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1 Sixth Mittweida Workshop on Computational Intelligence

From 02. Juli to 04. Juli 2014 we had the pleasure to organize and attend the sixth Mittweida Workshop on Computational Intelligence (MiWoCi 2014) as a satellite event of 10th Workshop on Self Organizing Maps (WSOM’14). Multiple scientists from the University of Bielefeld, HTW Dresden, the University of Groningen (NL), the SOM Japan Inc (Japan), the University of Birmingham (UK) and the University of Applied Sciences Mittweida met in Mittweida, Germany, to continue the tradition of the Mittweida Workshops on Computational Intelligence - MiWoCi’2014.

The aim was to present their current research, discuss scientific questions, and exchange their ideas. The seminar centered around topics in machine learning, signal processing and data analysis, covering fundamental theoretical aspects as well as recent applications, partially in the frame of innovative industrial cooperations. This volume contains a collection of extended abstracts and short papers which accompany some of the discussions and presented posters of the MiWoCi Workshop.

Apart from the scientific merits, this year’s seminar came up with the great chance to attend the 10th Workshop on Self Organizing Maps (WSOM’14). WSOM is the major anchor conference focusing on Self Organizing Maps and is not only a perfect chance to meet high renowned researchers in the field but also to attend the three invited plenary talks given during WSOM 2014:

- Prof. Dr. Michael Biehl, University Groningen (NL), Johann-Bernoulli-Institute of Mathematics and Computer Sciences
- Prof. Dr. Erzsebet Merenyi, Rice University Houston (USA), Department of Statistics and Department of Electrical and Computer Engineering
- Prof. Dr. Fabrice Rossi, Universite Paris1- Pantheon-Sorbonne, Department Statistique, Analyse, Modélisation Multidisciplinaire (SAMM)

This year the MiWoCi Workshop was also accompanied by a poster spotlight at the WSOM 2014 for each poster contribution and a best poster award was announced.

Our particular thanks for a perfect local organization of the workshop go to Thomas Villmann as spiritus movens of the seminar and his PhD and Master students.

Mittweida, July, 2014
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Interpretation of linear mappings employing $l_1$ regularization

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Abstract

In this contribution we propose a new technique to judge the relevance of features for a given linear mapping, thereby taking redundancy and interdependence of features into account.

We employ a two step optimization strategy: In the first step, we linearly minimize the $l_1$-norm of the linear mapping $\sum_i |w_i|$, while taking redundancies in the data distribution into account. Since the first step does not necessarily yield a unique solution, we search in this solution space by minimizing/maximizing the absolute value of each single feature, respectively.

Thus, we obtain a lower and upper bound of relevance for each feature, indicating how important it minimally and maximally is (similar to strong and weak relevance in the literature).

Acknowledgement

Funding by the CITEC center of excellence is gratefully acknowledged.
Hellinger divergence in information theoretic novelty detection

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Abstract
A novelty detection framework proposed in 2009 by M. Filippone and G. Sanguinetti [6] is considered, which is suitable for small training sample sizes and allows control over the false positive rate. It is based on estimating the information content a test sample yields via the Kullback-Leibler divergence. In case of a Gaussian density estimation this approach is analytically tractable and for Gaussian mixtures appropriate approximations are provided. Here the framework is expanded by allowing the use of the Hellinger divergence [10] instead, summarizing the work done in [16].

1 Introduction
Outlier detection is an important task in machine learning where outliers – observations which deviate markedly from a given sample of training data [9] – are to be identified. There are many applications such as fault detection [2, 5] or monitoring medical conditions [14, 17], where such problems arise. Novelty detection concerns the case that no anomalous data is available in the training phase of the system. This is the case when outliers are costly or difficult to obtain, or when anomalous data can not to be modeled in advance. For instance, it would be unreasonable to sabotage an aircraft engine just to obtain anomalous observation data [13] and a new method of fraud is unlikely to be modeled in advance [4, 11].

Since outliers (true positives) are rare by definition, the accuracy alone is not sufficient for evaluating a novelty detection system. The framework presented here allows control over the false positive rate (fpr), which is the rate at which normal data samples (true negatives) give rise to an outlier alarm.

The key idea of the information theoretic approach is to first model the training data alone, and to train a second model which also takes a test point into account. The two models are then compared using a divergence. This is in [6] the Kullback-Leibler divergence. Here we consider the Hellinger divergence instead, which is symmetric and therefore easier to be interpreted as a distance-like measure. If the test point is a true negative, the two models are expected to be similar, resulting in a low divergence; and if it is a true positive the second model is expected to be strongly adapted, hence inducing a high divergence. Since the divergences considered here are defined for probability density functions, it is necessary to model the data via a probabilistic approach.

The goal is then to find a divergence threshold of acceptance for a test sample, which is found via Monte Carlo simulation. In this simulation phase a statistical test – in this work referred to as the F-test – is implemented, which significantly improves the performance of the framework. The framework is restricted to Gaussian mixture models (GMMs), hence assuming the data to be distributed normally. In case of single-component Gaussian densities it is analytically tractable.

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The paper is structured as follows: In Section 2 the process of modeling data via GMMs is considered. In Section 3 the F-test is reviewed in order to incorporate it into the framework. In Section 4 the Hellinger divergence is approximated to allow an implementation. The performance of the framework is illustrated on an artificial dataset and validated on the well-known Iris dataset in Section 5, before a conclusion is given in Section 6.

2 Data model

Let \( X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d \) be the training set of samples, where each \( x_i \) is drawn from a normal distribution. Let \( f \) be the GMM with \( c \) components fitted to the training data (training model)

\[
f(x) = \sum_{k=1}^{c} \hat{\pi}_k N(x | \hat{m}_k, \hat{S}_k);
\]

\[
N(x | \hat{m}_k, \hat{S}_k) = \frac{1}{\sqrt{2\pi\hat{S}_k}} \exp \left( \frac{(x - \hat{m}_k)^T \hat{S}_k^{-1} (x - \hat{m}_k)}{2} \right),
\]

where the parameters \( \hat{\pi}_k \) denote the estimated mixing coefficients, \( \hat{m}_k \) the estimated means and \( \hat{S}_k \) the sample covariances for each component \( i \in [c] := \{1, \ldots, c\} \). The distinction between parameter estimations \( \hat{\pi}_i, \hat{m}_i, \hat{S}_i \) and the true parameters \( \pi_i, m_i, S_i \) of the generating density will become important in the next section. Such a GMM with maximal likelihood

\[
\sum_{i=1}^{n} f(x_i) \rightarrow \max
\]

can be obtained via the Expectation/Maximization (E/M) algorithm [3], where the user has to know the number of components \( c \) in advance. For a test sample \( x_\ast \) the training model \( f \) is adjusted to the adapted model \( f^\ast \)

\[
f^\ast(x) = \sum_{k=1}^{c} \hat{\pi}_k^\ast N(x | \hat{m}_k^\ast, \hat{S}_k^\ast),
\]

which is obtained by performing only a single E/M-step on \( X \cup \{x_\ast\} \), starting from the parameters of \( f \). Under the assumption that adding a single point to the fitted dataset leads to small changes in the parameter estimations of the GMM, it is reasonable that a single E/M step might already give a good estimate of the new parameters. The reason for doing this is that the updated parameters then can be denoted in closed form. It is then eventually possible to formulate an explicit divergence approximation which only depends on \( x_\ast \) and the parameters of \( f \).

The Expectation step does not affect any responsibility \( u_{ik} \) of component \( k \) for the training sample \( x_i \), whereas the responsibilities for \( x_\ast \) are:

\[
u_{ik} = \frac{\hat{\pi}_k N(x_\ast | \hat{m}_k, \hat{S}_k)}{\sum_{r=1}^{c} \hat{\pi}_r N(x_\ast | \hat{m}_r, \hat{S}_r)}
\]

The updated cardinality of component \( k \) is

\[
u_k^\ast = n_k + u_{ik} + u_{ik}^\ast = \sum_{i=1}^{n} u_{ik} + u_{ik}^\ast
\]

and the updated parameter estimates are

\[
\hat{\pi}_k = \frac{n_k^\ast + u_{ik}^\ast}{n_k + 1}; \quad \hat{m}_k^\ast = \hat{m}_k + \frac{u_{ik}^\ast}{n_k^\ast} \bar{x}_{ik}; \quad \hat{S}_k^\ast = \frac{n_k}{n_k^\ast} \left( \hat{S}_k + \frac{u_{ik}^\ast}{n_k^\ast} \bar{x}_{ik} \bar{x}_{ik}^T \right),
\]

where \( \bar{x}_{ik} := (x_\ast - \hat{m}_k) \).
3 The F-test

Let \( X = \{ x_1, \ldots, x_n \} \) be the training set, where each \( x_i \in \mathbb{R}^d \) is drawn from a multivariate Gaussian distribution \( \mathcal{N}(\mathbf{m}, \mathbf{S}) \). The maximum likelihood estimation of the generating distribution based on \( X \), \( \mathcal{N}(\hat{\mathbf{m}}, \hat{\mathbf{S}}) \), is unique and known explicitly with parameters

\[
\hat{\mathbf{m}} = \frac{1}{n} \sum_{i=1}^{n} x_i, \quad \hat{\mathbf{S}} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \hat{\mathbf{m}})(x_i - \hat{\mathbf{m}})^T.
\]

One could find a decision threshold for a test sample \( x_* \) via generating a user-specified number of vectors from this estimated density (Monte Carlo simulation). These simulated vectors yield a distribution of density evaluations, which allows to choose a threshold \( \theta \) based on the preferred false positive rate.

The major flaws of this approach are that (a) it is a multivariate test for the intrinsically one-dimensional decision \( f(x_*) \geq \theta \) and (b) the generating function of the simulated samples depends on the parameter estimations \( \hat{\mathbf{m}}, \hat{\mathbf{S}} \). These are random variables themselves and their prediction quality is significantly impaired for small values of \( n = |X| \):

\[
\hat{\mathbf{m}} \sim \mathcal{N}(\mathbf{m}, \frac{1}{n} \mathbf{S}), \quad n\hat{\mathbf{S}} \sim \mathcal{W}(n-1)(\mathbf{S}),
\]

where \( \mathcal{W}(\nu) \) denotes the Wishart distribution with \( \nu \) degrees of freedom. In order to improve the Monte Carlo simulation, the distribution of the squared Mahalanobis distance \( \hat{z}^2 \) between a test point \( x_* \) and the sample mean \( \hat{\mathbf{m}} \)

\[
\hat{z}^2 = (x_* - \hat{\mathbf{m}})^T \hat{\mathbf{S}}^{-1} (x_* - \hat{\mathbf{m}})
\]
is considered. The following result from statistics is used [1]:

Suppose that \( y \sim \mathcal{N}(0, aS) \) and \( A \sim \mathcal{W}_v(S) \). Then:

\[
y^T A^{-1} y \sim \frac{ad}{\nu - d + 1} F_{d, \nu - d + 1}
\]

The \( F \)-distribution, named after R. A. Fisher [7], is the distribution of the quotient of two \( \chi^2 \)-distributed variables. The degrees of freedom of these \( \chi^2 \)-distributed variables are the parameters of the \( F \)-distribution.

Under the null hypothesis that \( x_* \) was generated by the same distribution as the training set, we have

\[
(x_* - \hat{\mathbf{m}}) \sim \mathcal{N}(0, \left(1 + \frac{1}{n}\right)S)
\]

and therefore, eventually

\[
\hat{z}^2 \sim \frac{(n + 1)d}{n - d} F_{d, n - d}.
\]

The statistical test based on this result is referred to as the \( F \)-test. It takes the uncertainty caused by the number of training samples \( n \) and the number of dimensions \( d \) into account. It is furthermore optimal in the sense that the distribution of \( \hat{z}^2 \) is independent of the estimated parameters \( \hat{\mathbf{m}} \) and \( \hat{\mathbf{S}} \). Furthermore, since this imposes a univariate test, multidimensional calculations can be circumvented completely in the simulation phase for Gaussian density estimations.

When GMMs are used, however, certain multidimensional calculations are necessary. The position of a simulated point \( x_* \) determines all \( \hat{z}^2 \)'s

\[
\forall k \in [c] : \hat{z}^2_k = (x_* - \hat{\mathbf{m}}_k)^T \hat{\mathbf{S}}_k^{-1} (x_* - \hat{\mathbf{m}}_k),
\]

which makes it necessary to compute the corresponding Mahalanobis distances \( \hat{z}^2_i \), \( i \in [c] \setminus \{k\} \) when \( \hat{z}^2_k \) is generated. This can be done [6] via

\[
\hat{z}^2_j = \frac{1}{2} \left[ \hat{\mathbf{S}}_j^{-1/2} \hat{\mathbf{v}}_k \right]^2 + \left[ \hat{\mathbf{S}}_j^{-1/2} (\hat{\mathbf{m}}_k - \hat{\mathbf{m}}) \right]^2 + 2 \sqrt{\hat{z}^2_k (\hat{\mathbf{m}}_k - \hat{\mathbf{m}})} \hat{\mathbf{S}}_j^{-1/2} \hat{\mathbf{v}}_k,
\]

where \( \hat{\mathbf{v}}_k \) is a randomly generated unit norm vector.
4 $D_H$ approximation

In order to implement the information theoretic approach, it is necessary to compare a training model to an adapted model. This can be done via divergences. In [6] the well-known Kullback-Leibler divergence ($D_{KL}$) [12] is used, which is based on the concept of self-information introduced by Shannon [15]. We propose the Hellinger divergence

$$D_H(f||g) = 1 - \int_{\mathbb{R}^d} \sqrt{f \cdot g} \, dx,$$

(5)

to be implemented instead, which is defined for probability densities $f, g$. In contrast to $D_{KL}$, $D_H$ is symmetric, which makes it easier to be interpreted as a distance-like measure. It is not to be mistaken as a metric, however, since it violates the triangle inequality.

Now, the goal is to derive an explicit formula of the divergence between a training model $f$ and an adapted model $f^*$ fitted to $X \cup \{x_*\}$. In case the densities are GMMs, the integral in Equation (5) is not analytically tractable, making approximations necessary for efficient computing. For GMMs the above equation translates to:

$$D_H(f||f^*) = 1 - \int_{\mathbb{R}^d} \sqrt{f \cdot f^*} \, dx = 1 - \int_{\mathbb{R}^d} \sum_{k=1}^c \hat{\pi}_k \mathcal{N}_k \cdot \sum_{r=1}^c \hat{\pi}_r^* \mathcal{N}_r^* \, dx$$

$$\mathcal{N}_i := \mathcal{N}(x|\hat{\mu}_i, \hat{\Sigma}_i), \quad \mathcal{N}_r^* := \mathcal{N}(x|\hat{\mu}_r^*, \hat{\Sigma}_r^*)$$

The notation from the end of Section 2 is used.

The root of the sum is no further tractable analytically. *Jensen’s Inequality* is used to obtain an upper bound:

$$1 - \int_{\mathbb{R}^d} \sum_{k=1}^c \hat{\pi}_k \mathcal{N}_k \cdot \sum_{r=1}^c \hat{\pi}_r^* \mathcal{N}_r^* \, dx \leq 1 - \sum_{k=1}^c \sum_{r=1}^c \hat{\pi}_k \hat{\pi}_r^* \int_{\mathbb{R}^d} \sqrt{\mathcal{N}_k \cdot \mathcal{N}_r^*} \, dx$$

The remaining integral is analytically tractable [16]:

$$\int_{\mathbb{R}^d} \sqrt{\mathcal{N}_k \cdot \mathcal{N}_r^*} \, dx = \left( \frac{\exp \left( - (\hat{\mu}_k - \hat{\mu}_r^*)^T (\hat{\Sigma}_r^* + \hat{\Sigma}_k)^{-1} (\hat{\mu}_k - \hat{\mu}_r^*) \right)}{\left| \frac{1}{4} (\hat{\Sigma}_r^* + \hat{\Sigma}_k)^{-1} (\hat{\Sigma}_r^{-1} + \hat{\Sigma}_k^{-1}) \right|} \right)^{\frac{1}{4}}$$

(6)

This yields a formula for $D_H$ that depends on $x_*$ (implicitly) and the parameters of the model $f$. However, a framework based on this formula imposes questionable rejection regions, as discussed in [16]. A second approximation is done by neglecting the above term for $k \neq r$, leading to another upper bound for the Hellinger divergence:

$$D_H(f||f^*) \leq 1 - \sum_{k=1}^c \hat{\pi}_k \hat{\pi}_k^* \int_{\mathbb{R}^d} \sqrt{\mathcal{N}_k \cdot \mathcal{N}_k^*} \, dx$$

(7)

A similar approximation is done for $D_{KL}$ in [6]. The last approximation furthermore allows the following step: In order to incorporate the $F$-test it is necessary to reformulate the above formula in terms of $z^2_1, \ldots, z^2_d$ instead of $x_*$. The detailed calculation is rather intricate, applying the *Sherman-Morrison formula* and using a certain reasoning from [6] to explicitly evaluate the determinant in the denominator of the right-hand side of (6). It can be found in [16]. The resulting formula for the integral can then be expressed as:

$$\left( \int_{\mathbb{R}^d} \sqrt{\mathcal{N}_k \cdot \mathcal{N}_k^*} \, dx \right)^4 = \exp \left( \frac{(n_k - n_k^*)u_{kk}z^2_k - n_k^2u^{2*}_{kk}z^2_k}{(n_k + n_k^*)u_{kk}^2z^2_k} \right) \frac{(4n_k)^d n_k^{d-1}(n_k^* + u_{kk}z^2_k)(n_k + n_k^*)^{2(1-d)}}{[(n_k + n_k^*)^2 + (2(n_k + n_k^*) + u_{kk}z^2_k)u_{kk}z^2_k]}$$

(8)

The notation from the end of Section 2 is used.
5 Framework & Experiments

Algorithm 1 Novelty detection framework for $D_H$

 Require: training set $X$, #GMM components $c$, #Monte Carlo samples $m$, false positive rate $r$, test sample $x_*$

 Fit $GMM f$ to $X$ with the E/M algorithm

 /* Monte Carlo simulation */
 for $i = 1, \ldots, c$
 do
 generate $m\pi_i$ values of $\hat{z}_i^2$ using (2)
 generate $m\hat{\pi}_i$ unit norm vectors $\mathbf{v}_i$
 $\forall j \in [c]\{i\}$ : calculate $\hat{z}_j^2$'s using (4)
 end for

 evaluate $D_H$ with (7) and (8) for each sample
 return $(1-r)$-th quantile $\theta$ of these evaluations

 evaluate $D_H(x_*)$ using (3) and (8)
 if $D_H(x_*) \geq \theta$ then
 $x_*$ is outlier
 else
 $x_*$ is normal
 end if

5.1 Artificial dataset

In order to illustrate the behavior of the approximation $D_H$ of the Hellinger divergence, an artificial dataset is considered first. In this example 100 data points are drawn from $c = 3$ bivariate Gaussians (about 33 each), which resemble the letter "A" (Figure 1). A GMM is fitted to this data, and a Monte Carlo simulation according to the $F$-distribution from Section 3 is performed. This way, using the approximations from Section 4 for $D_H$ and those from [6] for $D_{KL}$, decision thresholds for $D_H$ and $D_{KL}$ are obtained. The statistical test $L_F$ from [16] is also considered. The false positive rate is chosen to be $fpr = 0.03$. The outlier decision is made for a $10^3 \times 10^3$ test grid of points over $[-5,5]^2$, which is depicted in Figure 2. The main differences between the three methods are visible in areas where the decision borders of components overlap or are in close proximity.

5.2 Iris

The framework is validated on the well-known Iris dataset, which was introduced by R. A. Fisher in 1936 [8]. The data consists of 150 data samples (Iris plants) in 3 classes -- "Iris setosa", "Iris versicolor" and "Iris virginica", each consisting of 50 samples. Each observation is made of $d = 4$ features -- sepal length, sepal width, petal length and petal width. The classes "versicolor" and "virginica" are combined into one pool of 100 normal datasamples and the 50 "setosa" class members are considered anomalous. A sample of size...
\( n \in \{30, 35, \ldots, 80\} \) is randomly drawn from the normal data and the remaining \( 150 - n \) points serve as the test set of samples. The GMM is chosen to have \( c = 2 \) components and the fpr is chosen to be 0.03; \( 10^6 \) Monte Carlo samples are simulated to obtain the corresponding decision threshold. For each \( n \), this experiment is repeated 100 times, the averages of the achieved accuracy and false positive rate are depicted in Figure 3. Three methods are considered: a purely statistical test \( L_F \) [16], as well as the above framework using the approximations of the Hellinger divergence \( D_H \) and the Kullback-Leibler divergence \( D_{KL} \) [6].

Other validation examples can be found in [16].
6 Conclusion

With the formulas presented here it is possible to use the symmetric Hellinger divergence instead of its Kullback-Leibler counterpart in the framework from [6]. The measures $D_H$ and $D_{KL}$ perform similarly, whereas the former is easier to interpret as a distance-like measure. However, the performance of both methods is questioned by that of a purely statistical approach based on (2) – both in robustness and in control of the fpr. This is discussed in more detail in [16].

References


The new proposal of the calculation for the significance degree by once SOM learning
-using iris, gene, and other data-

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Abstract—The significance degree of each component was calculated only by once SOM learning where the Spherical Self-Organizing-Map (SSOM) was used for the demonstration. In the method, kinds of specimens of the data are inserted in each column as each specimen. The method is first demonstrated using the iris data and then gene data. The method can be used for other data with successful results. The method can also be processed by the usual planar SOM.

Keywords—Self organizing map; Significance degree;

I. INTRODUCTION

Here, the aim of the new proposal is described. Table 1 is the explanation of the concept of the significance degree. Relation between the fatigue and the other components about it is shown in Table 1. There is fatigue in the A group but there is none in the B group.

Table 1 Experimental condition for testing presence or absence of fatigue among other components.

<table>
<thead>
<tr>
<th></th>
<th>Fatigue</th>
<th>Vividness</th>
<th>Vigor</th>
<th>Tired</th>
<th>Exhaustion</th>
</tr>
</thead>
<tbody>
<tr>
<td>A group</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>B group</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>A-B</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

This time, the way of allocating Table 2 is considered for being fatigued or not being fatigued like in the two dimensional space.

Table 2 Fatigue in Table 1 is separated by Yes and No

<table>
<thead>
<tr>
<th>Fatigue</th>
<th>Fatigue No</th>
<th>Vividness</th>
<th>Vigor</th>
<th>Tired</th>
<th>Exhaustion</th>
</tr>
</thead>
<tbody>
<tr>
<td>A group</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>B group</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

In the way in Table 2, the fatigue can be equally evaluated from the A group, as well as from the B group. In other words, if gathering the one where 1 stands in feeling fatigued, the significance degree of feeling fatigued is found from the each item. Also, if gathering the one where 1 stands feeling not fatigued, the significance degree of feeling not fatigued is found from the each item. This time, the proposed method is applied to the iris data which were used last time.

II. THE ALGORITHM OF CALCULATING THE SIGNIFICANCE DEGREE

The contents are first described using iris data [1]. Using Spherical Self-Organizing Maps (SSOM) method [2,3,4] The significance degree calculation was previously introduced [5]. This time, the proposed method is as follows that the significance degree between each label pairs is computed by the once learning a lot of label data groups. First, the contents are described by the iris data. Next, the generality of the concerned method is described by using Gene and Tof-SIMS data [6]. The part of the original iris data is shown in tables 3 and 4. The data are composed of 1 (setosa), 2 (versicolor), and 3 (virginica), (each 50 stocks of 1, 2, and 3). A learning result is shown in Fig. 1.
Table 3 Part of the original iris data with 4 components. The classifications are added as setosa, versicolor and virginica by 3 columns.

<table>
<thead>
<tr>
<th></th>
<th>1_set</th>
<th>2_ver</th>
<th>3_gnc</th>
<th>Sepal_length</th>
<th>Sepal_width</th>
<th>Petal_length</th>
<th>Petal_width</th>
</tr>
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<td>0</td>
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<td>3</td>
<td>1.4</td>
<td>0.3</td>
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<td>51</td>
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<td>0.2</td>
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<td>1</td>
<td>7</td>
<td>3.2</td>
<td>4.7</td>
<td>1.4</td>
</tr>
<tr>
<td>55</td>
<td>2.2</td>
<td>0</td>
<td>1</td>
<td>6.4</td>
<td>3.2</td>
<td>4.5</td>
<td>1.5</td>
</tr>
<tr>
<td>56</td>
<td>2.3</td>
<td>0</td>
<td>1</td>
<td>6.9</td>
<td>3.1</td>
<td>4.9</td>
<td>1.5</td>
</tr>
<tr>
<td>57</td>
<td>2.4</td>
<td>0</td>
<td>1</td>
<td>5.5</td>
<td>3.3</td>
<td>4</td>
<td>1.3</td>
</tr>
<tr>
<td>58</td>
<td>2.5</td>
<td>0</td>
<td>1</td>
<td>6.5</td>
<td>2.8</td>
<td>4.6</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Table 4 The border between 2 (versicolor) and 3 (virginica).

<table>
<thead>
<tr>
<th></th>
<th>1_set</th>
<th>2_ver</th>
<th>3_gnc</th>
<th>Sepal_length</th>
<th>Sepal_width</th>
<th>Petal_length</th>
<th>Petal_width</th>
</tr>
</thead>
<tbody>
<tr>
<td>98</td>
<td>2.46</td>
<td>0</td>
<td>1</td>
<td>5.7</td>
<td>3</td>
<td>4.2</td>
<td>1.2</td>
</tr>
<tr>
<td>100</td>
<td>2.47</td>
<td>0</td>
<td>1</td>
<td>5.7</td>
<td>2.9</td>
<td>4.2</td>
<td>1.3</td>
</tr>
<tr>
<td>101</td>
<td>2.48</td>
<td>0</td>
<td>1</td>
<td>6.2</td>
<td>2.9</td>
<td>4.3</td>
<td>1.3</td>
</tr>
<tr>
<td>102</td>
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<td>1</td>
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<td>2.5</td>
<td>3</td>
<td>1.1</td>
</tr>
<tr>
<td>103</td>
<td>2.50</td>
<td>0</td>
<td>1</td>
<td>5.7</td>
<td>2.8</td>
<td>4.1</td>
<td>1.3</td>
</tr>
<tr>
<td>104</td>
<td>3.1</td>
<td>0</td>
<td>0</td>
<td>6.3</td>
<td>3.3</td>
<td>6</td>
<td>2.5</td>
</tr>
<tr>
<td>105</td>
<td>3.2</td>
<td>0</td>
<td>0</td>
<td>5.8</td>
<td>2.7</td>
<td>5.1</td>
<td>1.9</td>
</tr>
<tr>
<td>106</td>
<td>3.3</td>
<td>0</td>
<td>0</td>
<td>7.1</td>
<td>3</td>
<td>5.9</td>
<td>2.1</td>
</tr>
<tr>
<td>107</td>
<td>3.4</td>
<td>0</td>
<td>0</td>
<td>6.3</td>
<td>2.9</td>
<td>5.6</td>
<td>1.8</td>
</tr>
<tr>
<td>108</td>
<td>3.5</td>
<td>0</td>
<td>0</td>
<td>6.5</td>
<td>3</td>
<td>5.8</td>
<td>2.2</td>
</tr>
</tbody>
</table>

The raw data are normalized in the column wise direction. As an example, when the comparison between the classification 1_set and 2_ver is carried out, 3_gnc in Table 3 must be erased. Leave the label, 1 and 2 of each 50 stocks, 100 stocks in amount as shown in Table 8. Then, continue the calculation.

The result is shown in Fig.1. (a) is the U-matrix display which shows the distances between the nodes. (b) is the color display where the boundaries among the clusters of 1, 2, and 3 are clearly classified. The red mark in (b) on the spherical surface is the one of iris classification 1(setosa) where the minimum value (0.981816) is shown. Also, 2_11 in classification 2 and 3_20, in classification 3, shows the minimum value where label code books have minimum value of 0.991068 in 2_11 and 0.987421 in 3_20. They are on the other side of the sphere.

Fig.1 (a) The U- matrix display at Griff value (0). (b) The boundary in coloring display of 1_set, 2_ver, and 3_gnc region.
Data processing is as follows. (a) Arrange the table in the descending order of a B column of 1_set in the code book vector of 642 nodes. Then, search the minimum value of 1_16. Above it, compute the average and the result in the 130th line. (b) Next, carry the same procedure of a) in C column of 2_ver And search the minimum code book label of 2_11. (c) In the same way, arrange and search the minimum value as 3_20 to the D column, in the descending order of 3_gnc. Then, computes the average values at 146th line, and 152th line, respectively.

Table 6 shows the summary of Table 5. Data processing is as follows. Copy the 130th line in (a), 146th line in (b) and 152th line in (c), in the previous Table 5 and multiply them by 100 times.
Table 7 shows the differences of 2ver-1set, 3gnc-1set and 2ver-3gnc. Those were calculated using the averaged values with each line, based on Table 6. The direction of the subtraction is for the comparison between the conventional method and the proposed method for the 2 clusters.

Table 7 The differences of 2ver-1set, 3gnc-1set and 2ver-3gnc

<table>
<thead>
<tr>
<th>g</th>
<th>1_set</th>
<th>2_ver</th>
<th>3_gnc</th>
<th>Sepal_length</th>
<th>Sepal_width</th>
<th>Petal_length</th>
<th>Petal_width</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>1.46</td>
<td>1.00</td>
<td>0.133888889</td>
<td>0.416666667</td>
<td>0.087979661</td>
<td>0.083333333</td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>1.47</td>
<td>0.00</td>
<td>0.223222222</td>
<td>0.75</td>
<td>0.101694951</td>
<td>0.041666667</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>1.48</td>
<td>1.00</td>
<td>0.083333333</td>
<td>0.5</td>
<td>0.077979661</td>
<td>0.041666667</td>
<td></td>
</tr>
<tr>
<td>51</td>
<td>1.49</td>
<td>1.00</td>
<td>0.277777778</td>
<td>0.708333333</td>
<td>0.087979661</td>
<td>0.041666667</td>
<td></td>
</tr>
<tr>
<td>52</td>
<td>1.50</td>
<td>1.00</td>
<td>0.194444444</td>
<td>0.541666667</td>
<td>0.087979661</td>
<td>0.041666667</td>
<td></td>
</tr>
<tr>
<td>53</td>
<td>2.1</td>
<td>0.00</td>
<td>0.583333333</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
<td></td>
</tr>
<tr>
<td>54</td>
<td>2.2</td>
<td>0.00</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>2.3</td>
<td>0.00</td>
<td>0.333333333</td>
<td>0.125</td>
<td>0.508474576</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>56</td>
<td>2.4</td>
<td>0.00</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
<td></td>
</tr>
<tr>
<td>57</td>
<td>2.5</td>
<td>0.00</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
<td></td>
</tr>
</tbody>
</table>

Next, normalization of the iris raw data of Table 3 and 4 was carried out. Those are shown in Table 8. Normalization data of only setosa 1 and versicolor 2, with 100 stocks are used.

Table 8 Normalization of the iris data of 1_set and 2_ver (yellow columns)

<table>
<thead>
<tr>
<th>g</th>
<th>1_set</th>
<th>2_ver</th>
<th>Sepal_length</th>
<th>Sepal_width</th>
<th>Petal_length</th>
<th>Petal_width</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>1.46</td>
<td>1.00</td>
<td>0.133888889</td>
<td>0.416666667</td>
<td>0.087979661</td>
<td>0.083333333</td>
</tr>
<tr>
<td>49</td>
<td>1.47</td>
<td>0.00</td>
<td>0.223222222</td>
<td>0.75</td>
<td>0.101694951</td>
<td>0.041666667</td>
</tr>
<tr>
<td>50</td>
<td>1.48</td>
<td>1.00</td>
<td>0.083333333</td>
<td>0.5</td>
<td>0.077979661</td>
<td>0.041666667</td>
</tr>
<tr>
<td>51</td>
<td>1.49</td>
<td>1.00</td>
<td>0.277777778</td>
<td>0.708333333</td>
<td>0.087979661</td>
<td>0.041666667</td>
</tr>
<tr>
<td>52</td>
<td>1.50</td>
<td>1.00</td>
<td>0.194444444</td>
<td>0.541666667</td>
<td>0.087979661</td>
<td>0.041666667</td>
</tr>
<tr>
<td>53</td>
<td>2.1</td>
<td>0.00</td>
<td>0.583333333</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
<tr>
<td>54</td>
<td>2.2</td>
<td>0.00</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
<tr>
<td>55</td>
<td>2.3</td>
<td>0.00</td>
<td>0.333333333</td>
<td>0.125</td>
<td>0.508474576</td>
<td>0.5</td>
</tr>
<tr>
<td>56</td>
<td>2.4</td>
<td>0.00</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
<tr>
<td>57</td>
<td>2.5</td>
<td>0.00</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
</tbody>
</table>

Table 9 shows the same data of Table 8. The classification column is different as the class identifier allocated to one column.

Table 9 Same data of Table 8. Class identifier column is different

<table>
<thead>
<tr>
<th>g</th>
<th>2_ver-1_set</th>
<th>Sepal_length</th>
<th>Sepal_width</th>
<th>Petal_length</th>
<th>Petal_width</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>1.46</td>
<td>0.133888889</td>
<td>0.416666667</td>
<td>0.087979661</td>
<td>0.083333333</td>
</tr>
<tr>
<td>49</td>
<td>1.47</td>
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<td>0.75</td>
<td>0.101694951</td>
<td>0.041666667</td>
</tr>
<tr>
<td>50</td>
<td>1.48</td>
<td>0.083333333</td>
<td>0.5</td>
<td>0.077979661</td>
<td>0.041666667</td>
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<tr>
<td>51</td>
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<td>0.041666667</td>
</tr>
<tr>
<td>52</td>
<td>1.50</td>
<td>0.194444444</td>
<td>0.541666667</td>
<td>0.087979661</td>
<td>0.041666667</td>
</tr>
<tr>
<td>53</td>
<td>2.1</td>
<td>0.583333333</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
<tr>
<td>54</td>
<td>2.2</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
<tr>
<td>55</td>
<td>2.3</td>
<td>0.333333333</td>
<td>0.125</td>
<td>0.508474576</td>
<td>0.5</td>
</tr>
<tr>
<td>56</td>
<td>2.4</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
<tr>
<td>57</td>
<td>2.5</td>
<td>0.664016667</td>
<td>0.5</td>
<td>0.593220339</td>
<td>0.583333333</td>
</tr>
</tbody>
</table>

The results of the proposed method are shown in Fig. 2. In Fig. 2(b), the proposed method is applied only to two cases of Table 9.

Fig. 2 (a) The significance degree among versicolor : setosa calculated using Tables 3 and 4 (b) using Table 9
Fig. 3 is moreover compared adding with the conventional method in Table 9. Hereinafter, other combinations of the significance degree of virginica : versicolor and also of virginica : setosa are included. The comparison among the total 3 methods of the proposed 2 methods and a conventional method is shown for these 3 cases in Fig. 3. The significance degree are calculated and compared among 2-ver-1set of versicolor: setosa, 3gnc-1set of versinica : setosa, and 3gnc-2ver of virginica : versicolor. The significance degree among gnc-ver of virginica : versicolor doesn't agree only a little as shown in the figure.

In case of the iris data, in the first, the data of three kinds of the total 150 stocks were normalized in the column direction. In the case of the computations for 2 methods, this original normalized data were used and computed. In this case, all 3 methods approximately fully agreed as shown in Fig. 3.

III. THE APPLICATION TO THE GENE DATA

Here, we have the data where the relation between the breast cancer and the gene are examined, respectively. Breast cancer is classified into 4 steps to the breast cancer level 5, 4, 2-3 from 1 of the health. Here, 1 of the health and 5 of the breast cancer are compared in the significance degree. 40 cases are classified into 1-5 level of the cancer by the doctor. Each of the gene of 40 cases was named in 1-831. Further, the level 2 and 3 are gathered altogether as 2-3 for simplicity. By the method which is described in the Tables 3 and 4, the flags of 4 steps of 1, 2-3, 4, and 5 were put up as shown in Table 10. The data of Table 10 was studied by the Spherical SOM. Incidentally, the gene data was normalized at the maximum-the minimum of the gene to 1-831 in each sample. This is the so-called line normalization. The number of component is large as 831. Therefore, the number of the flags was set as the weight. Total 20 columns in amount are the flags of 4 clusters with five lines of each cluster as shown in Table 10. Four kinds of the label of 1, 2-3, 4, and 5 are used as classification. Learning data and a learning result are shown in Table 10, and Fig. 4, respectively.

---

**Table 10** The learning data normalized at the line (row) direction

| A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | X | Y | Z |
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
| 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 2 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 3 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 4 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 6 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 7 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 8 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 9 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 10 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 11 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 12 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 13 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 14 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 15 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 16 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 17 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 18 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 19 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 20 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

---
Using the learning codebook vector of Fig. 4, the calculation of the same as Tables 5 and 6 was carried out. The average of each cluster was calculated. The 5th line was subtracted from the 9th line. The significance degree of 5-1 is tabled on the 12th line. The colored flags of the clusters at the 12th line were deleted here. Only the significance degree of the gene was graphed. The results are shown in Table 11.

Table 11 The significance degree of 5-1

|    | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | X | Y | Z | AA | AB | AC |
| 2  |   | 2.5| 2.5| 2.3| 2.3| 1 | 1 | 1 | 1 | 1 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 |
| 4  | 1 | 2.3| 2.3| 2.3| 2.3| 1 | 1 | 1 | 1 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 |
| 6  | 1.0| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02| 0.02|
| 8  | 4.0| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01|
| 10 | 4.0| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01|
| 12 | 5.0| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01| 0.01|

Only the part of the gene with the 12th line of Table 11 was graphed in Fig. 5. In Fig. 5(a), To the 1-150th gene and skipping a little interval, (b) To 301-450th gene. + side is intentional gene with 5, the breast cancer. - side is the healthily intentional gene with 1 cluster.

![Fig. 4 The SOM learning result using the data in Table 10. (a) 1 cluster, (b) 2-3 cluster, (c) 4 cluster, and (d) 5 cluster](image)

![Fig. 5 The SOM learning result using the data in Table 10. (a) 1 cluster, (b) 2-3 cluster, (c) 4 cluster, and (d) 5 cluster](image)

![Fig. 5 Graph of significance degree of Table 8. (a) to 1-150th gene, (b) to 301-450th gene](image)
The characteristics of the significance degree between 5-1 can be seen from Figs. 5 and 6. It has begun with Fig. 5(a) already, but the bigger the gene number becomes, the smaller significance degree becomes on the healthy 1 side. Specifically, in figure 6(b), most peaks are on the 5 sides of the breast cancer.

![Fig. 6 Significance degree. (a) to 601-750th gene, (b) to 751-831th gene. A little interval is skipped.](image_url)

Table 12 shows the significance degree on the 5 side of the breast cancer equal to or more than 40 degree was chosen in each gene number range. The number of the higher significance degree is especially high in 1-150th gene number range. The green color range shows equal to or more than 45.

<table>
<thead>
<tr>
<th>Gene Range</th>
<th>Significance Degree</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-150</td>
<td>(a) to 601-750th gene</td>
</tr>
<tr>
<td>751-831</td>
<td>(b) to 751-831th gene</td>
</tr>
<tr>
<td></td>
<td>A little interval is skipped.</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 12 The significance degree on the 5 side of the breast cancer</th>
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<tbody>
<tr>
<td>Gene Range</td>
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<tr>
<td>------------</td>
</tr>
<tr>
<td>1-150</td>
</tr>
<tr>
<td>751-831</td>
</tr>
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<td></td>
</tr>
</tbody>
</table>

Next, the side of 1 health is shown in Table 13. In the range of 1-151, the number of the genes which have the absolute value of the significance degree equal to or more than -40 is more than on the side above of 5 breast cancer (cf. 65). Equal to or less than 40 genes are equally distributed approximately compared with Table 12. On the significance degree for the side of the health, it can be seen that the high significance gene is the 47th and 741st gene from the table.

<table>
<thead>
<tr>
<th>Table 13 Significance degree of the side of 1 health</th>
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<tbody>
<tr>
<td>Gene Range</td>
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<tr>
<td>------------</td>
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<tr>
<td>1-150</td>
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<td>751-831</td>
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Machine Learning Reports
Tables 12 and 13 are generalized. The genetic code which shows the characteristic of the gene is next to the gene number. For the gene of the higher strength of the green color, the highest value for the 1 health side shows -65. In other words, the healthy gene has the clear characteristics. However, there are many, too, numbers of the manifestation in the genes on the 5 side of the breast cancer. The strength is uniformly, too. The gene comparison between the breast cancer and the health, was evaluated using the method of this significance degree. As for the manifestation gene of the breast cancer, both the manifestation quantity and the number of the manifestation are high compared with the side of the health. In this way, it is possible to diagnose breast cancer from the genetic code.

Incidentally, it was examined the breast cancer of which level the strange sample is in. By considering in which area of 4 areas of Fig. 4 there is a sample of strange (UK), the cancer level of the sample can be distinguished.

IV. CONCLUSIONS

Thus, a new method for calculating the significance degree was proposed using the Spherical Self-Organizing Maps (SSOM). It was verified by the iris 3 data. The procedure is of leaving the same flag which is equal to each label of 3 kinds of data. In this way, each label (the classification) could be equally compared. When the significance degree which was sought in this method of using all 3 data and the significance degree which were sought in two combinations, were compared, the results reasonably agreed as shown in Fig. 3. Also, using this method of the significance degree, the gene comparison between the breast cancer (stage 5) and the health (stage 1), was evaluated. As for the breast cancer, both the manifestation quantity and the number of the manifestation of the gene are high compared with the side of the health. Thus, it is possible to diagnose breast cancer from the gene examination. The iris, and the gene data are the examples which the human being classified a cluster by some procedure. However, in case of the ToF-SIMS data of the unknown clustering, it was automatically classified using Spherical SOM. However, the results of the analysis for the TOF-SIMS data are deleted due to insufficient space.

As the conclusion, a general procedure is described as follows:

1. Any data can be learned by the Spherical SOM.
2. The spherical surface was deformed considering the distance (U-matrix) among the learned nodes. Then, a classification is carried out and a dendrogram is constructed.
3. Here, the optional group to be analyzed can be chosen. 1 or 0 of the classification was assigned to the chosen group for the number of the classification like Tables 3, 4, and 8.
4. This data is once again, learned by the Spherical SOM method. The significance degree among two kinds of classification for each is evaluated by the procedure which is shown in Tables 5, 6, and 7.

Incidentally, a little, the precision falls however, it is possible to compute the significance degree by the plane SOM. When the classification becomes three kinds for example, in multiple regression [7], it cannot avoid allocating the classification with -1, 0, 1 (or 0, 1, 2). To the group which doesn't have an order, it is improper to allocate an order having to do with a number. It is possible to be solved if making the classification of three-dimensional as (1,0,0 ••• ) as having proposed this time.

REFERENCES

LEARNING ALGORITHMS FOR NON-METRIC SPACES - A SHORT SURVEY -

Frank-M. Schleif and Peter Tino

1 Department of Computer Science, University of Birmingham, UK

1. INTRODUCTION

Machine learning is a key element in data analysis systems and often used to analyze standard vectorial data with the Euclidean distance.

With the advent of web and social media data this has rapidly changed. Many data are now given as

NEW non-standard or structured data with indefinite proximities

by means of dedicated, often non-metric proximity measures. Due to the mathematical power and efficiency of the Euclidean space only few methods were proposed for non-Euclidean data and even less for non-metric data analysis. In this contribution we provide a short review of the few available algorithms and concepts for non-metric data analysis as available today.

OLD in metric spaces similarities between two objects \( x, y \in X \) calculated as a mapping \( \phi: X \to F \) using the kernel trick [21], \( k: X \times X \to F \) with \( k(x, x') = \phi(x)^T \phi(x') \), \( \forall x, x' \in X \). Thereby it is assumed that the kernel function \( k(x, x') \) is positive semi definite (psd).

NEW For non-psd \((\cdot, \cdot)\) a Krein space has to be used which for finite dimensions is a pseudo-Euclidean space \((P_2)\). We can always embed \( X \) into \( P_2 \) for symmetric dissimilarities with constant zero diagonal [9].

Definition 1 (Pseudo-Euclidean space [16]) A pseudo-Euclidean space \((P_2)\) is a real vector space equipped with a non-degenerate, indefinite inner product \((\cdot, \cdot)_p\). \((\cdot, \cdot)_p\) admits a direct orthogonal decomposition \( \xi = \xi_+ \oplus \xi_- \) where \( \xi_+ \subset \mathbb{R}^n \) and \( \xi_- \subset \mathbb{R}^m \) and the inner product is positive definite on \( \xi_+ \) and negative definite on \( \xi_- \).

A symmetric bilinear form in this space is given by

\[
(x, y)_p = \sum_{i=1}^{p} x_i y_i - \sum_{i=p+1}^{q} x_i y_i = X^T L_p Y
\]

where \( L_p \) is a diagonal matrix with \( p \) entries 1 and \( q \) entries -1. The eigendecomposition of \( S = U A U^T \) provides a vectorial representation \( \mathbf{V} \) in \( P_2 \):

\[
\mathbf{V} = U [A]^{1/2}_p
\]

For symmetric (non-psd) similarities with low intrinsic dimension this can be calculated exact and in linear time [20].

USAGE:

- use the decomposition to learn the model in \( \xi_+ \) and \( \xi_- \) by late recombination [14];
- incriments of the model (e.g. scatter matrix) can be calculated on the decomposition [18, 24];
- just learn e.g. a generic regression function \( f(x) = \sum_{i=1}^{p} w_i \phi_i(x) + b \) which can be related to the indefinite \( k(x, \cdot) \) [11, 3];
- local metric adaptations [2, 5] to correct violated triangle inequalities.

1. Learning in non-metric spaces is relevant [7, 16, 19, 13]
2. Only few approaches around - still often limited (theory, runtime, scalability, .).
3. Specific effects of transformations not really understood [8, 12, 15]
4. First steps on establishing a theory on learning in non-metric spaces [1, 23]
5. Most approaches focus on supervised learning or retrieval

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2. COMMON (NON-METRIC) SIMILARITY MEASURES

Non-metric proximities (similarities and dissimilarities) are frequent if domain specific measures are used. There is often not even an explicit vector space available.

- alignment (Bioinformatics)
- Levenshtein (Textprocessing)
- Hamming (Information theory)
- Geodesic distance (Geometry)
- jaccard index (Statistics)
- Compression distance
- dynamic time warping (time-series)

Other examples for indefinite proximities:

- Manhattan kernel \( k(x, x') = -||x - x'||_1 \)
- indefinite sigmoid kernel \( k(x, x') = \tanh(a(x^T x') + r) \) (for some parameters \( a, r \))
- Many divergence measures popular in the field of spectroscopy

Outcome: (non-)metric proximities with negative eigenvalues in the eigenspectrum.

3. CURRENT APPROACHES - MAKE IT GLOBAL PSD

Consider negative eigenvalues as noise - correct the eigenpsd to noise.

(1) Eigenspectrum correction

(2) Proxy alignment (find a similar psd matrix)

(3) Similarity space approach

(4) Do nothing (can easily fail)

(1) Eigenspectrum correction

(2) Proxy alignment (find a similar psd matrix)

(3) Similarity space approach

(4) Do nothing (can easily fail)

Construct a vector space from the proximity matrix [27]

4. SUMMARY

1. Learning in non-metric spaces is relevant [7, 16, 19, 13]
2. Only few approaches around - still often limited (theory, runtime, scalability, .).
3. Specific effects of transformations not really understood [8, 12, 15]
4. First steps on establishing a theory on learning in non-metric spaces [1, 23]
5. Most approaches focus on supervised learning or retrieval

REFERENCES


ROC-Optimization and Statistical Quality Measures in Learning Vector Quantization Classifiers

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¹Johann-Bernoulli-Institute for Mathematics and Computer Sciences, University Groningen, The Netherlands
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Abstract

This paper deals with the integration of statistical measures into the framework of prototype-based learning vector quantization for learning of binary classification problems. In particular, the evaluation and optimization of the confusion matrix by means of a learning vector quantizer is considered keeping the Hebbian learning paradigm for prototype adaptation. In a further step, receiver operating characteristic curves are investigated. The area under the respective curves, which can be equivalently interpreted by a rank-statistics model, serves as an alternative quality measure for parametrized classifiers. As we show, this statistical approach can also be integrated into the learning vector quantization scheme whereas the precision-recall-curve counterpart is not suitable for such a model approach.

1 Introduction - Classification by Learning Vector Quantization

Learning vector quantization (LVQ) models are prototype-based adaptive classifiers for processing vectorial data [15]. Training samples are assumed to be of the form \( \mathbf{v} \in V \subseteq \mathbb{R}^n \) with class labels \( x_\mathbf{v} = x(\mathbf{v}) \in \mathcal{C} = \{1, \ldots, C\} \). The set of prototypes \( W = \{w_j \in \mathbb{R}^n, j = 1 \ldots M\} \) contains representatives of the classes carrying prototype

∗supported by the European Social Foundation Saxony (ESF)
†corresponding author - email: thomas.villmann@hs-mittweida.de
labels $y_j \in C$. Classification decisions for unknown data samples $\tilde{v}$ are usually made according to a winner take all rule, i.e.

$$x_{\tilde{v}} := y_{s(\tilde{v})} \text{ with } s(\tilde{v}) = \arg\min_j (d(\tilde{v}, w_j))$$

where $d(\tilde{v}, w_j)$ is a dissimilarity measure in the data space, frequently chosen as the Euclidean distance. IVQ training amounts to distributing the prototypes in the data space such that the classification error is minimized. Stochastic gradient descent learning have been introduced which is based on objective function

$$E(W, f) = \frac{1}{2} \sum_{v \in V} f(\mu(v))$$

approximating the classification error [22]. Here, the function

$$\mu(v) = \frac{d^+(v) - d^-(v)}{d^+(v) + d^-(v)}$$

is the so-called classifier function. This approach is known as Generalized LVQ (GLVQ) [22]. Here $d^+(v) = d(v, w^+)$ denotes the dissimilarity between the data vector $v$ and the closest prototype $w^+ = w_{s+}$ with the same class label $y_{s+} = x_v$, while $d^-(v) = d(v, w^-)$ is the distance from the best matching prototype $w^-$ with a class label $y_{s-}$ different from $x_v$. The modulation function $f$ in (1) is a monotonically increasing function usually chosen as a sigmoid or the identity function. A typical choice is the Fermi function

$$f_{\theta}(x) = \frac{1}{1 + a \cdot \exp\left(-\frac{(x-x_0)}{\theta^2}\right)}$$

with $x_0 = 0$ and $a = 1$ as standard parameter values. The parameter $\theta$ determines the slope of $f_{\theta}$ but is frequently fixed as $\theta = 1$.

Stochastic gradient learning performs update steps of the form

$$\Delta w^\pm \propto -\frac{\partial f_{\theta}(\mu(v))}{\partial \mu(v)} \cdot \frac{\partial \mu(v)}{\partial d^+(v)} \cdot \frac{\partial d^\pm(v)}{\partial w^\pm}$$

for a randomly chosen data sample $v$.

## 2 Classification Accuracy and Statistical Measures in GLVQ

In the following we demonstrate how to realize a classifier optimizing a statistical measure based on the confusion matrix by means of GLVQ. GLVQ is the preferred choice to keep the intuitive approach of prototype based classification.
Table 1: Contingency / Confusion matrix: TP - true positives, FP - false positives, TN - true negatives, FN - false negatives, \( \hat{N}_+ \) - number of positive/negative data, \( \hat{N} \) - number of predicted positive/negative samples.

<table>
<thead>
<tr>
<th>labels</th>
<th>true</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>( C_+ )</td>
</tr>
<tr>
<td>predicted</td>
<td>( C_+ )</td>
</tr>
<tr>
<td></td>
<td>( C_- )</td>
</tr>
<tr>
<td></td>
<td>( \hat{N}_+ )</td>
</tr>
</tbody>
</table>

In this view, first we observe that the classifier function \( \mu(v) \) from (2) becomes negative if the data point \( v \) is correctly classified, i.e. if \( x_v = y_{s(v)} \) is valid. Further, in the limit \( \theta \downarrow 0 \) the sigmoid \( f_\theta(3) \) becomes the Heaviside function

\[
H(x) = \begin{cases} 
0 & \text{if } x \leq 0 \\
1 & \text{else}
\end{cases}
\]

such that border sensitive classification learning takes place [13]. Thus, in this limit, \( E(W,H) \) counts the misclassifications. Considering a two-class problem with a positive class \( C_+ \) labeled by \( \oplus \) and a negative class \( C_- \) with class label \( \ominus \), these misclassifications are distinguished as the false positives (\( FP \)) and false negatives (\( FN \)) according to the contingency table Tab. 1.

Yet, counting of misclassifications is not always an appropriate evaluation of classifier, in particular, if the data are imbalanced [21]. In statistical analysis contingency table evaluations are well-known to deal with this problem more properly. Several measures were developed to judge the classification quality based on the confusion matrix emphasizing different aspects. For example, precision \( \pi \) and recall \( \rho \), defined as

\[
\pi = \frac{TP}{TP + FP} = \frac{TP}{\hat{N}_+} \tag{6}
\]

and

\[
\rho = \frac{TP}{TP + FN} = \frac{TP}{\hat{N}_+} \tag{7}
\]

respectively, are used in the widely applied \( F_\beta \)-measure

\[
F_\beta = \frac{(1 + \beta^2) \cdot \pi \cdot \rho}{\beta^2 \cdot \pi + \rho} \tag{8}
\]

developed by C.J. van Rijsbergen [20].

To integrate these contingency quantities into a GLVQ-like cost function, we have to approximate them properly while ensuring their dependence on the prototypes is differentiable. For this purpose we introduce the quantity \( \hat{\mu}(v) = f_\theta(-\mu(v)) \) with
\( \hat{\mu}(v) \approx 1 \) iff the data point \( v \) is correctly classified and \( \hat{\mu}(v) \approx 0 \) otherwise for small values \( \theta \), with the derivative

\[
\frac{\partial \hat{\mu}(v)}{\partial w^\pm} = -\frac{\partial \hat{\mu}(v)}{\partial f_\theta} \cdot \frac{\partial f_\theta}{\partial \mu} \cdot \frac{\partial \mu}{\partial d^\pm(v)} \cdot \frac{\partial d^\pm(v)}{\partial w^\pm}.
\]

Thus we can express all quantities of the confusion matrix in terms of the new classifier function \( \hat{\mu}(v) \):

\[
TP = \sum_v \delta_{\oplus,v} \cdot \hat{\mu}(v),
\]

\[
FP = \sum_v \delta_{\ominus,v} \cdot (1 - \hat{\mu}(v)),
\]

\[
FN = \sum_v \delta_{\oplus,v} \cdot (1 - \hat{\mu}(v))
\]

and

\[
TN = \sum_v \delta_{\ominus,v} \cdot \hat{\mu}(v)
\]

with \( \delta_{\oplus,v} \) is the Kronecker symbol and \( \delta_{\ominus,v} = 1 - \delta_{\oplus,v} \). Obviously, all these quantities are also differentiable with respect to \( \hat{\mu}(v) \) and, hence, also with respect to the prototypes \( w_k \). In consequence, an arbitrary general statistical measure can be optimized by a GLVQ-like stochastic gradient learning of the prototypes, if it is continuous and differentiable with respect to \( TP, FP, FN, \) and \( TN \). Clearly, the above mentioned quantities precision \( \pi \) and recall \( \rho \) as well as the \( F_\beta \)-measure belong to this function class and, therefore, can be plugged into the GLVQ learning scheme.

3 Receiver Operation Characteristic Optimization and GLVQ

The Receiver Operation Characteristic (ROC) is an important tool for performance comparison of binary classifiers. A classifier is considered superior if it delivers a higher value of the area under the ROC-curve (AUC). Following [4], the AUC refers to the true distribution of positive and negative instances, but it can be estimated using a sample. The normalized Wilcoxon-Mann-Whitney statistic [25, 18] reveals the maximum likelihood of the true AUC for a given classifier [26]. Several method were developed to maximize AUC directly including gradient descent learning [11], approximated AUC optimization [5], reject option optimization [17], AUC optimization by linear programming [1] or ranking based optimization [8], to name just a few of the recently proposed approaches. Yet, for prototype based classification based on LVQ, which can be seen as a robust variant of the nearest-neighbor classifier [12], a direct optimization scheme for AUC is not known so far. As we will show in this chapter, the GLVQ variant of the basic LVQ scheme can be easily adapted for AUC optimization.
3.1 Probability Interpretation of AUC

Suppose the binary classification problem for classes \(A\) and \(B\) and related datasets \(V_A\) and \(V_B\) with cardinalities \(#V_A\), \(#V_B\), respectively. Further assume that a classifier delivers a continuous output (discriminant function) \(\vartheta\) used for the classification decision. Then the AUC can be interpreted as the probability \(P_{AB}\) that a classifier will rank a randomly chosen \(A\)-instance \(v_A \in V_A\) higher than a randomly chosen \(B\)-instance \(v_B \in V_B\) \([7]\). In this view we can formulate an equivalent cost function introducing the (local) ordering function

\[
O_\theta (v_A, v_B) = f_\theta (\vartheta (v_A) - \vartheta (v_B))
\]

for an ordered pair \((v_A, v_B)\) of vectors. We approximate \(P_{AB}\) by

\[
P_{AB} (\theta) = \frac{1}{#V_{AB}} \sum_{(v_A, v_B)} O_\theta (v_A, v_B)
\]

depending on the slope parameter \(\theta\) of the sigmoid function \(f_\theta (x)\) from (3). If \(\theta \downarrow 0\) holds, \(P_{AB} (\theta)\) converges to \(P_{AB}\) for \(#V_{AB} \rightarrow \infty\) according to the underlying rank statistics \([18, 25]\) and paying attention to the functional limit \(f_\theta \rightarrow H\) for \(\theta \downarrow 0\) with the Heaviside function \(H\) from (5).

3.2 A cost function for AUC based on GLVQ

The probabilistic interpretation of the AUC introduced in the previous subsection can be facilitated in the GLVQ-framework. To this end, the discriminant function \(\vartheta\) in (9) is replaced by a discriminant function \(\mu_{AB}\) specifically designed for the GLVQ and, hence based on the prototypes used in GLVQ. In particular, we define

\[
\mu_{AB} (v, \gamma) = \frac{d^B (v) - d^A (v)}{d^A (v) + d^B (v)} - \gamma
\]

with \(d^A (v) = d^A (v, w_A^* (v))\) where \(w_A^* (v)\) is the closest prototype to \(v\) responsible for class \(A\). Analogously, \(w_B^* (v)\) and \(d^B (v)\) are defined in the same manner. The parameter \(\gamma \in [-1, 1]\) defines a threshold shifting the decision boundary between \(w_A^*\) and \(w_B^*\), which plays the role of the varying parameter for the ROC-curve. The unbiased case is obtained for the choice \(\gamma = 0\). With these settings the ROC cost function for a respective GLVQ-scheme reads as

\[
E_{ROC} (\theta, V_A, V_B, W) = \frac{1}{#V_{AB}} \sum_{(v_A, v_B)} f_\theta (\mu_{AB} (v_A, \gamma) - \mu_{AB} (v_B, \gamma))
\]

again depending on the slope parameter \(\theta\) of the sigmoid function \(f_\theta (x)\) from (3). Hence, border sensitive learning in this ROC-GLVQ, i.e. forcing \(\theta \downarrow 0\) in (9), leads to the limit

\[
E_{ROC} (\theta, V_A, V_B, W) \xrightarrow{\theta \downarrow 0} P_{AB}.
\]
Further, using the derivatives
\[
\frac{\partial \mu_{AB}(v, \gamma)}{\partial w_A^*(v)} = \frac{dB(v)}{(d^A(v) + d^B(v))^2} \cdot \frac{\partial d^A(v)}{\partial w_A^*(v)}
\]
and
\[
\frac{\partial \mu_{AB}(v, \gamma)}{\partial w_B^*(v)} = -\frac{d^A(v)}{(d^A(v) + d^B(v))^2} \cdot \frac{\partial d^B(v)}{\partial w_B^*(v)}
\]
we can calculate the gradients of the GLVQ-adapted ordering function
\[
O_{\theta}^{\mu AB}(v_A, v_B) = f_\theta (\mu_{AB}(v_A, \gamma) - \mu_{AB}(v_B, \gamma))
\]
regarding to both \( v_A \) and \( v_B \), respectively:
\[
\frac{\partial O_{\theta}^{\mu AB}(v_A, v_B)}{\partial w_A^*(v_A)} = \frac{\partial f_\theta}{\partial z}\bigg|_z \cdot \left( \frac{\partial \mu_{AB}(v_A, \gamma)}{\partial w_A^*(v_A)} - \frac{\partial \mu_{AB}(v_B, \gamma)}{\partial w_A^*(v_A)} \right)
\]
\[
\frac{\partial O_{\theta}^{\mu AB}(v_A, v_B)}{\partial w_B^*(v_B)} = \frac{\partial f_\theta}{\partial z}\bigg|_z \cdot \left( \frac{\partial \mu_{AB}(v_B, \gamma)}{\partial w_B^*(v_B)} - \frac{\partial \mu_{AB}(v_B, \gamma)}{\partial w_B^*(v_B)} \right)
\]
\[
\frac{\partial O_{\theta}^{\mu AB}(v_A, v_B)}{\partial w_A^*(v_B)} = \frac{\partial f_\theta}{\partial z}\bigg|_z \cdot \left( \frac{\partial \mu_{AB}(v_A, \gamma)}{\partial w_A^*(v_B)} - \frac{\partial \mu_{AB}(v_B, \gamma)}{\partial w_A^*(v_B)} \right)
\]
\[
\frac{\partial O_{\theta}^{\mu AB}(v_A, v_B)}{\partial w_B^*(v_A)} = \frac{\partial f_\theta}{\partial z}\bigg|_z \cdot \left( \frac{\partial \mu_{AB}(v_B, \gamma)}{\partial w_B^*(v_A)} - \frac{\partial \mu_{AB}(v_B, \gamma)}{\partial w_B^*(v_A)} \right)
\]
with \( z = \mu_{AB}(v_A, \gamma) - \mu_{AB}(v_B, \gamma) \).

In consequence, GLVQ-like stochastic gradient learning is possible also for the ROC cost function \( E_{ROC} \) from (12). However, for this purpose a \textit{structured input}
\[
v_{AB} = (v_A, v_B)
\]
is required in GLVQ learning. Thus, stochastic gradient descent learning on \( E_{ROC-GLVQ} \) takes place with respect to \( w_A^*(v_A), w_A^*(v_B), w_B^*(v_A), \) and \( w_B^*(v_B) \) using the gradients (15)–(18) of the GLVQ-adapted ordering function \( O_{\theta}^{\mu AB} \) from (14) depending on the randomly selected structured input \( v_{AB} \). We emphasize at this point that the ROC-GLVQ delivers an AUC-optimizing scheme only in the limit \( \theta \searrow 0 \) of border sensitive learning.

### 3.3 The ROC-LVQ model

In the previous section we introduced a cost function for AUC based on the GLVQ-paradigm. Although frequently assumed, the standard GLVQ does not guarantees the prototypes to being class representative after learning [19, 9]. To enhance this property a generative cost function amount
\[ E_{\text{GEN}}(\theta, V_A, V_B, W) = \sum_{(v_A, v_B)} d^A(v_A) + d^B(v_B) \]  

has to be added to \( E_{\text{ROC}} \) from (12) such that the overall ROC-GLVQ cost function becomes

\[ E_{\text{ROC-GLVQ}}(\theta, V_A, V_B, W, \alpha) = (1 - \alpha) \cdot E_{\text{GEN}} + \gamma \cdot E_{\text{ROC}} \]  

with the balancing parameter \( \alpha \in [0, 1] \) weighting both aspects classification-separation versus description of class distribution [12].

4 Precision-Recall-Curves and GLVQ

Precision-Recall-Curves (PR-curves) are closely related to ROC but do not provide the identical information [2, 6, 16]. Therefore, they can provide additional insides. Precision and recall as introduced in (6) and (7), respectively, are intensively used for test statistics and classification problems in medical applications. In this area, the recall \( \rho \) is often denoted as sensitivity describing the ability of the classifier to detect positive samples accurately. The counterpart of the sensitivity is the specificity value

\[ \varsigma = \frac{TN}{TN + FP} = \frac{TN}{N} \]  

judging the ability for detecting negative samples. Precision-recall-relations are frequently investigated taking the \( F_\beta \)-measure from (8) with \( \beta = 1 \) [16]. This is just the ratio of the arithmetic and the geometric mean of precision and recall, i.e.

\[ F_1 = \frac{2 \cdot \pi \cdot \rho}{\pi + \rho} \]  

However, for evaluation of PR-curves, only a few approaches were proposed [3, 2, 16]. In the following we will identify the difficulties arising, if one would like to adapt the ideas of AUC-maximization learning in GLVQ to PR-curve optimization by GLVQ.

4.1 Basic Definitions and Notations

We follow the explanations in [3]: We denote the class \( A \) as positive class and \( B \) is the negative. The real-valued model output for the positive samples \( v_A \) is \( y^A \) and, analogously, negative samples \( v_B \) generate \( y^B \). The class skew \( S \) is defined as the probability \( S = P(A) \) and also known as prevalence or a prior class distribution. The recall can be written as a probability

\[ \rho(c) = P(y^A > c) \]  

whereas the precision \( \pi \) is a conditional probability

\[ \pi(c) = P(v \in A | z > c) . \]
In this formula, \( z = z(v) \) is the overall real-valued output of the classifier model for a given unclassified sample \( v \) being a mixture of \( y^A \) and \( y^B \). With this definitions, the precision-recall-curve \( PR \) is the set

\[
PR = \{(\rho(c), \pi(c)), \ -\infty < c < \infty\}.
\]

We assume larger outputs to be associated with positive samples. In consequence, as \( c \) decreases, the recall \( \rho(c) \) increases to one and the precision \( \pi(c) \) approaches to \( S \). The area \( \Theta \) under the precision-recall-curve (AUCPR) is an average of the precision weighted by the probability of a given threshold \( c \):

\[
\Theta = \int_{-\infty}^{\infty} \pi(c) dP(y^A \leq c)
\]  

(25)

Since, \( \pi(c) \) and \( P(y^A \leq c) \) are both bounded on the unit square, the inequality \( 0 \leq \Theta \leq 1 \) holds. Therefore, \( \Theta \) can be interpreted as a probability. According to [3], the integral (25) can be interpreted as the fraction of positive examples among those examples whose output values exceed a randomly selected threshold \( c \). Eq.(25) can be written equivalently as

\[
\Theta = \int_{0}^{1} \pi(c) d\rho(c)
\]  

(26)

paying attention to the fact that for \( -\infty \leq c \leq \infty \) the range \( \rho(c) \in [0, 1] \) is valid [16, 14].

There exist several estimators for \( \Theta \) in case of real datasets \( V = V_A \cup V_B \) [3]. One powerful estimator avoiding the explicit determination of the empirical curve \( PR \) is the the averaged precision

\[
\hat{\Theta} = \frac{1}{\#V_A} \sum_{i=1}^{\#V_A} \hat{\pi}(y^A_i)
\]  

(27)

and

\[
\hat{\pi}(x) = \frac{S \cdot \hat{\rho}(x)}{S \cdot \hat{\rho}(x) + \frac{(1-S)}{\#V_B} \sum_{j=1}^{\#V_B} I(y^B_j > x)}
\]  

(28)

is the empirical precision estimate with

\[
\hat{\rho}(x) = \frac{1}{\#V_A} \sum_{i=1}^{\#V_A} I(y^A_i > x)
\]  

(29)

being the empirical estimate of the recall \( \rho(x) \) and \( I(E) \) is the indicator function of the event \( E \).

4.2 PRC-LVQ

According to the previous ROC-GLVQ model assumptions we have to define a GLVQ-output in the sense of a discriminat function. For this purpose we make use of the already declared and define

\[
\hat{\mu}_{AB}(v) = -\mu_{AB}(v)
\]  

(30)
as PR-LVQ discriminant function, which is in agreement with the assumption that larger outputs should be associated with positive samples. Further, we replace the indicator function \( I(y > x) \) by the Heaviside-function \( H(y - x) \) from (5) and approximate the latter one by the sigmoid function \( f_\theta \) from (3). Doing so and estimating the skew \( S = \frac{\#V_A}{\#V_B} \), the estimator \( \hat{\Theta} \) from (27) for the AUCPR can be written as a cost function

\[
E_{PRC}(\theta, V_A, V_B, W) = \frac{1}{\#V_A} \sum_{i=1}^{\#V_A} \frac{1}{1 + \frac{(1-S)\sum_{j=1}^{\#V_B} f_\theta(\hat{\mu}_{AB}(v_B^j) - \hat{\mu}_{AB}(v_A^i))}{\sum_{k=1}^{\#V_A} f_\theta(\hat{\mu}_{AB}(v_A^k) - \hat{\mu}_{AB}(v_A^i))}}
\]

(31)

to be minimized in dependence on the prototype set \( W \). In analogy to the above ROC-LVQ cost function we finally obtain the formal PRC-LVQ cost function as

\[
E_{PRC-LVQ}(\theta, V_A, V_B, W, \gamma) = (1 - \gamma) \cdot E_{GEN} + \gamma \cdot E_{PRC}
\]

(32)

with \( E_{GEN} \) being the generative part (19).

However, this cost function \( E_{PRC} \) contains nested sums over the single events \( v_A^k \) and \( v_B^j \) in contrast to the pairwise events \( (v_A, v_B) \) considered in the cost function (12) of AUCs for GLVQ. Thus stochastic gradient descent learning would become complicate for this model, because of the nested sums. Therefore, other optimization strategies like Expectation-Maximization should be investigated instead. However, this is behind the scope of this introduction article and will be studied in the future.

5 Conclusion

We present in this article the mathematical framework for learning of prototype-based LVQ-classifiers to optimize statistical quality measures based on the confusion matrix or receiver operating characteristic. We further obtained a GLVQ modification for maximizing explicitly the area under the ROC-curve, whereas a derivation of a similar method for precision-recall-curve optimization failed.

Obviously, the obtained approaches can be easily combined with other advanced GLVQ-techniques like relevance and matrix learning or kernelized variants [10, 23, 24].
References


About the Generalization of the Eigen-Problem for Semi-Inner Products in Minkowski-\(\ell_p\)-Spaces

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Abstract

Semi-inner products as generalization of inner products are recently discussed in several machine learning approaches for classification and vector quantization. This technical paper considers the eigen-problem from the perspective of semi-inner products and discusses related numerical and algebraic problems for its solution.

1 Introduction - the Usual Eigen-Problem

We start introducing the usual eigen-problem (EP) based on the usual inner product. This is done to clarify notations and to relate the later eigen-problem in case of semi-inner products to the usual ones.

For this purpose let \( V \) be a vector space over the field \( \mathbb{K} \) assumed to be \( \mathbb{R} \) or \( \mathbb{C} \). The linear map \( f : V \rightarrow V \) is supposed to be an endomorphism. The EP consists in determination of a pair \((\lambda, v)\) such that \( f(v) = \lambda v \) is valid with \( \lambda \in \mathbb{K} \), \( v \in V \) and \( v \neq 0 \). Then \( v \) is denoted as eigenvector of \( f \) and \( \lambda \) the respective eigenvalue. If we further assume that \( \dim(V) = n < \infty \) is finite then \( f \) uniquely corresponds to a \( n \times n \)-matrix \( A \) over the field \( \mathbb{K} \), i.e. \( A \in \mathbb{K}^{n \times n} \) and the EP becomes

\[
Av = \lambda v
\]

also denoted more precisely as the right-side EP (REP) with \( v \) being a column vector. Analogously, we can define the left-side EP (LEP) as

\[
v^T A = \lambda v^T
\]
where \( v^T \) denotes the transposed vector.

In this paper we will use the following notations for a given matrix \( B \in K^{m \times n} \):

- \( B_{i,:} \): row \( i \in \{1,2,...,m\} \) of the matrix \( B \)
- \( B_{:,j} \): column \( j \in \{1,2,...,n\} \) of the matrix \( B \)
- \( B_{i,j} = (B)_{i,j} \) matrix element at the position \( i, j \) of the matrix \( B \)
- \( I \) is the \( n \)-dimensional unity matrix

The vector space as \( V := \mathbb{C}^n \) together with the Euclidean inner product \( \langle \cdot, \cdot \rangle_E \) is a Hilbert space. Thus the REP (1.1) writes as

\[
Av = \lambda v \iff \begin{pmatrix}
\langle A^T_{1\to}, v \rangle_E \\
\langle A^T_{2\to}, v \rangle_E \\
\vdots \\
\langle A^T_{n\to}, v \rangle_E 
\end{pmatrix} = \lambda v
\]

with the induced norm \( \|x\|_2 = \sqrt{\langle x, x \rangle_E} \).

Several numerical methods were developed to solve the REP, like

- v.-Mises-iteration with deflation
- inverse v.-Mises-iteration
- the QR-algorithm
- Krylov-subspace-method

to name just a few. They make intensively use of the Hermitian symmetry of the inner product \( \langle \cdot, \cdot \rangle_E \), which implies the sesqui-linearity, i.e.

\[
\langle v, \lambda \cdot w \rangle_E = \lambda \cdot \langle v, w \rangle_E
\]

and linearity in the first argument. We refer to \([3, 8]\), for further reading.

## 2 The Eigen Problem in the Minkowski-\( p \)-Space

Now we turn to consider normed complete vector spaces, i.e. Banach spaces. A prominent example is the \( n \)-dimensional Minkowski-\( p \)-space \( \ell_p^n \) over the complex numbers \( \mathbb{C} \) equipped with the Minkowski-\( p \)-norm

\[
\|x\|_p = \left( \sum_{k=1}^{n} |x_k|^p \right)^{1/p}
\]

for \( 1 \leq p \leq \infty \).

For Banach spaces does not necessarily exist an inner product. However, a weaker concept can be identified - semi-inner products (SIPs) as introduced by G. Lumer \([5]\):
**Definition 1** A semi-inner product \([\cdot,\cdot]\) of a vector spaces \(V\) over the field \(K\) is a map

\[
[\cdot,\cdot] : V \times V \longrightarrow K
\]

with the following properties

1. \([\cdot,\cdot]\) is semi-definite
   \[
   \forall x \in V : [x,x] \geq 0 \quad \text{and} \quad [x,x] = 0 \iff x = 0
   \]

2. \([\cdot,\cdot]\) is linear with respect to the first argument, i.e.
   \[
   \forall x, y, z \in V, \forall \xi \in K : \xi \cdot [x,z] + [y,z] = [\xi \cdot x + y, z]
   \]

3. \([\cdot,\cdot]\) fulfills the Cauchy-Schwarz inequality
   \[
   \forall x, y \in V : |[x,y]|^2 \leq [x,x][y,y]
   \]

Note that the Hermitian symmetry, as it is valid for inner products according to (1), is not required for SIPs and the triangle inequality for inner products is replaced by the Cauchy-Schwarz inequality. Lumer has shown that each Banach space \(B\) with norm \(\|\cdot\|_B\) can be equipped with a SIP \([\cdot,\cdot]_B\) such that the norm is generated, i.e.

\[
\|x\|_B = \sqrt{[x,x]_B}.
\]

Generally, several SIPs may deliver the same norm. Uniqueness can be obtained by additional requirements, like differentiability in the second argument and other. We refer to [2] for details.

The previously mentioned Banach space \(\ell_p^n\) obeys the unique SIP

\[
[x,y]_p = \frac{1}{(\|y\|_p^{p-2})} \sum_{k=1}^{n} x_k \cdot \bar{y}_k \cdot |y_k|^{p-2}
\]

(2.1)

as shown in [2]. In the next step we introduce for this space an analog procedure to the Euclidean matrix multiplication from (1.2). For matrices \(A \in K^{m \times l}\) and \(B \in K^{l \times n}\) we define the operation \(\diamond\) with respect to the SIP (2.1) for the \(\ell_p^n\)-space as

\[
A \diamond B := \begin{pmatrix}
[AT_{1 \to}, B_{11}]_p & [AT_{1 \to}, B_{21}]_p & \cdots & [AT_{1 \to}, B_{n1}]_p \\
[AT_{2 \to}, B_{11}]_p & [AT_{2 \to}, B_{21}]_p & \cdots & [AT_{2 \to}, B_{n1}]_p \\
\vdots & \vdots & \ddots & \vdots \\
[AT_{m \to}, B_{11}]_p & [AT_{m \to}, B_{21}]_p & \cdots & [AT_{m \to}, B_{n1}]_p
\end{pmatrix}
\]

(2.2)

denoted as SIP-matrix-multiplication (SIP-MM). The following lemma can be stated:
**Lemma 2** Let \(A \in \mathbb{K}^{m \times k}, B \in \mathbb{K}^{k \times l}\) and \(C \in \mathbb{K}^{l \times n}\) be matrices. Then
\[
A \cdot (B \circ C) = (A \cdot B) \circ C
\]
is valid, whereby \(A \cdot B\) denotes the Euclidean matrix multiplication (EMM) with respect to the Euclidean inner product in agreement with (1.2).

**Proof.** We consider an arbitrary matrix element \((A \cdot (B \circ C))_{i,j}\) and show that
\[
(A \cdot (B \circ C))_{i,j} = ((A \cdot B) \circ C)_{i,j} \quad \forall i = 1, \ldots, m \text{ and } \forall j = 1, \ldots, n
\]
is valid: Using the linearity of the SIP with respect to the first argument we derive
\[
(A \cdot (B \circ C))_{i,j} = A_{i} \cdot \left( \begin{bmatrix} [B_{1 \rightarrow}^{T}, C_{j \downarrow}]_{p} \\ [B_{2 \rightarrow}^{T}, C_{j \downarrow}]_{p} \\ \vdots \\ [B_{k \rightarrow}^{T}, C_{j \downarrow}]_{p} \end{bmatrix} \right)
\]
\[
= \sum_{h=1}^{k} A_{i,h} \cdot [B_{h \rightarrow}^{T}, C_{j \downarrow}]_{p}
\]
\[
= \sum_{h=1}^{k} [A_{i,h} \cdot B_{h \rightarrow}^{T}, C_{j \downarrow}]_{p}
\]
\[
= \left[ \left( \sum_{h=1}^{k} A_{i,h} \cdot B_{h \rightarrow} \right)^{T}, C_{j \downarrow} \right]_{p}
\]
\[
= \left[ (A_{i} \cdot B)^{T}, C_{j \downarrow} \right]_{p}
\]
\[
= ((A \cdot B) \circ C)_{i,j}
\]
showing the stated property. \(\blacksquare\)

Now we are able to define the REP and the LEP in Banach spaces with respect to a given SIP:

**Definition 3** Let \(\mathbb{B}\) be a \(n\)-dimensional Banach space over the field \(\mathbb{K}\) with the norm \(\| \cdot \|_{\mathbb{B}}\). Let \([\cdot, \cdot]_{\mathbb{B}}\) be a SIP with \(\|x\|_{\mathbb{B}} = \sqrt{[x, x]_{\mathbb{B}}}\). The REP for a matrix \(A \in \mathbb{K}^{n \times n}\) with respect to the SIP \([\cdot, \cdot]_{\mathbb{B}}\) is defined as the determination of the pair \((\lambda, \mathbf{v})\) with \(\lambda \in \mathbb{K}\) and \(\mathbf{v} \in \mathbb{B}\) such that
\[
A \circ \mathbf{v} = \lambda \mathbf{v} \iff \begin{bmatrix} [A_{1 \rightarrow}^{T}, \mathbf{v}]_{\mathbb{B}} \\ [A_{2 \rightarrow}^{T}, \mathbf{v}]_{\mathbb{B}} \\ \vdots \\ [A_{n \rightarrow}^{T}, \mathbf{v}]_{\mathbb{B}} \end{bmatrix} = \lambda \mathbf{v} \quad (2.3)
\]
is valid. The related LEP reads as
\[ v^T \odot A = \lambda v^T \iff ( [v, A_{1\downarrow}]_B, [v, A_{2\downarrow}]_B, \cdots, [v, A_{n\downarrow}]_B ) = \lambda v^T \] (2.4)
and we refer to these as sREP and sLEP, respectively. \((\lambda, v)\) is denoted as an eigen-pair.

3 Numerical Approaches for the sREP and the sLEP

The sREP introduced in (2.3) offers a serious difficulty for its numerical solution. As it was explained above, most of the known numerical methods for the REP in Hilbert spaces utilize the Hermitian linearity (1) of the inner product in the second argument, which is not valid in case of SIPs. To our best knowledge, there is no general way to solve this problem so far by means of classical numerical approaches. An alternative was proposed in [1, 4] based on Hebbian learning for the special case of covariance matrices for a given set \( S \subset \mathbb{R}^n \) of data vectors \( s \in S \): For randomly presented \( s \) and randomly initialized vector \( w \in \mathbb{R}^n \) the adaptation
\[ w = w + \Delta w \]
with
\[ \Delta w = \varepsilon \cdot [s, w]_p \left( s - [s, w]_p \cdot w \right) \] (3.1)
is applied. The positive learning rate \( \varepsilon \) has to be small and decreasing during time, i.e. \( 1 \gg \varepsilon > 0 \) and \( \lim_{t \to \infty} \varepsilon (t) = 0 \) with \( \sum_t (\varepsilon (t))^2 = \infty \). The update scheme (3.1) is known as Oja’s rule in the literature originally introduced for the REP [6, 7]. It delivers the eigenvector belonging to the maximum eigenvalue and can be extended also to calculate more than one eigenvector [9, 1, 4].

For the sLEP the situation is easier, because we can use the linearity of the SIP with respect to the first argument. As the main result of this paper we state the following theorem:

**Theorem 4 (Saralajew & Villmann)** Let \( Q \in \mathbb{K}^{n \times n} \) be a regular matrix over the field \( \mathbb{K} \) and \((\lambda, v)\) be an eigen-pair of the matrix \( A \in \mathbb{K}^{n \times n} \) with respect to the sLEP defined in (2.4). Then \((\lambda, w)\) is an eigen-pair of LEP for the matrix \( B = (Q^{-1} \odot A) \) \( Q \) with respect to the *Euclidean* inner product and \( w = Q^T v \) holds.

**Proof.** Using Lemma 2 we calculate
\[ w^T B = (Q^T v)^T B \]
\[ = v^T Q (Q^{-1} \odot A) Q \]
\[ = v^T (I \odot A) Q \]
\[ = (v^T \odot A) Q \]
\[ = \lambda v^T Q \]
\[ = \lambda w^T , \]
which is the desired result. □

This theorem allows to transfer the sLEP to the usual Euclidean REP:

**Corollary 5 (Saralajew & Villmann)** We consider the matrix \( C = (I \odot A)^T \) for \( A \in \mathbb{K}^{n \times n} \) being a matrix over the field \( \mathbb{K} \). Then the sLEP \( v^T \odot A = \lambda v^T \) can be translated equivalently into the Euclidean REP \( Cv = \lambda v \), i.e.

\[
v^T \odot A = \lambda v^T \iff Cv = \lambda v
\]

holds.

**Proof.** The corollary immediately follows according to

\[
Cv = \lambda v \iff (I \odot A)^T v = \lambda v \\
\iff v^T (I \odot A) = \lambda v^T \\
\iff v^T \odot A = \lambda v^T
\]

applying the previous theorem with \( Q := I \). □

Thus it is possible to solve the sLEP using an arbitrary numerical approach for the Euclidean REP.

4 Conclusion

In this paper we briefly investigate the numerical solution of eigen-problems in Banach spaces, where no inner product is available as they are known from Hilbert spaces. Instead, semi-inner products with weaker requirements are the counterparts there. Whereas the right eigen-problem is difficult to handle, we present a solution for the left-side problem translating it to a right-side problem in an Euclidean space equipped with the Euclidean inner product.
References


