Metric and Kernel Learning

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Metric Learning

- Goal: "Learn" Distance Metric between Data
- Important problem in Data Mining & Machine Learning
- Can govern success or failure of data mining algorithm

Metric Learning: Example I

Similarity by Person(identity) or by Pose

Metric Learning: Example II

- Consider a set of text documents
- Each document is a review of a classical music piece
- Might be clusterable in one of two ways
  - By Composer (Beethoven, Mozart, Mendelssohn)
  - By Form (Symphony, Sonata, Concerto)
- Similarity by Composer or by Form

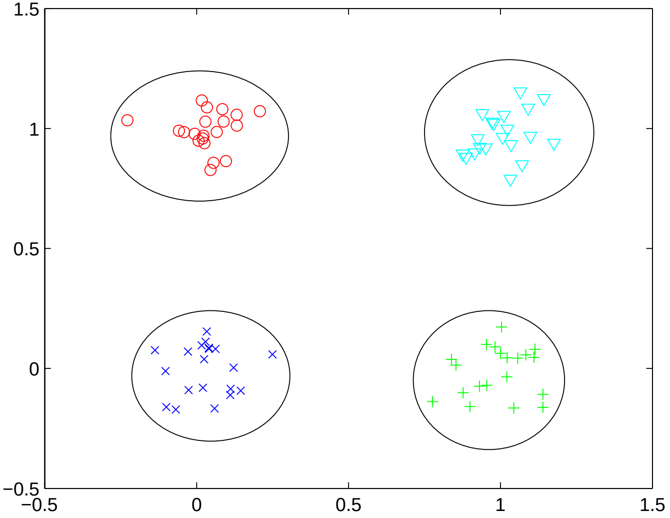
Mahalanobis Distances

- We restrict ourselves to learning *Mahalanobis distances*:
  - Distance parameterized by positive definite matrix $\mathbf{\Sigma}$:

$$d_{\mathbf{\Sigma}}(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 - \mathbf{x}_2)^T \mathbf{\Sigma}(\mathbf{x}_1 - \mathbf{x}_2)$$

  - Often $\mathbf{\Sigma}$ is the inverse of the covariance matrix
  - Generalizes squared Euclidean distance ($\mathbf{\Sigma} = I$)
  - Rotates and scales input data

Example: Four Blobs



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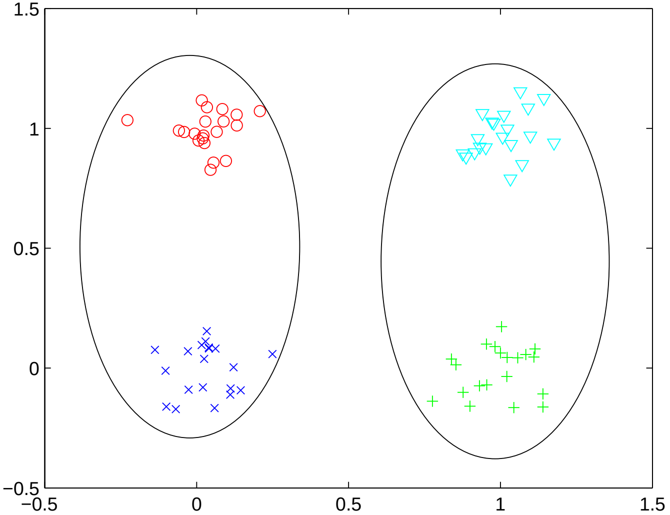

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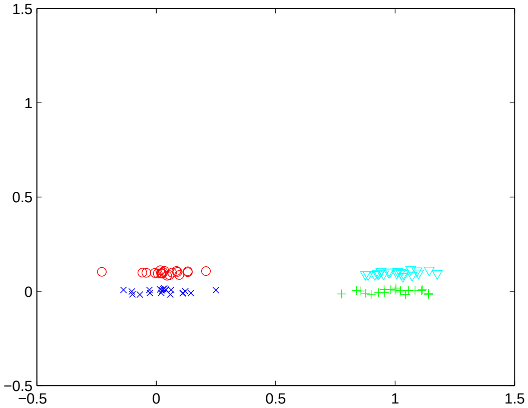

- Want to learn:

$$\boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & \epsilon \end{pmatrix}$$

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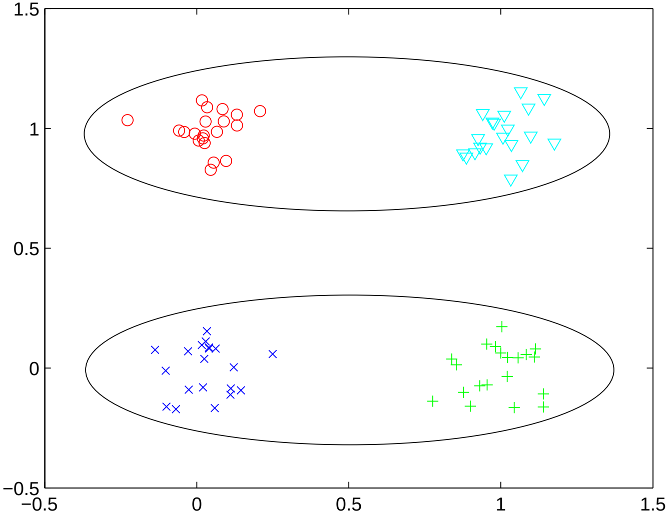

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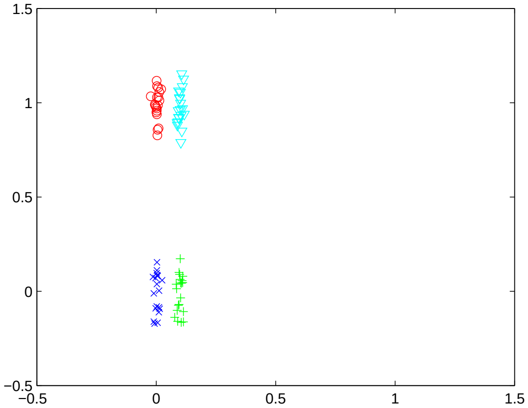

- Want to learn:

$$\Sigma = \begin{pmatrix} \epsilon & 0 \\ 0 & 1 \end{pmatrix}$$

Problem Formulation

- **Metric Learning Goal:**

$$\begin{array}{ll} \min_{\boldsymbol{\Sigma}} \mathrm{dist}(\boldsymbol{\Sigma}, \boldsymbol{\Sigma}_0) & \\ (\mathbf{x}_i - \mathbf{x}_j)^T \boldsymbol{\Sigma} (\mathbf{x}_i - \mathbf{x}_j) \leq u & \text{if } (i,j) \in S \text{ [similarity constraints]} \\ (\mathbf{x}_i - \mathbf{x}_j)^T \boldsymbol{\Sigma} (\mathbf{x}_i - \mathbf{x}_j) \geq \ell & \text{if } (i,j) \in D \text{ [dissimilarity constraints]} \end{array}$$

- Learn spd matrix $\boldsymbol{\Sigma}$ that is "close" to the baseline spd matrix $\boldsymbol{\Sigma}_0$
- Other linear constraints on $\boldsymbol{\Sigma}$ are possible
- Constraints can arise from various scenarios
  - Unsupervised: Click-through feedback
  - Semi-supervised: must-link and cannot-link constraints
  - Supervised: points in the same class have "small" distance, etc.

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- Learn spd matrix $\boldsymbol{\Sigma}$ that is "close" to the baseline spd matrix $\boldsymbol{\Sigma}_0$
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- Constraints can arise from various scenarios
  - Unsupervised: Click-through feedback
  - Semi-supervised: must-link and cannot-link constraints
  - Supervised: points in the same class have "small" distance, etc.
- QUESTION: What should "dist" be?

LogDet Divergence

- We use $\text{dist}(\boldsymbol{\Sigma}, \boldsymbol{\Sigma}_0)$ to be the Log-Determinant Divergence:

$$D_{\ell d}(\boldsymbol{\Sigma}, \boldsymbol{\Sigma}_0) = \text{trace}(\boldsymbol{\Sigma}\boldsymbol{\Sigma}_0^{-1}) - \log\det(\boldsymbol{\Sigma}\boldsymbol{\Sigma}_0^{-1}) - d$$

- **Our Goal:**

$$\begin{array}{ll} \min_{\boldsymbol{\Sigma}} D_{\ell d}(\boldsymbol{\Sigma}, \boldsymbol{\Sigma}_0) & \\ (\mathbf{x}_i - \mathbf{x}_j)^T \boldsymbol{\Sigma} (\mathbf{x}_i - \mathbf{x}_j) \leq u & \text{if } (i,j) \in S \text{ [similarity constraints]} \\ (\mathbf{x}_i - \mathbf{x}_j)^T \boldsymbol{\Sigma} (\mathbf{x}_i - \mathbf{x}_j) \geq \ell & \text{if } (i,j) \in D \text{ [dissimilarity constraints]} \end{array}$$

Preview

- Salient points of our Approach:
  - Metric Learning is equivalent to "Kernel Learning"
  - Generalizes to Unseen Data Points
  - Can improve upon an input metric or kernel
  - No expensive eigenvector computation or semi-definite programming
- Most existing methods fail to satisfy one or more of the above

Brief Digression

Bregman Divergences

- Let $\varphi : S \rightarrow \mathbb{R}$ be a differentiable, strictly convex function of "Legendre type" ($S \subseteq \mathbb{R}^d$)
- The Bregman Divergence $D_\varphi : S \times \text{relint}(S) \rightarrow \mathbb{R}$ is defined as

$$D_\varphi(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x}) - \varphi(\mathbf{y}) - (\mathbf{x} - \mathbf{y})^T \nabla \varphi(\mathbf{y})$$

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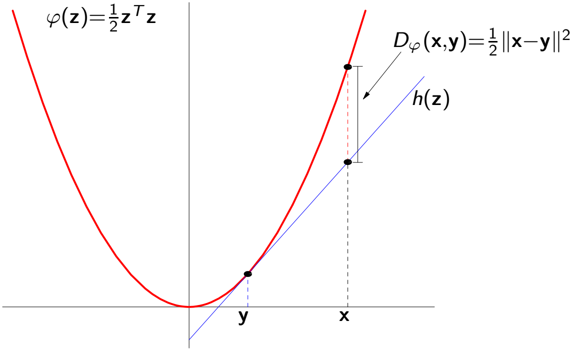

Squared Euclidean distance is a Bregman divergence

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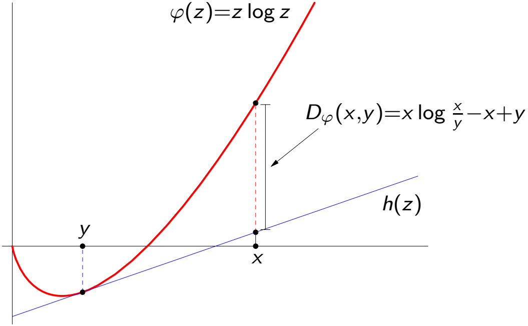

Relative Entropy (or KL-divergence) is another Bregman divergence

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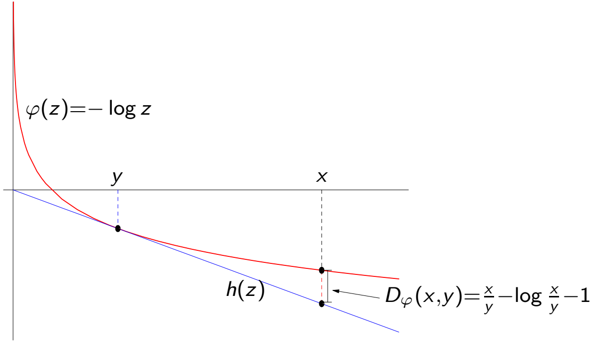

Itakura-Saito Dist.(used in signal processing) is also a Bregman divergence

Examples of Bregman Divergences

Function Name	$\varphi(x)$	$D_\varphi(x,y)$
Squared norm	$\frac{1}{2}x^2$	$\frac{1}{2}(x-y)^2$
Shannon entropy	$x\log x - x$	$x\log\frac{x}{y} - x + y$
Bit entropy	$x\log x + (1-x)\log(1-x)$	$x\log\frac{x}{y} + (1-x)\log\frac{1-x}{1-y}$
Burg entropy	$-\log x$	$\frac{x}{y} - \log\frac{x}{y} - 1$
Hellinger	$-\sqrt{1-x^2}$	$(1-xy)(1-y^2)^{-1/2} - (1-x^2)^{1/2}$
ℓ_p quasi-norm	$-x^p \qquad (0<p<1)$	$-x^p + p\,xy^{p-1} - (p-1)\,y^p$
ℓ_p norm	$\lvert x\rvert^p \qquad (1<p<\infty)$	$\lvert x\rvert^p - p\,x\,\mathrm{sgn}\,y\lvert y\rvert^{p-1} + (p-1)\lvert y\rvert^p$
Exponential	e^x	$e^x - (x-y+1)e^y$
Inverse	$1/x$	$1/x + x/y^2 - 2/y$

Bregman Matrix Divergences

- Define

$$D_{\varphi}(X, Y) = \varphi(X) - \varphi(Y) - \text{trace}((\nabla\varphi(Y))^T(X - Y))$$

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$$D_\varphi(X, Y) = \frac{1}{2}\|X - Y\|_F^2$$

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$$D_\varphi(X, Y) = \frac{1}{2}\|X - Y\|_F^2$$
- von Neumann Divergence: For $X \succeq 0$, $\varphi(X) = \text{trace}(X \log X)$. Then
$$D_\varphi(X, Y) = \text{trace}(X \log X - X \log Y - X + Y)$$
  - also called quantum relative entropy

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- LogDet divergence: For $X \succ 0$, $\varphi(X) = -\log\det X$. Then

$$D_\varphi(X, Y) = \mathrm{trace}(XY^{-1}) - \log\det(XY^{-1}) - d$$

LogDet Divergence: Properties I

$$D_{\ell d}(X, Y) \quad = \quad \text{trace}(XY^{-1}) - \log\det(XY^{-1}) - d$$

- Properties:
  - Not symmetric
  - Triangle inequality does not hold
  - Can be unbounded
  - Convex in first argument (not in second)
  - Pythagorean Property holds:

$$D_{\ell d}(X, Y) \geq D_{\ell d}(X, P_\Omega(Y)) + D_{\ell d}(P_\Omega(Y), Y)$$

  - Divergence between inverses:

$$D_{\ell d}(X, Y) = D_{\ell d}(Y^{-1}, X^{-1})$$

LogDet Divergence: Properties II

$$\begin{aligned} D_{\ell d}(X, Y) &= \operatorname{trace}(XY^{-1}) - \log\det(XY^{-1}) - d, \\ &= \sum_{i=1}^{d}\sum_{j=1}^{d}(\mathbf{v}_i^T\mathbf{u}_j)^2\left(\frac{\lambda_i}{\theta_j} - \log\frac{\lambda_i}{\theta_j} - 1\right) \end{aligned}$$

- Properties:
  - Scale-invariance

$$D_{\ell d}(X, Y) = D_{\ell d}(\alpha X, \alpha Y), \quad \alpha \geq 0$$

  - In fact, for any invertible M

$$D_{\ell d}(X, Y) = D_{\ell d}(M^T X M, M^T Y M)$$

LogDet Divergence: Properties II

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  - Definition can be extended to rank-deficient matrices
  - Finiteness:

$$D_{\ell d}(X,Y) \text{ is finite iff } X \text{ and } Y \text{ have the same range space}$$

Information-Theoretic Interpretation

- Differential Relative Entropy between two Multivariate Gaussians:

$$\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}_0) \log \left(\frac{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}_0)}{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})} \right) d\mathbf{x} = \frac{1}{2} D_{\ell d}(\boldsymbol{\Sigma}, \boldsymbol{\Sigma}_0)$$

- Thus, the following two problems are equivalent

Relative Entropy Formulation		**LogDet Formulation**
$\min_{\boldsymbol{\Sigma}} \int \mathcal{N}(\mathbf{x}\vert\boldsymbol{\mu}, \boldsymbol{\Sigma}_0) \log \frac{\mathcal{N}(\mathbf{x}\vert\boldsymbol{\mu}, \boldsymbol{\Sigma}_0)}{\mathcal{N}(\mathbf{x}\vert\boldsymbol{\mu}, \boldsymbol{\Sigma})} d\mathbf{x}$		$\min_{\boldsymbol{\Sigma}} D_{\ell d}(\boldsymbol{\Sigma}, \boldsymbol{\Sigma}_0)$
$\mathrm{tr}(\boldsymbol{\Sigma}(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j^T) \le u$	$\Leftrightarrow$	$\mathrm{tr}(\boldsymbol{\Sigma}(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j^T) \le u$
$\mathrm{tr}(\boldsymbol{\Sigma}(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \ge \ell$		$\mathrm{tr}(\boldsymbol{\Sigma}(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \ge \ell$
$\boldsymbol{\Sigma} \succeq 0$		$\boldsymbol{\Sigma} \succeq 0$

Stein's Loss

- LogDet divergence is known as Stein's loss in the statistics community
- Stein's loss is the unique *scale invariant* loss-function for which the uniform minimum variance unbiased estimator is also a minimum risk equivariant estimator

Quasi-Newton Optimization

- LogDet Divergence arises in the BFGS and DFS updates
  - Quasi-Newton methods
  - Approximate Hessian of the function to be minimized
- [Fletcher, 1991] BFGS update can be written as:

$$\begin{array}{ll} \min_{B} & D_{\ell d}(B, B_t) \\ \text{subject to} & B\, s_t = y_t \quad (\text{“Secant Equation”}) \end{array}$$

- $s_t = x_{t+1} - x_t$, $y_t = \nabla f_{t+1} - \nabla f_t$
- Closed-form solution:

$$B_{t+1} = B_t - \frac{B_t s_s s_t^T B_t}{s_t^T B_t s_t} + \frac{y_t y_t^T}{s_t^T y_t}$$

- Similar form for DFS update

Algorithm: Bregman Projections for LogDet

- Algorithm: Cyclic Bregman Projections (successively onto each linear constraint) — converges to globally optimal solution
- Use Bregman projections to update the Mahalanobis matrix:

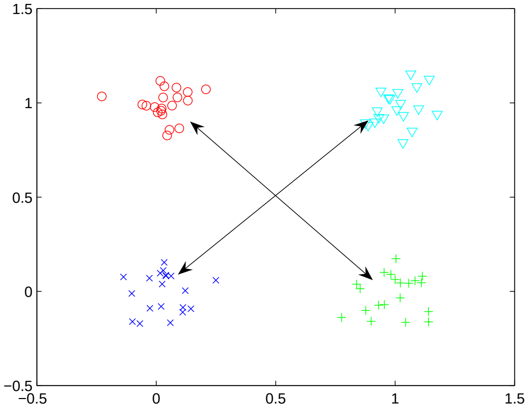
$$\begin{array}{ll} \min_{\boldsymbol{\Sigma}} & D_{\ell d}(\boldsymbol{\Sigma}, \boldsymbol{\Sigma}_t) \\ \text{s.t.} & (\mathbf{x}_i - \mathbf{x}_j)^T \boldsymbol{\Sigma} (\mathbf{x}_i - \mathbf{x}_j) \leq u \end{array}$$

- Can be solved by rank-one update:

$$\boldsymbol{\Sigma}_{t+1} = \boldsymbol{\Sigma}_t + \beta_t \boldsymbol{\Sigma}_t (\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T \boldsymbol{\Sigma}_t$$

- Advantages:
  - Automatic enforcement of positive semidefiniteness
  - Simple, closed-form projections
  - No eigenvector calculation
  - Easy to incorporate slack for each constraint

Example: Noisy XOR



- No linear transformation for XOR grouping

Kernel Methods

- Map input data to higher-dimensional "feature" space:

$$\mathbf{x} \rightarrow \varphi(\mathbf{x})$$

- Idea: Run machine learning algorithm in feature space

- Noisy XOR Example:

$$\mathbf{x} \rightarrow \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}$$

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- Map input data to higher-dimensional "feature" space:

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- Noisy XOR Example:

$$\mathbf{x} \longrightarrow \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}$$

- Kernel function: $K(\mathbf{x}, \mathbf{y}) = \langle \varphi(\mathbf{x}), \varphi(\mathbf{y}) \rangle$
- "Kernel trick" — no need to explicitly form high-dimensional features
- Noisy XOR Example: $\langle \varphi(\mathbf{x}), \varphi(\mathbf{y}) \rangle = (\mathbf{x}^T \mathbf{y})^2$

Connection to Kernel Learning

LogDet Formulation (1)

$$\begin{aligned} \min_{\mathbf{\Sigma}} \quad & D_{\ell d}(\mathbf{\Sigma}, \mathbf{\Sigma}_0) \\ \text{s.t.} \quad & \operatorname{tr}(\mathbf{\Sigma}(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \leq u \\ & \operatorname{tr}(\mathbf{\Sigma}(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \geq \ell \\ & \mathbf{\Sigma} \succeq 0 \end{aligned}$$

Kernel Formulation (2)

$$\begin{aligned} \min_{K} \quad & D_{\ell d}(K, K_0) \\ \text{s.t.} \quad & \operatorname{tr}(K(\mathbf{e}_i - \mathbf{e}_j)(\mathbf{e}_i - \mathbf{e}_j)^T) \leq u \\ & \operatorname{tr}(K(\mathbf{e}_i - \mathbf{e}_j)(\mathbf{e}_i - \mathbf{e}_j)^T) \geq \ell \\ & K \succeq 0 \end{aligned}$$

- (1) optimizes w.r.t. the $d \times d$ Mahalanobis matrix $\mathbf{\Sigma}$
- (2) optimizes w.r.t. the $N \times N$ kernel matrix K
- Let $K_0 = X^T \mathbf{\Sigma}_0 X$, where X is the input data
- Let $\mathbf{\Sigma}^*$ be optimal solution to (1) and K^* be optimal solution to (2)
- **Theorem:** $K^* = X^T \mathbf{\Sigma}^* X$
    - In fact, $\mathbf{\Sigma}^* = UKU^* + WW^*$, where UU^* is the orthogonal projector onto Range(X), and WW^* onto Null(X)

Kernelization

- Metric learning in kernel space
  - Assume input kernel function $\kappa(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x})^T \varphi(\mathbf{y})$
  - Want to learn

$$d_{\mathbf{\Sigma}}(\varphi(\mathbf{x}), \varphi(\mathbf{y})) = (\varphi(\mathbf{x}) - \varphi(\mathbf{y}))^T \mathbf{\Sigma}(\varphi(\mathbf{x}) - \varphi(\mathbf{y}))$$

  - Equivalently: learn a new kernel function of the form

$$\tilde{\kappa}(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x})^T \mathbf{\Sigma} \varphi(\mathbf{y})$$

  - How to learn this only using $\kappa(\mathbf{x}, \mathbf{y})$?
- Learned kernel can be shown to be of the form

$$\tilde{\kappa}(\mathbf{x}, \mathbf{y}) = \kappa(\mathbf{x}, \mathbf{y}) + \sum_i \sum_j \sigma_{ij} \kappa(\mathbf{x}, \mathbf{x}_i) \kappa(\mathbf{y}, \mathbf{x}_j)$$

- Can update σ_{ij} parameters while optimizing the kernel formulation

Related Work

- Distance Metric Learning [Xing, Ng, Jordan & Russell, 2002]
- Large margin nearest neighbor(LMNN) [Weinberger, Blitzer & Saul, 2005]
- Collapsing Classes (MCML) [Globerson & Roweis, 2005]
- Online Metric Learning (POLA) [Shalev-Shwartz, Singer & Ng, 2004]
- Many others!

Experimental Results

Framework

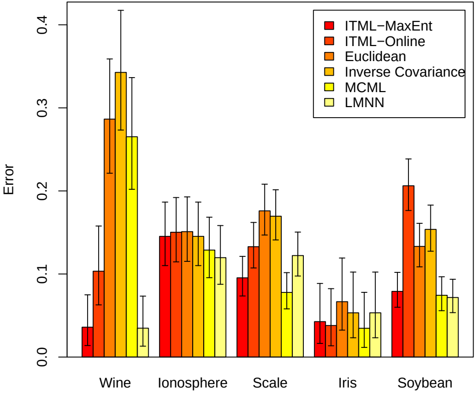
- k-nearest neighbor ($k = 4$)
- ℓ and u determined by 5th and 95th percentile of distribution
- $20c^2$ constraints, chosen randomly
- 2-fold cross validation

Algorithms

- Information-theoretic Metric Learning (offline and online)
- Large-Margin Nearest Neighbors (LMNN) [Weinberger et al.]
- Metric Learning by Collapsing Classes (MCML) [Globerson and Roweis]
- Baseline Metrics: Euclidean and Inverse Covariance

Results: UCI Data Sets

- Ran ITML with $\Sigma_0 = I$ (ITML-MaxEnt) and the inverse covariance (InverseCovariance)
- Ran online algorithm for 10^5 iterations



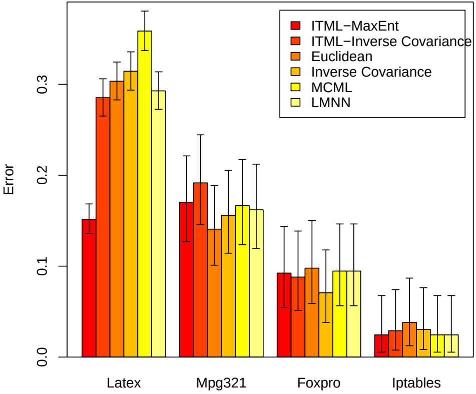
Application 1: "Clarify"

"Clarify" improves error reporting for software that uses black box components

- Motivation: Black box components complicate error messaging
- Solution: Error diagnosis via machine learning
- Representation: System collects program features during run-time
  - Function counts
  - Call-site counts
  - Counts of program paths
  - Program execution represented as a vector of counts
- Class labels: Program execution errors
- Nearest neighbor software support
  - Match program executions with others
  - Underlying distance measure should reflect this similarity

Results: Clarify

- Very high dimensionality
- Feature selection reduces the number of features to 20



Application 2: Learning Image Similarity

Goal: Learn a metric to compare images

- Start with a baseline measure
  - Use the **pyramid match kernel** [Grauman and Darrell]
  - Compares sets of image features
  - Efficient and effective measure of similarity between images
- Application of metric learning in kernel space
  - Other metric learning methods (LMNN, etc) cannot be applied
  - Does metric learning work in kernel space?

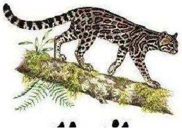
Caltech 101 Results

Data Set: Caltech 101

- Standard benchmark for multi-category image recognition
- 101 classes of images
- Wide variance in pose etc.
- Challenging data set

Experimental Setup

- 15 images per class in training set; rest in test set (2454 images)
- Performed 1-NN using original PMK and learned PMK



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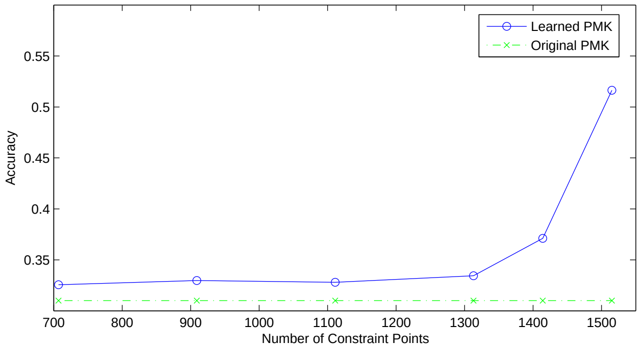


- When constraints are drawn from all training data, kNN accuracy is 52%, versus 32% for original PMK ([Jain, Kulis & Grauman, 2007])
- Data set is well-studied—best performance with 15 training images per class is 60%
  - Uses different features (geometric-blur)

Metric Learning in High Dimensions

Text analysis & Software analysis: Feature sets larger than 1,000

- Learning full distance matrix requires over 1 million parameters!
- Overfitting problems, intractable

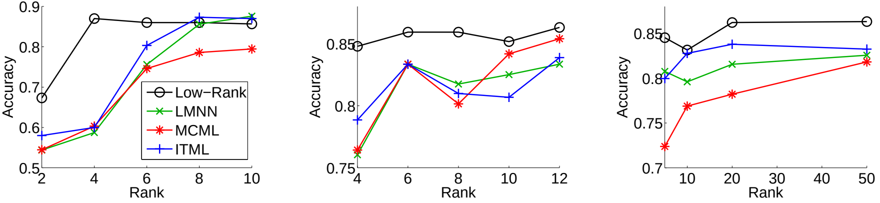
Solution: Learning low-rank Mahalanobis matrices

- LogDet divergence can be generalized to low-rank matrices
- $D_{\ell d}(X, Y)$ is finite $\leftrightarrow$ X and Y have the same range space
- Extending ITML to the low-rank case
  - If $\boldsymbol{\Sigma}_0$ is low-rank $\rightarrow$ $\boldsymbol{\Sigma}$ is low-rank
  - Clustered Mahalanobis matrices
  - If $\boldsymbol{\Sigma}_0$ is a block matrix, then $\boldsymbol{\Sigma}$ will also be a block matrix

Low-rank Metric Learning: Preliminary Results

Classification accuracy for Low-Rank ITML

- Classic3: Text dataset, PCA basis
- Mpg321, Gcc: Software analysis, Clustered basis



Classic3 Mpg321 Gcc

Conclusions

Metric Learning Formulation

- Uses LogDet divergence
- Information-theoretic interpretation
- Equivalent to kernel learning problem
  - Can improve upon input metric or kernel
  - Generalizes to unseen data points

Algorithm

- Bregman projections result in simple rank-one updates
- Can be kernelized
- Online variant has provable regret bounds

Empirical Evaluation

- Method is competitive with existing techniques
- Scalable to large data sets
- Applied to nearest-neighbor software support & image recognition

References

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