## Information-Theoretic Metric Learning

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## Introduction

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- Information-theoretic viewpoint
- Bijection between Gaussian distributions and Mahalanobis distances
- Natural entropy-based objective
- Connections with kernel learning
- Fast and simple methods
- Based on Bregman's method for convex optimization
- No eigenvalue computations are needed!


## Learning a Mahalanobis Distance

- Given $n$ points $\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}$ in $\Re^{d}$
- Given inequality constraints relating pairs of points
- Similarity constraints: $d_{A}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right) \leq u$
- Dissimilarity constraints: $d_{A}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right) \geq \ell$


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

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d_{A}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}\right)=\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right)^{T} A\left(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}}\right)
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- Applications
- k-means clustering
- Nearest neighbor searches


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

$$
\mathrm{KL}\left(p\left(\mathbf{x} ; \mathbf{m}_{1}, A_{1}\right) \| p\left(\mathbf{x} ; \mathbf{m}_{2}, A_{2}\right)\right)=\int p\left(\mathbf{x} ; \mathbf{m}_{1}, A_{1}\right) \log \frac{p\left(\mathbf{x} ; \mathbf{m}_{1}, A_{1}\right)}{p\left(\mathbf{x} ; \mathbf{m}_{2}, A_{2}\right)} d \mathbf{x}
$$

## Problem Formulation

Goal: Minimize differential relative entropy subject to pairwise inequality constraints

$$
\begin{array}{rll}
\min & \mathrm{KL}(p(\mathbf{x} ; \mathbf{m}, A) \| p(\mathbf{x} ; \mathbf{m}, I)) \\
\text { subject to } & d_{A}\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) \leq u \quad(i, j) \in S \\
& d_{A}\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) \geq \ell & (i, j) \in D \\
& A \succ 0
\end{array}
$$

## 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
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- 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


## Low-Rank Kernel Learning

- Given $X=\left[\begin{array}{llll}\mathbf{x}_{1} & \mathbf{x}_{2} & \ldots & \mathbf{x}_{n}\end{array}\right], \mathbf{x}_{i} \in \Re^{d}$, define $K_{0}=X^{\top} X$
- Constraints: similarity $(S)$ or dissimilarity $(D)$ between pairs of points
- Objective: Learn $K$ that minimizes the divergence to $K_{0}$


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- Constraints: similarity $(S)$ or dissimilarity $(D)$ between pairs of points
- Objective: Learn $K$ that minimizes the divergence to $K_{0}$ $\min \quad D_{\text {Burg }}\left(K, K_{0}\right)$ subject to $\quad K_{i i}+K_{j j}-2 K_{i j} \leq u \quad(i, j) \in S$, $K_{i i}+K_{j j}-2 K_{i j} \geq \ell \quad(i, j) \in D$, $K \succeq 0$
- $D_{\text {Burg }}$ is the Burg divergence

$$
D_{\text {Burg }}\left(K, K_{0}\right)=\operatorname{Tr}\left(K K_{0}^{-1}\right)-\log \operatorname{det}\left(K K_{0}^{-1}\right)-n
$$

## 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 $K_{0}$
- $K=X^{T} W^{\top} W X$


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

- Then $A=W^{T} W$ is an optimal solution to the corresponding metric learning problem


## Proof Sketch

Lemma 1: $D_{\text {Burg }}\left(K, K_{0}\right)=2 K L(p(\mathbf{x} ; \mathbf{m}, A) \| p(\mathbf{x} ; \mathbf{m}, I))+c$

- 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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- 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]
Lemma 2: Given $K=X^{T} A X, A$ is feasible if and only if $K$ is feasible


## 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
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- Requires no eigenvalue decomposition


## Extensions

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- Minimizing $K L$-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]


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- Sample 100 such constraints
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- 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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| 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 |

## 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!

