Indefinite proximity learning - A review

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Abstract

Efficient learning of a data analysis task strongly depends on the data representation. Most methods rely on (symmetric) similarity or dissimilarity representations by means of *metric* inner products or distances, providing easy access to powerful mathematical formalisms like kernel or branch-and-bound approaches. Similarities and dissimilarities are however often naturally obtained by non-metric proximity measures which can not easily be handled by classical learning algorithms. In the last years major efforts have been undertaken to provide approaches which can either directly be used for such data or to make standard methods available for these type of data. We provide a comprehensive survey for the field of learning with non-metric proximities. First we introduce the formalism used in non-metric spaces and motivate specific treatments for non-metric proximity data. Secondly we provide a systematization of the various approaches. For each category of approaches we provide a comparative discussion of the individual algorithms and address complexity issues and generalization properties. In a summarizing

chapter we provide a larger experimental study for the majority of the algorithms on standard datasets. We also address the problem of large scale proximity learning which is often overlooked in this context and of major importance to make the method relevant in practice. **The algorithms discussed in this paper are in general applicable for proximity based clustering, one-class classification, classification, regression or embedding approaches**. In the experimental part we focus on classification tasks.

1 Introduction

The notion of pairwise proximities plays a key role in most machine learning algorithms. The comparison of objects by a *metric*, often Euclidean, distance measure is a standard element in basically every data analysis algorithm. This is mainly due to the easy access to powerful mathematical models in metric spaces. Based on work of (Schoelkopf & Smola, 2002) and others, the usage of similarities by means of metric inner products or kernel matrices has lead to a great success of similarity based learning algorithms. Thereby the data are represented by metric pairwise similarities only. We can distinguish similarities, indicating how close or similar two items are to each other and dissimilarities as measures of the unrelatedness of two items. Given a set of N data items, their pairwise proximity (similarity or dissimilarity) measures can be conveniently summarized in a $N \times N$ proximity matrix. In the following we will refer to similarity and dissimilarity type proximity matrices as $\mathbf{S}$ and $\mathbf{D}$, respectively. For some methods symmetry of the proximity measures is not strictly required, while some other methods add additional constraints, such as non-negativity of the proximity matrix. These notions enter into models by means of similarity or dissimilarity functions $f(\mathbf{x}, \mathbf{y}) \in \mathbb{R}$ where $\mathbf{x}$ and $\mathbf{y}$ are the compared objects. The objects $\mathbf{x}, \mathbf{y}$ may exist in a d-dimensional vector space, so that $\mathbf{x} \in \mathbb{R}^d$, but can also be given without an explicit vectorial representation, e.g. biological sequences (see Figure 1). However, as pointed out in (Pekalska & Duin, 2005), proximities often occur to be non-metric and their us-

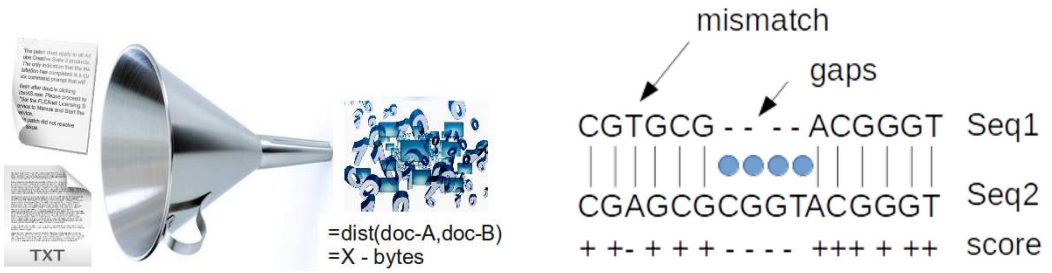


Figure 1: Left: Illustration of a proximity (in this case dissimilarity) measure between pairs of documents - the compression distance (Cilibrasi & Vitányi, 2005). It is based on the difference between the total information theoretic complexity of two documents considered in isolation and the complexity of the joint document obtained by concatenation of the two documents. In its standard form it violates the triangle inequality. Right: a simplified illustration of the blast sequence alignment providing symmetric but non-metric similarity scores in comparing pairs of biological sequences.

age in standard algorithms leads to invalid model formulations.

The function $f(\mathbf{x}, \mathbf{y})$ may violate the metric properties to different degrees. Symmetry is in general assumed to be valid because a large number of algorithms become meaningless for asymmetric data. However, especially in the field of graph analysis, asymmetric weightings have already been considered. Asymmetric weightings have also been used in the fields of clustering and data embedding (Strickert et al., 2014; Olszewski & Ster, 2014). Examples of algorithms capable of processing asymmetric proximity data in supervised learning are exemplar based methods (Nebel et al., 2014). A recent article focusing on this topic is available in (Calana et al., 2013). More frequently, proximities are symmetric, but the triangle inequality is violated, proximities are negative, or self-dissimilarities are not zero. Such violations can be attributed to different sources. While some authors attribute it to noise (Luss & d'Aspremont, 2009), for some proximities and proximity functions f this may be purposely caused by the measure itself. If noise is the source, often a simple eigenvalue correction (Y. Chen, Garcia, et al., 2009a) can be used, although this can become costly for large

datasets. A recent analysis of the possible sources of negative eigenvalues is provided in (Xu et al., 2011). Such analysis can be potentially helpful in, for example, selecting the appropriate eigenvalue correction method applied to the proximity matrix. Prominent examples for genuine non-metric proximity measures can be found in the field of bioinformatics where classical sequence alignment algorithms (e.g. smith-waterman score (Gusfield, 1997)) produce non-metric proximity values. For such data some authors argue that the non-metric part of the data contains valuable information and should not be removed (Pekalska et al., 2004).

For non-metric inputs the support vector machine formulation (Vapnik, 2000) no longer leads to a convex optimization problem. Prominent solvers. such as sequential minimization (SMO) will converge to a local optimum (J. C. Platt, 1999; tien Lin & Lin, 2003) and other kernel algorithms may not converge at all. Accordingly, dedicated strategies for non-metric data are very desirable.

A previous review on non-metric learning was given in (Y. Chen, Garcia, et al., 2009b) with a strong focus on support vector classification and eigenspectrum corrections for similarity data evaluated on multiple small world data sets. While we include and update these topics, our focus is on a broader context general supervised learning. Most approaches can be transferred to the unsupervised setting in a straightforward manner.

Besides eigenspectrum corrections making the similarity matrix positive semi definite (psd), we also consider generic novel proxy approaches (which learn a psd matrix from a non-psd representation), different novel embedding approaches and, crucially, natural indefinite learning algorithms, which are not restricted to psd matrices. We also address the issue of out of sample extension and the widely ignored topic of larger scale data processing (given the quadratic complexity in sample size).

The paper is organized as follows. In Section 2 we outline the basic notation and some mathematical formalism, related to machine learning with non-metric proximities. Section 3 discusses different views and sources of indefinite proximities and addresses

the respective challenges in more detail. A taxonomy of the various approaches is proposed in Section 4, followed by Section 5-6, which detail the two families of methods. In Section 7 we discuss some techniques to improve the scalability of the methods for larger datasets. Section 8 provides experimental results comparing the different approaches for various classification tasks and Section 8.1 concludes this paper.

2 Notation and basic concepts

We now briefly review some concepts typically used in proximity based learning.

2.1 Kernels and kernel functions

Let $\mathcal{X}$ be a collection of N objects x_i, $i = 1, 2, ..., N$, in some input space. Further, let $\phi : \mathcal{X} \mapsto \mathcal{H}$ be a mapping of patterns from $\mathcal{X}$ to a high-dimensional or infinite dimensional Hilbert space $\mathcal{H}$ equipped with the inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. The transformation ϕ is in general a non-linear mapping to a high-dimensional space $\mathcal{H}$ and may in general not be given in an explicit form. Instead a kernel function $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is given which encodes the inner product in $\mathcal{H}$. The kernel k is a positive (semi) definite function such that $k(x, x') = \phi(x)^\top \phi(x')$ for any $x, x' \in \mathcal{X}$. The matrix $K := \Phi^\top \Phi$ is an $N \times N$ kernel matrix derived from the training data, where $\Phi : [\phi(x_1), \ldots, \phi(x_N)]$ is a matrix of images (column vectors) of the training data in $\mathcal{H}$. The motivation for such an embedding comes with the hope that the non-linear transformation of input data into higher dimensional $\mathcal{H}$ allows for using linear techniques in $\mathcal{H}$. Kernelized methods process the embedded data points in a feature space utilizing only the inner products $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ (kernel trick) (Shawe-Taylor & Cristianini, 2004), without the need to explicitly calculate ϕ. The specific kernel function can be very generic. Most prominent are the linear kernel with $k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$ where $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$ is the Euclidean inner product or the rbf kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2\sigma^2}\right)$, with σ as a free parameter. Thereby it is assumed that the kernel function $k(\mathbf{x}, \mathbf{x}')$ is positive semi definite (psd).

2.2 Krein and Pseudo-Euclidean spaces

A Krein space is an *indefinite* inner product space endowed with a Hilbertian topology. Let $\mathcal{K}$ be a real vector space. An inner product space with an indefinite inner product $\langle \cdot, \cdot \rangle_{\mathcal{K}}$ on $\mathcal{K}$ is a bi-linear form where all $f, g, h \in \mathcal{K}$ and $\alpha \in \mathbb{R}$ obey the following conditions. Symmetry: $\langle f, g \rangle_{\mathcal{K}} = \langle g, f \rangle_{\mathcal{K}}$; linearity: $\langle \alpha f + g, h \rangle_{\mathcal{K}} = \alpha \langle f, h \rangle_{\mathcal{K}} + \langle g, h \rangle_{\mathcal{K}}$; and $\langle f, g \rangle_{\mathcal{K}} = 0$ implies $f = 0$. An inner product is positive definite if $\forall f \in \mathcal{K}$, $\langle f, f \rangle_{\mathcal{K}} \geq 0$, negative definite if $\forall f \in \mathcal{K}$, $\langle f, f \rangle_{\mathcal{K}} \leq 0$, otherwise it is indefinite. A vector space $\mathcal{K}$ with inner product $\langle \cdot, \cdot \rangle_{\mathcal{K}}$ is called an inner product space.

An inner product space $(\mathcal{K}, \langle \cdot, \cdot \rangle_{\mathcal{K}})$ is a Krein space if we have two Hilbert spaces $\mathcal{H}_+$ and $\mathcal{H}_-$ spanning $\mathcal{K}$ such that $\forall f \in \mathcal{K}$ we have $f = f_+ + f_-$ with $f_+ \in \mathcal{H}_+$ and $f_- \in \mathcal{H}_-$ and $\forall f, g \in \mathcal{K}$, $\langle f, g \rangle_{\mathcal{K}} = \langle f_+, g_+ \rangle_{\mathcal{H}_+} - \langle f_-, g_- \rangle_{\mathcal{H}_-}$.

Indefinite kernels are typically observed by means of domain specific non-metric similarity functions (such as alignment functions used in biology (Smith & Waterman, 1981)), by specific kernel functions - e.g. the Manhattan kernel $k(\mathbf{x}, \mathbf{y}) = -\|\mathbf{x} - \mathbf{y}\|_1$, tangent distance kernel (Haasdonk & Keysers, 2002) or divergence measures plugged into standard kernel functions (Cichocki & Amari, 2010). Another source of non-psd kernels are noise artifacts on standard kernel functions (Haasdonk, 2005). A finite-dimensional Krein-space is a so called pseudo Euclidean space.

For such spaces vectors can have negative squared "norm", negative squared "distances" and the concept of orthogonality is different from the usual Euclidean case. Given a symmetric *dissimilarity* matrix with zero diagonal, an embedding of the data in a pseudo-Euclidean vector space determined by the eigenvector decomposition of the associated similarity matrix $\mathbf{S}$ is always possible (Goldfarb, 1984) [1]. Given the eigendecomposition of $\mathbf{S}$, $\mathbf{S} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$, we can compute the corresponding vectorial

[1] The associated similarity matrix can be obtained by double centering (Pekalska & Duin, 2005) of the dissimilarity matrix. $\mathbf{S} = -\mathbf{JDJ}/2$ with $\mathbf{J} = (\mathbf{I} - \mathbf{1}\mathbf{1}^\top/N)$, identity matrix $\mathbf{I}$ and vector of ones $\mathbf{1}$.

representation $\mathbf{V}$ in the pseudo-Euclidean space by

$$\mathbf{V} = \mathbf{U}_{p+q+z} \left| \mathbf{\Lambda}_{p+q+z} \right|^{1/2} \tag{1}$$

where $\mathbf{\Lambda}_{p+q+z}$ consists of p positive, q negative non-zero eigenvalues and z zero eigenvalues. $\mathbf{U}_{p+q+z}$ consists of the corresponding eigenvectors. The triplet (p, q, z) is also referred to as the signature of the Pseudo-Euclidean space. A detailed presentation of similarity and dissimilarity measures, and mathematical aspects of metric and non-metric spaces is provided in (Pekalska & Duin, 2005; Deza & Deza, 2009; Ong et al., 2004).

3 Indefinite proximities

Proximity functions can be very generic but are often restricted to fulfill metric properties to simplify the mathematical modeling and especially the parameter optimization. In (Deza & Deza, 2009) a large variety of such measures was reviewed and basically most nowadays public methods make use of metric properties. While this appears to be a reliable strategy researchers in the field of e.g. psychology (Hodgetts & Hahn, 2012; Hodgetts et al., 2009), vision (Kinsman et al., 2012; Xu et al., 2011; Van Der Maaten & Hinton, 2012; Scheirer et al., 2014) and machine learning (Pekalska et al., 2004; R. P. W. Duin & Pekalska, 2010) have criticized this restriction as inappropriate in multiple cases. In fact in (R. P. W. Duin & Pekalska, 2010) multiple examples from real problems show that many real life problems are better addressed by proximity measures which are not restricted to be metric.

The triangle inequality is most often violated if we consider object comparisons in daily life problems like the comparison of text documents, biological sequence data, spectral data or graphs (Y. Chen, Garcia, et al., 2009b; Kohonen & Somervuo, 2002; Neuhaus & Bunke, 2006). These data are inherently compositional and a feature rep-

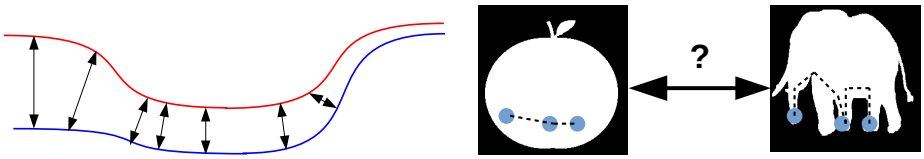


Figure 2: Visualization of two non-metric distance measures which are frequently used. Left: Dynamic time warping (DTW) - a frequently used measure to align one dimensional time series(Sakoe & Chiba, 1978); Right: Inner distance - a common measure in shape retrieval (Ling & Jacobs, 2005)

resentation leads to information loss. As an alternative, tailored dissimilarity measures such as pairwise alignment functions, kernels for structures or other domain specific similarity and dissimilarity functions can be used as the interface to the data (Gärtner et al., 2004; Poleksic, 2011). But also for vectorial data, non-metric proximity measures are common in some disciplines. An example of this type is the use of divergence measures (Cichocki & Amari, 2010; Z. Zhang et al., 2009; Schnitzer et al., 2012) which are very popular for spectral data analysis in chemistry, geo- and medical sciences (Mwebaze et al., 2010; Nguyen et al., 2013; Tian et al., 2013; van der Meer, 2006; Bunte, Haase, et al., 2012), and are not metric in general. Also the popular Dynamic Time Warping (DTW) (Sakoe & Chiba, 1978) algorithm provides a non-metric alignment score which is often used as a proximity measure between two one-dimensional functions of different length. In image processing and shape retrieval indefinite proximities are often obtained by means of the inner distance. It specifies the dissimilarity between two objects which are solely represented by their shape. Thereby a number of landmark points is used and the shorted paths *within* the shape are calculated in contrast to the Euclidean distance between the landmarks. Further examples can be found in physics where problems of the special relativity theory naturally lead to indefinite spaces.

Examples of indefinite measures can be easily found in many domains, some of them are exemplary shown in Figure 2. A list of non-metric proximity measures is given

Measure	Application field
Dynamic Time Warping (DTW) (Sakoe & Chiba, 1978)	Time series or spectral alignment
Inner distance (Ling & Jacobs, 2005)	Shape retrieval e.g. in robotics
Compression distance (Cilibrasi & Vitányi, 2005)	Generic used also for text analysis
Smith Waterman Alignment (Gusfield, 1997)	Bioinformatics
Divergence measures (Cichocki & Amari, 2010)	Spectroscopy and audio processing
Generalized Lp norm (Lee & Verleysen, 2005)	Time series analysis
Non-metric modified Hausdorff (Dubuisson & Jain, 1994)	Template matching
(Domain specific) alignment score (Maier et al., 2006)	Mass spectrometry

Table 1: List of commonly used non-metric proximity measures in various domains

in Table 1. Most of these measures are very popular but often violate the symmetry or triangle inequality condition or both. Hence many standard proximity based machine learning methods like kernel methods are not easy accessible for these data.

3.1 Why is a non-metric proximity function a problem?

A large number of algorithmic approaches assume that the data are given in a metric vector space, typically an Euclidean vector space, motivated by the strong mathematical framework which is available for metric Euclidean data. But with the advent of new measurement technologies and many non-standard data this strong constraint is often violated in practical applications and non-metric proximity matrices are more and more common.

This is often a severe problem for standard optimization frameworks as used e.g. for the Support Vector Machines (SVM), where psd matrices or more specific mercer kernels, are expected (Vapnik, 2000). The naive usage of non-psd matrices in such a context invalidates the guarantees of the original approach (like ensured convergence to a convex or stationary point or the expected generalization accuracy to new points).

In (Haasdonk, 2005) it was shown that the SVM not any longer optimizes a global convex function but is minimizing the distance between reduced convex hulls in a pseudo-Euclidean space leading to a local optimum. In (Laub, 2004) and (Filippone, 2009) different cost functions for clustering where analyzed and the authors point out

that the spectrum shift operation (discussed in the following) was found to be very robust with respect to the used optimization function.

Currently, the vast majority of approaches encodes such comparisons by enforcing metric properties into these measures or by using alternative, in general less expressive measures, which do obey metric properties. With the continuous increase of non-standard and non-vectorial data sets non-metric measures and algorithms in Krein or pseudo-euclidean spaces are getting more popular and have recently raised wide interest in the research community (Gnecco, 2013; J. Yang & Fan, 2013; Liwicki et al., 2013; Kanzawa, 2012; Gu & Guo, 2012; Zafeiriou, 2012; Miranda et al., 2013; Epifanio, 2013; Kar & Jain, 2012). In this article we review major research directions in the field of non-metric proximity learning where data are given by pairwise proximities only.

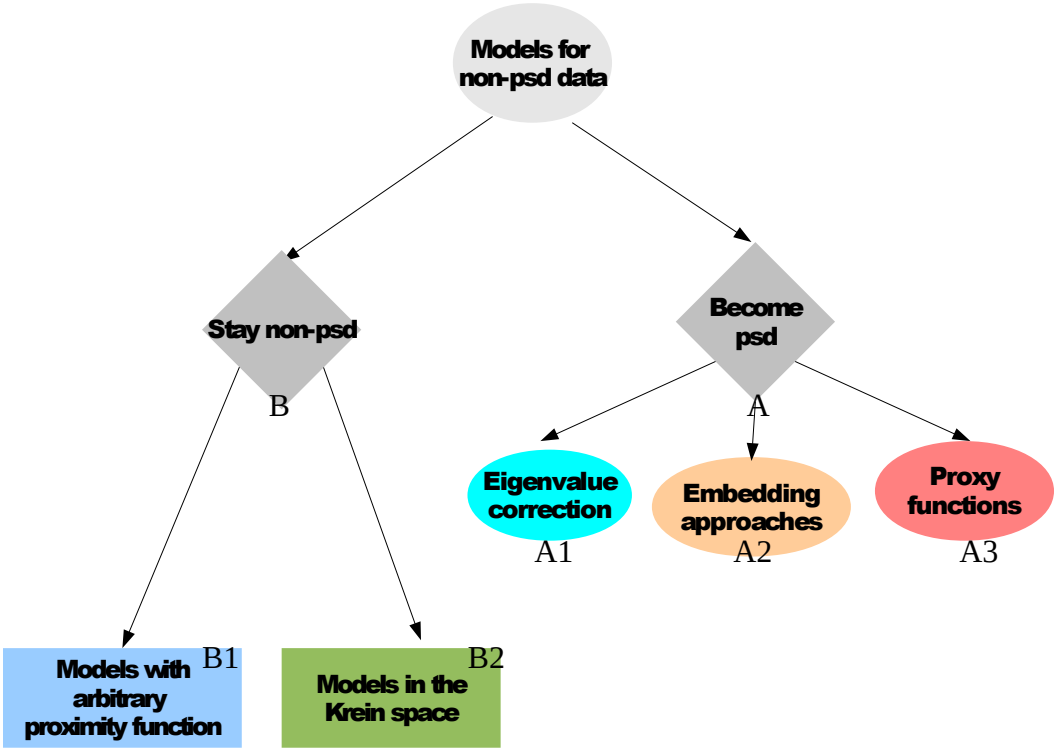


Figure 3: Schematic view of different approaches to analyze non-psd data

4 A systematization of non-metric proximity learning

The problem of non-metric proximity learning has been addressed before by some research groups and multiple approaches were proposed within the last years. A schematic view summarizing the major research directions is show in Figure 3 and in Table 2 and Table 3.

Basically, there exist two main directions:

(A) Transforming the non-metric proximities to become metric

(B) Stay in the non-metric space by providing a method which is insensitive to metric violations or can naturally deal with non-metric data

The first direction can again be divided to the following sub-strategies:

A.1 *Applying direct eigenvalue corrections*. The original data are decomposed by an

Turn non-metric proximities into metric ones (Sec. 5)		
(A1) Eigenvalue corrections (like clipping, flipping, shifting) are applied to the eigenspectrum of the data (Muoz & De Diego, 2006; Roth et al., 2002; Y. Chen, Garcia, et al., 2009a; Filippone, 2009). This can also be effectively done for dissimilarities by a specific pre-processing (Schleif & Gisbrecht, 2013)	(A2) Embedding approaches like (variants of MDS (Cox & Cox, 2000; Choo et al., 2012), t-SNE (Van Der Maaten & Hinton, 2012), NeRV (Venna et al., 2010) can be used to obtain an Euclidean embedding in a lower dimensional space but also the (dis-)similarity (proximity) space is a kind of embedding leading to a vectorial representation (Pekalska & Duin, 2008a, 2002, 2008b; Pekalska et al., 2001, 2006; Kar & Jain, 2011; R. P. W. Duin et al., 2014), as well as non-metric locality sensitive hashing (Mu & Yan, 2010) and local embedding or triangle correction techniques (L. Chen & Lian, 2008)	(A3) Learning of a proxy function is frequently used to obtain an alternative psd proximity matrix which has maximum alignment with the original non-psd matrix. (J. Chen & Ye, 2008; Luss & d'Aspremont, 2009; Y. Chen, Gupta, & Recht, 2009; Gu & Guo, 2012; Lu et al., 2005; Brickell et al., 2008; Li et al., 2015)

Table 2: Classification of the methods which have been reviewed in Sections 5–6. The table provides a brief summary and the most relevant references.

Algorithms for learning on non-metric data (Sec. 6)		
(B1) Algorithms with a decision function which can be based on non-metric proximities: (Kar & Jain, 2012; M. Tipping, 2001a; H. Chen et al., 2014, 2009a; Graepel et al., 1998)	(B2) Algorithms which define their models in the pseudo-Euclidean space: (Haasdonk & Pkalska, 2008; Pekalska & Haasdonk, 2009; Liwicki et al., 2013, 2012; Zafeiriou, 2012; Kowalski et al., 2009; Xue & Chen, 2014; J. Yang & Fan, 2013; Pekalska et al., 2001)	
Theoretical work for indefinite data analysis and related overviews		
Focusing on SVM: (Haasdonk, 2005; Mierswa & Morik, 2008; tien Lin & Lin, 2003; Ying et al., 2009), indefinite kernels and pseudo-euclidean spaces (Balcan et al., 2008; Wang et al., 2009; Brickell et al., 2008; Schleif & Gisbrecht, 2013; Schleif, 2014; Pekalska & Duin, 2005; Pekalska et al., 2004, 2001; Ong et al., 2004; Laub et al., 2006; D.-G. Chen et al., 2008; R. P. W. Duin & Pekalska, 2010; Gnecco, 2013; Xu et al., 2011; Higham, 1988; Goldfarb, 1984; Graepel & Obermayer, 1999; Zhou & Wang, 2011; Alpay, 1991; Haasdonk & Keysers, 2002), indexing, retrieval and metric modification techniques (Z. Zhang et al., 2009; Skopal & Loko, 2008; Bustos & Skopal, 2011; Vojt & Eckhardt, 2009; Jensen et al., 2010), overview papers and cross discipline studies (Y. Chen, Garcia, et al., 2009a; Muoz & De Diego, 2006; R. P. W. Duin, 2010; Kinsman et al., 2012; Laub, 2004; Hodgetts & Hahn, 2012; Hodgetts et al., 2009; Kanzawa, 2012)		

Table 3: Classification (continued) of the methods which have been reviewed in Sections 5–6. The table provides a brief summary and the most relevant references.

Eigenvalue decomposition and the eigenspectrum is corrected in different ways to obtain a corrected psd matrix.

A.2 *Embedding of the data in a metric space*. Here, the input data are embedded into a (in general Euclidean) vector space. A very simple strategy is to use Multi-Dimensional Scaling (MDS) to get a two- dimensional representation of the distance relations encoded in the original input matrix.

A.3 *Learning of a proxy function to the proximities*. These approaches learn an alternative (proxy) psd representation with maximum alignment to the non-psd input data.

while the second branch is less diverse but one can identify at least two sub-strategies:

B.1 *Model definition based on the non-metric proximity function*. Recent theoretical work on generic dissimilarity and similarity functions is used to define models which can directly employ the given proximity function with only very moderate assumptions.

B.2 *Krein space model definition*. The Krein space is the natural representation for non-psd data and some approaches have been formulated within this much less restrictive, but hence more complicated, mathematical space.

In the following we detail the different strategies and their advantages and disadvantages. As a general comment the approaches covered in B stay closer to the original input data whereas for the strategy A the input data are in parts substantially modified which can lead to a reduced interpretability and also limits a valid out-of sample extension in many cases.

5 Make the input space metric

5.1 Eigenspectrum approaches (A1)

The metric violations cause negative eigenvalues in the eigenspectrum of **S** leading to non-psd proximity matrices. Many learning algorithms are based on kernels yielding symmetric and psd similarity (kernel) matrices. The mathematical meaning of a kernel is the inner product in some Hilbert space (Shawe-Taylor & Cristianini, 2004). However, it is often loosely considered simply as a pairwise "similarity" measure between data items. If a particular learning algorithm requires the use of Mercer kernels and the similarity measure does not fulfill the kernel conditions, steps must be taken to ensure a valid model.

A natural way to address this problem and to obtain a psd similarity matrix is to correct the eigenspectrum of the original similarity matrix **S**. Popular strategies include *flipping, clipping, shift correction*. The non-psd similarity matrix **S** is decomposed as

$$\mathbf{S} = U\Lambda U^{\top}, \tag{2}$$

where U contains the eigenvectors of **S** and Λ contains the corresponding eigenvalues.

Clip eigenvalue correction: all negative eigenvalues in Λ are set to 0. Spectrum clip leads to the nearest psd matrix **S** in terms of the Frobenius norm (Higham, 1988). The clip transformation can also be expressed as (Gu & Guo, 2012):

$$\mathbf{S}^{*} = \mathbf{S}\mathbf{V}_{\text{clip}}\mathbf{V}_{\text{clip}}^{\top}\mathbf{S}, \tag{3}$$

with $\mathbf{V}_{\text{clip}} = U|\Lambda|^{-\frac{1}{2}}diag(I_{\Lambda_1>0}, \ldots, I_{\Lambda_N>0})$, where $I_{\cdot}$ is an indicator function[2].

[2]The validity of the transformation function can be easily shown by: $\mathbf{S}^{*} = U\Lambda(U^{\top}U)|\lambda|^{-1}diag(I_{\Lambda_1>0}, \ldots, I_{\Lambda_N>0})(U^{\top}U)\Lambda U^{\top} = U\Lambda|\Lambda|^{-1}diag(I_{\Lambda_1>0}, \ldots, I_{\Lambda_N>0})\Lambda U^{\top} = U\Lambda diag(I_{\Lambda_1>0}, \ldots, I_{\Lambda_N>0})U^{\top}$. Similar derivations can also be found for the other transformation functions (flip, shift, square).

Flip eigenvalue correction: all negative eigenvalues in Λ are set to $\Lambda_i := |\Lambda_i| \ \forall i$ which at least keeps the absolute values of the negative eigenvalues and can be relevant if these eigenvalue contain important information (Pekalska et al., 2004). The flip transformation can be expressed as (Gu & Guo, 2012):

$$\mathbf{S}^* = \mathbf{S}\mathbf{V}_{\text{flip}}\mathbf{V}_{\text{flip}}^\top\mathbf{S}, \tag{4}$$

with $\mathbf{V}_{\text{flip}} = U|\Lambda|^{-\frac{1}{2}}$.

Shift eigenvalue correction: the shift operation was already discussed earlier by different researchers (Laub, 2004; Filippone, 2009) and modifies Λ such that $\Lambda := \Lambda - \min_{ij}\Lambda$. The shift transformation can also be expressed as (Gu & Guo, 2012):

$$\mathbf{S}^* = \mathbf{S}\mathbf{V}_{\text{shift}}\mathbf{V}_{\text{shift}}^\top\mathbf{S}, \tag{5}$$

with $\mathbf{V}_{\text{shift}} = U|\Lambda|^{-1}(\Lambda - \nu I)^{\frac{1}{2}}$ with $\nu = \min_{ij}\Lambda$. Spectrum shift enhances all the self-similarities by the amount of ν and does not change the similarity between any two different data points.

Square and bending eigenvalue correction: further strategies where recently discussed in (Muoz & De Diego, 2006) and contain the *square transformation* where Λ is changed to $\Lambda := \Lambda^2$ (taking the square elementwise) which leads to the following transformation matrix

$$\mathbf{S}^* = \mathbf{S}\mathbf{V}_{\text{square}}\mathbf{V}_{\text{square}}^\top\mathbf{S} = \mathbf{S}\mathbf{S}^\top \tag{6}$$

with $\mathbf{V}_{\text{square}} = U(\Lambda^2)^{-\frac{1}{2}}$ and *bending*, where in an iterative process the matrix is updated such that the influence of points (causing the metric violation) is down-weighted. In the same work also a brief comparison to some transformation approaches can be found. The prior transformations can be applied to symmetric *similarity* matrices. If the input is a symmetric dissimilarity matrix one has first to apply a double centering

(Pekalska & Duin, 2005) step. The obtained potentially non-psd similarity matrix can be converted as shown above and subsequently converted back to dissimilarities using Eq. (7), if needed.

Complexity: all of these approaches are applicable to similarity (as opposed to dissimilarity) data and require eigenvalue decomposition of the full matrix. The eigendecomposition (EVD) in Eq. (2) has a complexity of $O(N^3)$ using standard approaches. In (Gisbrecht & Schleif, 2014) a linear EVD was proposed which is based on the Nyström approximation and can also be used for indefinite low rank matrices **S**.

To apply these approaches to dissimilarity data one first needs to apply double centering (Pekalska & Duin, 2005) to the dissimilarity matrix **D**:

$$\begin{aligned} \mathbf{S} &= -\mathbf{JDJ}/2 \\ \mathbf{J} &= (\mathbf{I} - \mathbf{1}\mathbf{1}^\top/N) \end{aligned}$$

with identity matrix **I** and vector of ones **1**. To get from **S** to **D** is obviously also possible by calculating the dissimilarity between items i and j as follows:

$$\mathbf{D}_{ij} = \mathbf{S}_{ii} + \mathbf{S}_{jj} - 2\mathbf{S}_{ij}. \tag{7}$$

The same approach was used in (Graepel et al., 1998) for indefinite dissimilarity data followed by a flipping transformation. A more efficient strategy combining double centering and eigenvalue correction for symmetric dissimilarity matrices was provided in (Schleif & Gisbrecht, 2013) and uses the Nyström approximation to get efficient non-psd to psd conversions for low-rank matrices with linear costs.

Out of sample extension to new test points: in general, one would like to modify the training *and* test similarities in a consistent way, that is, to modify the underlying similarity *function* and not only modifying the training matrix **S**. Using the transformation

strategies mentioned above, one can see that the spectrum modification are in general based on a transformation matrix applied to **S**. Using this transformation matrix one can obtain corrected and consistent test samples in a straightforward way. We calculate the similarities of the new test point to all N training sample and obtain a row-vector $\mathbf{s_t} \in \mathbb{R}^{1xN}$ which replaces **S** in the above equations. For clip we would get:

$$\mathbf{s_t^*} = \mathbf{s_t}\mathbf{V}_{\text{clip}}\mathbf{V}_{\text{clip}}^{\top}\mathbf{s_t} \tag{8}$$

with $\mathbf{V}_{\text{clip}}$ as defined before on the training matrix **S**.

5.2 Learning of alternative metric representations (A3)

As mentioned before many algorithmic optimization approaches become invalid for non-metric data. An early approach to address this problem used an optimization framework to address the violation of assumptions in the input data. A prominent way is to optimize not on the original proximity matrix but on a proxy matrix which is ensured to be psd and is aligned to the original non-psd proximity matrix.

Proxy matrix for noisy kernels: the proxy matrix learning problem for indefinite kernel matrices is addressed in (Luss & d'Aspremont, 2009) for support vector classification (SVC), regression (SVR) and 1-class classification. The authors attribute the indefiniteness to noise effecting the original kernel and propose to learn a psd proxy matrix. The SVC or SVR problem is reformulated to be based on the proxy kernel with additional constraints to keep the proxy kernel psd and aligned to the original non-psd kernel. A similar conceptually related proxy learning algorithm for indefinite kernel regression was recently proposed in (Li et al., 2015). The specific modification is done as an update on the cone of psd matrices which effectively removes the negative eigenvalues of the input kernel matrix.

A similar but more generic approach was proposed for dissimilarities in (Lu et al.,

2005). Thereby the input can be a noisy, incomplete and inconsistent dissimilarity matrix. A convex optimization problem is established, estimating a regularized psd kernel from the given dissimilarity information. Also in (Brickell et al., 2008) potentially asymmetric but non-negative dissimilarity data are considered. Thereby a proxy matrix is searched for such that the triangle violations for triple points sets of the data are minimized or removed. This is achieved by specifying a convex optimization problem on the cone of metric dissimilarity matrices constrained to obey all triangle inequality relations for the data. Various triangle inequality fixing algorithms are proposed to solve the optimization problem at reasonable costs for moderate data sets. The benefit of (Brickell et al., 2008) is that as few distances as possible are modified to obtain a metric solution. Another approach is to learn a metric representation based only on given conditions on the data point relations, such as linked or unlinked. In (Davis et al., 2007) a Mahalanobis type metric is learned such that $d(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{(\mathbf{x}_i - \mathbf{x}_j)^\top \mathbf{G}(\mathbf{x}_i - \mathbf{x}_j)}$ where the user given constraints are optimized with the matrix $\mathbf{G}$.

Proxy matrix guided by eigenspectrum correction: in (J. Chen & Ye, 2008) the work of (Luss & d'Aspremont, 2009) was adapted to a semi-infinite quadratic constraint linear program with an extra pruning strategy to handle the large number of constraints. Further approaches following this line of research were recently reviewed in (Muoz & De Diego, 2006).

In (Luss & d'Aspremont, 2009) the indefinite kernel K_0 is considered to be a noise disturbed realization of a psd kernel K. They propose a joint optimization of a proxy kernel aligned to K_0 and the (dual) SVM classification problem [3]:

$$\max_{(\alpha^\top y=0, 0\leq\alpha\leq C)} \min_{(K\succeq 0)} \alpha^\top \mathbf{1} - \frac{1}{2} Tr(K(\mathbf{Y}\alpha)(\mathbf{Y}\alpha)^\top) + \gamma \|K - K_0\|_F^2$$

where α are the Lagrange variables, K is the proxy kernel, $\mathbf{Y}$ is a diagonal label matrix

[3] Later extended to regression and one-class SVM

and C, γ are control parameters. For the Frobenius norm the closest psd kernel to K_0 is the corresponding clipped kernel, accordingly in (Luss & d'Aspremont, 2009) the proxy kernel can be calculated explicit (for given α) as:

$$K^* = (K_0 + (\mathbf{Y}\alpha)(\mathbf{Y}\alpha)^\top)/(4\gamma))_+ \tag{9}$$

where $_+$ indicates the clipping operation as discussed before. Accordingly, for $\gamma \to \infty$ the optimal kernel is obtained by zeroing out negative eigenvalues. We can also see in Eq (9) that similarities for points with different labels are shifted to zero (and finally clipped) and similarities for points in the same class are lifted.

Another work based on (Luss & d'Aspremont, 2009) was introduced in (Y. Chen, Gupta, & Recht, 2009), where the proxy or surrogate kernel is restricted to result from few specific transformations. such as eigenvalue flipping, clipping or shifting, leading to a second-order cone program. In (Y. Chen, Gupta, & Recht, 2009) the optimization problem is similar to the one proposed in (Luss & d'Aspremont, 2009) but the regularization is handled differently. Instead a computationally simpler method restricting K^* to be a spectrum modification of K_0 is suggested, based on indicator variables a. This approach also leads to an easier out of sample extension. The suggested problem in the primal domain was given as:

$$\begin{aligned} \underset{c,b,\xi,\alpha}{\text{minimize}} \quad & \tfrac{1}{N}\mathbf{1}^\top\xi + \eta c^\top K_a c + \gamma h(a) \\ s.t. \quad & \text{diag}(y)(K_a c + b\mathbf{1}) \geq \mathbf{1} - \xi, \\ & \xi \geq 0, \Lambda a \geq 0 \end{aligned} \tag{10}$$

where $K_a = U\text{diag}(a)\Lambda U^\top$ with $K = U\Lambda U^\top$ as the eigenvalue decomposition of the kernel matrix and $h(a)$ is a convex regularizer of a e.g. $\|a - a_{\text{clip}}\|_2$ or $\|a - a_{\text{flip}}\|_2$, which is chosen by cross-validation. The regularizer is controlled by a balancing parameter γ having the same role as in Eq (9). The other parameters are with respect to a standard SVM problem (for details see (Y. Chen, Gupta, & Recht, 2009)).

A similar strategy coupling the SVM optimization with a modified kernel PCA was

proposed recently in (Gu & Guo, 2012). Here the basic idea is to modify the eigenspectrum of the non-psd input matrix as discussed in (Y. Chen, Gupta, & Recht, 2009), but based on a kernel PCA for indefinite kernels. The whole problem was formalized in a multi-class SVM learning scheme.

For all those methods the common idea is to convert the non-psd proximity matrix into a psd similarity matrix by using a numerical optimization framework. The approach of (Lu et al., 2005) learns the psd matrix independently of the algorithm which subsequently uses the matrix. The other approaches solve jointly the matrix conversion and the model-specific optimization problem.

Complexity: while the approaches of (Luss & d'Aspremont, 2009) and (J. Chen & Ye, 2008) appear to be quite resource demanding, the approaches of (Gu & Guo, 2012) and (Y. Chen, Gupta, & Recht, 2009) are more tractable by constraining the matrix conversion to few possible strategies and providing a simple out of sample strategy for mapping new data points. The approaches of (Luss & d'Aspremont, 2009) uses a full eigenvalue decomposition in the first step ($\mathcal{O}(N^3)$). Further the full kernel matrix is approximated by a psd proxy matrix with $\mathcal{O}(N^2)$) memory complexity. The approach by (J. Chen & Ye, 2008) has similar conditions. The approach in (Brickell et al., 2008) shows $\mathcal{O}(N^3)$ runtime complexity. All these approaches have a rather high computational complexity and do not scale to larger datasets with $N \gg 1e5$.

Out of sample extension to new test points: the work in (Luss & d'Aspremont, 2009; J. Chen & Ye, 2008) and (Lu et al., 2005) extends to new test points by employing an extra optimization problem. (J. Chen & Ye, 2008) proposed to find aligned test similarities using a quadratically constrained quadratic program (QCQP). Given new the test similarities s and an optimized kernel K^* aligned to $\mathbf{S}$ an optimized $\tilde{k}$ is found

by solving

$$\begin{aligned} \min_{k,r} \quad & \left\| \begin{pmatrix} K^* & \tilde{k} \\ \tilde{k}^\top & r \end{pmatrix} - \begin{pmatrix} \mathbf{S} & s \\ s^\top & \Delta s \end{pmatrix} \right\|_F \\ \text{s.t.} \quad & \left[\begin{pmatrix} K^* & \tilde{k} \\ \tilde{k}^\top & r \end{pmatrix} \right] \geq 0 \end{aligned}$$

The optimized kernel values are given in $\tilde{k}$ with self similarities in r, $\Delta s = S(x, x)$ and $\|\cdot\|_F$ is the Frobenius norm. As pointed out in more detail in (J. Chen & Ye, 2008) one finally obtains the following rather simple optimization problem:

$$\begin{aligned} \min_{k,r} \quad & 2\|\tilde{k} - s\|_2^2 + (r - \Delta s)^2 \\ \text{s.t.} \quad & \tilde{k}^\top (K^*)^{-1} \tilde{k} - r \leq 0 \\ & (I - K^*(K^*)^{-1})\tilde{k} = 0 \end{aligned}$$

which can be derived from (Boyd & Vandenberghe, 2004) (Appendix A.5.5).

In (Gu & Guo, 2012) the extension is directly available by use of a projection function within a multiclass optimization framework.

5.3 Experimental evaluation

The formerly mentioned approaches are all similar to each other but from the published experiments it is not clear how they compare. Subsequently we give a brief study comparing the approach of (Luss & d'Aspremont, 2009) and (J. Chen & Ye, 2008). We consider different non-psd standard datasets processed by the two methods, systematically varying the penalization parameter $\gamma \in [1e-4, \ldots, 1000]$ at a logarithmic scale with 200 steps. The various kernel matrices form a manifold in the cone of the psd matrices. We compared these kernel matrices pairwise using the Frobenius norm. The obtained distance matrix is embedded into two dimensions using the t-SNE algorithm

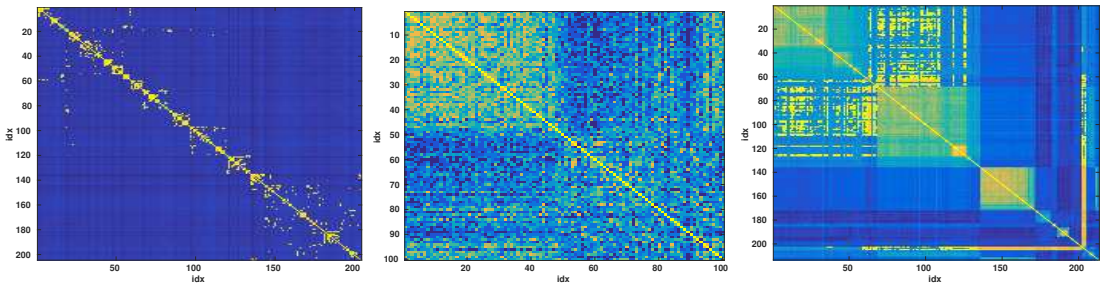


Figure 4: Visualization of the proxy kernel matrices (amazon, aural sonar, protein).

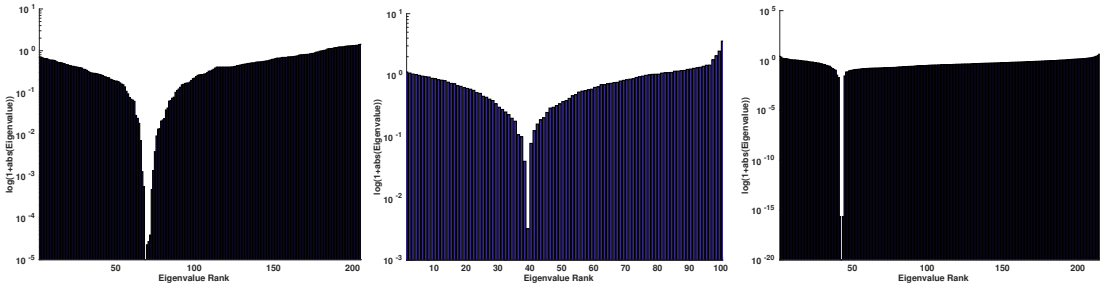


Figure 5: Eigenspectra of the proxy kernel matrices (amazon, aural sonar, protein).

(van der Maaten & Hinton, 2008) and an manually adapted penalty term. As anchor points we also included the clip, flip, shift, square and the original kernel solution.

The considered data are the Amazon47 data (204pts, two classes), the Aural Sonar data (100pts, two classes) and the Protein data (213pts, two classes). The similarity matrices are shown in Figure 4 with indices sorted according to the class labels. For all datasets the labeling has been changed to a two class scheme by combining odd or even class labels, respectively. All datasets are then quite simple classification problems leading to an empirical error of close to 0 in the SVM model trained on the obtained proxy kernels. However they are also strongly non-psd as can be seen from the eigenspectra plots in Figure 5.

An exemplary embedding is shown in Figure 7 with arbitrary units (so we omit the axis labeling). There are basically two trajectories of kernel matrices (each represented by a circle) where the penalty parameter value is indicated by a red or blue shading. We also see some separate clusters which are caused by the embedding procedure. We see the kernel matrices for the protein data set. In the left we have the trajectory of the

approach provided by Chen and in the right the one as obtained by the method of Luss. We see that the clip solution is close to the crossing point of the two trajectories. The square, shift and flip solutions are near to the original kernel matrix (light green circle). We can find the squared solution quite close to the original kernel matrix but also some points of the Luss trajectory are close to this matrix. Similar observations can be made for the other datasets. [4]. We would also like to mention again that both algorithms are not only optimizing with respect to the Frobenius norm but also in the line of the SVM optimization.

From the plots we can conclude that both method calculate psd kernel matrices along a smooth trajectory with respect to the penalty parameter finally leading to the clip solution. The square, shift and original kernel solution appear to be very similar and are close but in general not crossing the trajectory of Luss or Chen. The flip solution is typically less similar to the other kernel matrices.

5.4 A geometric view of eigenspectrum and proxy approaches

As seen in the previous section the surrogate or proxy kernel is not learned from scratch but is often restricted to be in a set of valid psd kernels originating from some standard spectrum modification approaches (such as flip or clip) applied to K. The approach in (Luss & d'Aspremont, 2009) is formulated primary with respect to an increase of the class separation by the proxy kernel and, as the second objective, to ensure that the obtained kernel matrix is still psd. This can be easily seen in Equation Eq (9). If a pair (i, j) of data items are form the same class, i.e. $y_i = y_j$, the corresponding similarities in the kernel matrix are emphasized (increased), otherwise they are decreased. If by doing this the kernel becomes indefinite, it is clipped back to the boundary of the space of

[4] It should be noted that the two dimensional embedding is neither unique nor perfect because the intrinsic dimensionality of the observed matrix space is larger and t-SNE is a stochastic embedding technique. But also with different parameter settings and multiple runs at different random start points we consistently observe similar results. As only local relations are valid within the t-SNE embedding the Chen solutions can also be close to e.g. the squared matrix in the high dimensional manifold and may have been potentially teared apart in the plot

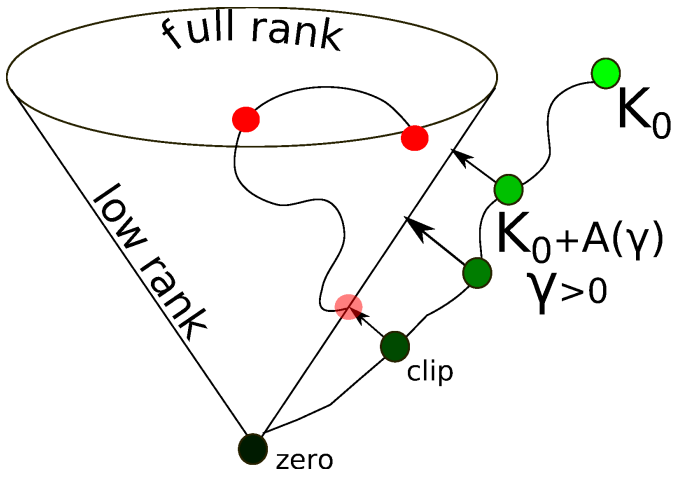


Figure 6: Schematic visualization of the eigenspectrum and proxy matrix approaches with respect to the cone of psd matrices. The cone interior covers the full rank psd matrices and the cone boundary contains the psd matrices having at least one zero eigenvalue. In the origin we have the matrix with all eigenvalues zero. Out of the cone are the non-psd matrices. Both strategies project the matrices to the cone of psd-matrices. The γ parameter controls how strong the matrices are regularized towards a clipping solution with a matrix update A. Depending on the penalizer and the rank of S the matrices follow various trajectories (an exemplary one is shown by the curved line in the cone). If $\gamma = \infty$ the path reaches the clipping solution at the boundary of the cone.

psd kernel matrices[5]. This approach can also be considered as a type of kernel matrix learning (Lanckriet et al., 2004).

In (Y. Chen, Gupta, & Recht, 2009) the proxy matrix is restricted to be a combination of clip or flip operations on the eigenspectrum of the matrix K. We denote the cone of $N \times N$ positive semi-definite matrices by C (see figure 6). Further, we define the kernel matrix obtained by the approach of Eq. (9) as K^L and at Eq. (10) as K^C. The approaches of Eq. (9) and Eq. (10) can be interpreted as a smooth path in C. Given, the balancing parameter $\gamma \in (0, \infty)$, the optimization problems in Eq. (9) and Eq. (10) have unique solutions $K^L(\gamma)$ and $K^C(\gamma)$, respectively. In the interior of C, a small

[5] In general a matrix with negative entries can still be psd

perturbation of γ will lead to small perturbations in K^L and K^C, meaning that the optimization problems in Eq. (9) and Eq. (10) defines continuous paths $K^L(0,\infty) \to C_{\geq 0}$ and $K^C(0,\infty) \to C_{\geq 0}$, respectively. It has been shown that as γ grows, $K^L(\gamma)$ approaches K^{clip} (Y. Chen, Gupta, & Recht, 2009). Note that for the approach of Chen the vector a (see Eq. 10) defines the limiting behavior of the path $K^C(\gamma)$. This can be easily seen by defining $\lambda = (\lambda_1, \ldots, \lambda_N)$ and $a = (a_1, \ldots, a_N)$ as follows: If $\lambda_i = 0$, then $a_i = 0$. Otherwise,

- clip : $a_i = 1$ if $\lambda_i \geq 0$ and $a_i = 0$ otherwise
- flip : $a_i = \frac{|\lambda_i|}{\lambda_i}$
- square: $a_i = \lambda_i$

Depending on the setting of the vector a, $K^C(\gamma)$ converges to either K^{clip}, K^{flip}, K^{square}.

Following the idea of eigendecomposition by Chen, $K = U\Lambda U^\top$, we suggest a unified intuitive interpretation of proximity matrix psd corrections. Applying an eigendecomposition to the kernel $K_0 = \sum \lambda_i u_i u_i^\top$, we can view K_0 is a weighted mixture of N rank-1 "expert proximity suggestions"[6] K_i: $K_0 = \sum_{i=1}^N \lambda_i K_i$, where $K_i = u_i u_i^\top$.

Different proximity matrix psd corrections result in different weights of the experts K_i, $K = \sum_{i=1}^N \omega_i K_i$:

- no correction: $\omega_i = \lambda_i$
- clip : $\omega_i = [\lambda_i]_+$
- flip : $\omega_i = |\lambda_i|$
- square: $\omega_i = \lambda_i^2$
- shift $\omega_i = \lambda_i - \min_j \lambda_j$

[6] It can effectively be less then N experts if $\text{rank}(K) < N$.

Each expert provides an opinion $[K_i]_{(a,b)}$ about the similarity for an object pair (a, b), weighted by ω_i. Note that in some cases the similarities $[K_i]_{(a,b)}$ and the weights ω_i can be negative. If *both* terms are positive or negative, the contribution of the i-th expert increases the overall similarity $K_{(a,b)}$, otherwise it is decreased. If we consider a classification task, we can now analyze the misclassifications in more detail by inspecting the similarities of misclassified entries for individual experts. Depending on the used eigenvalue correction one gets information whether similarities are increased or decreased. In the experiments given in Section 8.1 and Section 8 we see that clipping is in general worse than flipping or square. Clipping removes some of the experts opinions. Consider a negative similarity value $[K_i]_{(a,b)}$ from the i-th expert. Negative eigenvalue λ_i of K_0 causes the contribution from expert i to increase the overall similarity $K_{(a,b)}$ between items a and b. Flipping corrects this by enforcing the contribution from expert i to decrease $K_{(a,b)}$. Square in addition enhances and suppresses weighting all experts with $|\lambda_i| > 1$ and $|\lambda_i| < 1$, respectively. On the other hand, Shift consistently ranks up unimportant experts (weights in K_0 close to 0), explaining the (in general) bad results for shift in Table 6.

An exemplary visualization of the proximity matrix trajectories for the approaches of (Y. Chen, Gupta, & Recht, 2009) and (Luss & d'Aspremont, 2009) is shown in Figure 7. Basic eigenspectrum approaches project the input matrix K_0 on the boundary of the cone C if the matrix has low rank, or project it in the interior of C when the transformed matrix has still full rank. Hence, the clip and shift approaches give always a matrix on the boundary and are quite restricted. The other approaches can lead to projections in the cone and may still permit additional modifications of the matrix e.g. to enhance inner-class similarities. However the additional modifications may lead to low rank matrices such that they are projected back to the boundary of the cone.

Having a look at the protein data (see Figure 5) we see that the eigenspectrum of K_0 shows strong negative components. We know that the proximities of the protein data are generated by a non-metric alignment algorithm, errors in the triangle inequalities

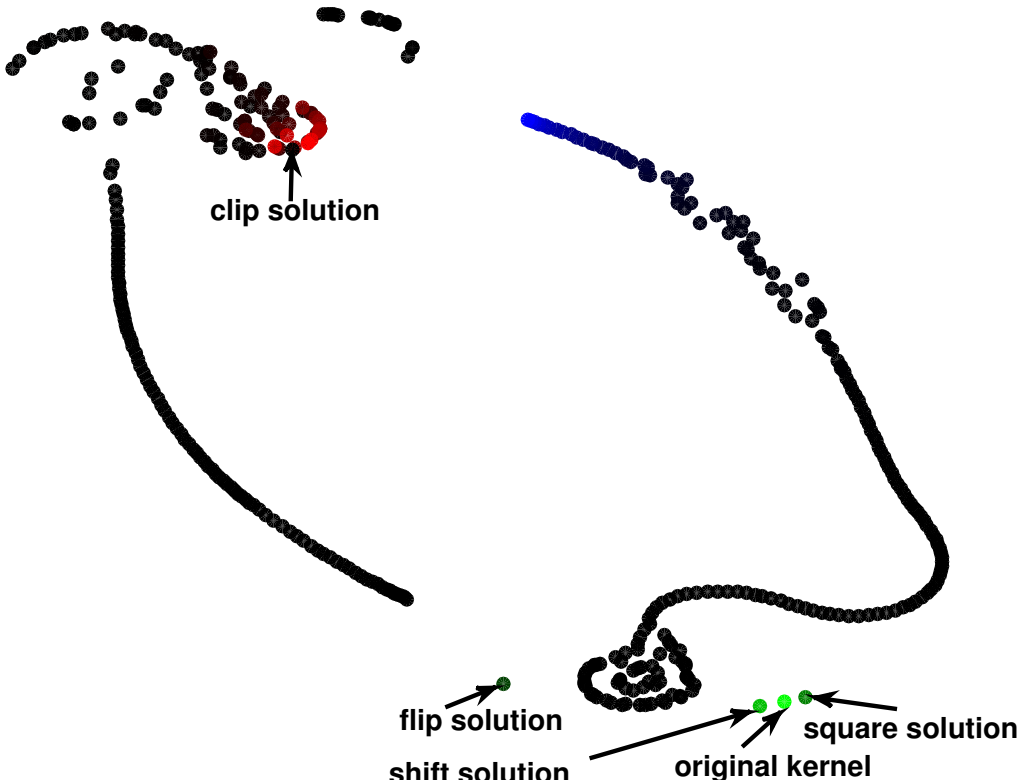


Figure 7: Embedding of adapted proxy kernel matrices for the protein data as obtained by Luss (blue shaded) and Chen (red shaded). One sees typical proximity matrix trajectories for the approaches of (Y. Chen, Gupta, & Recht, 2009) and (Luss & d'Aspremont, 2009), both using the clip strategy. The embedding was obtained by t-distributed stochastic neighbor embedding (t-SNE) (van der Maaten & Hinton, 2008), where the Frobenius norm was used as a similarity measure between two matrices. Although the algorithms start from different initialization points of the proximity matrices, the trajectories roughly end in the clip solution for increasing γ.

are therefore most likely caused by the algorithm and not by numerical errors (noise). For simplicity we reduce the protein data to a two class problem by focusing on the two largest classes. We obtain a proximity matrix with 144×144 entries and an eigenspectrum which is very similar to the one of the original protein data. The smallest eigenvalue is -12.41 and the largest 68.77. Now we identify those points which show a stronger alignment to the eigenvector of the dominant *negative* eigenvalue - i.e. points with high absolute values in the corresponding co-ordinates of the eigenvector. We collected the top 61 of such points in a set $\mathcal{B}$. Training SVM on the two-class problem without eigenvalue correction lead to 57% training error. We observed that 52% of data items from $\mathcal{B}$ were misclassified. By applying an eigenvalue correction we still have misclassifications (flip - 5%, clip - 14%), but for flip none of the misclassified items and for clip 15% of them are in $\mathcal{B}$. This shows again that the negative eigenvalues can contain relevant information for the decision process.

5.5 Embedding and mapping strategies (A2)

Global proximity embeddings: an alternative approach is to consider different types of embeddings or local representation models to effectively deal with non-psd matrices. After the embedding into an (in general low dimensional) Euclidean space standard data analysis algorithms e.g. to define classification functions can be used. While many embedding approaches are applicable to non-metric matrix data the embedding can lead to a substantial information loss (Wilson & Hancock, 2010). Some embedding algorithms like laplacian eigenmaps (Belkin & Niyogi, 2003) can not be calculated based on non-metric input data and pre-processings as mentioned before are needed to make the data psd.

Data embedding methods follow a general principle (Bunte, Biehl, & Hammer, 2012): for a given finite set of N data items some characteristics $\text{char}_{\mathbf{X}}$ are derived and the aim

is to match them as well as possible with corresponding characteristics $\text{char}_{\mathbf{Y}}$ in the low dimensional embedding space:

$$\text{tension}(\mathbf{X}, \mathbf{Y}) = \sum_{i=1}^{N} \mathfrak{m}(\text{char}_{\mathbf{X}}(\mathbf{X}, \mathbf{x}_i), \text{char}_{\mathbf{Y}}(\mathbf{Y}, \mathbf{y}_i)) \quad . \tag{11}$$

Here $\mathfrak{m}(\cdot)$ denotes a measure of mismatch between the characteristics, and the index i refers to the i^{th} data object $\mathbf{x}_i$ and its low-dimensional counterpart $\mathbf{y}_i$. The source matrix contains pairwise similarity information about the data items. Optimization of usually low-dimensional point coordinates $\{\mathbf{y}_i\}_{i=1}^{N}$ or of parameters θ of a functional point placement model $\mathbf{Y} = F_\theta(\mathbf{X})$ allows for minimization of the overall tension.

Using the above formalism with Multi-Dimensional-Scaling (MDS) (Kruskal, 1964) $\mathfrak{m} = \mathfrak{m}_{\text{MDS}}$ being the sum of squares and $\text{char}(\cdot, \cdot)$ picking pairwise distances $\mathbf{D}_{ij}$, classical MDS can be expressed as

$$\text{tension}_{\text{MDS}}(\mathbf{X}, \mathbf{Y}) = \sum_{i=1}^{N} \sum_{j=1}^{N} (\mathbf{D}_{ij}^{\mathbf{X}} - \mathbf{D}_{ij}^{\mathbf{Y}})^2 \quad . \tag{12}$$

In practice, eigen-decomposition is used for solving this classical scaling problem efficiently. However, a large variety of modification exists for modeling embedding stress in customized, e.g. scale sensitive, ways by iterative optimization of suitably designed tension functions $\mathfrak{m}$ (France & Carroll, 2011).

In a comparison of distance distributions of high-dimensional Euclidean data points and low-dimensional points it turns out that the former one is shifted to higher average distances with relatively low standard deviation. This phenomenon is referred to as concentration of the norm (Lee & Verleysen, 2007).

In order to embed such distances with their specific properties properly in a low-dimensional space, versions of stochastic neighbor embedding (SNE) (van der Maaten & Hinton, 2008) and the neighbor retrieval visualizer NeRV (Venna et al., 2010) apply different input and output distributions. Gaussian distributions $\mathbf{P}(\mathbf{X})$ are used in in the high-

dimensional input space and Student t-distributions $\mathbf{Q}(\mathbf{Y})$ in the low-dimensional output space aiming at minimizing the Kullback-Leibler divergence (KL) between them by adapting low-dimensional points $\mathbf{Y}$. Mismatch between per-object neighborhood probabilities is thus modeled by $\mathfrak{m}_{\text{t-SNE}} = \mathsf{KL}(\mathbf{P}||\mathbf{Q}(\mathbf{Y}))$:

$$\text{tension}_{\text{t-SNE}}(\mathbf{X}, \mathbf{Y}) = \sum_{i=1}^{N} \mathsf{KL}(\mathbf{P}_i(\mathbf{X})||\mathbf{Q}_i(\mathbf{Y})) \quad . \tag{13}$$

Neighborhoods are expressed in terms of σ_i-localized Gaussian transformations of squared Euclidean distances:

$$\mathbf{P}_{ij} = \frac{\exp(-||\mathbf{x}_i - \mathbf{x}_j||^2/2\sigma_i)}{\sum_{k \neq i} \exp(-||\mathbf{x}_i - \mathbf{x}_k||^2/2\sigma_i)} \quad . \tag{14}$$

The neighborhood probability is modeled indirectly by setting the bell shape width σ_i for each point to capture to which degree nearby points are considered as neighbors for a fixed radius of 'effective' neighbors. This number is referred to as perplexity parameter and is usually set to $5 \leq p \leq 50$. Naturally, variations in data densities lead to different σ_i and, consequently, to asymmetric matrices $\mathbf{P}$. Gaussian distributions could be used in the embedding space too, but in order to embed large input distances with relatively low variability in a low-dimensional space, the heavy-tailed Student t-distribution

$$\mathbf{Q}_{ij}(\mathbf{Y}) = \frac{(1 + ||\mathbf{y}_i - \mathbf{y}_j||^2)^{-1}}{\sum_{k \neq l}^{N} (1 + ||\mathbf{y}_k - \mathbf{y}_l||^2)^{-1}} \tag{15}$$

turned out to be a more suitable characteristics (van der Maaten & Hinton, 2008).

The priorly mentioned multidimensional scaling technique (MDS) takes a symmetric dissimilarity matrix $\mathbf{D}$ as input and calculates a $d-$ dimensional vector space representation such that for the $N \times N$ dissimilarities the new N points $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, with $X \in \mathbb{R}$ are close to those of the original dissimilarity measure using some stress function. In classical MDS (cMDS) this stress function is the Euclidean distance. During this procedure, details see (Kruskal, 1964), negative eigenvalues are clipped and a psd

kernel can be obtained as $\mathbf{S}^* = XX^\top$, where $X = U\Lambda^{\frac{1}{2}}$. The approach is exact if the input data can be embedded into a Euclidean space without any extra loss, which is not always possible (Wilson & Hancock, 2010).

Local embeddings: in (L. Chen & Lian, 2008) an unsupervised retrieval problem is considered where the used distance function is non-metric. A model is defined, such that the data can be divided into disjoint groups and the triangle inequality holds within each group by constant shifting[7]. Similar approaches where recently discussed in (Bustos & Skopal, 2011) and the same authors proposed a specific distance modification approach in (Skopal & Loko, 2008). Local concepts in the line of non-metric proximities where also recently analyzed for the visualization a non-metric proximity data by (Van Der Maaten & Hinton, 2012) where different (local) maps are defined to get different views on the data. Another interesting approach was proposed in (Goldfarb, 1984) where the non-metric proximities are mapped in a pseudo-Euclidean space.

Proximity feature space: finally also the so called similarity or dissimilarity space representation (Graepel et al., 1998; Pekalska & Duin, 2008a, 2005) has found wide usage. In (Graepel et al., 1998) a SVM in pseudo-Euclidean space is proposed and a generalized nearest mean classifier and Fisher linear discriminant classifier was proposed in (Pekalska & Duin, 2008a, 2005) also using the feature space representation.

Thereby the proximity matrix is considered to be a feature matrix with rows as the data points (cases) and columns as the features. Accordingly each point is represented in an N dimensional feature space where the features are the proximities of the considered point to all other points. This few on proximity learning is also conceptually related to a more advanced theory proposed in (Balcan et al., 2008).

The former mentioned approaches are either transforming the given proximities by a local strategy or completely change the data space representation as in the last case. The

[7] Unrelated to the eigenspectrum shift approach mentioned before.

approach by (Pekalska & Duin, 2005) is cheap but a feature selection problem is raised because in general it is not acceptable to use all N features to represent a point during training but also for out of sample extensions in the test phase (Pekalska et al., 2006). Further this type of representation radically changes the original data representation.

The embedding, suggested in (Goldfarb, 1984) is rather costly because it involves an eigenvalue decomposition (EVD) of the proximity matrix which can be done effectively only by using some novel strategies for *low rank* approximations which also provide an out of sample approach (Schleif & Gisbrecht, 2013).

In (Balcan et al., 2008) a theoretical analysis for using similarities as features was provided with similar findings for dissimilarities in (Wang et al., 2009). The authors in (Balcan et al., 2008) provide criteria for a good similarity function to be used in a discrimination function. Roughly they call a similarity as good if the expected intra-class similarity is sufficiently large compared to the expected interclass similarity (more specific in Theorem 4 of (Balcan et al., 2008)). Given N training points and a good similarity function, there exists a linear separator on the similarities as features that has a specifiable maximum error at a margin that depends on N (Balcan et al., 2008).

Wang et al. (2007) show that under slightly less restrictive assumptions on the similarity function there exists with high probability a convex combination of simple classifiers on the similarities as features which has a maximum specifiable error.

Complexity: the classical MDS has a complexity of $O(N^3)$ but using Landmark MDS (de Silva & Tenenbaum, 2002; J. Platt, 2005) (L-MDS) the complexity can be reduced to $O(Nm^2)$ with m as the number of landmarks. L-MDS is however double centering the input data on the small landmark matrix only and applies a clipping of the eigenvalues obtained on the $m \times m$ similarity matrix. It has therefore two sources of inaccuracy, namely in the double centering and the eigenvalue estimation step (the eigenfunction of $\mathbf{S}$ are only estimated on the $m \times m$ Landmark matrix $\mathbf{D}_{m \times m}$). Further the clipping may remove relevant information as pointed out before. In (Gisbrecht & Schleif, 2014)

a generalization of L-MDS was proposed which is more accurate and flexible in these two points.

The before mentioned local approaches can not directly be used in e.g. a classification or standard clustering context but are method specific for a retrieval or inspection task. The proximity feature space approaches has basically no extra costs (given the proximity matrix is fully available) but defines a finite dimensional space of size d with d determined by the number of (in this context) called prototypes or reference points. So often d is simple chosen as $d = N$ which can lead to a high dimensional vectorial data representation and costly distance calculations.

Out of sample extension to new test points: To obtain the corrected similarities for MDS one can calculate $\mathbf{s}_t^* = \mathbf{s}_t U \Lambda^{\frac{-1}{2}} \Lambda^{\frac{1}{2}} U^\top = \mathbf{s}_t U U^\top$. If this operation is to costly also approximative approaches as suggested in (Gisbrecht, Lueks, et al., 2012; Gisbrecht et al., 2015; Vladymyrov & Carreira-Perpiñán, 2013) can be used. The local embedding approaches typically generate a model which has to be regenerated from scratch to be completely valid or specific insertion concepts can be used as shown in (Skopal & Loko, 2008). The proximity space representation is directly extended to new samples by providing the proximity scores to the corresponding prototypes, which however can be costly for a large number of prototypes.

6 Natural Non-metric learning approaches

An alternative to correct the non-psd matrix is to use the additional information in the negative eigenspectrum in the optimization framework. This is in agreement with research done by (Pekalska et al., 2004). The most simple strategy is to use a nearest neighbor classifier (NNC) as discussed in (R. P. W. Duin et al., 2014). The NNC is optimal if $N \to \infty$ but is also very costly because for a new item all potential neighbors have to be evaluated in the worst case. The organization into a tree structure can resolve

this issue for the average case using e.g. the NM-Tree as proposed in (Skopal & Loko, 2008) but is complicated to maintain for life long learning and suffers from the shortcomings of NN for a final N.

There are models that functionally resemble kernel machines, such as SVM, but do not require Mercer kernels for their model formulation and fitting, e.g. the Relevance Vector Machine (RVM) (M. Tipping, 2001a), Radial-Basis-Function networks (RBF) (Buhmann, 2003) (with kernels positioned on top of each training point) or the Probabilistic Classification Vector Machine (PCVM) (H. Chen et al., 2009a). In such approaches kernels expressing "similarity" between data pairs are treated as non-linear basis functions $\phi_i(x) = K(\cdot, x_i)$ transforming input x into its non-linear image $\phi(x) = (\phi_1(x), ..., \phi_N(x))^\top$, making the out-of-sample extension straightforward, while not requiring any additional conditions on K. The main part of the models is formed by the projection of the data image $\phi(x)$ onto the parameter weight vector $\mathbf{w}$: $\mathbf{w}^\top\phi(x)$. Subsequently we detail some of these methods.

6.1 Approaches using the Indefinite krein or pseudo Euclidean space (B2)

Some approaches are formulated using the Krein space and avoid costly transformations of the given indefinite similarity matrices. Pioneering work about learning with indefinite or non-positive kernels can be found in (Ong et al., 2004; Haasdonk, 2005). In (Ong et al., 2004) the authors noticed that if the kernels are indefinite one can not any longer minimize the loss of standard kernel algorithms but instead stabilize the loss in average. In (Ong et al., 2004) it is shown that for every kernel there is an associated Krein space, and for every reproducing kernel krein space (RKKS) (Alpay, 1991), there is a unique kernel. In the same work a list of indefinite kernels like the linear combination of Gaussians with negative combination coefficients is provided and initial work for learning algorithms in RKKS combined by Rademacher Bounds was proposed. In

(Haasdonk, 2005) a geometric interpretation of SVMs with indefinite kernel functions is provided. It was shown that indefinite SVMs are optimal hyperplane classifiers not by margin maximization, but by minimization of distances between convex hulls in pseudo-Euclidean spaces. The approach is solely defined on distances and convex hulls which can be fully defined in the pseudo-Euclidean space. This approach is very appealing as it shows that SVMs can be learned for indefinite kernels although not as a convex problem. However it is also mentioned that the approach is inappropriate for proximity data with a large number of negative eigenvalues. Based on the priorly address theory multiple kernel approaches have been extended to be applicable for indefinite kernels.

Indefinite fisher and kernel quadratic discriminant: in (Haasdonk & Pkalska, 2008; Pekalska & Haasdonk, 2009) indefinite kernel fisher discriminant analysis (iKFDA) and indefinite kernel quadratic discriminant analysis (iKQDA) was proposed focusing on classification problems, recently extended by a weighting scheme in (J. Yang & Fan, 2013).

The initial idea is to embed the training data into a Krein space and apply a modified kernel fisher discriminant analysis (KFDA) or kernel quadratic discriminant analysis (KQDA) for indefinite kernels.

Given the indefinite kernel matrix K and the embedded data in a pseudo-Euclidean space (pE), the linear Fisher Discriminant function $f(x) = \langle w, \Phi(x) \rangle_{pE} + b$ is based on a weight vector $\mathbf{w}$ such that the between-class scatter is maximized while the within-class scatter is minimized along w. This direction is obtained by maximizing the Fisher criterion:

$$J(\mathbf{w}) \frac{\langle \mathbf{w}, \Sigma_b \mathbf{w} \rangle}{\langle \mathbf{w}, \Sigma_w \mathbf{w} \rangle}_{pE}$$

where Σ_b is the between and Σ_w the within scatter matrix. In (Haasdonk & Pkalska, 2008) it is shown that the Fisher Discriminant in the pE space $\in \mathbb{R}^{(p,q,z)}$ is identical to the Fisher Discriminant in the associated Euclidean space $\mathbb{R}^{p+q+z}$. To avoid the explicit embedding into the pE space a kernelization is considered such that the weight

vector $w \in \mathbb{R}^{p,q,z}$ is expressed as a linear combination of the training data $\phi(x_i)$, which transferred to the Fisher criterion allows to use the kernel trick. A similar strategy can be used for KQDA. Different variations of these algorithms are discussed and also the indefinite kernel PCA is briefly addressed.

In (Zafeiriou, 2012; Liwicki et al., 2012) an indefinite kernel PCA was proposed and integrated in the Fisher discriminant framework to get a low-dimensional feature extraction for indefinite kernels. The basic idea is to define an optimization problem similar to the psd kernel PCA but using the squared indefinite kernel which has no effect on the eigenvectors but only on the eigenvalues. In the corresponding derivation of the principal components the eigenvalues are only considered as $|\Lambda|$ such that those principal components are found corresponding to the largest *absolute* eigenvalues. Later on this approach was applied in the context of slow-feature analysis for indefinite kernels (Liwicki et al., 2013). A *multiple* indefinite kernel learning approach was recently proposed in (Kowalski et al., 2009) another recent work about indefinite kernel machines was proposed in (Xue & Chen, 2014). Recently also the kernelized version of localized sensitive hashing was extended to indefinite kernels (Mu & Yan, 2010) by combining kernelized hash functions on the associated Hilbert spaces of the decomposed pseudo Euclidean space.

Complexity: all these methods have a runtime complexity of $\mathbb{O}(N^2) - \mathbb{O}(N^3)$ and do not directly scale to large data sets. The test phase complexity is linear in the number of used points to represent $\mathbf{w}$. Accordingly sparsity concepts as suggested in (M. E. Tipping, 2000) can be employed to further reduce the complexity for test cases.

Out of sample extension to new test points: the models of iKFD, iKPCA and iKQDA allow a direct and easy out of sample extension by calculating the (indefinite) similarities of a new test point to the corresponding training points used in the linear combination of $\mathbf{w} = \sum_i^N \alpha_i \phi(x_i)$.

6.2 Learning of decision functions using indefinite proximities (B1)

In (Balcan et al., 2008) a theory for learning with similarity function was proposed with extensions for dissimilarity data in (Wang et al., 2009). The authors in (Balcan et al., 2008) discussed necessary properties of proximity functions to ensure good generalization capabilities for learning tasks. This theory motivates generic learning approaches purely based on in general symmetric, potentially non-metric proximity functions minimizing the hinge loss, relative to the margin. They show that such a similarity function can be used in a two-stage algorithm. First the data are represented by creating a *empirical similarity map* by selecting a subset of data points as landmarks and then representing each data point using the similarities to those landmarks. Subsequently standard methods can be employed to find a large-margin linear separator in this new space. Indeed in recent years multiple approaches have been proposed which could be covered by these theoretical frameworks although most often not explicitly considered in this way.

Probabilistic classification vector machine: in (H. Chen et al., 2009a) and (H. Chen et al., 2014) the authors propose the *Probabilistic Classification Vector Machine* (PCVM) which can deal also with asymmetric indefinite proximity matrices[8]. Within a Bayesian approach a linear classifier function is learned such that each point can be represented by a sparse weighted linear combination of the original similarities. Similar former approaches like the Relevance Vector Machine (RVM) (M. Tipping, 2001b) were found to be unstable without early stopping during learning. In order to tackle this problem, a signed and truncated Gaussian prior is adopted over every weight in PCVMs, where the sign of prior is determined by the class label, i.e. $+1$ or -1. The truncated Gaussian prior not only restricts the sign of weights but also leads to a sparse estimation of weight vectors, and thus controls the complexity of the model. Thereby the empirical feature map is automatically generated by a sparse adaptation scheme using the EM algorithm.

[8] In general the input is a symmetric kernel matrix, but the method is not restricted in this way.

As other kernel methods PCVM uses a kernel regression model $\sum_{i=1}^{N} w_i \phi_{i,\theta}(\mathbf{x}) + b$ to which a link function is applied, with w_i being the weights of the basis functions $\phi_{i,\theta}(\mathbf{x})$ and b as a bias term. The basis functions will correspond to kernels evaluated at data items. Consider binary classification and a data set of input-target training pairs $D = \{\mathbf{x}_i, y_i\}_{i=1}^{N}$, where $y_i \in \{-1, +1\}$. The implementation of PCVM (H. Chen et al., 2014) uses the probit link function, i.e.

$$\Psi(x) = \int_{-\infty}^{x} \mathcal{N}(t|0,1)dt,$$

where $\Psi(x)$ is the cumulative distribution of the normal distribution $\mathcal{N}(0,1)$. Parameters are optimized by an Expectation Maximization (EM) scheme.

After incorporating the probit link function, the PCVM model becomes:

$$l(\mathbf{x}; \mathbf{w}, b) = \Psi\left(\sum_{i=1}^{N} w_i \phi_{i,\theta}(\mathbf{x}) + b\right) = \Psi\left(\Phi_\theta(\mathbf{x})\mathbf{w} + b\right) \tag{16}$$

Where $\Phi_\theta(\mathbf{x})$ is a vector of basis function evaluations for data item $\mathbf{x}$.

In the PCVM formulation (H. Chen et al., 2009b), a truncated Gaussian prior N_t with mode at 0 is introduced for each weight w_i. Its support is restricted to $[0, \infty)$ for entries of the positive class and $(-\infty, 0]$ for entries of the negative class as shown in Eq. (17). A zero-mean Gaussian prior is adopted for the bias b. The priors are assumed to be mutually independent.

$$\begin{aligned} p(\mathbf{w}|\alpha) &= \prod_{i=1}^{N} p(w_i|\alpha_i) = \prod_{i=1}^{N} N_t(w_i|0, \alpha_i^{-1}), \\ p(b|\beta) &= \mathcal{N}(b|0, \beta^{-1}), \end{aligned}$$

where α_i and β are inverse variances:

$$\begin{aligned} p(w_i|\alpha_i) &= \begin{cases} 2\mathcal{N}(w_i|0,\alpha_i^{-1}) & \text{if } y_i w_i > 0 \\ 0 & \text{otherwise} \end{cases} \\ &= 2\mathcal{N}(w_i|0,\alpha_i^{-1}) \cdot \delta(y_i w_i). \end{aligned} \tag{17}$$

where $\delta(\cdot)$ is the indicator function $\mathbf{1}_{x>0}(x)$.

We follow the standard probabilistic formulation and assume that $z_\theta(\mathbf{x}) = \Phi_\theta(\mathbf{x})\mathbf{w}+b$ is corrupted by an additive random noise ϵ , where $\epsilon \sim \mathcal{N}(0,1)$. According to the probit link model, if $h_\theta(\mathbf{x}) = \Phi_\theta(\mathbf{x})\mathbf{w}+b+\epsilon \geq 0, y = 1$ and if $h_\theta(\mathbf{x}) = \Phi_\theta(\mathbf{x})\mathbf{w}+b+\epsilon < 0, y = -1$. We obtain:

$$p(y = 1|\mathbf{x},\mathbf{w},b) = p(\Phi_\theta(\mathbf{x})\mathbf{w} + b + \epsilon \geq 0) = \Psi(\Phi_\theta(\mathbf{x})\mathbf{w} + b). \tag{18}$$

$h_\theta(\mathbf{x})$ is a latent variable because ϵ is an unobservable variable. We collect evaluations of $h_\theta(\mathbf{x})$ at training points in a vector $\mathbf{H}_\theta(\mathbf{x}) = (h_\theta(\mathbf{x_1}),\ldots,h_\theta(\mathbf{x_N}))^\top$. In the expectation step the expected value $\bar{\mathbf{H}}_\theta$ of $\mathbf{H}_\theta$ with respect to the posterior distribution over the latent variables is calculated (given old values $\mathbf{w}^{\text{old}}, b^{\text{old}}$). In the maximization step the parameters are updated through

$$\mathbf{w}^{\text{new}} = M(M\Phi_\theta^\top(\mathbf{x})\Phi_\theta(\mathbf{x})M + I_N)^{-1} \tag{19}$$

$$M(\Phi_\theta^\top(\mathbf{x})\bar{\mathbf{H}}_\theta - b\Phi_\theta^\top(\mathbf{x})\mathbf{I}) \tag{20}$$

$$\mathbf{b}^{\text{new}} = t(1 + tNt)^{-1}t(\mathbf{I}^\top\bar{\mathbf{H}}_\theta - \mathbf{I}^\top\Phi_\theta(\mathbf{x})\mathbf{w}) \tag{21}$$

where I_N is a N-dimensional identity matrix and $\mathbf{I}$ a all-ones vector, the diagonal ele-

ments in the diagonal matrix M are:

$$m_i = (\bar{\alpha}_i)^{-1/2} = \begin{cases} \sqrt{2}w_i & \text{if} \quad y_i w_i \geq 0 \\ 0 & \text{else} \end{cases} \tag{22}$$

and the scalar $t = \sqrt{2}|b|$. For further details see (H. Chen et al., 2009b).

Supervised Learning with Similarity Functions: the theoretical foundations for classifier construction based on generic (ϵ_0, B)-good similarity functions was proposed in (Balcan et al., 2008). The theory in this paper suggests a constructive approach to derive a classifier. After a mapping, like the one described already before, the similarity functions are normalized and this representation is used in a linear SVM to find a large margin classifier.

Another approach directly relating to the work of (Balcan et al., 2008) was proposed by (Kar & Jain, 2012) and showed a practical realization of the ideas outlined in (Balcan et al., 2008) and how to generate a classifier function based on symmetric (non-)psd similarity functions. The procedure takes label vectors $y \in \{-1, 1\}$, with $Y = \{y_1, \ldots, y_N\}$ a (ϵ_0, B)-good similarity function K see (Balcan et al., 2008), and a loss function $l_S : \mathbb{R} \times Y \rightarrow \mathbb{R}^+$ as input, providing a classifier function $f : \mathbf{x} \mapsto \langle \mathbf{w}, \Psi(\mathbf{x}) \rangle$. First a d-dimensional landmarks set (columns) $\mathcal{L} = \{\mathbf{x}_1 \rightarrow \mathbf{x}_d\}$ is selected from the similarity map K and a mapping function $\Psi_{\mathcal{L}}\mathbf{x} \mapsto \frac{1}{\sqrt{d}}(K(\mathbf{x}, \mathbf{x}_1), \ldots, K(\mathbf{x}, \mathbf{x}_d)) \in \mathbb{R}^d$ is defined. Subsequently a weight-vector $\mathbf{w}$ is optimized such that the following minimization problem is solved:

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w} \in \mathbb{R}^d : \|\mathbf{w}\|_2 \leq B} \sum_{i=1}^{N} l_S(\langle \mathbf{w}, \Psi(\mathbf{x}) \rangle, y_i)$$

Reasonable loss functions for classification and regression problems are provided in (Kar & Jain, 2012). In contrast to the work given in (H. Chen et al., 2009a), the identification of the empirical feature-map or landmark selection is just realized by a random

selection procedure instead of a systematic approach. A major limitation is the random selection of the landmarks which leads to large standard-deviation in the obtained models. Although the used theory guarantees to get a large margin classifier from a good similarity measure the random procedure used in (Kar & Jain, 2012) may not necessarily find such a model. In general the solution gets better for larger landmarks sets but due to the used $l-2$ norm in the optimization $\mathbf{w}$ is in general not sparse, such that a complex model is obtained and the out of sample extension becomes costly.

In (Wang et al., 2009) a similar approach was proposed for dissimilarity functions whereby the landmarks set is optimized by a boosting procedure.

Some other related approaches are given by so called median algorithms. Thereby the model parameters are specific data points of the original training, identified during the optimization and considered as cluster centers or prototypes, which can be used to assign new points. One may consider this also as a sparse version of 1-nearest neighbor and it can also be related to the nearest mean classifier for dissimilarities proposed in (Wilson & Hancock, 2010). An example for such median approaches can e.g. be found in (Nebel et al., 2014) and (Hammer & Hasenfuss, 2010). Approaches in the same line but with a weighted linear combination where proposed in (D. Hofmann et al., 2014; Hammer et al., 2014; Gisbrecht, Mokbel, et al., 2012) for dissimilarity data. Similar as discussed in (Haasdonk, 2005) these approaches may converge only to a saddle point for indefinite proximities.

Complexity: algorithms which derive decision functions in the former way are in general very costly involving $O(N^2)$ to $O(N^3)$ operations or make use of random selection strategies which can lead to models of very different generalization accuracy if the selection procedure is included in the evaluation. The approaches directly following (Balcan et al., 2008) are however very efficient if the similarity measure already separates the classes very well, regardless of the specific landmark set.

Table 4: Overview of the complexity (worst case) and application aspects of the former methods. Most often the approaches are in average less complicated. For MDS like approaches the complexity depends very much on the used method and whether the data are given as vectors or as proximities. The proximity space approach may generate further costs if e.g. a classification model has to be calculated for the representation. Proxy matrix approaches are very costly due to the raised optimization problem and the classical solver used. Some proxy approaches solve a similar complex optimization problem also for out of sample extensions. For low rank proximity matrices the above mentioned costs can often be reduced by a magnitude or more - see section 7.

Method	**memory complexity**	**runtime complexity**	**out of sample**
Eigenvalue correction (A1)	$O(N^2)$	$O(N^3)$	$O(N)$
Proxy matrix (A3)	$O(N^2)$	$O(N^3)$	$O(N) - O(N^3)$
Proximity space (A2)	$O(N)$	$O(C)$	$O(N)$
Embeddings (like MDS) (A2)	$O(N) - O(N^2)$	$O(N^2) - O(N^3)$	$O(N) - O(N^2)$
iKFD (B2)	$O(N)$	$O(N^3)$	$O(N)$
PCVM (B1)	$O(m)$ (sparse, $m \ll N$)	$O(N^3)$ (fst steps)	$O(m)$
(linear) similarity function (B1)	$O(m)$ (sparse, $m \ll N$)	$O(N^2)$ - $O(N^3)$	$O(m)$

Out of sample extension to new test points: for PCVM and the median approaches the weight vector $\mathbf{w}$ is in general very sparse such that out of sample extensions are easily calculated by just finding the few similarities $\{K(\mathbf{x}, \mathbf{w}_1), \ldots, K(\mathbf{x}, \mathbf{w}_d)\}$. As all approaches in the former section can naturally deal with non-metric data additional modifications of the similarities are avoided and the out of sample extension is consistent.

7 Scaling up approaches of proximity learning for larger datasets

A major issue with the application of the aforementioned approaches is the scalability to large N. While we already provided a brief complexity analysis for each major branch

recent research has focused on improving the scalability of the approaches to reduce memory or runtime costs, or both. Subsequently we briefly sketch some of the more recent approaches which are used in this context and have been already proposed in the line of non-metric proximity learning or can be easily transferred.

7.1 Nyström approximation

The Nyström approximation technique has been proposed in the context of kernel methods in (Williams & Seeger, 2000). Here, we give a short review of this technique before it is employed in PCVM. One well known way to approximate a $N \times N$ Gram matrix, is to use a low-rank approximation. This can be done by computing the eigendecomposition of the kernel matrix $K = U\Lambda U^T$, where U is a matrix, whose columns are orthonormal eigenvectors, and Λ is a diagonal matrix consisting of eigenvalues $\Lambda_{11} \geq \Lambda_{22} \geq ... \geq 0$, and keeping only the m eigenspaces which correspond to the m largest eigenvalues of the matrix. The approximation is $\tilde{K} \approx U_{N,m}\Lambda_{m,m}U_{m,N}$, where the indices refer to the size of the corresponding submatrix restricted to the larges m eigenvalues. The Nyström method approximates a kernel in a similar way, without computing the eigendecomposition of the whole matrix, which is an $O(N^3)$ operation.

By the Mercer theorem kernels $k(\mathbf{x}, \mathbf{y})$ can be expanded by orthonormal eigenfunctions φ_i and non negative eigenvalues λ_i in the form

$$k(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{\infty} \lambda_i \varphi_i(\mathbf{x}) \varphi_i(\mathbf{y}).$$

The eigenfunctions and eigenvalues of a kernel are defined as the solution of the integral equation

$$\int k(\mathbf{y}, \mathbf{x}) \varphi_i(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} = \lambda_i \varphi_i(\mathbf{y}),$$

where $p(\mathbf{x})$ is the probability density of $\mathbf{x}$. This integral can be approximated based on

the Nyström technique by an i.i.d. sample $\{\mathbf{x}^k\}_{k=1}^m$ from $p(\mathbf{x})$:

$$\frac{1}{m}\sum_{k=1}^{m} k(\mathbf{y},\mathbf{x}^k)\varphi_i(\mathbf{x}^k) \approx \lambda_i\varphi_i(\mathbf{y}).$$

Using this approximation we denote with $K^{(m)}$ the corresponding $m\times m$ Gram sub-matrix and get the corresponding matrix eigenproblem equation as:

$$K^{(m)}U^{(m)} = U^{(m)}\Lambda^{(m)}$$

with $U^{(m)} \in \mathbb{R}^{m\times m}$ is column orthonormal and $\Lambda^{(m)}$ is a diagonal matrix.

Now we can derive the approximations for the eigenfunctions and eigenvalues of the kernel k

$$\lambda_i \approx \frac{\lambda_i^{(m)}\cdot N}{m}, \quad \varphi_i(\mathbf{y}) \approx \frac{\sqrt{m/N}}{\lambda_i^{(m)}}\mathbf{k}_y^\top \mathbf{u}_i^{(m)}, \tag{23}$$

where $\mathbf{u}_i^{(m)}$ is the ith column of $U^{(m)}$. Thus, we can approximate φ_i at an arbitrary point $\mathbf{y}$ as long as we know the vector $\mathbf{k}_y = (k(\mathbf{x}^1,\mathbf{y}),...,k(\mathbf{x}^m,\mathbf{y}))$. For a given $N\times N$ Gram matrix K we randomly choose m rows and respective columns. The corresponding indices are called landmarks, and should be chosen such that the, data distribution is sufficiently covered. A specific analysis about selection strategies was recently given in (K. Zhang et al., 2008). We denote these rows by $K_{m,N}$. Using the formulas (23) we obtain $\tilde{K} = \sum_{i=1}^m 1/\lambda_i^{(m)}\cdot K_{m,N}^T(\mathbf{u}_i^{(m)})^T(\mathbf{u}_i^{(m)})K_{m,N}$, where $\lambda_i^{(m)}$ and $\mathbf{u}_i^{(m)}$ correspond to the $m\times m$ eigenproblem. Thus we get, $K_{m,m}^{-1}$ denoting the Moore-Penrose pseudoinverse,

$$\tilde{K} = K_{N,m}K_{m,m}^{-1}K_{m,N}. \tag{24}$$

as an approximation of K. This approximation is exact, if $K_{m,m}$ has the same rank as K.

7.2 Linear time eigenvalue decomposition using the Nyström approximation

For a matrix approximated by Eq. (24) it is possible to compute its exact eigenvalue decomposition in linear time. To compute the eigenvectors and eigenvalues of an *indefinite* matrix we first compute its squared form, since the eigenvectors in the squared matrix stay the same and only the eigenvalues are squared. Let K be a psd similarity matrix, for which we can write its decomposition as

$$\begin{aligned}\tilde{K} &= K_{N,m}K_{m,m}^{-1}K_{m,N} \\ &= K_{N,m}U\Lambda^{-1}U^{\top}K_{N,m}^{\top} \\ &= BB^{\top},\end{aligned}$$

where we defined $B = K_{N,m}U\Lambda^{-1/2}$ with U and Λ being the eigenvectors and eigenvalues of $K_{m,m}$, respectively. Further it follows for the *squared* $\tilde{K}$

$$\begin{aligned}\tilde{K}^2 &= BB^{\top}BB^{\top} \\ &= BVAV^{\top}B^{\top},\end{aligned}$$

where V and A are the eigenvectors and eigenvalues of $B^{\top}B$, respectively. The corresponding eigenequation can be written as $B^{\top}Bv = av$. Multiplying it with B from left we get the eigenequation for $\tilde{K}$

$$\underbrace{BB^{\top}}_{\tilde{K}}\underbrace{(Bv)}_{u} = a\underbrace{(Bv)}_{u}$$

It is clear that A must be the matrix with the eigenvalues of $\tilde{K}$. The matrix Bv is the matrix of the corresponding eigenvectors, which are orthogonal but not necessary or-

thonormal. The normalization can be computed from the decomposition:

$$\begin{aligned}\tilde{K} &= BVV^\top B^\top \\ &= BVA^{-1/2}AA^{-1/2}V^\top B^\top \\ &= CAC^\top,\end{aligned}$$

where we defined $C = BVA^{-1/2}$ as the matrix of orthonormal eigenvectors of K. The eigenvalues of $\hat{K}$ can be obtained using $A = C^\top \hat{K} C$. The above mentioned strategies can now be used in a variety of the above discussed algorithm to safe computation and memory costs, given the matrix is low rank. An example is the Nyström approximated PCVM as proposed in (Schleif, 2015), which makes use of the above concept in a non-trivial way. As shown in (Schleif, 2015) these concept can also be used to approximate a singular value decomposition (SVD) for large (indefinite) matrices or other algorithms which can be based on eigenvalue decompositions.

7.3 Approximation concepts for low dimensional embeddings

Recently various strategies have been proposed to reduce the in general $\mathcal{O}(N^3)$ run-time complexity of various embedding approaches. Two general ideas have been suggested. One is based on the Barnes-Hut concepts, widely known in the analysis of astro-physical data (Barnes & Hut, 1986) and the second one is based on a representer concept where latent projection of each point are constrained to be a local linear function of latent projections. of some landmarks(Vladymyrov & Carreira-Perpiñán, 2013). Both approaches assume that mapped data have an intrinsic group structure in the input and the output space which can be effectively employed to reduce computation costs. As a consequence they are in general only efficient if the target embeddings are really in a low-dimensional space, such that an efficient data structure for low dimensions can be employed.

In (Z. Yang et al., 2013) a Barnes-Hut approach was proposed as a general frame-

work for a multitude of embedding approaches. A specific strategy for t-SNE was recently presented in (van der Maaten, 2013). Here we briefly summarize the main ideas suggested in (Z. Yang et al., 2013), we refer to the corresponding journal papers for more details.

The computational complexity in neighbor embeddings (NE) is essentially due to the coordinates and pairwise distances in the output space, which change at every step of optimization. The idea is to summarize pairwise interaction costs, which are calculated for each data point i with respect to its neighbors by grouping. The terms in the respective sum of the NE cost function are partitioned into several groups G_t^i and each group will be approximated as an interaction with a representative point of the group. The authors in (Z. Yang et al., 2013) consider the following typical summation used in NE objectives:

$$\sum_j f\left(||y_i - y_j||^2\right) = \sum_t \sum_{j \in G_t^i} f\left(||y_i - y_j||^2\right) \tag{25}$$

$$\approx \sum_t |G_t^i| f\left(||y_i - \hat{y}_t||^2\right), \tag{26}$$

where i is the starting data point, j are its neighbors, G_t^i are groups (subsets) of the neighbors j, $|G_t^i|$ is the size of the group, and $\hat{y}_t^i$ is the representative, e.g. mean, of the points in group G_t^i. Similarly, we can approximate the gradient of the above sum. Denote $g_{ij} = f'\left(||y_i - y_j||^2\right)$. We have

$$\sum_j g_{ij}\left(y_i - y_j\right) = \sum_t \sum_{j \in G_t^i} g_{ij}\left(y_i - y_j\right) \approx \sum_t |G_t^i| f'\left(||y_i - \hat{y}_t^i||^2\right)\left(y_i - \hat{y}_t^i\right). \tag{27}$$

The approximation within each group G_t^i is accurate when all points in the group are far enough from y_i. Otherwise the group is divided into subgroups and the approximation principle is used recursively to each subgroup, until the group contains a single point j. There one directly calculates $f\left(||y_i - y_j||^2\right)$ or g_{ij}. This grouping hierarchy forms a tree-like structure. In general a quadtree is used for embedding into $2d$ or a octree for three

dimensional embeddings. First the root node is assigned to the smallest bounding box that contains all data points, and a representative which is the mean of all points. If the bounding box contains more than one data point, it is divided into four smaller boxes of equal size, and a child node is constructed at each smaller bounding box if it contains at least one data point. The splitting is done recursively until all leaf nodes contain exactly one data point. The tree (re-)construction costs are neglectable compared with the standard embedding approaches. During the optimization of the point embedding in 2 or 3 dimensions the tree is reconstructed and employed to identify compact point groups in the embedding which can be summarized also in the summations of the NE cost function.

In (Gisbrecht & Schleif, 2014; Schleif & Gisbrecht, 2013) a generalization of Landmark-MDS is proposed which is also very efficient for non-metric proximity data. Using the same concepts it is also possible to obtain linear runtime complexity of Laplacian Eigenmaps for (corrected) non-metric input matrices.

7.4 Random projection and sparse models

The proximity (dis-similarity) space - discussed in sub section 5.5 makes use of all N similarities for a point i. To reduce the computational costs for generating a model this N dimensional space can be reduced in various ways. Various heuristics and multi-objective criteria have been employ to select an appropriate set of similarities, which are also sometimes called prototypes (Pekalska et al., 2006).

Random projection is another effective way and widely studied in recent publications also in the context of classification see e.g. (Durrant & Kaban, 2013, 2010; Mylavarapu & Kaban, 2013). It is based on the Johnson-Lindenstrauss lemma which states that a (random) mapping of N points from a high-dimensional (D) to a $O(\frac{1}{\epsilon^2}\log N)$ low-dimensional feature space distorts the length of the vector by at most $1 \pm \epsilon$. More recent work can be found in (Kane & Nelson, 2014). Another option is to derive the de-

cision function directly only on a subset of the proximities where theoretically work discussing this option is available in (Balcan et al., 2008; Wang et al., 2009; Guo & Ying, 2014).

8 Experiments

In Table 6 we compared multiple of the priorly discussed methods on various non-psd datasets with different attributes. As a baseline we use the k-Nearest-Neighbor (kNN) algorithm with k as the number of considered neighbors, optimized on an independent hold out meta-parameter tuning set. We modified k in the range $[1 \ldots, 10]$. It should be noted that kNN is known to be very efficient in general but requests the storage of the full training set and is hence very unattractive in the test phase due to high memory load and computation costs. In case of proximity data a new test sample has to compared to all training points to get mapped in the kNN model. We also compare to a SVM with different eigenvalue corrections, the SVM-Proxy approach as proposed by (J. Chen & Ye, 2008) and two native methods namely the formerly discussed iKFD and PCVM approach.

8.1 Dataset

We consider datasets as already used in (Y. Chen, Garcia, et al., 2009a; R. P. Duin, 2012) and additional larger scale problems. All data are used as similarity matrices (dissimilarities have been converted to similarities by Double-Centering in advance) and shown in Figure 9 and Figure 12. The datasets are from very different practical domains such as sequence alignments, image processing or audio data analysis.

Aural Sonar: the *Aural Sonar* data set is taken from (Philips et al., 2006), investigating the human ability to distinguish different types of sonar signals by ear. The signals were returns from a broadband active sonar system, with 50 target-of-interest signals

and 50 clutter signals. Every pair of signals was assigned a similarity score from 1 to 5 by two randomly chosen human subjects unaware of the true labels, and these scores were added to produce a 100×100 similarity matrix with integer values from 2 to 10 (Y. Chen, Garcia, et al., 2009a) with a signature of $(62, 38, 0)$

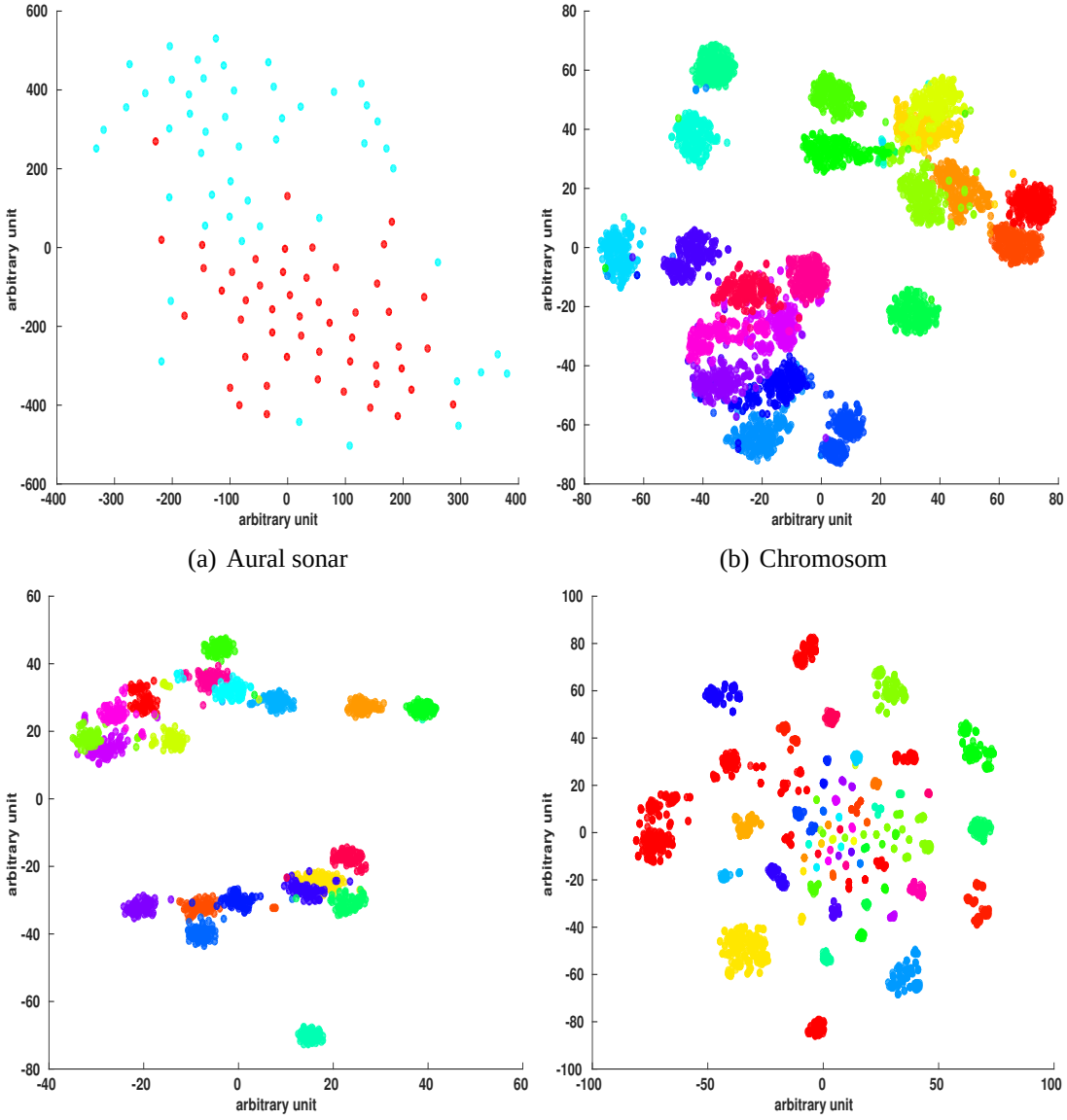
Chromosom: the *Copenhagen Chromosomes* data constitute a benchmark from cytogenetics. 4,200 human chromosomes from 21 classes are represented by grey-valued images. These are transferred to strings measuring the thickness of their silhouettes. An example pattern representing a chromosome has the form

$$11332444222333323322223332233233322226662223311 11 .$$

The string indicates the thickness of the gray levels of the image. These strings can be directly compared using the edit distance based on the differences of the numbers and insertion/deletion costs 4.5 (Neuhaus & Bunke, 2006). The obtained proximity matrix has a signature of $(2258, 1899, 43)$. The classification problem is to label the data according to the chromosome type.

Delft: the Delft gestures (DS5, 1500 points, 20 classes, balanced, signature: $(963, 536, 1)$) taken from (R. P. Duin, 2012) is a set of dissimilarities generated from a sign-language interpretation problem. It consists of 1500 points with 20 classes and 75 points per class. The gestures are measured by two video cameras observing the positions of the two hands in 75 repetitions of creating 20 different signs. The dissimilarities are computed using a dynamic time warping procedure on the sequence of positions (Lichtenauer et al., 2008).

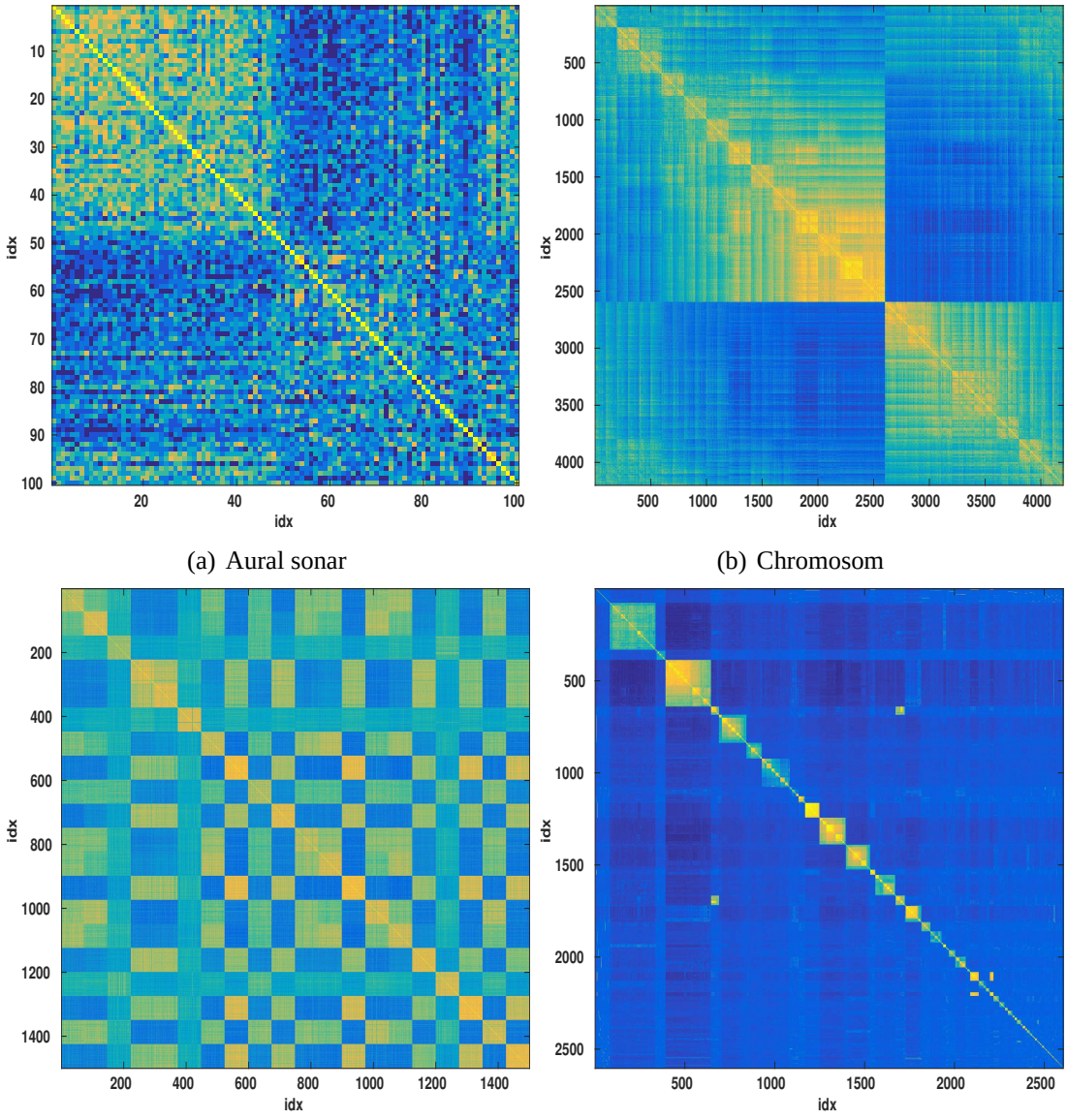
Face Rec: the Face Rec data set consists of 945 sample faces of 139 people from the NIST Face Recognition Grand Challenge data set. There are 139 classes, one for each person. Similarities for pairs of the original three-dimensional face data were computed



(a) Aural sonar (b) Chromosom

(c) Delft (d) Prodom

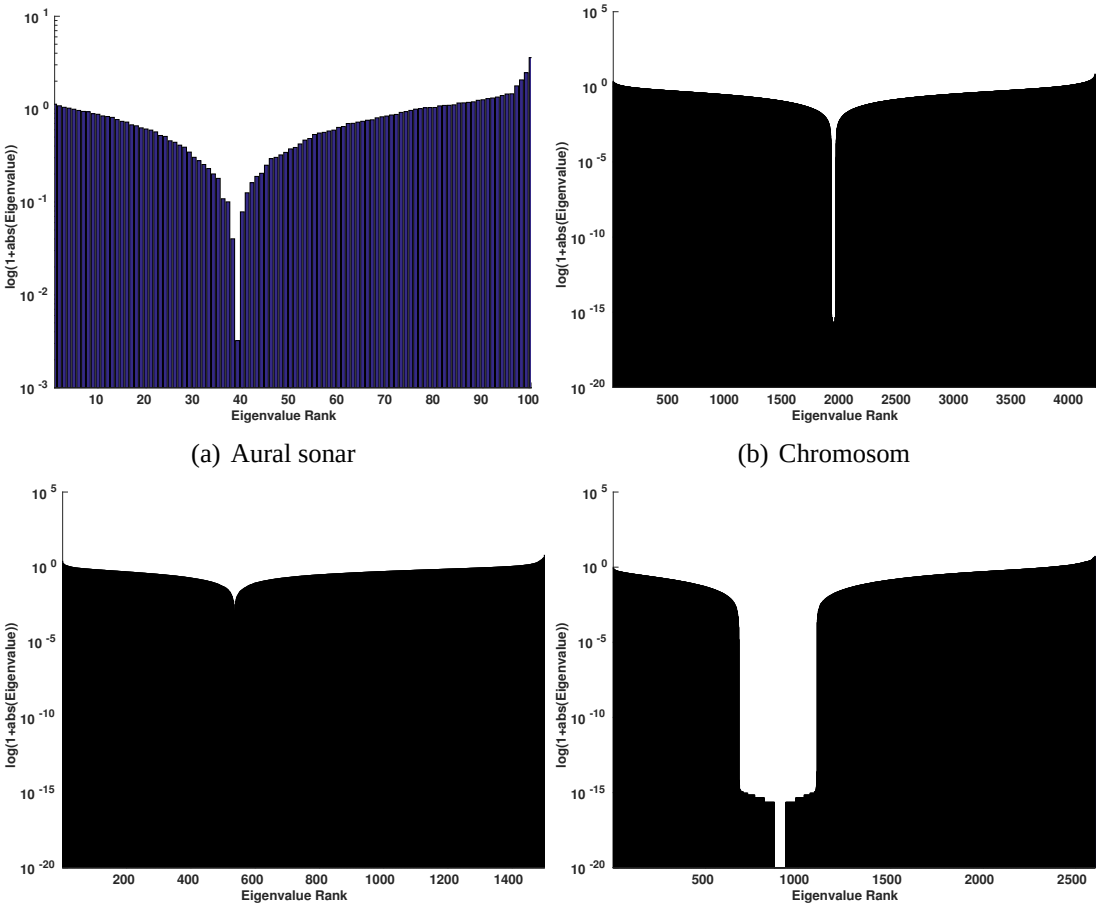
Figure 8: Embeddings of the similarity matrices of Aural sonar, Chromosom, Delft and Prodom using t-SNE



(a) Aural sonar (b) Chromosom

(c) Delft (d) Prodom

Figure 9: Visualization of the proxy kernel matrices of Aural sonar, Chromosom, Delft and Prodom.



(a) Aural sonar (b) Chromosom

(c) Delft (d) Prodom

Figure 10: Eigenspectra of the proxy kernel matrices of Aural sonar, Chromosom, Delft and Prodom.

as the cosine similarity between integral invariant signatures based on surface curves of the face (Feng et al., 2007) with a a signature of $(794, 150, 1)$

ProDom: the *ProDom* dataset with signature $(1502, 680, 422)$ consists of 2604 protein sequences with 53 labels. It contains a comprehensive set of protein families and appeared first in the work of (Roth et al., 2002). The pairwise structural alignments are computed by (Roth et al., 2002). Each sequence belongs to a group labeled by experts, here we use the data as provided in (R. P. Duin, 2012).

Protein: the Protein data set has sequence-alignment similarities for 213 proteins from 4 classes, where class one through four contains $72, 72, 39$, and 30 points, respectively (T. Hofmann & Buhmann, 1997). The signature is $(170, 40, 3)$.

Sonatas: the *Sonatas* data set contains complex symbolic data with a signature $(1063, 4, 1)$ taken from (Mokbel et al., 2009). It is comprised of pairwise dissimilarities between 1,068 sonatas from the classical period (by Beethoven, Mozart and Haydn) and the baroque era (by Scarlatti and Bach). The musical pieces were given in the MIDI file format, taken from the online MIDI collection *Kunst der Fuge*[9]. Their mutual dissimilarities were measured with the normalized compression distance (NCD), see (Cilibrasi & Vitányi, 2005). The musical pieces are classified according to their composer.

SwissProt: the *SwissProt* data set with a signature $(8487, 2500, 1)$, consists of 5,791 points of protein sequences in 10 classes taken as a subset from the popular SwissProt database of protein sequences (Boeckmann et al., 2003). The considered subset of the SwissProt database refers to the release 37. A typical protein sequence consists of a string of amino acids, and the length of the full sequences varies between 30 to more than 1000 amino acids depending on the sequence. The 10 most common classes such as Globin, Cytochrome b, Protein kinase st, etc. provided by the Prosite labeling

[9] `http://www.kunstderfuge.com`

(Gasteiger et al., 2003) where taken leading to 5,791 sequences. Due to this choice, an associated classification problem maps the sequences to their corresponding Prosite labels. These sequences are compared using Smith-Waterman which computes a local alignment of sequences (Gusfield, 1997). This database is the standard source for identifying and analyzing protein sequences such that an automated classification and processing technique would be very desirable.

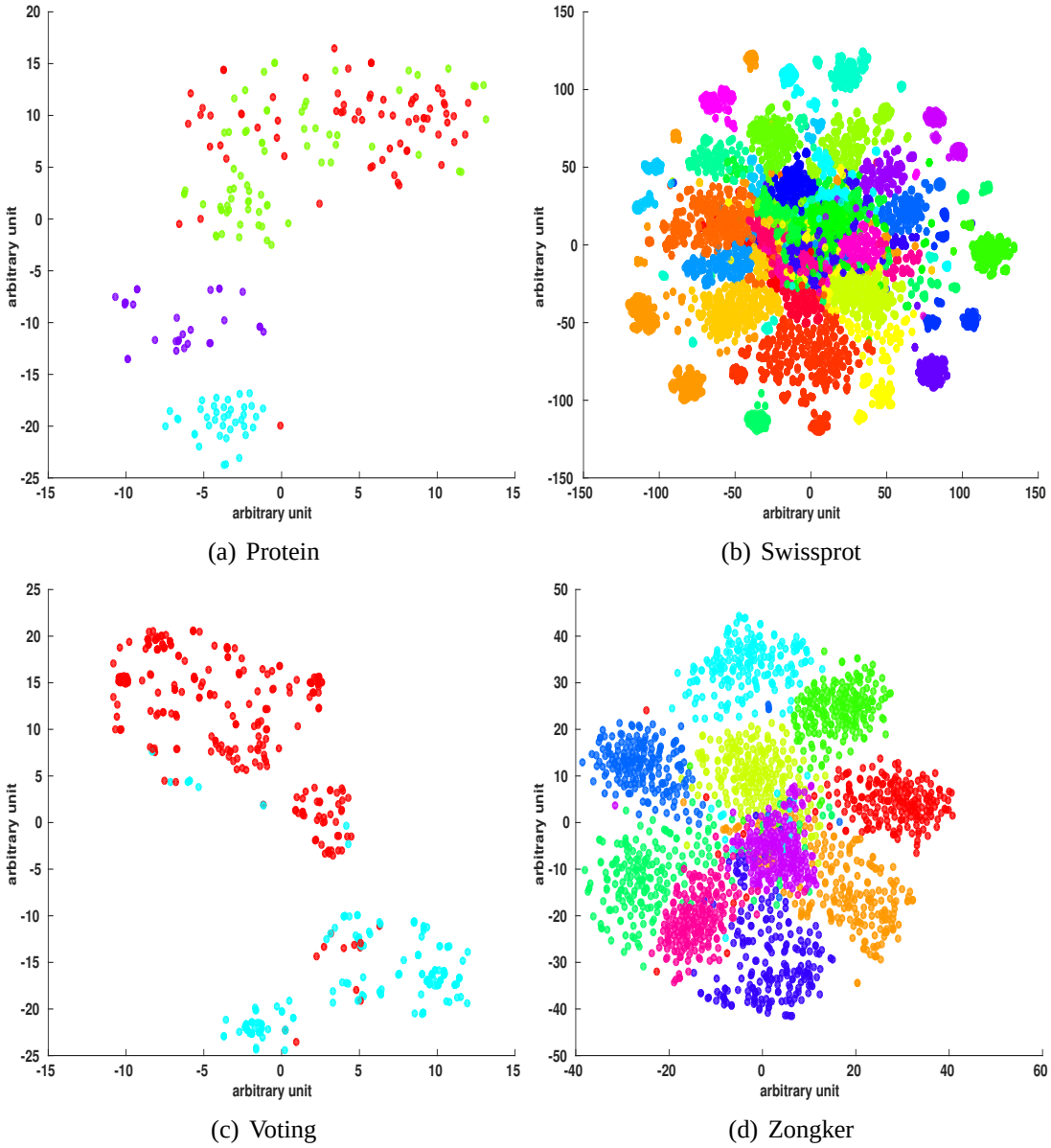
Voting: the Voting data set comes from the UCI Repository. It is a two- class classification problem with 435 points, where each sample is a categorical feature vector with 16 components and three possibilities for each component. We compute the value difference metric (Stanfill & Waltz, 1986) from the categorical data, which is a dissimilarity that uses the training class labels to weight different components differently so as to achieve maximum probability of class separation. The signature is $(178, 163, 94)$.

Zongker: the Zongker digit dissimilarity data (2000 points in 10 classes) from (R. P. Duin, 2012) is based on deformable template matching. The dissimilarity measure was computed between 2000 handwritten NIST digits in 10 classes, with 200 entries each, as a result of an iterative optimization of the non-linear deformation of the grid (Jain & Zongker, 1997). The signature is $(1039, 961, 0)$.

We also show the eigenspectra of the datasets in Figure 10 and Figure 13 indicating already how strong a dataset violates the metric properties. Additionally some summarizing information about the datasets is provided in Table 5 and t-SNE embeddings of the data in Figure 8 and Figure 11 to get a rough estimate whether the data are classwise multimodal. Further we can interpret *local* neighborhood relations and whether datasets are more overlapping or well separated[10].

We observe that there is no clear winning method but we find an advance for SVM-square (4 times best) and kNN (3 times best). If we remove kNN from the ranking due

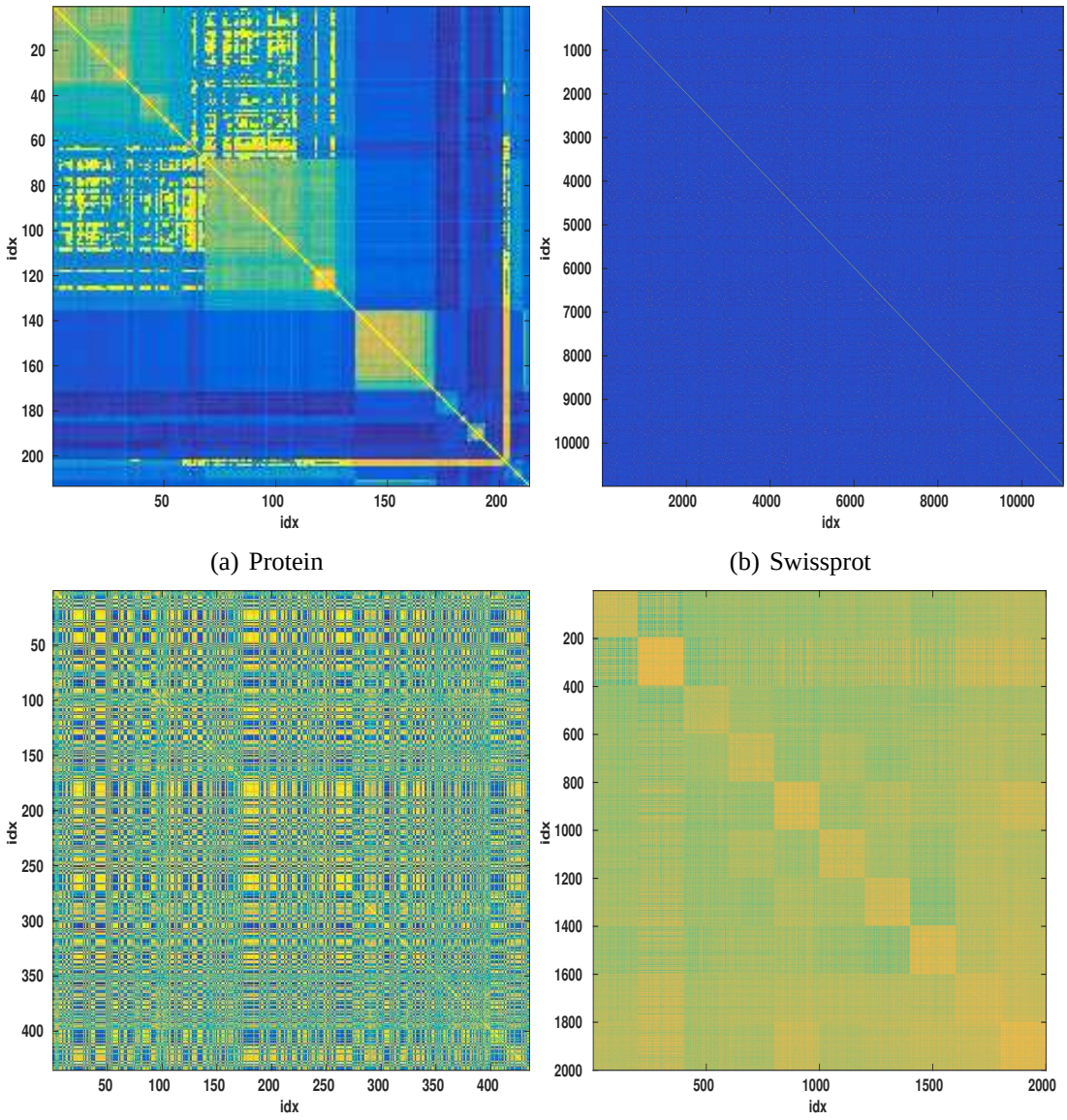
[10] T-SNE visualizations are not unique and we have adapted the perplexity parameter to get reasonable visualization in general as $\lfloor \log(N)^2 \rfloor$



(a) Protein (b) Swissprot

(c) Voting (d) Zongker

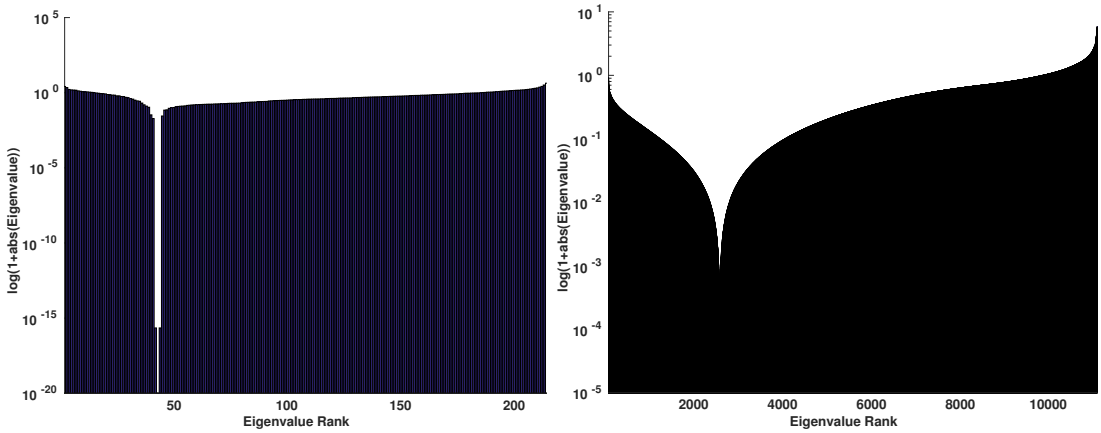
Figure 11: Embeddings of the similarity matrices of Protein, Swissprot, Voting and Zongker using t-SNE



(a) Protein (b) Swissprot

(c) Voting (d) Zongker

Figure 12: Visualization of the proxy kernel matrices of Protein, Swissprot, Voting and Zongker.



(a) Protein (b) Swissprot

(c) Voting (d) Zongker

Figure 13: Eigenspectra of the proxy kernel matrices of Protein, Swissprot, Voting and Zongker.

Table 5: Overview of the datasets. The last two columns refer to the number of positive and negative eigenvalues, respectively.

Data set	Points	Classes	Balanced	+EV	-EV
Aural Sonar	100	2	yes	62	38
Chromosoms	4200	21	yes	2258	1899
Delft	1500	20	yes	963	536
FaceRec	945	139	no	794	150
Prodom	2604	53	no	1502	680
Protein	213	4	no	170	40
Sonatas	1068	5	no	1063	4
SwissProt	10988	30	no	8487	2500
Voting	435	2	no	178	163
Zongker	2000	10	yes.	1039	961

Table 6: Comparison of different priorly discussed methods for various non-psd data sets.

Method	PCVM (B1)	IKFD (B2)	kNN	SVM	SVM-Flip (A1)	SVM-Clip	SVM-Squared	SVM-Shift	SVM-Proxy (A3)
Aural Sonar	84.00 ± 11.74	87.00 ± 10.59	80.00 ± 11.48	85.00 ± 11.79	88.00 ± 11.35	91.00 ± 8.76	87.00 ± 9.49	**91.00 ± 7.38**	88.00 ± 4.85
Chromosoms	85.48 ± 3.65	97.36 ± 1.09	95.11 ± 0.88	97.10 ± 1.00	**97.64 ± 0.79**	97.48 ± 0.72	96.81 ± 0.68	97.10 ± 0.92	n.a.
Delft	71.20 ± 11.84	98.20 ± 1.48	95.93 ± 1.65	97.73 ± 0.76	98.40 ± 0.90	**98.53 ± 0.75**	97.47 ± 1.58	97.47 ± 0.91	n.a.
FaceRec	54.18 ± 6.62	67.73 ± 6.34	**95.29 ± 1.84**	21.59 ± 7.56	21.59 ± 7.56	21.59 ± 7.56	37.78 ± 9.11	21.59 ± 7.56	n.a.
Prodom	99.62 ± 0.60	99.46 ± 0.55	99.87 ± 0.21	not converged	99.65 ± 0.56	99.65 ± 0.56	**99.92 ± 0.22**	98.96 ± 0.99	n.a.
Protein	95.76 ± 4.17	**99.05 ± 2.01**	59.13 ± 12.44	61.50 ± 10.64	98.59 ± 2.30	89.67 ± 9.75	98.59 ± 3.21	61.97 ± 9.83	97.07 ± 2.73
Sonatas	90.45 ± 3.84	90.17 ± 2.00	89.07 ± 3.68	87.36 ± 3.88	90.07 ± 3.90	89.61 ± 3.78	**92.60 ± 2.82**	87.17 ± 3.64	n.a.
SwissProt	97.78 ± 0.48	96.81 ± 0.79	**98.59 ± 0.35**	97.38 ± 0.36	97.33 ± 0.42	97.38 ± 0.37	98.37 ± 0.33	97.37 ± 0.38	n.a.
Voting	95.39 ± 2.70	95.62 ± 4.01	93.62 ± 4.54	95.63 ± 3.13	95.63 ± 3.13	95.63 ± 3.13	**95.86 ± 2.99**	95.63 ± 3.13	95.28 ± 1.96
Zongker	94.45 ± 1.64	97.10 ± 1.13	73.17 ± 3.29	not converged	**97.30 ± 1.21**	96.40 ± 1.39	97.00 ± 1.53	92.00 ± 2.55	n.a.

to the high costs in the test phase the best two approaches would be SVM-squared and iKFD.

If we analyze the prediction accuracy with respect to the negativity fraction (NF) of the data: $NF = \sum_{i=q}^{N} |\lambda_i| / \sum_{i=1}^{N} |\lambda_i|$ as shown in Figure 14 one can see that with increasing NF the performance variability of the methods increases. In a further experiment we take the Protein data and actively vary the negativity of the eigenspectrum, by varying the number of negative eigenvalues fixed to zero. We analyze the behavior of an SVM classifier by using the different eigenvalue correction methods discussed before. The results are shown in Figure 15 We see that for vanishing negativity the accuracy is around 87%. With increasing negativity the differences between the eigenvalue correction methods become more pronounced. When the negativity reaches 0.2 larger negative eigenvalues are included in the data and we observe that flip and square show a beneficial behavior. Without any corrections (blue dotted line), the accuracy drops significantly with increasing negativity. The shift approach is the worst. With

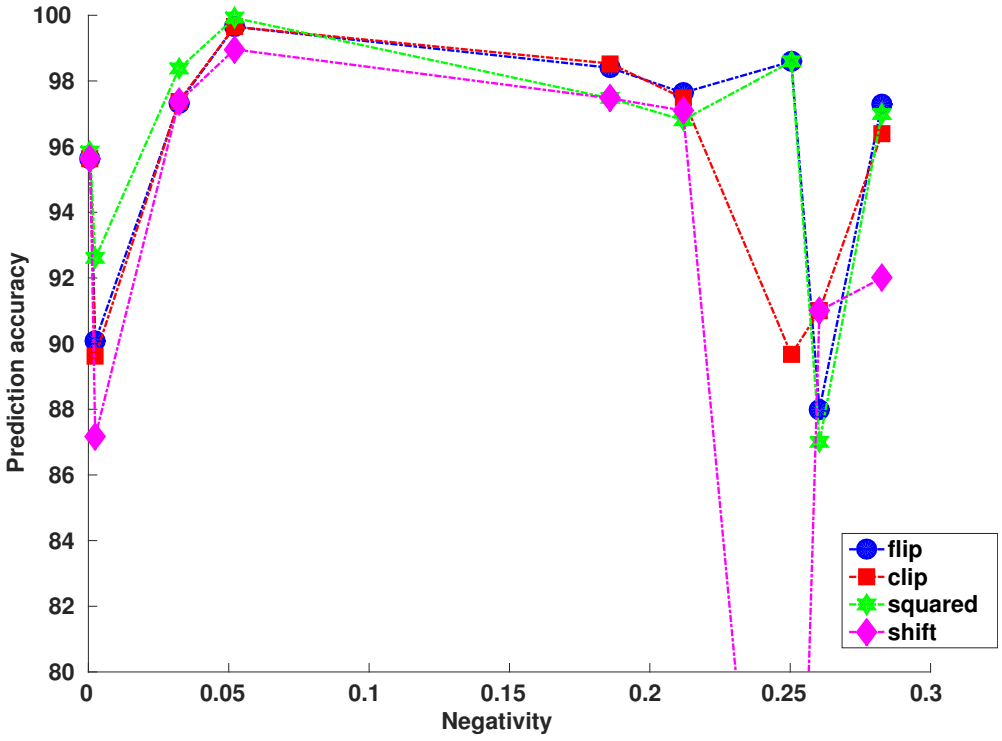


Figure 14: Analysis of eigenvalue correction approaches with respect to the negativity of the considered datasets. For each dataset and each correction method we show the prediction accuracy of the SVM with respect to the negativity of the data. The performance variability of the methods increases with increasing negativity of the eigen spectrum.

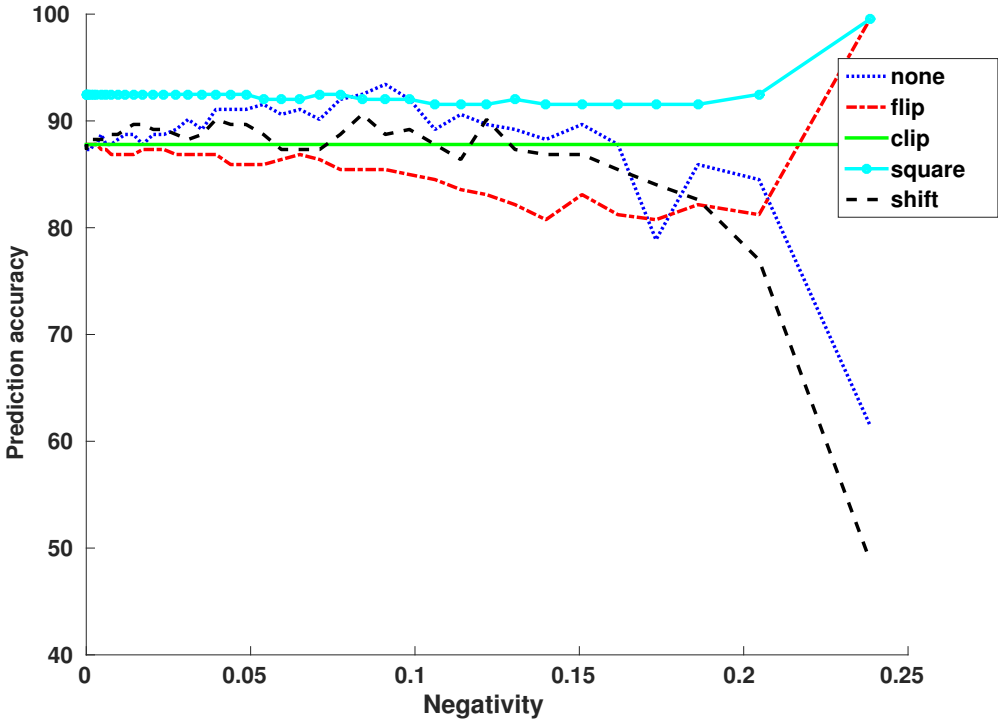


Figure 15: Analysis of eigenvalue correction approaches using the Protein data with varying negativity. The prediction accuracies have been obtained by using SVM. An increase in the negativity, such that the dataset is less metric, leads to stronger errors in the SVM model. This effect is severe for larger negativity and especially the shift correction or if no correction is applied.

respect to the discussion in section 5.4 this can now be easily explained. For the Protein data the largest negative eigenvalues are obviously encoding relevant information and smaller negative eigenvalues appear to encode noise. The shift approach removes the largest negative eigenvalue, suppress the second etc., while increasing all originally non-negative eigenvalue contributions, including those which were close to zero. Similar observations hold for the other datasets.

Discussion

This review shows that learning with indefinite proximities is a complex task which can be addressed by a variety of methods. We discussed the sources of indefiniteness in proximity data and have outlined a taxonomy of the different algorithmic approaches. Thereby we identified two major methodological directions namely approaches modifying the input proximities such that a metric representation is obtained and algorithmic formulations of dedicated methods which are insensitive to metric violations. The ”metric” direction is the most established field with a variety of approaches and algorithms. From our experiments in Section 8 we found that for many datasets the differences between algorithms of the ”metric” direction are only minor regarding the prediction accuracy on the test data. Small advantages could be found for the square and flipping approach. Especially *shift* is in general worse than the other approaches followed by clip. From the experiments one can conclude that the correction of indefinite proximities to metric ones is in general effective. If the indefiniteness can be attributed to a significant amount of noise a clipping operation is preferable, as it will reduce the noise in the input. If the indefiniteness is due to relevant information it is obviously better to keep this information in the data representation e.g. by using the square operation. Beside of the effect on the model accuracy the methods also differ in the way how out-of sample extensions are treated and with respect to the overall complexity of the approaches. We have addressed these topics in the respective sections and provided also

efficient approximation schemes for some of the methods given the input data have low rank. If the rank of the input data is rather high, approximations are inappropriate and the methods have $O(N^3)$ complexity.

The alternative direction is to preserve the input data in its given form and to generate models which are insensitive to indefinite proximities or can be directly derived in the pseudo-Euclidean space. Comparing the results in Table 6 we observe that those methods which avoid modifications of the input proximities are in general competitive but at a complexity of $O(N) - O(N^3)$. But for many of these methods low rank approximation schemes can be applied as well. As a very simple alternative we also considered the nearest-neighbor classifier which worked reasonable well. However NN is known to be very sensitive to outliers and requires the storage of all training points to calculate out of sample extensions.

In conclusion, the machine learning expert has to know a bit about the underlying data and especially the used proximity function to make an educated decision. In particular:

- If the proximity function is derived from a mathematical distance or inner product, the presence of negative eigenvalues is likely caused by numerical errors. In this case, a very simple eigenvalue correction of the proximity matrix (e.g. clipping) (A1) may be sufficient.

- If the given proximity function is domain specific and non-metric, more careful modifications of the proximity matrix are in order (as discussed in Sections 5.1-5.2 and shown in the experiments - in Section 8).

- For asymmetric proximity measures, we have provided links to the few existing methods capable of dealing with asymmetric proximity matrices (see A2, B1). However, all of them are either costly in the model generation or in the out-of-sample extension (application to new test points). Fortunately, some form of symmetrization of the proximity matrix is often acceptable. For example, in

the analysis of biological sequences, the proximity scores are in general “almost symmetric” and a symmetrization leads to no performance degradation.

- If rank of the proximity matrix is rather high (e.g. FaceRec data), low-rank approximations (Sec. 7) will lead to information loss.

There are many open research questions in the field of indefinite proximity learning. As already seen in the former sections the handling of non-metric data is still not very comfortable, although meanwhile a compact set of efficient methods is available. As indefinite proximities can occur due to numerical errors or noise it would be desirable to have a more systematic procedure isolating these components from those which carry relevant information. It would be also very desirable to have a larger benchmark of indefinite proximity data similar as within the UCI database for (most often) vectorial datasets. Also in the pre-mentioned algorithms we can find various open topics: the set of algorithms with explicit formulations in the Krein space like (Haasdonk & Pkalska, 2008; Pekalska & Haasdonk, 2009; Liwicki et al., 2013; Zafeiriou, 2012) is still very limited. Further the runtime performance for the processing of large scale data is often inappropriate. It would also be of interest whether some of the methods can be extended to asymmetric input data or if concepts from the analysis of large asymmetric graph networks can be transferred to the analysis of indefinite proximities.

Datasets and implementations

The datasets used in this paper have been made available at the following web page `http://promos-science.blogspot.de/p/blog-page.html`. Parts of the implementations of the algorithms discussed before can be accessed at `http://www.techfak.uni-bielefeld.de/~fschleif/review/`. An implementation of the Probabilistic Classification Vector Machine is available at `https://mloss.org/software/view/610/`.

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