A Scalable Deterministic Global Optimization Algorithm for Clustering Problems

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Problem Setup

We consider the following optimization problem:

$$\min_{\mu,d,b} \sum_{s\in\mathcal{S}} d_{s,*} \tag{1a}$$

$$\text{s.t.} \quad -N(1-b_{s,k}) \leq d_{s,*} - d_{s,k} \leq N(1-b_{s,k}) \tag{1b}$$

$$\boxed{d_{s,k} \geq ||x_s - \mu_k||^2} \tag{1c}$$

$$\sum_{k\in\mathcal{K}} b_{s,k} = 1 \tag{1d}$$

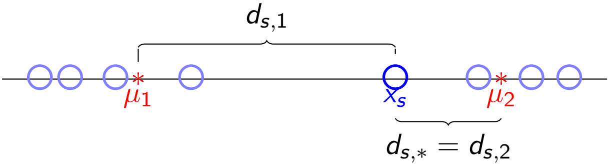
$$b_{s,k} \in \{0,1\} \tag{1e}$$

$$s \in \mathcal{S}, k \in \mathcal{K} \tag{1f}$$

$$b_{s,k} = \begin{cases} 1 & \text{If } x_s \text{ is in cluster } k \\ 0 & \text{otherwise} \end{cases}$$

$d_{s,k}$ is the distance between x_s and the cluster center μ_k

$d_{s,*}$ is $\min_k d_{s,k}$, $k \in \mathcal{K}$



Branch and Bound (BB) on Clustering Problem

Given a dataset D with m features and n samples, to cluster it into K clusters:

- The scale of such problem has $m(2n+K)$ variables
- A three-cluster, two dimensional dataset with 1000 samples consists of 4006 variables.
- BB in off-the-shelf solvers (CPLEX or Gurobi): branching on all (integer) variables.
- Our approach: branching only on space of centers (μ) is enough to guarantee the convergence. (# of branching variables: 6.)

LB Strategy: Scenario Decomposition

Problem 1 can be reformulated as following optimization problem:

$$z(M) = \min_{\mu \in M} \sum_{s \in \mathcal{S}} Q_s(\mu) \tag{2}$$

$$\begin{aligned} Q_s(\mu) = \min_{d_s, b_s} \; & d_{s,*} \\ \text{s.t.} \; & -N(1 - b_{s,k}) \leq d_{s,*} - d_{s,k} \leq N(1 - b_{s,k}) \\ & d_{s,k} \geq ||x_s - \mu_k||^2 \\ & \sum_{k \in \mathcal{K}} b_{s,k} = 1 \\ & b_{s,k} \in \{0, 1\}, k \in \mathcal{K} \end{aligned} \tag{3}$$

which is equivalent to:

$$\min_{\mu_s \in M} \quad \sum_{s \in \mathcal{S}} Q_s(\mu_s) \tag{4a}$$

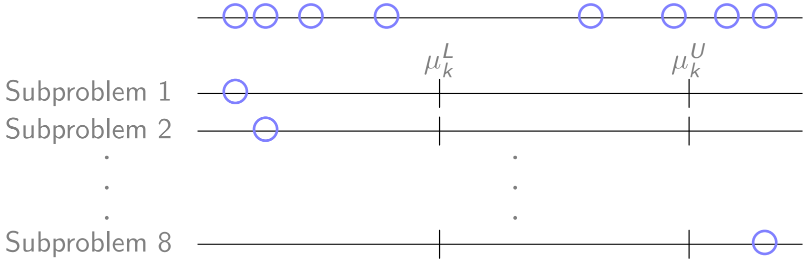
$$\text{s.t.} \quad \mu_s = \mu_{s+1}, s \in \{1, \cdots, \mathcal{S} - 1\} \tag{4b}$$

LB Strategy 1: Closed Form Solution

By relaxing the non-antipativity constraints 4b, we can obtain the lower bounding problem as follow:

$$\beta(M) = \sum_{s \in \mathcal{S}} \beta_s(M) = \min_{\mu_s \in M} \sum_{s \in \mathcal{S}} Q_s(\mu_s) \tag{LB1}$$

It is easy to decompose the Problem LB1 into n subproblems, where n is the number of samples of a dataset.



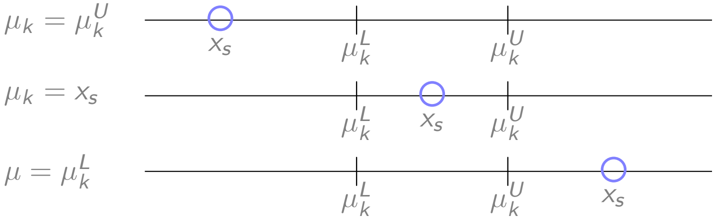
LB Strategy 1: Closed Form Solution

For each scenario s, the lower bound function β_s can be solved as follow:

$$\beta_s(M) = \min_k \beta_{s,k}(M_k) = \min_k \min_{\mu_k \in M_k} ||x_s - \mu_k||^2, \tag{5}$$

where $M_k := \{\mu_k \mid \mu_k^L \leq \mu_k \leq \mu_k^U\}$
Advantage: $\beta_{s,k}$ has a closed form solution:

$$\mu_{k,i} = \text{mid}\{\mu_{k,i}^L, x_{s,i}, \mu_{k,i}^U\}, \forall i \in \{1 \cdots m\} \tag{6}$$



LB Strategy 2: Lagrangean Decomposition

We dualized the non-anticipativity constraints and added to the objective functions with Lagrange multipliers λ:

$$\beta^{LD}(M,\lambda) := \min_{\mu \in M} \{ \sum_{s \in \mathcal{S}} Q_s(\mu_s) + \sum_{s=1}^{S-1} \lambda_s(\mu_s - \mu_{s+1}) \} \tag{7}$$

Thus we solve the lagrangean dual problem:

$$\beta^{LD}(M) = \max_{\lambda} \beta^{LD}(M,\lambda). \tag{LB2}$$

Lemma

$$\beta(M) = \beta^{LD}(M,0) \leq \beta^{LD}(M) \leq z(M)$$

LB Strategy 3: Adaptive Sample Grouping

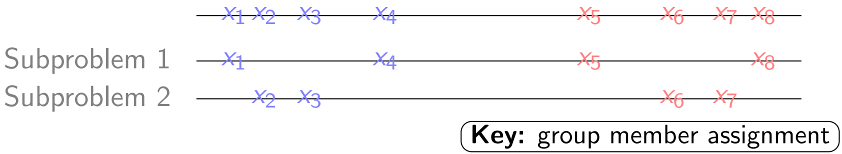
We assign group of samples into one subproblem

$$\min_{\mu_g \in M} \sum_{g \in \mathcal{G}} Q_g(\mu_g) \tag{8a}$$

$$\text{s.t.} \quad \mu_g = \mu_{g+1}, g \in \{1, \cdots, \mathcal{G} - 1\}. \tag{8b}$$

Thus, we have lower bounding problem by relaxing 8b:

$$\beta^{SG}(M) = \sum_{g \in \mathcal{G}} \beta_g^{SG}(M) = \min_{\mu_g \in M} \sum_{g \in \mathcal{G}} Q_g(\mu_g) \tag{LB3}$$



Lemma

$$\beta(M) \leq \beta^{SG}(M) \leq z(M)$$

Upper Bounding Problem

Two strategies to construct upper bound:

- Fix μ at a candidate solution $\hat{\mu} \in M$, we get an upper bound:

$$\alpha(M) = \sum_{s \in S} Q_s(\hat{\mu}) \tag{UB1}$$

- Solve the following NLP problem to local minimum:

$$\begin{aligned} \alpha(M) = \min_{\mu \in M, b} & \sum_{s \in \mathcal{S}} \sum_{k \in \mathcal{K}} b_{s,k} ||x_s - \mu_k||^2 \\ & \sum_{k \in \mathcal{K}} b_{s,k} = 1 \\ & 0 \leq b_{s,k} \leq 1, s \in \mathcal{S}, k \in \mathcal{K} \end{aligned} \tag{UB2}$$

Theorem

Construct $LB \in \{LB1, LB2, LB3\}$, $UB \in \{UB1, UB2\}$, the BB procedure converges by branching only on μ (center of clusters).

Experiment Analysis

Table 1: Comparison on datasets with state of the art. ($k = 2$)

Methods	UB	Nodes	Gap(%)
Padberg and Rinald's Dataset ($n = 2,392, d = 2$)			
Aloise et al., 2012	2.967×10^{10}	1	i[1] (50h)
serial	2.967×10^{10}	7	1.32 (4h)
serial	2.967×10^{10}	253	0.1 (11h)
20 cores	2.967×10^{10}	247	0.1 (1h)
Glass Identification ($n = 214, d = 9$)			
Aloise et al., 2012	cannot be solved		
serial	819.63	85	28.65 (4h)
serial	819.63	339	0.1 (9h)
20 cores	819.63	415	0.1 (1h)

Table 2: Performance of large dataset in parallel. (200 cores, $k = 3$)

Dataset	UB	Nodes	Gap(%)
Syn-210000	2.43×10^{6}	6	2.55

[1] Solved at the root node.

Contributions

Our work contributes for the following benefits:

- We provided a guaranteed global optimal solution for the minimum sum-of-squares clustering problem.
- By reformulating the clustering problem as a two-stage stochastic program problem, we proposed a tailed reduced space BB clustering algorithm that enables insensitivity to the scale of samples.
- By constructing proper upper and lower bounding problem, we are able to deal with datasets over 200,000 samples in a relatively short time ($\leqslant 4h$).