Integrating Constraints and Metric Learning in Semi-Supervised Clustering

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Machine Learning Seminar

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:

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

- Semi-supervised clustering with constraints

$$Minimize \underbrace{\sum_{x_i \in \mathcal{X}} ||x_i - \mu_{l_i}||^2}_{\text{Typical k-means}} + \underbrace{\sum_{(x_i, x_j) \in \mathcal{M}} w_{ij} \mathbf{1}[l_i \neq l_j]}_{\text{must-link}} + \underbrace{\sum_{(x_i, x_j) \in \mathcal{C}} \bar{w}_{ij} \mathbf{1}[l_i = l_j]}_{\text{cannot-link}}$$

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Metric-based Method

- Euclidean distance:

$$||x_i - x_j|| = \sqrt{(x_i - x_j)^T (x_i - x_j)}$$

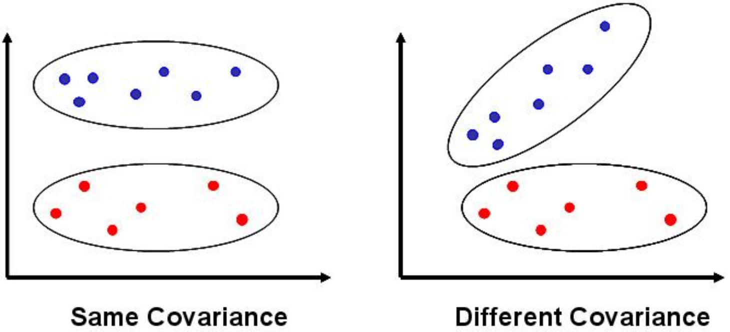
- Mahalanobis distance:

$$||x_i - x_j||_{\mathbf{A}} = \sqrt{(x_i - x_j)^T \mathbf{A} (x_i - x_j)}$$

  where **A** is a covariance matrix.
- $\mathbf{A} \succeq 0$
- If a **A** is used for calculate distance, then each cluster is modeled as a multivariate Gaussian distribution with covariance $\mathbf{A}^{-1}$.

Clustering with different shape

What if the shape of clusters are different?



- Use different **A** for each cluster(Assign different covariance).
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$$Minimize \quad \sum_{x_i \in \mathcal{X}} \left(||x_i - \mu_{l_i}||^2_{\mathbf{A}_{l_i}} - log(det\mathbf{A}_{l_i}) \right)$$

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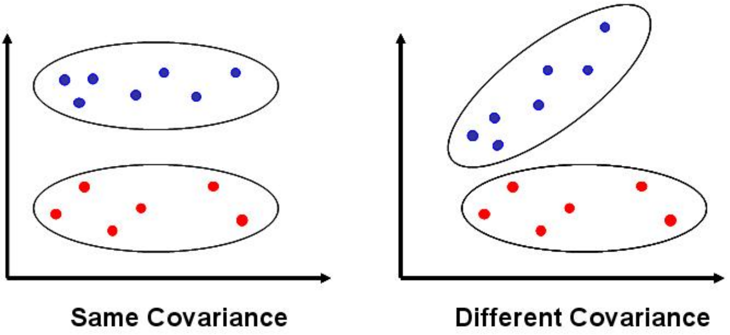

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Intuitively, the penality w_{ij} and $\bar{w}_{ij}$ should be based on distance of two data points.

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Penality based on distance

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

$$f_M(x_i, x_j) = \underbrace{\frac{1}{2}(||x_i - x_j||^2_{A_{l_i}} + ||x_i - x_j||^2_{A_{l_j}})}_{Average}$$

The further away two data are, the more penality.

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

$$f_C(x_i, x_j) = \underbrace{||x'_{l_i} - x''_{l_i}||^2_{\mathbf{A}_{l_i}}}_{\text{Maximum distant points}} - ||x_i - x_j||^2_{\mathbf{A}_{l_i}}$$

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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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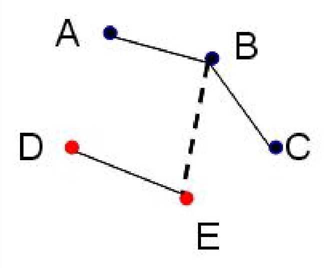
Initialization

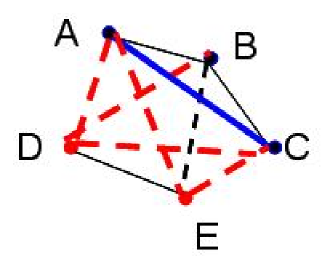
Basic idea

- 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};





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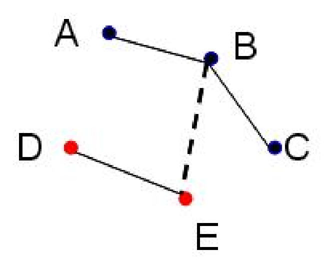

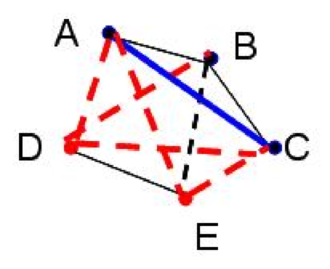

Cluster Assignment

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

$$\mathit{Minimize} \qquad \mathcal{J} = \sum_{x_i \in \mathcal{X}} [||x_i - \mu_{l_i}||^2_{\mathbf{A}_{l_i}} - log(det \mathbf{A}_{l_i})]$$
$$+ \sum_{(x_i, x_j) \in \mathcal{M}} f_M(x_i, x_j) \mathbf{1}[l_i \neq l_j] + \sum_{(x_i, x_j) \in \mathcal{C}} f_c(x_i, x_j) \mathbf{1}[l_i = l_j]$$

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:

$$
\begin{aligned}
\mathbf{A}_h \quad = \quad |\mathcal{X}_h| \Bigg\{ & \sum_{x_i \in \mathcal{X}_h} (x_i - \mu_i)(x_i - \mu_i)^T \\
& + \sum_{(x_i, x_j) \in \mathcal{M}_h} \frac{1}{2} w_{ij} (x_i - x_j)(x_i - x_j)^T \mathbf{1}[l_i \neq l_j])
\end{aligned}
$$

$$
+ \sum_{(x_i, x_j) \in \mathcal{C}_h} \bar{w}_{ij} \left((x'_h - x''_h)(x'_h - x''_h)^T - (x_i - x_j)(x_i - x_j)^T \right) \mathbf{1}[l_i = l_j] \Bigg\}^{-1}
$$

Some issues

1. Singularity: If the sum is singular, Set $\mathbf{A}_h^{-1} = \mathbf{A}_h^{-1} + \epsilon tr(\mathbf{A}_h^{-1})\mathbf{I}$ to ensure nonsiguarity.
2. Semi-positive definiteness: If $\mathbf{A}_h$ is negative definite, project it into set $C = \{\mathbf{A} : \mathbf{A} \succeq 0\}$ 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.

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Experiment Results(1)

A single diagonal matrix is used.

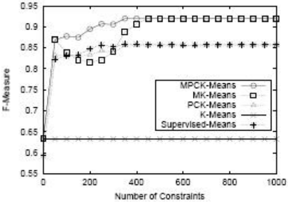


Figure 2. *Iris*: ablations

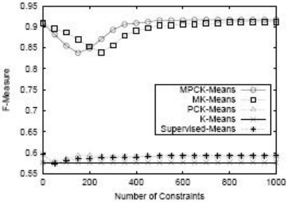


Figure 3. *Wine*: ablations

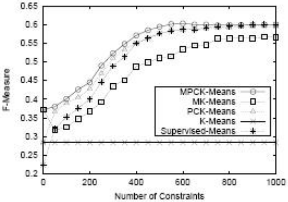


Figure 4. *Protein*: ablations

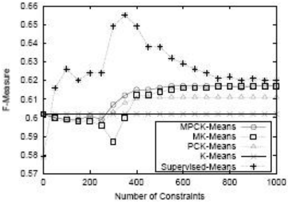


Figure 5. *Ionosphere*: ablations

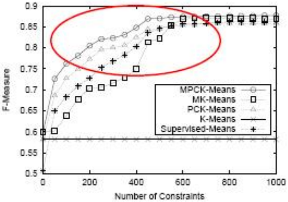


Figure 6. *Digits-389*: ablations

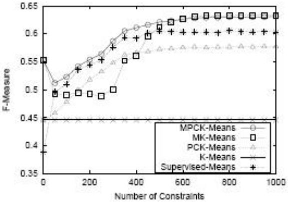


Figure 7. *Letters-IJL*: ablations

Experiment Results(2)

A single diagonal matrix compared with multiple full matrix.

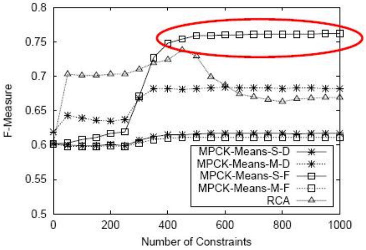
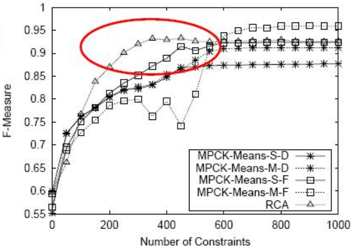


Figure 11. *Ionosphere*: metric learning



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- When the constraints are few, RCA seems working better than MPCK-means. Why?

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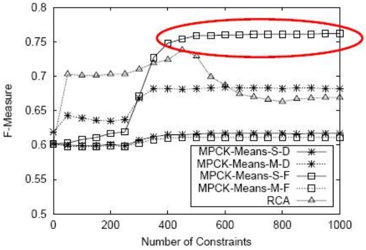

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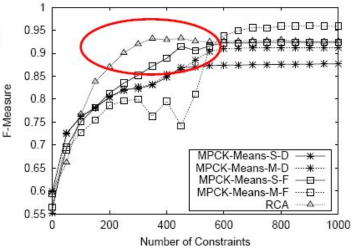

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