Structure Preserving Encoding of Non-euclidean Similarity Data

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Abstract: Domain-specific proximity measures, like divergence measures in signal processing or alignment scores in bioinformatics, often lead to non-metric, indefinite similarities or dissimilarities. However, many classical learning algorithms like kernel machines assume metric properties and struggle with such metric violations. For example, the classical support vector machine is no longer able to converge to an optimum. One possible direction to solve the indefiniteness problem is to transform the non-metric (dis-)similarity data into positive (semi-)definite matrices. For this purpose, many approaches have been proposed that adapt the eigenspectrum of the given data such that positive definiteness is ensured. Unfortunately, most of these approaches modify the eigenspectrum in such a strong manner that valuable information is removed or noise is added to the data. In particular, the shift operation has attracted a lot of interest in the past few years despite its frequently re-occurring disadvantages. In this work, we propose a modified *advanced shift correction method* that enables the preservation of the eigenspectrum structure of the data by means of a low-rank approximated nullspace correction. We compare our advanced shift to classical eigenvalue corrections like eigenvalue clipping, flipping, squaring, and shifting on several benchmark data. The impact of a low-rank approximation on the data's eigenspectrum is analyzed.

1 INTRODUCTION

Learning classification models for structured data is often based on pairwise (dis-)similarity functions, which are suggested by domain experts. However, these domain-specific (dis-)similarity measures are typically not positive (semi-)definite (*non-psd*). These so-called *indefinite kernels* are a severe problem for many kernel-based learning algorithms because classical mathematical assumptions such as positive (semi-)definiteness (psd), used in the underlying optimization frameworks, are violated. For example, the modified Hausdorff-distance for structural pattern recognition, various alignment scores in bioinformatics, and also many others generate non-metric or indefinite similarities or dissimilarities.

As a consequence, e.g., the classical Support Vector Machine (SVM) (Vapnik, 2000) has no longer a convex solution - in fact, most standard solvers will not even converge for this problem (Loosli et al., 2016). Researchers in the field of, e.g., psychology (Hodgetts and Hahn, 2012), vision (Scheirer et al., 2014; Xu et al., 2011), and machine learning (Duin and Pekalska, 2010) have criticized the typical restriction to metric similarity measures. (Duin and Pekalska, 2010) pointed out many real-life problems to be better addressed by, e.g., kernel functions that are not restricted to be based on a metric. The use of divergence measures (Schnitzer et al., 2012; Zhang et al., 2009) is very popular for spectral data analysis in chemistry, geo- and medical sciences (van der Meer, 2006), and are in general not metric. Also, the popular Dynamic Time Warping (DTW) (Sakoe and Chiba, 1978) algorithm provides a non-metric alignment score, which is commonly used as a proximity measure between two one-dimensional functions of different length. In image processing and shape retrieval, indefinite proximities are frequently obtained in the form of the inner distance (Ling and Jacobs, 2007) - another non-metric measure. Further prominent examples of genuine non-metric proximity measures can be found in the field of bioinformatics where

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classical sequence alignment algorithms (e.g., smith-waterman score (Gusfield, 1997)) produce non-metric proximities. Those domain-specific measures are effective but not particularly accessible in the mathematical context. The importance of preserving the non-metric part of the data is emphasized by many authors. Multiple authors argue that the non-metric part of the data contains valuable information and should not be removed (Scheirer et al., 2014; Pekalska and Duin, 2005).

There are two main directions to handle the problem of indefiniteness: using insensitive methods like indefinite kernel fisher discrimination (Haasdonk and Pekalska, 2008), empirical feature space approaches (Alabdulmohsin et al., 2016), or correcting the eigenspectrum to psd.

Due to its strong theoretical foundations, Support Vector Machine (SVM) has been extended for indefinite kernels in several ways (Haasdonk, 2005; Luss and d'Aspremont, 2009; Gu and Guo, 2012). A recent survey on indefinite learning is given in (Schleif and Tiňo, 2015). In (Loosli et al., 2016), a stabilization approach was proposed to calculate a valid SVM model in the Krĕin space, which can be directly applied to indefinite kernel matrices. This approach has shown great promise in several learning problems but used the so-called flip approach to correct the negative eigenvalues, which is a substantial modification of the structure of the eigenspectrum. In (Loosli, 2019), a similar approach was proposed using the classical shift technique.

The present paper provides a shift correction approach that preserves the eigenstructure of the data and avoids cubic eigendecompositions. We also address the limitation of the classical shift correction, which renders to be impracticable and error-prone in practical settings.

2 LEARNING WITH NON-PSD KERNELS

Learning with non-psd kernels can be a challenging problem and may occur very quickly when using domain-specific measures or noise occurs in the data. The metric violations cause negative eigenvalues in the eigenspectrum of the kernel matrix K, leading to non-psd similarity matrices or indefinite kernels. Many learning algorithms are based on kernel formulations, which have to be symmetric and psd. The mathematical meaning of a kernel is the inner product in some Hilbert space (Shawe-Taylor and Cristianini, 2004). However, it is often loosely considered simply as a pairwise "similarity" measure between data items, leading to a similarity matrix S.

If a particular learning algorithm requires the use of Mercer kernels and the similarity measure does not fulfill the kernel conditions, then one of the mentioned strategies have to be applied to ensure a valid model.

2.1 Background and Basic Notation

Consider a collection of N objects $\mathbf{x}_i$, $i = \{1,2,...,N\}$, in some input space $\mathcal{X}$. Given a similarity function or inner product on $\mathcal{X}$, corresponding to a metric, one can construct a proper Mercer kernel acting on pairs of points from $\mathcal{X}$. For example, if $\mathcal{X}$ is a finite-dimensional vector space, a classical similarity function is the Euclidean inner product (corresponding to the Euclidean distance) - a core component of various kernel functions such as the famous radial basis function (RBF) kernel. Now, let $\phi : \mathcal{X} \mapsto \mathcal{H}$ be a mapping of patterns from $\mathcal{X}$ to a 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 $k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle_{\mathcal{H}}$, for any $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$. The matrix $K_{i,j} := k(\mathbf{x}_i, \mathbf{x}_j)$ is an $N \times N$ kernel (Gram) matrix derived from the training data. For more general similarity measures, subsequently, we also use $\mathbf{S}$ to describe a similarity matrix. Such an embedding is motivated by the non-linear transformation of input data into higher dimensional $\mathcal{H}$ allowing linear techniques in $\mathcal{H}$. Kernelized methods process the embedded data points in a feature space utilizing only the inner products $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ (Shawe-Taylor and Cristianini, 2004), without the need to explicitly calculate ϕ, known as *kernel trick*. The 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 and ϕ is the identity mapping, or the RBF kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x}-\mathbf{x}'||^2}{2\sigma^2}\right)$, with $\sigma > 0$ as a free scale parameter. In any case, it is always assumed that the kernel function $k(\mathbf{x}, \mathbf{x}')$ is psd. However, this assumption is not always fulfilled and the underlying similarity measure may not be metric and hence not lead to a Mercer kernel. Examples can be easily found in domain-specific similarity measures, as mentioned before and detailed later on. Such similarity measures imply *indefinite* kernels, preventing standard "kernel-trick" methods developed for Mercer kernels to be applied.

2.2 Eigenspectrum Approaches

A natural way to address the indefiniteness problem and to obtain a psd similarity matrix is to correct the eigenspectrum of the original similarity matrix S. Popular strategies include eigenvalue correction by *flipping, clipping, squaring*, and *shifting*. The non-psd similarity matrix S is decomposed by an eigendecomposition: $S = U\Lambda U^\top$, where U contains the eigenvectors of S and Λ contains the corresponding eigenvalues λ_i. Now, the eigenvalues in Λ can be manipulated to eliminate all negative parts. Following the operation, the matrix can be reconstructed, now being psd.

Clip Eigenvalue Correction. All negative eigenvalues in Λ are set to 0. Such a spectrum clip leads to the nearest psd matrix S in terms of the Frobenius norm (Higham, 1988). Such a correction can be achieved by an eigendecomposition of the matrix S, a clipping operator on the eigenvalues, and the subsequent reconstruction. This operation has a complexity of $O(N^3)$. The complexity might be reduced by either a low-rank approximation or the approach shown by (Luss and d'Aspremont, 2009) with roughly quadratic complexity.

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 keeps the relevant information (Pekalska and Duin, 2005). This operation can be calculated with $O(N^3)$ or $O(N^2)$ if low-rank approaches are used.

Square Eigenvalue Correction. All negative eigenvalues in Λ are set to $\lambda_i := \lambda_i^2 \; \forall i$ which amplifies large and very small eigenvalues. The square eigenvalue correction can be achieved by matrix multiplication (Strassen, 1969) with $\approx O(N^{2.8})$.

Classical Shift Eigenvalue Correction. The shift operation was already discussed earlier by different researchers (Filippone, 2009) and modifies Λ such that $\lambda_i := \lambda_i - \min_{ij}\Lambda \; \forall i$. The classical shift eigenvalue correction can be accomplished with linear costs if the smallest eigenvalue $\lambda_{\min}$ is known. Otherwise, some estimator for $\lambda_{\min}$ is needed. A few estimators for this purpose have been suggested: analyzing the eigenspectrum on a subsample, making a reasonable guess, or using some low-rank eigendecomposition. In our approach, we suggest employing a power iteration method, for example the *von Mises* approach, which is fast and accurate.

Spectrum shift enhances all the self-similarities and therefore the eigenvalues by the amount of λ_{min} and does not change the similarity between any two different data points, but it may also increase the intrinsic dimensionality of the data space and amplify noise contributions.

2.3 Limitations

Multiple approaches have been suggested to correct the eigenspectrum of a similarity matrix and to obtain a psd matrix (Pekalska and Duin, 2005; Schleif and Tiňo, 2015). Most approaches modify the eigenspectrum in a very powerful way and are also costly due to an involved cubic eigendecomposition. In particular, the clip, flip, and square operator have an apparent strong impact. While the clip method is useful in case of noise, it may also remove valuable contributions. The clip operator only *removes* eigenvalues, but generally keeps the majority of the eigenvalues unaffected. The flip operator, on the other hand, affects all negative eigenvalues by changing the sign and this will additionally lead to a reorganization of the eigenvalues. The square operator is similar to flip but additionally emphasizes large eigencontributions while fading out eigenvalues below 1. The classical shift operator is only changing the diagonal of the similarity matrix leading to a shift of the whole eigenspectrum by the provided offset. This may also lead to reorganizations of the eigenspectrum due to new non-zero eigenvalue contributions. While this simple approach seems to be very reasonable, it has the major drawback that all (!) eigenvalues are shifted, which also affects small or even 0 eigenvalue contributions. While 0 eigenvalues have no contribution in the original similarity matrix, they are artificially upraised by the classical shift operator. This may introduce a large amount of noise in the eigenspectrum, which could potentially lead to substantial numerical problems for employed learning algorithms, for example, kernel machines. Additionally, the intrinsic dimensionality of the data is increased artificially, resulting in an even more challenging problem.

3 ADVANCED SHIFT CORRECTION

To address the aforementioned challenges, we suggest an alternative formulation of the shift correction, subsequently referred to as *advanced shift*. In particular, we would like to keep the original eigenspectrum structure and aim for a sub-cubic eigencorrection.

3.1 Algorithmic Approach

As mentioned in Sec. 2.3 the classical shift operator introduces noise artefacts for small eigenvalues. In the advanced shift procedure, we will remove these artificial contributions by a null space correction. This is particularly effective if non-zero, but small eigenvalues are also taken into account. Accordingly, we apply a low-rank approximation of the similarity matrix as an additional pre-processing step. The procedure is summarized in Algorithm 1.

Algorithm 1: Advanced shift eigenvalue correction.

Advanced_shift(S,k)
if approximate to low rank **then**
  $S :=$ LowRankApproximation(S,k)
end if
$\lambda :=$ |ShiftParameterDetermination(S)|
$\mathbf{B} :=$ NullSpace(S)
$\mathbf{N} := \mathbf{B} \cdot \mathbf{B}'$
$S^* := S + 2 \cdot \lambda \cdot (I - \mathbf{N})$
return S^*

The first part of the algorithm applies a low-rank approximation on the input similarities S using a restricted SVD or other techniques (Sanyal et al., 2018). If the number of samples $N \leq 1000$, then the rank parameter $k = 30$ and $k = 100$, otherwise. The shift parameter λ is calculated on the low-rank approximated matrix, using a *von Mises* or power iteration (Mises and Pollaczek-Geiringer, 1929) to determine the respective largest negative eigenvalue of the matrix. As shift parameter, we use the absolute value of λ for further steps. This procedure provides an accurate estimate of the largest negative eigenvalue instead of making an educated guess as suggested. This is particular relevant because the scaling of the eigenvalues can be very different between the various datasets, which may lead to an ineffective shift (still remaining negative eigenvalues) if the guess is incorrect. The basis $\mathbf{B}$ of the nullspace is calculated, again by a restricted SVD. The nullspace matrix $\mathbf{N}$ is obtained by calculating a product of $\mathbf{B}$. Due to the low-rank approximation, we ensure that small eigenvalues, which are indeed close to 0 due to noise, are shrunk to 0 (Ilic et al., 2007). In the final step, the original S or the respective low-rank approximated matrix $\hat{S}$ is shifted by the largest negative eigenvalue λ that is determined by von Mises iteration. By combining the shift with the nullspace matrix $\mathbf{N}$ and the identity matrix I, the whole matrix will be affected by the shift and not only the diagonal matrix. At last, the doubled shift factor 2 ensures that the largest negative eigenvalue $\hat{\lambda}^*$ of the new matrix $\hat{S}^*$ will not become 0, but remains a contribution.

Table 1: Overview of the different datasets. Details are given in the textual description.

Dataset	#samples	#classes
Balls3d	200	2
Balls50d	2,000	4
Gauss	1,000	2
Chromosomes	4,200	21
Protein	213	10
SwissProt	10,988	10
Aural Sonar	100	2
Facerec	945	10
Sonatas	1,068	5
Voting	435	2
Zongker	2,000	10

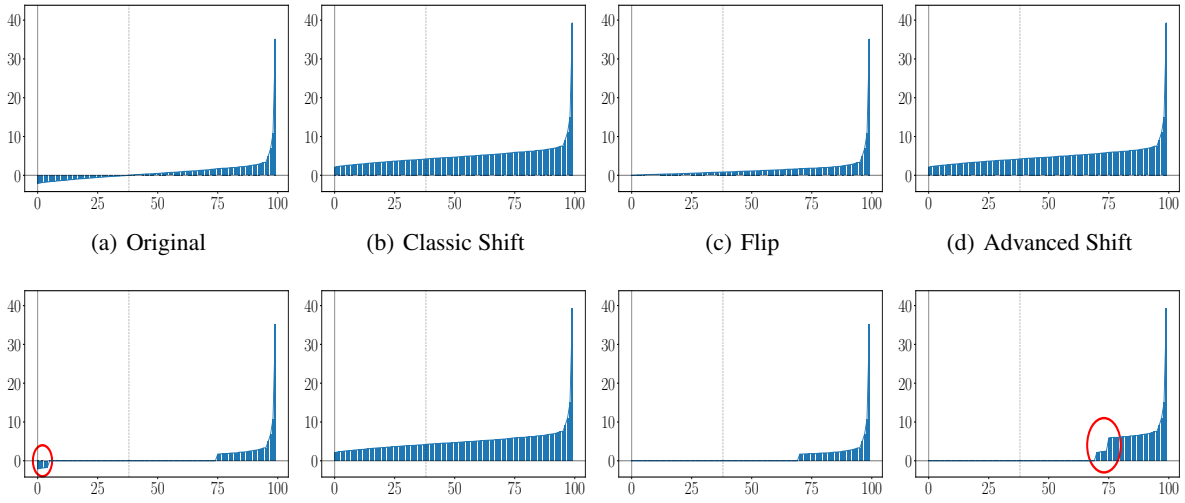
Complexity: The advanced shift approach shown in Algorithm 1 is comprised of various subtasks with different complexities. The low-rank approximation can be achieved with $O(N^2)$ as well as the nullspace approximation. The shift parameter is calculated by *von Mises* iteration with $O(N^2)$. Since $\mathbf{B}$ is a rectangular $N \times k$ matrix, the matrix $\mathbf{N}$ can be calculated with $O(N^2)$.

The final eigenvalue correction to obtain $\hat{S}^*$ is also $O(N^2)$. In summary, the low-rank advanced shift eigenvalue correction can be achieved with $O(N^2)$ operations. If no low-rank approximation is employed, the calculation of $\mathbf{N}$ will cost $O(N^{2.8})$ using Strassen matrix multiplication.

In the experiments, we analyze the effect of our new transformation method with and without a low-rank approximation and compare it to the aforementioned alternative methods.

3.2 Structure Preservation

In our context, the term *structure preservation* refers to the structure of the eigenspectrum. Those parts of the eigenspectrum which are not to be corrected to make the matrix psd should be kept unchanged. The various eigen correction methods have a different impact on the eigenspectrum as a whole and often change the structure of the eigenspectrum. Those changes are: changing the sign of an eigenvalue, changing its magnitude, removing an eigenvalue, introducing a new eigenvalue (which was 0 before), or changing the position of the eigenvalue with respect to a ranking. The last one is particularly relevant if only a few eigenvectors are used in some learning models, like kernel PCA or similar methods. To illustrate the various impact on the eigenspectrum, the plots (a)-(d) of Figure 1 plots (a)-(d), we show the eigencorrection methods on the original of an exemplary similarity matrix, here the Aural-Sonar dataset. Obviously,



(a) Original (b) Classic Shift (c) Flip (d) Advanced Shift

(e) Original low-rank (f) Classic Shift low-rank (g) Flip low-rank (h) Advanced Shift low-rank

Figure 1: Eigenspectrum plots of the protein data set using the different eigenspectrum corrections. Plots (e) - (h) are generated using a low-rank processing. The x-axis represents the index of the eigenvalue while the y-axis illustrates the value of the eigenvalue. The dashed vertical bar indicates the transition between negative and non-negative eigenvalues. The classical shift clearly shows an increase in the intrinsic dimensionality by means of non-zero eigenvalues. For flip and the advanced shift we also observe a reorganization of the eigenspectrum.

the classical shift increases the number of non-zero eigencontributions introducing artificial noise in the data. The same is also evident for the advanced shift (without low-rank approximation), but this is due to a very low number of zero eigenvalues for this particular dataset and can be cured in the low-rank approach. The plots (e)-(h) show the respective corrections on a low-rank representation of the Aural-Sonar dataset. Obviously, the classical shift is still inappropriate whereas the advanced shift correction preserves the structure of the spectral information. In contrast to (f) and (g), the small negative eigenvalues from (e) are still taken into account in (h), which can be recognized by the abrupt eigenvalue step in the circle. In any case, clipping removes the negative eigencontributions leading to a plot similar to (a),(e) but without negative contributions. The spectrum of the square operations looks very similar to the results for the flip method. Flip and square effect the ranks of the eigenvalues, but square additionally changes the magnitudes.

Although we only show results for the Aural-Sonar data in this section, we observed similar findings for the other datasets as well. This refers primarily to the structure of the eigenspectrum, with hardly eigenvalues close to zero. In particular, a more elaborated treatment of the eigenspectrum becomes evident, motivating our approach in favour of more simple approaches like classical shift or flip.

4 EXPERIMENTS

This part contains the results of the experiments aimed at demonstrating the effectiveness of our proposed advanced shift correction in combination with low-rank approximation. The used data are briefly described in the following and summarized in Table 1, with details given in the references.

4.1 Datasets

We use a variety of standard benchmark data for similarity-based learning. All data are indefinite with different spectral properties. If the data are given as dissimilarities, a corresponding similarity matrix can be obtained by double centering (Pekalska and Duin, 2005): $S = -JDJ/2$ with $J = (I - \mathbf{1}\mathbf{1}^\top/N)$, with identity matrix I and vector of ones $\mathbf{1}$.
For evaluation, we use three synthetic datasets:

Balls3d/Balls50d consist of 200/2000 samples in two/four classes. The dissimilarities are generated between two constructed balls using the shortest distance on the surfaces. The original data description is provided in (Pekalska et al., 2006).

For working with **Gauss** data, we create two datasets X, each consisting of 1000 data points in two dimensions divided into two classes. Data of the first dataset are linearly separable, whereas data of the second dataset are overlapping. To calculate dissimilarity

Table 2: Results using various eigen-correction methods on the original matrix. Best results are given in bold.

Dataset	Advanced Shift	Classic Shift	Flip	Clip	Square
Aural Sonar	88.0 ± 0.07	90.0 ± 0.1	89.0 ± 0.08	$\mathbf{91.0 \pm 0.12}$	89.0 ± 0.09
Balls3d	42.5 ± 0.15	36.0 ± 0.06	$\mathbf{98.0 \pm 0.04}$	76.5 ± 0.08	55.0 ± 0.1
Balls50d	23.35 ± 0.03	20.5 ± 0.01	$\mathbf{40.95 \pm 0.02}$	28.45 ± 0.04	25.45 ± 0.04
Chromosomes	1.86 ± 0.0	not converged	$\mathbf{97.86 \pm 0.0}$	34.29 ± 0.03	96.71 ± 0.01
Facerec	$\mathbf{88.99 \pm 0.03}$	87.1 ± 0.03	85.61 ± 0.04	86.46 ± 0.04	85.82 ± 0.03
Gauss with overlap	89.3 ± 0.03	17.0 ± 0.02	$\mathbf{91.4 \pm 0.03}$	88.8 ± 0.02	91.2 ± 0.03
Gauss without overlap	98.5 ± 0.01	2.2 ± 0.01	$\mathbf{100.0 \pm 0.0}$	99.8 ± 0.0	$\mathbf{100.0 \pm 0.0}$
Protein	52.12 ± 0.06	55.37 ± 0.08	$\mathbf{99.52 \pm 0.01}$	93.46 ± 0.05	98.59 ± 0.02
Sonatas	82.87 ± 0.02	85.11 ± 0.02	91.01 ± 0.02	90.54 ± 0.03	$\mathbf{93.45 \pm 0.03}$
SwissProt	95.03 ± 0.01	96.2 ± 0.01	97.46 ± 0.0	97.46 ± 0.0	$\mathbf{98.44 \pm 0.0}$
Voting	95.65 ± 0.03	95.87 ± 0.03	$\mathbf{96.79 \pm 0.02}$	96.09 ± 0.02	96.78 ± 0.03
Zongker	92.15 ± 0.02	92.75 ± 0.02	$\mathbf{97.65 \pm 0.01}$	97.4 ± 0.01	97.25 ± 0.01

Table 3: Results using various eigen-correction methods on a low-rank approximated matrix. Best accuracies are given in bold.

Dataset	Advanced Shift	Classic Shift	Flip	Clip	Square
Aural Sonar	88.0 ± 0.13	$\mathbf{89.0 \pm 0.08}$	88.0 ± 0.06	86.0 ± 0.11	87.0 ± 0.11
Balls3d	$\mathbf{100.0 \pm 0.0}$	37.0 ± 0.07	96.0 ± 0.04	78.5 ± 0.05	55.0 ± 0.09
Balls50d	$\mathbf{48.15 \pm 0.04}$	20.65 ± 0.02	41.15 ± 0.03	27.2 ± 0.04	25.05 ± 0.02
Chromosomes	96.45 ± 0.01	not converged	$\mathbf{97.29 \pm 0.0}$	38.95 ± 0.02	96.07 ± 0.01
Facerec	62.33 ± 0.05	62.22 ± 0.07	63.27 ± 0.05	61.92 ± 0.07	$\mathbf{86.13 \pm 0.02}$
Gauss with overlap	$\mathbf{91.6 \pm 0.03}$	17.1 ± 0.03	91.5 ± 0.02	88.6 ± 0.03	91.3 ± 0.02
Gauss without overlap	$\mathbf{100.0 \pm 0.0}$	2.2 ± 0.01	$\mathbf{100.0 \pm 0.0}$	99.7 ± 0.0	$\mathbf{100.0 \pm 0.0}$
Protein	$\mathbf{99.07 \pm 0.02}$	58.31 ± 0.09	99.05 ± 0.02	98.59 ± 0.02	98.61 ± 0.02
Sonatas	$\mathbf{94.29 \pm 0.02}$	90.73 ± 0.02	94.19 ± 0.02	93.64 ± 0.04	93.44 ± 0.03
SwissProt	$\mathbf{97.55 \pm 0.01}$	96.48 ± 0.0	96.54 ± 0.0	96.42 ± 0.0	97.43 ± 0.0
Voting	$\mathbf{97.24 \pm 0.03}$	95.88 ± 0.03	96.77 ± 0.03	96.59 ± 0.04	96.77 ± 0.02
Zongker	$\mathbf{97.7 \pm 0.01}$	92.85 ± 0.01	97.2 ± 0.01	96.85 ± 0.01	96.75 ± 0.01

matrix D, we use $D = \tanh(-2.25 \cdot X \cdot X^T + 2)$.
Further, we use three biochemical datasets:

The Kopenhagen **Chromosomes** data set constitutes 4,200 human chromosomes from 21 classes represented by grey-valued images. These are transferred to strings measuring the thickness of their silhouettes. These strings are compared using edit distance. Details are provided in (Neuhaus and Bunke, 2006).

Protein consists of 213 measurements in four classes. From the protein sequences, similarities were measured using an alignment scoring function. Details are provided in (Chen et al., 2009).

SwissProt consists of 10,988 samples of protein sequences in 10 classes taken as a subset from the SwissProt database. The considered subset of the SwissProt database refers to the release 37 mimicking the setting as proposed in (Kohonen and Somervuo, 2002).
Another four datasets are taken from signal processing:

Aural Sonar consists of 100 signals with two classes, representing sonar signals dissimilarity measures to investigate the human ability to distinguish different types of sonar signals by ear. Details are provided in (Chen et al., 2009).

Facerec dataset consists of 945 sample faces with 139 classes, representing sample faces of people, compared by the cosine similarity as measure. Details are provided in (Chen et al., 2009).

Sonatas dataset consists of 1068 sonatas from five composers (classes) from two consecutive eras of western classical music. The musical pieces were taken from the online MIDI database *Kunst der Fuge* and transformed to similarities by normalized compression distance (Mokbel, 2016).

Voting contains 435 samples in 2 classes, representing categorical data, which are compared based on the value difference metric (Chen et al., 2009).

Zongker dataset is a digit dissimilarity dataset. The dissimilarity measure was computed between 2000 handwritten digits in 10 classes, with 200 entries in each class (Jain and Zongker, 1997).

4.2 Performance in Supervised Learning

We evaluate the performance of the proposed advanced shift correction on the mentioned datasets against other eigenvalue correction methods using a standard SVM classifier. The correction approaches ensure that the input similarity, herein used as a kernel matrix, is psd. Within all experiments, we measured the algorithm's accuracy and its standard deviation in a ten-fold cross-validation shown in Table 2 and Table 3. The parameter C has been selected for each correction method by a grid search on independent data not used during testing.

In Table 2, we show the classification performance for the considered data and correction approaches. The flip correction performed best, followed by the square correction, which is in agreement with former findings by (Loosli et al., 2016). The clip correction is also often effective. Both shift approaches struggle on a few datasets, in particular, those having a more complicated eigenspectrum (see e.g. (Schleif and Tiňo, 2015)) and if the matrix is close to a full rank structure.

In Table 3, which includes the low-rank approximation, we observe similar results to Table 2, but the advanced shift correction performs much better also in comparison to the other methods (also to the ones without low-rank approximation). In contrast to Table 2, the low-rank approximation leads to a large number of truly zero eigenvalues making the advanced shift correction effective. It becomes evident that besides the absolute magnitude of the larger eigenvalues also the overall structure of the eigenspectrum is important for both shift operators. The proposed approach benefits from eigenspectra with many close to zero eigenvalues which occurs in many practical data. In fact, many datasets have an intrinsic low-rank nature, which we employ in our approach. In any case, the classical shift increases the intrinsic dimensionality also if many eigenvalues have been zero in the original matrix. This leads to substantial performance loss in the classification models, as seen in Table 2 but also in Table 3. Surprisingly, the shift operator is still occasionally preferred in the literature (Filippone, 2009; Laub, 2004; Loosli, 2019) but not on a large variety of data, which would have shown the observed limitations almost sure. The herein proposed advanced shift overcomes the limitations of the classical shift. Considering the results of Table 3, the advanced shift correction is almost preferable in each scenario but should be avoided if low-rank approximations have a negative impact on the information content of the data. One of those rare cases is the Facerec dataset which has a large number of small negative eigenvalues and many possibly meaningful positive eigenvalues. Any kind of correction of the eigenspectrum of this dataset addressing the negative part has almost no effect - the largest negative eigenvalue is $-7e10^{-4}$. In this case, a low-rank approximation removes large parts of the positive eigenspectrum resulting in information loss. As already discussed in former work, there is no simple answer to the correction of eigenvalues. One always has to consider characteristics like the relevance of negative eigenvalues, the ratio between negative and positive eigenvalues, the complexity of the eigenspectrum, and the properties of the desired machine learning model. The results clearly show that the proposed advanced shift correction is particularly useful if the negative eigenvalues are meaningful and a low-rank approximation of the similarity matrix is tolerable.

5 CONCLUSIONS

In this paper, we presented an alternative formulation of the classical eigenvalue shift, preserving the structure of the eigenspectrum of the data. Furthermore, we pointed to the limitations of the classical shift induced by the shift of all eigenvalues, including those with small or zero eigenvalue contributions.

Surprisingly, the classical shift eigenvalue correction is nevertheless frequently recommended in the literature pointing out that only a suitable offset needs to be applied to shift the matrix to psd. However, it is rarely mentioned that this shift affects the entire eigenspectrum and thus increases the contribution of eigenvalues that had no contribution in the original matrix. As a result of our approach, the eigenvalues that had vanishing contribution before the shift remain irrelevant after the shift. Those eigenvalues with a high contribution keep their relevance, leading to the preservation of the eigenspectrum but with a positive (semi-)definite matrix. In combination with the low-rank approximation, our approach was, in general, better compared to the classical methods.

Future work on this subject will include a possible adoption of the advanced shift to unsupervised scenarios. Another field of interest is the reduction of the computational costs using advanced matrix approximation and decomposition (Musco and Woodruff, 2017; Sanyal et al., 2018) in the different sub-steps.

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