Activation Functions for Generalized Learning Vector Quantization - A Performance Comparison

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Abstract. An appropriate choice of the activation function plays an important role in the performance of (deep) multilayer perceptrons (MLP) for classification and regression learning. Prototype-based classification learning methods like (generalized) learning vector quantization (GLVQ) are powerful alternatives. These models also deal with activation functions but here they are applied to the so-called classifier function instead. In this paper we investigate successful candidates of activation functions known for MLPs for application in GLVQ and their influence on the performance.

Keywords: learning vector quantization, classification, activation function, ReLU, swish, sigmoid, perceptron, prototype-based networks

1 Introduction

Prototype-based classification learning like learning vector quantization (LVQ) was introduced by T. Kohonen in \cite{1} and belongs to robust and stable classification models in machine learning \cite{2}. One of the most prominent variants is

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generalized learning vector quantization (GLVQ, [3]). The GLVQ cost function to be minimized by stochastic gradient descent learning (SGDL) is an approximation of the overall classification error. Further, GLVQ belongs to the family of margin optimizers for classification learning, because GLVQ maximizes the hypothesis margin [4].

Beside the usually taken geometric perspective for GLVQ interpretation, the neural network perspective of LVQ gains more and more attraction, because it allows to combine LVQ models with techniques of deep learning [5,6]. In this perspective the LVQ prototypes, as elements of the Euclidean space, are interpreted as weight vectors of linear perceptrons, such that the maximum perceptron excitation by a data vector corresponds to minimum Euclidean distance according to the nearest prototype principle realized in vector quantization approaches [7]. GLVQ performance crucially depends on the activation function for the so-called classifier function of the GLVQ costs, usually chosen as a parametrized sigmoid function [8].

A hot topic in deep network design is the search for appropriate perceptron activation functions improving standard sigmoid or ReLU [9,10]. Yet, recent studies show that ReLU-units can be further improved using more sophisticated activation function like \textit{swish}, \textit{soft+} and others [11,12,13].

For GLVQ, to our best knowledge, only linear and sigmoid activation functions were considered as activation functions for the (GLVQ-) classifier function regarding their classification behavior whereas convergence behavior was not in the focus so far.

Therefore, the aim of this contribution is to investigate several prominent state-of-the-art activation functions of (deep) MLPs regarding their convergence behavior and resulting final classification performance when applied in GLVQ.

2 Generalized Learning Vector Quantization - from a Multilayer Network Perspective

We start considering GLVQ from the geometric perspective.

In GLVQ, a set $W = \{w_1, w_2, ..., w_N\}$ of prototypes $w_k \in \mathbb{R}^p$ is assumed as well as (training) data $x \in X \subseteq \mathbb{R}^n$ equipped with class labels $c(x)$. Each prototype is uniquely responsible for a certain class $c_k = c(w_k)$. The data are projected by means of a projection $\pi : \mathbb{R}^n \to \mathbb{R}^p$ into the prototype space $\mathbb{R}^p$ also denoted as projection space in this context. The vector quantization mapping $x \mapsto \kappa(x)$ takes place as a winner-takes-all (WTA) rule according to

$$\kappa(x, W) = \arg\min_{k : w_k \in W} \{d(\pi(x), w_k) | k = 1, 2, ..., N\}.$$  \hspace{1cm} (1)
realizing the nearest prototype principle with respect to a predefined dissimilarity measure \( d \). The value \( \kappa(x, W) \) is called the index of the best matching (winner) prototype with respect to the set \( W \). An unknown data vector \( u \) is assigned to the class \( c_{\kappa(u)} = c \left( w_{\kappa(u)} \right) \).

Usually, the (squared) Euclidean distance is used, which can be written as

\[
d_{\pi}(x, w_k) = -2 \langle \pi(x), w_k \rangle_E - b_k(x)
\]

where \( \langle z, w \rangle_E \) denotes the Euclidean inner product and

\[
b_k(x) = \langle \pi(x), \pi(x) \rangle + \langle w_k, w_k \rangle_E
\]

collects the squared norm values of \( x \) and \( w \). Let \( w^+ \in W^+ \) and \( w^- \in W^- \) be the best matching prototypes according to \( W^+(x) = \{ w_k | w_k \in W \land c_k = c(x) \} \subset W \) and \( W^-(x) = W \setminus W^+ \), respectively. The local loss in GLVQ is defined as

\[
l(x, W, \gamma) = f \left( \frac{d^+_\pi(x) - d^-_\pi(x)}{\eta(x)} - \gamma \right)
\]

with \( d^+_\pi(x) = d_\pi(x, w^+) \). The GLVQ-activation function \( f \) is a monotonically increasing and differentiable function, which is denoted as activation function for the classifier function

\[
\mu(x, \gamma) = \frac{d^+_\pi(x) - d^-_\pi(x)}{\eta(x)} - \gamma.
\]

The quantity \( \eta(x) = d^+_\pi(x) + d^-_\pi(x) \) is the local normalization, and \( \gamma \in \mathbb{R} \) is a shifting variable frequently set to zero. The difference quantity \( h(x) = \frac{1}{2} |d^-_\pi(x) - d^+_\pi(x)| \) is denoted as (local) hypothesis margin \([4]\), which is related to the hypothesis margin vector

\[
h(x) = w^- - w^+
\]

via the triangle \( \triangle(x, w^+, w^-) \). The classifier function yields negative values only for correctly classified training samples.

The cost function to be minimized by stochastic gradient descent learning (SGDL) becomes

\[
E_{GLVQ}(X, W) = \sum_{x \in X} l(x, W)
\]

as explained in \([3]\). Doing so, the stochastic gradient of the cost function involves the derivative \( \frac{\partial f(\mu(x, \gamma))}{\partial \mu(x, \gamma)} \) of the activation function.

The choice \( \pi(x) = x \) yields the standard GLVQ whereas for the linear mapping \( \pi_{\Omega}(x) = \Omega x \) the matrix variant GMLVQ is obtained, which reduces to relevance GLVQ (GRLVQ) for a diagonal matrix \( \Omega \) \([14,15]\). If \( \pi(x) \) is realized by a deep network, DeepGLVQ is resulted \([6,5]\).
In the following we reconsider GLVQ taking the neural network perspective. For this purpose, remark that the squared Euclidean distance $d^2$ can be seen as a linear perceptron with weight vector $w_k$ and the bias $b_k(x)$ regarding the projected input vector $\pi(x) \in \mathbb{R}^p$. As shown in [17], we get for the local costs $l(x, W) = f(\langle \hat{\pi}(x), h(x) \rangle_E + B^\pm(x, \gamma))$ with the scaled data mapping $\hat{\pi}(x) = \frac{2\pi(x)}{\pi(x)}$ and hypothesis margin vector $h(x)$.

Thus, the local loss can be seen as a linear perceptron with hypothesis margin vector $h(x)$ as the weight vector and a parameterized bias $B^\pm(x, \gamma)$ for the projected data $\hat{\pi}(x)$. In this sense, the GLVQ activation function can be interpreted as an activation function for the special GLVQ-perceptron $\Pi_f(x, W)$. Note that the GLVQ-perceptron $\Pi_f(x, W)$ delivers maximum local costs for maximum excitation, such that GLVQ-classification-learning relates to minimum excitation learning for GLVQ-perceptrons $\Pi_f(x, W)$. In GLVQ, standard choices for the activation function are identity $id(x) = x$ and the sigmoid $sgd(x, \beta)$ with $\beta = 1$, see Tab. 1.

### 2.1 Activation Function for MLP and GLVQ-MLN

As we have explained in the previous subsection, the local loss in GLVQ can be described as a particular perceptron structure. Hence, the consideration of the respective activation function becomes inevitable. Many considerations for (deep) MLPs have shown that the appropriate choice of activation functions is essential for convergence behavior and final network performance [13]. Originally, sigmoid functions like tangens-hyperbolicus or standard sigmoid function $sgd(x, \beta)$ with $\beta = 1$ (see Tab. 1) were preferred to ensure non-linearity and differentiability together with easy analytical computation of derivatives. Later, Rectified linear Units (ReLU) $ReLU(x) = \max(0, x)$ became popular due to its performance and computational simplicity [9]. Recently, a systematic study of activation functions was proposed [11]. It turns out that the swish-function $swish(x, \beta) = x \cdot sgd(x, \beta)$ introduced in [18] is, in average, the most successful although not always the best choice. It can be seen as an intermediate between ReLU($x$) and the scaled identity $id(x)$ according to functional limits

\[
swish(x, \beta) \xrightarrow{\beta \to \infty} ReLU(x) \text{ and } swish(x, \beta) \xrightarrow{\beta \searrow 0} id(x) \tag{8}
\]

respectively. Yet, other activation functions like $m(x, \beta) = \max(x, sgd(x, \beta))$ also perform very well for deep MLP as outlined in [11]. Further, the choice of the activation also affects the classification robustness [19]. A collection of promising
activation functions together with their derivatives is given in Table 1. Note that for \( \beta = 0 \) the Leaky ReLU \( \text{LReLU}(x, \beta) \) introduced in [22] simply becomes ReLU \( (x) \), whereas \( \text{swish}_\tau(x, \beta) \) and \( m_\tau(x, \beta) \) are variants of \( \text{swish}(x, \beta) \) and \( m(x, \beta) \) replacing the sigmoid \( \text{sgd}(x, \beta) \) by the tangens-hyperbolicus function \( \tau(x, \beta) \).

The neural network perspective of GLVQ and, particularly, the GLVQ-perceptrons \( \Pi_f(x, W) \) interpretation motivates to consider the impact of the activation functions regarding the GLVQ performance.

3 Numerical Results

We performed numerical investigations regarding the performance of the activation functions from Table 1 for four widely used standard data sets. These are

- the Tecator Data Set comprising 215 spectra measured for several meat probes. The spectral range is 850 - 1050 nm with \( D = 100 \) spectral bands. The data set is labeled according to the fat content (high/low) The data set is provided as a training set \( (N_{V_{\text{train}}}= 172) \) and a test set \( (N_{V_{\text{test}}} = 43) \) [23].

- the Indian Pine Data Set, which is a spectral data set from remote sensing. It was generated by an AVIRIS sensor capturing an area corresponding to \( 145 \times 145 \) pixels in the Indian Pine test site in the northwest of Indiana [24]. The spectrometer operates in the visible and mid-infrared wavelength range \( 0.4 - 2.4 \mu \text{m} \) with \( D = 220 \) equidistant bands. The area includes 16 different kinds of forest or other natural perennial vegetation and non-agricultural sectors, which are also denoted as background. These background pixels are removed.

3 The derivative of the maximum function \( m(x, \beta) \) could be approximated using the quasi-max function \( Q_{\alpha}(x, \beta) = \frac{1}{\alpha} \log \left( \frac{e^{\alpha x} + e^{\alpha \cdot \text{sgd}(x, \beta)}}{e^{\alpha x} + e^{\alpha \cdot \tau(x, \beta)}} \right) \) proposed by J.D. Cook [20] with \( \alpha \gg 0 \). The respective consistent derivative approximation is

\[
\frac{d m(x, \beta)}{dx} \approx \frac{\left( \exp(\alpha x) + \frac{d \text{sgd}(x, \beta)}{dx} \cdot \exp(\alpha \cdot \text{sgd}(x, \beta)) \right)}{\left( \exp(\alpha x) + \frac{d \tau(x, \beta)}{dx} \cdot \exp(\alpha \cdot \tau(x, \beta)) \right)} \quad (9)
\]

as provided in [21]. Analogously, the quasi-max approximation \( m_\tau(x, \beta) \approx \frac{1}{\alpha} \log \left( \exp(\alpha x) + \exp(\alpha \cdot \tau(x, \beta)) \right) \) is valid with

\[
\frac{d m_\tau(x, \beta)}{dx} \approx \frac{\left( \exp(\alpha x) + \frac{d \tau(x, \beta)}{dx} \cdot \exp(\alpha \cdot \tau(x, \beta)) \right)}{\left( \exp(\alpha x) + \exp(\alpha \cdot \tau(x, \beta)) \right)} \quad (10)
\]

as the derivative approximation.

4 Tecator data set is available at StaLib: [http://lib.stat.cmu.edu/datasets/tecator](http://lib.stat.cmu.edu/datasets/tecator)

5 The data set can be found at www.ehu.es/ccwintco/uploads/2/22/Indian_pines.mat}
Table 1. Successful Activation functions for MLP according to [11] together with their derivatives.
from the data set as usual. Additionally, we remove 20 wavelengths, mainly affected by water content (around 1.33µm and 1.75µm). Finally, all spectral vectors were normalized according to the $l_2$-norm. This overall preprocessing is usually applied to this data set [24]. Data classes with less than 100 samples were removed yielding a 12-class-problem.

– the Wisconsin-Breast-Cancer-data (WBCD) and the Indian diabetes data set (PIMA) contain 562 and 768 data vectors with 32 and 8 data dimensions, respectively, and each divided into two classes (healthy/ill). A detailed description can be found in [25].

3.1 Results

The results reported here were obtained for GLVQ with only one prototype per class.

For each data set and each activation function from Tab.1 we performed 100 runs for several parameter configurations $\beta$ by a grid search where the averaged accuracy was the evaluation criterion. The learning rate as well as a maximum number of 10000 epochs per training experiment were maintained uniformly for all experiments. We report the results regarding the best parameter configurations.

The detailed results can be found in [17]. Here we give the results averaged over all four data sets. For this purpose we take ReLU-accuracies as references and calculate the respective ratios. Ratios greater than one indicate better accuracies, whereas lower ratios refer to worse results. The ratios averaged over all data sets together with their standard deviations are depicted in Tab.2 Additionally, we give the averaged ratios and standard deviations for convergence performance. The convergence performance is measured considering the number of training epochs until the averaged gradient becomes approximately zero. Thus, ratios lower than one refer to higher convergence rate than ReLU whereas greater values indicate slower convergence.

From this experiments we can conclude that soft+, sgd and swish achieve best results with almost similar accuracies for an appropriate parameter choice $\beta$, all improving standard ReLU. Among them, swish clearly outperforms the others regarding the convergence performance. Further, both standard activation functions for GLVQ, id and sgd with $\beta = 1$, are significantly weaker than ReLU and, hence, also weaker than the leading activation functions. Hence they should be avoided.

Yet, also the maximum function $m(x, \beta)$ achieves high accuracies. However, these results are obtained for values $\beta \gg 1$. In this case, $m(x, \beta)$ behaves like sgd($x, \beta$). Therefore, it is not mentioned explicitly in the list of best functions.

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Table 2. Results for the activation functions compared to ReLu. The best accuracy results are in bold font. Among them, the best respective convergence ratio is also depicted in bold font. For further explanations see text.

| activation function | av. accuracy ratio | st. dev | av. convergence ratio | st. dev |
|---------------------|--------------------|---------|-----------------------|---------|
| ReLU ($x$)          | 1                  | 0       | 3.292611899           | 4.382405967 |
| sgd ($x, \beta$)   | 1.058588283        | 0.065044863 | 3.292611899           | 4.382405967 |
| sgd ($x, \beta = 1$)| 0.855523844       | 0.166406655 | 0.17755527            | 0.089233988 |
| $\tau (x, \beta)$  | 0.896820407        | 0.150230939 | 0.021782303           | 0.172070555 |
| swish ($x, \beta$) | 1.05793573         | 0.058660376 | 0.553609888           | 0.275164898 |
| swish, ($x, \beta$)| 0.936386328       | 0.160171911 | 0.184983626           | 0.1057056 |
| LRelu ($x, \beta$) | 1.028269063        | 0.089099257 | 1.023108516           | 0.928273831 |
| $m (x, \beta)$     | 1.057855692        | 0.069498943 | 4.519976424           | 5.838384012 |
| $m, (x, \beta)$    | 0.894020574        | 0.153118782 | 0.392754746           | 0.385784308 |
| cosxx($\beta, x$) | 0.990139782        | 0.10838342  | 0.375625059           | 0.179953065 |
| soft+ ($\beta, x$)| 1.078091745        | 0.058366659 | 4.595046404           | 3.698125022 |
| id ($x$)            | 0.85092197         | 0.16492968  | 0.141372141           | 0.109199298 |

4 Conclusions

In this paper we studied the influence of several MLP activation function candidates regarding their performance influence for GLVQ. Motivation for this investigation is the fact that the classifier function of GLVQ can be described as a generalized perceptron and, hence, the GLVQ activation function plays the role of a perceptron activation function. The numerical experiments have shown that soft+, sgd and swish achieve the best accuracy performance better than ReLU as it is also frequently the case for (deep) MLP networks [11]. Yet, regarding the convergence speed swish has to be highly favored. Moreover, the standard activation functions of GLVQ are clearly outperformed.

Summarizing these experiments we suggest to switch over from id and sgd (with $\beta = 1$) to swish for GLVQ activation.

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