Balanced Clustering with Least Square Regression

Team7 (Onkar Verma, Navdeep Singh Chahal, Ashish Kumar & Priyansh Agrawal)

Introduction

- Clustering algorithms find use in many applications.
- Problems occurs when we want clusters to be balanced. Clustering algorithms often produce unbalanced structures or trees that are difficult to navigate.
- Examples like, Energy Load Balance of wireless sensor networks where unbalanced cluster structure may cause unbalanced energy consumption and shorten the network lifetime. Similarly, in case of photo query system, retail chain problem etc. Balanced clusters plays an important role in order to produce best results more quickly.

Introduction (Cont.)

- In this paper, the authors proposed a novel and simple method for clustering (BCLS), to minimize least square linear regression with balance constraint to regularize the clustering model.
- The algorithm proposed is best among all state-of-art algorithms so far.

Related Work

- Over the past decades, many clustering algorithms have been proposed and extended, such as **K-means, fuzzy C-means, spectral clustering methods,** and **projected clustering**.
- Some of closely related work includes clustering algorithms that are able to produce balanced clusters. These algorithms can be categorized into two types, namely, **Hard-balanced clustering algorithms** in which ‘cluster size’ is strictly required by setting fixed number of samples in the clusters and **Soft-balanced clustering algorithms** in which balancing is the aim but not mandatory requirement.

Related Work (Cont.)

- Algorithms like ‘Constraint K-means’ (Bradly, Benneet, Demiriz 2000) and ‘Balanced K-means’ (Malinen and Franti, 2014) are two Hard-balanced clustering algorithms. Where as works of Banerjee and Ghosh (2002 and 2004), Zhong and Ghosh (2003) and Chang et.al (2014) are some of the evidence based on Soft-Balanced Clustering.

How current work is better than previous

- The aim of paper is to have balanced result i.e, balanced number of clusters and higher cluster quality i.e, high clustering accuracy at the same time without compromising either one.
- Consider a balance constraint to regularize the clustering model, which belongs to the soft-balanced algorithms, in order to have a balanced result and maintain good clustering performance simultaneously.

How current work is better than previous (Cont.)

- Incorporated least square linear regression as it can provide the model of dissimilarity for clustering to guide the partitioning. Also, it can estimate the class-specific hyperplanes dividing each class of data from others.
- Experimented on 7 benchmarks datasets and observed that the proposed approach not only produces good clustering performance but also guarantees balanced clustering result.

Least Square Linear Regression

- In regression, the estimation error is minimized as follows: $\min \sum_{i=1}^{n} e(f(x_i), y_i)$, where $f(x_i) = x_i^T w + b$ for 2-class dataset $\{(x_i, y_i)\}_{i=1}^{n}$. Each $x_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$.
- In general, for dataset with c classes, Multivariate linear regression problem is given as: $\min_{W,b} \sum_{i=1}^{n} ||W^T x_i + b - y_i||_2^2 + \gamma R(W)$. Here W is the projection matrix or matrix whose columns are normals of class-specific hyperplanes. b is the bias vector and R(W) = $||W||_F^2$

Augmented Lagrange Multipliers(ALM) Method

- ALM are a series of algorithms for solving constrained optimization problems.
- Given constraint OP of following kind:
  min f(X), s.t. H(X) = 0 ,where $f : \mathbb{R}^{mxn} \rightarrow \mathbb{R}$ and $H : \mathbb{R}^{mxn} \rightarrow \mathbb{R}^{mxn}$.
  The augmented lagrangian function is defined as:
  $L(X, \wedge, \mu) = f(X) + \langle \wedge, H(X) \rangle + \frac{\mu}{2} ||H(X)||_F^2$
  , where μ is the positive scalar that gets updated after each iteration and $\wedge$ is an estimate of the Lagrange multiplier with the estimation accuracy improved at every step.

Background (Cont.)

- The constraint OP becomes an unconstraint problem by minimizing the Lagrangian function L(X,$\wedge, \mu$) with updating parameters μ and $\wedge$.
- The indication of convergence of the method is H(X) $\rightarrow$ 0 or $\wedge$ remains unchanged.

Notations and Variables used in the paper

- M=(m_{ij}) $\in \mathbb{R}^{pxq}$, m_{ij} denotes the (i,j)-th entry of M, M^T denotes the transpose of M, and tr(M) denotes the trace of M. The F-norm of M is denoted by $||M||_F$ and the l_2-norm is denoted by $||M||_2$. The inner product of matrices A and B is denoted by $\langle A.B \rangle$. **1** denotes the vector with all elements as 1, and **0** denotes the vector with all elements 0.
- X = $[x_1, x_2, ..., x_n] \in \mathbb{R}^{dxn}$, where n is the number of samples and d is the data dimension. Each $x_i \in \mathbb{R}^d$. This is the mean centered data-matrix.
- Y = $[y_1, y_2, ..., y_n]^T \in \mathbb{R}^{nxc}$, is the label matrix also known as class indicator matrix ($Y \in$ Ind).

Notations and Variables used in the paper (Cont.)

- W = $[w_1, w_2, ..., w_c] \in \mathbb{R}^{dxc}$, is the projection matrix where the w_k denotes normal vector to the hyperplane that partition the k-th class from the others.
- R(W) is the regularization term of standard least square linear regression. This value equals to $||W||_F^2$.
- b $\in \mathbb{R}^c$, is the bias vector.
- γ is the regularization parameter.
- λ is the balance parameter.

Approach to the problem (Timeline)

- Finding the balance constraint which is responsible for balanced clustering.
- Incorporating balance constraint in the optimization problem of least square linear regression.
- Solving the resultant OP using Augmented Lagrange Multiplier method (ALM).
- Performing experiment on datasets and comparing the results.

Balance Constraint

- Defining s = $[s_1, s_2, ..., s_c] \in \mathbb{R}^{1xc}$, where s_i denotes the number of samples in i-th cluster. It can be observed that s=$\mathbf{1}^T$Y , where Y is the indicator matrix.
- Average number of clusters in each cluster is $\frac{n}{c}$.
- Objective is to partition the samples into balanced clusters i.e, to make the cluster size as close to $\frac{n}{c}$ as possible. This is equivalent to minimize variance (σ^2) of s_k.

Problem Formulation (Cont.)

$$\begin{aligned}\min_s \sigma^2 &\Leftrightarrow \min_s \frac{1}{c}\sum_{k=1}^{c}(s_k - \frac{n}{c})^2 \\ &\Leftrightarrow \min_s \sum_{k=1}^{c}(s_k^2 - 2s_k\frac{n}{c} + \frac{n^2}{c^2}) \\ &\Leftrightarrow \min_s(\sum_{k=1}^{c} s_k^2 - \frac{n^2}{c}) \\ &\Leftrightarrow \min_s \sum_{k=1}^{c} s_k^2\end{aligned} \tag{1}$$

- From above deduction, we can see that

$$\sum_{k=1}^{c} s_k^2 = ||s||_2^2 = ||\mathbf{1}^T Y||_2^2 = tr(Y^T \mathbf{1}\mathbf{1}^T Y) \tag{2}$$

Problem Formulation (Cont.)

- This means to minimize the variance, we need to minimize the $tr(Y^T \mathbf{1}\mathbf{1}^T Y)$. Thus this value indicates the balance degree of our clustering algorithm.
- By minimizing the $tr(Y^T \mathbf{1}\mathbf{1}^T Y)$, the data samples tend to be clustered into c balanced classes with $\frac{n}{c}$ samples in each class.

Objective Function

- Traditional least square regression model:

$$\min_{W,b} ||X^T W + \mathbf{1}b^T - Y||_F^2 + \gamma ||W||_F^2 \tag{3}$$

- Including balance constraint as another regularization term in our clustering model, we proposed BCLS with the following objective function:

$$\min_{W,b,Y\in Ind} ||X^T W + \mathbf{1}b^T - Y||_F^2 + \gamma ||W||_F^2 + \lambda tr(Y^T \mathbf{1}\mathbf{1}^T Y) \tag{4}$$

Problem Formulation (Cont.)

- In the objective function in Eq.(4), the minimization of the least square regression term guides the clustering process to partition data points into c clusters. Meanwhile, minimizing the balance regularization term guarantees the balanced partitioning among different categories.

Solving OP using ALM

- Problem is NP-hard. To solve it in polynomial time we first apply Alternating Direction Method of Multipliers (ADMM) proposed in Eckstein and Bertsekas, 1992. We replace Y with Z that has entries with continuous values, so as to transfer Eq.(4) into an equality constraint OP and approximately obtain the optimal solution by alternatively solving Y with Z fixed and solving Z with Y fixed.
- Converted equation thus becomes:

$$\min_{\substack{W,b,Y\in Ind,\\ Y=Z}} ||X^TW + \mathbf{1}b^T - Y||_F^2 + \gamma||W||_F^2 + \lambda tr(Z^T\mathbf{1}\mathbf{1}^TZ) \tag{5}$$

st. Y-Z=0

Solving OP using ALM (Cont.)

- The resultant problem in Eq.(5) is non-convex and since objective function has multiple unknown variables (W,b,Y,Z). It can be solved by alternating updating the unknown variables.
- Final solutions obtained are:

$$\begin{cases} W & = (XX^T + \gamma I_d)^{-1} XY \\ b & = \frac{1}{n} Y^T \mathbf{1} \end{cases} \tag{6}$$

Solving OP using ALM (Cont.)

$$Z = (\mu I_n + 2\lambda \mathbf{1}\mathbf{1}^T)^{-1}(\mu Y + \wedge) \tag{7}$$

- Inverse of $\mu I_n + 2\lambda \mathbf{1}\mathbf{1}^T$ can be given by $\frac{(\mu+2n\lambda)I_n - 2\lambda \mathbf{1}\mathbf{1}^T}{(\mu^2+2n\lambda\mu)}$
- Y=$(y_{ik}) \in \mathbb{R}^{nxc}$ and its entries y_{ik} is given by:

$$y_{ik} = \begin{cases} 1 & \text{if } k = arg\max_k \{v_{ik}\}_{k=1}^{c} \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

  where, v_{ik} are the entries of matrix V = $(v_{ik}) \in \mathbb{R}^{nxc}$ and V is given by:

$$V = \frac{2}{2+\mu}(X^T W + \mathbf{1}b^T) + \frac{1}{2+\mu}(\mu Z - \wedge) \tag{9}$$

- This is obtained by solving following OP:

$$\min_{Y \in Ind} ||Y - V||_F^2 + const. \tag{10}$$

Experiment

- We have done experiment on 3 datasets namely, Ionosphere, Wine and UMIST
- Optimal values are chosen for different parameters as given in original paper.
- The time complexity in a single iteration is $O(n^2c + d^2c)$

Principal Component Analysis

Dataset	Samples	Orinigal Dim.	PCA Dim.	#Class
Wine	178	13	10	3
UMIST	380	10304	50	20
Ionosphere	351	34	20	2

Experiment (Cont.)

- Clustering accuracy (ACC) [Cai, He, and Han 2005] is used to evaluate clustering performance.
- To evaluate balancing performance, Normalized entropy (N_{entro}) [Zhong and Ghosh 2003] is incorporated.
- N_{entro} of 1 means perfectly balanced clusters and 0 means extremely unbalanced clusters.
- Below given is table for each performance metrics evaluated for each of 3 datasets.

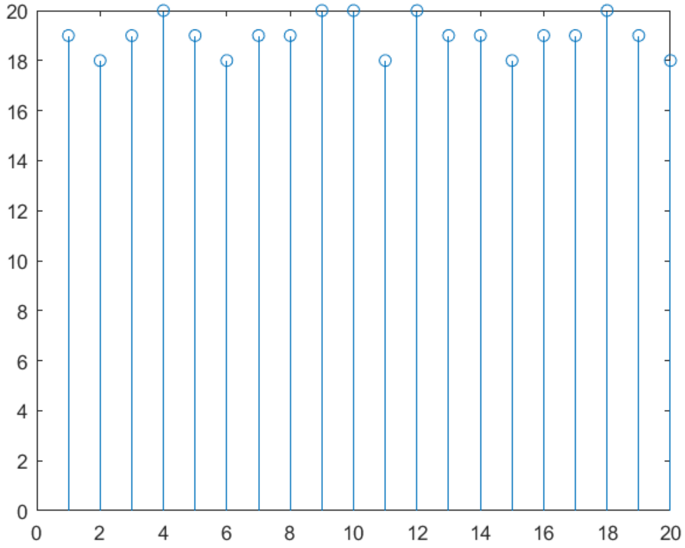
Accuracy

Dataset	correct	n	ACC	N_{entro}
Ionoshpere	239	351	68.09%	1.0
Wine	167	178	93.82%	0.9998
UMIST	224	380	61.57%	1.0

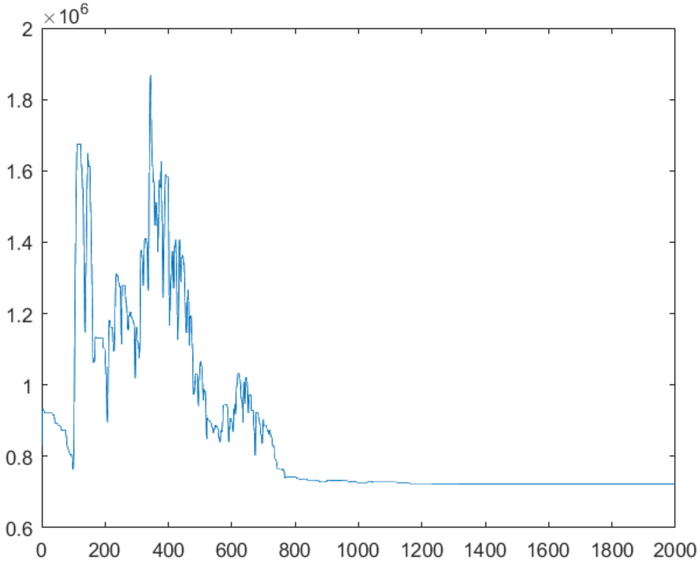
Optimal parameters

Dataset	γ	λ	μ
Ionoshpere	10^{-5}	1000	0.1
Wine	10^{-5}	10	1
UMIST	10^{-5}	100	0.1

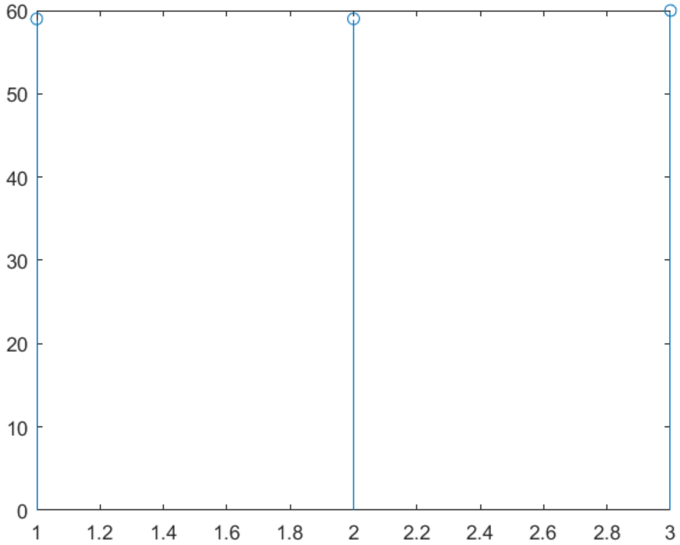
UMIST Dataset Cluster distribution



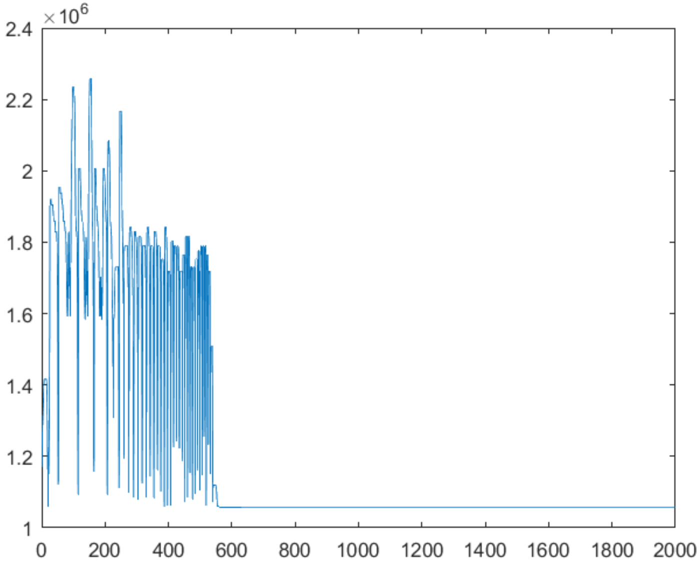
UMIST Dataset Cluster distribution



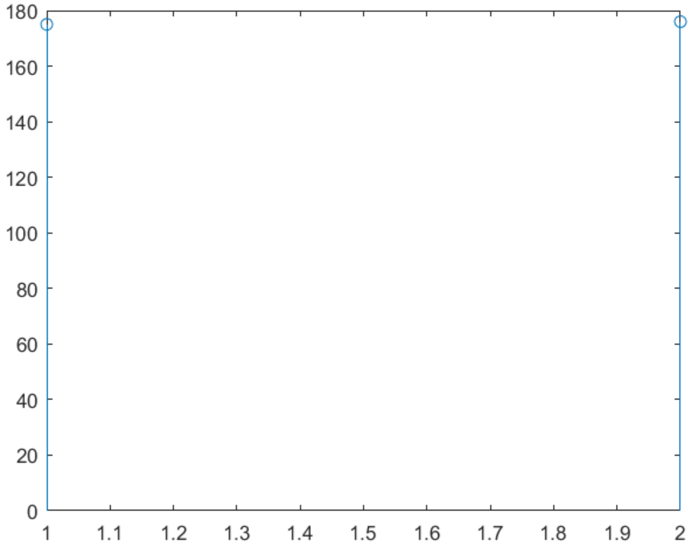
Wine Dataset Cluster distribution



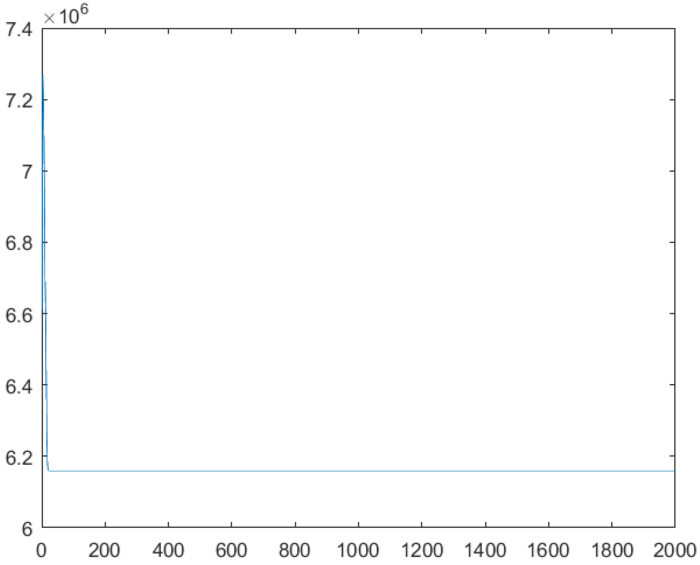
Wine Dataset Objective Function



Iono Dataset Cluster distribution



Iono Dataset Object Function



Conclusion

- Proposed a conceptually simple but effective clustering algorithm that produces balanced clusters.
- Estimated the class-specific hyperplanes that partition the data points into different clusters by iteratively minimizing the least square error of the linear regression.
- Balance constraint is introduced in order to achieve a balanced clustering result.

Conclusion (Cont.)

- ALM along with ADMM is applied for obtaining good approximate solutions of the resultant OP.
- Experiments is performed on benchmarks datasets from which we observed that BCLS produces good clustering and balancing performances simultaneously.