Information-theoretic Metric Learning

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Introduction

Metric Learning

- Important problem in machine learning
  - Metric governs success or failure of learning algorithm
  - Exploit distance information intrinsically available
  - Useful in many domains
- Several existing approaches
  - SDP approach [Xing et al.]
  - Large-margin nearest neighbor (LMNN) [Weinberger et al.]
  - Collapsing Classes (MCML) [Globerson and Roweis]
  - Online Metric Learning (POLA) [Shalev-Shwartz et al.]
  - Many others!

Our Approach

- Contributions
  - Simple and scalable
  - Incorporates a variety of constraints
  - Online learning variant with regret bounds
  - Allows kernelization for learning a kernel function
- Existing methods fail to satisfy all the above

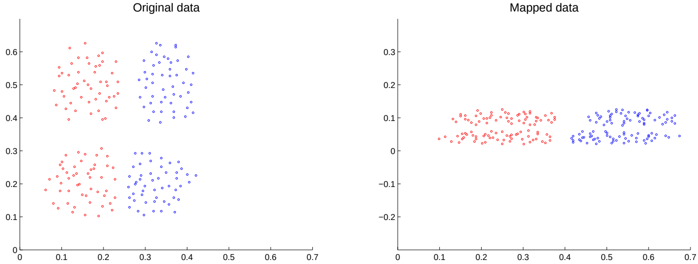
Mahalanobis Distances

Like many others, we consider learning *Mahalanobis distances*

- Distance parameterized by p.d. $d \times d$ matrix A:

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

- Often A is inverse of the covariance matrix
- Generalizes squared Euclidean distance ($A = I$)
- Rotates and scales input data
- Standard for metric learning



Problem Formulation

Introduce constraints—Examples:

- Assume pairwise similarity and dissimilarity constraints

$$\begin{aligned} d_A(\mathbf{x}_i, \mathbf{x}_j) &\leq u \quad \text{if } (i,j) \in S \text{ [similarity constraints]} \\ d_A(\mathbf{x}_i, \mathbf{x}_j) &\geq \ell \quad \text{if } (i,j) \in D \text{ [dissimilarity constraints]} \end{aligned}$$

- Other linear constraints on A possible

Goal:

- Learn a metric d_A which is "close" to some starting metric d_{A_0}
  - d_A satisfies additional prespecified constraints
  - Need notion of distance between metrics

The Gaussian Connection

- Exploit connection to Gaussian distributions:

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A) = \frac{1}{Z}\exp\left(-\frac{1}{2}d_A(\mathbf{x}, \boldsymbol{\mu})\right)$$

- Bijection between set of Mahalanobis distances and set of Gaussians with fixed $\boldsymbol{\mu}$
- Compare Gaussians using relative entropy

$$\begin{array}{ccc} d_A(\mathbf{x}, \mathbf{y}) & & d_{A_0}(\mathbf{x}, \mathbf{y}) \\ \updownarrow & & \updownarrow \\ \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A) & \leftrightarrow & \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A_0) \\ & \uparrow & \\ & \textbf{Differential Relative Entropy} & \end{array}$$

The Optimization Problem

$$\begin{aligned} \min_A \quad & \int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A_0) \log \left(\frac{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A_0)}{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A)} \right) d\mathbf{x} \\ \text{subject to} \quad & d_A(\mathbf{x}_i, \mathbf{x}_j), \ \leq u, \ (i,j) \in S \\ & d_A(\mathbf{x}_i, \mathbf{x}_j) \geq \ell, \ (i,j) \in D \\ & A \succeq 0 \end{aligned}$$

- Utilize connection between KL-divergence and the LogDet divergence (assume $\boldsymbol{\mu}$ fixed)

$$\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A_0) \log \left(\frac{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A_0)}{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A)} \right) d\mathbf{x} = \frac{1}{2} D_{\ell d}(A, A_0)$$

$$D_{\ell d}(A, A_0) = \text{trace}(AA_0^{-1}) - \log\det(AA_0^{-1}) - d$$

The Optimization Problem

KL Formulation		**LogDet Formulation**
$\min_A \quad \int \mathcal{N}(\mathbf{x}\vert\boldsymbol{\mu}, A_0) \log \frac{\mathcal{N}(\mathbf{x}\vert\boldsymbol{\mu}, A_0)}{\mathcal{N}(\mathbf{x}\vert\boldsymbol{\mu}, A)} d\mathbf{x}$		$D_{\ell d}(A, A_0)$
$\text{s.t.} \quad d_A(\mathbf{x}_i, \mathbf{x}_j) \leq u$	$\Leftrightarrow$	$\mathrm{tr}(A(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \leq u$
$d_A(\mathbf{x}_i, \mathbf{x}_j) \geq \ell$		$\mathrm{tr}(A(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \geq \ell$
$A \succeq 0$		$A \succeq 0$

- Utilize connection between KL-divergence and the LogDet divergence (assume $\boldsymbol{\mu}$ fixed)

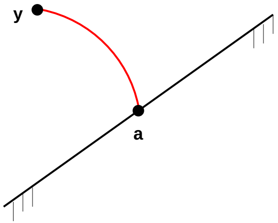
$$\int \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A_0) \log \left(\frac{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A_0)}{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, A)} \right) d\mathbf{x} = \frac{1}{2} D_{\ell d}(A, A_0)$$

$$D_{\ell d}(A, A_0) = \mathrm{trace}(AA_0^{-1}) - \log\det(AA_0^{-1}) - d$$

Bregman's Method

- Use the "Bregman" projection of **y** onto affine set $\mathcal{H}$,

$$P_{\mathcal{H}}(\mathbf{y}) = \underset{\mathbf{a}\in\mathcal{H}}{\operatorname{argmin}}\, D_{\varphi}(\mathbf{a}, \mathbf{y})$$



- Method projects onto each constrain and applies correction
- Dual Coordinate Ascent
- A has rank-one update (no eigenvector calculation):

$$A_{t+1} = A_t + \beta_t A_t (\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T A_t$$

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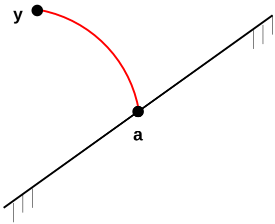


- Advantages:
  - Scalable
  - Automatic enforcement of positive semidefiniteness
  - Simple, closed-form projections
  - No eigenvector calculation

Connection to Kernel Learning

LogDet Formulation (1)

$$\begin{aligned} \min_A \quad & D_{\ell d}(A, A_0) \\ \text{s.t.} \quad & \mathrm{tr}(A(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \leq u \\ & \mathrm{tr}(A(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T) \geq \ell \\ & A \succeq 0 \end{aligned}$$

Kernel Formulation (2)

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

- (1) opt. w.r.t. the Mahalanobis matrix, (2) w.r.t. the kernel matrix
- Let $K_0 = X^T A_0 X$, where X is the input data
- Let A^* be the opt. solution to (1) and K^* be the opt. solution to (2)
- **Theorem:** $K^* = X^T A^* X$

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

$$d_A(\varphi(\mathbf{x}), \varphi(\mathbf{y})) = (\varphi(\mathbf{x}) - \varphi(\mathbf{y}))^T A(\varphi(\mathbf{x}) - \varphi(\mathbf{y}))$$

  - Equivalently: learn a new kernel function of the form

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

  - 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

Online Metric Learning

Setup

- Want to learn metric in online setting
- Every timestep t, receive pair of points $(\mathbf{x}_t, \mathbf{y}_t)$
- Predict distance between $\mathbf{x}_t$ and $\mathbf{y}_t$, then receive "true" distance
- Record loss at step t, update A_t to A_{t+1}
- **Goal:** minimize total loss

Regret Bounds

- L_{OML}: total loss of online metric learning algorithm
- L_{A^*}: total loss of best offline algorithm

$$L_{OML} \leq r_1 L_{A^*} + r_2 D_{\ell d}(A^*, I)$$

- r_1, r_2 functions of the learning rate of the algorithm

Experimental Results

Framework

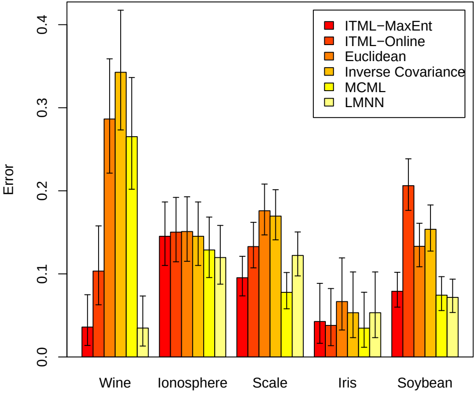
- k-nearest neighbor ($k = 4$)
- ℓ and u determined by 5th and 95th percentile of distribution
- $20c^2$ constraints, chosen randomly
- 2-fold cross validation
- Binomial confidence intervals at the 95% level

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

UCI Data Sets

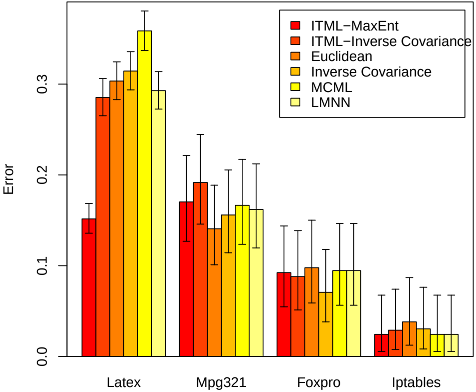
- Ran ITML with $A_0 = I$ (ITML-MaxEnt) and the inverse covariance (InverseCovariance)
- Ran online algorithm for 10^5 iterations



- ITML-MaxEnt is the best performing algorithm (within the 95% confidence intervals) across all data sets

Clarify Data Sets

- Classification for nearest-neighbor software support
- Clarify monitors predefined program features
- Each program run is one data point
- Very high dimensionality
- Feature selection reduces the number of features to 20



- ITML-MaxEnt is the best performing algorithm (within the 95% confidence intervals) across all data sets

Conclusions

Formulation

- Minimizes the relative entropy between 2 Gaussians
- Connection to LogDet divergence
- Many different constraints may be enforced

Algorithm

- Applies Bregman projections—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
- Application to nearest-neighbor software support