Information-Theoretic Metric Learning

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Presenter: Jason V. Davis

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Introduction

 Problem: Learn a Mahalanobis distance function subject to linear constraints

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- Problem: Learn a Mahalanobis distance function subject to linear constraints
- Information-theoretic viewpoint
 - Bijection between Gaussian distributions and Mahalanobis distances

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Natural entropy-based objective

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- Natural entropy-based objective
- Connections with kernel learning

Introduction

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- Information-theoretic viewpoint
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 - Natural entropy-based objective
- Connections with kernel learning
- Fast and simple methods
 - Based on Bregman's method for convex optimization

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No eigenvalue computations are needed!

Learning a Mahalanobis Distance

- Given *n* points $\{\mathbf{x}_1, ..., \mathbf{x}_n\}$ in \Re^d
- Given inequality constraints relating pairs of points
 - Similarity constraints: $d_A(\mathbf{x_i}, \mathbf{x_j}) \le u$
 - Dissimilarity constraints: $d_A(\mathbf{x_i}, \mathbf{x_j}) \ge \ell$

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- Problem: Learn a Mahalanobis distance that satisfies these constraints:

$$d_A(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i - \mathbf{x}_j)^T A(\mathbf{x}_i - \mathbf{x}_j)$$

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- Applications
 - k-means clustering
 - Nearest neighbor searches

Mahalanobis Distance and the Multivariate Gaussian

Problem: How to choose the 'best' Mahalanobis distance from the feasible set?

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Mahalanobis Distance and the Multivariate Gaussian

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- Solution: Regularize by choosing that which is 'closest' to Euclidean distance

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Mahalanobis Distance and the Multivariate Gaussian

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- Bijection between the multivariate Gaussian and the Mahalanobis Distance

$$p(\mathbf{x};\mathbf{m},A) = \frac{1}{Z} \exp\left(-\frac{1}{2}(\mathbf{x}-\mathbf{m})^T A(\mathbf{x}-\mathbf{m})\right)$$

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$$p(\mathbf{x};\mathbf{m},A) = \frac{1}{Z} \exp\left(-\frac{1}{2}(\mathbf{x}-\mathbf{m})^T A(\mathbf{x}-\mathbf{m})\right)$$

- Allows for comparison of two Mahalanobis distances
- Differential relative entropy between the associated Gaussians:

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$$\mathsf{KL}(p(\mathbf{x};\mathbf{m}_1,A_1)\|p(\mathbf{x};\mathbf{m}_2,A_2)) = \int p(\mathbf{x};\mathbf{m}_1,A_1)\log\frac{p(\mathbf{x};\mathbf{m}_1,A_1)}{p(\mathbf{x};\mathbf{m}_2,A_2)}\,d\mathbf{x}.$$

Problem Formulation

Goal: Minimize differential relative entropy subject to pairwise inequality constraints

$$\begin{array}{ll} \min & \mathsf{KL}(p(\mathbf{x};\mathbf{m},A) \| p(\mathbf{x};\mathbf{m},I)) \\ \text{subject to} & d_A(\mathbf{x}_i,\mathbf{x}_j) \leq u \qquad (i,j) \in S, \\ & d_A(\mathbf{x}_i,\mathbf{x}_j) \geq \ell \qquad (i,j) \in D \\ & A \succ 0 \end{array}$$

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Equivalence to Kernel Learning Optimization via Bregman's Method Extensions

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Overview: Optimizing the Model

- Show an equivalence between our problem and a low-rank kernel learning problem [Kulis, 2006]
 - > Yields closed-form solutions to compute the problem objective
 - Shows that the problem is convex

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Overview: Optimizing the Model

- Show an equivalence between our problem and a low-rank kernel learning problem [Kulis, 2006]
 - > Yields closed-form solutions to compute the problem objective
 - Shows that the problem is convex
- Use this equivalence to solve our problem efficiently

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Low-Rank Kernel Learning

- Given $X = [\mathbf{x}_1 \ \mathbf{x}_2 \ ... \ \mathbf{x}_n], \ \mathbf{x}_i \in \Re^d$, define $K_0 = X^T X$
- Constraints: similarity (S) or dissimilarity (D) between pairs of points
- Objective: Learn K that minimizes the divergence to K_0

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Low-Rank Kernel Learning

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- Constraints: similarity (S) or dissimilarity (D) between pairs of points
- Objective: Learn K that minimizes the divergence to K_0

$$\begin{array}{ll} \min & D_{\mathsf{Burg}}(K, K_0) \\ \text{subject to} & K_{ii} + K_{jj} - 2K_{ij} \leq u \qquad (i,j) \in S, \\ & K_{ii} + K_{jj} - 2K_{ij} \geq \ell \qquad (i,j) \in D, \\ & K \succeq 0 \end{array}$$

► *D*_{Burg} is the Burg divergence

$$D_{\text{Burg}}(K, K_0) = \text{Tr}(KK_0^{-1}) - \log \det(KK_0^{-1}) - n$$

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Equivalence to Kernel Learning

[Kulis, 2006] Let K be the optimal solution to the low-rank kernel learning problem.

- ▶ Then K has the same range space as K₀
- $\blacktriangleright K = X^T W^T W X$

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Equivalence to Kernel Learning

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Theorem: Let $K = X^T W^T W X$ be an optimal solution to the low-rank kernel learning problem.

Then A = W^TW is an optimal solution to the corresponding metric learning problem

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Proof Sketch

Lemma 1: $D_{\text{Burg}}(K, K_0) = 2\text{KL}(p(\mathbf{x}; \mathbf{m}, A) || p(\mathbf{x}; \mathbf{m}, I)) + c$

- Establishes that the objectives for the problem are the same
- Builds on a recent connection relating the relative entropy between Gaussians and the Burg divergence [Davis, 2006]

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Proof Sketch

Lemma 1: $D_{\text{Burg}}(K, K_0) = 2\text{KL}(p(\mathbf{x}; \mathbf{m}, A) || p(\mathbf{x}; \mathbf{m}, I)) + c$

- Establishes that the objectives for the problem are the same
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Lemma 2: Given $K = X^T A X$, A is feasible if and only if K is feasible

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Optimization via Bregman's Method

- Solve the associated kernel learning problem via Bregman's method
 - Dual ascent method
 - Iteratively projects onto one constraint at a time
 - Closed-form updates are known for this projection

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Optimization via Bregman's Method

- Solve the associated kernel learning problem via Bregman's method
 - Dual ascent method
 - Iteratively projects onto one constraint at a time
 - Closed-form updates are known for this projection
- Running time per iteration: $O(cd^2)$
 - Works on the kernel in factored form
 - Uses closed-form Bregman projections

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Optimization via Bregman's Method

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- Running time per iteration: $O(cd^2)$
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- Requires no eigenvalue decomposition

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Extensions

- Minimizing KL-divergence to a different Mahalanobis matrix
 - inverse of the sample covariance matrix

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- Minimizing KL-divergence to a different Mahalanobis matrix
 - inverse of the sample covariance matrix
- Slack variables

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Extensions

- Minimizing KL-divergence to a different Mahalanobis matrix
 - inverse of the sample covariance matrix
- Slack variables
- General linear inequality constraints
 - e.g. Relative distance comparisons [Schutz, 2003]

Experimental Methodology

► Goal: learn a Mahalanobis function for *kNN* classification

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Experimental Methodology

- ► Goal: learn a Mahalanobis function for *kNN* classification
- Approach:
 - Constrain points in the same class to be similar
 - Constrain points in different class to be dissimilar
 - Upper and lower bounds determined empirically

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Experimental Methodology

- ► Goal: learn a Mahalanobis function for *kNN* classification
- Approach:
 - Constrain points in the same class to be similar
 - Constrain points in different class to be dissimilar
 - Upper and lower bounds determined empirically
 - Sample 100 such constraints
 - No parameter tuning

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Experimental Methodology

- ► Goal: learn a Mahalanobis function for *kNN* classification
- Approach:
 - Constrain points in the same class to be similar
 - Constrain points in different class to be dissimilar
 - Upper and lower bounds determined empirically
 - Sample 100 such constraints
 - No parameter tuning
- Evaluate via cross-validation

Experimental Results

- ITML: Information-Theroetic Metric Learning
- Sample Cov: parametrize Mahalanobis distance by the inverse of the sample covariance of the data
- LDA: Linear Discriminant Analysis
- MCML: Maximally Collapsing Metric Learning [Globerson, 2005]

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Experimental Results

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Dataset	ITML	Sample Cov	Euclidean	LDA	MCML
Balance-scale	0.9312	0.9072	0.9120	0.9312	.9536
Wine	0.8315	0.8258	0.8427	0.7303	.8034
Iris	1.0000	0.9733	0.9667	1.0000	.9600
lonosphere	0.9915	0.9858	0.9829	0.5128	.9915
Soybean	0.9283	0.9429	0.9283	0.9385	.9590

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Conclusion

- Presented an information-theoretic formulation for metric learning
- Given an equivalence between this problem and low-rank kernel learning
- Provided efficient algorithms
- Experiments are promising, but much more work is needed!

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