Outline

1. Introduction
2. Unsupervised Metric Learning
3. Supervised Metric Learning
4. Relation to Other Methods
5. An application
Outline

1 Introduction

2 Unsupervised Metric Learning

3 Supervised Metric Learning

4 Relation to Other Methods

5 An application
Motivation

- How do we measure similarity?
- What is a metric?
- Why to learn a metric?
- How to learn a metric?
How do we measure similarity?

Most algorithms that intend to extract knowledge from data, have to, at some stage, compute *distances* between data points. Thus, their performance, often critically, depends on their *definition of similarity* between objects.
What is a metric?

A **metric** or **distance function** is a function that defines a distance between each pair of elements of a set.

Formally, it is a mapping $\mathcal{D} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$ over a vector space $\mathcal{X}$, where the following conditions are satisfied $\forall x_i, x_j, x_k \in \mathcal{X}$:

1. $\mathcal{D}(x_i, x_j) \geq 0$  
   **Non-negativity**
2. $\mathcal{D}(x_i, x_j) = \mathcal{D}(x_j, x_i)$  
   **Symmetry**
3. $\mathcal{D}(x_i, x_j) \leq \mathcal{D}(x_i, x_k) + \mathcal{D}(x_k, x_j)$  
   **Triangle inequality**
4. $\mathcal{D}(x_i, x_j) = 0 \iff x_i = x_j$  
   **Identity of indiscernibles**

If condition 4 is not met, we are referring to a **pseudo-metric**. Usually we do not distinguish between metrics and pseudo-metrics.
Why learn a metric?

“The greatest thing by far is to be a master of metaphor; it is the one thing that cannot be learned from others; and it is also a sign of genius, since a good metaphor implies an intuitive perception of the similarity of the dissimilar.”

Aristotle
Why learn a metric?

- Sometimes, the problem implicitly defines a suitable similarity measure, e.g. Euclidean distance for depth estimation:

- In many interesting problems however, the similarity measure is not easy to find. It is preferable then to learn the similarity from data, together with other parameters of the model.
A family of metrics

A family of metrics over \( X \) is defined by computing Euclidean distances after applying a linear transformation \( L \) such that \( x \rightarrow Lx \). These metrics compute squared distances as

\[
D_L(x_i, x_j) = \|Lx_i - Lx_j\|^2_2
\]

Equation (1) defines a valid metric if \( L \) is full rank and a valid pseudo-metric otherwise.

Intuitively, we want to \textit{stretch} the dimensions that contain more information and \textit{contract} the ones that explain less of the data.
A family of metrics - An example

Consider two data points $x_1 = (1, 1)$ and $x_2 = (3, 2)$ that are known to be dissimilar. The transformation $L = \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}$ maps the points to $x'_1 = (3, 1)$ and $x'_2 = (9, 2)$ as it weights distances along the first axis 3 times more than the second. The squared distance of the points changed from $(3 - 1)^2 + (2 - 1)^2 = 5$ to $(9 - 3)^2 + (2 - 1)^2 = 37$. 

\[ D = \sqrt{5} \]

\[ D = \sqrt{37} \]
Another view: Mahalanobis metrics

Expanding the squared distances equation:

$$D_L(x_i, x_j) = \|Lx_i - Lx_j\|_2^2 = (x_i - x_j)^T L^T L (x_i - x_j)$$ (2)

This allows us to express squared distances in terms of the square matrix $M = L^T L$ which is guaranteed to be positive semidefinite. In terms of $M$ we denote squared distances as

$$D_M(x_i, x_j) = (x_i - x_j)^T M (x_i - x_j)$$ (3)

We refer to pseudo-metrics of this form as Mahalanobis metrics.

It is easy to see that by setting $M$ equal to the identity matrix, we fall back to common Euclidean distances.
To learn $L$ or $M$

Thus, we have two options on what to learn, which gives rise to two approaches in DML:

- Learn a linear transformation $L$ of the data
  - $M = L^T L$ is then uniquely defined
  - Optimization is unconstrained

- Learn a Mahalanobis metric $M$
  - $M$ defines $L$ up to rotation (does not influence distances)
  - Constraint: $M$ must be positive semidefinite
  - But has certain advantages
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Principal Component Analysis [Pearson, 1901]

The main goal of PCA is to find the linear transformation $\mathbf{L}$ that projects the data to a subspace that maximizes the variance.

The variance is expressed with the covariance matrix

$$
\mathbf{C} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)(x_i - \mu)^T
$$

(4)

where $\mu = \frac{1}{n} \sum_{i=1}^{n} x_i$ is the sample mean.

It turns out that $\mathbf{C} = \frac{1}{n} \mathbf{XX}^T$ (assuming zero-mean $\mathbf{X} \in \mathbb{R}^{d \times n}$).

The covariance of the projected inputs is then

$$
\mathbf{C'} = \frac{1}{n} (\mathbf{LX})(\mathbf{LX})^T = \frac{1}{n} \mathbf{LXX}^T \mathbf{L}^T = \frac{1}{n} \mathbf{LCL}^T
$$

(5)
Principal Component Analysis - Illustration

In red: The first two eigenvectors of the covariance matrix, scaled by the square roots of the two largest eigenvalues respectively.
Principal Component Analysis (cont’d)

We can formulate PCA as an optimization problem:

$$\max_L \text{Tr}(LCL^T) \quad \text{subject to} \quad LL^T = I$$ (6)

*Closed-form solution*: Rows of $L$ are the eigenvectors of $C$.
*Eigen-decomposing $C$ is equivalent to computing the SVD of $X$.*

Remarks around PCA

- Is an unsupervised method (does **not** use data labels)
- Is widely used for dimensionality reduction: $L \in \mathbb{R}^{p \times d}, p < d$
- Can be used for:
  - *De-noising*: By removing the bottom eigenvectors
  - Speeding up search of nearest neighbors.
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Unlike PCA, LDA is supervised: it uses labels of the inputs.

**Goal:** Find the $L$ that maximizes the between-class variance w.r.t. the within-class variance.

Assuming we have $m$ classes, the covariance matrices are

$$C_b = \frac{1}{m} \sum_{c=1}^{m} \mu_c \mu_c^T \quad (7)$$
$$C_w = \frac{1}{n} \sum_{c=1}^{m} \sum_{i \in \Omega_c} (x_i - \mu_c)(x_i - \mu_c)^T \quad (8)$$

where $\Omega_c$ is the set of indices of inputs that belong to class $c$, $\mu_c$ is the sample mean of class $c$.

We assume that the data are globally centered.
Linear Discriminant Analysis - Illustration

Original IRIS dataset

IRIS dataset after LDA

setosa
versicolor
virginica

setosa
versicolor
virginica
Linear Discriminant Analysis (cont’d)

Corresponding optimization problem:

\[
\max_L \text{Tr}(\frac{L C_b L^T}{L C_w L^T}) \quad \text{subject to} \quad LL^T = I \tag{9}
\]

*Closed form solution:* Rows of \( L \) are the eigenvectors of \( C_w^{-1} C_b \).

**Remarks around LDA**

- Is a supervised method (makes use of label information)
- Is widely used as a preprocessing step for pattern classification
- Works well when class distributions are Gaussians
Neighborhood Component Analysis [Goldberger et al., 2004]

Idea: Learn a Mahalanobis metric explicitly to improve \textit{k-nn} classification.

Goal: Estimate the $L$ that minimizes the expected LOO error.

Observations

- LOO error is highly discontinuous w.r.t. the distance metric. 😞
- In particular, an infinitesimal change in the metric can alter the neighbour graph and thus change the validation performance.
- We need a smoother (or at least continuous) function

Idea 2: Instead of picking a fixed number of $k$ nearest neighbors, select a single neighbor \textit{stochastically} and count the expected votes.
Neighborhood Component Analysis (cont’d)

The reference samples $x_j$ for each point $x_i$ are drawn from a softmax pdf:

$$ p_{ij} = \begin{cases} 
\frac{\exp\left(-\|L_{x_i} - L_{x_j}\|^2\right)}{\sum_{k\neq i} \exp\left(-\|L_{x_i} - L_{x_k}\|^2\right)} & \text{if } i \neq j \\
0 & \text{if } i = j 
\end{cases} \quad (10) $$

The fraction of the time that $x_i$ will be correctly labeled is:

$$ p_i^+ = \sum_{j \in C_i} p_{ij} \quad (11) $$

The expected error then is

$$ \varepsilon_{NCA} = 1 - \frac{1}{n} \sum_{ij} p_{ij} y_{ij} \quad \text{where} \quad y_{ij} = \begin{cases} 
1 & \text{if } y_i = y_j \\
0 & \text{otherwise} 
\end{cases} \quad (12) $$
Neighborhood Component Analysis (cont’d)

- We don’t have to choose a parameter $k$ 😊
- The stochastic nature makes $\varepsilon_{NCA}$ differentiable w.r.t. $L$ 😊
- But $\varepsilon_{NCA}$ is not convex $\rightarrow$ no globally optimal $L$ 😐

$k$-nn classification accuracy
### Dimensionality Reduction - PCA vs LDA vs NCA

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Dimensions</th>
</tr>
</thead>
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<tr>
<td>concentric rings</td>
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<td>faces</td>
<td>560</td>
</tr>
<tr>
<td>digits</td>
<td>256</td>
</tr>
</tbody>
</table>

![Images of dimensionality reduction](image.png)

**Notes:**
- **PCA**: Principal Component Analysis
- **LDA**: Linear Discriminant Analysis
- **NCA**: Neighborhood Components Analysis
Large Margin Nearest Neighbor [Weinberger et al., 2005]

- **Idea**: Enforce the **maximum margin** possible between intra-class and inter-class samples (as in SVMs)
- **Target neighbors** of $\vec{x}_i$: samples desired to be closest to $\vec{x}_i$
- **Impostors**: samples that violate the margin
- **Loss function**
  - Pulling target neighbors together
    \[
    \varepsilon_{\text{pull}}(L) = \sum_{i,j \sim i} ||L(\vec{x}_i - \vec{x}_j)||^2.
    \]
  - Pushing impostors away
    \[
    \varepsilon_{\text{push}}(L) = \sum_{i,j \sim i} \sum_l (1 - y_{il}) [1 + ||L(\vec{x}_i - \vec{x}_j)||^2 - ||L(\vec{x}_i - \vec{x}_l)||^2]_+.
    \]
  - Convex combination
    \[
    \varepsilon(L) = \mu \varepsilon_{\text{pull}}(L) + (1 - \mu) \varepsilon_{\text{push}}(L), \quad \mu \in [0, 1]
    \]
Large Margin Nearest Neighbor (cont’d)

- Supervised Distance Metric Learning for classification
- Considers triplets of points at a time.

- Goal: Find a metric to maximize $k$-NN accuracy
- Advantage: Convex formulation 😊

Euclidean Metric  Mahalanobis Metric
Metric Learning Variants

Most metric learning algorithms improve by looking at pairs, triplets or even quadruplets of points. Many noteworthy algorithms exist:

- Relevant Component Analysis (RCA)
- Information Theoretic Metric Learning (ITML)
- Pseudo-metric Online Batch Learning Algorithm (POLA)
- LogDet Exact Gradient Online (LEGO)
- BoostMetric (combines boosting and metric learning)
- Large Scale Online Learning of Image Similarity Through Ranking (OASIS)

This is definitely not an exhaustive list.
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Metric Learning and Kernel Methods

Kernel methods

- Express similarity with the Gram matrix $K$ which is $n \times n$.
- The feature space $\Phi$ is usually high-dimensional (theoretically can be infinite-dimensional).
- The training takes place in the kernel space. The algorithm no longer sees the raw inputs $X$.

Metric Learning

- Learns a transformation $L$, which is $p \times d$ or a Mahalanobis matrix $M$ which is $d \times d$, like the covariance matrix $C$.
- Usually $p < d \rightarrow$ learning also results in dimensionality reduction.
- Therefore usually more efficient than kernel methods.

Metric learning can be combined with kernel methods for better results.
Multidimensional Scaling [Torgerson, 1952]

**Inverse Problem**: Given dissimilarities, find an embedding. Goal of MDS is to find coordinates of the data points in some subspace of $\mathbb{R}^n$ such that the given distances are preserved.

A famous problem in cartography: Find a 2-dimensional map of the earth, so that distances between cities are distorted as little as possible. Notice that the original distances are not Euclidean, but measured along the earth's surface.
Multi-dimensional Scaling (cont’d)

We are given an \( n \times n \) matrix \( D \) of distances \( d_{ij} \) between all pairs of points. Metric MDS minimizes the distortion of distances in terms of a residual sum of squares, called the “stress”:

\[
\text{stress}(x_1, x_2, \ldots, x_n) = \sqrt{\frac{\sum_{i,j} (d_{ij} - \|x_i - x_j\|)^2}{\sum_{i,j} d_{ij}^2}}
\]  

(13)

so

\[
\{x_1, x_2, \ldots, x_n\}^* = \arg \min_{\{x_i\}} \text{stress}(x_1, x_2, \ldots, x_n)
\]  

(14)

- No unique solution. For example, all rotations of a solution would produce the same distances.

- MDS is often used for data visualization.
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Non-rigid 3D Shape Retrieval via LMNN [Chiotellis et al., 2016]

Dataset: SHREC’14 [Pickup et al., 2014]
Synthetic dataset: 300 models
(15 persons × 20 poses)

Real dataset: 400 models
(40 persons × 10 poses)
Non-rigid 3D Shape Retrieval via LMNN (cont’d)

Retrieval Example

Non-rigid 3D Shape Retrieval via LMNN (cont’d)

Embeddings Visualization

Dataset

$y_f(S)$ before learning

learned $L \cdot y_f(S)$

SHREC’14
Real

SHREC’14
Synthetic
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