# Distance Metric Learning

# Outlines

- I Introduction
- II Application of DML

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How to measure distance?

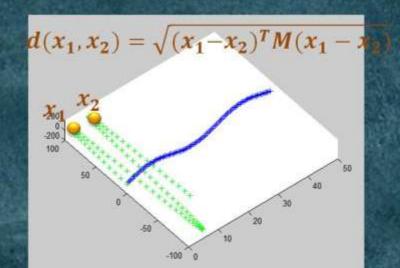
$$d(x_1, x_2) = \sqrt{(x_1 - x_2)^T M(x_1 - x_2)}$$

$$d(x_{1},x_{2}) = \sqrt{(x_{1}-x_{2})^{T}(x_{1}-x_{2})} \qquad M = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$d(x_{1},x_{2}) = |x_{11}-x_{21}| \qquad M = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

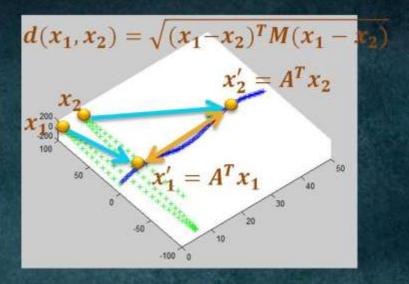
$$d(x_{1},x_{2}) = |x_{12}-x_{22}| \qquad M = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$d(x_{1},x_{2}) = 0 \qquad M = \begin{bmatrix} \sin^{2}(\alpha) - \cos^{2}(\alpha) & 2\sin(\alpha)\cos(\alpha) \\ 0 & -\cos^{2}(\alpha) + \sin^{2}(\alpha) \end{bmatrix}$$





How to measure distance?



learn A generate M apply M to new sample x

$$d(x_1,x) = \sqrt{(x_1-x)^T M(x_1-x)}$$

$$d(x_1, x_2) = \sqrt{(A^T x_1 - A^T x_2)^T (A^T x_1 - A^T x_2)}$$

$$d(x_1, x_2) = \sqrt{(x_1 - x_2)^T A A^T (x_1 - x_2)}$$



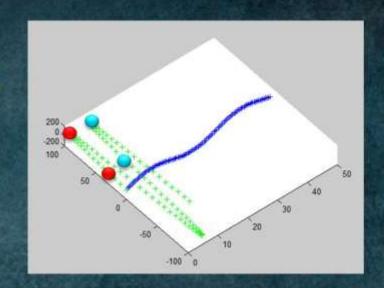
### Categorization

- Unsupervised DML
  - Linear Model
    - PCA,
    - MDS
  - Nonlinear Model
    - LLE,
    - ISOMAP,
    - Laplacian
       Eigenmaps
    - Kernel PCA

- Supervised DML
  - Global Distance Metric Learning
    - Probabilistic Global Distance Metric Learning (PGDM)
  - Local Distance Metric Learning
    - Neighborhood Components Analysis (NCA)
    - Relevant Component Analysis (RCA)
    - Discriminative Component Analysis (DCA)
    - Probabilistic Relevant Component Analysis (pRCA)
    - Large Margin Nearest Neighbor (LMNN)
    - Information-Theoretic Metric Learning (ITML)
    - Bregman Distance Function Learning (BDFL)
  - Certain Constraint
    - NCA, RCA, DCA, LMNN, ITML, BDFL, etc
  - Uncertain Constraint
    - pRCA
  - Matrix Form
    - NCA, RCA, DCA, LMNN, ITML, pRCA, etc
  - Functional Form
    - BDFL

Supervised metric learning?

$$d(x_1, x_2) = \sqrt{(x_1 - x_2)^T M(x_1 - x_2)}$$



**Object function** 

L(M)

Side information

Similar pairs

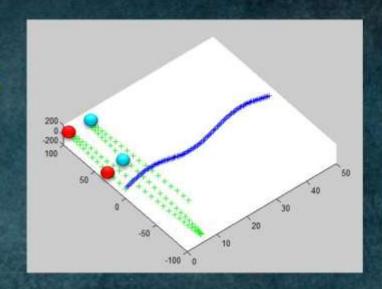
• •

Dissimilar pairs Regularization

R(M)

Supervised metric learning?

$$d(x_1, x_2) = \sqrt{(x_1 - x_2)^T M(x_1 - x_2)}$$



**Object function** 

L(M)

Side information

Similar • • Dissimilar pairs • • pairs

Regularization

R(M)

### Probabilistic Global Distance Metric Learning (PGDM)

Map similar points close to each other

Minimize the distance between similar samples

$$\min_{A} \sum_{(x_i,x_j)\in S} ||x_i-x_j||$$

$$s. t. \sum_{(x_i, x_i) \in D} \left| \left| x_i - x_j \right| \right|_A \ge 1$$

Preserve certain distance between others

### **Extended Reading:**

E. P. Xing, A. Y. Ng, M. I. Jordan, and S. Russell, Distance metric learning, with application to clustering with side-information, *Advances in Neural Information Processing Systems* 15, vol. 15, 2002, pp. 505-512.

### **Neighborhood Components Analysis (NCA)**

Neighbors should gain probability to be in the same class

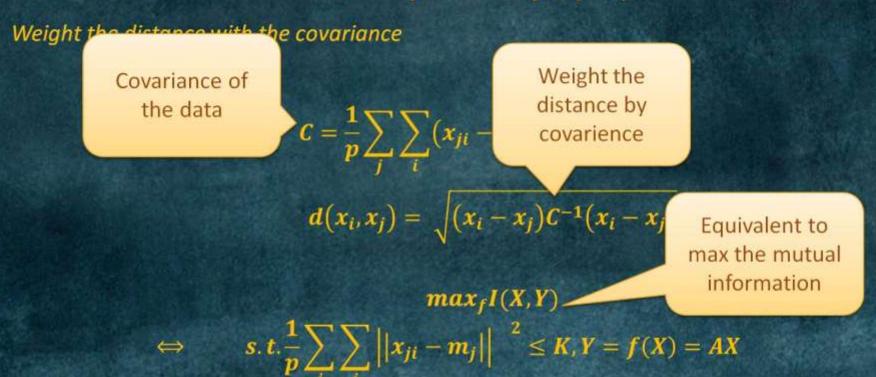
$$p_{ij} = \frac{exp(-||Ax_i - Ax_j||^2)}{\sum_{k \neq i} exp(-||Ax_i - Ax_k||^2)}$$

$$max_A \sum_{t=1}^n log(\sum_{j \in C_i} p_{ij})$$
Minimize the distance between neighbors
$$j \text{ is neighbor of } i$$

**Extended Reading:** 

J. Goldberger, S. Roweis, G. Hinton, and R. Salakhutdinov, "Neighbourhood components analysis," in *Proc. NIPS*, 2005.

### Relevant Component Analysis (RCA)



### Extended Reading:

N. Shental and D. Weinshall, Learning distance functions using equivalence relations, In Proceedings of the Twentieth International Conference on Machine Learning, vol. 21, 2003, pp. 11-18.

Information maximiz

Find a mapping that maximize the mutual info and that in transformed space

Mutual information between original data and embedded data

$$\max_{A} I(X,Y)$$

$$s. t. \frac{1}{p} \sum_{j} \sum_{i} ||y_{ji} - m_{j}||^{2} \leq K \qquad Y = AX$$

$$I(X,Y) = H(Y) - H(Y|X) \Rightarrow max I(X,Y) = max H(Y) \Rightarrow max |A| \Rightarrow max |M|$$

$$p(y) = \frac{p(x)}{|J(x)|} \Rightarrow H(Y) = -\int p(y) \log p(y) dy = -\int p(x) \log \frac{p(x)}{|J(x)|} dx = H(X) + \log |J(X)|$$

$$max_{M}|M$$

$$s. t. \frac{1}{p} \sum_{j} \sum_{i} ||x_{ji} - m_{j}||_{M}^{2} \leq K, \quad M > 0$$

$$M = \frac{K}{N}C^{-1}$$

# **Extended Reading:**

A. Bar-Hillel, T. Hertz, N. Shental, and D. Weinshall, "Learning distance functions using equivalence relations," in *Proc. International Conference on Machine Learning*, 2003.

### Discriminative Component Analysis (DCA)

dictance within each chunklet and maximize the distance between Minimize

chunkle Covariance between chunklets

$$C_b = \frac{1}{k} \sum_i \sum_j (m_i - m_j) (m_i - m_j)^T$$

Covariance within chunklet

$$C_b = \frac{1}{k} \sum_{i} \sum_{j} (m_i - m_j) (m_i - m_j)^T$$

$$C_w = \frac{1}{n} \sum_{i} \sum_{j} (x_{ji} - m_j) (x_{ji} - m_j)^T$$

$$J(A) = argmax_A \frac{A^T C_b A}{A^T C_w A}$$

### Extended Reading:

Steven C. H. Hoi, Wei Liu, Michael R. Lyu, and Wei-Ying Ma. 2006. Learning Distance Metrics with Contextual Constraints for Image Retrieval. In Proceedings of the 2006 IEEE Computer Society Conference on Computer Vision and Pattern Recognition -Volume 2 (CVPR '06), 2006.

well as Metric

# probabilistic Relevance Component Analysis (pRCA)

Learning the distance based on probabilistic side information. Minimize the distance Optimize the membership probability to belong to same chunklet and maximize the vith low probability with same chunklets Probabilistic side

Probabilistic side information

$$min_{M>0,P,m} \sum_{i} \sum_{j} p_{ij} \|x_i - m_j\|_M^2 - \lambda log|M|$$
 $s.t. \|P - P_0\| < \gamma,$ 
 $\sum_{i} p_{ij} = 1, p_{ij} > 0$ 

### **Extended Reading:**

Lei Wu, Steven C.H. Hoi, Rong Jin, Jianke Zhu, Nenghai Yu, "Distance Metric Learning from Uncertain Side Information with Application to Automated Photo Tagging", ACM International Conference on Multimedia (MM'09), 2009.

### Large Margin Nearest Neighbor (LMNN)

Maximize the margin between the distance of similar samples and the distance of dissimilar samples

$$\min_{M>0} \sum_{ij} \eta_{ij} \|x_i - x_j\|_{M}^2 + c \sum_{ijl} \eta_{ij} (1 - y_{il}) \left(1 + \|x_i - x_j\|_{M}^2 - \|x_i - x_l\|_{M}^2\right)_{+}$$

Select neighbor

ij are the ne neighbor in the label

penalizes large distances between each input and its target neighbors Select samples with different labels

penalizes small distances between each input and all other inputs that do not share the same Jabel

**Extended Reading:** 

Kilian Q. Weinberger and Lawrence K. Saul. 2009. Distance Metric Learning for Large Margin Nearest Neighbor Classification. J. Mach. Learn. Res. 10 (June 2009), 207-244.

### Information-Theoretic Metric Learning (ITML)

Regularize the Mahalanobis matrix M to be as close as possible to a given

Mahalanobis distance function, parameterized by  $M_0$ 

$$min_{M>0}KL(p(x,M_0)||p(x,M))-$$
s.t.  $d_M(x_i,x_j) < u, (x_i,x_j) \in S$ 

$$d_M(x_i,x_j) > l, (x_i,x_j) \in D$$

$$p(x,M) = \sum_{M=0}^{\infty} \frac{1}{2} d_M(x,u)$$

Minimize the KL divergence to the predefined distance

Make the distance between Similar samples smaller than u

Make the distance between dissimilar samples larger than I

### **Extended Reading:**

Jason V. Davis, Brian Kulis, Prateek Jain, Suvrit Sra, and Inderjit S. Dhillon. 2007. Information-theoretic metric learning. In *Proceedings of the 24th international conference on Machine learning* (ICML '07),2007.

### **Bregman Distance Function Learning (BDFL)**

Extend the Mahalanobis matrix M to Bregman functional form  $\mathbb{Z}^2$ 

Use a function form rather than matrix form for distance metric

$$d(x_1, x_2) = \varphi(x_1) - \varphi(x_2) - (x_1 + x_2)^{\mathsf{T}} \nabla^2 \varphi(\widehat{x})(x_1 - x_2)$$

$$\Rightarrow d(x_1, x_2) = (x_1 - x_2)^{\mathsf{T}} \nabla^2 \varphi(\widehat{x})(x_1 - x_2)$$

$$\min_{\varphi \in \Omega(\mathcal{H}_k), b \in R^+} \frac{1}{2} |\varphi|_{\mathcal{H}_k}^2 + C \sum_i \ell(y^i [d(x_1^i, x_2^i) - b^i])$$

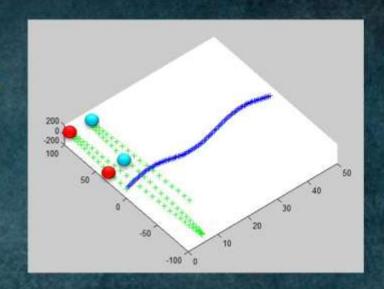
Search for an optimal convex function from a Reproducing Kernel Hilbert Space

### **Extended Reading:**

Lei Wu, Rong Jin, Steven C.H. Hoi, Jianke Zhu, Nenghai Yu, "Learning Bregman Distance Functions and Its Application for Semi-Supervised Clustering", Advances in Neural Information Processing Systems (NIPS'09), 2009.

Supervised metric learning?

$$d(x_1, x_2) = \sqrt{(x_1 - x_2)^T M(x_1 - x_2)}$$



**Object function** 

L(M)

Side information

Similar pairs

• •

Dissimilar pairs

Regularization

R(M)

### Probabilistic Global Distance Metric Learning (PGDM)

Map similar points close to each other

$$\begin{aligned} \min_{A} & \sum_{(x_i, x_j) \in S} \left| \left| x_i - x_j \right| \right|_A^2 \\ s. t. & \sum_{(x_i, x_j) \in D} \left| \left| x_i - x_j \right| \right| \geq 1 \end{aligned}$$
S, D: hard side info

### **Extended Reading:**

E. P. Xing, A. Y. Ng, M. I. Jordan, and S. Russell, Distance metric learning, with application to clustering with side-information, *Advances in Neural Information Processing Systems* 15, vol. 15, 2002, pp. 505-512.

### **Neighborhood Components Analysis (NCA)**

### Pairwise hard constraint

$$p_{ij} = \frac{exp(-||Ax_i - Ax_j||^2)}{\sum_{k \neq i} exp(-||Ax_i - Ax_k||^2)}$$

$$max_A \sum_{t=1}^{n} log(\sum_{j \in C_i} p_{ij})$$

side info:  $j \in C_i \text{ or } j \notin C_i$ 

### **Extended Reading:**

J. Goldberger, S. Roweis, G. Hinton, and R. Salakhutdinov, "Neighbourhood components analysis," in *Proc. NIPS*, 2005.

### Information maximization RCA

Find a mapping that maximize the mutual information of sample in original space and that in transformed space

 $max_AI(X,Y)$ 

$$s. t. \frac{1}{p} \sum_{j} \sum_{i} ||y_{ji} - m_{j}||^{2} \leq K \quad Y = AX$$

$$I(X,Y) = H(Y) - H(Y|X) \Rightarrow \max I(X,Y) = \max H(Y) \Rightarrow \max |A| \Rightarrow \max |M|$$

$$p(y) = \frac{p(x)}{|J(x)|} \Rightarrow H(Y) = -\int p(y) \log p(y) dy = -\int p(x) \log \frac{p(x)}{|J(x)|} dx = H(X) + \log |J(X)|$$

$$\implies \max_{M} |M|$$

$$s. t. \frac{1}{p} \sum_{j} \sum_{i} ||x_{ji} - m_{j}||_{M}^{2} \leq K, \quad M > 0$$

 $M = \frac{K}{N}C^{-1}$ 

 $M = \frac{K}{N}C^{-1}$   $x_{ji}$  i-th sample in j-th chunklet

Hard constraint

# **Extended Reading:**

A. Bar-Hillel, T. Hertz, N. Shental, and D. Weinshall, "Learning distance functions using equivalence relations," in *Proc. International Conference on Machine Learning*, 2003.

### Discriminative Component Analysis (DCA)

Minimize the distance within each chunklet and maximize the distance between chunklets

$$C_{b} = \frac{1}{k} \sum_{i} \sum_{j} (m_{i} - m_{j}) (m_{i} - m_{j})^{T}$$

$$C_{w} = \frac{1}{n} \sum_{i} \sum_{j} (x_{ji} - m_{j}) (x_{ji} - m_{j})^{T}$$

$$J(A) = argmax_{A A^{TC}}$$

$$x_{ji} \text{ i-th sample in j-th chunklet}$$

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$$+ C_{w} = \frac{1}{n} \sum_{$$

### **Extended Reading:**

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### Large Margin Nearest Neighbor (LMNN)

Maximize the margin between the distance of similar samples and the distance of dissimilar samples

$$\min_{M > 0} \sum \eta_{ij} \|x_i - x_j\|_M^2 + c \sum_{ijl} \eta_{ij} (1 - y_{il}) \left(1 + \|x_i - x_j\|_M^2 - \|x_i - x_l\|_M^2\right)_+$$
Nearest neighbor + hard constraints

# **Extended Reading:**

Kilian Q. Weinberger and Lawrence K. Saul. 2009. Distance Metric Learning for Large Margin Nearest Neighbor Classification. J. Mach. Learn. Res. 10 (June 2009), 207-244.

### Information-Theoretic Metric Learning (ITML)

Regularize the Mahalanobis matrix M to be as close as possible to a given Mahalanobis distance function, parameterized by  $M_0$ 

$$\begin{aligned} &\min_{M > 0} KL(p(x, M_0) || p(x, M)) \\ &s.t. \ d_M(x_i, x_j) < u, (x_i, x_j) \in S \\ &d_M(x_i, x_j) > l, (x_i, x_j) \in D \\ &p(x, M) = \frac{1}{Z} exp(-\frac{1}{2} d_M(x, u)) \end{aligned} \qquad \text{S and D are hard constraints}$$

### **Extended Reading:**

Jason V. Davis, Brian Kulis, Prateek Jain, Suvrit Sra, and Inderjit S. Dhillon. 2007. Information-theoretic metric learning. In *Proceedings of the 24th international conference on Machine learning* (ICML '07),2007.

### **Bregman Distance Function Learning (BDFL)**

#### Pairwise hard constraints

$$d(x_1, x_2) = \varphi(x_1) - \varphi(x_2) - (x_1 - x_2)^{\top} \varphi^2(x_2)$$
  

$$\Rightarrow d(x_1, x_2) = (x_1 - x_2)^{\top} \nabla^2 \varphi(\widehat{x})(x_1 - x_2)$$

$$\min_{\varphi \in \Omega(\mathcal{H}_k), b \in \mathbb{R}^+} \frac{1}{2} |\varphi|_{\mathcal{H}_k}^2 + C \sum_i \ell(y^i [d(x_1^i, x_2^i) - b^i])$$

Side info:  $x_1 x_2$  similar: y = 1 $x_1 x_2$  dissimilar: y = -1

### Extended Reading:

Lei Wu, Rong Jin, Steven C.H. Hoi, Jianke Zhu, Nenghai Yu, "Learning Bregman Distance Functions and Its Application for Semi-Supervised Clustering", Advances in Neural Information Processing Systems (NIPS'09), 2009.

# probabilistic Relevance Component Analysis (pRCA)

Probabilistic constraints

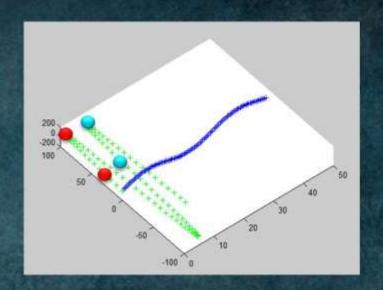
$$\min_{M > 0, P, m} \sum_{i} \sum_{j} p_{ij} \|x_i - m_j\|_{M}^2 - \lambda log |M|$$
Probabilistic side information  $> 0$ 

### **Extended Reading:**

Lei Wu, Steven C.H. Hoi, Rong Jin, Jianke Zhu, Nenghai Yu, "Distance Metric Learning from Uncertain Side Information with Application to Automated Photo Tagging", ACM International Conference on Multimedia (MM'09), 2009.

Supervised metric learning?

$$d(x_1, x_2) = \sqrt{(x_1 - x_2)^T M(x_1 - x_2)}$$



**Object function** 

L(M)

Side information

Similar • • Dissimilar pairs • • pairs

Regularization

R(M)

### Regularization

Introducing additional information in order to solve an ill-posed problem or to prevent overfitting

### **Basic regularizers:**

- Bayesian information criterion || M || 0
  - Equal to minimum description length criterion (MDL)
- Least absolute shrinkage and selection operator (Lasso) ||M||<sub>1</sub>
  - Fundamental to compressed sensing
- Tikhonov regularization (ridge regression)  $||M||_2$ 
  - Common method to handle ill posed problem

### **Extended Reading:**

A. Neumaier, Solving ill-conditioned and singular linear systems: A tutorial on regularization, SIAM Review 40 (1998), 636-666.

### Regularization

Introducing additional information in order to handle specific requirements, such as sparsity

### Some other regularizers:

- tr(M)
  - Regularize diagonals
- log det(M)
  - Equal to tr(exp(M))
- $||M||_{(2,1)} = \sum_{i} (\sum_{j} |m_{ij}|^{2})^{\frac{1}{2}}$ 
  - Regularize columns

### **Extended Reading:**

Guo-Jun Qi, Jinhui Tang, Zheng-Jun Zha and Tat-Seng Chua and Hong-Jiang Zhang, An Efficient Sparse Metric Learning in High-Dimensional Space via I1-Penalized Log-Determinant Regulaization, ICML 2009

### Regularization

Introducing additional information in order to handle specific requirements, such as sparsity

### Generalized regularizers for metric learning:

- tr(LM)
  - If  $L = I \Rightarrow tr(M) \Rightarrow$  Generalized Sparese metric learning
  - If  $L = \sum \Rightarrow \sum_{x_i x_j} (x_i x_j)^{\top} M(x_i x_j)$
  - if  $L = I, M = v^{T}v \Rightarrow ||v||_{2} \Rightarrow D ranking vector machine$
  - if L = M,  $\Rightarrow tr(MM) \Rightarrow ||M||_{Fro}^2 \Rightarrow Pair wise SVM$

• 
$$||M||_{Fro} = \sqrt{\sum_{i} \sum_{j} |m_{ij}|^2} = \sqrt{tr(MM)}$$

### Extended Reading:

Kaizhu Huang, Yiming Ying, and Colin Campbell. 2009. GSML: A Unified Framework for Sparse Metric Learning. In *Proceedings of the 2009 Ninth IEEE International Conference on Data Mining* (ICDM '09). IEEE Computer Society, Washington, DC, USA, 189-198.

What is the dimension of Metric M?

 $d \times d$ 

Metric M must be symmetric or can be represented as a nonsymmetric form?

$$M = \frac{M + M^{\mathsf{T}}}{2} + \frac{M - M^{\mathsf{T}}}{2}$$

Metric M must positive semi-definite (PSD)?

$$if x^{\top} M x \leq 0$$

$$x = y - z \Leftrightarrow ||y - z||_{M} \leq ||y - y||_{M}$$

# Metric M must meet the triangular inequality?

$$||x - y||_M \le ||x - z||_M + ||z - y||_M$$
If  $y = x$ ?

# What property should distance preserve?

$$d(x_1,x_2)=d(x_2,x_1)$$

$$d(x_1,x_2)=0 \Leftrightarrow x_1=x_2$$

$$d(x_1,x_3) \leq d(x_1,x_2) + d(x_2,x_3)$$

What is the relation between Metric learning and support vector machine?

DML

$$min_{M} \sum_{i} y_{i} (||(x_{i1} - x_{i2})A||^{2} - b_{i}) + log|M|$$

SVM

$$min_{w,b,\alpha} \frac{1}{2} ||w||^2 - \sum_i \alpha_i \left[ y_i (w_i x_i - b_i) - 1 \right]$$

$$\iff \max_{\alpha} -\frac{1}{2} \sum_{i,j} y_i y_j K(x_i, x_j) \alpha_i \alpha_j + \sum_j \alpha_j$$

$$s.t. \sum_{i} \alpha_{i} y_{i} = 0, \qquad 0 \leq \alpha_{i} \leq C, \forall i$$

$$K(x_i, x_j) = \left| \left| x_i - x_j \right| \right|^2 - c$$

What is the relation between Metric learning and Embedding?

DML: pair-wise constraints, preserve the supervised side info

$$M^* = argmin_M \sum_{(x_{i1}, x_{i2}) \in S} ||Ax_{i1} - Ax_{i2}||^2$$

Embeding: preserve the geodesic distance between samples

$$W^* = argmin_W \sum_{i} \left\| x_i - \sum_{x_j \in N(x_i)} W_j x_j \right\|^2$$

Exploration of Distance Function Learning (BDFL)
(Learning Bregman Distance Functions and Its Application for Semi-Supervised Clustering (NIPS09))

$$d(x_1,x_2) = \sqrt{(x_1-x_2)^T M(x_1-x_2)}$$

Drawbacks: M is a dxd matrix

### Advantage:

1.  $\varphi(\widehat{x})$  is a function  $\mathbb{R}^d o \mathbb{R}$ , and  $\nabla \varphi(x_1)$  is a vector rather than a matrix  $\mathcal{O}(dxd) o \mathcal{O}(d)$ 

**2.**  $\varphi(\widehat{x})$  is local sensitive. Hessian matrix of convex function  $\nabla^2 \varphi(\widehat{x})$  depends on the location of  $x_1$  and  $x_2$ 

### **Any Problem?**

# Exploration of Distance Function Learning (Learning Bregman Distance Functions and Its Application for Semi-Supervised Clustering (NIPS09))

$$d(x_1, x_2) = \sqrt{(x_1 - x_2)^T M(x_1 - x_2)} \leftarrow d(x_1, x_2) = (x_1 - x_2)^T \nabla^2 \varphi(\widehat{x})(x_1 - x_2)$$

**Property of Mahalanobis distance** 

$$d(x_1, x_2) = d(x_2, x_1)$$
 $d(x_1, x_2) = 0 \Leftrightarrow x_1 = x_2$ 
 $d(x_1, x_3) \le d(x_1, x_2) + d(x_2, x_3)$ 

Property of Bregman distance function  $\nabla^2 \varphi(\widehat{x})$ 

$$d(x_1, x_2) = d(x_2, x_1)$$
 $d(x_1, x_2) = 0 \Leftrightarrow x_1 = x_2$ 
 $d(x_1, x_3) \le d(x_1, x_2) + d(x_2, x_3)$ 
?

Let  $\Omega$  be the closed domain for x. If  $\exists m, M \in \mathbb{R}, M > m > 0$ , and  $mI \leqslant \min_{x \in \Omega} \nabla^2 \varphi(x) \leqslant \max_{x \in \Omega} \nabla^2 \varphi(x) \leqslant MI$  where I is identity matrix, we have the following inequality

$$\sqrt{d(x_a, x_b)} \le \sqrt{d(x_a, x_c)} + \sqrt{d(x_c, x_b)} + (\sqrt{M} - \sqrt{m})(d(x_a, x_c)d(x_c, x_b))^{\frac{1}{4}}$$

Let  $\Omega$  be the closed domain for x. If  $\exists m, M \in \mathbb{R}, M > m > 0$ , and  $mI \leq \min_{x \in \Omega} \nabla^2 \varphi(x) \leq \max_{x \in \Omega} \nabla^2 \varphi(x) \leq MI$  where I is identity matrix, we have the following inequality

$$\sqrt{d(x_a,x_b)} \leq \sqrt{d(x_a,x_c)} + \sqrt{d(x_c,x_b)} + \left(\sqrt{M} - \sqrt{m}\right)\left(d(x_a,x_c)d(x_c,x_b)\right)^{\frac{1}{4}}$$

*Proof.* First, let us denote by f as follows:

$$f = (\sqrt{M} - \sqrt{m})[d(x_a, x_c)d(x_c, x_b)]^{1/4}$$

The square of the right side of Eq. (2) is

$$(\sqrt{d(x_a, x_c)} + \sqrt{d(x_c, x_b)} + f^{1/4})^2 = d(x_a, x_b) - \eta(x_a, x_b, x_c) + \delta(x_a, x_b, x_c)$$

where

$$\delta(x_a, x_b, x_c) = f^2 + 2f\sqrt{d(x_a, x_c)} + 2f\sqrt{d(x_c, x_b)} + 2\sqrt{d(x_a, x_c)d(x_c, x_b)} 
\eta(x_a, x_b, x_c) = (\nabla\varphi(x_a) - \nabla\varphi(x_c))(x_c - x_b) + (\nabla\varphi(x_c) - \nabla\varphi(x_b))(x_a - x_c).$$

From this above equation, the proposition holds if and only if  $\delta(x_a, x_b, x_c) - \eta(x_a, x_b, x_c) \geq 0$ . From the fact that

$$=\frac{\delta(x_{a},x_{b},x_{c})-\eta(x_{a},x_{b},x_{c})}{\frac{(\sqrt{M}-\sqrt{m})^{2}+2(\sqrt{M}-\sqrt{m})\left(d(x_{a},x_{c})^{\frac{3}{4}}d(x_{c},x_{b})^{\frac{1}{4}}+d(x_{c},x_{b})^{\frac{3}{4}}d(x_{a},x_{c})^{\frac{1}{4}}\right)+2d(x_{a},x_{c})d(x_{c},x_{b})}{\sqrt{d(x_{a},x_{c})d(x_{c},x_{b})}}$$

since  $\sqrt{M} > \sqrt{m}$  and the distance function  $d(\cdot) \geq 0$ , we get  $\delta(x_a, x_b, x_c) - \eta(x_a, x_b, x_c) \geq 0$ .  $\square$ 

Exploration of Distance Function Learning
(Learning Bregman Distance Functions and Its Application for Semi-Supervised Clustering (NIPS09))

$$d(x_1,x_2) = (x_1 - x_2)^{\mathsf{T}} \nabla^2 \varphi(\widehat{\mathbf{x}})(x_1 - x_2)$$

$$\min_{\varphi,b} \frac{1}{2} |\varphi|_{\mathcal{H}_k}^2 + C \sum_{i=1}^n \ell(y_i [d(x_i^1, x_i^2) - b])$$

How to solve?

$$\varphi(x) = \int dy \kappa(x, y) q(y) = \int dy \exp(x^{T}y) q(y)$$
$$= \int du \exp(x^{T}Xu) q(u)$$

Assume 
$$q(y) = \sum_{i} \alpha_{i} \delta(y - x_{i})$$

$$Min_{\alpha \in \mathbb{R}^{N}_{+}, b} \mathcal{L} = \frac{1}{2} \alpha^{\top} K \alpha + C \sum_{i} \ell(y_{i}[z_{i}^{\top} \alpha - b])$$

$$z_{i} = \left[ exp(x_{i}^{1}) - exp(x_{i}^{2}) \right] \circ \left[ X^{\top}(x_{i}^{1} - x_{i}^{2}) \right]$$

Extended Reading:

Lei Wu, Rong Jin, Steven C.H. Hoi, Jianke Zhu, Nenghai Yu, "Learning Bregman Distance Functions and Its Application for Semi-Supervised Clustering", Advances in Neural Information Processing Systems (NIPS'09), 2009.

The function that minimizes

$$\min_{\varphi,b} \frac{1}{2} |\varphi|_{\mathcal{H}_k}^2 + C \sum_{i=1}^n \ell(y_i [d(x_i^1, x_i^2) - b])$$

Admits the following form:

$$\begin{split} \varphi(x) \in \mathcal{H}_\parallel &= \int_{y \in A} dy q(y) h(x^\top y) = \int du \; h(x^\top X u) q(u) \\ \textit{Where } u \in R^N, \textit{and } X = (x_1, \cdots, x_N). \end{split}$$

*Proof.* We write  $\varphi(x) = \varphi_{\parallel}(x) + \varphi_{\perp}(x)$  where

$$\varphi_{\parallel}(x) \in \mathcal{H}_{\parallel} = \int\limits_{y \in \mathcal{A}} dy q(y) h(x^{\top}y), \ \varphi_{\perp}(x) \in \mathcal{H}_{\perp} = \int\limits_{y \in \bar{\mathcal{A}}} dy q(y) h(x^{\top}y)$$

Thus, the distance function defined in (1) is then expressed as

$$d(x_{a}, x_{b}) = (x_{a} - x_{b})^{\top} \left(\nabla \varphi_{\parallel}(x_{a}) - \nabla \varphi_{\parallel}(x_{b})\right) + (x_{a} - x_{b})^{\top} \left(\nabla \varphi_{\perp}(x_{a}) - \nabla \varphi_{\perp}(x_{b})\right)$$

$$= \int_{y \in \mathcal{A}} q(y)(h'(x_{a}^{\top}y) - h'(x_{b}^{\top}y))y^{\top} (x_{a} - x_{b}) + \int_{y \in \bar{\mathcal{A}}} q(y)(h'(x_{a}^{\top}y) - h'(x_{b}^{\top}y))y^{\top} (x_{a} - x_{b})$$

$$= \int_{y \in \mathcal{A}} q(y)(h'(x_{a}^{\top}y) - h'(x_{b}^{\top}y))y^{\top} (x_{a} - x_{b}) = (x_{a} - x_{b})^{\top} \left(\nabla \varphi_{\parallel}(x_{a}) - \nabla \varphi_{\parallel}(x_{b})\right)$$

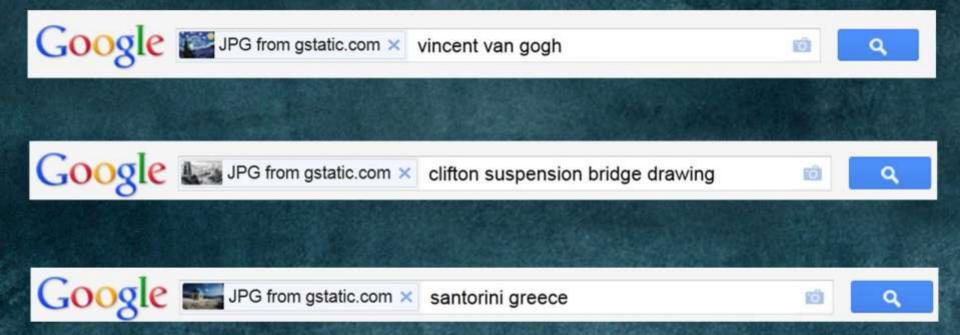
Since  $|\varphi(x)|_{\mathcal{H}_{\kappa}}^2 = |\varphi_{\parallel}(x)|_{\mathcal{H}_{\kappa}}^2 + |\varphi_{\perp}(x)|_{\mathcal{H}_{\kappa}}^2$ , the minimizer of (1) should have  $|\varphi_{\perp}(x)|_{\mathcal{H}_{\kappa}}^2 = 0$ . Since  $|\varphi_{\perp}(x)| = \langle \varphi_{\perp}(\cdot), \kappa(x, \cdot) \rangle_{\mathcal{H}_{\kappa}} \leq |\kappa(x, \cdot)|_{\mathcal{H}_{\kappa}} |\varphi_{\perp}|_{\mathcal{H}_{\kappa}} = 0$ , we have  $\varphi_{\perp}(x) = 0$  for any x. We thus have  $\varphi(x) = \varphi_{\parallel}(x)$ , which leads to the result in the theorem.



Distance Metric Learning II

Application of DML

Lei Wu University of Pittsburgh Distance measurement is important.



#### Background

- Annotation/tagging is essential to making images accessible to Web users
- Social media data in social websites enjoy rich tagging information provided by Web users











Taken the tagged images as knowledge, is it possible to automatically tag the billions of images?

- Annotation by Search (Wang et al. 2006)
  - resolve the challenge of auto-photo annotation by leveraging the emerging huge amount of rich image surrounding text

### Main problems which limit the Annotation by Search

- Web noise
- Semantic gap



Sun Bird Sky Blue ...



Bird Fly White Cloud



Sun Cloud Hawk Fly Eagle

....

$$d_M(x_i, x_j) = \sqrt{((x_i - x_j)^\top M(x_i - x_j))}$$

- Distance Metric Learning
  - Learning to optimize the metric M
  - Side Information (a.k.s. "Pairwise Constraints")
    - Similar pairs  $S(x_1, x_2)$ :  $x_1$  and  $x_2$  belong to the same category
    - Dissimilar pairs D(x<sub>1</sub>, x<sub>2</sub>): x<sub>1</sub> and x<sub>2</sub> belong to different categories

#### Motivation

- Certain side information
  - Generated by humans
  - Noise free
  - Hard constraints: similar=1; dissimilar=0
- How about learning a better soft constraints automatically from uncertain info of the Web?
  - Small-scale
  - Inaccurate

#### Motivation

#### **Certain Side Info**

#### Pros:

- Simple
- Easy to Adopt

#### Cons:

- Manual
- Expensive



#### **Uncertain Side Info**

#### Pros:

- Learn from Web
- Large amount

#### Cons:

- Complicated
- Noisy



Author: Lei

Tags:

Sun, Bird Sky, Blue

...

Author: Lei

Tags:

Bird, Fly

White, Cloud

...

#### Motivation

- Annotation by Search from Social Media
  - NO explicit pairwise side information available
  - But rich information is available with social images
- Ideas of our research
  - To discover implicit pairwise relationship between social images via a probabilistic approach
  - To learn effective distance metrics from uncertain side information that is discovered from social images implicitly

Probabilistic Relevance Component Analysis (pRCA)

## The objective function of pRCA:

Minimize Sum of square distances of examples from their chunklet's centers

$$\min_{M\succeq 0,\mu,P} \qquad \sum_{i=1}^n \sum_{k=1}^m p_i^{(k)} \|x_i - \mu_k\|_M^2 - \lambda \log |M|$$
 
$$s.t. \qquad \|P - P_0\|_F^2 \leq \gamma,$$
 
$$\sum_k p_i^{(k)} = 1 \qquad \text{regularization preventing the trivial solution}$$

**Corollary 1.** When fixing the means of chunklets  $\mu$  and the matrix of probability assignments P (assuming with hard assignments of 0 and 1), the Probabilistic Relevance Component Analysis (pRCA) formulation reduces to the regular RCA learning.

 To evaluate the time efficiency performance of the proposed DML algorithm on the same dataset

Table 1: Time cost of different DML methods.

(s)	baseline	RCA	DCA	ITML
Time	N/A	731.63	865.58	1185.27
(s)	LMNN	NCA	RDML	pRCA
Time	1673.23	28989.78	824.81	891.15

## Findings

- The most efficient method is the regular RCA approach
- The most time-consuming one is NCA
- pRCA is quite competitive, which is worse than RCA,DCA, and RDML, but is considerably better than ITML, LMNN, and NCA

#### Some Good Examples

# **Query Photo** Top Recommended Tags autumn, fall, forest, trees, nature, tree wood, germany, path, creative sunset, clouds, sky, sea, beach, abigfave, sun, water, landscape, ocean tiger, zoo, specanimal, impressedbeauty, abigfave, nature, animal, cat, animals, aplusphoto garden, flowers, yellow, nature, hdr, nikon, spring, festival, impressed beauty

## Some Poor Examples

Query Photo	Top Recommended Tags
	macro, nikon, bokeh, nature, flower, canon, storm, eos, plane, flickrsbest
	nikon, street, water, sport, blue, bike, lebanon, kids, eric mckenna, krissy mckenna
	winter, photography, art , beach usa, fashion, portrait , travel, party, snow
The state of the s	park, river, travel, trees, lake, hiking, winter, green, vacation, water

#### Conclusions

- Distance metric learning (DML) is very useful tool in solving distance based applications
- There are quite a lot of interesting research problems in DML
- A little step on DML will make great impact to many applications
- This lecture is only an introduction. More details please refer to the reference papers
- Think hard and maybe a great idea will come out to change the world

#### References

- J. Goldberger, S. Roweis, G. Hinton, and R. Salakhutdinov, "Neighbourhood components analysis," in *Proc. NIPS*, 2005.
- E. P. Xing, A. Y. Ng, M. I. Jordan, and S. Russell. Distance metric learning with application to clustering with side-information. In NIPS2002, 2002
- A. Bar-Hillel, T. Hertz, N. Shental, and D. Weinshall, "Learning distance functions using equivalence relations," in *Proc. International Conference on Machine Learning*, 2003.
- Steven C. H. Hoi, Wei Liu, Michael R. Lyu, and Wei-Ying Ma. 2006. Learning Distance Metrics with Contextual Constraints for Image Retrieval. (CVPR '06), 2006.
- Lei Wu, Steven C.H. Hoi, Rong Jin, Jianke Zhu, Nenghai Yu, "Distance Metric Learning from Uncertain Side Information with Application to Automated Photo Tagging", ACM International Conference on Multimedia (MM'09), 2009.
- Kilian Q. Weinberger and Lawrence K. Saul. 2009. Distance Metric Learning for Large Margin Nearest Neighbor Classification. J. Mach. Learn. Res. 10 (June 2009), 207-244.
- Jason V. Davis, Brian Kulis, Prateek Jain, Suvrit Sra, and Inderjit S. Dhillon. 2007. Information-theoretic metric learning. In Proceedings of the 24th international conference on Machine learning (ICML '07),2007.
- Lei Wu, Rong Jin, Steven C.H. Hoi, Jianke Zhu, Nenghai Yu, "Learning Bregman
  Distance Functions and Its Application for Semi-Supervised Clustering", Advances in
  Neural Information Processing Systems (NIPS'09), 2009.

# Thanks

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