Integrating Constraints and Metric Learning in Semi-Supervised Clustering

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Machine Learning Seminar
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Semi-supervised Clustering

1. Constrained-based method
   - *Seeded KMeans, Constrained KMeans* given partial label information.
   - *COP KMeans* given pairwise constraint (must-link, cannot-link)

2. Metric-based method
   - Learn a metric to satisfy the constraint, such that the data of the same cluster gets closer, whereas data of different clusters gets further away

Limitations
- Previous metric learning excludes unlabeled data during metric training.
- A single distance metric is used for all clusterings, forcing them to have the same shape.
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Constrait-based method

- **K-means clustering:**
  
  $$\text{Minimize} \quad \sum_{x_i \in X} \| x_i - \mu_{l_i} \|^2$$

- Semi-supervised clustering with constraints

  $$\text{Minimize} \quad \sum_{x_i \in X} \| x_i - \mu_{l_i} \|^2 + \sum_{(x_i, x_j) \in M} w_{ij} \mathbf{1}[l_i \neq l_j] + \sum_{(x_i, x_j) \in C} \bar{w}_{ij} \mathbf{1}[l_i = l_j]$$

  - Typical k-means
  - must-link
  - cannot-link
K-means clustering:

$$\text{Minimize} \quad \sum_{x_i \in \mathcal{X}} \|x_i - \mu_{l_i}\|^2$$

Semi-supervised clustering with constraints

$$\text{Minimize} \quad \sum_{x_i \in \mathcal{X}} \|x_i - \mu_{l_i}\|^2 + \sum_{(x_i, x_j) \in \mathcal{M}} w_{ij}1[l_i \neq l_j] + \sum_{(x_i, x_j) \in \mathcal{C}} \bar{w}_{ij}1[l_i = l_j]$$

Typical k-means

must-link

cannot-link
Metric-based Method

- Euclidean distance:
  \[ ||x_i - x_j|| = \sqrt{(x_i - x_j)^T(x_i - x_j)} \]

- Mahalanobis distance:
  \[ ||x_i - x_j||_A = \sqrt{(x_i - x_j)^T A (x_i - x_j)} \]

  where \( A \) is a covariance matrix.

- \( A \succeq 0 \)

- If a \( A \) is used for calculate distance, then each cluster is modeled as a multivariate Gaussian distribution with covariance \( A^{-1} \).
Clustering with different shape

What if the shape of clusters are different?

- Use different $A$ for each cluster (Assign different covariance).
- To Maximize the likelihood boils down to:

$$
\text{Minimize } \sum_{x_i \in \mathcal{X}} \left( \|x_i - \mu_i\|_A^2 - \log(\det A_i) \right)
$$
Clustering with different shape

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- To Maximize the likelihood boils down to:

$$\text{Minimize} \sum_{x_i \in \mathcal{X}} \left( \| x_i - \mu_l \|^2_{A_l} - \log(\det A_l) \right)$$
Combine Constraints and Metric Learning

**Minimize**

\[
\sum_{x_i \in X} \left[ \| x_i - \mu_{l_i} \|_{A_{l_i}}^2 - \log(\det A_{l_i}) \right] + \sum_{(x_i, x_j) \in M} w_{ij} 1[l_i \neq l_j] + \sum_{(x_i, x_j) \in C} \bar{w}_{ij} 1[l_i = l_j]
\]

**Metric Learning**

**Constraints**

Intuitively, the penalty \( w_{ij} \) and \( \bar{w}_{ij} \) should be based on distance of two data points.

**Minimize**

\[
\sum_{x_i \in X} \left[ \| x_i - \mu_{l_i} \|_{A_{l_i}}^2 - \log(\det A_{l_i}) \right] + \sum_{(x_i, x_j) \in M} f_M(x_i, x_j) 1[l_i \neq l_j] + \sum_{(x_i, x_j) \in C} f_c(x_i, x_j) 1[l_i = l_j]
\]
Combine Constraints and Metric Learning

Minimize

\[
\sum_{x_i \in X} \left[ \| x_i - \mu_{l_i} \|_{A_{l_i}}^2 - \log(\det A_{l_i}) \right]
\]

Metric Learning

\[+ \sum_{(x_i, x_j) \in M} w_{ij} \mathbf{1}[l_i \neq l_j] + \sum_{(x_i, x_j) \in C} \bar{w}_{ij} \mathbf{1}[l_i = l_j]\]

Constraints

Intuitively, the penalty \( w_{ij} \) and \( \bar{w}_{ij} \) should be based on distance of two data points.
Penalty based on distance

- Must-link: Violations means data belongs to different cluster.

\[ f_M(x_i, x_j) = \frac{1}{2} \left( \|x_i - x_j\|_{A_{l_i}}^2 + \|x_i - x_j\|_{A_{l_j}}^2 \right) \]

The further away two data are, the more penalty.

- Cannot-link: Violations means data belongs to the same cluster.

\[ f_C(x_i, x_j) = \|x_i' - x_i''\|_{A_{l_i}}^2 - \|x_i - x_j\|_{A_{l_i}}^2 \]

The closer two data are, the more penalty.
Penalty based on distance

- **Must-link**: Violations means data belongs to different cluster.

\[
f_M(x_i, x_j) = \frac{1}{2}(\|x_i - x_j\|_{A_i}^2 + \|x_i - x_j\|_{A_j}^2)
\]

The further away two data are, the more penalty.

- **Cannot-link**: Violations means data belongs to the same cluster.

\[
f_C(x_i, x_j) = \underbrace{\|x'_i - x''_i\|_{A_i}^2}_{\text{Maximum distant points}} - \underbrace{\|x_i - x_j\|_{A_i}^2}_{\text{Average}}
\]

The closer two data are, the more penalty.
Metric pairwise constrained K-means (MPCK)

General Framework of MPCK algorithm based on EM

- Initialize clusters
- Repeat until convergence:
  - Assign Cluster to minimize the objective goal.
  - Estimate the mean
  - Update the metric

Difference with k-means

- Cluster assignment takes constraint into consideration.
- The metric is updated in each round.
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Initialization

Basic idea
- Construct traversive closure of the must-link
- Choose the mean of each component as the seed.
- Extend the sets of must-link and cannot-link.

Construct traversive closure of the must-link
Must-link: \{AB, BC, DE\}; Cannot link: \{BE\};
Initialization

Basic idea
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Construct traversive closure of the must-link
Must-link: \{AB, BC, DE\}; Cannot link: \{BE\};
Cluster Assignment

1. Randomly re-order the data points
2. Assign each data point to a cluster that minimize the objective function:

Minimize \( J = \sum_{x_i \in \mathcal{X}} \left[ ||x_i - \mu_{l_i}||_{\mathbf{A}_{l_i}}^2 - \log(\det \mathbf{A}_{l_i}) \right] \)

\[ + \sum_{(x_i, x_j) \in \mathcal{M}} f_M(x_i, x_j) \mathbf{1}[l_i \neq l_j] + \sum_{(x_i, x_j) \in \mathcal{C}} f_c(x_i, x_j) \mathbf{1}[l_i = l_j] \]
Update the metric

1. Update the centroid of each cluster

2. Update the distance metric of each cluster; Take the derivative of the goal function and set it to 0 to get the new metric:

\[
\mathbf{A}_h = |\mathcal{X}_h| \left\{ \sum_{x_i \in \mathcal{X}_h} (x_i - \mu_i)(x_i - \mu_i)^T + \sum_{(x_i,x_j) \in \mathcal{M}_h} \frac{1}{2} w_{ij} (x_i - x_j)(x_i - x_j)^T 1[l_i \neq l_j] \right\}^{-1}
\]

\[
+ \sum_{(x_i,x_j) \in \mathcal{C}_h} \tilde{w}_{ij} \left( (x_h' - x_h'')(x_h' - x_h'')^T - (x_i - x_j)(x_i - x_j)^T \right) 1[l_i = l_j]
\]
1 Singularity: If the sum is singular, set $A_h^{-1} = A_h^{-1} + \epsilon tr(A_h^{-1})I$ to ensure nonsingularity.

2 Semi-positive definiteness: If $A_h$ is negative definite, project it into set $C = \{A: A \succeq 0\}$ by setting negative eigenvalues to 0.

3 Computational cost: Use diagonal matrix. Or the same distance metric for all clusters.

4 Convergence: Theoretically, each step reduce the objective goal. But if singularity and semi-positive definiteness are involved, the algorithm might not converge in theory. Anyhow, it works fine in reality.
Some issues

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A single diagonal matrix is used.
Experiment Results (2)

A single diagonal matrix compared with multiple full matrix.

![Graphs showing F-measure vs. number of constraints for different methods: Ionosphere and Digits-389.](image)

*Figure 11. Ionosphere: metric learning*  
*Figure 12. Digits-389: metric learning*

Some phenomenons

- Use different matrix and cluster and use full matrix definitely increase the performance.
- When the constraints are few, RCA seems working better than MPCK-means. Why?
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- When the constraints are few, RCA seems working better than MPCK-means. Why?
By integrating metric learning and constraints during clustering, it outperforms each single approach.

Questions?

Thank you!!
Conclusions

By integrating metric learning and constraints during clustering, it outperforms each single approach.

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