SIMILARITY AND DISTANCE METRIC LEARNING

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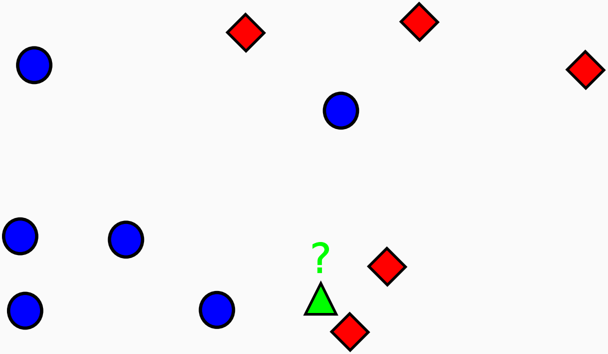
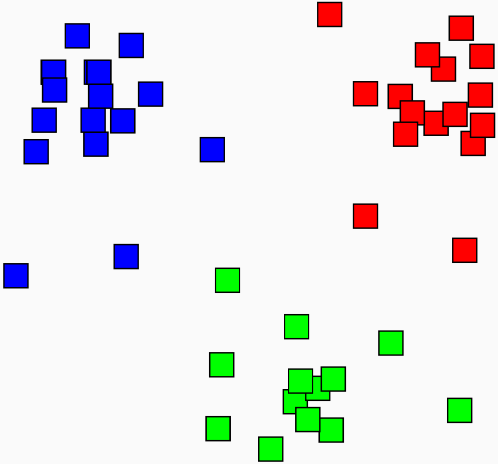
INTRODUCTION

- Similarity / distance judgments are essential components of many human cognitive processes
    - Compare perceptual or conceptual representations
    - Perform recognition, categorization...
- Underlie most machine learning and data mining techniques

Nearest neighbor classification



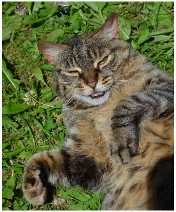
Clustering



MOTIVATION

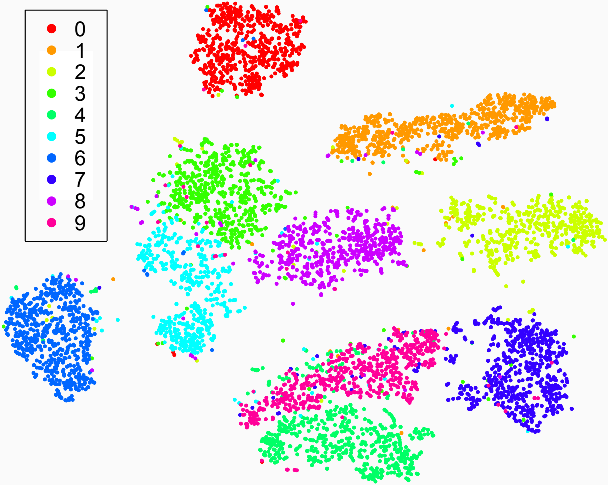
Information retrieval

Query document



Most similar documents

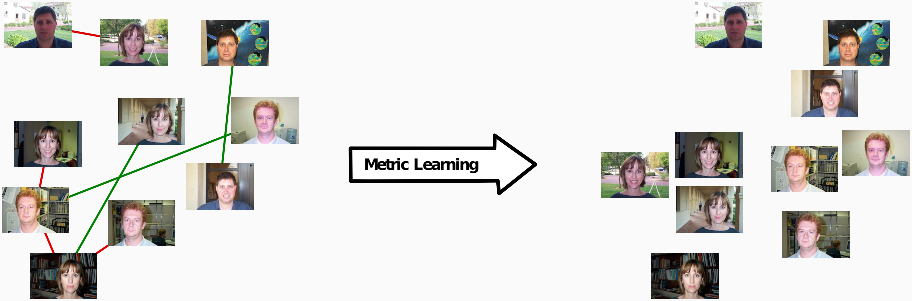
Data visualization



(image taken from [van der Maaten and Hinton, 2008])

- Choice of similarity is crucial to the performance
- Humans weight features differently depending on context
  - Facial recognition vs. determining facial expression
- Fundamental question: how to appropriately measure similarity or distance for a given task?
- Metric learning $\rightarrow$ infer this automatically from data
- Note: we will refer to *distance* or *similarity* indistinctly as *metric*

METRIC LEARNING IN A NUTSHELL



Basic recipe

1. Pick a parametric distance or similarity function
    - Say, a distance $D_M(x, x')$ function parameterized by a matrix M
2. Collect similarity judgments on data pairs/triplets
    - $\mathcal{S} = \{(x_i, x_j) : x_i \text{ and } x_j \text{ are similar}\}$
    - $\mathcal{D} = \{(x_i, x_j) : x_i \text{ and } x_j \text{ are dissimilar}\}$
    - $\mathcal{R} = \{(x_i, x_j, x_k) : x_i \text{ is more similar to } x_j \text{ than to } x_k\}$
3. Estimate parameters s.t. metric best agrees with judgments
    - Solve an optimization problem of the form

$$M^* = \arg\min_M \left[\underbrace{\ell(M, \mathcal{S}, \mathcal{D}, \mathcal{R})}_{\text{loss function}} + \underbrace{\lambda reg(M)}_{\text{regularization}} \right]$$

LINEAR METRIC LEARNING

Definition (Distance function)

A distance over a set $\mathcal{X}$ is a pairwise function $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ which satisfies the following properties $\forall x, x', x'' \in \mathcal{X}$:

(1) $d(x, x') \geq 0$ (nonnegativity)

(2) $d(x, x') = 0$ if and only if $x = x'$ (identity of indiscernibles)

(3) $d(x, x') = d(x', x)$ (symmetry)

(4) $d(x, x'') \leq d(x, x') + d(x', x'')$ (triangle inequality)

- Note: a pseudo-distance satisfies the above except (2)

Minkowski distances

- A family of distances induced by L_p norms ($p \geq 1$)

$$d_p(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_p = \left(\sum_{i=1}^{d} |x_i - x_i'|^p \right)^{1/p}$$

- When $p = 2$: "ordinary" Euclidean distance

$$d_{euc}(\mathbf{x}, \mathbf{x}') = \left(\sum_{i=1}^{d} |x_i - x_i'|^2 \right)^{1/2} = \sqrt{(\mathbf{x} - \mathbf{x}')^T (\mathbf{x} - \mathbf{x}')}$$

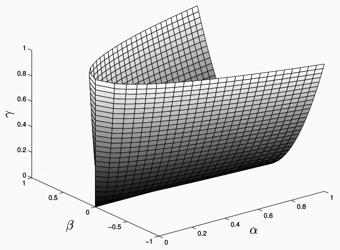
- When $p = 1$: Manhattan distance $d_{man}(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{d} |x_i - x_i'|$
- When $p \to \infty$: Chebyshev distance $d_{che}(\mathbf{x}, \mathbf{x}') = \max_i |x_i - x_i'|$

- Mahalanobis (pseudo) distance:

$$D_M(x, x') = \sqrt{(x - x')^T M (x - x')}$$

where $M \in \mathbb{R}^{d \times d}$ is symmetric positive semi-definite (PSD)

- Denote by $\mathbb{S}_+^d$ the cone of symmetric PSD $d \times d$ matrices



- A symmetric matrix $\boldsymbol{M}$ is in $\mathbb{S}_+^d$ (also denoted $\boldsymbol{M} \succeq 0$) iff:
    - Its eigenvalues are all nonnegative
    - $\boldsymbol{x}^T\boldsymbol{M}\boldsymbol{x} \geq 0, \forall \boldsymbol{x} \in \mathbb{R}^d$
    - $\boldsymbol{M} = \boldsymbol{L}^T\boldsymbol{L}$ for some $\boldsymbol{L} \in \mathbb{R}^{k \times d}$, $k \leq d$
- Equivalent to Euclidean distance after linear transformation:

$$D_M(x, x') = \sqrt{(x - x')^T L^T L(x - x')} = \sqrt{(Lx - Lx')^T(Lx - Lx')}$$

- If $\text{rank}(\boldsymbol{M}) = k \leq d$, then $\boldsymbol{L} \in \mathbb{R}^{k \times d}$ does dimensionality reduction
- For convenience, we often work with the squared distance

A first approach with pairwise constraints [Xing et al., 2002]

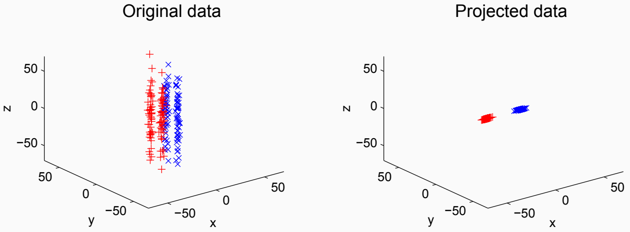
- Targeted task: clustering with side information

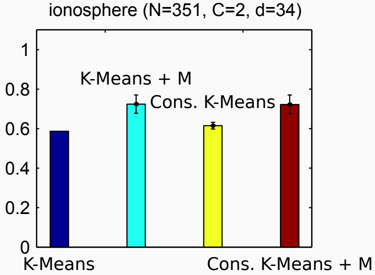
Formulation

$$\max_{M \in \mathbb{S}^d_+} \quad \sum_{(x_i, x_j) \in \mathcal{D}} D_M(x_i, x_j)$$
$$\text{s.t.} \quad \sum_{(x_i, x_j) \in \mathcal{S}} D^2_M(x_i, x_j) \leq 1$$

- Problem is convex in M and always feasible (take $M = \mathbf{0}$)
- Solved with projected gradient descent
    - Project onto distance constraint: $O(d^2)$ time
    - Project onto $\mathbb{S}^d_+$: $O(d^3)$ time
- Only look at sums of distances

A first approach with pairwise constraints [Xing et al., 2002]





A first approach with triplet constraints [Schultz and Joachims, 2003]

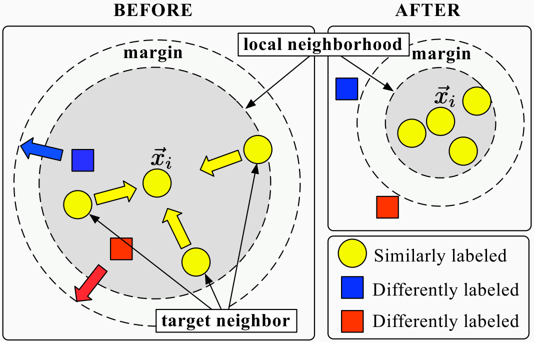
Formulation

$$\min_{M \in \mathbb{S}_+^d, \boldsymbol{\xi} \geq 0} \quad \|M\|_{\mathcal{F}}^2 \quad + \quad \lambda \sum_{i,j,k} \xi_{ijk}$$
$$\text{s.t.} \quad D_M^2(\mathbf{x}_i, \mathbf{x}_k) - D_M^2(\mathbf{x}_i, \mathbf{x}_j) \geq 1 - \xi_{ijk} \quad \forall (\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k) \in \mathcal{R}$$

- Regularization by Frobenius norm $\|M\|_{\mathcal{F}}^2 = \sum_{i,j=1}^{d} M_{ij}^2$
- Formulation is convex
- One large margin soft constraint per triplet
- Can be solved with similar techniques as SVM

Large Margin Nearest Neighbor [Weinberger et al., 2005]

- Targeted task: k-NN classification
- Constraints derived from labeled data
  - $\mathcal{S} = \{(\mathbf{x}_i, \mathbf{x}_j) : y_i = y_j, \mathbf{x}_j$ belongs to k-neighborhood of $\mathbf{x}_i\}$
  - $\mathcal{R} = \{(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k) : (\mathbf{x}_i, \mathbf{x}_j) \in \mathcal{S}, y_i \neq y_k\}$



Large Margin Nearest Neighbor [Weinberger et al., 2005]

Formulation

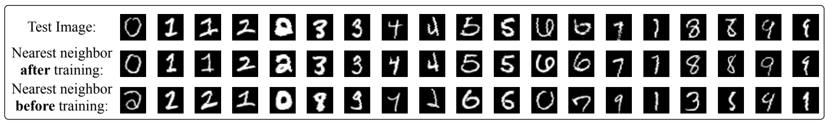
$$\min_{M \in \mathbb{S}_+^d, \boldsymbol{\xi} \geq 0} \quad (1-\mu) \sum_{(x_i, x_j) \in \mathcal{S}} D_M^2(x_i, x_j) \quad + \quad \mu \sum_{i,j,k} \xi_{ijk}$$

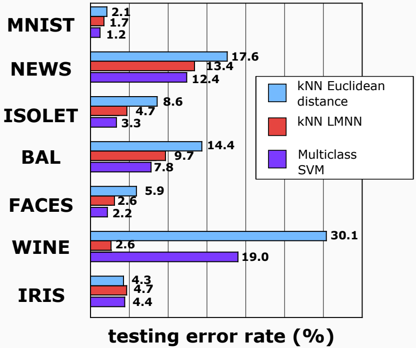
$$\text{s.t.} \quad D_M^2(x_i, x_k) - D_M^2(x_i, x_j) \geq 1 - \xi_{ijk} \quad \forall (x_i, x_j, x_k) \in \mathcal{R}$$

$\mu \in [0, 1]$ trade-off parameter

- Convex formulation, unlike NCA [Goldberger et al., 2004]
- Number of constraints in the order of kn^2
  - Solver based on projected gradient descent with working set
  - Simple alternative: only consider closest "impostors"
- Chicken and egg situation: which metric to build constraints?

Large Margin Nearest Neighbor [Weinberger et al., 2005]





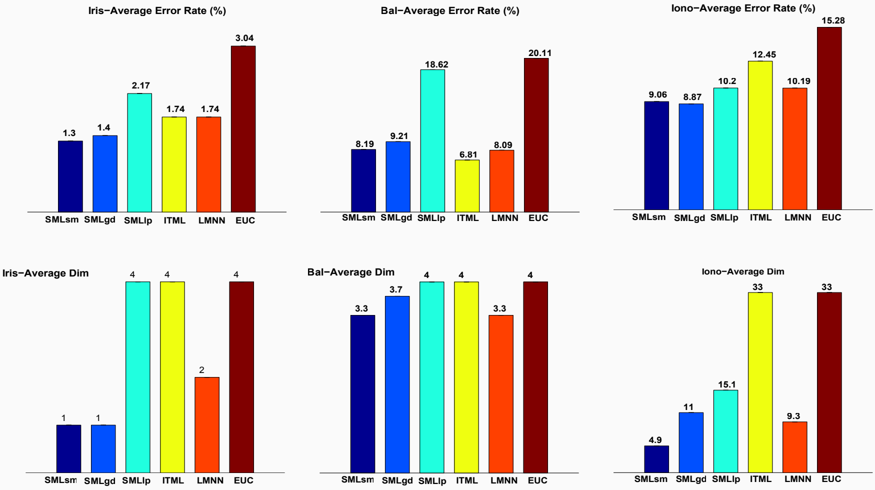
Pointers to metric learning algorithms for other tasks

- Learning to rank [McFee and Lanckriet, 2010]
- Multi-task learning [Parameswaran and Weinberger, 2010]
- Transfer learning [Zhang and Yeung, 2010]
- Semi-supervised learning [Hoi et al., 2008]

Interesting regularizers

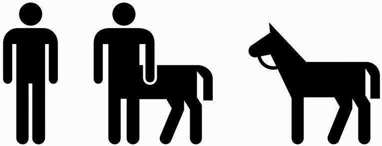
- Add regularization term to prevent overfitting
- We have already seen the Frobenius norm $\|M\|_{\mathcal{F}}^2 = \sum_{i,j=1}^d M_{ij}^2$
  - Convex, smooth $\rightarrow$ easy to optimize
- Mixed $L_{2,1}$ norm: $\|M\|_{2,1} = \sum_{i=1}^d \|M_i\|_2$
  - Tends to zero-out entire columns $\rightarrow$ feature selection
  - Convex but nonsmooth
  - Efficient proximal gradient algorithms
- Trace (or nuclear) norm: $\|M\|_* = \sum_{i=1}^d \sigma_i(M)$
  - Favors low-rank matrices $\rightarrow$ dimensionality reduction
  - Convex but nonsmooth
  - Efficient Frank-Wolfe algorithms

$L_{2,1}$ norm illustration



(image taken from [Ying et al., 2009])

- Mahalanobis distance satisfies some distance properties
  - Nonnegativity, symmetry, triangle inequality
  - Natural regularization, required by some applications
- In practice, these properties may not be satisfied
  - By human similarity judgments



  - By some good visual recognition systems
- Alternative: learn bilinear similarity function $S_M(x, x') = x^T M x'$
  - Example: OASIS algorithm (presented later)
  - No PSD constraint on M $\rightarrow$ computationally easier

NONLINEAR EXTENSIONS

Definition (Kernel function)

A symmetric function K is a kernel if there exists a mapping function $\phi : \mathcal{X} \to \mathbb{H}$ from the instance space $\mathcal{X}$ to a Hilbert space $\mathbb{H}$ such that K can be written as an inner product in $\mathbb{H}$:

$$K(x, x') = \langle \phi(x), \phi(x') \rangle \,.$$

Equivalently, K is a kernel if it is positive semi-definite (PSD), i.e.,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j K(x_i, x_j) \geq 0$$

for all finite sequences of $x_1, \ldots, x_n \in \mathcal{X}$ and $c_1, \ldots, c_n \in \mathbb{R}$.

Kernel trick for metric learning

- Notations
  - Kernel $K(x, x') = \langle \phi(x), \phi(x') \rangle$, training data $\{x_i\}_{i=1}^n$
  - $\boldsymbol{\phi}_i \stackrel{def}{=} \phi(x_i) \in \mathbb{R}^D$, $\boldsymbol{\Phi} \stackrel{def}{=} [\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n] \in \mathbb{R}^{n \times D}$
- Mahalanobis distance in kernel space

$$D_{\boldsymbol{M}}^2(\boldsymbol{\phi}_i, \boldsymbol{\phi}_j) = (\boldsymbol{\phi}_i - \boldsymbol{\phi}_j)^T \boldsymbol{M}(\boldsymbol{\phi}_i - \boldsymbol{\phi}_j) = (\boldsymbol{\phi}_i - \boldsymbol{\phi}_j)^T \boldsymbol{L}^T \boldsymbol{L}(\boldsymbol{\phi}_i - \boldsymbol{\phi}_j)$$

- Setting $\boldsymbol{L}^T = \boldsymbol{\Phi} \boldsymbol{U}^T$, where $\boldsymbol{U} \in \mathbb{R}^{D \times n}$, we get

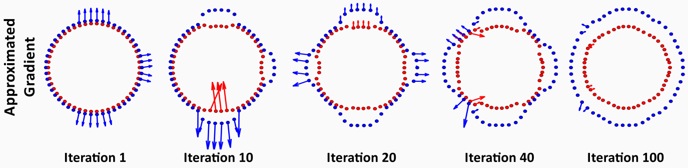
$$D_{\boldsymbol{M}}^2(\phi(x), \phi(x')) = (\boldsymbol{k} - \boldsymbol{k}')^T \boldsymbol{M}(\boldsymbol{k} - \boldsymbol{k}')$$

  - $\boldsymbol{M} = \boldsymbol{U}^T \boldsymbol{U} \in \mathbb{R}^{n \times n}$, $\boldsymbol{k} = \boldsymbol{\Phi}^T \phi(x) = [K(x_1, x), \ldots, K(x_n, x)]^T$
- Theoretically justified (representer theorem)

Kernel trick for metric learning

- Similar trick as kernel SVM
    - Use a nonlinear kernel (e.g., Gaussian RBF)
    - Inexpensive computations through the kernel
    - Nonlinear metric learning while retaining convexity
- Need to learn $O(n^2)$ parameters
- Linear metric learning algorithm must be kernelized
    - Interface to data limited to inner products only
    - Several algorithms shown to be kernelizable
- General trick (simple and works well in practice):
    1. Kernel PCA: nonlinear mapping to low-dimensional space
    2. Apply linear metric learning algorithm to transformed data

LEARNING A NONLINEAR METRIC

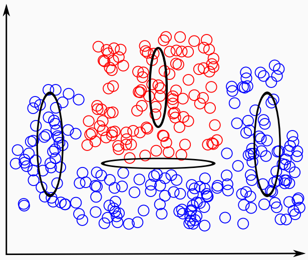


- More flexible approach: learn nonlinear mapping ϕ to optimize

$$D_\phi(x, x') = \|\phi(x) - \phi(x')\|_2$$

- Possible parameterizations for ϕ:
    - Regression trees
    - Deep neural nets
    - ...
- Typically nonconvex formulations

- Simple linear metrics perform well locally
- Idea: different metrics for different parts of the space



Multiple Metric LMNN [Weinberger and Saul, 2009]

- Group data into C clusters
- Learn a metric for each cluster in a coupled fashion

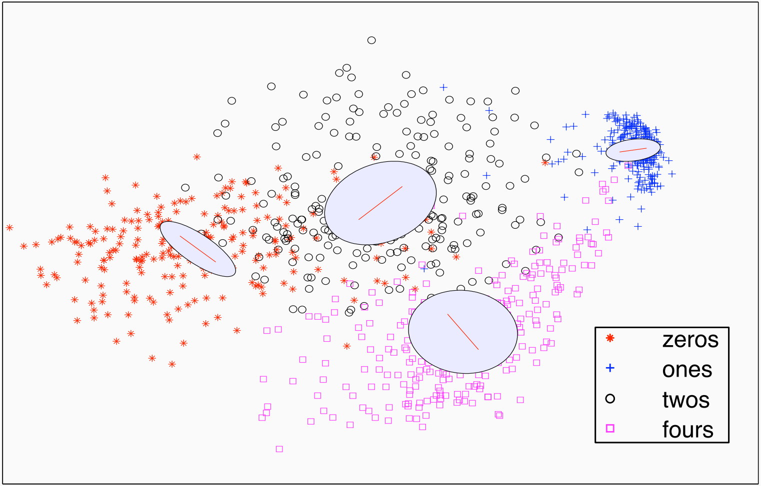
Formulation

$$\min_{\substack{M_1,\dots,M_C \\ \boldsymbol{\xi}\geq 0}} \quad (1-\mu)\sum_{(x_i,x_j)\in\mathcal{S}} D^2_{M_{C(x_j)}}(\mathbf{x}_i,\mathbf{x}_j) \quad + \quad \mu\sum_{i,j,k}\xi_{ijk}$$

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

- Remains convex
- Computationally more expensive than standard LMNN
- Subject to overfitting (many parameters)

Multiple Metric LMNN [Weinberger and Saul, 2009]



LARGE-SCALE METRIC LEARNING

MAIN CHALLENGES

- How to deal with large datasets?
  - Number of similarity judgments can grow as $O(n^2)$ or $O(n^3)$
- How to deal with high-dimensional data?
  - Cannot store $d \times d$ matrix
  - Cannot afford computational complexity in $O(d^2)$ or $O(d^3)$

Online learning

- Online algorithm
    - Receive *one* similarity judgment
    - Suffer loss based on current metric
    - Update metric and iterate
- Goal: minimize regret

$$\sum_{t=1}^{T} \ell_t(M_t) - \sum_{t=1}^{T} \ell_t(M^*) \leq f(T),$$

- ℓ_t: loss suffered at time t
- M_t: metric learned at time t
- M^*: best metric in hindsight

OASIS [Chechik et al., 2010]

Formulation

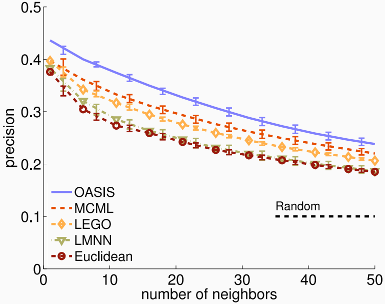
- Set $M^0 = I$
- At step t, receive $(x_i, x_j, x_k) \in \mathcal{R}$ and update by solving

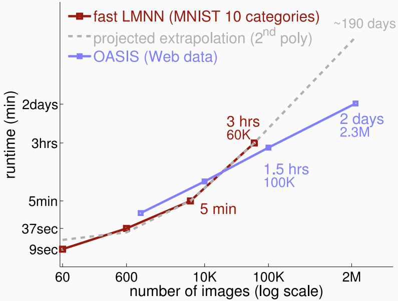
$$\begin{aligned} M^t = \quad & \arg\min_{M,\xi} \quad \frac{1}{2}\|M - M^{t-1}\|_{\mathcal{F}}^2 + C\xi \\ & \text{s.t.} \quad 1 - S_M(x_i, x_j) + S_M(x_i, x_k) \leq \xi \\ & \qquad \xi \geq 0 \end{aligned}$$

  - $S_M(x, x') = x^T M x'$, C trade-off parameter

- Simple closed-form solution at each iteration
- Trained with 160M triplets in 3 days on 1 CPU

OASIS [Chechik et al., 2010]





Stochastic and distributed optimization

- Assume metric learning problem of the form

$$\min_{M} \quad \frac{1}{|\mathcal{R}|} \sum_{(x_i, x_j, x_k) \in \mathcal{R}} \ell(M, x_i, x_j, x_k)$$

- Can use Stochastic Gradient Descent
    - Use a random sample (mini-batch) to estimate gradient
    - Better than full gradient descent when n is large
- Can be combined with distributed optimization
    - Distribute triplets on workers
    - Each worker use a mini-batch to estimate gradient
    - Coordinator averages estimates and updates

Simple workarounds

- Learn a diagonal matrix
  - Learn d parameters
  - Only a weighting of features!
- Learn metric after dimensionality reduction (e.g., PCA)
  - Used in many papers
  - Potential loss of information
  - Learned metric difficult to interpret

Matrix decompositions

- Low-rank decomposition $\boldsymbol{M} = \boldsymbol{L}^T \boldsymbol{L}$ with $\boldsymbol{L} \in \mathbb{R}^{r \times d}$
  - Learn $r \times d$ parameters
  - Generally nonconvex, must tune r
- Rank-1 decomposition $\boldsymbol{M} = \sum_{i=1}^{K} w_k \boldsymbol{b}_k \boldsymbol{b}_k^T$
  - Learn K parameters
  - Must choose good basis set
- Special case: sparse data [Liu et al., 2015]
  - Decomposition as rank-1 4-sparse matrices
  - Greedy algorithm incorporating a single basis at each iteration
  - Computational cost independent of d

METRIC LEARNING FOR STRUCTURED DATA

- Each data instance is a structured object
  - Strings: words, DNA sequences
  - Trees: XML documents
  - Graphs: social network, molecules

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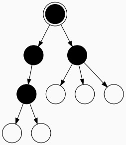
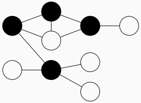




- Metrics on structured data are convenient
  - Act as proxy to manipulate complex objects
  - Can use any metric-based algorithm

MOTIVATION

- Could represent each object by a feature vector
  - Idea behind many kernels for structured data
  - Could then apply standard metric learning techniques
  - Potential loss of structural information
- Instead, focus on edit distances
  - Directly operate on structured object
  - Variants for strings, trees, graphs
  - Natural parameterization by cost matrix

- Notations
  - Alphabet Σ: finite set of symbols
  - String x: finite sequence of symbols from Σ
  - $|x|$: length of string x
  - \$: empty string / symbol

Definition (Levenshtein distance)

The Levenshtein string edit distance between x and x' is the length of the shortest sequence of operations (called an *edit script*) turning x into x'. Possible operations are insertion, deletion and substitution of symbols.

- Computed in $O(|x| \cdot |x'|)$ time by Dynamic Programming (DP)

Parameterized version

- Use a nonnegative $(|\Sigma|+1) \times (|\Sigma|+1)$ matrix C
  - C_{ij}: cost of substituting symbol i with symbol j

Example 1: Levenshtein distance

C	\$	a	b
\$	0	1	1
a	1	0	1
b	1	1	0

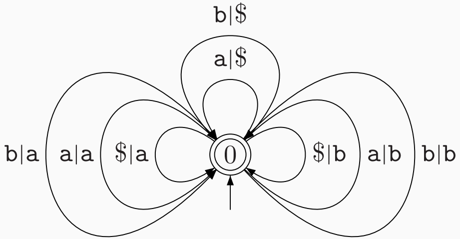
$\Longrightarrow$ edit distance between abb and aa is 2 (needs at least two operations)

Example 2: specific costs

C	\$	a	b
\$	0	2	10
a	2	0	4
b	10	4	0

$\Longrightarrow$ edit distance between abb and aa is 10 ($\mathtt{a} \to \$,\ \mathtt{b} \to \mathtt{a},\ \mathtt{b} \to \mathtt{a}$)

- Interdependence issue
  - The optimal edit script depends on the costs
  - Updating the costs may change the optimal edit script
- Consider edit probability $p(\mathrm{x}'|\mathrm{x})$ [Oncina and Sebban, 2006]
  - Cost matrix: probability distribution over operations
  - Corresponds to summing over all possible scripts
- Represent process by a stochastic memoryless transducer
- Maximize expected log-likelihood of positive pairs

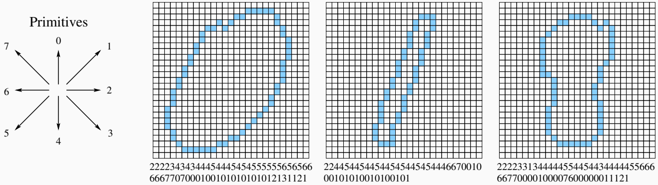


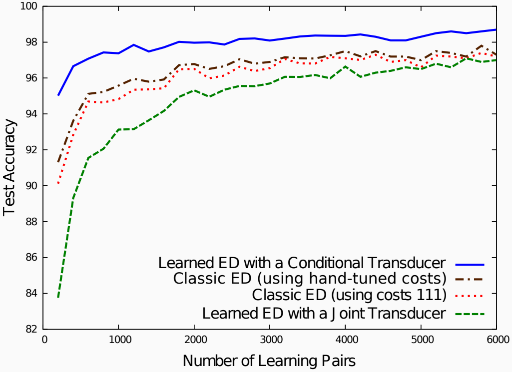
Iterative Expectation-Maximization algorithm [Oncina and Sebban, 2006]

- Expectation step
  - Given edit probabilities, compute frequency of each operation
  - Probabilistic version of the DP algorithm
- Maximization step
  - Given frequencies, update edit probabilities
  - Done by likelihood maximization under constraints

$$\forall u \in \Sigma, \sum_{v \in \Sigma \cup \{\$\}} c_{v|u} + \sum_{v \in \Sigma} c_{v|\$} = 1, \quad \text{with} \sum_{v \in \Sigma} c_{v|\$} + \underbrace{c(\#)}_{\text{exit prob.}} = 1,$$

Application to handwritten digit recognition [Oncina and Sebban, 2006]





Some remarks

- Advantages
  - Elegant probabilistic framework
  - Enables data generation
  - Generalization to trees [Bernard et al., 2008]
- Drawbacks
  - Convergence to local minimum
  - Costly: DP algorithm for each pair at each iteration
  - Cannot use negative pairs

GESL [Bellet et al., 2012]

- Inspired from successful algorithms for non-structured data
  - Large-margin constraints
  - Convex optimization
- Requires key simplification: fix the edit script

$$e_C(\mathrm{x}, \mathrm{x}') = \sum_{u,v \in \Sigma \cup \{\$\}} C_{uv} \cdot \#_{uv}(\mathrm{x}, \mathrm{x}')$$

  - $\#_{uv}(\mathrm{x}, \mathrm{x}')$: nb of times $u \to v$ appears in Levenshtein script
- e_C is a linear function of the costs

GESL [Bellet et al., 2012]

Formulation

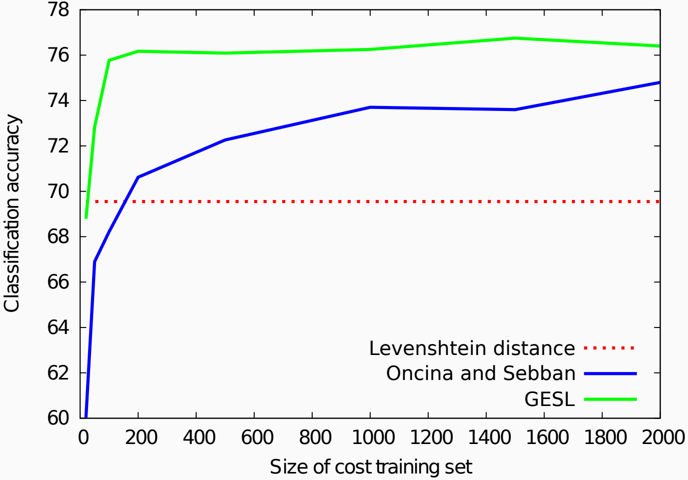
$$\min_{\mathbf{C}\geq 0, \boldsymbol{\xi}\geq 0, B_1\geq 0, B_2\geq 0} \quad \sum_{i,j} \xi_{ij} \quad + \quad \lambda \|\mathbf{C}\|_{\mathcal{F}}^2$$

$$\begin{aligned} \text{s.t.} \quad & e_{\mathbf{C}}(\mathrm{x}, \mathrm{x}') \geq B_1 - \xi_{ij} & \forall (\mathrm{x}_i, \mathrm{x}_j) \in \mathcal{D} \\ & e_{\mathbf{C}}(\mathrm{x}, \mathrm{x}') \leq B_2 + \xi_{ij} & \forall (\mathrm{x}_i, \mathrm{x}_j) \in \mathcal{S} \\ & B_1 - B_2 = \gamma \end{aligned}$$

γ margin parameter

- Convex, less costly and use of negative pairs
- Straightforward adaptation to trees and graphs
- Less general than proper edit distance
  - Chicken and egg situation similar to LMNN

Application to word classification [Bellet et al., 2012]



- Distance / similarity: key component of machine learning
- Metric learning often requires only weak supervision
- Many algorithms:
  - For classification, clustering, ranking...
  - Linear, nonlinear, local metrics
  - Scalable methods
- Very successful in practical applications
- More details: can refer to [Bellet et al., 2015]

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