Large-Scale Similarity and Distance Metric Learning

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Séminaire Criteo
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A bit about me

- PhD in Computer Science (Dec 2012)
  - Université Jean Monnet, Saint-Etienne
  - Advisors: Marc Sebban, Amaury Habrard
- Postdoc in 2013–2014 (18 months)
  - University of Southern California, Los Angeles
  - Working with Fei Sha
- Joined Télécom ParisTech in October
  - Chaire "Machine Learning for Big Data"
  - Working with Stéphan Clémençon

Outline of the talk

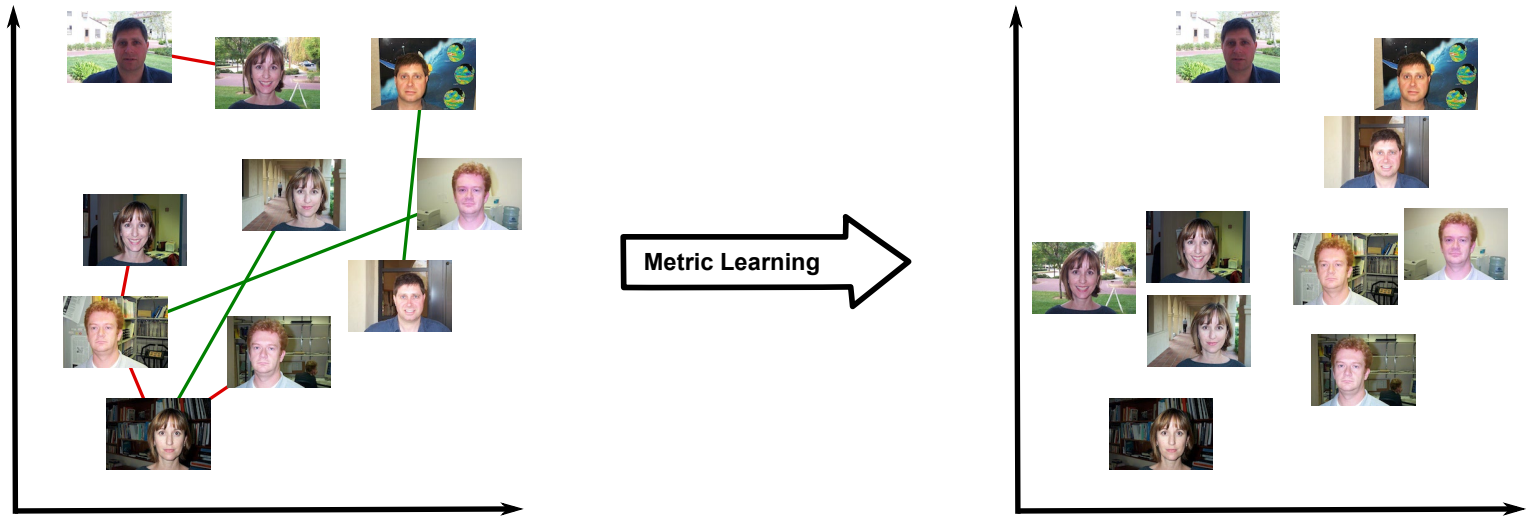
1. Introduction to Metric Learning
2. Learning (Infinitely) Many Local Metrics
3. Similarity Learning for High-Dimensional Sparse Data
4. Scaling-up ERM for Metric Learning

Introduction

Metric learning

Motivation

- How to assign a similarity score to a pair of objects?
  - Basic component of many algorithms: k-NN, clustering, kernel methods, ranking, dimensionality reduction, data visualization
  - Crucial to performance of the above
  - Obviously problem-dependent
- The machine learning way: let's learn it from data!
  - We'll need some examples of similar / dissimilar things
  - Learn to approximate the latent notion of similarity
  - Can be thought of as representation learning



Metric learning

Basic recipe

1. Pick a parametric form of distance or similarity function
   - (Squared) Mahalanobis distance

     $d^2_{\boldsymbol{M}}(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}-\boldsymbol{x}')^{\mathrm{T}} \boldsymbol{M} (\boldsymbol{x}-\boldsymbol{x}')$ with $\boldsymbol{M} \in \mathbb{R}^{d \times d}$ symmetric PSD

   - Bilinear similarity

     $$S_{\boldsymbol{M}}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^{\mathrm{T}} \boldsymbol{M} \boldsymbol{x}' \text{ with } \boldsymbol{M} \in \mathbb{R}^{d \times d}$$

2. Collect similarity judgments on data pairs/triplets
   - $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ are similar (or dissimilar)
   - $\boldsymbol{x}_i$ is more similar to $\boldsymbol{x}_j$ than to $\boldsymbol{x}_k$

3. Estimate parameters such that metric best satisfies them
   - Convex optimization and the like

Metric learning

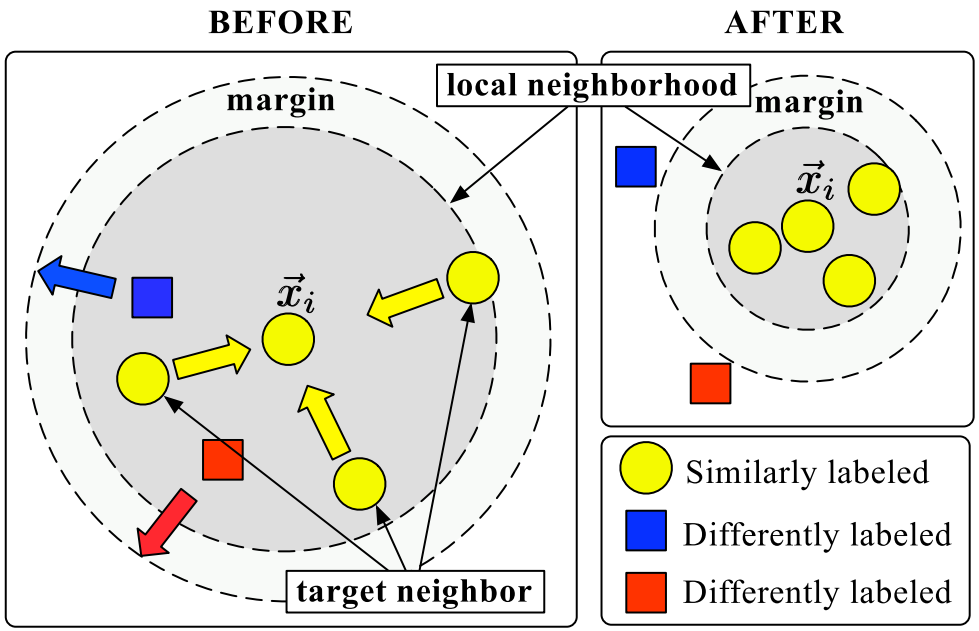
A famous algorithm: LMNN [Weinberger et al., 2005]

Large Margin Nearest Neighbors

$$\min_{\mathbf{M}\in\mathbb{S}_+^d,\xi\geq 0} \quad (1-\mu)\sum_{(\mathbf{x}_i,\mathbf{x}_j)\in\mathcal{S}} d^2_{\mathbf{M}}(\mathbf{x}_i,\mathbf{x}_j) \quad + \quad \mu\sum_{i,j,k}\xi_{ijk}$$

$$\text{s.t.} \quad d^2_{\mathbf{M}}(\mathbf{x}_i,\mathbf{x}_k) - d^2_{\mathbf{M}}(\mathbf{x}_i,\mathbf{x}_j) \geq 1-\xi_{ijk} \quad \forall(\mathbf{x}_i,\mathbf{x}_j,\mathbf{x}_k)\in\mathcal{R},$$

$\mathcal{S} = \{(\mathbf{x}_i,\mathbf{x}_j) : y_i = y_j$ and $\mathbf{x}_j$ belongs to the k-neighborhood of $\mathbf{x}_i\}$
$\mathcal{R} = \{(\mathbf{x}_i,\mathbf{x}_j,\mathbf{x}_k) : (\mathbf{x}_i,\mathbf{x}_j)\in\mathcal{S}, y_i \neq y_k\}$



Metric learning

Large-scale challenges

- How to efficiently learn multiple metrics?
  - Multi-task learning
  - Local linear metrics
- How to efficiently learn a metric for high-dimensional data?
  - Full $d \times d$ matrix not feasible anymore
- How to deal with large datasets?
  - Number of terms in the objective can grow as $O(n^2)$ or $O(n^3)$

Learning (Infinitely) Many Local Metrics

[Shi et al., 2014]

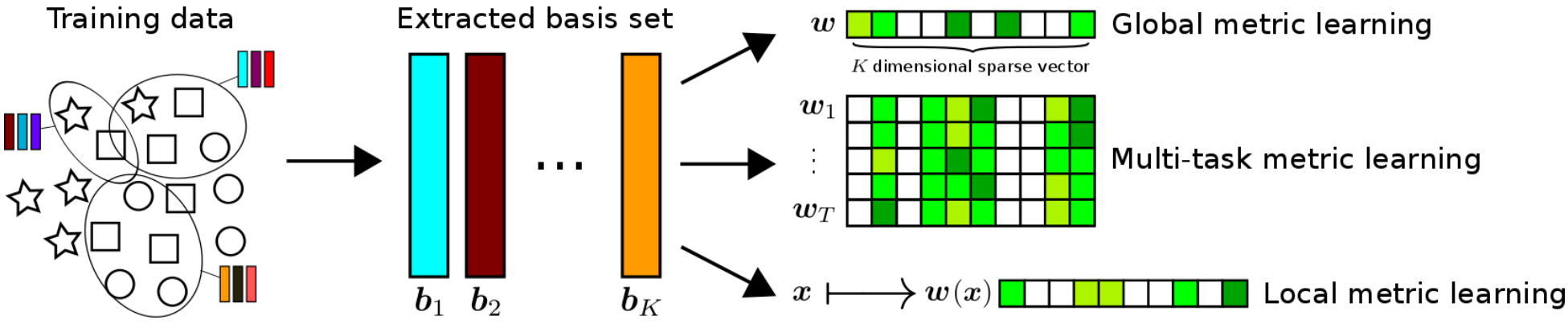
Learning (infinitely) many local metrics

Main idea

- Assume we are given a basis dictionary $B = \{\boldsymbol{b}_k\}_{k=1}^K$ in $\mathbb{R}^d$
- We will learn $d_{\boldsymbol{w}}^2(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x} - \boldsymbol{x}')^{\mathrm{T}} \boldsymbol{M} (\boldsymbol{x} - \boldsymbol{x}')$ where

$$\boldsymbol{M} = \sum_{k=1}^{K} w_k \boldsymbol{b}_k \boldsymbol{b}_k^{\mathrm{T}}, \quad \boldsymbol{w} \geq 0$$

- Use sparsity-inducing regularizer to do basis selection



Learning (infinitely) many local metrics

Global and multi-task convex formulations

$$\mathcal{C} = \left\{ \boldsymbol{x}_i, \boldsymbol{x}_i^+, \boldsymbol{x}_i^- : d^2_{\boldsymbol{w}}(\boldsymbol{x}_i, \boldsymbol{x}_i^+) \text{ should be smaller than } d^2_{\boldsymbol{w}}(\boldsymbol{x}_i, \boldsymbol{x}_i^-) \right\}_{i=1}^{C}$$

SCML-Global

$$\min_{\boldsymbol{w} \in \mathbb{R}^K_+} \quad \frac{1}{C} \sum_{i=1}^{C} \left[1 + d^2_{\boldsymbol{w}}(\boldsymbol{x}_i, \boldsymbol{x}_i^+) - d^2_{\boldsymbol{w}}(\boldsymbol{x}_i, \boldsymbol{x}_i^-) \right]_+ \quad + \quad \beta \|\boldsymbol{w}\|_1,$$

where $[\cdot]_+ = \max(0, \cdot)$

mt-SCML : extension to T tasks

$$\min_{\boldsymbol{W} \in \mathbb{R}^{T \times K}_+} \quad \sum_{t=1}^{T} \frac{1}{C_t} \sum_{i=1}^{C_t} \left[1 + d^2_{\boldsymbol{w}_t}(\boldsymbol{x}_i, \boldsymbol{x}_i^+) - d^2_{\boldsymbol{w}_t}(\boldsymbol{x}_i, \boldsymbol{x}_i^-) \right]_+ + \beta \|\boldsymbol{W}\|_{2,1}$$

- $\|\boldsymbol{W}\|_{2,1}$: induce column-wise sparsity
- Metrics are task-specific but regularized to share features

Learning (infinitely) many local metrics

Local metric learning

- Learn multiple local metrics : more flexibility
  - One metric per region or class
  - One metric per training instance
- Many issues
  - How to define the local regions?
  - How to generalize at test time?
  - How to avoid a growing number of parameters?
  - How to do avoid overfitting?
- Proposed approach : learn a metric for each point in space

Learning (infinitely) many local metrics

Local nonconvex formulation

- We use the following parameterization :

$$d_w(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x} - \boldsymbol{x}')^{\mathrm{T}} \left(\sum_{k=1}^{K} w_k(\boldsymbol{x}) \boldsymbol{b}_k \boldsymbol{b}_k^{\mathrm{T}} \right) (\boldsymbol{x} - \boldsymbol{x}'),$$

  - $w_k(\boldsymbol{x}) = (\boldsymbol{a}_k^{\mathrm{T}} \phi(\boldsymbol{x}) + c_k)^2$: weight of basis k
  - $\phi(\boldsymbol{x}) \in \mathbb{R}^{d'}$: (nonlinear) projection of $\boldsymbol{x}$ (e.g., kernel PCA)
  - $\boldsymbol{a}_k \in \mathbb{R}^{d'}$ and $c_k \in \mathbb{R}$: parameters to learn for each basis

SCML-Local

$$\min_{\tilde{\boldsymbol{A}} \in \mathbb{R}_+^{(d'+1) \times K}} \quad \frac{1}{C} \sum_{i=1}^{C} \left[1 + d_w^2(\boldsymbol{x}_i, \boldsymbol{x}_i^+) - d_w^2(\boldsymbol{x}_i, \boldsymbol{x}_i^-) \right]_+ + \beta \|\tilde{\boldsymbol{A}}\|_{2,1}$$

- $\tilde{\boldsymbol{A}}$: stack $\boldsymbol{A} = [\boldsymbol{a}_1 \dots \boldsymbol{a}_K]^{\mathrm{T}}$ and $\boldsymbol{c}$
- If $\boldsymbol{A} = \boldsymbol{0}$, recover the global formulation

Learning (infinitely) many local metrics

Efficient optimization

- Nonsmooth objective with large number of terms
  - Use stochastic proximal methods
- SCML-Global and mt-SCML are convex
  - Regularized Dual Averaging [Xiao, 2010]
- SCML-Local is nonconvex
  - Forward-backward algorithm [Duchi and Singer, 2009]
  - Initialize with solution of SCML-Global

Learning (infinitely) many local metrics

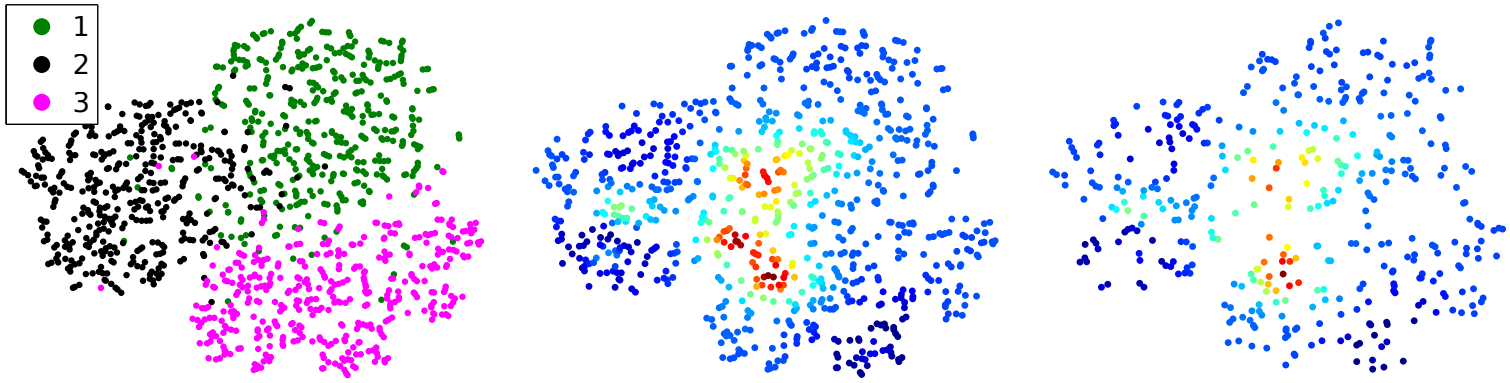
Experiments

Dataset	Euc	LMNN	BoostML	SCML-Global
Vehicle	29.7±0.6	23.5±0.7	**19.9±0.6**	21.3±0.6
Vowel	**11.1±0.4**	**10.8±0.4**	11.4±0.4	**10.9±0.5**
Segment	5.2±0.2	4.6±0.2	**3.8±0.2**	**4.1±0.2**
Letters	14.0±0.2	11.6±0.3	10.8±0.2	**9.0±0.2**
USPS	10.3±0.2	**4.1±0.1**	7.1±0.2	**4.1±0.1**
BBC	8.8±0.3	**4.0±0.2**	9.3±0.3	**3.9±0.2**
Avg. rank	3.3	2.0	2.3	**1.2**

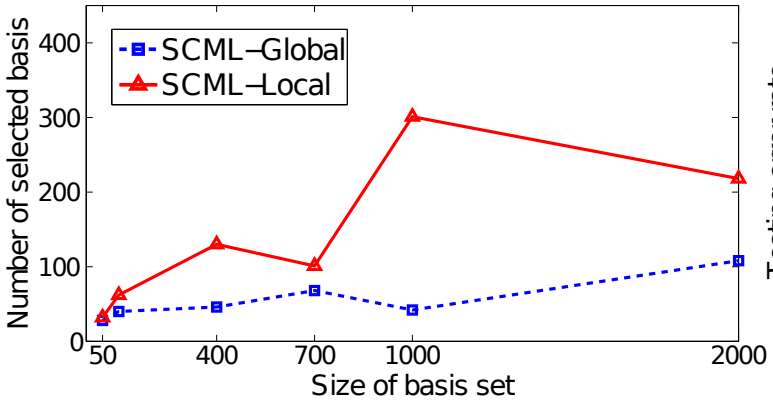
Dataset	M^2LMNN	GLML	PLML	SCML-Local
Vehicle	23.1±0.6	23.4±0.6	22.8±0.7	**18.0±0.6**
Vowel	6.8±0.3	**4.1±0.4**	8.3±0.4	6.1±0.4
Segment	**3.6±0.2**	**3.9±0.2**	**3.9±0.2**	**3.6±0.2**
Letters	9.4±0.3	10.3±0.3	**8.3±0.2**	**8.3±0.2**
USPS	**4.2±0.7**	7.8±0.2	4.1±0.1	**3.6±0.1**
BBC	4.9±0.4	5.7±0.3	**4.3±0.2**	**4.1±0.2**
Avg. rank	2.0	2.7	2.0	**1.2**

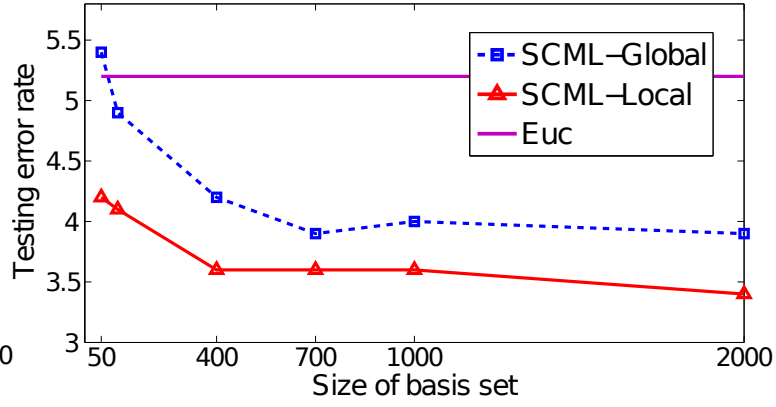
Learning (infinitely) many local metrics

Experiments



(a) Class membership (b) Trained metrics (c) Test metrics





Similarity Learning for High-Dimensional Sparse Data

[Liu et al., 2015]

Similarity learning for high-dimensional sparse data

Problem setting

- Assume data points are high-dimensional ($d > 10^4$) but D-sparse (on average) with $D \ll d$
  - Bags-of-words (text, image), bioinformatics, etc
- Existing metric learning algorithms fail
  - Intractable: training cost $O(d^2)$ to $O(d^3)$, memory $O(d^2)$
  - Severe overfitting
- Practitioners use dimensionality reduction (PCA, RP)
  - Poor performance in presence of noisy features
  - Resulting metric difficult to interpret for domain experts
- Contributions of this work
  - Learn similarity in original high-dimensional space
  - Time/memory costs independent of d
  - Explicit control of similarity complexity

Similarity learning for high-dimensional sparse data

A very large basis set

- We want to learn a similarity function $S_{\boldsymbol{M}}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^{\mathrm{T}} \boldsymbol{M} \boldsymbol{x}'$
- Given $\lambda > 0$, for any $i, j \in \{1, \ldots, d\}$, $i \neq j$ we define

$$\boldsymbol{P}_{\lambda}^{(ij)} = \begin{pmatrix} \ddots & \vdots & \ddots & \vdots & \ddots \\ \cdots & \lambda & \cdots & \lambda & \cdots \\ \ddots & \vdots & \ddots & \vdots & \ddots \\ \cdots & \lambda & \cdots & \lambda & \cdots \\ \ddots & \vdots & \ddots & \vdots & \ddots \end{pmatrix} \quad \boldsymbol{N}_{\lambda}^{(ij)} = \begin{pmatrix} \ddots & \vdots & \ddots & \vdots & \ddots \\ \cdots & \lambda & \cdots & -\lambda & \cdots \\ \ddots & \vdots & \ddots & \vdots & \ddots \\ \cdots & -\lambda & \cdots & \lambda & \cdots \\ \ddots & \vdots & \ddots & \vdots & \ddots \end{pmatrix}$$

$$\mathcal{B}_{\lambda} = \bigcup_{ij} \left\{ \boldsymbol{P}_{\lambda}^{(ij)}, \boldsymbol{N}_{\lambda}^{(ij)} \right\}$$

$$\boldsymbol{M} \in \mathcal{D}_{\lambda} = \mathrm{conv}(\mathcal{B}_{\lambda})$$

- One basis involves only 2 features:

$$S_{\boldsymbol{P}_{\lambda}^{(ij)}}(\boldsymbol{x}, \boldsymbol{x}') = \lambda(x_i x_i' + x_j x_j' + x_i x_j' + x_j x_i')$$

$$S_{\boldsymbol{N}_{\lambda}^{(ij)}}(\boldsymbol{x}, \boldsymbol{x}') = \lambda(x_i x_i' + x_j x_j' - x_i x_j' - x_j x_i')$$

Similarity learning for high-dimensional sparse data

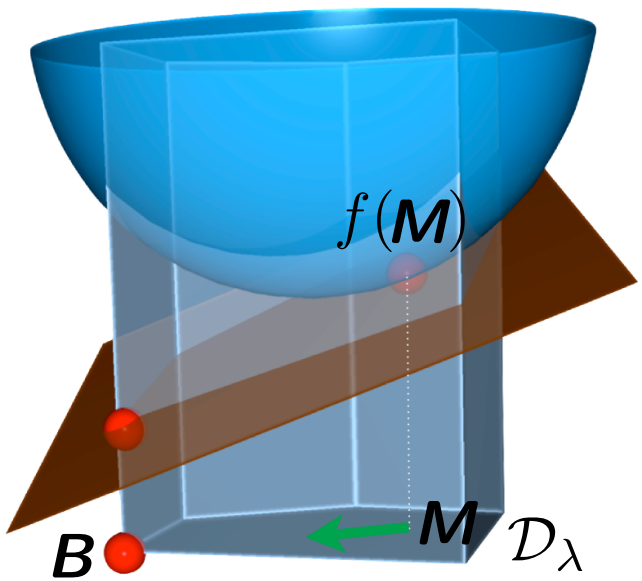
Problem formulation and algorithm

Optimization problem (smoothed hinge loss ℓ)

$$\min_{\boldsymbol{M} \in \mathbb{R}^{d \times d}} \quad f(\boldsymbol{M}) = \frac{1}{C} \sum_{i=1}^{C} \ell\left(1 - \boldsymbol{x}_i^T \boldsymbol{M} \boldsymbol{x}_i^+ + \boldsymbol{x}_i^T \boldsymbol{M} \boldsymbol{x}_i^-\right)$$

$$\text{s.t.} \quad \boldsymbol{M} \in \mathcal{D}_\lambda$$

- Use a Frank-Wolfe algorithm [Jaggi, 2013] to solve it



Let $\boldsymbol{M}^{(0)} \in \mathcal{D}_\lambda$

for $k = 0, 1, \ldots$ **do**

$\boldsymbol{B}^{(k)} = \arg\min_{\boldsymbol{B} \in \mathcal{B}_\lambda} \left\langle \boldsymbol{B}, \nabla f(\boldsymbol{M}^{(k)}) \right\rangle$

$\boldsymbol{M}^{(k+1)} = (1 - \gamma)\boldsymbol{M}^{(k)} + \gamma \boldsymbol{B}^{(k)}$

end for

Figure adapted from [Jaggi, 2013]

Similarity learning for high-dimensional sparse data

Convergence and complexity analysis

Convergence

Let $L = \frac{1}{C}\sum_{i=1}^{C} \|\boldsymbol{x}_i(\boldsymbol{x}_i^+ - \boldsymbol{x}_i^-)^T\|_F^2$. At any iteration $k \geq 1$, the iterate $\boldsymbol{M}^{(k)} \in \mathcal{D}_\lambda$ of the FW algorithm:

- has at most rank $k+1$ with $4(k+1)$ nonzero entries
- uses at most $2(k+1)$ distinct features
- satisfies $f(\boldsymbol{M}^{(k)}) - f(\boldsymbol{M}^*) \leq 16L\lambda^2/(k+2)$

- An optimal basis can be found in $O(CD^2)$ time and memory
- An approximately optimal basis can be found in $O(mD^2)$ with $m \ll C$ using a Monte Carlo approximation of the gradient
  - Or even $O(mD)$ using a heuristic (good results in practice)
- Storing $\boldsymbol{M}^{(k)}$ requires only $O(k)$ memory
  - Or even the entire sequence $\boldsymbol{M}^{(0)}, \ldots, \boldsymbol{M}^{(k)}$ at the same cost

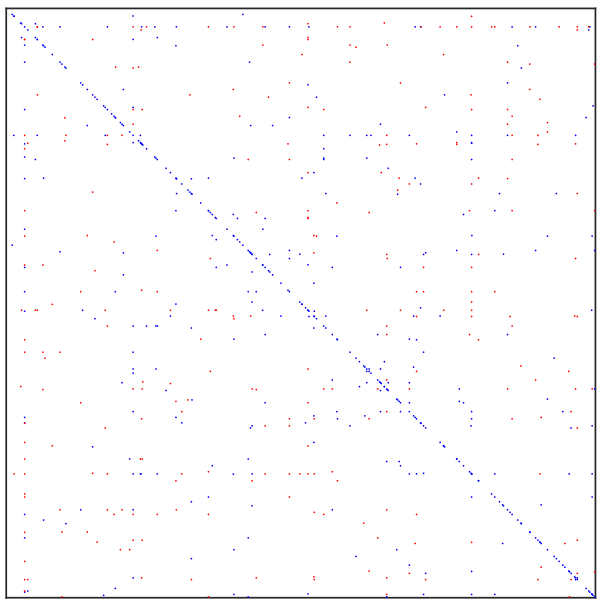
Similarity learning for high-dimensional sparse data

Experiments

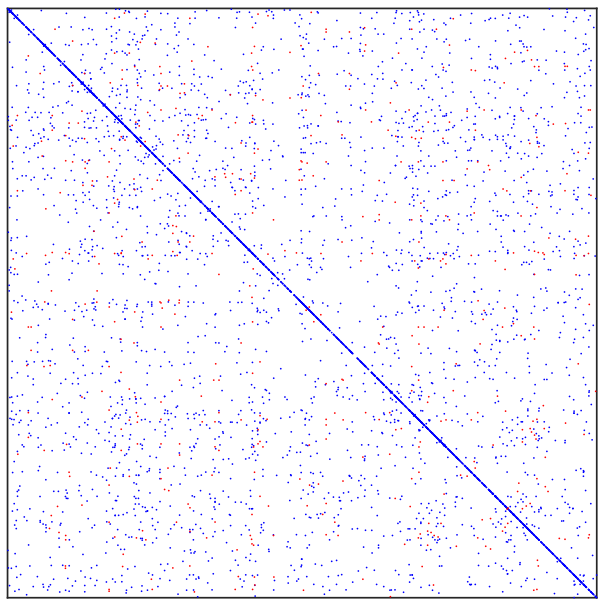
- K-NN test error on datasets with d up to 10^5

Datasets	IDENTITY	RP+OASIS	PCA+OASIS	DIAG-ℓ_2	DIAG-ℓ_1	HDSL
dexter	20.1	24.0	9.3	8.4	8.4	**6.5**
dorothea	9.3	11.4	9.9	6.8	6.6	**6.5**
rcv1_2	6.9	7.0	4.5	3.5	3.7	**3.4**
rcv1_4	11.2	10.6	6.1	6.2	7.2	**5.7**

- Sparsity structure of the matrices



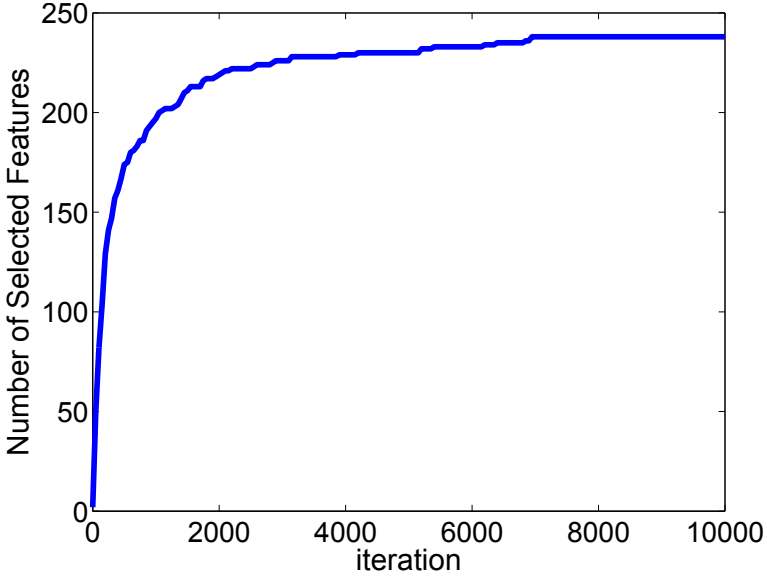
(a) dexter ($20,000 \times 20,000$ matrix, 712 nonzeros)



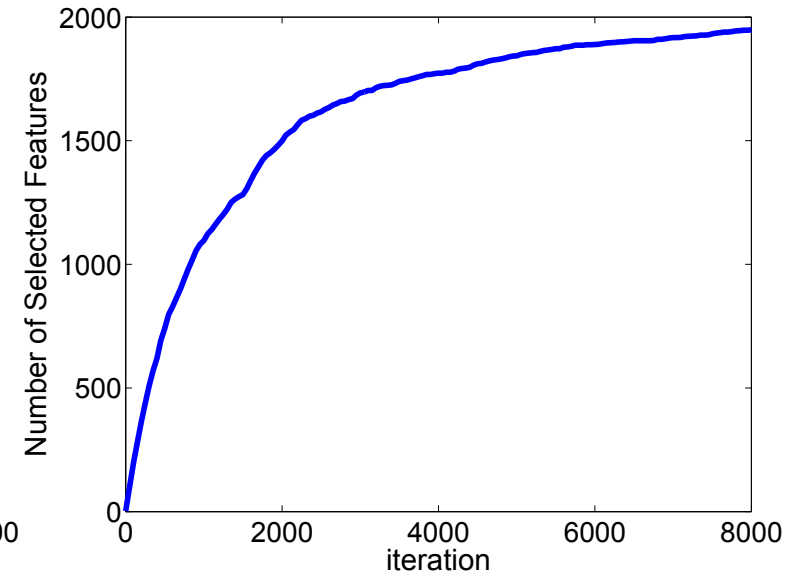
(b) rcv1_4 ($29,992 \times 29,992$ matrix, 5263 nonzeros)

Similarity learning for high-dimensional sparse data

Experiments



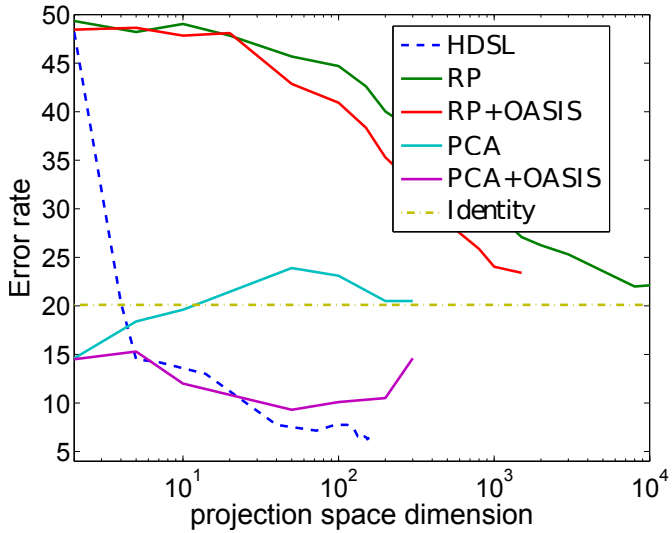
(a) dexter dataset



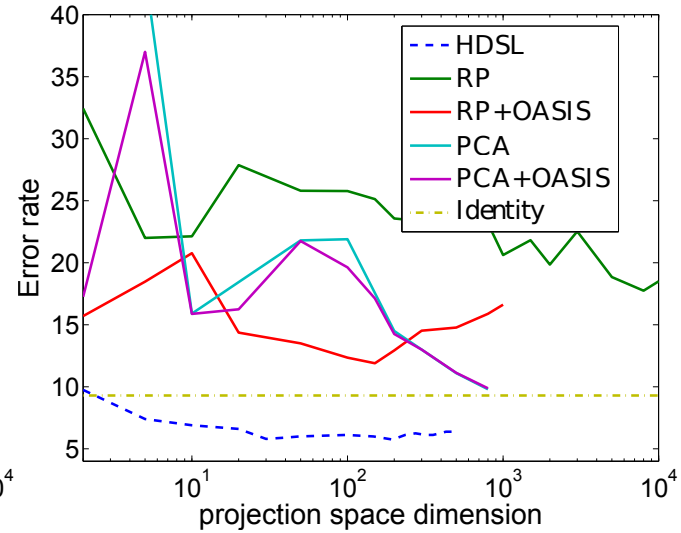
(b) rcv1_4 dataset

Similarity learning for high-dimensional sparse data

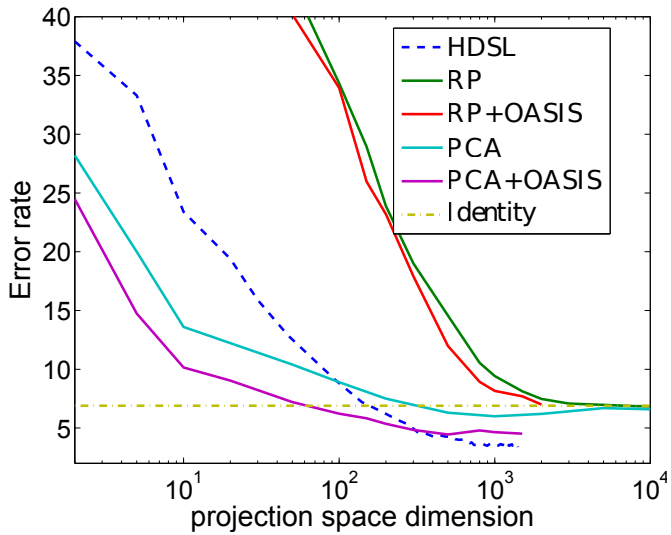
Experiments



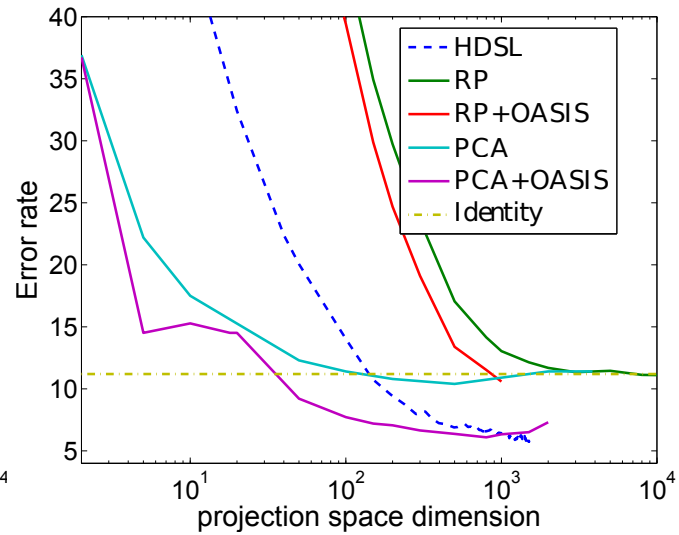
(a) dexter dataset



(b) dorothea dataset



(c) rcv1_2 dataset



(d) rcv1_4 dataset

Scaling-up ERM for Metric Learning

[Clémençon et al., 2015]

Scaling-up ERM for metric learning

Empirical Minimization of U-Statistics

- Given an i.i.d. sample $X_1, \ldots, X_n$, the U-statistic of degree 2 with kernel H is given by

$$U_n(H;\theta) = \frac{2}{n(n-1)} \sum_{i<j} H(X_i, X_j; \theta)$$

  - Can be generalized to higher degrees and multi-samples

- Empirical Minimization of U-statistic: $\min_{\theta \in \Theta} U_n(H;\theta)$
  - Applies to metric learning for classification
  - Also pairwise clustering, ranking, etc

- Number of terms quickly becomes huge
  - MNIST dataset : $n = 60000 \rightarrow 2 \times 10^9$ pairs

Scaling-up ERM for metric learning

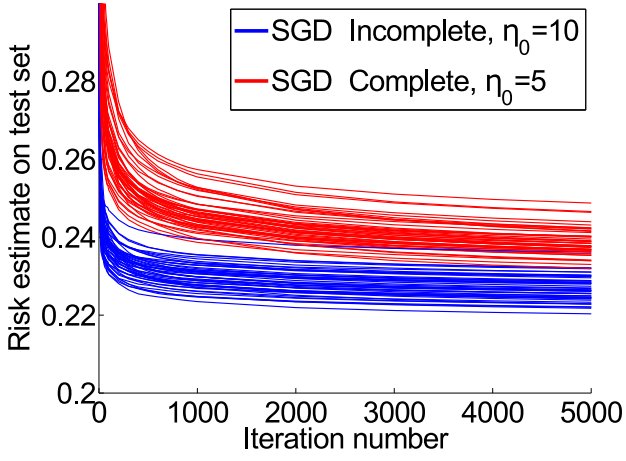
Main idea and results

- Approximate $U_n(H)$ by an incomplete version $\tilde{U}_B(H)$
  - Uniformly sample B terms (with replacement)
- Main result : if $B = O(n)$, the learning rate is preserved
  - $O(1/\sqrt{n})$ convergence in the general case
  - Objective function has only $O(n)$ terms v.s. $O(n^2)$ initially
  - Due to high dependence in the pairs
- Naive strategy : use complete U-statistic with fewer samples
  - Uniformly sample $O(\sqrt{n})$ samples
  - Form all possible pairs : $O(n)$ terms
  - Learning rate is only $O(1/n^{1/4})$
- Can use similar ideas in mini-batch SGD
  - Reduce variance of gradient estimates

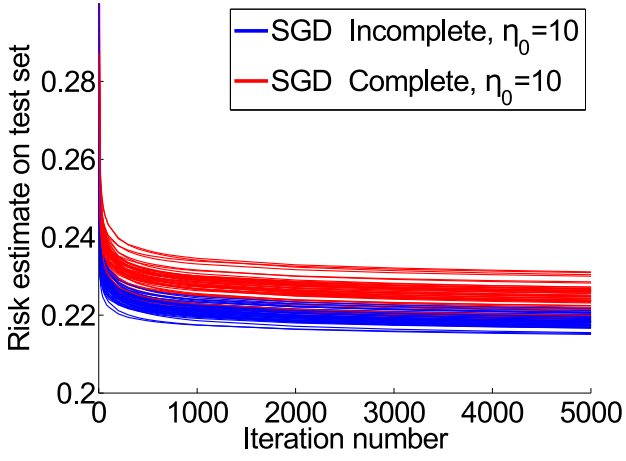
Scaling-up ERM for metric learning

Experiments

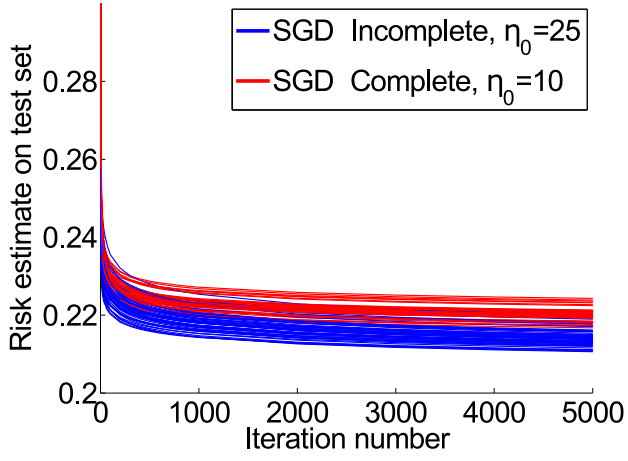
- MNIST dataset : $n = 60000 \rightarrow 2 \times 10^9$ pairs
- Mini-batch SGD
  - Step size tuning
  - 50 random runs



(a) $B = 10$



(b) $B = 55$



(c) $B = 253$

Conclusion and perspectives

- Metric learning: useful in a variety of setting
- Ideas to overcome some key limitations
  - Large datasets
  - High dimensionality
  - Learn many local metrics
- Details and more results in the papers
- One interesting challenge : distributed metric learning
  - Existing work [Xie and Xing, 2014] too restrictive

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