

# Applications of $l_p$ -Norms and their Smooth Approximations for Gradient Based Learning Vector Quantization

M. Lange<sup>1</sup>, D. Zühlke<sup>2</sup>, O. Holz<sup>3</sup>, and T. Villmann<sup>1</sup>

1- University of Appl. Sciences Mittweida - Dept. of Mathematics  
Mittweida, Saxonia - Germany

2- Fraunhofer-IAIS - Dep. of Organized Knowledge  
Sankt Augustin, Germany

3- Fraunhofer-ITEM - Hannover, Germany

**Abstract.** Learning vector quantization applying non-standard metrics became quite popular for classification performance improvement compared to standard approaches using the Euclidean distance. Kernel metrics and quadratic forms belong to the most promising approaches. In this paper we consider Minkowski distances ( $l_p$ -norms). In particular,  $l_1$ -norms are known to be robust against noise in data, such that, if this structural knowledge is available in advance about the data, this norm should be utilized. However, application in gradient based learning algorithms based on distance evaluations need to calculate the respective derivatives. Because  $l_p$ -distance formulas contain the absolute approximations thereof are required. We consider in this paper several approaches for smooth consistent approximations for numerical evaluations and demonstrate the applicability for exemplary real world applications.

## 1 Introduction

Utilization of non-standard (non-Euclidean) metrics is one of the key ideas in learning vector quantization to improve the performance of classification learning. Whereas in traditional vector quantization the Euclidean distance is standard, kernel methods like support vector machines make use of kernel similarities [20]. Other examples are weighted Euclidean distances [8], general bilinear forms [22], correlations [23], functional norms and Sobolev distances [14, 18], divergences [4, 24] or kernel distances [20, 25], to name just a few.

Recently,  $l_p$ -norms with  $p \neq 2$  became popular as alternative dissimilarities in machine learning approaches [1, 6, 16]. Depending on the parameter  $p$ ,  $l_p$ -norms show different behavior, which makes them interesting for many applications [2, 17]. For example, the larger the  $p$ -value, the greater is the influence of noise for the receptive  $p$ -norm. Thus, for noisy data  $l_1$ -norms are more appropriate than the Euclidean norm [7].

Yet, differentiation of general  $l_p$ -norms and their induced dissimilarity measures suffers from the inconsistency for the origin  $\mathbf{x} = \mathbf{0}$  due to the inherent absolute value calculation. Therefore, the application of  $l_p$ -norms in gradient based machine learning approaches requires smooth consistent approximations of the derivatives.

The aim of the paper is twofold: First we consider several smooth approximations of dissimilarities induced by  $l_p$ -norms and semi-norms and provide consistent approximations of their derivatives. Thus, they can immediately be applied in gradient based learning vector quantization (GLVQ,[19]). Second, we show in two real world examples the successful application of  $l_1$ -norms for LVQ.

## 2 $l_p$ -Norms, derivatives and approximations thereof

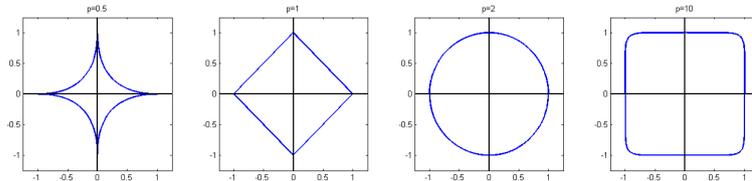
### 2.1 Basic notations and properties

In this section we provide useful approximations of the  $l_p$ -norms such that derivatives become available also at the origin  $\mathbf{x} = \mathbf{0}$ . For this purpose, we consider the Minkowski  $l_p$ -norm  $\|\mathbf{x}\|_p = \sqrt[p]{\sum_{i=1}^n |x_i|^p}$  for  $1 \leq p < \infty$  with the corresponding *Minkowski distance*  $d_p^*(\mathbf{v}, \mathbf{w}) = \|\mathbf{v} - \mathbf{w}\|_p$ . The frequently used quantity

$$d_p(\mathbf{v}, \mathbf{w}) = \left(\|\mathbf{v} - \mathbf{w}\|_p\right)^p \quad (1)$$

is only a dissimilarity measure violating the triangle-inequality and the linearity of distances. However, it is frequently considered in machine learning.

The choice of the  $p$ -value causes different behavior of the dissimilarities. The larger  $p$  the more important great variations become in a single dimension. For  $p < 1$  small variations, are emphasized and the unit 'circle' becomes concave, see Fig.1.



**Figure 1:** Unit circles for several Minkowski- $p$ -norms  $\|\mathbf{x}\|_p$ : from left to right  $p = 0.5$ ,  $p = 1$  (Manhattan),  $p = 2$  (Euclidean),  $p = 10$ .

For  $0 < p < 1$ ,  $d_p^*$  is only a *quasi-norm* [15] fulfilling  *$p$ -triangle inequality*  $\|\mathbf{v}\|_p^p + \|\mathbf{w}\|_p^p \leq \|\mathbf{v} + \mathbf{w}\|_p^p$ . However, now (1) is a *translation-invariant distance* [11]. The *weighted dissimilarities*

$$d_p^\lambda(\mathbf{v}, \mathbf{w}) = \sum_{i=1}^n \lambda_i |v_i - w_i|^p \quad \text{and} \quad d_p^\Omega(\mathbf{v}, \mathbf{w}) = \sum_{i=1}^m (|\Omega(\mathbf{v} - \mathbf{w})|_i)^p \quad (2)$$

with  $\lambda_i \geq 0$  subject to  $\sum_{i=1}^n \lambda_i = 1$  and  $\Omega \in \mathbb{R}^{m \times n}$ , respectively, were proposed for  $p = 2$  in relevance learning for learning vector quantization [8, 22]. Thereby, we denoted  $[\mathbf{x}]_i = x_i$ .

### 2.2 Formal derivatives for $d_p(\mathbf{v}, \mathbf{w})$

Utilization of those dissimilarities with in gradient based machine learning methods like self-organizing maps or GLVQ requires the calculation of the derivatives  $\frac{\partial d_p(\mathbf{v}, \mathbf{w})}{\partial \mathbf{w}}$ , where  $\mathbf{v} \in \mathbb{R}^n$  is a data vector  $\mathbf{w} \in \mathbb{R}^n$  is a prototype. Supposing  $0 < p < \infty$ , the formal derivative is

$$\frac{\partial d_p(\mathbf{v}, \mathbf{w})}{\partial w_k} = -p \cdot |z_k|^{p-1} \cdot \frac{\partial |z_k|}{\partial w_k} \quad (3)$$

with  $\mathbf{z} = \mathbf{v} - \mathbf{w}$ . The gradient (3) can be written in vectorized form as

$$\frac{\partial d_p(\mathbf{v}, \mathbf{w})}{\partial \mathbf{w}} = -p \cdot |\mathbf{z}|^{*(p-1)} \circ \frac{\partial |\mathbf{z}|}{\partial \mathbf{z}} \quad (4)$$

where  $\mathbf{x} \circ \mathbf{y} = (x_1 \cdot y_1, \dots, x_n \cdot y_n)^\top$  denotes the Hadamard product. Further,  $\mathbf{x}^{*k}$  denotes the componentwise power of  $\mathbf{x} = (x_1^k, \dots, x_n^k)^\top$  and  $\frac{\partial |\mathbf{z}|}{\partial \mathbf{w}} = -\frac{\partial |\mathbf{z}|}{\partial \mathbf{z}}$  holds. Analogously, we find

$$\frac{\partial d_p^\lambda(\mathbf{v}, \mathbf{w})}{\partial \mathbf{w}} = -p \cdot \lambda \circ |\mathbf{z}|^{*(p-1)} \circ \frac{\partial |\mathbf{z}|}{\partial \mathbf{z}} \quad \text{and} \quad \frac{\partial d_p^\Omega(\mathbf{v}, \mathbf{w})}{\partial \mathbf{w}} = -p \cdot \Omega^\top \left( |\mathbf{s}|^{*(p-1)} \circ \frac{\partial (|\mathbf{s}|)}{\partial \mathbf{s}} \right) \quad (5)$$

with  $\mathbf{s} = \Omega \mathbf{z} \in \mathbb{R}^m$ . We observe that we need the derivative of the absolute value function, which has to be approximated for the origin.

For  $p = \infty$  the above dissimilarity formulas (2) involve the maximum function  $\max(\mathbf{x}) = \max_i(x_i)$ . Thus we get

$$\frac{\partial d_\infty^\lambda(\mathbf{v}, \mathbf{w})}{\partial \mathbf{w}} = -\frac{\partial \max(\lambda \circ |\mathbf{z}|)}{\partial \mathbf{z}} \quad \text{and} \quad \frac{\partial d_\infty^\Omega(\mathbf{v}, \mathbf{w})}{\partial \mathbf{w}} = -\Omega^\top \frac{\partial \max(|\mathbf{s}|)}{\partial \mathbf{s}} \quad (6)$$

analogously. Here, the derivative of the maximum function is required. The derivatives for the relevance weights  $\lambda_i$  and the  $\Omega_{k,j}$  in case of the weighted dissimilarities (2) are obtained analogously for relevance or matrix learning and can be found in [13].

### 2.3 Approximations for the functions $\max(\mathbf{x})$ and $|\mathbf{x}|$

In the following we consider smooth approximation for the function  $\max(\mathbf{x})$  and  $|\mathbf{x}|$  as well as their derivatives.

At least two variants for the the maximum function easily are well-known: The first is the  $\alpha$ -softmax function

$$\mathcal{S}_\alpha(\mathbf{x}) = \frac{\sum_{i=1}^n x_i e^{\alpha x_i}}{\sum_{i=1}^n e^{\alpha x_i}} \quad (7)$$

with  $\alpha > 0$ , frequently applied in optimization and neural computation [3, 9]. A value  $\alpha < 0$  in (7) yields a smooth minimum approximation whereas for  $\alpha \rightarrow 0$  a soft approximation of the mean is obtained. The second frequently applied variant is the  $\alpha$ -quasimax function

$$\mathcal{Q}_\alpha(\mathbf{x}) = \frac{1}{\alpha} \log \left( \sum_{i=1}^n e^{\alpha x_i} \right) \quad (8)$$

proposed by J.D. COOK [5]. This  $\alpha$ -quasimax can be seen as a kind of a *generalized functional mean* or *quasi-arithmetic mean* discussed in [12]. One can easily verify that  $\mathcal{Q}_\alpha(\mathbf{x}) \leq \max(\mathbf{x}) + \frac{\log(n)}{\alpha}$  is always valid.

A smooth approximation of the absolute value function was proposed in [21]:

$$|x|_\alpha = (x)_\alpha^+ + (-x)_\alpha^+ \quad (9)$$

with  $(y)_\alpha^+ = \max(\mathbf{y}_0)$  for  $\mathbf{y}_0 = (y, 0)^\top$ . CHENG&MANGASARIAN proposed a convex  $\alpha$ -approximation  $(y)_\alpha^+ = y + \frac{1}{\alpha} \log(1 + e^{-\alpha y})$ . One verifies that this is equivalent to

$$(y)_\alpha^+ = y + \mathcal{Q}_\alpha(\mathbf{y}_0) \quad (10)$$

using the  $\alpha$ -quasimax function  $Q_\alpha$  from (8) [13]. Inserting these formulas in (9), we obtain an approximation

$$|x|_\alpha^Q = \frac{1}{\alpha} \log(2 + e^{-\alpha x} + e^{\alpha x}) \quad (11)$$

referred as  $\alpha$ -quasi-absolute. Hence,  $|x|_\alpha^Q$  is consistent with  $Q_\alpha(\mathbf{x})$  with the upper bound  $||x| - |x|_\alpha^Q| \leq 2 \frac{\log(2)}{\alpha}$  [17].

Alternatively, we can replace in (10) the  $\alpha$ -quasimax function  $Q_\alpha$  by the  $\alpha$ -softmax function  $S_\alpha$  which leads to

$$|x|_\alpha^S = \frac{x \cdot (e^{\alpha x} - e^{-\alpha x})}{2 + e^{\alpha x} + e^{-\alpha x}} \quad (12)$$

denoted as  $\alpha$ -soft-absolute.

### 2.3.1 Approximation of the derivatives

If the above introduced smooth approximations are used in gradient based numerical methods, neural networks or other methods in machine learning the derivatives have to be known. We provide the respective formulas in the following: In particular, we obtain

$$\frac{\partial |x|_\alpha^Q}{\partial x} = \tanh\left(\frac{\alpha}{2}x\right) \quad \text{and} \quad \frac{\partial |x|_\alpha^S}{\partial x} = \tanh\left(\frac{\alpha}{2}x\right) + \frac{\alpha x}{2 \left(\cosh\left(\frac{\alpha}{2}x\right)\right)^2}$$

for the  $\alpha$ -quasi-absolute  $|x|_\alpha^Q$  and for the  $\alpha$ -soft-absolute  $|x|_\alpha^S$ , respectively. Although  $|x|_\alpha^Q$  and  $|x|_\alpha^S$  look quite different, their derivatives differ only slightly by the additive deviation term

$$\Delta_{S_Q}(\alpha x) = \frac{\alpha x}{2 \left(\cosh\left(\frac{\alpha x}{2}\right)\right)^2}. \quad (13)$$

For the  $\alpha$ -softmax function  $S_\alpha(\mathbf{x})$  from (7), the gradient can be expressed in terms of  $S_\alpha(\mathbf{x})$  itself

$$\frac{\partial S_\alpha(\mathbf{x})}{\partial x_k} = \frac{e^{\alpha x_k}}{\sum_{i=1}^n e^{\alpha x_i}} [1 + \alpha(x_k - S_\alpha(\mathbf{x}))] \quad (14)$$

whereas for the  $\alpha$ -quasimax function  $Q_\alpha(\mathbf{x})$  from (8) we simply obtain

$$\frac{\partial Q_\alpha(\mathbf{x})}{\partial x_k} = \frac{e^{\alpha x_k}}{\sum_{i=1}^n e^{\alpha x_i}}. \quad (15)$$

Again, we observe only a slight variation  $\frac{\partial S_\alpha(\mathbf{x})}{\partial x_k} = \frac{\partial Q_\alpha(\mathbf{x})}{\partial x_k} \cdot \nabla_{S_Q}$  with the multiplicative corrector  $\nabla_{S_Q} = [1 + \alpha(x_k - S_\alpha(\mathbf{x}))]$ .

## 3 Applications

We applied the dissimilarity  $d_p^\Omega(\mathbf{v}, \mathbf{w})$  from (2) in the matrix variant of GLVQ (GMLVQ, [22]) for two different datasets. The first one is a set of 4120 tiling microarray (data dimension  $n = 24$ ) of corresponding to exonic and intronic/intragenic regions in chromosome 3 of *C.elegans*. Tiling micro array data usually contain a lot of noise

such that learning of these data is difficult. A detailed description of the data can be found in [1]. In the investigation described in this publication, the standard LVQ1 algorithm was applied for prototype learning, which is based on the (weighted) Euclidean norm  $d_2^\lambda(\mathbf{v}, \mathbf{w})$ . However, inherent prototype selection as well as relevance parameters  $\lambda_i$  optimization were done using the  $l_1$ -distance  $d_1^\lambda(\mathbf{v}, \mathbf{w})$  to deal with the noisy data. Thus, there is an inconsistency in the approach. The best performance was obtained for 6 prototypes per class: 89.3%. In our application we used the same number of prototypes (6 per class). We applied GMLVQ with  $d_p^\Omega(\mathbf{v}, \mathbf{w})$  for  $p = 1$  and  $p = 2$  consistently used for prototype learning and matrix adaptation in a 4-fold cross-validation. The achieved test accuracies are 90.8% and 88.8%, respectively. Thus consistent  $l_1$ -learning improves the result. Further, we did not recognize any significant difference regarding the used approximation ( $\alpha$ -quasi-absolute or  $\alpha$ -soft-absolute,  $\alpha = 20$ ).

In a second application we analyzed spectral data obtained from a gas chromatography–mass spectrometry (GC-MS) analysis of volatile organic components in exhaled breath for detection of inflammatory processes in the lung. The GC-MS spectra were delivered as 334-dimensional spectra covering a measurement time interval of 20min. The dataset contains 48 spectra partitioned into two classes. A detailed data description can be found in [10]. We used only one prototype per class in GMLVQ and conducted a 8-fold cross-validation. Again we applied  $d_p^\Omega(\mathbf{v}, \mathbf{w})$  for  $p = 1$  and  $p = 2$  consistently for prototype learning and matrix adaptation. We achieved the test accuracies 85.4% and 81.3%, respectively. The better  $l_1$ -result clearly emphasizes this choice of dissimilarity. This is in agreement with the knowledge about the noise influence for GC-MS spectra regarding the peak height [26] and the above mentioned robust behavior of  $l_p$ -distances for smaller  $p$ -values also reported in [7].

## 4 Conclusion

In this paper we consider  $l_p$ -distances and discuss smooth approximation thereof, which are required when used in gradient based learning methods based on dissimilarity evaluations between data and reference vectors. Generally,  $l_p$ -distances contain the absolute value function, which causes difficulties for the (numerical) calculation of the derivatives. We provide smooth approximations and explain the respective derivatives. We compare the utilization of the weighted  $l_1$ -distance with the weighted Euclidean distance for two applications. The first one is also in comparison to an earlier but inconsistent approach. We demonstrate that  $l_1$ -distances can be successfully applied using the described approximation techniques.

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