Strong bounds for large-scale Minimum Sum-of-Squares Clustering

Veronica Piccialli

Sapienza University of Rome

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FAIR project

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Sapienza: Spoke 5 High Quality AI:

Task 5.7.3 – High Quality AI by means of Optimization

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NextGenerationEU

Ministero dell'Università e della Ricerca

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PIANO NAZIONALE DI RIPRESA E RESILIENZA

Future Artificial Intelligence Research

Minimum Sum of Squares Clustering

It starts from a visit of Angelika Wiegele[a] in 2019:
V. Piccialli, A. M. Sudoso and A. Wiegele.
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V. Piccialli and A. M. Sudoso. Global optimization for cardinality-constrained minimum sum-of-squares clustering via semidefinite programming, **Mathematical Programming** (2023)

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Large scale MSSC

Idea

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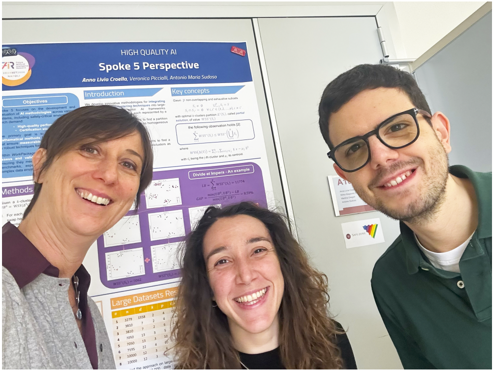

Joint work with Anna Livia Croella Assistant Professor at Mercatorum and Antonio Maria Sudoso my colleague at DIAG-Sapienza

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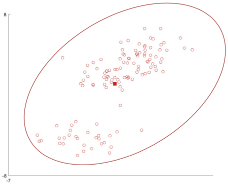
MSSC Clustering

We focus on the **Minimum Sum of Squares Clustering** problem.
Given n data points $x_1, \ldots, x_n$ in $\mathbb{R}^d$, partition them into k clusters by minimizing the total squared distance between each point and the cluster center.



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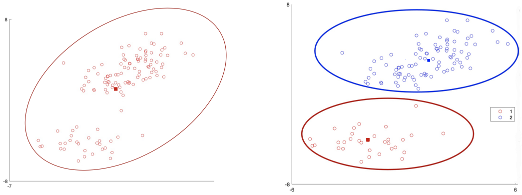

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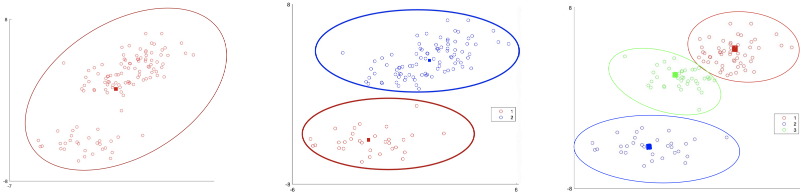

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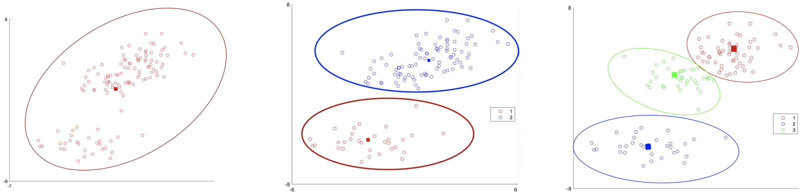

Given a cluster assignment, the optimal cluster center is the average of the points in the cluster.

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Mathematical formulation

The mathematical formulation is

$$\begin{aligned} \min \quad & \sum_{i=1}^{n}\sum_{j=1}^{k} \delta_{ij}||x_i - m_j||_2^2 \\ & \sum_{j=1}^{k} \delta_{ij} = 1 \quad i = 1, \ldots, n \\ & \delta_{ij} \in \{0.1\},\; m_j \in \mathbb{R}^d \quad i = 1, \ldots, n,\; j = 1, \ldots, k \end{aligned} \tag{MSSC}$$

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(MSSC) is NP-hard even for $k = 2$ or $d = 2$ (Aloise, Deshpande, Hansen, and Popat 2009)

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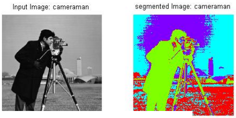
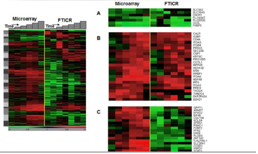
Applications

1. Image segmentation

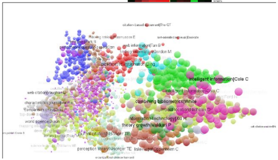


2. credit risk evaluation

3. biology



4. document clustering



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Literature Review

Heuristic methods

✓ *k*-means (MacQueen 1967; Lloyd 1982) heuristic ($\approx$ 3M references in Google Scholar 2024) is the most popular heuristic for solving MSSC.

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- ✓ Standard metaheuristic algorithms:simulated annealing (Lee and Perkins 2021), tabu search (Al-Sultan 1995), variable neighborhood search (Hansen and Mladenovic 2001; Orlov, Kazakovtsev, Rozhnov, Popov, and Fedosov 2018), iterated local search (Likas, Vlassis, and Verbeek 2003), evolutionary algorithms (Maulik and Bandyopadhyay 2000; Karmitsa, Bagirov, and Taheri 1997).

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- ✓ DC (Difference of Convex functions) programming for clustering large datasets (Tao et al. 2014; Bagirov, Taheri, and Ugon 2016; Karmitsa, Bagirov, and Taheri 2017; Karmitsa, Bagirov, and Taheri 2018).

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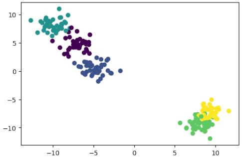
- ✓ The k-means algorithm is also used as a local search subroutine in various algorithms, such as population-based metaheuristics (Mansueto and Schoen 2021)

The importance of the global minimum

200 points in the plane $k = 5$



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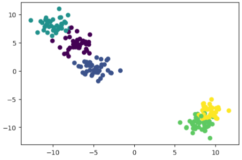
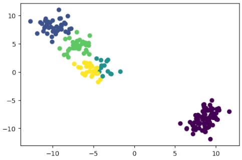


Heuristic solution



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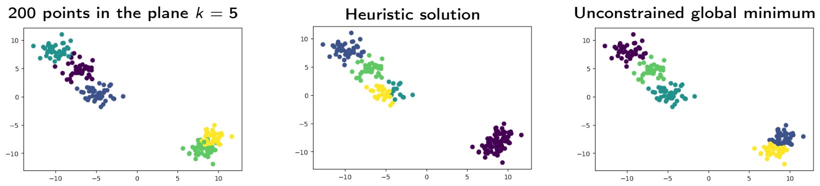

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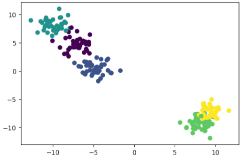

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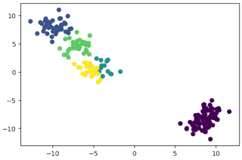
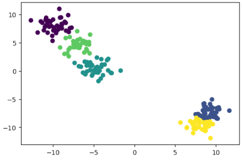


Unconstrained global minimum



Interpretation derived by the heuristic solution can be completely wrong!

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Literature Review - Exact

Three main approaches:

B& B (Koontz, Narendra, and Fukunaga 1975), (Diehr 1985), and RBBA (Brusco 2006) are B& B algorithms where the lower bound is computed by solving smaller instances and exploiting the properties of MSSC. (Sherali and Desai 2005) employs the reformulation-linearization technique (RLT) to derive lower bounds by transforming the non-linear problem into a 0-1 mixed-integer program. (Burgard, Moreira Costa, Hojny, Kleinert, and Schmidt 2023) focus on mixed-integer programming techniques to improve solver performance.

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SDP Peng (Peng and Xia 2005; Peng and Wei 2007) showed the equivalence between MSSC and a 0-1 SDP reformulation. Aloise and Hansen 2009 developed a branch-and-cut algorithm based on the linear programming relaxation of the 0-1 SDP model. Piccialli, Sudoso, and Wiegele 2022 proposed SOS-SDP, a branch-and-bound algorithm using SDP relaxation and polyhedral cuts, capable of solving real-world instances with up to 4.000 data points.

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3. a branching rule based on the problem
4. We manage to exploit the must link constraints to reduce the size of the SDPs for computing the lower bound

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SDP reformulation

Unconstrained Problem (MSSC) can be reformulated as a **nonlinear** SDP problem [Peng & Wei 2007]:

$$\begin{aligned} \min \quad & \sum_{i=1}^{n}\sum_{j=1}^{k} \delta_{ij} ||x_i - m_j||_2^2 \\ & \sum_{j=1}^{k} \delta_{ij} = 1 \quad i = 1, \dots, n \\ & \delta_{ij} \in \{0.1\} \\ & m_j \in \mathbb{R}^d \quad i = 1, \dots, n, \; j = 1, \dots, k \end{aligned} \qquad \text{(MSSC)}$$

$$\begin{aligned} \min \quad & \langle WW^T, I - Z \rangle \\ & Ze = e \\ & \text{trace}(Z) = k \\ & Z \geq 0 \\ & Z = Z^T \\ & Z^2 = Z \end{aligned} \qquad \text{(SDP} - \text{MSSC)}$$

where $W \in \mathbb{R}^{n \times d}$ is the data matrix obtained by stacking the data points x_i for all i, $e \in \mathbb{R}^n$ is the vector of all ones and $I \in \mathbb{R}^{n \times n}$ is the identity matrix.

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Problem (MSSC) and (SDP-MSSC) are equivalent.

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  - $x_1, x_2, x_3, x_4, x_5, x_6,$ $\quad Z = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}$

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SDP relaxation

Problem (SDP-MSSC) can be rewritten as an SDP with an additional rank constraint:

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By dropping the non-convex constraint $rank(Z) = k$, we obtain the Semidefinite Programming (SDP) relaxation [Peng, Wei 2007]

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$$\begin{aligned} \min \quad & \langle WW^T, I - Z\rangle \\ & Ze = e \\ & \mathrm{trace}\,(Z) = k \\ & \mathrm{rank}\,(Z) = k \\ & Z \geq 0 \\ & Z \succeq 0 \end{aligned} \qquad \text{(SDP} - \text{MSSC)}$$

By dropping the non-convex constraint $rank(Z) = k$, we obtain the Semidefinite Programming (SDP) relaxation [Peng, Wei 2007]

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In order to tighten the bound, we add valid inequalities of different classes with a cutting plane procedure.

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Triangle if i and j are in the same cluster and i and h are in the same cluster, then j and h must be in the same cluster [Peng, Wei 2007], that translates into

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Clique if the number of clusters is k, given any subset Q of $k + 1$ points, it must hold that at least two points have to be in the same cluster:

$$\sum_{(i,j) \in Q, i<j} Z_{ij} \geq \frac{1}{n - k + 1} \quad \forall Q \subset \{1, \dots, n\}, |Q| = k + 1$$

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We remove at each iteration the added inequalities that are not active to keep the size of the SDP tractable

Branching Decision

Cannot Link Node Points i and j in different clusters:

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In a matrix Z corresponding to a clustering, for each pair (i, j) either $Z_{ij} = 0$ or $Z_{i\cdot} = Z_{j\cdot}$. Select a pair of data points to branch on:

$$\max_{i,j}\{\min\{Z_{ij}, \|Z_{i\cdot} - Z_{j\cdot}\|^2\}\}$$

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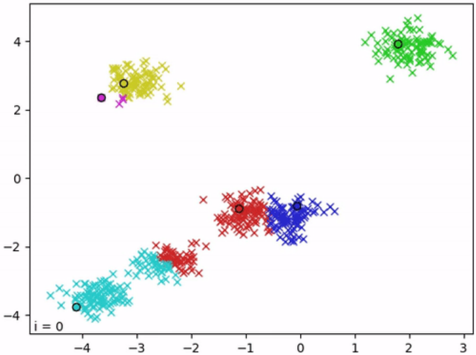
Note:

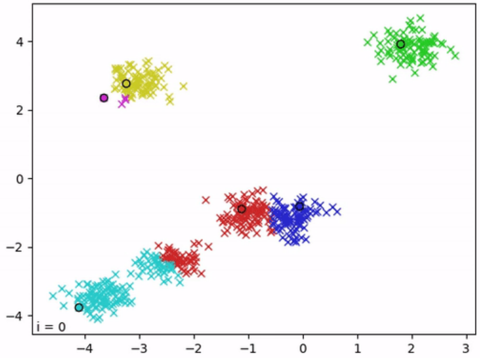
In the B&B nodes we add **instance level constraints**!

K-means Algorithm



Kmeans alternates two phases:

K-means Algorithm



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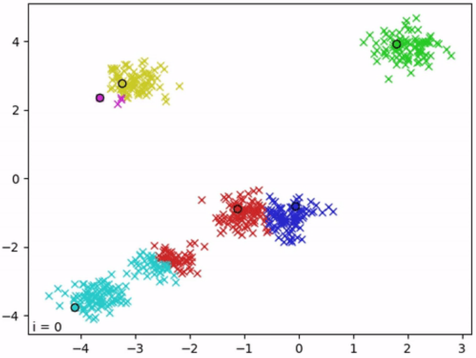

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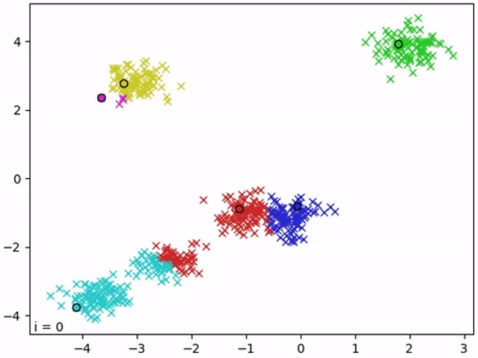

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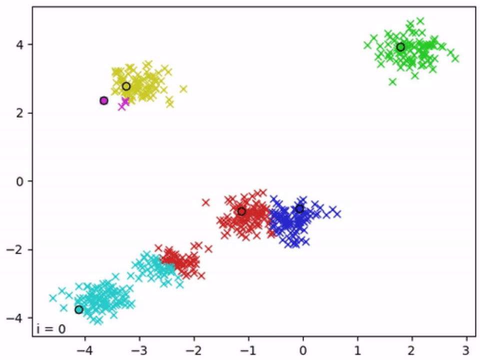

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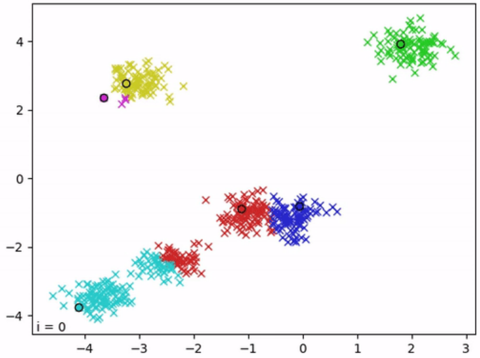

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At each node, we have additional constraints (must link and cannot link), we need a **constrained version**!

IPC-k-means (Baumann 2020)

Input Data points $p_1, \ldots, p_n$, initial cluster centers $m_1, \ldots, m_k$, must-link $\mathcal{ML}$ and cannot-link $\mathcal{CL}$ constraints

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Center Initialization

The center initialization is based on the SDP solution

Results

SOS-SDP solves instances up to **4000** points, before up to 1000 only in the plane or 2300 but for $k \geq 230$ (n/k small) (Aloise, Hansen, and Liberti 2012b). Recent paper by Aloise and Sudoso up to 6000 datapoints on the plane. Our code: `https://github.com/antoniosudoso/sos-sdp`

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Can we exploit SOS-SDP to give some optimality guarantees for large scale (10000 points) instances?

Lower bound

Let the dataset $O = \{p_1, \ldots, p_N\}$ be partitioned into T subsets $\{S_1, \ldots, S_T\}$ such that $\cup_{t=1}^{T} S_t = O$ and $S_i \cap S_j = \emptyset$

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Assume also that the optimal value of the MSSC problem on each subset is available, i.e. let

$$MSSC(S_t, k) = \min_{\delta_{ij}^t} \sum_{j=1}^{K} \sum_{i \in S_t} \delta_{ij}^t \|p_i - \mu_j^t\|^2 \tag{1a}$$

$$\text{s.t.} \sum_{j=1}^{K} \delta_{ij}^t = 1, \quad \forall i \in S_t \tag{1b}$$

$$\sum_{i \in S_t} \delta_{ij}^t \geq 1, \quad \forall j \in \{1, \ldots, K\} \tag{1c}$$

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Lower Bound

$$MSSC(O, k) \geq \sum_{t=1}^{T} MSSC(S_t, k) \geq \sum_{t=1}^{T} LB(S_t, k). \qquad LB$$

for any valid lower bound $LB(S_t, k)$ on the objective of Problem (1).

Literature

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The bound is used again in (Brusco 2006), where the algorithm begins with the application of branch-and-bound for $k + 1$ objects and subsequently adds objects, one at a time, until all n objects are included. Each time a new object is added, the branch-and-bound algorithm is repeated (or reapplied). The algorithm is improved by a smart ordering of the data points

Idea: decomposition in smaller instances

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Good news: We can use SOS-SDP to compute $MSSC(S_t, k)$ or $LB(S_t, k)$ (few nodes of the B&B tree) **as long as the size of S_t is not too large**

Less good news: The quality of the bound heavily depends on the partition!

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Research question

How to choose the partitions S_t in order to have a very good bound (possibly optimal)??

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Anticlustering

Ideally, we would like to **find the partition of O in subsets of equal size providing the best bound**, that is solving the following problem:

$$\max_{\xi_{it}} \sum_{t=1}^{T} MSSC(S_t, k) \tag{2a}$$

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Too hard, the lower level problem is NP-hard already

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Using the lower bound for validation

In general, the computation of the lower bound is needed to prove the validity of a certain heuristic solution.

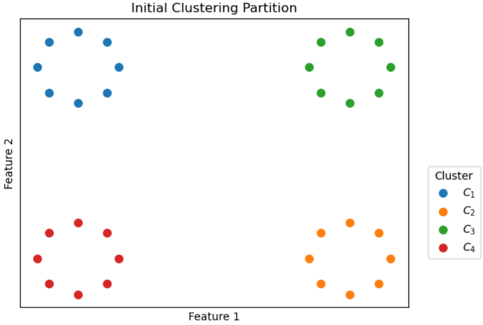

Figure: $MSSC(O, 4) = 287.82$

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Assume we have the optimal solution (δ_{ij}^*) of the original MSSC problem, and a partition of O.

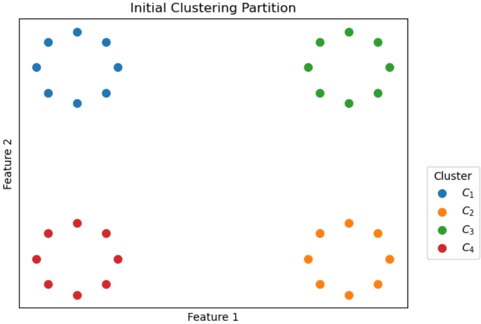
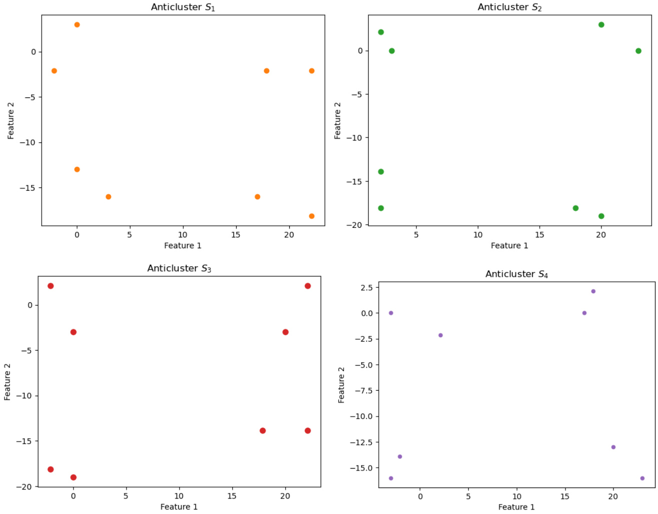
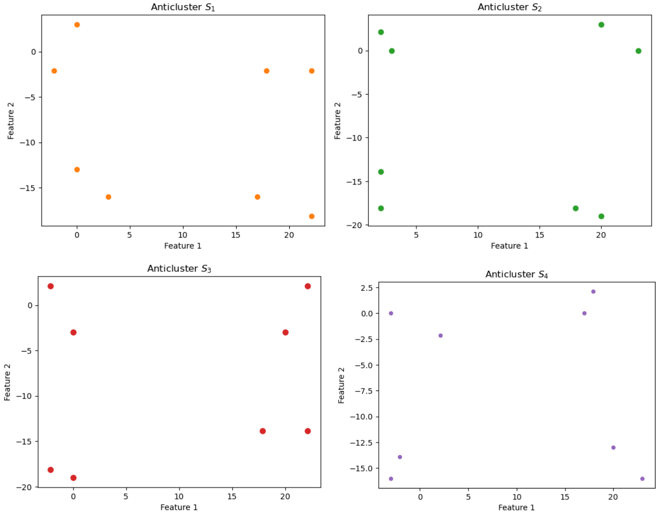


Figure: $MSSC(O, 4) = 287.82$

Partition


Anticluster S_1
Anticluster S_2
Anticluster S_3
Anticluster S_4
Feature 1
Feature 2

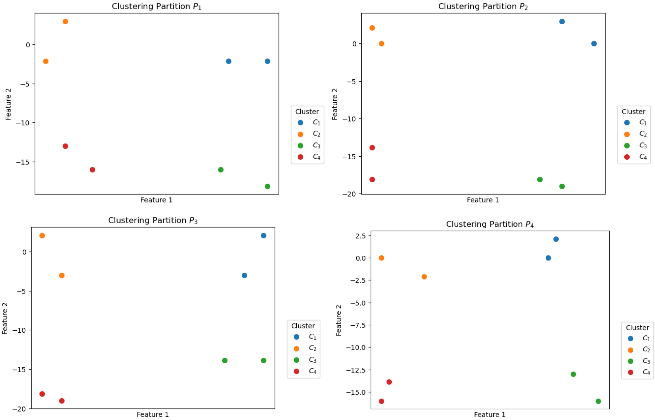
Partition



We can define the projection of the optimal solution on the single partition.

Projection

We can define the projection of δ_{ij}^*:



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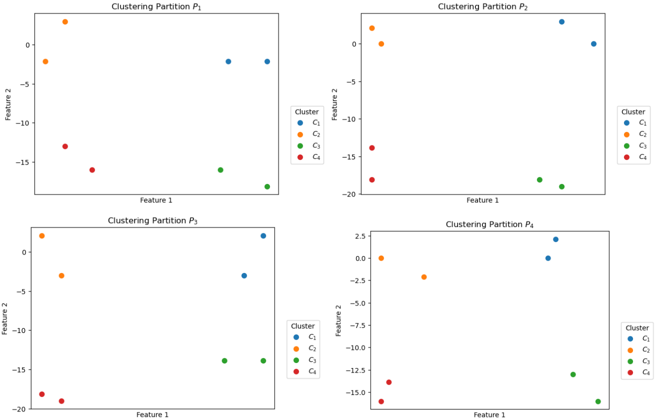
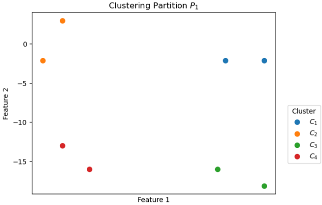


If the clusters are well separated, the projection is optimal for each subset (as in this example)

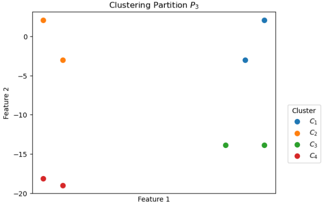
Quality of the bound

What is the quality of this partition?:

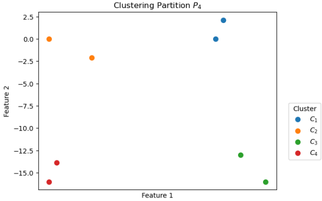


(a) $MSSC(S_{\mathbf{1}}, 4) = 48.69695$

(b) $MSSC(S_{\mathbf{2}}.4) = 23.25395$



(c) $MSSC(S_{\mathbf{3}}.4) = 42.33187$



(d) $MSSC(S_{\mathbf{3}}.4) = 29.62268$

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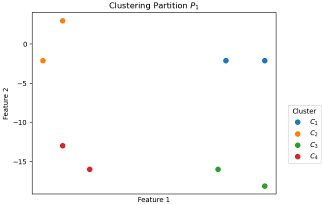

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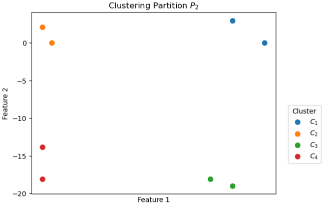

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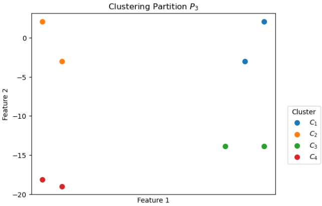

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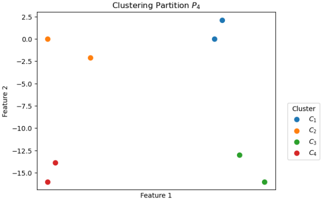

(d) $MSSC(S_{\mathbf{3}}.4) = 29.62268$

Summing up the different contribution of each subset we get a lower bound $LB = 143.90546$ with a gap of around 50%!!!

Our problem

What makes a partition "good"?

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Let's look at the objective function of MSSC:

$$\sum_{j=1}^{K} \sum_{i \in S_t} \delta_{ij}^t \|p_i - \mu_j^t\|^2$$

with

$$\mu_j^t = \frac{\sum_{i=1}^{N} p_i \delta_{ij}^t}{\sum_{i=1}^{N} \delta_{ij}^t}$$

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It can be rewritten as

$$\sum_{j=1}^{K} \frac{\sum_{i=1}^{N} \sum_{i'=1}^{N} \delta_{ij}^t \delta_{i'j}^t ||p_i - p_{i'}||^2}{\sum_{i=1}^{N} \delta_{ij}^t}$$

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The contribution of the single anticluster is larger for larger distances among points in the same cluster (in that anticluster)

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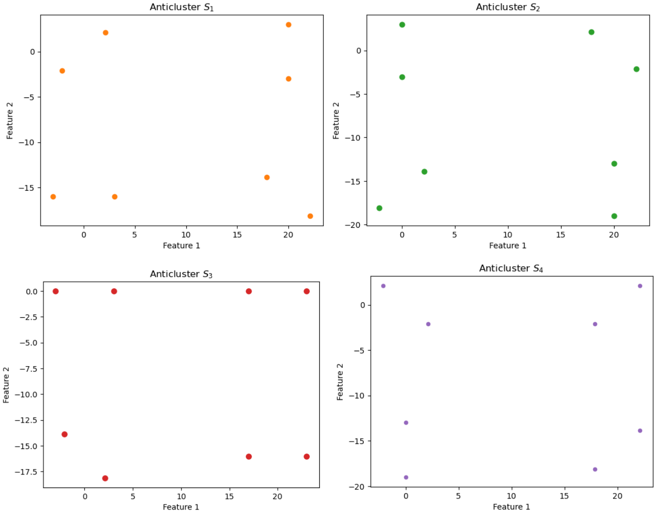
A different partition



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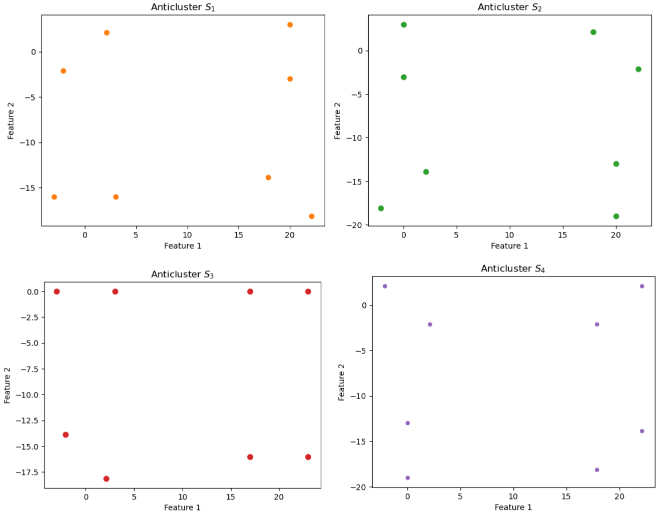
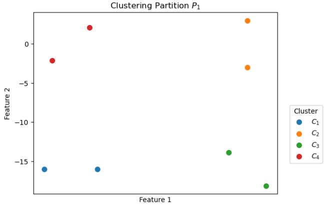


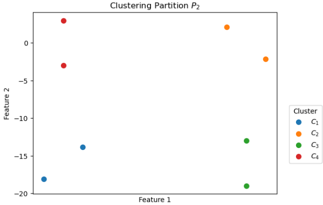
The single anticluster better "represents" the original dataset

Quality of the bound

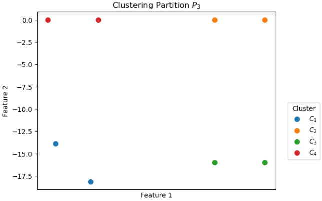
What is the quality of this partition?:



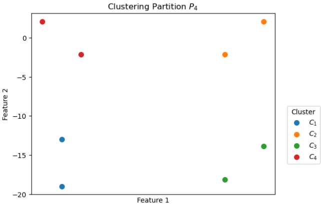
(a) $MSSC(S_{\mathbf{1}}, 4) = 71.97703$



(b) $MSSC(S_{\mathbf{2}}.4) = 71.93196$



(c) $MSSC(S_{\mathbf{3}}.4) = 71.97695$



(d) $MSSC(S_{\mathbf{4}}.4) = 71.93248$

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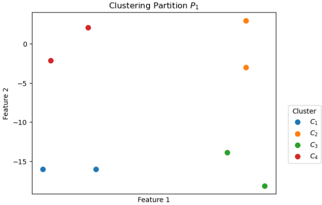

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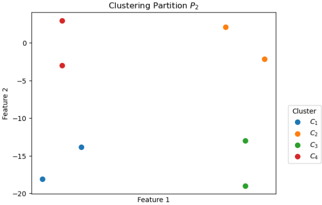

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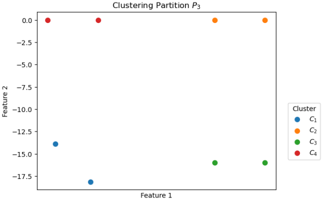

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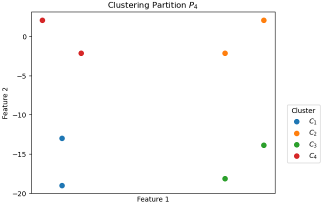

(d) $MSSC(S_{\mathbf{4}}.4) = 71.93248$

Summing up the different contribution of each subset we get a lower bound $LB = 287.81842$ with a gap of around 0%!!!

Assumption

Assume that we have a feasible (possibly optimal) solution (δ^*_{ij}) of the original MSSC problem, and that for any partition of the dataset the projection of δ^* on the partition is still optimal. This implies that the optimal solution of the MSSC(S_t) is still δ^* restricted to S_t.

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Under this assumption, problem 2 can be written as follow:

$$\max_{\xi_{it}} \sum_{t=1}^{T} \sum_{k=1}^{K} \sum_{i \in C(k)} \sum_{j \in C(k): j \neq i} \frac{\|p_i - p_j\|^2}{N_k / T} \cdot \xi_{it} \cdot \xi_{jt} \tag{3a}$$

$$\text{s.t.} \sum_{t=1}^{T} \xi_{it} = 1, \quad \forall i \in \{1, \dots, N\} \tag{3b}$$

$$\sum_{i \in C(k)} \xi_{it} = \frac{|C(k)|}{T}, \quad \forall t \in \{1, \dots, T\} \, \forall k \in \{1, \dots, K\} \tag{3c}$$

$$\xi_{it} \in \{0, 1\}, \quad \forall i \in \{1, \dots, N\} \, \forall t \in \{1, \dots, T\}. \tag{3d}$$

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Problem 3 can be decomposed in K independent subproblems, one for each cluster $C(k)$ with $k \in \{1, \cdots, K\}$. We have that:

$$\max_{\xi_{it}} \sum_{t=1}^{T} \sum_{i \in C(k)} \sum_{j \in C(k): j \neq i} \frac{\|p_i - p_j\|^2}{N_k / T} \cdot \xi_{it} \cdot \xi_{jt} \tag{4a}$$

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Each subproblem (4) can be linearized by introducing a binary variable for every pair of points and for every anticluster $t \in \{1, \cdots, T\}$.

Related literature

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The idea is to partition elements into disjoint groups with the goal of obtaining **high between-group similarity** and **high within-group heterogeneity**.

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Anticlustering

One of the most common objective functions is the sum of the (squared) distances of the points in the anticluster (group) that is exactly our objective function

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Our idea

We define our heuristic for our version of the anticlustering problem

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Our evaluation algorithm

S1. Compute a heuristic solution by k-means with objective value $UB(\delta^*_{ij})$

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S2. Compute a partition of the dataset $\{S_1, \ldots, S_T\}$ by heuristically solving problems (4)

S3. Compute the lower bound $(LB(\delta^*_{ij}))$

S4. Return the optimality gap

$$\gamma_{\mathrm{LB}} = \frac{UB(\delta^*_{ij}) - LB(\delta^*_{ij})}{UB(\delta^*_{ij})}$$

Anticlustering heuristic

We aim to find a good feasible solution for the following problems (one for each $C(k)$ induced by the solution δ^*_{ij}, they can be solved in parallel)

$$\max_{\xi_{it}} \sum_{t=1}^{T} \sum_{i \in C(k)} \sum_{j \in C(k): j \neq i} \frac{\|p_i - p_j\|^2}{N_k / T} \cdot \xi_{it} \cdot \xi_{jt}$$

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$$\xi_{it} \in \{0, 1\}, \quad \forall i \in C(k)\ \forall t \in \{1, \dots, T\}. \tag{5a}$$

Random Generate a random balanced partition for each $C(k)$.

Mounting Solve a MILP for finding the optimal "mounting" of the generated anticlusters

Improve Try to improve the current partition by a swap procedure: we try to swap points exchanging points close to the centroid of the cluster in the anticluster with points far away from the center in the same cluster but in a different anticluster (larger contribution to the objective)

Swap evaluation

How to decide whether a swap improves my lower bound?

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$$\tilde{LB} = \sum_{t=1}^{T} \tilde{UB}_t$$

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If the bound improves, the swap is implemented and the procedure keeps going until no improvement is achieved (or a time limit is reached)

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Actual lower bound computation

Once we have the final anticlusters,with corresponding estimated gap $\gamma^+ = \frac{UB - LB^+}{UB}$, we compute the real lower bound by applying SOS-SDP on each anticluster (in parallel)

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We need to choose whether to run it only at the root node, or allowing for some branching to improve the lower bound, there is a trade off related also to the size of each subproblem (number of anticlusters)

We need to choose the number of anticlusters, the quality of the bound can oscillate

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Experimental setup

We run SOS-SDP on each anticluster only at the root node, allowing the default cutting plane procedure for computing the bound:

1. As for the pair and triangle inequalities, we randomly separate at most 100000 valid cuts, we sort them in decreasing order with respect to the violation, and we select the first 10% of violated ones, yielding at most 10000 pairs and at most 10000 triangles added in each cutting-plane iteration.

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3. Finally, we set the accuracy tolerance of SDPNAL+ to 10^{-4}
4. The lower bound is valid since we postprocess the output of the SDP solver (to be improved)

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Two toy examples

Table: Toy datasets

Dataset	N	D	K
pr1002	1002	2	4
Synthetic	900	2	9

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Dataset	N	D	K
`pr1002`	1002	2	4
`Synthetic`	900	2	9

The two instances are on the plane. We use them to visualize what happens in two very different cases: one where the clusters are well separated and one where they are not well separated

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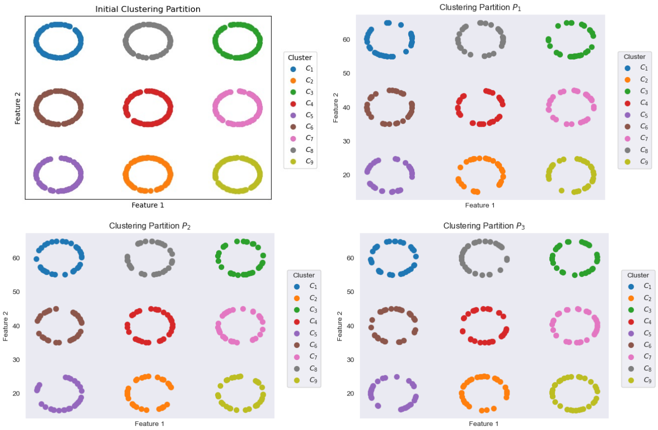
Synthetic- Random Initial Partition

900 points, 9 cluster each with 100 points, 3 anticlusters



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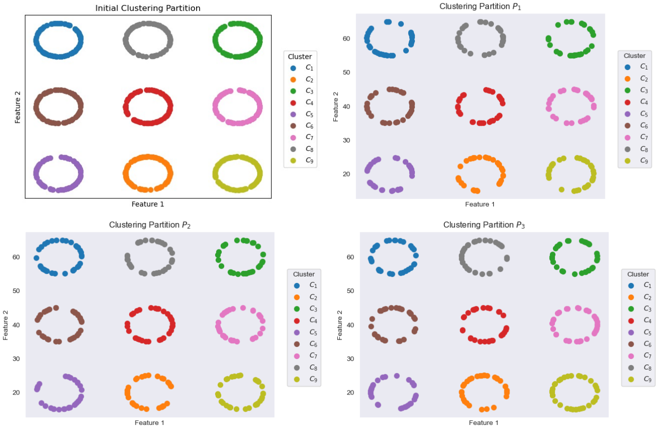
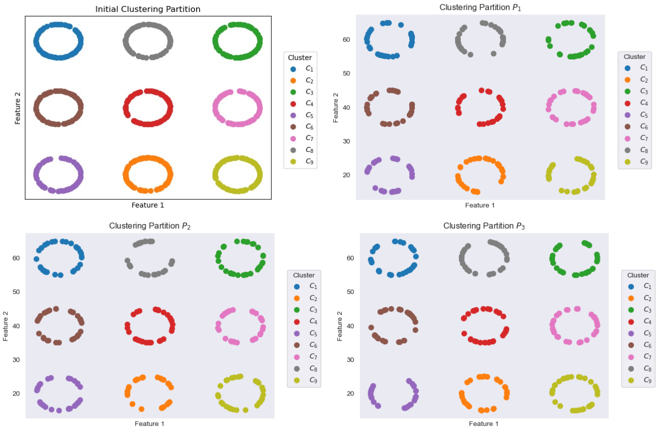


Gap (estimated with k-means) $= 1.65$ %

Synthetic- Final Partition

900 points, 9 cluster each with 100 points, 3 anticlusters



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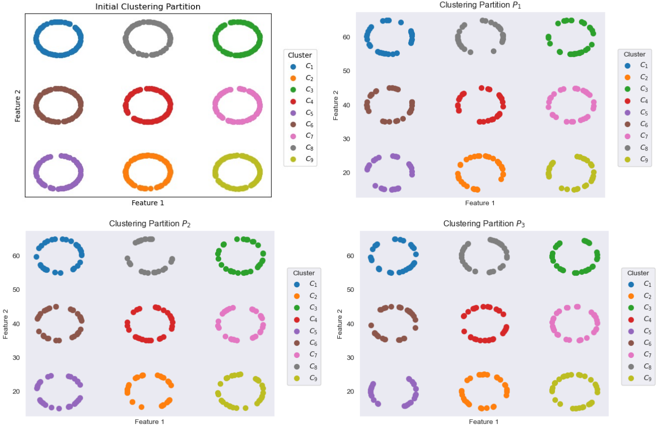
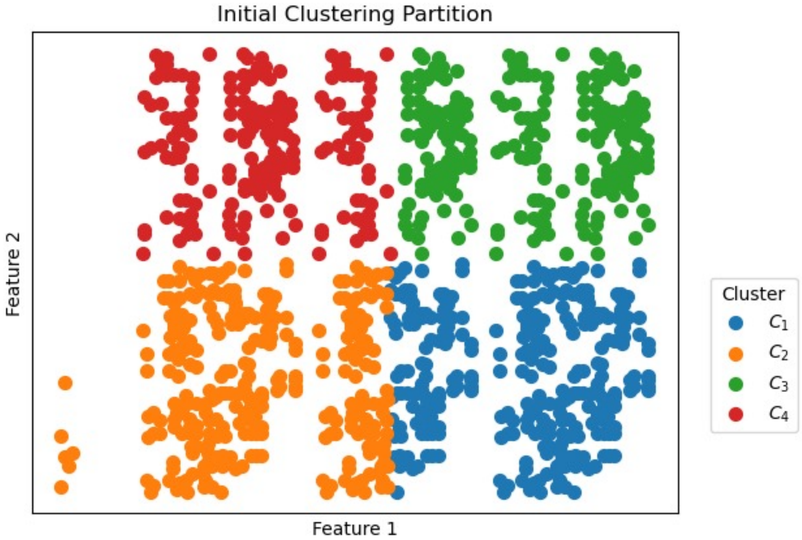
900 points, 9 cluster each with 100 points, 3 anticlusters



Gap (with respect to the lower bound computed by SOS-SDP) = 0.29 %

pr1002- Random Initial Partition

1002 points, 4 clusters, 4 anticlusters



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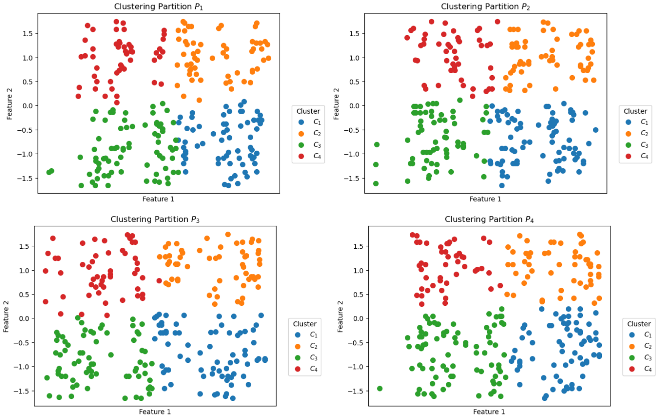

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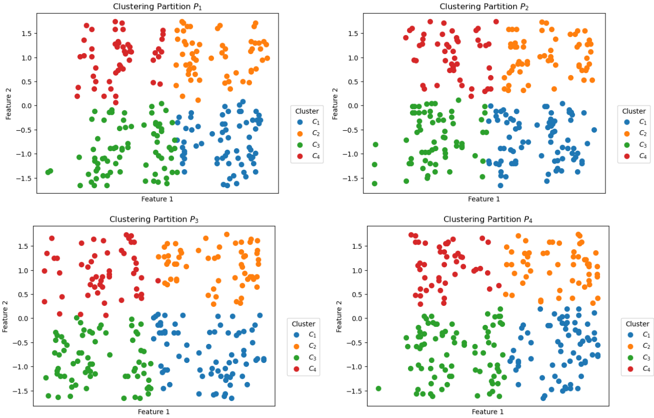
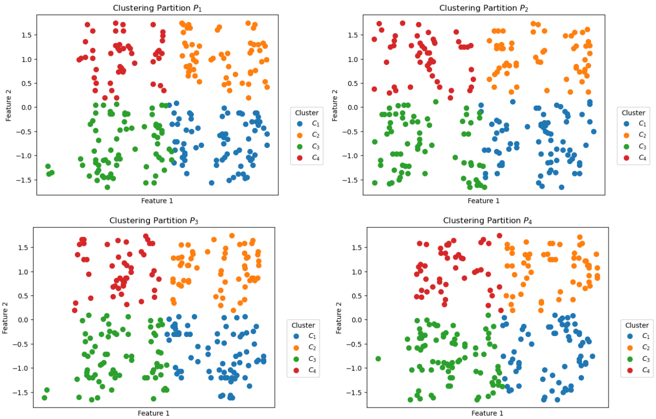


Gap (estimated with k-means) =2.516 %

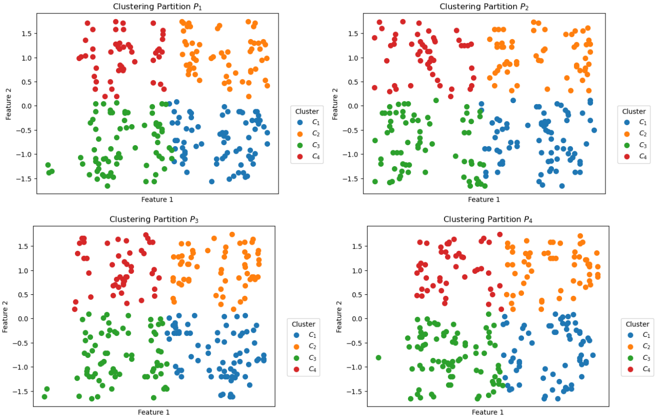
pr1002- Final Partition

1002 points, 4 clusters, 4 partitions



pr1002- Final Partition

1002 points, 4 clusters, 4 partitions



Gap (with respect to the lower bound computed by SOS-SDP) = 1.49%, with the UB = 0.06%

Artificial Instances

- We generate large-scale Gaussian datasets comprising $N = 10.000$ data points in a two-dimensional space ($D = 2$).

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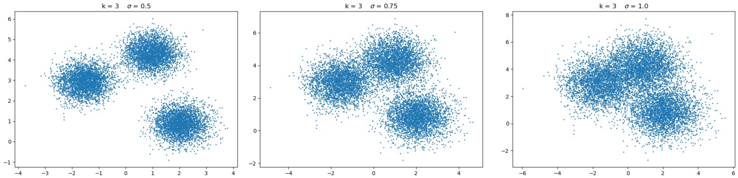
- The standard deviation σ varies among $\{0.50, 0.75, 1.00\}$, representing different noise levels. Cluster centers μ_j are drawn from a uniform distribution within the interval $[-10.10]$.



Results on artificial datasets : 2 clusters

Noise	T	GAP(LB)	$\tilde{GAP}$(UB)	Time(min)
0.5	10	0.18%	0.18%	43.27
0.5	12	0.29%	0.29%	61,9
0.5	15	0.36%	0.36%	37.58
0.5	17	0.33%	0.33%	38,92
0.5	20	0.4%	0.4%	37.05
0.75	10	0.28%	0.26%	127.68
0.75	12	0.25%	0.22%	102.4
0.75	15	0.32%	0.3%	73.18
0.75	17	0.38%	0.36%	92.07
0.75	20	0.4%	0.38%	65.47
1	10	0.47%	0.26%	198,25
1	12	0.41%	0.23%	130.32
1	15	0.41%	0.32%	146.32
1	17	0.75%	0.65%	126.68
1	20	0.56%	0.5%	105.87

Results on artificial datasets : 3 clusters

Noise	T	GAP(LB)	$\tilde{GAP}$(UB)	Time(min)
0.5	10	0.31%	0.3%	95.62
0.5	12	0.38%	0.38%	88.85
0.5	15	0.58%	0.58%	67.47
0.5	17	0.53%	0.53%	50.8
0.5	20	0.62%	0.61%	57.3
0.75	10	0.43%	0.37%	138.12
0.75	12	0.56%	0.48%	178.25
0.75	15	0.61%	0.56%	94.38
0.75	17	0.65%	0.62%	122.68
0.75	20	0.8%	0.77%	63.98
1	10	1.43%	0.43%	184.53
1	12	1.44%	0.52%	217.72
1	15	1.24%	0.58%	89.18
1	17	0.93%	0.4%	115.2
1	20	1.29%	0.78%	114.52

Results on artificial datasets : 4 clusters

Noise	T	GAP(LB)	$\tilde{GAP}$(UB)	Time(min)
0.5	10	0.51%	0.51%	110.57
0.5	12	0.68%	0.68%	75.18
0.5	15	0.83%	0.83%	70.7
0.5	17	0.99%	0.98%	53.35
0.5	20	0.87%	0.87%	60.83
0.75	10	0.54%	0.47%	155.62
0.75	12	0.58%	0.53%	100.4
0.75	15	0.61%	0.58%	104.32
0.75	17	0.83%	0.79%	76.22
0.75	20	0.91%	0.88%	72.5
1	10	1.58%	0.73%	201.72
1	12	1.25%	0.57%	120.13
1	15	1.31%	0.86%	105.27
1	17	1.24%	0.92%	121.32
1	20	1.16%	0.87%	83.85

Datasets

We select some large scale datasets that cannot be solved directly by SOS-SDP:

Dataset	N	D	K	$\lvert C_1\rvert \dots \lvert C_K\rvert$			
Abalone	4,177	10	3	1,308	1,341	1,528	
Facebook	7,050	13	3	218	2,558	4,274	
Frogs	7,195	22	4	605	670	2,367	3,553
Electric	10,000	12	3	2,886	3,537	3,577	
Pulsar	17,898	8	2	2,057	15,841		

Table: Characteristics of real-world datasets.

- Each dataset has been tested for 5 different values of the number of anticlusters T, depending on the number of data points N and on the size of the clusters of the initial solution.
- The choice of T is influenced by two key requirements: (i) the size of each anticluster must be tractable, i.e., less than 1,000 data points; (ii) each cluster must be adequately represented in each anticluster
- The smallest instance Abalone was solved exactly in 2.6 hours
- Solving an instance of around 1,000 data points to global optimality requires several hours of computational time

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Results on real world datasets

Inst (K)	T	γ_{LB} (%)	γ_{UB} (%)	γ^{+} (%)	MILP (s)	Heur (s)	SOS (s)	Time (min)
Ab (3)	4	**0.003**	0.001	0.001	0	172	424	10
	5	0.007	0.001	0.001	0	154	314	8
	6	0.004	0.001	0.001	0	205	213	7
	8	0.009	0.001	0.001	0	546	198	12
	10	0.004	0.001	0.002	0	591	158	12
El (3)	10	2.880	0.460	0.001	2	1,384	5,467	114
	15	**2.198**	0.757	0.001	4	1,759	6,417	136
	20	2.329	0.944	0.001	9	5,118	3,915	151
	25	2.482	1.270	0.002	21	5,062	3,218	138
	30	2.837	1.393	0.003	45	6,856	2,248	152
FB (3)	7	**2.428**	0.321	0.014	0	1,694	4,813	108
	8	2.881	0.923	0.029	1	1,937	3,155	85
	10	3.820	2.107	0.034	1	2,439	4,130	110
	13	5.157	3.306	0.093	1	3,155	2,423	93
	18	7.639	6.373	0.285	5	4,343	2,349	112
Frogs (4)	8	5.147	2.008	1.824	1	2,032	5,558	127
	10	4.824	2.252	1.807	1	2,443	2,639	85
	13	**4.121**	1.881	1.795	4	3,202	2,217	90
	15	4.339	2.397	1.788	9	3,714	1,885	93
	16	4.131	2.323	1.780	10	3,849	1,758	94
Pulsar (2)	18	2.625	0.165	0.001	7	4,059	19,012	385
	20	2.727	0.206	0.002	7	4,884	19,502	407
	25	2.562	0.020	0.002	7	6,031	11,727	296
	30	2.390	0.159	0.002	8	7,275	10,435	295
	35	**2.274**	0.524	0.003	7	8,523	7,873	273

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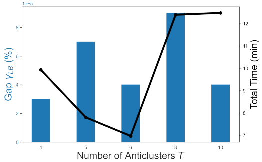
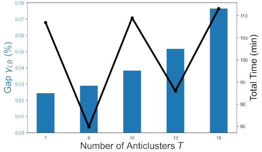
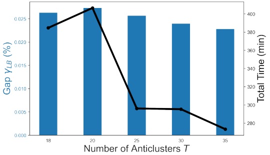
Results



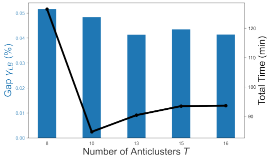
(a) Abalone



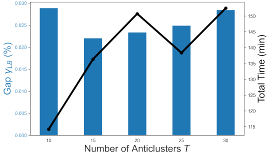
(b) Facebook



(c) Pulsar



(d) Frogs



(e) Electric

Figure: Performance comparison for different numbers of anticlusters. The bar chart represents the lower bound gap (γ_{LB}), while the black line with markers indicates the total computation time in minutes (Time (min)).

Conclusions and future work

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