,5)^{T}$ $(1,0)^{T}$ $(5,1)^{T}$ $(7,2)^{T}$ $(1,4)^{T}$ $(3,5)^{T}$

$$(1,1)^T$$
 $(5,2)^T$ $(6,3)^T$

$$(0,1)^{T}$$

$$\boldsymbol{\sigma}_{1} = \begin{pmatrix} 0.500 \\ 0.500 \end{pmatrix}, \ \boldsymbol{\sigma}_{2} = \begin{pmatrix} 0.471 \\ 0.471 \end{pmatrix}, \ \boldsymbol{\sigma}_{3} = \begin{pmatrix} 0.471 \\ 0.816 \end{pmatrix}, \boldsymbol{\sigma}_{4} = \begin{pmatrix} 0.500 \\ 0.500 \end{pmatrix}, \boldsymbol{\sigma}_{5} = \begin{pmatrix} 0.500 \\ 0.000 \end{pmatrix}$$

Step 8. Trying to split. Set S(it) = 0. For every cluster denote the cluster center and the cluster samples by

$$\mathbf{y}_{j} = (y_{j}^{(1)}, y_{j}^{(2)}, ..., y_{j}^{(n)})^{T}, 1 \le j \le c$$
 (3.4.5)

$$\mathbf{x}_{l_{kj}} = \left(x_{l_{kj}}^{(1)}, x_{l_{kj}}^{(2)}, \dots, x_{l_{kj}}^{(n)}\right)^{T}, \ 1 \le j \le c, \ 1 \le k \le m_{j}$$
(3.4.6)

respectively. Calculate the standard deviation vectors

$$\sigma_j = \left(\sigma_j^{(1)}, \sigma_j^{(2)}, \dots, \sigma_j^{(n)}\right)^T, \quad 1 \le j \le c$$
 (3.4.7)

where

$$\sigma_j^{(i)} = \left(\frac{\sum_{k=1}^{m_j} \left(x_{l_{i_j}}^{(i)} - y_j^{(i)}\right)^2}{m_j}\right)^{1/2}, \ 1 \le j \le c, \ 1 \le i \le n$$
(3.4.8)

Each $\sigma_i^{(i)}$ is the standard deviation of the j-th cluster population along the i-th coordinate. Denote $\sigma_j^{(i_0)} = \max \sigma_j^{(i)}, \quad 1 \le i \le n \text{ (clearly } i_0 \text{ depends on } j \text{)}.$

 Considere las observaciones y centros dados en la figura

$$Y = \begin{cases} (0,0)^T, (1,0)^T, (1,1)^T, (0,1)^T, \\ (4,1)^T, (5,1)^T, (5,2)^T, (7,1)^T, \\ (7,2)^T, (6,3)^T, (2,3)^T, (1,4)^T, \\ (2,5)^T, (3,5)^T \end{cases}$$

- $Y = \{(0,0)^T, (4,1)^T, (7,2)^T, (2,3)^T, (3,5)^T\}$
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 - c = 5
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$$\overline{d}_1 = 0.707, \overline{d}_2 = 0.654, \overline{d}_3 = 0.863, \overline{d}_4 = 0.707, \overline{d}_5 = 0.500$$

$$\boldsymbol{\sigma}_{1} = \begin{pmatrix} 0.500 \\ 0.500 \end{pmatrix}, \ \boldsymbol{\sigma}_{2} = \begin{pmatrix} 0.471 \\ 0.471 \end{pmatrix}, \ \boldsymbol{\sigma}_{3} = \begin{pmatrix} 0.471 \\ 0.816 \end{pmatrix}, \boldsymbol{\sigma}_{4} = \begin{pmatrix} 0.500 \\ 0.500 \end{pmatrix}, \boldsymbol{\sigma}_{5} = \begin{pmatrix} 0.500 \\ 0.000 \end{pmatrix}^{-3}.$$

Step 9. For $j: 1 \le j \le c$ if $\sigma_j^{(i_0)} \le \sigma_0$ do not split the j-th cluster; otherwise split it, provided that *at least* one of the relations

$$c \le \left[\frac{k+1}{2}\right] \tag{3.4.9}$$

$$\overline{d}_j > \overline{d}$$
 and $m_j \ge 2m_0$ (3.4.10)

holds. Splitting the j-th cluster is done as follows. The cluster center y_j is deleted while two new cluster centers y_{j+}, y_{j-} defined as

$$\mathbf{y}_{i+} = \left(y_i^{(1)}, \dots, y_i^{(i_0-1)}, y_i^{(i_0)} + \lambda \sigma_i^{(i_0)}, y_i^{(i_0+1)}, \dots, y_i^{(n)}\right)$$
(3.4.11)

$$y_{j-} = \left(y_j^{(i)}, \dots, y_j^{(i_0-1)}, y_j^{(i_0)} - \lambda \sigma_j^{(i_0)}, y_j^{(i_0+1)}, \dots, y_j^{(n)}\right)$$
(3.4.12)

are created, and we set $c \leftarrow c+1$. Thus, y_j is splitted along the i_0 -th coordinate. The splitting is controlled by the parameter λ which ensures a noticeable but not dramatic change in the cluster centers arrangement. If splitting occurred, set S(it) = 1 and go to Step 2. Otherwise:

- 1. If it > 1, L(it-1) = 0 and NC = 0 go to Step 12.
- 2. If it > 1, L(it-1) = 0 and NC = 1 go to Step 2.
- 3. If it > 1, $L(it-1) \neq 0$ continue.
- 4. If it = 1 continue.

Considere las observaciones y centros dados en la figura

$$Y = \begin{cases} (0,0)^T, (1,0)^T, (1,1)^T, (0,1)^T, \\ (4,1)^T, (5,1)^T, (5,2)^T, (7,1)^T, \\ (7,2)^T, (6,3)^T, (2,3)^T, (1,4)^T, \\ (2,5)^T, (3,5)^T \end{cases}$$

- $Y = \{(0,0)^T, (4,1)^T, (7,2)^T, (2,3)^T, (3,5)^T\}$
- Los parámetros
 - c = 5
 - k = 3
 - $m_0 = 2$
 - $\sigma_0 = 1.5$
 - $\lambda = 0.5$
 - $d_0 = 2.5$
 - l = 2
 - N = 10

Step 10. Lumping. Set L(it) = 0. If c < 2, S(it) = 0 and NC = 0, go to Step 12. If c < 2 S(it) = 0 and NC = 1, go to Step 2. If

c < 2 and S(it) = 2, go to Step 2; otherwise calculate all the distances between arbitrary two cluster centers, i.e.

$$d_{ij} = \|\mathbf{y}_i - \mathbf{y}_j\|, 1 \le i \le c - 1, i + 1 \le j \le c \tag{3.4.13}$$

Rearrange $\{d_{ij}\}$ as a monotonic increasing sequence and denote by l' the number of $d_{ij}'s$ which do not exceed d_0 . Consider now the first $l^* = \min(l, l')$ numbers of this sequence which satisfy

$$d_{i_1 j_1} \le d_{i_2 j_2} \le \dots \le d_{i_1 * j_1 *} \le d_0 \tag{3.4.14}$$

If $l^* = 0$ no lumping occurs: if S(it) = 2 go to Step 2 and if S(it) = 0 go to Step 12. If $l^* \neq 0$ set L(it) = 1 and continue.

Ejemplo: Paso 11-13

Considere las observaciones y centros dados en la figura

$$X = \begin{cases} (0,0)^T, (1,0)^T, (1,1)^T, (0,1)^T, \\ (4,1)^T, (5,1)^T, (5,2)^T, (7,1)^T, \\ (7,2)^T, (6,3)^T, (2,3)^T, (1,4)^T, \\ (2,5)^T, (3,5)^T \end{cases}$$

- $Y = \{(0,0)^T, (4,1)^T, (7,2)^T, (2,3)^T, (3,5)^T\}$
- · Los parámetros
 - *c* = 5
 - k = 3
 - $m_0 = 2$
 - $\sigma_0 = 1.5$
 - $\lambda = 0.5$
 - $d_0 = 2.5$
 - l = 2
 - N = 10

Step 11. The lumping starts with the pair of cluster centers (i_1, j_1) and terminates with (i_{l^*}, j_{l^*}) . Each two cluster centers are lumped together and if a given pair (i_r, j_r) is such that either the i_r - th or the j_r - th cluster center had already been lumped, this pair is ignored. The lumping is done by replacing the i_r - th and the j_r - th cluster centers by

$$\mathbf{y}_{(i_r,j_r)} = \frac{m_{i_r} \mathbf{y}_{i_r} + m_{j_r} \mathbf{y}_{j_r}}{m_{i_r} + m_{j_r}}$$
(3.4.15)

i.e. by their center of gravity based on their current populations. Since y_{i_r} and y_{j_r} are deleted we also set $c \leftarrow c-1$. When the lumping is completed go to Step 2.

- **Step 12.** Output $\{y_j\}$, $1 \le j \le c$; it and stop.
- **Step 13.** Output y_i , $1 \le j \le c$; 'number of iterations exceeded' and stop.

Comentarios

- Para una implementación exitosa de ISODATA es necesario experimentar con σ_0 , λ , d_0 para encontrar valores apropiados
- Valores inapropiados pueden llevar a oscilaciones (secuencias infinitas de divisiones y agrupamientos)
- Esto puede suceder cuando $2\lambda\sigma_0 < d_0$

Ejercicio

- Revisar el algoritmo de Isodata
- Implementar el algoritmo en Python
- Ejecute el algoritmo de Isodata con los datos del ejemplo y grafique la solución encontrada
- De su opinión del algoritmo y contesté las 4 preguntas típicas de análisis y diseño de algoritmos

Bibliografía

 Introduction to Pattern Recognition: Statistical, Structural, Neural, and Fuzzy Logic Approaches. Libro de Abraham Kandel y Menachem Friedman

Para la otra vez...

 Agrupamiento y reconocimiento de patrones



