Large-Scale Similarity and Distance Metric Learning

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Joint work with K. Liu, Y. Shi and F. Sha (USC), S. Clémençon and I. Colin (Télécom ParisTech)

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
     \[ d_M^2(x, x') = (x - x')^T M (x - x') \text{ with } M \in \mathbb{R}^{d \times d} \text{ symmetric PSD} \]
   ▶ Bilinear similarity
     \[ S_M(x, x') = x^T M x' \text{ with } M \in \mathbb{R}^{d \times d} \]

2. Collect similarity judgments on data pairs/triplets
   ▶ \( x_i \) and \( x_j \) are similar (or dissimilar)
   ▶ \( x_i \) is more similar to \( x_j \) than to \( x_k \)

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**

\[
\min_{M \in S^d_+, \xi \geq 0} \quad (1 - \mu) \sum_{(x_i, x_j) \in S} d_M^2(x_i, x_j) + \mu \sum_{i,j,k} \xi_{ijk}
\]

\[
\text{s.t.} \quad d_M^2(x_i, x_k) - d_M^2(x_i, x_j) \geq 1 - \xi_{ijk} \quad \forall (x_i, x_j, x_k) \in \mathcal{R},
\]

\[
S = \{(x_i, x_j) : y_i = y_j \text{ and } x_j \text{ belongs to the } k\text{-neighborhood of } x_i\}
\]

\[
\mathcal{R} = \{(x_i, x_j, x_k) : (x_i, x_j) \in S, y_i \neq y_k\}
\]
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 \( B = \{ b_k \}_{k=1}^{K} \) in \( \mathbb{R}^d \)
- We will learn \( d^2_w(x, x') = (x - x')^T M (x - x') \) where
  \[
  M = \sum_{k=1}^{K} w_k b_k b_k^T, \quad w \geq 0
  \]
- Use sparsity-inducing regularizer to do basis selection
Learning (infinitely) many local metrics

Global and multi-task convex formulations

\[ C = \{ x_i, x_i^+, x_i^- : d_w^2(x_i, x_i^+) \text{ should be smaller than } d_w^2(x_i, x_i^-) \} \]

\[ C_i = 1 \]

SCML-Global

\[
\min_{w \in \mathbb{R}^K_+} \frac{1}{C} \sum_{i=1}^{C} \left[ 1 + d_w^2(x_i, x_i^+) - d_w^2(x_i, x_i^-) \right]_+ + \beta \| w \|_1,
\]
where \([\cdot]_+ = \max(0, \cdot)\)

mt-SCML : extension to \(T\) tasks

\[
\min_{W \in \mathbb{R}^{T \times K}_+} \sum_{t=1}^{T} \frac{1}{C_t} \sum_{i=1}^{C_t} \left[ 1 + d_{w_t}^2(x_i, x_i^+) - d_{w_t}^2(x_i, x_i^-) \right]_+ + \beta \| W \|_{2,1}
\]

- \(\| W \|_{2,1}\) : 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 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:

\[
d_w(x, x') = (x - x')^T \left( \sum_{k=1}^{K} w_k(x) b_k b_k^T \right) (x - x'),
\]

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

SCML-Local

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

- \(\tilde{A}\) : stack \(A = [a_1 \ldots a_K]^T\) and \(c\)
- If \(A = 0\), 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

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Euc</th>
<th>LMNN</th>
<th>BoostML</th>
<th>SCML-Global</th>
</tr>
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<tbody>
<tr>
<td>Vehicle</td>
<td>29.7±0.6</td>
<td>23.5±0.7</td>
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<td>7.1±0.2</td>
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<tr>
<td>BBC</td>
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<td>4.0±0.2</td>
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<td>3.9±0.2</td>
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<tr>
<td>Avg. rank</td>
<td>3.3</td>
<td>2.0</td>
<td>2.3</td>
<td>1.2</td>
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</table>

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<thead>
<tr>
<th>Dataset</th>
<th>M²LMNN</th>
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<th>PLML</th>
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<tr>
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<tr>
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<td>2.0</td>
<td>1.2</td>
</tr>
</tbody>
</table>
Learning (infinitely) many local metrics

Experiments

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

\[
\text{Number of selected basis vs Size of basis set}
\]

\[
\text{Testing error rate vs Size of basis set}
\]
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 $S_M(x, x') = x^T M x'$

- Given $\lambda > 0$, for any $i, j \in \{1, \ldots, d\}$, $i \neq j$ we define

  $P^{(ij)}_{\lambda} = \begin{pmatrix} \lambda & \lambda & \ldots & \lambda \\ \lambda & \lambda & \ldots & \lambda \\ \ldots & \ldots & \ldots & \ldots \\ \lambda & \lambda & \ldots & \lambda \end{pmatrix}$

  $N^{(ij)}_{\lambda} = \begin{pmatrix} \lambda & \ldots & \lambda \\ \cdot & \ldots & \cdot \\ \cdot & \ldots & \cdot \\ \cdot & \ldots & \cdot \\ \cdot & \ldots & \cdot \\ \lambda & \ldots & \lambda \\ \cdot & \ldots & \cdot \\ \cdot & \ldots & \cdot \\ \cdot & \ldots & \cdot \\ \lambda & \ldots & \lambda \end{pmatrix}$

  $B_{\lambda} = \bigcup_{ij} \{P^{(ij)}_{\lambda}, N^{(ij)}_{\lambda}\}$

  $M \in D_{\lambda} = \text{conv}(B_{\lambda})$

- One basis involves only 2 features:

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

  $S_{N^{(ij)}_{\lambda}}(x, x') = \lambda(x_i x'_i + x_j x'_j - x_i x'_j - x_j x'_i)$
Similarity learning for high-dimensional sparse data

Problem formulation and algorithm

Optimization problem (smoothed hinge loss $\ell$)

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

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

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

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

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

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

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

end for

Figure adapted from [Jaggi, 2013]
### Convergence

Let $L = \frac{1}{C} \sum_{i=1}^{C} \|x_i(x_i^+ - x_i^-)^T\|_F^2$. At any iteration $k \geq 1$, the iterate $M^{(k)} \in \mathcal{D}_\lambda$ 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 $f(M^{(k)}) - f(M^*) \leq \frac{16L\lambda^2}{(k + 2)}$

- 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 $M^{(k)}$ requires only $O(k)$ memory
  - Or even the entire sequence $M^{(0)}, \ldots, M^{(k)}$ at the same cost
Similarity learning for high-dimensional sparse data

Experiments

- **K-NN test error on datasets with** \( d \) **up to** \( 10^5 \)

<table>
<thead>
<tr>
<th>Datasets</th>
<th>IDENTITY</th>
<th>RP+OASIS</th>
<th>PCA+OASIS</th>
<th>DIAG-( \ell_2 )</th>
<th>DIAG-( \ell_1 )</th>
<th>HDSL</th>
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</thead>
<tbody>
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<td>24.0</td>
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<td>8.4</td>
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<td>6.5</td>
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<td>rcv1_2</td>
<td>6.9</td>
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<td>3.4</td>
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<tr>
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<td>6.1</td>
<td>6.2</td>
<td>7.2</td>
<td>5.7</td>
</tr>
</tbody>
</table>

- **Sparsity structure of the matrices**

(a) dexter (20,000 × 20,000 matrix, 712 nonzeros)  
(b) rcv1_4 (29,992 × 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

\( B = 10 \)

\( B = 55 \)

\( B = 253 \)
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
References


References II

Dual Averaging Methods for Regularized Stochastic Learning and Online Optimization.

Large Scale Distributed Distance Metric Learning.