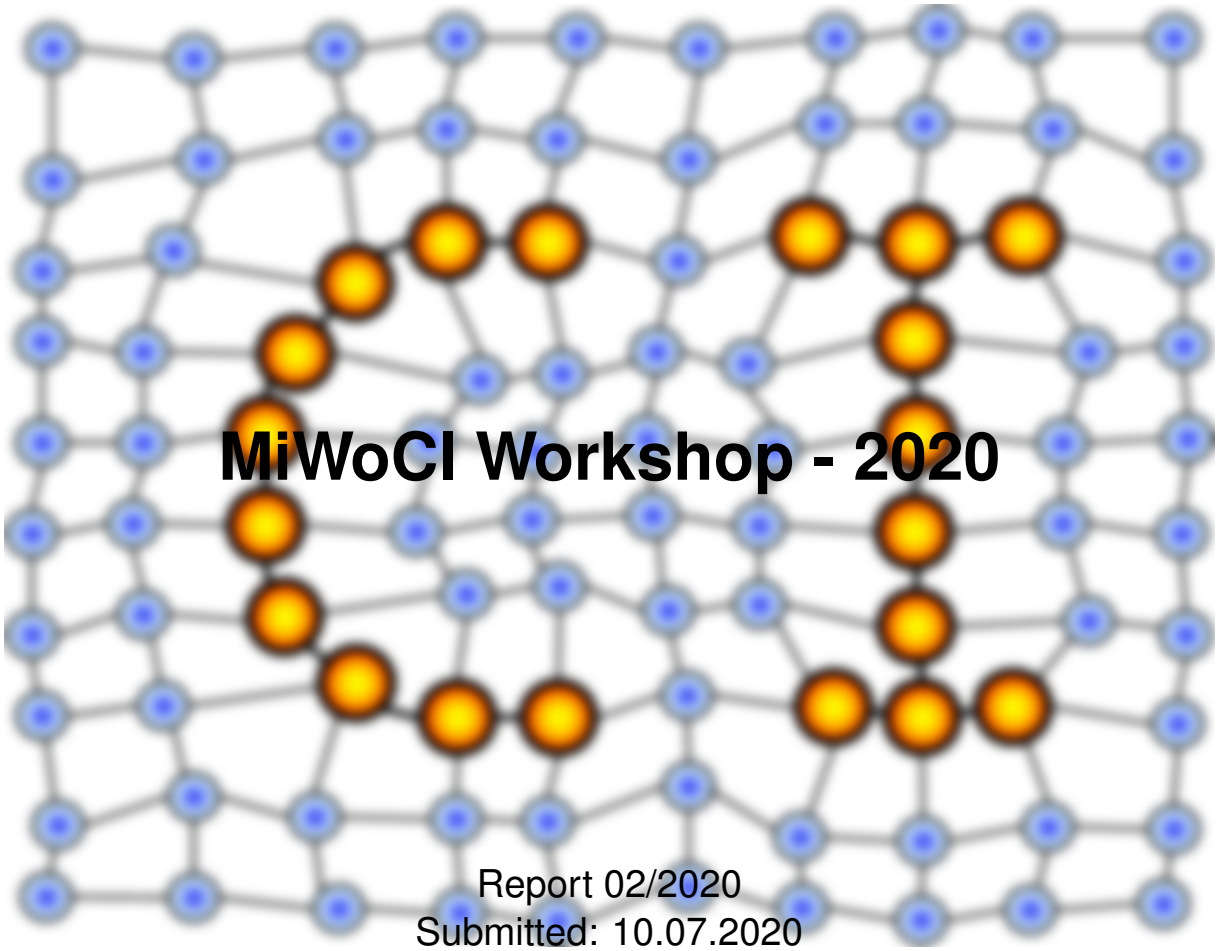
MACHINE LEARNING REPORTS



MiWoCI Workshop - 2020

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Abstracts of the 12^{th} Mittweida Workshop on Computational Intelligence - MiWoCI 2020 -

Frank-Michael Schleif, Marika Kaden, and Thomas Villmann

Machine Learning Report 02/2020

Preface

The 12 th international *Mittweida Workshop on Computational Intelligence* (MiWoCI) gathering together more than 50 scientists from different universities including Bielefeld, Groningen, UAS Mittweida, UAS Würzburg-Schweinfurt, UAS Zwickau, University of Sydney, and IFF Fraunhofer in Magdeburg. This year it was a little bit special, instead of all scientist coming to Mittweida, Germany, the Workshop was digital. Nevertheless, from 1.7.- 3.7.2020 the tradition of scientific presentations, vivid discussions, and exchange of novel ideas at the cutting edge of research was continued. They were connected to diverse topics in computer science, automotive industry, and machine learning.

This report is a collection of abstracts and short contributions about the given presentations and discussions, which cover theoretical aspects, applications, as well as strategic developments in the fields.

Contents

LVQ meets RNN

Jensun Ravichandran

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Abstract

Learning Vector Quantization (LVQ) methods have been popular choices of classification models ever since its introduction by T. Kohonen in the 90s [1]. Since then, a plethora of improvements have been made to the original formulation of the LVQ algorithm to handle several shortcomings. However, techniques to model recurrent relationships in the data using prototype methods still remain quite unsophisticated. In this paper, we propose the use of the Siamese architecture to not only model recurrent relationships within the prototypes but also the ability to handle prototypes of different dimensions simultaneously.

References

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DeepView: A toolbox to visualize deep neural network classifiers and others

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Abstract

Recent progress in the field of deep neural networks produces increasingly powerful models which are able to achieve human level and partially even super human performance [4, 3]. However, these networks are growing in complexity making them increasingly difficult to comprehend and more vulnerable to adversarial attacks [5]. To increase the understanding of a trained classification model, such as a deep network, we present the toolbox *DeepView*[1] [2], which provides a visualization of the classification function together with a data set. This is in contrast to most of the present literature, which focusses on explaining the investigated model with respect to individual data samples [1].

This toolbox is written in python and requires only a function that, given the classifier and a new data point, computes the prediction and a certainty of the latter. Based on this, DeepView computes a discriminative dimensionality reduction of the given data that is tuned for the classifier at hand and embeds the decision function therein. We demonstrate DeepView for deep networks with poisened data and for different classifiers.

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[1] Code available at `https://github.com/LucaHermes/DeepView`

Visualisation and knowledge discovery from interpretable models

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Abstract

Increasing number of anthropocentric sectors are using Machine Learning (ML) tools. Hence the need for understanding their working mechanism, evaluating their fairness in decision-making, and ensuring their trustworthiness are becoming paramount, ushering in the era of Explainable AI (XAI) [1, 2]. Recently we introduced a few intrinsically interpretable models which provide visualisation of the classifier and decision boundaries, in addition to extracting knowledge from the dataset and about the problem. They are also capable of dealing with missing values: they are the angle based variants of Learning Vector Quantization. We have demonstrated the algorithms on a synthetic dataset and a real-world one (heart disease dataset from the UCI repository). The newly developed angle LVQ variants helped in investigating the complexities of the UCI dataset as a multiclass problem. The performance of the developed classifiers were comparable to those reported in literature for this dataset, with additional value of interpretability, when the dataset was treated as a binary class problem. [2]

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[2] Visualisation and knowledge discovery from interpretable models, Ghosh, Sreejita and Tino, Peter and Bunte, Kerstin, accepted at IJCNN 2020, 2020

Document Embedding to Explain AI Components

Philip Kenneweg, Robert Feldhans, Sarah Schröder

Abstract

We analyze the performance of state of the art text embeddings on AI descriptions. With the recent popularity of AI and data science, there are plenty of researchers and providers for such solutions. These are met by the demand for automation and "intelligent" solutions in countless use cases. Identifying the proper solution for a certain application is not trivial and far from automated. Not without reason there have been many publications in the field of AutoML recently.
We address this issue from another perspective by examining the possibility to interpret description texts for AI components in order to explain their functionality, find similar solutions or match solutions with a user's requirements. In this context, we compare the performance of different text embeddings applied to descriptions from the scikit-learn[1] and ROS[2] documentation.
Using different visualization and clustering methods, we aim to explain how well existing text embeddings represent these descriptions and whether it is possible to identify functionally similar components.

References

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Understanding Sign Language: Is OpenPose Suitable?

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Abstract

Teaching sign language is a time consuming task which requires constant interaction with the students. During many training sessions the signs are repeated multiple times and the teacher has to respond to each student individually. Up to now, there are no technologies available which allow for distant self-reliant learning by students as known from audio and video support for common spoken language study. Due to the three dimensional features and the temporal aspect of the signs no training material for self-study are available.

We want to develop a tool which allows students to practice sign language in an off-classroom setting without intervention by a teacher. In a first step the signs should be recognized and translated to spoken language. Next steps involve gradual sign recognition (*This sign could mean xyz, but it could also stand for abc.*) and feedback to the learner with hints for improvement (*The sign for xyz is almost correct. The hand movement in the end is not quite right.*). For the analysis and evaluation of the data different algorithms for clustering and classification will be used. We are still at the very beginning of our research and are not sure yet, which algorithm will be the most suitable to perform this kind of sign classification, since besides the movement data we also have to consider the timing aspects.

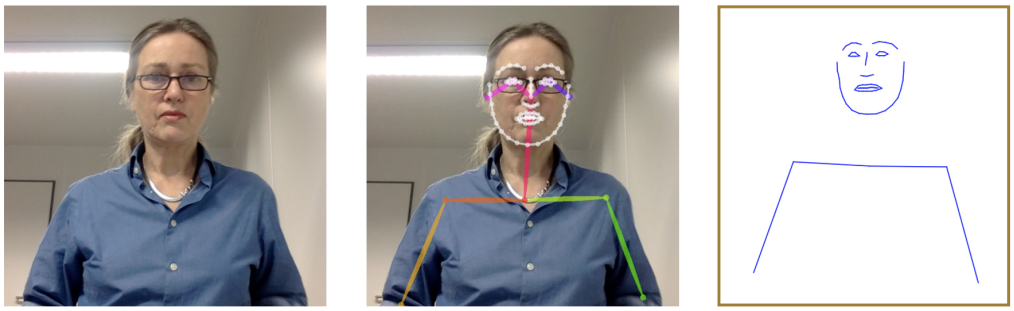

Figure 1: Extracting movement features with Open Pose based on body, hand, and face recognition.

For feature extraction from video sequences we plan to use Open Pose [1], which is an open source software detecting body, hand, and face movements in video sequences in real-time. First experiments performed on a small set of sequences indicate that this

toolbox is suitable in our context to extract enough relevant movement data and timing information of signers. Figure 1 depicts an example. The labelling of the data will be provided by professional signers.

Experimental settings found in literature always include elaborate equipment like 3d-cameras, kinect, or infra-red sensors. We want to keep it simple and affordable for students and teachers relying on smartphone / tables or build in computer cameras only.

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Automated Evaluation of Classification Models for Spectral Data with Discriminative Dimensionality Reduction Methods

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Abstract

The usage of hyperspectral data for food inspection gained a lot of attention in the past years due to the rather easy data collection in comparison to e.g. laboratory analyses. Nevertheless, these analyses are only promising if the data contains the property of interest and the model applied is capable of representing these properties. Due to measurement biases, especially in field data, normalization techniques should be considered before modelling. Common model choices are e.g. multi-layer perceptrons (MLP), convolutional neural networks (CNN), or radial basis function networks (RBF). Accuracy of prediction is commonly used to score these models in hope of achieving generalisation and therefore predicting future data. While accuracy is good in providing a basic idea of the quality of a model, it does not deliver any information about the specific representation of data in different models. For this purpose, techniques to visualise the decision boundaries of models have been developed. One recently developed technique based on discriminative dimensionality reduction is implemented in the package "Deepview" [1]. It embeds the data in a space of features that are important for the model's predictions and visualises the model's decisions in this feature space. We adapt this technique, which was developed and evaluated on the base of image data, to spectral data classification problems. Therefore, we adjust the colouring of the model's decisions in the embedding space by normalising it based on the entropy of the underlying model. Furthermore, the distribution of the network's certainty and related quantities in the embedding space are summarised and analysed to build a base for the evaluation and comparison of different models. With this approach, different models with different data normalisations are compared.

References

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*presenter

Domain Invariant Representations with Deep Spectral Alignment

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Abstract

Similar as traditional algorithms, deep learning networks struggle in generalizing across domain boundaries. A current solution is the simultaneous training of the classification model and the minimization of domain differences in the deep network. In this work, we propose a new *un*supervised deep domain adaptation architecture, which trains a classifier and minimizes the difference of spectral properties of the co-variance matrix of the data. Evaluated against standard architectures and datasets, the approach shows an alignment with respect to the data variance between related domains.

Evaluation of the Potential of Machine Learning Methods in Motion Analysis Using alaska/DYNAMICUS

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Abstract

The bio-mechanical human model alaska/DYNAMICUS, developed at the Institute of Mechatronics e.V. in Chemnitz, is a multi-body dynamics-based simulation model of humans with individualization anthropometric properties [1]. The system processes recorded motion data from (optical) motion capturing as well as force measurement systems. Results of the simulation are kinematic and dynamic quantities such as joint angles, speeds, and forces (joint moments). DYNAMICUS is used in several areas, e. g. product and process ergonomics in the automotive industry, sports, and human-technology interaction [2]. In a cooperation project[1] with UAS Mittweida (SICIM) the potential of machine learning methods is analyzed. Thereby, learning approaches are evaluated with the already existing statistical and rule-based models in different aspects like performance, runtime in the application phase, the effort to create the model and the robustness/stability of the models. A first basic problem is the detection of simple movements (sitting, standing, sitting down) using kinematic quantities (joint angles and speeds). The challenge here is that the labeling of the data is automatically done by the existing system and not manually. This results in uncertainties in labeling, but also in difficulties in the evaluation of the models. Furthermore, in the future not only individual movements should be detected, but also overlapping movements. This type of problem can be transferred in machine learning to so called multi-label classification. Another promising application is the prediction of the maximum strength of the leg stretching muscles during squats with weights. The aim is to use the movement data, measured below the maximum range to predict the maximum strength of the proband, i. e. the maximum weight with which it can still perform the squat. The maximum force is an essential problem, especially in junior top-class sport, and previous statistical methods provide only an imprecise results. A first feasibility study showed promising results [3]. In the presentation the human model is briefly introduced and the two applications mentioned above are described. In addition, questions and challenges for the application as well as for the machine learning models are discussed.

[1]alaska/KIML is support by European Social Fund; This measure is co-financed by taxes on algae in the budget adopted by the Saxon state parliament

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Sensors performance evaluation in classification tasks - ToF/Radar fusion system use case -

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Abstract

This work is a part of my research topic, which is about applying sensor fusion in industry for enhancing the human/robotic collaboration. The aim of this work first is to apply prototype-based machine learning algorithms in creating a model for human classification (classify whether an image contains a human or not). Second, during the training, the algorithm learns several parameters, which reflect the importance of the usage of each of the sensors for human classification purposes.

The dual functionality of the proposed approach is illustrated in the chart Figure 1. We present an example where we collect images from 3 different sensors and feed them separately into a pre-trained network for features extraction. These features are normally used to train prototypes (distances d) used later for new data classification. However, in this approach, distances are trained together with new parameters (new distance D). As an output from the distance layer, we obtain a model with trained distances to each of the two classes as well as an information about the contribution of each of the three sensors in the classification task. This information is relevant for making decision about which sensors should be fused for which purpose.

The whole training and evaluation is running on a CPU and based on the Protoflow package and keras.

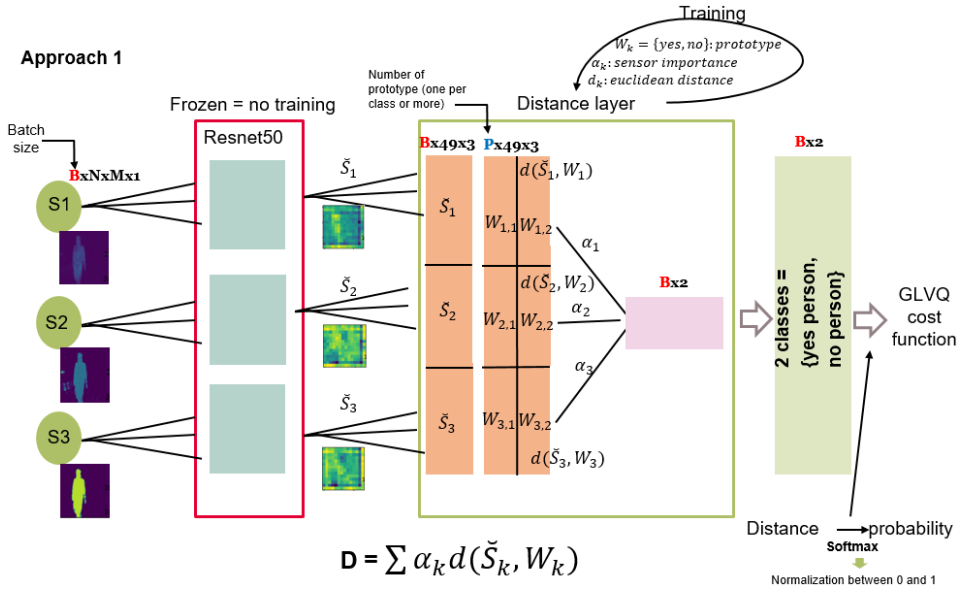

Figure 1: Illustration of the dual functionally

From tiny ants to mighty Cosmic-web

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Abstract

The preliminary step for many different machine learning projects is dimensionality reduction or clustering. Nonetheless, the results of this step are highly sensitive to noise and outliers. Many studies suggest solutions for detecting and removing few noise points close to a manifold [1, 2] or merging them in the manifold [3]. However, in many applications such as astronomical datasets, the density varies alongside manifolds that are buried in a noisy background, and previous techniques cannot handle the amount of noise in these datasets. We propose a denoising method based on the ideas of Ant colony optimization to extract manifolds, which instead of seeking high-density structures, it captures the points which are locally aligned with a manifold direction. Moreover, we empirically show that the biologically inspired formulation of ant pheromone reinforces this behavior, enabling the method to recover multiple manifolds embedded in extremely noisy data clouds. The demonstration of the proposed method on the simulation of the Cosmic-web [4] is a valuable example of how this method can be advantageous for detecting many low dimensional manifolds in the presence of noise.

References

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An Application of Generalized Matrix Learning Vector Quantization in Neuroimaging

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June 29, 2020

Abstract

We present an application of prototype-based Generalized Matrix Learning Vector Quantization (GMLVQ) in combination with the scaled sub-profile model principal component analysis (SSM/PCA) methodology as a novel approach to analyze [^{18}F]fluorodeoxyglucose positron emission tomography image data. Specifically, we show how to use GMLVQ to produce an understandable low-dimensional discriminative representation of the image data set. Furthermore, by exploiting the linearity of the SSM/PCA transformation in combination with the prototypes and relevance matrix found by GMLVQ we are able to produce and visualize disease typical residual activity profiles within the original voxel space. In other words, this analysis enables the identification of specific subgroups in the studied data set. To show this, we present a study including scans of patients suffering from Parkinson's disease collected from three different neuroimaging centers. We conclude that the approach shows promising results with respect to the better understanding of the disease classifications and the inner workings of the GMLVQ model and therefore could be a useful tool for medical specialists working within this domain.

Analysis of SARS-CoV-2 RNA-Sequences by Interpretable Machine Learning Models

Marika Kaden[1], Katrin Sophie Bohnsack[1], Mirko Weber[1], Mateusz Kudla[1,2], Kaja Gutowska[2,3,4], Jacek Blazewicz[2,3,4], and Thomas Villmann[1]

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Abstract

We present in our talks our contribution of [1]. In this paper we investigate SARS-CoV-2 virus sequences based on alignment-free methods for RNA sequence comparison. In particular, we verify a given clustering result for the GISAID data set, which was obtained analyzing the molecular differences in coronavirus populations by phylogenetic trees. For this purpose, we use alignment-free dissimilarity measures for sequences and combine them with learning vector quantization classifiers for virus type discriminant analysis and classification. Those vector quantizers belong to the class of interpretable machine learning methods, which, on the one hand side provide additional knowledge about the classification decisions like discriminant feature correlations, and on the other hand can be equipped with a reject option. This option gives the model the property of self controlled evidence if applied to new data, i. e. the models refuses to make a classification decision, if the model evidence for the presented data is not given. After training such a classifier for the GISAID data set, we apply the obtained classifier model to another but unlabeled SARS-CoV-2 virus data set. On the one hand side, this allows us to assign new sequences to already known virus types and, on the other hand, the rejected sequences allow speculations about new virus types with respect to nucleotide base mutations in the viral sequences.

References

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Interactive Machine Learning und Process Mining

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June 25, 2020

Abstract

Many real-world problems invoke remarkable complexity and still need to be understood, evaluated, and maybe controlled by humans. Combining the best of human and computational abilities can only be done using interactive and interpretable modeling. A further property of real-world problems is their unfolding in time. Often they are neither real snapshots nor straight time series. In contrast, we see several events emerging irregularly in time. Here process mining comes into play (see e.g. [1]). It allows us e.g., to look into the development of patients based on their visits to the doctor, the learning progress of students based on tests and exams, or the ideal communication strategy to customers in their sales life cycle based on singular communication events. Interactive process mining has gained interest, especially in the last years [2, 3, 4]. But still, it offers a lot of open questions. We will look into some of them.

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Drift Detection Using Coresets Over Sliding Windows

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June 23, 2020

Abstract

The change of underlying data is one of the biggest challenges in non-stationary environments. While several algorithms have been proposed to detect these changes, substantial problems remain in the case of higher dimensional data. Thus, we propose a novel Concept Drift detector based on Minimum Enclosing Balls, with the capability to quickly process higher dimensional data. Additionally a kernelized version of this detector is derived, to process non-linear streaming data. We also propose a method to measure the performance of drift detectors with a binary classification evaluation technique, the confusion matrix, which enables calculating statistics like the F1 score.

On-line learning in the presence of concept drift

Michiel Straat

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Abstract

In numerous applications data is available in the form of streams and machine learning models are adapted in an incremental fashion (on-line learning), as opposed to models that are trained on fixed datasets (off-line learning). In these situations *concept drift* may be present: The task at hand is subject to a statistical change in the input data, known as *virtual drift*, and/or a change in the rule itself, referred to as *real drift*. Very often in practical situations, a combination of the two types of drift is present. In one of the model scenarios considered in [1], we study on-line gradient descent learning of a regression scheme that exhibits real concept drift. The regression scheme is defined by a *teacher* Soft Committee Machine (SCM) that models the drift by randomly changing weight vectors. A *student* SCM learns the regression scheme from a stream of random and independent examples of which the target outputs are provided by the drifting teacher SCM. We have studied for both the ReLU-SCM and the Erf-SCM the sensitivity of the learning performance to the strength of the drift and the effectiveness of introducing a weight decay as a mechanism of forgetting. Results show significant differences between the two types of SCM.

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Online Learning with Imbalanced Data

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Abstract

Recently, machine learning techniques are often applied in real world scenarios where learning signals are provided as a stream of data points. Models need to be adapted online in this setting, and two issues have to be considered. First, a severe problem are changes in the underlying data distribution which occur over time due to concept drift. Second, the available data is often imbalanced since signals for rare classes are particularly sparse.

In the last years, a number of learning technologies, which can reliably learn in the presence of drift, have been proposed. Non-parametric approaches such as the recent model SAM-kNN [1] can deal particularly well with heterogeneous or priorly unknown types of drift. However, these methods share the deficiencies of the underlying vanilla-kNN classifier when dealing with imbalanced classes. In this contribution, we propose intuitive extensions of SAM-kNN, which incorporate successful balancing techniques for kNN, namely SMOTE-sampling [2] and kENN [3]. Besides, we propose a new method, Informed Downsampling, for solving class imbalance in non-stationary settings with underlying drift, and demonstrate its superiority in a number of benchmarks.

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Mirror, Mirror on the Wall - Are You Native or at All?

Julia Abel, Marika Kaden, Thomas Villmann

University of Applied Sciences Mittweida, Saxonian Institute for Computational Intelligence and Machine Learning

Abstract

Proteins can have two conformations: the L-enantiomeric conformation and the D-enantiomeric conformation. The first represents the natural form (further known as native) of a protein, whereas the latter represents an exact mirror-image of it [2, 5, 7, 9]. The differentiation of native and mirror proteins is crucial for further analysis and research in the fields of drug discovery and synthetic biology [6, 8]. *Ramachandran plots* (R-plots) display the dihedral angles Φ and Ψ of a protein's backbone to visualize their distribution [3]. R-plots provide an easily inspectable tool to detect underlying properties of the secondary structure in that protein [1].
In this contribution the discrimination between native and mirror models of proteins according to their chirality is tackled based on the structural protein information. This information is contained in the R-plots of the protein models. We provide an approach to classify those plots by means of an interpretable machine learning classifier - the Generalized Matrix Learning Vector Quantizer [4]. Applying this tool, we are able to distinguish with high accuracy between mirror and native structures just evaluating the R-plots. The classifier model provides additional information regarding the importance of regions, e.g. α-helices and β-strands, to discriminate the structures precisely. This importance weighting differs for several considered protein classes.

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How to Compare RNA/DNA Sequences - a Systematic Approach

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Abstract

The automatic comparison of RNA/DNA or rather nucleotide sequences in data mining and data classification is a complex task requiring careful design due to the computational complexity. While alignment-based models suffer from computational costs in time, alignment-free models have to deal with appropriate data preprocessing and consistently designed mathematical data comparison [8].

The proposed consideration deals with the latter strategy. In particular, a systematic categorization is suggested, which emphasizes two key concepts that have to be combined for a successful comparison analysis: 1) the data transformation comprising adequate mathematical sequence coding and feature extraction, and 2) the subsequent (dis-)similarity evaluation of the transformed data by means of problem specific but mathematically consistent proximity measures.

Respective approaches of different categories of the introduced scheme are examined with regard to their suitability to distinguish natural RNA virus sequences from artificially generated ones encompassing varying degrees of biological feature preservation [7]. The challenge in this application is the limited additional biological information available, such that the decision has to be made solely on the basis of the sequences and their inherent structural characteristics.

To address this, the present work focuses on interpretable, dissimilarity based classification models of machine learning, namely variants of Learning Vector Quantizers [5, 4]. These methods are known to be robust and highly interpretable, and therefore, allow to evaluate the applied data transformations together with the chosen proximity measure with respect to the given discrimination task. We will present preleminary results for the above mentioned discrimination task for artificial and biological RNA virus sequences [1].

These first analysis results should be taken as a starting point for more in-depth analysis of this problem in the future research. In particular, a promising ansatz could be to integrate statistical information into the proximity measure or into the probabilistic model to achieve a more problem-specific classifier [6]. Another perspective based on the systematic use of appropriate proximities could be to integrate them into a LVQ classifier model, which serves as a discriminator in a Generative Adversarial Network (GAN) [2, 3]. If the

discriminator of the GAN would be able to make use of the interpretability of the LVQ model this could lead to task specific and better interpretable generator networks within the GAN providing more statistical and other inside information about the considered DNA/RNA sequences.

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Evidence for tissue specific ribosomes in normal and cancer samples: machine learning analysis of human ribosomal protein levels

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Abstract

This contribution presents selected results obtained in an interdisciplinary collaboration of physicists, computer scientists and biomedical researchers [1].

Ribosomes are molecular machines which perform translation, i.e. protein synthesis in all living cells. They are composed of ribosomal RNA (rRNA) and structural ribosomal proteins (RP). Traditionally, RPs are believed to be hightly constant and conserved across tissues and external conditions. However, a growing body of recent work suggests ribosome heterogeneity at several levels, see [1, 2] and references therein.

We present and discuss results from a detailed analysis of human ribosomal protein (RP) levels in normal and cancer samples. Here, emphasis is on the application of a variety of unsupervised and supervised machine learning techniques, including Learning Vector Quantization (LVQ) and relevance learning, Self-Organizing-Maps (SOM), Uniform Manifold Approximation and Projection (UMAP) and t-Distributed Stochastic Neighbor Embedding (t-SNE).

We find highly consistent, tissue specific RP-mRNA signatures in normal and tumor samples. Moreover, multiple RP-mRNA subtypes are found to exist in several cancers, which display significantly different survival rates.

Our results suggest that heterogeneous RP levels play a significant functional role in cellular physiology, in both normal and disease states.

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Recursive Tree Grammar Autoencoders

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Abstract

Machine learning for tree-structured data has made impressive progress in recent years with advanced tree kernels [1], distances [2], and neural networks [3]. However, most methods to date are limited to trees as input data and can not produce trees as output [4]. Yet, tree-structured output would be very helpful for interesting tasks such as molecule design in chemistry [5] or hint provision in intelligent tutoring systems [6]. In this talk, we will cover one way to elegantly enable trees both as input and output, namely autoencoders for trees. The key ingredients for this approach are recursive neural networks [7] and regular tree grammars [8]. In more detail, we encode trees to vectors using a tree parser and decode vectors to trees using a tree grammar, both guided by a recursive neural network. We also provide two training schemes. First, for small datasets, we suggest to initialize the recursive nets as tree echo state networks [9] and only train the output layer of the decoder via a linear SVM, thus achieving nontrivial results within seconds of training. Second, for large datasets, we suggest to train the model end-to-end based on the variational autoencoder loss [5] and backpropoagation. In this way, we achieve a proper generative model for trees which can improve both the autoencoding error as well as the optimization performance beyond state-of-the art models.

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Quantum-Inspired Learning Vector Quantization – Basic Concepts and Beyond

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Abstract

Interpretable machine learning classifiers like prototype based models are a promising alternative to deep neural networks and regarding efforts to make them explainable [1, 9]. Among those interpretable models the family of learning vector quantizers (LVQ) is one of the most intuitive approaches realizing a simple scheme of attraction and repelling if the Euclidean distance is used as the underlying data proximity measure [8]. Although heuristically motivated, today mathematically well-defined variants based on cost functions are available, which approximate the classification error [10]. Remarkable extensions of the basic scheme are the incorporation of metric adaptation schemes as well as the utilization of more sophisticated proximity measures like divergences [5, 12, 19].

Otherwise, support vector machines (SVM) became powerful classifier systems benefiting from fast adaptation due to the convexity of the respective cost function formulated as a constrained optimization problem [13]. Another key ingredient of SVMs is the kernel trick: The data $\mathbf{x} \in X \subseteq \mathbb{C}^n$ are implicitly mapped into a *Reproducing Kernel Hilbert space* $\mathcal{H}$ (RKHS) by a generally non-linear map $\Phi_{\mathcal{H}}$ but the data evaluation is still done in the data space using the kernel function $\kappa_{\mathcal{H}}$. This non-linear mapping together with the usually infinite dimensionality of $\mathcal{H}$ provides a great flexibility of SVM which frequently leads to excellent classification performance. In some sense, SVMs also may be seen as a prototype based approach, where the support vectors take over the role of prototypes [17, 18]. The kernel, in fact, determines just an inner product in the RKHS $\mathcal{H}$ and, hence, defines a kernel distance $d_{\mathcal{H}}$, which can be still evaluated in the original data space X. Using this observation, kernel methods can also be plugged into LVQ to improve their flexibility [20]. Thus, the prototypes in kernelized LVQ (KGLVQ) are implicitly adapted in the RKHS adjusting their origins in the data space followed by the subsequent implicit mapping by means of $\Phi_{\mathcal{H}}$.

An interesting new perspective to this kernel approach is provided by quantum-inspired computing. Suppose quantum state vectors $\mathbf{q} \in \mathcal{Q}^n \subseteq \mathbb{Q}^n$ where $\mathbb{Q}^n = \{|\mathbf{x}\rangle\}$ is the set of

quantum bit vectors $|\mathbf{x}\rangle = (|x_1\rangle, \ldots, |x_n\rangle)^T$ with quantum bits (qubits)

$$|x_k\rangle = \alpha_k \cdot |0\rangle + \beta_k \cdot e^{i \cdot \phi_k} \cdot |1\rangle \tag{1}$$

where the amplitudes $\alpha_k, \beta_k \in \mathbb{R}$ fulfill the normalization condition

$$|\alpha_k|^2 + |\beta_k|^2 = 1 \tag{2}$$

and $\phi_k \in \mathbb{R}$ gives the phase information. Hence, the qubits are elements of the *Bloch-sphere* or, more mathematically, the *Riemann-sphere* [24]. The quantum space $\mathbb{Q}^n$ is a *Hilbert space* equipped with the inner product $\langle \mathbf{x}|\mathbf{w}\rangle$ [11].

Taking prototypes in LVQ as well as data just as qubit vectors $|\mathbf{x}\rangle$ and $|\mathbf{w}\rangle$, respectively, prototype adaptation can be realized by means of stochastic gradient descent learning like in generalized LVQ ([10], GLVQ) in terms of derivatives with respect to the amplitudes and the phases of the qubits $|w_k\rangle$ contained in a prototype vector $|\mathbf{w}\rangle$ [21].

According to the postulates of quantum mechanics, the update of a quantum prototype, which is realized by the gradient of the local cost of GLVQ, has to be an unitary transformation (Hermitean transformation). Note at this point that an arbitrary unitary operator $\mathbf{U} \in \mathbb{C}^{2\times 2}$ of a qubit $|x\rangle$ can be expressed as a linear combination

$$\mathbf{U} = \sum_{k=0}^{3} z_k \cdot \boldsymbol{\sigma}_k$$

where the coefficients z_k are obtained as

$$z_0 = \frac{u_{00} + u_{11}}{2}, \quad z_1 = \frac{u_{01} + u_{10}}{2}, \quad z_2 = i\frac{u_{01} - u_{10}}{2}, \quad z_3 = \frac{u_{00} - u_{11}}{2}$$

and, the matrices $\boldsymbol{\sigma}_k \in \mathbb{C}^{2\times 2}$

$$\boldsymbol{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the *Pauli matrices* forming a basis $B = \{\boldsymbol{\sigma}_0, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3\}$ of the unitary group $\mathfrak{SU}(2) \subset \mathbb{C}^{2\times 2}$ [11]. Consequently, the unitary transformations can be realized by respective quantum gates [16]. Moreover, $\mathbb{C}^{2\times 2}$ is an Hilbert space equipped with the *Frobenius inner product* for matrices [22].

The main step to formulate an usual classification task in terms of quantum-inspired LVQ (Qu-GLVQ) is to transform the data appropriately by a suitable mapping $\Phi_{\mathcal{Q}^n} : \mathbf{x} \to |\mathbf{x}\rangle$. For example, the generally complex components x_k could be mapped non-linearly onto the Riemann-sphere by means of a stereographic projection [22].

Comparing the QU-GLVQ with KGLVQ the similarities are striking: non-linear mappings transform the data into a Hilbert space where the prototype adjustments take place. Whereas in KGLVQ (and SVM) these are done implicitly applying the kernel trick in Qu-GLVQ the processing is explicitly done in the mapping space $\mathbb{Q}^n$. This observation was first made in [15, 14] and, independently, in [21]. Further, an angle based GLVQ variant was proposed in [2], which also should be considered in the context of QU-GLVQ.

In the next research steps we will integrate the GROVER'S algorithm according to the quantum nearest neighbor method to determine the best matching prototypes [3, 4, 23] and consider, how the Qu-GLVQ could be related to known quantum k-means approaches [7, 25]. Finally, quantum entanglement has to be integrated [26] and should be compared with the entangled kernel approach [6].

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Comparing Activation Functions Using A Statistical Physics Approach

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Abstract

One of the elements which determines the performance of an artificial neural network is the activation function. Originally, the sigmoidal activation function was used in the hidden units of such networks. Nowadays, the Rectified Linear Unit activation (ReLU) is arguably the most popular choice, due to the function's computational ease and higher training rate compared to networks employing sigmoidal activation. Initially, claims about its increased performance were mostly based on empirical evidence, but recently theoretical arguments have been provided which confirm this idea. In the meanwhile, several other activation functions have been proposed, all of which acclaimed to have a better performance than its predecessors. A theoretical foundation that explains the fundamental differences between activation functions is lacking, however. In our study, which is a continuation of [1], we have borrowed concepts from statistical physics to research the learning behaviour of artificial neural networks in the context of off-line learning. We compare five activation functions: sigmoidal activation, Rectified Linear Unit activation, Leaky Rectified Linear Unit (LReLU) activation [2], Piecewise Linear Unit (PLU) activation [3], and a novel activation function, dubbed Bounded Rectified Linear Unit (BReLU). The activation functions studied have been selected based on their comparability, in order to give an answer to the question: what makes one activation function better than the other? Specifically, we are interested in what characteristic determines the type of *phase transition*, as this is a defining factor of the training speed.

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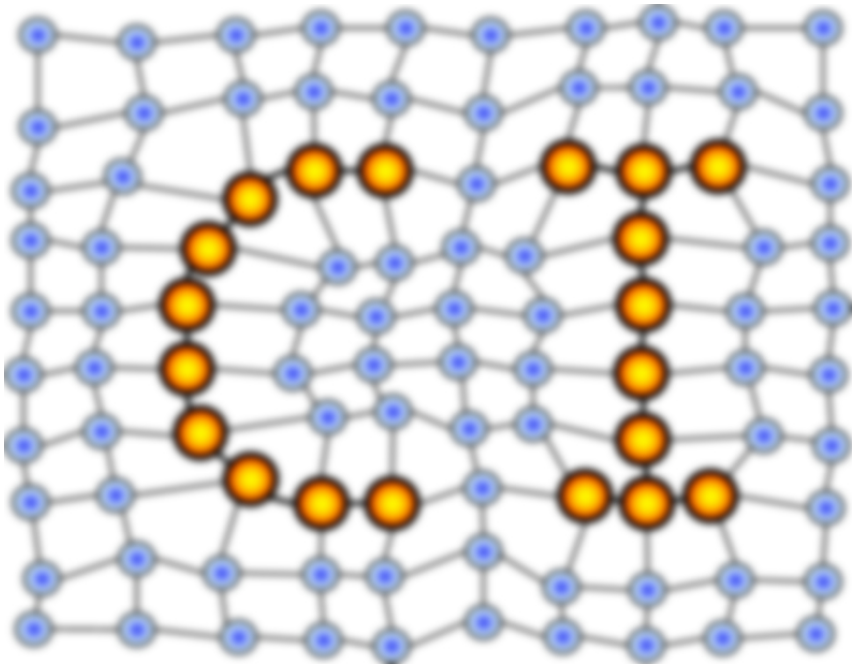

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