



CIMPA-UCR

Clasificación Bimodal

Metodos clásicos

Uso de Metaheurísticas

Uso de un índice difuso

Experimento de Monte Carlo

Clasificación bimodal

	B ₁	B ₂	B ₃
A ₁			
A ₂			
A ₃			

- Minimizar

con

$$W(P) = \sum_{k=1}^r \sum_{l=1}^m \sum_{i \in A_k} \sum_{j \in B_l} (x_{ij} - g_{kl})^2$$

$$g_{kl} = \frac{1}{|A_k| |B_l|} \sum_{i \in A_k} \sum_{j \in B_l} x_{ij}$$

Notación

- Data set: $X = (x_{ij})_{n \times m}$ with modes I, J ($|I| = n$, $|J| = m$, $I \cap J = \emptyset$), $x_{ij} \geq 0$
- $P = \{A_k | k = 1, \dots, K\}$: partition of mode I
- $Q = \{B_l | l = 1, \dots, L\}$: partition of mode J
- $A_k \times B_l$: two-mode class of $I \times J$
- (P, Q) is a **two-mode partition** of $I \times J$ in K, L classes
- P, Q : indicator classes of partitions P, Q

Notación

$$\mathbf{X}_{n \times m} = (x_{ij})_{n \times m}$$

Two-mode data matrix of n rows and m columns.

$$\mathbf{P}_{n \times K} = (p_{ik})_{n \times K}$$

Cluster membership matrix of the rows with K the number of row clusters, $p_{ik} = 1$ if row i belongs to row cluster k , and $p_{ik} = 0$ otherwise.

$$\mathbf{Q}_{m \times L} = (q_{jl})_{m \times L}$$

Cluster membership matrix of the columns with L the number of column clusters, $q_{jl} = 1$ if column j belongs to column cluster l , and $q_{jl} = 0$ otherwise.

$$\mathbf{V}_{K \times L} = (v_{kl})_{K \times L}$$

Matrix with cluster centers for row cluster k and column cluster l .

$$\mathbf{E}_{n \times m} = (e_{ij})_{n \times m}$$

Matrix with errors from cluster centers.



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Criterio

Given the two-mode matrix X and fixing K and L , the problem is to find partitions $P = (p_{ik})_{n \times K}$ and $Q = (q_{jl})_{m \times L}$, and an association matrix $V = (v_{kl})_{K \times L}$ such that

$$Z = Z(P, Q, V) = \sum_{i \in I} \sum_{j \in J} \left(x_{ij} - \sum_{k=1}^K \sum_{l=1}^L p_{ik} q_{jl} v_{kl} \right)^2$$

is **minimum**,

where the x_{ij} are centered ($x_{ij} \leftarrow x_{ij} - \bar{x}$) and

$$\hat{x}_{ij} = \sum_k \sum_l p_{ik} q_{jl} v_{kl}.$$

Simplificación

Z can be written in the form (Gaul & Schader (1996)):

$$Z = \sum_{k=1}^K \sum_{l=1}^L \sum_{i=1}^n \sum_{j=1}^m p_{ik} q_{jl} (x_{ij} - v_{kl})^2. \quad (1)$$

Given P and Q , the matrix V that minimizes Z is obtained for (see Gaul & Schader (1996)):

$$w_{kl} = \frac{1}{a_k b_l} \sum_{i \in A_k} \sum_{j \in B_l} x_{ij}, \quad (2)$$

where $a_k = |A_k|$ and $b_l = |B_l|$ are the cardinalities of the classes.

Simplificación

- We can write:

$$X = PVQ' + E,$$

- Hence, the criterion is:

$$f(P, Q, V) = \|X - PVQ'\|^2 = \sum_{k=1}^K \sum_{l=1}^L \sum_{i=1}^n \sum_{j=1}^m p_{ik} q_{jl} (x_{ij} - v_{kl})^2.$$



Métodos comparados

- Alternating exchanges (Gaul & Schader 1996)
- Two-mode K-means (Govaert 83; Baier, Gaul & Schader 1997)
- Simulated annealing (Trejos & Castillo 2000)
- Tabu search (Castillo & Trejos 2002)
- Fuzzy approach (Groenen, Roosmalen, Trejos & Castillo 2008)

Métodos existentes

- Intercambios alternantes (Gaul & Schader 96): transferencias en cada modo, iteraciones mientras el criterio mejora
- *K*-medias (Govaert 83; Baier, Gaul, Schader 97): fases de asignación y representación, hasta estabilización

Notación

- $A_k \xrightarrow{i} A_{k'}$: transfer of the row mode i from class A_k to class $A_{k'}$
- $B_l \xrightarrow{j} B_{l'}$: transfer of column object j from class B_l to class $B_{l'}$

All the following algorithms begin with an initial two-mode partition (P, Q) , which can be generated at random or it can be the result of some previous knowledge on the data

Intercambios Alternantes

1. Initialize P, Q ; compute W according to (2).
2. Alternate the following steps until Z does not improve:
 - a) Make $A_k \xrightarrow{i} A_{k'}$ for i and k' chosen at random; if $\Delta Z := Z^{\text{new}} - Z^{\text{current}} < 0$ accept the transfer, redefine P and compute W using (2).
 - b) Make $B_l \xrightarrow{j} B_{l'}$ for j and l' chosen at random; if $\Delta Z < 0$ accept the transfer, redefine Q and compute W using (2).



K-medias Bimodal

1. Initialize P^0, Q^0 ; compute W^0 according to (2); let $t := 0$.
2. Repeat the following steps until Z does not improve:

a) Given $W := W^t$ and $Q := Q^t$, define $\tilde{P}$ by

$$\tilde{A}_k := \{i \in I \mid \sum_l \sum_{j \in B_l} (x_{ij} - w_{kl})^2 \rightarrow \min_{k'} \sum_l \sum_{j \in B_l} (x_{ij} - w_{k'l})^2\}$$

b) Given $W := W^t$ and $P := P^t$, define $\tilde{Q}$ by

$$\tilde{B}_l := \{j \in J \mid \sum_k \sum_{i \in A_k} (x_{ij} - w_{kl})^2 \rightarrow \min_{l'} \sum_k \sum_{i \in A_k} (x_{ij} - w_{kl'})^2\}$$

c) Calculate W^t according to (2).

d) Let $t := t + 1$, $P^t := \tilde{P}$, $Q^t := \tilde{Q}$.

Uso de Sob.Sim.

- Vecindario generado por la transferencia en uno de los dos modos (escogido al azar)
- Si se escoge el modo fila: escoger al azar (unif.) i , escoger al azar (unif.) k' , hacer la transferencia de i de su clase actual a la clase k'
- Idem para columnas



Sobrecalentamiento Simulado

1. Initialize P, Q ; calculate W according to (2).
2. Estimate the initial temperature c_0 using the initial acceptance rate χ_0 .
3. For $t := 0$ until λ do:
 - a) choose at random a mode (I or J) with uniform probability $1/2$
 - b) make $A_k \xrightarrow{i} A_{k'}$ or $B_l \xrightarrow{j} B_{l'}$ in the following way:
 - choose at random i or j (according to the chosen mode);
 - choose at random k' or l' , different from the current class of i or j , noted k or l , depending on the corresponding case;
 - calculate ΔZ .
 - c) Accept the transfer if $\Delta Z < 0$, otherwise accept it with probability $\exp(-\Delta Z/c_t)$.
4. Make $c_{t+1} := \gamma c_t$ and return to step 1, until $c_t \approx 0$.

Uso de BT

- Movimiento: transferencia de un objeto fila o un objeto columna a una nueva clase
- Lista tabú contiene los valores de $W(P)$
- Generar una muestra del vecindario
- No se aplica un criterio de aspiración



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Búsqueda Tabú

1. Start with an initial partition (P, Q) and an empty tabu list. Set $(P, Q)_{opt} = (P, Q)$.
2. Choose the number of iterations S and a maximum length of the tabu list.
3. Perform the following steps S times.
 - (a) Generate a neighborhood of partitions N , consisting of the partitions that can be constructed by transferring one row or column object from (P, Q) to another cluster.
 - (b) Choose the partition $(P, Q)_{cand}$ as the partition in N with the lowest value of $Z(P, Q)$ that is not on the tabu list.
 - (c) Set $(P, Q) = (P, Q)_{cand}$. If $Z((P, Q)_{cand}) < Z((P, Q)_{opt})$, then $(P, Q)_{opt} = (P, Q)_{cand}$.
 - (d) Add (P, Q) to the tabu list. Remove the oldest item from the tabu list, if the list exceeds its maximum length.

Enfoque Difuso

We handle fuzzy two-mode partitions (P, Q) where $p_{ik}, q_{jl} \in [0, 1]$ instead of $p_{ik}, q_{jl} \in \{0, 1\}$. Let $s > 1$ be a real number. The criterion to be minimized is

$$f_s(\mathbf{P}, \mathbf{Q}, \mathbf{V}) = \sum_{k=1}^K \sum_{l=1}^L \sum_{i=1}^n \sum_{j=1}^m p_{ik}^s q_{jl}^s (x_{ij} - v_{kl})^2$$

and it is proved that, for fixed s, P and Q the best matrix V is given by

$$v_{kl} = \frac{\sum_{i=1}^n \sum_{j=1}^m p_{ik}^s q_{jl}^s x_{ij}}{\sum_{i=1}^n \sum_{j=1}^m p_{ik}^s q_{jl}^s} \quad (12)$$

Enfoque Difuso (2)

$$L_i(\mathbf{P}, \mathbf{Q}, \mathbf{V}, \lambda) = \sum_{k=1}^K p_{ik}^s \sum_{l=1}^L \sum_{j=1}^m q_{jl}^s (x_{ij} - v_{kl})^2 - \lambda \left(\sum_{k=1}^K p_{ik} - 1 \right).$$

Defining $c_{ik} = \sum_{l=1}^L \sum_{j=1}^m q_{jl}^s (x_{ij} - v_{kl})^2$ and taking partial derivatives of L_i gives

$$\frac{\partial L_i}{\partial p_{ik}} = s p_{ik}^{s-1} c_{ik} - \lambda \quad \text{and} \quad \frac{\partial L_i}{\partial \lambda} = \sum_{k=1}^K p_{ik} - 1.$$

Setting these derivatives to zero and solving for p_{ik} yields

$$p_{ik} = \frac{c_{ik}^{1/(1-s)}}{\sum_{k=1}^K c_{ik}^{1/(1-s)}}.$$

C-Medias Difuso Bimodal

1. Choose initial $\mathbf{P}$ and $\mathbf{Q}$, which can be either crisp or fuzzy, and calculate $\mathbf{V}$ according to (12).
2. Repeat the following, until the decrease in $f_s(\mathbf{P}, \mathbf{Q}, \mathbf{V})$ is small.
 - (a) Calculate $c_{ik} = \sum_{l=1}^L \sum_{j=1}^m q_{jl}^s (x_{ij} - v_{kl})^2$ and update $\mathbf{P}$ as $p_{ik} = \frac{c_{ik}^{1/(1-s)}}{\sum_{k=1}^K c_{ik}^{1/(1-s)}}$.
 - (b) Calculate $d_{jl} = \sum_{k=1}^K \sum_{i=1}^n p_{ik}^s (x_{ij} - v_{kl})^2$ and update $\mathbf{Q}$ as $q_{ik} = \frac{d_{jl}^{1/(1-s)}}{\sum_{k=1}^K d_{jl}^{1/(1-s)}}$.
 - (c) Update $\mathbf{V}$ according to (12).

This algorithm lowers the value of $f_s(\mathbf{P}, \mathbf{Q}, \mathbf{V})$ in each iteration, until convergence has been achieved. Therefore, the algorithm always converges to a saddle point or a local minimum, which may or may not be a global minimum.

Pasos difusos

1. Choose an initial value of s , a fuzzy step size $\gamma < 1$, and a threshold value s_{min} .
2. Choose initial P_0 and Q_0 and calculate V_0 according to (12). The initial P_0 and Q_0 can be either crisp or fuzzy.
3. Repeat the following while $s > s_{min}$.
 - (a) Perform the two-mode fuzzy c -means algorithm starting with P_0 , Q_0 , and V_0 . The results are in P_1 , Q_1 , and V_1 .
 - (b) Set $s = 1 + \gamma(s - 1)$ and set $P_0 = P_1$, $Q_0 = Q_1$, and $V_0 = V_1$.
4. Apply the two-mode k -means algorithm starting from P_0 , Q_0 , and V_0 .

Algunos resultados

	K-medias		Inter Alter.		Sob. Sim	
	#	τ	#	τ	#	τ
Cognac	1000	5%	500	10%	150	85%
Cigarros 1	1000	12%	500	35%	150	80%
Cigarros 2	1000	8%	500	40%	150	100%

$$r = m = 3$$

Datos de sanitarios (82x25)

$r=m$	Int.Alt.	k-means	SS	Fuzzy	BT
2	0.2289	0.2289	0.2289	0.2289	0.2289
3	0.3234	0.3234	0.3234	0.3234	0.3234
4	0.3729	0.3729	0.3804	0.3703	0.3804
5	0.4293	0.4293	0.4293	0.4293	0.4293
6	0.4635	0.4579	0.4651	0.4641	0.4651



Estudio de Simulación

- Simulate **P**, **Q**, **V**, **E**
- Generate **$X = PVQ^t + E$**
- 4 factors with 3 levels each: 81 combinations
- We simulate 50 data sets for each combination
- All 5 methods are performed for each data set
- Computation time is balanced



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Factores

1. Size of data: ($n=m=60$; $n=150, m=30$; $n=m=120$)
2. Number of clusters ($K=L=3$; $K=L=5$, $K=L=7$)
3. Size of error perturbations: elements of **E** are independent normally distributed with mean 0 and sta dev 0.5, 1 or 2
4. Distribution of the objects over the clusters:
 - Objects divided over the clusters with = probab
 - One cluster contains 10% of the objects
 - One cluster contains 60% of the clusters

Centros

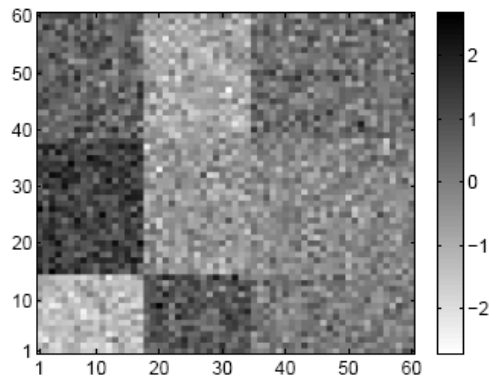
- Assign randomly the numbers

$$\Phi\left(\frac{i}{K \times L + 1}\right), i = 1, \dots, K \times L$$

to the elements of $\mathbf{V}$, where $\Phi(.)$ is the inverse standard normal cumulative distribution function

- As a result, the elements of $\mathbf{V}$ appear standard normally distributed, and a fixed minimum distance between the cluster centers is ensured

Representación Visual



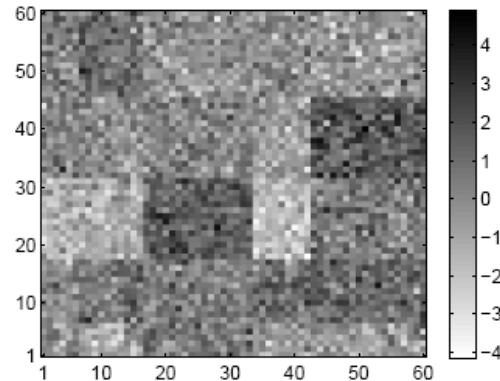
$$n = m = 60,$$

$$K = L = 3,$$

error s.d.=0.5

unif dist over clusters

Easy to recognize



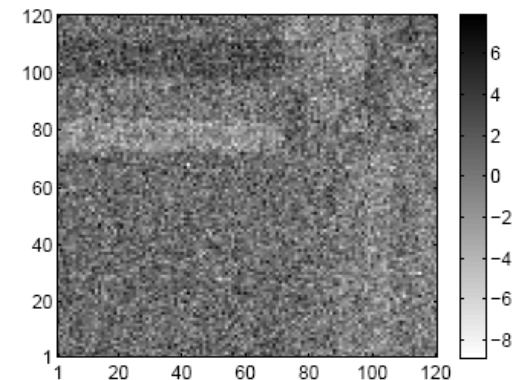
$$n = m = 60$$

$$K = L = 5$$

error s.d.=1

10% of obj in 1 cluster

Difficult to recognize



$$n = m = 120,$$

$$K = L = 7$$

error s.d.=2

60% of obj in 1 cluster

Impossible to recognize

Parámetros

- Alt.Exch.: 30 times for every simulated data set
- Two-mode K-Means: 500 times
- Sim.Annealing: $T = 1$, $\gamma = 0.95$, $t_{\max} = 10$,
 $R = (n(K-1) + m(L-1))/4$
- Tabu S.: number of iterations
 $S = 3(n(K-1) + m(L-1))^{1/2}$, length of tabu list = $S/3$
- Fuzzy steps: $s_0 = 1.05$, $\gamma = 0.85$, $s_{\min} = 1.001$, run 20 times



Criterios de comparación

- Variance accounted for (*VAF*)
- Adjusted Rand index (*ARI*)
- Average CPU time

Variance accounted for

$$VAF = 1 - \frac{\sum_{k=1}^K \sum_{l=1}^L \sum_{i=1}^n \sum_{j=1}^m p_{ik} q_{jl} (x_{ij} - v_{kl})^2}{\sum_{i=1}^n \sum_{j=1}^m (x_{ij} - \bar{x})^2}$$

where $\bar{x} = \frac{1}{nm} \sum_{i=1}^n \sum_{j=1}^m x_{ij}$

$$VAF \in [0,1]$$

$$VAF \rightarrow \max$$

Resultados de Simulación

Table 1: Average VAF for data sets with different error variances and numbers of rows and columns.

Size of data set	$n = 60, m = 60$			$n = 150, m = 30$			$n = 120, m = 120$		
Error st. dev.	.5	1	2	.5	1	2	.5	1	2
Alternating exchanges	.7260	.4128	.1685	.7288	.4140	.1750	.7251	.4058	.1532
Two-mode k -means	.7283	.4134	.1667	.7322	.4146	.1733	.7293	.4082	.1535
Simulated annealing	.7092	.4068	.1668	.7166	.4078	.1739	.7108	.3987	.1518
Tabu search	.6823	.4003	.1642	.6904	.4015	.1660	.6703	.3853	.1496
Fuzzy steps	.7248	.4129	.1688	.7299	.4143	.1755	.7199	.4064	.1531
Original partition	.7292	.4126	.1540	.7326	.4122	.1531	.7308	.4088	.1515

Resultados de Simulación

Table 2: Average VAF for data sets with different error variances and numbers of clusters.

Numbers of clusters Error st. dev.	$K = 3, L = 3$			$K = 5, L = 5$			$K = 7, L = 7$		
	.5	1	2	.5	1	2	.5	1	2
Alternating exchanges	.6843	.3558	.1294	.7399	.4260	.1725	.7557	.4508	.1948
Two-mode k -means	.6843	.3558	.1296	.7440	.4276	.1724	.7614	.4529	.1915
Simulated annealing	.6804	.3525	.1284	.7221	.4186	.1706	.7340	.4422	.1935
Tabu search	.6584	.3476	.1259	.6868	.4066	.1663	.6980	.4329	.1876
Fuzzy steps	.6838	.3558	.1288	.7394	.4264	.1725	.7515	.4515	.1960
Original partition	.6843	.3549	.1214	.7442	.4265	.1601	.7640	.4522	.1771

Resultados de Simulación

Table 3: Average VAF for data sets with different error variances and distributions of the objects over the clusters.

Object distribution Error st. dev.	uniform distribution			10% in one cluster			60% in one cluster		
	.5	1	2	.5	1	2	.5	1	2
Alternating exchanges	.7460	.4293	.1695	.7330	.4171	.1666	.7009	.3862	.1606
Two-mode <i>k</i> -means	.7467	.4294	.1683	.7336	.4174	.1655	.7094	.3894	.1596
Simulated annealing	.7352	.4255	.1684	.7199	.4105	.1650	.6814	.3774	.1593
Tabu search	.6858	.4127	.1641	.6818	.3993	.1606	.6755	.3751	.1552
Fuzzy steps	.7419	.4291	.1698	.7299	.4170	.1668	.7029	.3875	.1608
Original partition	.7467	.4288	.1602	.7337	.4167	.1566	.7121	.3881	.1418

Índice Ajustado de Rand

$$\text{ARI} = \frac{\sum_{i=1}^R \sum_{j=1}^R \binom{a_{ij}}{2} - \sum_{i=1}^R \binom{a_{i.}}{2} \sum_{j=1}^R \binom{a_{.j}}{2} / \binom{a}{2}}{[\sum_{i=1}^R \binom{a_{i.}}{2} + \sum_{j=1}^R \binom{a_{.j}}{2}] / 2 - \sum_{i=1}^R \binom{a_{i.}}{2} \sum_{j=1}^R \binom{a_{.j}}{2} / \binom{a}{2}}$$

where a_{ij} is the number of elements of $\mathbf{X}$ that simultaneously belong to cluster i of the original partition and cluster j of the retrieved partition, R is the total number of clusters, $a_{i.} = \sum_{j=1}^R a_{ij}$, $a_{.j} = \sum_{i=1}^R a_{ij}$, and $a = \sum_{i=1}^R \sum_{j=1}^R a_{ij} = nm$. Here we consider a pair of elements to be in the same cluster only if they belong to same row cluster and to the same column cluster, so that $R = K \times L$.



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Clasificación Bimodal usando Metaheurísticas de Optimización Combinatoria

Table 4: Average adjusted Rand indices for each level of each factor.

Size of data set	$n = 60, m = 60$	$n = 150, m = 30$	$n = 120, m = 120$
Alternating exchanges	.739	.721	.846
Two-mode k -means	.759	.748	.893
Simulated annealing	.678	.673	.793
Tabu search	.636	.613	.729
Fuzzy steps	.745	.737	.851
Numbers of clusters	$K = 3, L = 3$	$K = 5, L = 5$	$K = 7, L = 7$
Alternating exchanges	.865	.772	.669
Two-mode k -means	.868	.815	.718
Simulated annealing	.830	.702	.612
Tabu search	.775	.637	.567
Fuzzy steps	.858	.783	.692
Error standard deviation	.5	1	2
Alternating exchanges	.915	.853	.538
Two-mode k -means	.974	.889	.537
Simulated annealing	.852	.788	.503
Tabu search	.782	.742	.454
Fuzzy steps	.934	.863	.537
Distribution of the objects	uniform distribution	10% in one cluster	60% in one cluster
Alternating exchanges	.874	.861	.571
Two-mode k -means	.873	.860	.668
Simulated annealing	.837	.805	.501
Tabu search	.741	.727	.510
Fuzzy steps	.868	.856	.610

Tiempo de CPU

Table 5: Average CPU times of all optimization methods in seconds.

Size of data sets	$n = 60, m = 60$			$n = 150, m = 30$			$n = 120, m = 120$		
Numbers of clusters (K, L)	3	5	7	3	5	7	3	5	7
Alternating exchanges	1.21	2.54	3.96	1.92	4.22	6.43	2.39	5.59	8.72
Two-mode k -means	1.54	2.36	3.09	1.96	3.58	4.57	2.50	5.31	7.66
Simulated annealing	1.08	2.30	3.54	1.75	3.82	5.78	2.42	5.47	8.49
Tabu search	0.82	2.16	3.74	1.47	3.82	6.77	2.34	6.04	10.75
Fuzzy steps	0.99	1.91	2.66	1.05	2.48	3.47	2.22	7.92	11.28

Conclusiones

- Error variance and relative sizes of the clusters strongly affect how well a clustering structure can be retrieved
- Two-mode *k*-means most often had the best performance, especially in favorable conditions
- When the optimal partition was hard to find, the AE and FS methods often performed well
- Sim. Annealing was also fairly well
- Tabu search had an inferior performance