Learning Similarities for Linear Classification: Theoretical Foundations and Algorithms

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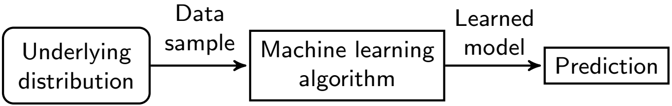
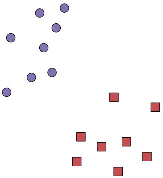
PhD Defense, December 2, 2016

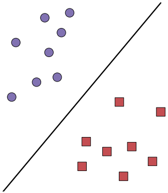
Scientific Context

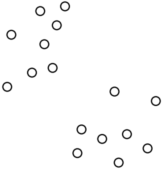
Machine Learning



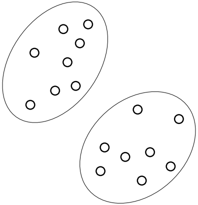


Supervised learning

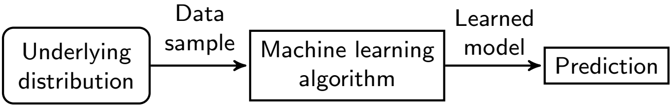


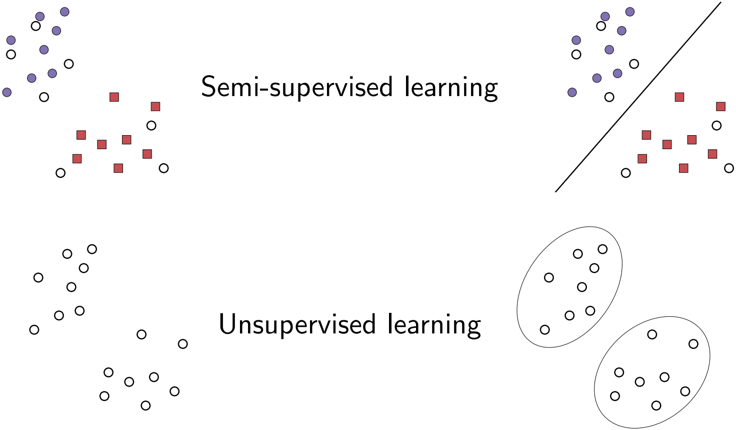


Unsupervised learning



Machine Learning

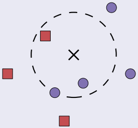




Metric Learning

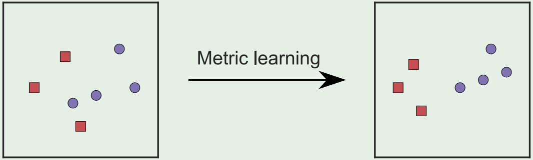
Performance depends on metrics

Most machine learning algorithms compare examples using a metric.



Adapting the metric to the problem

Learn a custom metric which better discriminates the examples.



Typically, it boils down to learning a new representation space.

Representation Learning

Importance

Representation learning is often key in machine learning algorithms.

Subfields of representation learning

- Kernel learning;
- Multiple kernel learning;
- Dictionary learning;
- Deep learning;
- Metric learning.

Differences come from:

- Orthogonality of the features;
- Implicit vs. explicit representation;
- Sparse vs. infinite representation space;
- Parametric vs. non parametric.

Background and Preliminaries

Input

A **sample** of n labeled examples $\mathcal{S} = \{z_i = (\mathbf{x}_i, y_i)\}_{i=1}^n$ independent and identically distributed (i.i.d.) according to an unknown distribution P.

Output

A model $h \in H$ that **best predicts** the labels of unseen examples.

Definition (True risk)

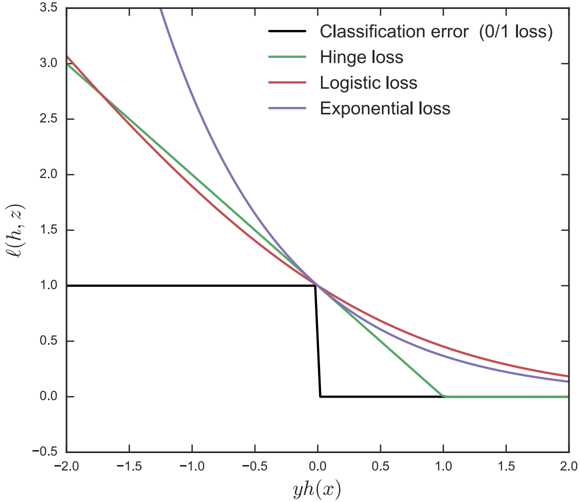
The expected loss suffered by h on the distribution P:
$R_P^\ell(h) = \mathbb{E}_{z \sim P}[\ell(h, z)]$.

Definition (Empirical risk)

The average loss incurred by h on the sample $\mathcal{S}$: $R_\mathcal{S}^\ell(h) = \frac{1}{n}\sum_{i=1}^n \ell(h, z_i)$.

Supervised Learning

Loss Functions for Binary Classification



Minimize an objective function of the form:

$$h_{\mathcal{S}} = \arg\min_{h \in H} R^{\ell}_{\mathcal{S}}(h) + \lambda ||h||.$$

PAC bounds

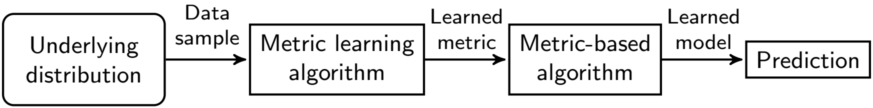
Bound the deviation of the empirical risk from the true risk of a hypothesis h, i.e. its **capacity to generalize** to an unseen sample:

$$|R^{\ell}_{P}(h) - R^{\ell}_{\mathcal{S}}(h)| \leq \mathcal{O}(complexity(h)/\sqrt{n}).$$

Theoretical frameworks

- Uniform convergence using VC dimension [VC71], Rademacher complexity [BM03] and other similar,
- Uniform stability [BE02],
- Algorithmic robustness [XM12].

Metric Learning



Mahalanobis distance learning

Find the positive semi-definite (PSD) matrix $\mathbf{M} \in \mathbb{R}^{d \times d}$ parameterizing a Mahalanobis distance $d^2_{\mathbf{M}}$ to best satisfy some constraints:

$$d_{\mathbf{M}}(\mathbf{x}, \mathbf{x}') = \sqrt{(\mathbf{x} - \mathbf{x}')^T \mathbf{M} (\mathbf{x} - \mathbf{x}')}.$$

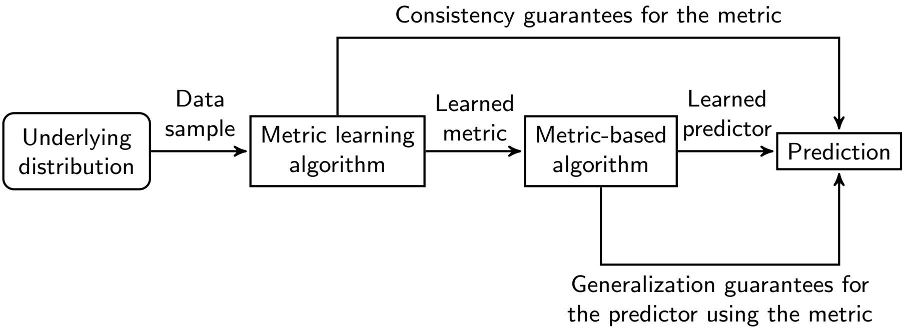
Similarity judgments (constraints)

- Pair-based: $\mathbf{x}$ and $\mathbf{x}'$ are (dis)similar;
- Triplet-based: $\mathbf{x}$ is more similar to $\mathbf{x}'$ than to $\mathbf{x}''$.

Existing methods differ in the choice of the **metric**, the **constraints**, the **loss function** and the **regularizer**.

Generalization Guarantees in Metric Learning

The question of the generalization capacity can be asked at two levels: the **metric** and the **predictor** using it.



Only a few methods provide generalization guarantees for:

- the **learned metric** $d_{\mathbf{M}}$ itself [JWZ09, BT11, CGY12];
- the **performance** of the algorithm using it [BBS08].

(ϵ, γ, τ)-Good Framework

(ϵ, γ, τ)-Good Similarity Functions

Some of the first results on how the properties of the **similarity function** influence its performance in **linear classification**.

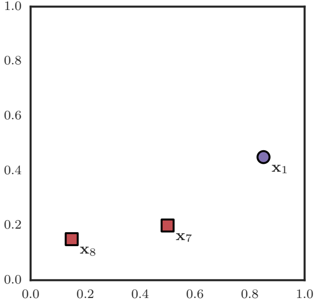
Definition

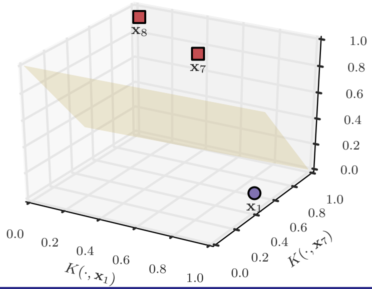
[BBS08] $K \in [-1, 1]$ is an (ϵ, γ, τ)-good similarity function in hinge loss for a learning problem P if there exists a random indicator function $R(\mathbf{x})$ defining a probabilistic set of landmarks such that the following conditions hold:

1. We have
$$\mathbb{E}_{(\mathbf{x},y)\sim P}\left[[1 - yg(\mathbf{x})/\gamma]_+\right] \leq \epsilon,$$
where $g(\mathbf{x}) = \mathbb{E}_{(\mathbf{x}',y'),R(\mathbf{x}')}[y'K(\mathbf{x},\mathbf{x}')|R(\mathbf{x}')]$.
2. $\Pr_{\mathbf{x}'}(R(\mathbf{x}')) \geq \tau$. $\qquad \epsilon, \gamma, \tau \in [0, 1]$

[BBS08] Maria-Florina Balcan, Avrim Blum, and Nathan Srebro. Improved Guarantees for Learning via Similarity Functions. In *COLT*, 2008.

Learning with (ϵ, γ, τ)-Good Similarity Functions





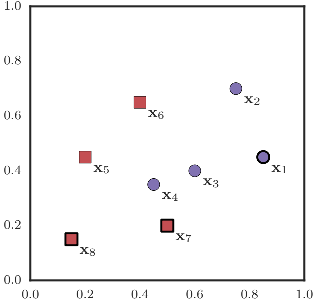
Theorem

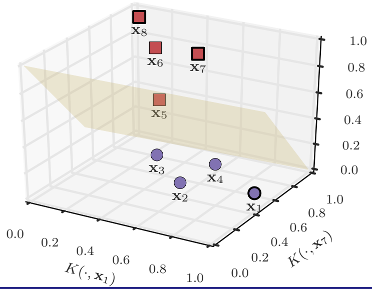
[BBS08] Given K is (ϵ, γ, τ)-good, there exists a linear separator α in the projection space that has error close to ϵ at margin γ.

Linear program (BBS)

$$\min_{\boldsymbol{\alpha}} \left\{ \sum_{i=1}^{m} \left[1 - \sum_{j=1}^{n} \alpha_j y_i K(\mathbf{x}_i, \mathbf{x}_j) \right]_+ : \sum_{j=1}^{n} |\alpha_j| \leq 1/\gamma \right\}$$

Learning with (ϵ, γ, τ)-Good Similarity Functions





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Summary

Advantages

- Theoretical guarantees on α;
- Semi-supervised framework.

Limitations

- Standard similarity functions might poorly satisfy the definition;
- No given method to find the suited similarity function.

Solution

- Learn the similarity function from a data sample;
- Directly optimize its **empirical goodness**;
- This implies **guarantees** for the linear classifier.

Contributions of the Thesis

- Optimize **similarity functions** instead of distances:
  - Less costly;
  - Gives access to a larger class of functions.
- Optimize the **goodness** of the similarities $\rightarrow$ generalization guarantees for the algorithm using the similarity.
- Derive **consistency guarantees** for the learned similarity.

More precisely

- Joint similarity and classifier learning for feature vectors.
- Similarity learning for multivariate time series classification.

Previous results using the (ϵ, γ, τ)-good framework

- String edit distance learning [BHS11];
- Learning a bilinear similarity for feature vectors [BHS12].

Joint Similarity and Classifier Learning for Feature Vectors

Optimizing the (ϵ, γ, τ)-Goodness in Metric Learning

(ϵ, γ, τ)-Goodness Criterion

$$\mathbb{E}_{(\mathbf{x},y)\sim P}\left[\left[1 - y\mathbb{E}_{(\mathbf{x}',y'),R(\mathbf{x}')}\left[yy'K_{\mathbf{M}}(\mathbf{x},\mathbf{x}'))|R(\mathbf{x}')\right]/\gamma\right]_+\right] \leq \epsilon.$$

To be satisfied on average.

Linear program (BBS)

$$\min_{\boldsymbol{\alpha}}\left\{\sum_{i=1}^{m}\left[1 - \sum_{j=1}^{n}\alpha_j y_i K(\mathbf{x}_i,\mathbf{x}_j)\right]_+ : \sum_{j=1}^{n}|\alpha_j| \leq 1/\gamma\right\}$$

Landmarks labels are not used.

Problem Formulation

Joint Similarity Learning (JSL)

$$\min_{\boldsymbol{\alpha},\mathbf{M}} \quad \sum_{i=1}^{m} \left[1 - \sum_{j=1}^{n} \alpha_j y_i K_{\mathbf{M}}(\mathbf{x}_i, \mathbf{x}_j)\right]_+ + \lambda ||\mathbf{M} - \mathbf{R}||$$

$$\text{s.t.} \quad \sum_{j=1}^{n} |\alpha_j| \leq 1/\gamma$$

Properties

- Semi-supervised setting $\rightarrow$ can use a small quantity of labeled data;
- Averaged constraints;
- Generic form of similarity and regularization;
- Convex for a large range of similarities and regularizers;
- Solved by alternating optimization steps over $\boldsymbol{\alpha}$ and $\mathbf{M}$.

Choice of Similarity and Regularization

Similarity functions

- $K^1_{\mathbf{M}}(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{M} \mathbf{x}'$;
- $K^2_{\mathbf{M}}(\mathbf{x}, \mathbf{x}') = 1 - (\mathbf{x} - \mathbf{x}')^T \mathbf{M} (\mathbf{x} - \mathbf{x}')$.

Regularizer $||\mathbf{M} - \mathbf{R}||$

- L_1 or L_2 norm;
- Value of $\mathbf{R} \in \mathbb{R}^{d \times d}$:
  - Identity matrix;
  - Empirical estimate of Kullback-Leibler divergence.

Theoretical Analysis using Rademacher Complexity

Rademacher average over $\mathcal{F}$

$$\hat{\mathfrak{R}}_{\mathcal{S}}(\mathcal{F}) := \mathbb{E}_\sigma \left[\sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i f(z_i) \right]$$

Rademacher complexity

$$\mathfrak{R}_n(\mathcal{F}) := \mathbb{E}_{\mathcal{S}} \hat{\mathfrak{R}}_{\mathcal{S}}(\mathcal{F}), \forall n$$

where

- $\mathcal{F}$ is a class of uniformly bounded functions;
- $\{\sigma_i : i \in \{1, \dots, n\}\}$ are independent Rademacher random variables, $\Pr(\sigma_i = 1) = \Pr(\sigma_i = -1) = \frac{1}{2}$.

Bounding True Risk with Rademacher Complexity

Definition ((β, c)-admissibility)

A similarity function $K_{\mathbf{M}} : \mathcal{X} \times \mathcal{X} \to [-1, 1]$ parameterized by $\mathbf{M} \in \mathbb{R}^{d \times d}$ is (β, c)-admissible if, for any matrix norm $|| \cdot ||$, there exist $\beta, c \in \mathbb{R}$ s.t. $\forall \mathbf{x}, \mathbf{x}' \in \mathcal{X}, |K_{\mathbf{M}}(\mathbf{x}, \mathbf{x}')| \leq \beta + c \cdot ||\mathbf{x}'\mathbf{x}^T|| \cdot ||\mathbf{M}||$.

Theorem (Generalization bound)

Let $(\mathbf{M}_{\mathcal{S}}, \boldsymbol{\alpha}_{\mathcal{S}})$ be the solution to JSL and $K_{\mathbf{M}}$ a (β, c)-admissible similarity function. Then, for any $0 < \delta < 1$, with probability at least $1 - \delta$, the following holds:

true risk *(β, c)-admissibility of $K_{\mathbf{M}}$* $X_* = \sup_{\mathbf{x}, \mathbf{x}' \in \mathcal{X}} ||\mathbf{x}'\mathbf{x}^T||_*$

$$|R_P^{\ell}(\mathbf{M}_{\mathcal{S}}, \boldsymbol{\alpha}_{\mathcal{S}}) - R_{\mathcal{S}}^{\ell}(\mathbf{M}_{\mathcal{S}}, \boldsymbol{\alpha}_{\mathcal{S}})| \leq 4\mathfrak{R}_m \left(\frac{cd}{\gamma}\right) + \left(\frac{\beta + cX_* d}{\gamma}\right) \sqrt{\frac{2 \ln \frac{1}{\delta}}{m}}.$$

empirical risk *Rademacher complexity* *convergence in $\mathcal{O}\left(\frac{1}{\sqrt{m}}\right)$*

Experimental Setup

Methods:

1. *Linear classifiers:*
   - Linear SVM with L_2 regularization;
   - BBS [BBS08];
   - SLLC [BHS12];
   - **JSL**;
2. *Nearest neighbor approaches:*
   - 3NN – euclidean distance;
   - ITML [DKJ$^+$07];
   - LMNN and LMNN-diag [WS08, WS09];
   - LRML [HLC10], semi-supervised setting.

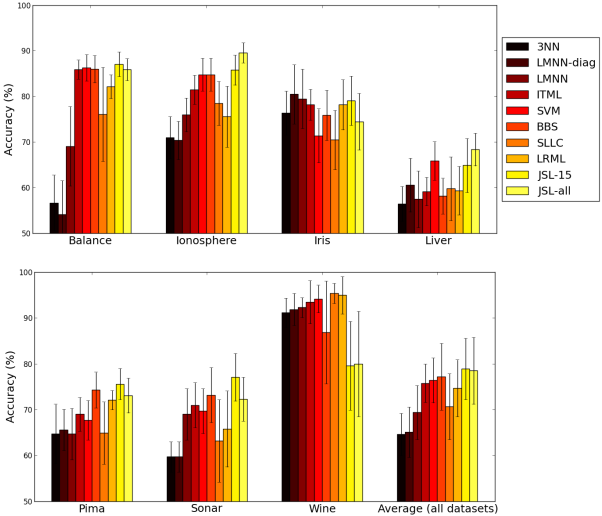
Settings:

- Small quantities of labeled data: 5, 10, 20 examples per class;
- 15 unlabeled examples, or the whole training set.

Datasets:

	Balance	Ionosphere	Iris	Liver	Pima	Sonar	Wine
# Instances	625	351	150	345	768	208	178
# Dimensions	4	34	4	6	8	60	13
# Classes	3	2	3	2	2	2	3

5 labeled points per class



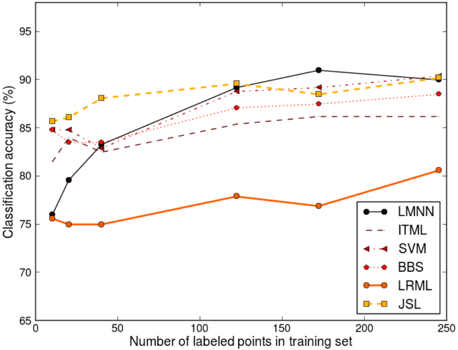
Experimental Results

Overall Accuracy Comparison

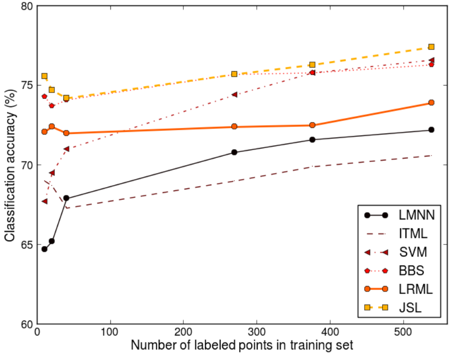
Method	5 pts./cl.	10 pts./cl.	20 pts./cl.
3NN	64.6±4.6	68.5±5.4	70.4±5.0
LMNN-diag	65.1±5.5	68.2±5.6	71.5±5.2
LMNN	69.4±5.9	70.9±5.3	73.2±5.2
ITML	75.8±4.2	76.5±4.5	76.3±4.8
SVM	76.4±4.9	76.2±7.0	77.7±6.4
BBS	77.2±7.3	77.0±6.2	77.3±6.3
SLLC	70.5±7.2	75.9±4.5	75.8±4.8
LRML	74.7±6.2	75.3±5.9	75.8±5.2
JSL-15	**78.9**±6.7	**77.6**±5.5	77.7±6.4
JSL-all	78.2±7.3	76.6±5.8	**78.4**±6.7

Experimental Results
Impact of the Amount of Labeled Data

15 unlabeled landmarks



(a) Ionosphere



(b) Pima

Summary of JSL

- New **semi-supervised** metric learning framework;
- **Joint learning** of a metric and a global separator;
- General similarity function and regularizer;
- **Theoretical guarantees** using Rademacher complexity and algorithmic robustness.

Publications

- M.-I. Nicolae, É. Gaussier, A. Habrard, and M. Sebban. Joint semi-supervised similarity learning for linear classification. In *ECML/PKDD*, 2015a.
- M.-I. Nicolae, M. Sebban, A. Habrard, É. Gaussier, and M.-R. Amini. Algorithmic Robustness for Semi-Supervised (ϵ, γ, τ)-Good Metric Learning. In *ICONIP*, pages 253–263, 2015b.
- M.-I. Nicolae, M. Sebban, A. Habrard, É. Gaussier, and M.-R. Amini. Algorithmic Robustness for Learning via (ϵ, γ, τ)-Good Similarity Functions. In *ICLR Workshop*, 2015.

Learning Similarities for Time Series Classification

Motivation

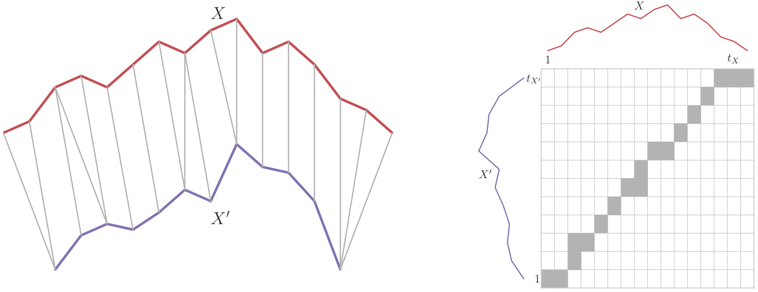
Time series

Vast presence of time series in real-world applications.

Metric learning for time series

- Little work in this field.
- Most of it focused on adapting known methods to the univariate case.

Dynamic Time Warping



Find the optimal alignment between two time series based on a cost matrix:

- **Quadratic complexity** in the length of the time series;
- Univariate case: often Euclidean distance;
- Multivariate case: need a measure for comparing time moments with multiple features.

Bilinear Similarity for Time Series

Time series **alignment** of length $t_{\mathbf{AB}}$ using DTW:

$$\mathbf{Y}_{\mathbf{AB}} = \mathrm{DTW}(\mathbf{A}, \mathbf{B}).$$

Affinity for aligning time moments $0 < i \leq t_{\mathbf{A}}$ and $0 < j \leq t_{\mathbf{B}}$ between series **A** and **B**:

$$\mathbf{C}_{\mathbf{M}}(\mathbf{A}, \mathbf{B})_{i,j} = \mathbf{a}_i^T \cdot \mathbf{M} \cdot \mathbf{b}_j.$$

Affinity matrix under metric $\mathbf{M} \in \mathbb{R}^{d \times d}$ for computing the cost of alignment:

$$\mathbf{C}_{\mathbf{M}}(\mathbf{A}, \mathbf{B}) = \mathbf{A} \cdot \mathbf{M} \cdot \mathbf{B}^T.$$

Bilinear similarity

Let $K_{\mathbf{M}} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ of form:

$$K_{\mathbf{M}}(\mathbf{A}, \mathbf{B}) = \mathrm{Tr}(\mathbf{C}_{\mathbf{M}}(\mathbf{A}, \mathbf{B})^T \cdot \mathbf{Y}_{\mathbf{AB}})/t_{\mathbf{AB}}.$$

Computes the score for aligning **A** and **B** under metric **M**.

Learning the Similarity

Improve the (ϵ, γ, τ)-goodness of $K_{\mathbf{M}}$:

$$\mathbb{E}_{(\mathbf{A},y)}\left[\left[1 - \mathbb{E}_{(\mathbf{B},y'),R(\mathbf{B})}\left[yy'K_{\mathbf{M}}(\mathbf{A},\mathbf{B}))|R(\mathbf{B})\right]/\gamma\right]_{+}\right] \leq \epsilon.$$

But we do not have access to expected values.

Similarity Learning for Time Series (SLTS)

Optimize the empirical value of the goodness criterion over sample $\mathcal{S}$ w.r.t. the set of landmarks $\mathcal{L}$:

$$\min_{\mathbf{M}} \frac{1}{m} \sum_{(\mathbf{A},y)\in\mathcal{S}} \left[1 - \frac{1}{n\gamma} \sum_{(\mathbf{B},y')\in\mathcal{L}} yy'K_{\mathbf{M}}(\mathbf{A},\mathbf{B})\right]_{+} + \lambda||\mathbf{M}||_{\mathcal{F}}^2.$$

Properties

- Convex formulation;
- Based on landmarks $\rightarrow$ does not need to compute DTW and the similarity for all pairs.

An algorithm is **stable** if its output is robust to small changes in its input. Uniform stability allows the derivation of generalization bounds.

Lemma

Given a training sample $\mathcal{S}$ of m examples drawn i.i.d. from P, our algorithm SLTS has uniform stability in κ/m with $\kappa = \frac{4d}{\gamma^2\lambda}$, that is:

$$\sup_{(\mathbf{A},l)\sim P} |\ell(\mathbf{M},(\mathbf{A},l)) - \ell(\mathbf{M}^i,(\mathbf{A},l))| \leq \frac{\kappa}{m},$$

where $\mathbf{M}^i$ is obtained by learning on $\mathcal{S}$ after replacing the ith example with a new one.

Bounding True Risk with Uniform Stability

Theorem (Generalization bound)

For any $0 < \delta < 1$, with probability $1 - \delta$, for any matrix $\mathbf{M}$ learned with SLTS, we have:

true risk — *# features*

$$|R_P^\ell(\mathbf{M}) - R_S^\ell(\mathbf{M})| \leq \frac{4d}{\gamma^2 \lambda m} + \left(\frac{4d}{\gamma^2 \lambda} + \frac{1}{\gamma}\sqrt{\frac{2d}{\lambda}} \right) \sqrt{\frac{2 \log \frac{2}{\delta}}{m}}.$$

empirical risk — *margin* — *convergence in $\mathcal{O}\left(\frac{1}{\sqrt{m}}\right)$*

- Independence from the length of the time series and the alignments.

Experimental Setup

Methods:

Nearest neighbor approaches:

- 1NN
- LDMLT

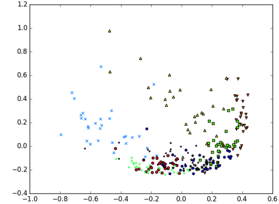
Linear classifiers:

- L_2 regularized SVM
- BBS
- **SLTS**.

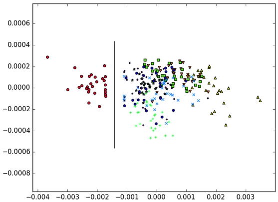
UCI Datasets [Lic13]:

Dataset	#Instances	Length	#Feat.	#Classes
Japanese vowels	640	7-29	12	9
Auslan	675	47-95	22	25
Arabic digits	8800	4-93	13	10
Robot execution failure				
LP1	88	15	6	4
LP2	47	15	6	5
LP3	47	15	6	4
LP4	117	15	6	3
LP5	164	15	6	5

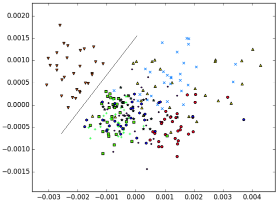
2D PCA on Japanese Vowels



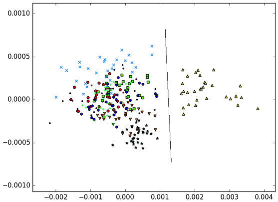
(a) No metric learning



(b) Metric for class 1



(c) Metric for class 2



(d) Metric for class 3

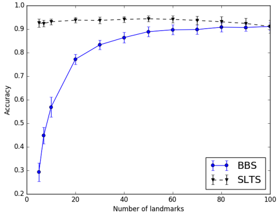
Experimental Results

Classification Accuracy (%)

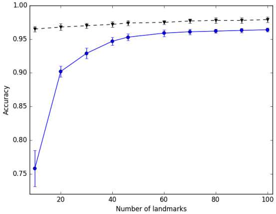
Method	Japanese vowels	Auslan	Arabic digits	Robot failure	Avg.
1NN	93.8	77.8±2.1	94.7	68.8±7.5	92.1
LDMLT	97.3	95.0±1.3	96.9	71.9±7.0	95.6
L_2 SVM	97.8±0.1	92.6±0.1	93.3±0.0	60.6±6.5	92.2
BBS	97.1±0.5	91.1±1.6	96.4±0.3	66.9±10.6	94.7
SLTS	97.1±0.4	91.1±2.7	97.9±0.4	67.0±7.8	**95.8**

- SLTS has comparable performance to the other methods;
- It has **theoretical guarantees** and does not need to compute all the alignments.

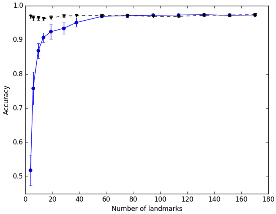
Classification accuracy for SLTS and BBS



(a) Auslan



(b) Arabic digits



(c) Japanese vowels

Summary of SLTS

- Novel method for **learning similarities** for multivariate time series classification.
- Metric consistency based on **uniform stability**.
- First method with **theoretical guarantees** for time series.

Publications

- M.-I. Nicolae, É. Gaussier, A. Habrard, and M. Sebban. Similarity Learning for Time Series Classification. Technical report, University of Saint-Etienne, 2016. arXiv:1610.04783. To be submitted to the journal track of *ECML/PKDD* 2017 and *MLJ*.

General Perspectives

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- Introduce nonlinearity by learning multiple local metrics.

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- Challenge the learning pairs.

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General Perspectives

- Introduce nonlinearity by learning multiple local metrics.
- Challenge the learning pairs.
- Goodness in similarity learning for local classification.
- Metric learning for an unsupervised setting with generalization guarantees.

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