Solving Medium and Large Size Problems of the Literature by the Accelerated Hyperbolic Smoothing Clustering Method

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Cluster Analysis

In the Cluster Analysis scope, algorithms use traditionally two main strategies:

- Hierarchical clustering methods
- Partition clustering methods...
- Here we introduce a New Approach for solving the problem...

Hyperbolic Smoothing Clustering Method - HSCM

General Problem Formulation:

$$S = \{S_1, \dots, S_m\}$$
 Set of m observations

$$x_i$$
, $i = 1,...,q$ Centroides of the clusters

$$z_j = \min_{i=1,\dots,n} ||s_j - x_i||$$
 Distance of the observation j to nearest centroide

Objective function specification

Minimize
$$\sum_{j=1}^{m} f(z_j)$$

where $f(z_j)$ is an arbitrary monotonic increasing function of the distance z_j .

Hyperbolic Smoothing Clustering Method - HSCM

General Problem Formulation:

Minimize
$$\sum_{j=1}^{m} f(z_j)$$

$$z_j = \min_{i=1,\dots,n} ||s_j - x_i||, j = 1,\dots,m$$

Trivial Examples of monotonic increasing functions:

$$\sum_{j=1}^{m} f(z_j) = \sum_{j=1}^{m} Z_j^2 \qquad \sum_{j=1}^{m} f(z_j) = \sum_{j=1}^{m} Z_j$$

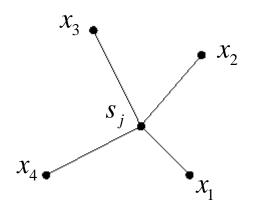
Possible Distance Metrics:

 L_2 (Euclidean) L_1 (Manhattan) L_∞ (Chebychev) L_p (Minkowshi)

1

HSCM: Resolution Methodology

The General Clustering Problem

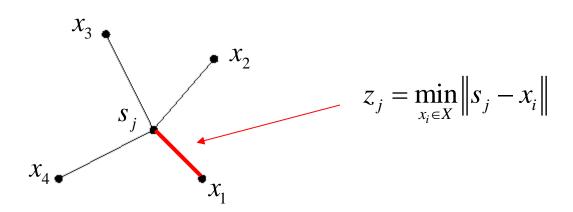


Consider a general observation point s_i .

Let be x_i , i=1,...,q, the centroids of clustersm where each set of these centroid coordinates will be represented by $X \in \mathbb{R}^{nq}$.

The General Clustering Problem

Consider a general observation point



Let be $x_i, i = 1, ..., q$, the centroids of clusters where each set of s_j these centroid coordinates will be represented by $X \in \Re^{nq}$. This procedure is strongly non differentiable.

Problem transformation

The general clustering problem is equivalent to the following problem:

(P1) Minimize
$$\sum_{j=1}^{m} f(z_j)$$
 Subject to:
$$z_j = \min_{i=1,\dots,q} \left\| s_j - x_i \right\| , \quad j = 1,\dots,m.$$

1

HSCM: Resolution Methodology

Problem transformation

From the problem (P1), it is obtained the relaxed problem:

(P2) Minimize
$$\sum_{j=1}^{m} f(z_{j})$$

Subject to: $z_{j} - ||s_{j} - x_{i}|| \le 0$, $j = 1,...,m$, $i = 1,...,q$.

Problem transformation

Let us use the auxiliary function

$$\psi(y) = \max\{0, y\}$$

From the inequalities

$$|z_j - ||s_j - x_i|| \le 0, \quad j = 1, ..., m, \quad i = 1, ..., q,$$

it follows:

$$\sum_{j=1}^{q} \Psi(z_{j} - ||s_{j} - x_{i}||) = 0, j = 1, \dots, m$$

4

HSCM: Resolution Methodology

Problem transformation

Using this set of equality constraints in place of the constraints in (P2), we obtain the following problem

(P3) Minimize
$$\sum_{j=1}^{m} f(z_j)$$
Subject to:
$$\sum_{i=1}^{q} \Psi(z_j - ||s_j - x_i||) = 0, j = 1, \dots, m$$

This problem corresponds also to a relaxation!!

Problem transformation

By performing a ε perturbation, it is obtained the problem:

(P4) Minimize
$$\sum_{j=1}^{m} f(z_{j})$$
Subject to:
$$\sum_{j=1}^{q} \Psi(z_{j} - ||s_{j} - x_{i}||) \ge \varepsilon, j = 1, \dots, m$$

4

HSCM: Resolution Methodology

Smoothing the problem

Let us define the auxiliary function

$$\phi(y,\tau) = (y + \sqrt{y^2 + \tau^2})/2$$

for
$$y \in \Re$$
 and $\tau > 0$.

Smoothing the problem

Function ϕ has the following properties:

(a)
$$\phi(y,\tau) > \Psi(y), \forall \tau > 0$$

(b)
$$\lim_{\tau \to 0} \phi(y, \tau) = \Psi(y)$$

(c) $\phi(y,\tau)$ is an increasing convex C^{∞} function.

Smoothing the problem

By using the Hyperbolic Smoothing approach for the problem (P4) it is obtained

(P5) Minimize
$$\sum_{j=1}^{m} f(z_{j})$$
Subject to:
$$\sum_{j=1}^{q} \phi(z_{j} - \|s_{j} - x_{i}\|, \tau) \ge \varepsilon, \quad j = 1, ..., m.$$



Smoothing the distance calculation

For the Euclidian metric, let us define the auxiliary function

$$\theta(s_j, x_i, \gamma) = \sqrt{\sum_{l=1}^{n} (s_{jl} - x_{il})^2 + \gamma^2}$$

for $\gamma > 0$.

Smoothing the Euclidian distance:

Function θ has the following properties:

(a)
$$\lim_{\gamma \to 0} \theta(s_j, x_i, \gamma) = ||s_j - x_i||_2;$$

(b) θ is a C^{∞} function.

Smoothing the problem

Therefore, it is now obtained the completely smooth problem:

(P6) Minimize
$$\sum_{j=1}^{m} f(z_{j})$$
Subject to:
$$\sum_{i=1}^{q} \phi(z_{j} - \theta(s_{j}, x_{i}, \gamma), \tau) \geq \varepsilon, \quad j = 1, ..., m.$$

Problem resolution

By considering the KKT conditions for the problem (P6), it is possible to conclude that all inequalities will certainly be active.

(P7) Minimize
$$\sum_{j=1}^{m} f(z_j)$$

Subject to:
$$h(x, z_j) = \sum_{i=1}^{q} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) - \varepsilon = 0, \quad j = 1, ..., m.$$

HS

HSCM: Resolution Methodology

Problem resolution

Therefore, by using the Implicit Function Theorem, it is obtained the unconstrained problem

(P8) Minimize
$$F(x) = \sum_{j=1}^{m} f(z_j)$$

where each z_j is obtained by the calculation of a zero of each equation

$$h(x,z_j) = \sum_{i=1}^{q} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) - \varepsilon = 0, \quad j = 1,...,m.$$

Problem resolution

Again, due to the Implicit Function Theorem, the functions $z_j(x)$ have all derivatives in relation to the variables x_i , i=1,...,q. So, it is possible to calculate the gradient of the objective function of the problem (P8)

$$\nabla F(x) = \sum_{j=1}^{m} \frac{df(z_j(x))}{dz_j} \nabla z_j(x)$$

where

$$\nabla z_{j}(x) = -\nabla h(x, z_{j}) / \frac{\partial h(x, z_{j})}{\partial z_{j}}.$$



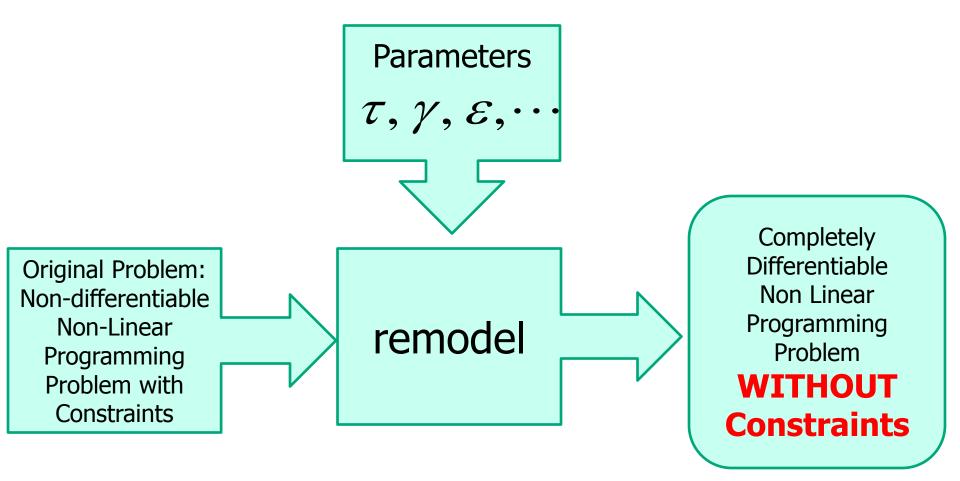
Problem resolution

Some remarks about the problem (P8):

It can be solved by making use of any method based in the first and second order derivatives information (conjugate gradient, quasi-Newton, Newton methods, etc).

It is defined in a *nq*-dimensional space, therefore a smaller dimension problem in relation to the original problem (P7).





Simplified HSC Algorithm

Initialization Step: Choose values $0 < \rho_1 < 1$, $0 < \rho_2 < 1$, $0 < \rho_3 < 1$; Choose initial values: x^0 , y^1 , τ^1 , ε^1 ; Let k = 1.

Main Step: Repeat indefinitely

Solve the unconstrained problem (P8)

minimize
$$F(x) = \sum_{j=1}^{m} f(z_j(x))$$

with $\gamma = \gamma^k$, $\tau = \tau^k$, $\varepsilon = \varepsilon^k$, starting at the initial point x^{k-1} , and let x^k be the solution obtained.

Let
$$\gamma^{k+1} = \rho_1 \gamma^k$$
, $\tau^{k+1} = \rho_2 \tau^k$, $\varepsilon^{k+1} = \rho_3 \varepsilon^k$, $k = k+1$.



Hyperbolic Smoothing Clustering Method

applied to:

Minimum Sum-of-Squares Clustering Problem



Hyperbolic Smoothing and Partition into Boundary and Gravitational Regions Applied to General Clustering Problem



The Computational Task of the HSC Algorithm

The most relevant computational task associated to HSC Algorithm is the determination of the zeros of m equations:

$$\sum_{i=1}^{q} \phi \left(z_j - \theta(s_j, x_i, \gamma), \tau \right) - \varepsilon = 0, \ j = 1, \dots, m$$



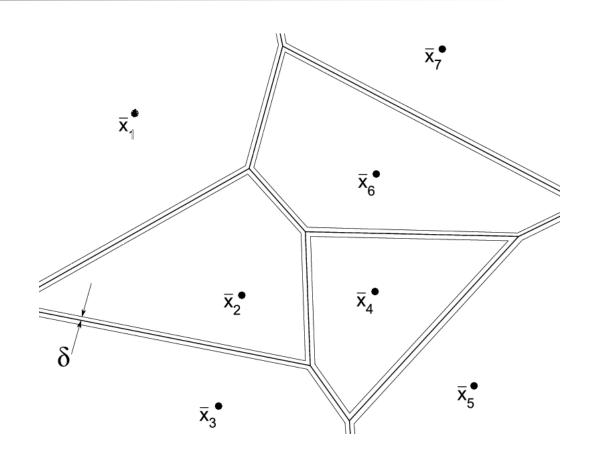
The Partition into Boundary and Gravitational Regions

The basic idea of the approach is the partition of the set of observations in two non overlapping parts:

- the first set corresponds to the observation points that are relatively close to two or more centroids;
- the second set corresponds to the observation points that are significantly close to a unique centroid in comparison with the other ones.



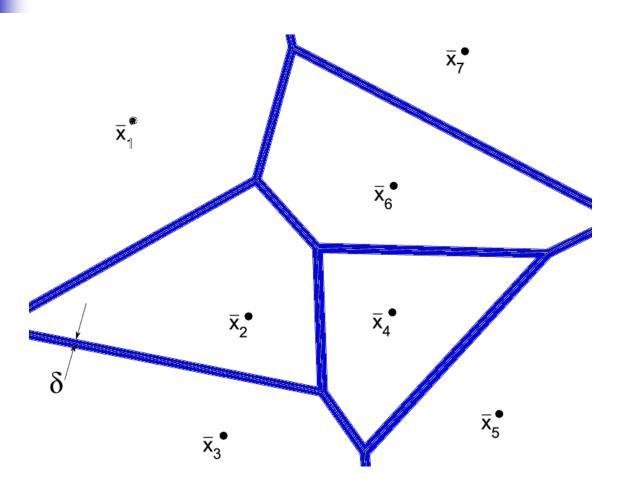
Partition of the Set of Observations



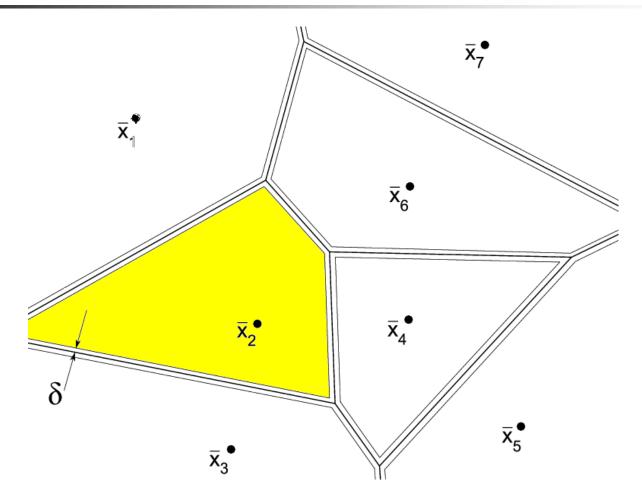
 \overline{x} : the referencial point

 δ : the band zone width

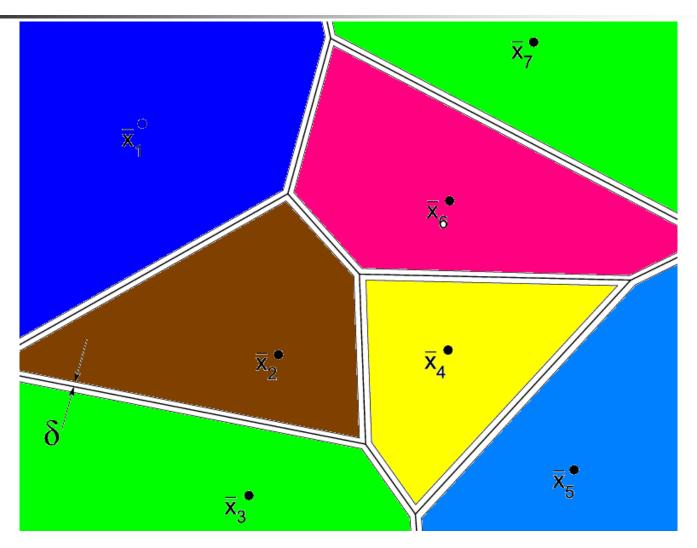
The Boundary Band Zone



Gravitational Region => \overline{x}_2



Gravitational Regions





The Partition of the Set of Observations

Let us define:

- J_R is the set of boundary observations;
- J_G is the set of gravitational observations.

Considering this partition, the objective function can be expressed in the following way:

Minimize
$$F(x) = \sum_{j=1}^{m} f(z_j) = \sum_{j \in J_B} f(z_j) + \sum_{j \in J_G} f(z_j)$$

So, the objective function can be expressed in the following way:

Minimize
$$F(x) = f_B(x) + f_G(x)$$

The First Component of the Objective Function

The component associated with the set of boundary observations, can be calculated by using the previous presented smoothing approach:

Minimize
$$F_B(x) = \sum_{j \in J_B} f(z_j)$$

where each z_i results from the calculation of a zero of each equation:

$$h(x,z_j) = \sum_{i=1}^{q} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) - \varepsilon = 0, j \in J_B$$



The component associated with the gravitational regions, can be calculated in a simpler form:

Minimize
$$F_G(x) = \sum_{i=1}^{q} \sum_{j \in J_i} f(||s_j - x_i||)$$

where J_i is the set of observations associated to cluster i .



Hyperbolic Smoothing and Partition into Boundary and **Gravitational Regions** Applied to Minimum Sum-of-Squares Clustering Problem



For The Minimum Sum-of-Squares Clustering formulation, the second component, associated with the gravitational regions, can be calculated in a direct form:

Minimize
$$F_G(x) = \sum_{i=1}^{q} \sum_{j \in J_i} \|s_j - v_i\|_2^2 + \sum_{i=1}^{q} |J_i| \|x_i - v_i\|_2^2$$

where J_i is the set of observations associated to centroid i v_i is the gravity center of cluster i.



The Gradient of the Second Component for the MSSC

The gradient of the second component, associated with the gravitational regions, can be calculated in an easy way:

$$\nabla F_G(x) = \sum_{i=1}^{q} 2|J_i| (x_i - v_i)$$

where J_i is the number the of observations associated to centroid i

Simplified Accelerated Algorithm: AHSCM

Initialization Step: Choose values $0 < \rho_1 < 1$, $0 < \rho_2 < 1$, $0 < \rho_3 < 1$;

Choose initial values: x^0 , γ^1 , τ^1 , ε^1 ; Let k = 1.

Specify the initial boundary band width: δ^1 .

Main Step: Repeat indefinitely

By using $\overline{x} = x^{k-1}$ and $\delta = \delta^k$ determine partitions J_B and J_G . Solve the problem

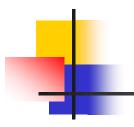
minimize
$$f(x) = \sum_{j \in J_B} z_j(x)^2 + \sum_{j \in J_G} z_j(x)^2$$

with $\gamma = \gamma^k$, $\tau = \tau^k$, $\varepsilon = \varepsilon^k$, starting at the initial point x^{k-1} , and let x^k be the solution obtained.

Redefine the boundary band width value δ^{k+1} .

Let
$$\gamma^{k+1} = \rho_1 \gamma^k$$
, $\tau^{k+1} = \rho_2 \tau^k$, $\varepsilon^{k+1} = \rho_3 \varepsilon^k$, $k = k+1$.





Hyperbolic Smoothing Clustering & Accelerated HSC Methods Results published in Pattern Recognion 44 (2011) 70-77

	£	Algorit	hm HSC	Algorithm	Speedun	
q	\mathbf{f}_{opt}	Error	Time (s)	Error	Time (s)	Speed up
2	0.31688E10	0.05	0.60	0.05	0.07	8.6
10	0.56025E09	0.01	16.16	0.01	0.28	57. 7
20	0.26681E09	-0.02	62.90	0.05	0.59	107
30	0.17557E09	-0.08	169.17	0.31	0.86	197
40	0.12548E09	-0.06	333.92	-0.11	1.09	306
50	0.98400E08	0.50	662.33	0.44	1.36	487
60	0.82006E08	-1.09	1049.97	-0.80	1.91	550
80	0.61217E08	-0.31	2038.31	-0.73	6.72	303
100	0.48912E08	-0.90	3499.76	-0.60	9.79	357

Comparison of Results: Pla85900

Hyperbolic Smoothing Clustering & Accelerated HSC Methods Results published in Pattern Recognion 44 (2011) 70-77

-	f	Algori	thm HSC	Algorithm	Speed up	
q	$ m f_{opt}$	Error	Time (s)	Error	Time (s)	speed up
2	0.37491E16	0.86	23.07	0.58	3.65	6.3
3	0.22806E16	0.00	47.41	0.04	4.92	9.6
4	0.15931E16	0.00	76.34	0.00	5.76	13.3
5	0.13397E16	0.80	124.32	1.35	7.78	16.0
6	0.11366E16	0.12	173.44	1.25	7.87	22.0
7	0.97110E15	0.42	254.37	0.87	9.33	27.3
8	0.83774E15	0.55	353.61	0.37	12.96	27.3
9	0.74660E15	0.68	438.71	0.25	13.00	33.8
10	0.68294E15	0.29	551.98	0.46	14.75	37.4



Hyperbolic Smoothing Applied to Minimum Sum-of-Squares Clustering Problem

Bagirov et al - December 2012



Computational Optimization and Applications

An incremental clustering algorithm based on hyperbolic smoothing

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Comparison Results

General k-means, Modified General, Hyperbolic Smoothing

D15112

		GKM			MGKM			SMOOTH		
q	f _{opt}	E	α	t	E	α	t	E	α	t
2	0.36840·10 ¹²	0.00	0.22	2.75	0.00	0.46	4.51	0.00	0.42	5.15
5	0.13271-10 ¹²	0.00	0.92	8.50	0.00	1.83	13.85	0.00	1.52	18.41
10	0.64892 - 10 ¹¹	0.78	2.07	14.87	0.78	4.12	24.98	0.00	3.44	41.50
15	0.43136-10 ¹¹	0.26	3.24	21.00	0.26	6.44	35.51	0.00	5.74	68.23
20	0.32177-10 ¹¹	0.25	4.43	26.99	0.25	8.77	45.68	0.00	8.65	101.82
25	0.25423-10 ¹¹	0.03	5.62	32.71	0.03	11.11	55.47	0.00	11.96	139.53

Comparison Results

General k-means, Modified General k-means, Hyperbolic Smoothing Pla85900

			GKI	И	MGKM			SMOOTH		
q	f_{opt}	Е	α	t	E	α	t	E	α	t
2	0.37491·10 ¹⁶	0.00	0.07	89.54	0.00	0.15	115.99	0.00	0.12	123.96
5	0.13397 - 10 ¹⁶	0.00	0.30	408.60	0.00	0.59	512.31	0.00	0.37	452.96
10	0.68294 - 10 ¹⁵	0.00	0.67	754.67	0.00	1.33	994.29	0.00	0.79	1011.17
15	0.46029-10 ¹⁵	0.51	1.04	1083.04	0.51	2.07	1448.94	0.00	1.24	1596.67
	$0.35087 \cdot 10^{15}$									
25	0.28323-10 ¹⁵	0.74	1.80	1570.37	0.73	3.57	2186.20	0.00	2.21	2863.18

Very Large Clustering Instances

Hyperbolic Smoothing and Partition into Boundary and Gravitational Regions Applied to Minimum Sum-of-Squares Clustering Problem

Synthetic Problems – 03/2013

Synthetic Problem 5.000.000 Observations Euclidian Space with n = 10 dimensions

q	f _{AHSC-L2}	Occur.	E _{Mean}	T _{Mean}
2	0.456807E7	3	0.94	16.12
3	0.373567E7	1	1.21	24.69
4	0.323058E7	1	0.91	32.90
5	0.274135E7	1	0.09	26.06
6	0.248541E7	1	0.04	36.55
7	0.222897E7	1	0.19	43.24
8	0.197977E7	2	0.12	45.38
9	0.173581E7	2	0.10	42.78
10	0.149703E7	10	0.00	32.98
С	0.150000E7	-	-	-

Medium and Large Clustering Instances

Hyperbolic Smoothing and Partition into Boundary and Gravitational Regions Applied to Minimum Sum-of-Squares Clustering Problem

Comparison with Bagirov et al

January-April 2014



Medium Size Instances Starting Point - Tight Way

		Gk	(M	мдкм		нѕсм		AHSCM	
k	F _{opt}	E	t	E	t	E	t	E	t
2	1,93E08	0	0	0	0.02	0	0.05	0.00	0.04
5	1,37E08	2.28	0.03	1.86	0.05	0	0.61	0.00	0.14
10	1,02E08	0.26	0.06	0.28	0.11	0	2.14	0.16	0.37
15	8,69E07	1.02	0.08	1.07	0.16	0	9.08	-0.36	0.62
20	7,65E07	3.64	0.11	1.80	0.20	0	27.36	-0.19	1.12
25	6,90E07	5.08	0.14	0.93	0.27	0	44.65	0.11	1.53



Medium Size Instances Starting Point - Tight Way

		GKM		МСКМ		нѕсм		AHSCM	
k	F _{opt}	E	t	E	t	E	t	Ε	t
2	3,17E13	0	0.06	0	0.11	0	0.25	0.06	0.11
5	1,20E13	0	0.25	0	0.39	0	0.98	0.00	0.21
10	5,60E12	2.78	0.48	0.58	0.81	0	2.64	0.56	0.69
15	3,56E12	0.07	0.70	1.06	1.20	0	5.16	0.03	1.40
20	2,67E12	2.00	0.94	0.48	1.61	0.11	8.86	0.22	2.39
25	2,15E12	0.78	1.20	0.23	1.98	0.01	14.01	0.18	3.84



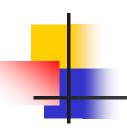
Pendigit (m=10992, n=16)

		GI	(M	MGKM		HSCM		AHSCM	
k	F _{opt}	E	t	Ε	t	E	t	E	t
2	1,28E12	0.39	2.56	0	5.23	0	5.37	0.00	0.38
5	7,53E11	0	9.73	0	18.72	0	22.60	0.00	1.76
10	4,93E11	0	20.45	0	39.31	0	61.71	0.00	4.99
15	3,91E11	0	30.79	0	59.19	0	120.46	0.00	10.33
20	3,41E11	0	41.25	0.17	78.37	0.16	250.80	-0.31	19.21
25	3,00E11	0.24	51.87	0.24	98.47	0	446.37	-0.12	33.06

Large Size Instances Starting Point - Tight Way

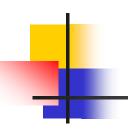
D15112 (m=15112, n=2)

		GI	ΚM	MGKM		нѕсм		AHSCM	
k	F _{opt}	E	t	Ε	t	E	t	Ε	t
2	3,68E15	0	2.75	0	4.51	0	5.15	0.00	0.31
5	1,33E15	0	8.50	0	13.85	0	18.41	0.00	1.36
10	6,49E14	0.78	14.87	0.78	24.98	0	41.50	-0.62	4.21
15	4,31E14	0.26	21.00	0.26	35.51	0	68.23	0.15	9.31
20	3,22E14	0.25	26.99	0.25	45.68	0	101.82	0.62	17.43
25	2,54E14	0.03	32.71	0.03	55.47	0	139.53	-0.49	30.22



Large Size Instances Starting Point - Tight Way

		S	huttle	(m=	58000	, n=9))		
		G	KM	MGKM		Н	SCM	AHSCM	
k	F _{opt}	E	t	E	t	E	t	E	t
2	2,13E13	0	63.20	0	123.82	0	86.74	0.00	0.20
5	7,24E12	0	251.65	0	521.81	0	351.50	0.00	1.35
10	2,83E12	0.02	581.28	0	1207.20	0	813.73	0.00	4.87
15	1,53E12	0	888.24	0	1776.88	0	1272.75	0.00	11.09
20	1,06E12	0	1195.84	0	2338.99	0	1798.88	-3.60	26.80
25	7,98E11	0.17	1512.55	0.17	2917.41	0	2396.82	-3.13	51.97



Large Size Instances Starting Point - Tight Way

Pla85900 (m=85900 , n=2)									
		GKM		МСКМ		HSCM		AHSCM	
k	F _{opt}	E	t	E	t	E	t	E	t
2	3,75E19	0	89.54	0	115.99	0	123.96	0.00	1.17
5	1,34E19	0	408.60	0	512.31	0	452.96	0.00	5.04
10	6,83E18	0	754.67	0	994.29	0	1011.17	0.00	15.66
15	4,60E18	0.51	1083.04	0.51	1448.94	0	1596.67	0.00	38.01
20	3,51E18	0.01	1355.85	0	1844.34	0	2210.91	0.00	73.09
25	2,83E18	0.74	1570.37	0.73	2186.20	0	2863.18	0.13	135.62



Conclusions



Conclusions

In view of the preliminary results obtained, where the proposed methodology performed efficiently and robustly, these algorithms can represent a possible approach for dealing with the solving of clustering of problems of real applications.



END