



# Supervised Metric Learning Liu



Data Mining Lab, Big Data Research Center, UESTC

Email: junmshao@uestc.edu.cn

http://staff.uestc.edu.cn/shaojunming

#### Overview



#### ▶1. Introduction

- Definition
- Application

#### ▶2.Comparing

- Similarity measure
- Dimensionality reduction

#### ➤ Supervised metric learning algorithms

- LDA
- MMDA
- ITML
- RCA
- NCA



## A Distance Metric if it satisfies the following four properties:

- Nonnegativity:  $D(x, y) \ge 0$
- Coincidence: D(x, y) = 0 if and only if x = y
- Symmetry: D(x, y) = D(y, x)
- Subadditivity:  $D(x, y) + D(y, z) \ge D(x, z)$

Where  $D: X \times X \rightarrow R$  and X represents a set of data points

#### What is metric learning



- ➤ Two important distance metric:
- 1. Euclidean distance, which measures the distance between x and y by

$$\mathcal{D}(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^{\top}(\mathbf{x} - \mathbf{y})}$$

2. Mahalanobis distance, which measures the distance between **x** and **y** by

$$\mathcal{D}(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^{\top} \mathbf{S}(\mathbf{x} - \mathbf{y})}$$

where S is the inverse of the data covariance matrix

#### What is metric learning



#### **Generalized** Mahalanobis distance

$$\mathcal{D}(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^{\top} \mathbf{M} (\mathbf{x} - \mathbf{y})}$$

where M is some arbitrary Symmetric Positive Semi-Definite (SPSD) matrix.

We can decompose M as  $M = U\Lambda U'$  and let  $W = U\Lambda^{1/2}$ 

$$\begin{split} \mathcal{D}(\mathbf{x}, \mathbf{y}) &= \sqrt{(\mathbf{x} - \mathbf{y})^{\top} \mathbf{W} \mathbf{W}^{\top} (\mathbf{x} - \mathbf{y})} = \sqrt{(\mathbf{W}^{\top} (\mathbf{x} - \mathbf{y}))^{\top} (\mathbf{W}^{\top} (\mathbf{x} - \mathbf{y}))} \\ &= \sqrt{(\widetilde{\mathbf{x}} - \widetilde{\mathbf{y}})^{\top} (\widetilde{\mathbf{x}} - \widetilde{\mathbf{y}})} \end{split}$$

where 
$$x = Wx$$



#### Distance Metric Learning:

The problem of learning a mapping function f (projection matrix W), such that f(x) and f(y) will be in the Euclidean space and D(x, y) = ||f(x) - f(y)||, where  $||\cdot||$  is the l2 norm.

#### Application



- ➤ Clustering
  - Similarity measure in K-means
- **≻**Classification
- KNN
- ➤ Image retrieval



- ➤ Similarity measure
  - -- similarity measures are in some sense the inverse of distance measure

$$s(x,y) = -||x - y||_2^2$$

- Dimensionality reduction
  - -- most of the existing metric learning approaches can be viewed as a standard Euclidean distance in some embedding space.

#### Supervised distance learning algorithms



| Local   | Global   |
|---|--|
| NCA Goldberger et al. (2004),<br>ANMM Wang and Zhang (2007),<br>LMNN Weinberger et al. (2005) | LDA Fukunaga (1990),<br>LSI Xing etal. (2002),<br>ITML Davis et al.(2007),<br>MMDA Kocsor et al.(2004),<br>RCA Shental et al. (2002) |



LDA defines the compactness matrix and scatterness matrix as

$$\Sigma_{\mathcal{C}} = \frac{1}{C} \sum_{c} \frac{1}{n_c} \sum_{\mathbf{x}_i \in c} (\mathbf{x}_i - \bar{\mathbf{x}}_c) (\mathbf{x}_i - \bar{\mathbf{x}}_c)^{\top}$$

$$\Sigma_{\mathcal{S}} = \frac{1}{C} \sum_{c} (\bar{\mathbf{x}}_c - \bar{\mathbf{x}}) (\bar{\mathbf{x}}_c - \bar{\mathbf{x}})^{\top}$$

The goal of LDA is to find a W which can be obtained by solving the following optimization problem

$$\min_{\mathbf{W}^{\top}\mathbf{W}=\mathbf{I}} \frac{tr(\mathbf{W}^{\top}\boldsymbol{\Sigma}_{\mathcal{C}}\mathbf{W})}{tr(\mathbf{W}^{\top}\boldsymbol{\Sigma}_{\mathcal{S}}\mathbf{W})}$$



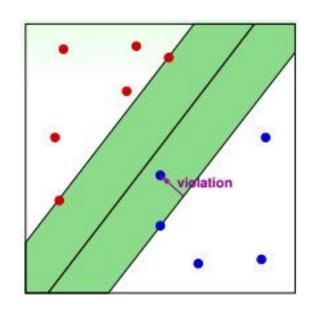
The goal of LDA is to find a W which can be obtained by solving the following optimization problem

$$\min_{\mathbf{W}^{\top}\mathbf{W}=\mathbf{I}} \frac{tr(\mathbf{W}^{\top}\boldsymbol{\Sigma}_{\mathcal{C}}\mathbf{W})}{tr(\mathbf{W}^{\top}\boldsymbol{\Sigma}_{\mathcal{S}}\mathbf{W})}$$

The learned distance between  $x_i$  and  $x_j$  is the Euclidean distance between  $Wx_i$  and  $Wx_j$ , and the computational technique involved is eigenvalue decomposition.

#### Motivation:

Intuitively what MMDA does is to find k **orthogonal** projection hyperplanes such that on each projection direction the two data clusters are separated as well as possible, where  $W = [w1, w2, \cdots, wk]$ .





## Margin maximizing discriminant analysis [DM] [DM]

The goal of MMDA is to find a W which can be obtained by solving the following optimization problem

$$\min_{\mathbf{W}, \mathbf{b}, \xi_r \ge 0} \frac{1}{2} \sum_{r=1}^{d} \|\mathbf{w}_r\|^2 + \frac{C}{n} \sum_{r=1}^{d} \sum_{i=1}^{n} \xi_{ri}$$

$$s.t. \ \forall i = 1, \dots, n, \ r = 1, \dots, d$$

$$l_i \left( \left( \mathbf{w}^r \right)^T \mathbf{x}_i + b \right) \ge 1 - \xi_{ri},$$

$$\mathbf{W}^T \mathbf{W} = \mathbf{I}$$

The learned distance between  $x_i$  and  $x_j$  is the Euclidean distance between  $Wx_i$  and  $Wx_j$ , and the computational technique involved is eigenvalue decomposition and quadratic programming.



#### **>** Assumption

- 1.Distance between point pairs in must-link set is less than u
- 2.Distance between point pairs in cannot-link set is larger than l
- 3.There exists priori metric matrix M<sub>0</sub> (if sample set satisfies Gaussian distribution, using covariance matrix parameterize M<sub>0</sub>).



#### ITML solves the following optimization problem

$$egin{aligned} \min_{M\succeq 0} & KL(p(oldsymbol{x};M_0) \| p(oldsymbol{x};M)) \ & ext{s.t.} \quad d_M(oldsymbol{x}_i,oldsymbol{x}_j) \leq u, \quad (oldsymbol{x}_i,oldsymbol{x}_j) \in S \ & d_M(oldsymbol{x}_i,oldsymbol{x}_j) \geq l, \quad (oldsymbol{x}_i,oldsymbol{x}_j) \in D \end{aligned}$$

The learned distance metric is the Mahalanobis distance with precision matrix **M**.



If M's and M0's distribution have the same mean value

$$KL(p(\boldsymbol{x}; M_0)||p(\boldsymbol{x}; M)) = \frac{1}{2}D_{ld}(M_0^{-1}, M^{-1})$$
  
 $D_{ld}(M, M_0) = \operatorname{tr}(MM_0^{-1}) - \log \det(MM_0^{-1}) - d$ 

ITML solves the following optimization problem

$$\min_{M \succeq 0} \ D_{ld}(M, M_0)$$
s.t.  $\operatorname{tr}(M(\boldsymbol{x}_i - \boldsymbol{x}_j)(\boldsymbol{x}_i - \boldsymbol{x}_j)^{\mathrm{T}}) \leq u, \ (\boldsymbol{x}_i, \boldsymbol{x}_j) \in S$ 
 $\operatorname{tr}(M(\boldsymbol{x}_i - \boldsymbol{x}_j)(\boldsymbol{x}_i - \boldsymbol{x}_j)^{\mathrm{T}}) \geq l, \ (\boldsymbol{x}_i, \boldsymbol{x}_j) \in D$ 



#### ITML solves the following optimization problem

$$\begin{aligned} & \min_{M\succeq 0} \ D_{ld}(M,M_0) \\ & \text{s.t.} \ \operatorname{tr}(M(\boldsymbol{x}_i-\boldsymbol{x}_j)(\boldsymbol{x}_i-\boldsymbol{x}_j)^{\mathrm{T}}) \leq u, \ (\boldsymbol{x}_i,\boldsymbol{x}_j) \in S \\ & \operatorname{tr}(M(\boldsymbol{x}_i-\boldsymbol{x}_j)(\boldsymbol{x}_i-\boldsymbol{x}_j)^{\mathrm{T}}) \geq l, \ (\boldsymbol{x}_i,\boldsymbol{x}_j) \in D \end{aligned}$$

Using an efficient Bregman projection approach to solve problem

$$M_{t+1} = M_t + \beta M_t (\boldsymbol{x}_i - \boldsymbol{x}_j) (\boldsymbol{x}_i - \boldsymbol{x}_j)^{\mathrm{T}} M_t$$

#### Relevant component analysis



The goal of RCA is to find a transformation that amplifies relevant variability and suppresses irrelevant variability.





#### Relevant component analysis



#### *Three steps of RCA:*

- Construct chunklets according to equivalence (must-link) constraints,
- -RCA computes the following weighted within-chunklet covariance matrix:

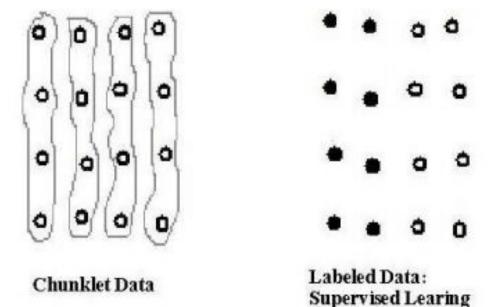
$$\mathbf{C} = \frac{1}{p} \sum_{j=1}^{k} \sum_{i=1}^{n_j} (\mathbf{x}_{ji} - \bar{\mathbf{m}}_j) (\mathbf{x}_{ji} - \bar{\mathbf{m}}_j)^{\top}$$

– Compute the whitening transformation  $W = C^1/2$ , and apply it to the original data points:  $\tilde{x} = Wx$ .

#### Relevant component analysis



#### Difference between labeled data and chunklet data



#### Neighborhood component analysis



▶each point xi selects another point xj as its neighbor with some probability pi j

$$p_{ij} = \frac{\exp\left(-\|\mathbf{W}^{\top}\mathbf{x}_i - \mathbf{W}^{\top}\mathbf{x}_j\|^2\right)}{\sum_{k \neq i} \exp\left(-\|\mathbf{W}^{\top}\mathbf{x}_i - \mathbf{W}^{\top}\mathbf{x}_k\|^2\right)}$$

➤ NCA computes the probability that point *i will* be correctly classified

$$p_i = \sum_i p_{ij}$$
 where  $\mathcal{L}_i = \{j | l_i = l_j\}$ )

#### Neighborhood component analysis



➤ The objective NCA maximizes is the expected number of points correctly classified

$$\mathcal{J}(\mathbf{W}) = \sum_{i} p_{i} = \sum_{i} \sum_{j \in \mathcal{L}_{i}} p_{ij}$$

The learned distance between *xi and xj* is the Euclidean distance between *Wxi and Wxj*. The computational technique involved is **eigenvalue decomposition**.

### Thanks

