# Neural networks in non-Euclidean metric spaces.

Włodzisław Duch and Rafał Adamczak, Department of Computer Methods, Nicholas Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland. E-mail: duch,raad@phys.uni.torun.pl

#### Abstract.

Multilayer Perceptrons (MLPs) use scalar products to compute weighted activation of neurons providing decision borders using combinations of soft hyperplanes. The weighted fun-in activation function corresponds to Euclidean distance functions used to compute similarities between input and weight vector. Replacing the fan-in activation function by non-Euclidean distance function offers a natural generalization of the standard MLP model, providing more flexible decision borders. An alternative way leading to similar results is based on renormalization of the input vectors using non-Euclidean norms in extended feature spaces. Both approaches influence the shapes of decision borders dramatically, allowing to reduce the complexity of MLP networks.

#### I. INTRODUCTION

TEURAL networks of the most popular multi-layer perceptron (MLP) type perform discrimination of the input feature space using hyperplanes. Many other transfer function have been proposed to increase the flexibility of contours used for estimation of decision borders [1] (for a recent review see [2]). Perhaps the best known alternative to sigmoidal functions are localized Gaussian functions and other radial basis functions. Viewing the problem of learning from geometrical point of view functions performed by neural nodes should enable tessellation of the input space in the most flexible way using a small number of adaptive parameters. Although neural networks with single hidden layer using sigmoidal or Gaussian functions can approximate an arbitrary continuous function on a compact domain with arbitrary precision given sufficient number of neurons [3], i.e. they are universal approximators, for some datasets a large (and hard to train) network using sigmoidal or Gaussian functions may be needed for tasks that could be solved with a small (and easy to train) networks using other transfer functions, providing more flexible borders.

Improvement in learning and architectures of neural networks may not be able to overcome inherent drawbacks of models that provide wrong decision borders for a given problem. Consider a simple classification problem in N dimensions, with spherical distribution of vectors belonging to class  $C_1$ , to be distinguished from vectors belonging to class  $C_2$ , lying outside the unit sphere. A single neuron performing multivariate Gaussian function with 2N adaptive parameters (specifying the center and dispersions in each dimension) is sufficient for this job and the training process is quite simple. Many hyperplanes provided by sigmoidal functions are needed to approximate spherical decision borders. The simplest approximation, using the standard multilayer perceptron (MLP) architecture, that captures any bound region of N-dimensional space, requires construction of a simplex using N sigmoids and an additional neuron to smooth the output of a combination of these neurons. Thus at least  $N^2 + N$  parameters are needed, compared with 2N parameters for localized functions. On the other hand if data vectors belonging to the first class are taken from the corner of the coordinate system bound by the (1, 1, ..., 1) plane a single sigmoidal function with N + 1 parameters is sufficient for perfect classification while Gaussian approximation will be quite difficult. A poor approximation may use one Gaussian in the center of the region and N + 1 Gaussians in the corners, using 2N(N+2) adaptive parameters.

In the first example the complexity of the training process is  $O(N^2)$  for MLP and O(N) for RBF, and in the second example the situation is reversed. One may easily create more complicated examples with more classes between concentric spheres of growing radii or with series of hyperplanes passing through (m,m,...,m) points. Improved learning algorithms or network architectures will not change the relative complexity of solutions as long as the decision borders provided by the transfer functions remain spherical (as in the first example) or planar (as in the second example). Artificial examples that are favorable for other types of functions are also easy to construct.

MLPs are similar to statistical discriminant techniques, although soft sigmoids allow for representation of more complex, nonlinear decision borders. This is usually considered to be a strength of the MLP model, although in cases when sharp decision borders are needed it may also become its weakness. For example, classification borders conforming to a simple logical rule  $x_1 > 1 \land x_2 > 1$  are easily represented by two hyperplanes, but there is no way to represent them accurately using soft sigmoidal functions. Increasing the slopes of sigmoidal functions to improve representation of such decision borders around the (1,1) point leads to problems with learning by backpropagation, or by any other gradientbased method, since the volume of the input space in which sigmoids change rapidly (and thus gradients are non-zero) is rapidly shrinking. In the limit sigmoidal functions become step-functions but gradient techniques like backpropagation cannot be used to make this transition. As a result for some datasets no change in learning rule or network architecture will improve the accuracy of neural solutions. A good realworld example is the hypothyroid dataset, for which the best optimized MLPs still give about 1.5% of error [4] while logical rules reduce it to 0.64% (since 3428 cases are provided for testing this is a significant improvement). Another example may be provided by the NASA Shuttle benchmark data [5], where MLP makes about 3.5% errors on the test set, RBF makes about 1.4% error while logical rules achieve 0.01% of errors (one or two vectors out of 14500 in the test set).

Most research on neural networks is concentrated on architectures and learning rules, but selection of neural transfer functions may be crucial to network performance [1]. Networks providing the most flexible decision borders with the lowest number of adaptive parameters may have an advantage over larger and more complex networks. There are two ways to create such networks. First, flexibility of transfer functions may be increased and second, inputs may be transformed in a non-linear way. Transfer functions  $o(I(\mathbf{X}))$ are compositions of the activation  $I(\mathbf{X})$  and the output function o(I). Output functions are usually either sigmoidal (S-shaped) squashing functions, preventing the unbounded growth of signals in the network, or localized, bell-shaped functions. Activation functions are almost always either fanin weighted scalar products  $\mathbf{W} \cdot \mathbf{X}$  used with sigmoidal functions or Euclidean distance functions used with bell-shaped functions. In this paper we will show how to change the activation functions to obtain more flexible decision borders. Flexibility of transfer functions is strongly correlated with the number of functions (and thus with the number of adaptive parameters available for training) necessary to model complex shapes of decision borders.

We will place our considerations in the general framework for similarity-based classification methods (SBMs) presented recently [6], [7]. Investigation of connections between neural network and similarity-based methods leads to a number of new neural network models. In particular the distancebased MLP (D-MLP) networks are obtained by replacing the weighted activation with a square of Euclidean distance [8]. Such networks improve upon the traditional approach by providing more flexible decision borders and by enabling a prototype-based interpretation of the results. Since the use of distance functions (instead of weighted activation) in neural network models is a novel idea it is described in the next section. In the third section transformation of the input data to the extended feature space is proposed, enabling the use of non-Euclidean distance functions in the standard MLP backpropagation programs without the need for coding the new transfer functions and their derivatives. The fourth section shows how to determine the architecture and parameters of such networks, including the slopes for each neuron. An illustration of this method on the Iris data is presented for pedagogical purposes in the fifth section. The paper is finished with a short discussion.

#### II. DISTANCE FUNCTIONS IN NEURAL NETWORKS

In the similarity-based framework the classification problem is solved using a set of class-labeled training vectors  $\{\mathbf{R}^{j}, C(\mathbf{R}^{j})\}, j = 1..N_{t}$ , where  $C(\mathbf{R}^{j})$  is the class of  $\mathbf{R}^{j}$ . The probability  $p(C_i | \mathbf{X}; M)$  that a given vector **X** belongs to class  $C_i$  is calculated using the information provided in the similarity measure  $D(\mathbf{X}, \mathbf{R}^{j})$ . M stands here for the classification model used, i.e. values of all parameters and procedures employed. A general similarity-based model [6] of an adaptive system used for classification may include various types of parameters and procedures, such as: the set  $\{\mathbf{R}^j\}$ of reference vectors created from the set of training vectors  $\{\mathbf{X}^i\}$  by selection and/or optimization procedure; a similarity function  $D(\cdot)$  (frequently a distance function or an activation function in neural networks) parameterized in various ways, or a table used to compute similarities for nominal attributes; a weighting function  $G(D(\mathbf{X}, \mathbf{R}))$ , estimating contribution of the reference vector  $\mathbf{R}$  to the classification probability depending on its similarity to the vector X; the total cost function  $E[\cdot]$  optimized during training. The cost function may include regularization terms, hints [3], it may depend upon a kernel function  $K(\cdot)$ , scaling the influence of the error, for a given training example, on the total cost, it may use a risk matrix  $R(C_i|C_i)$  of assigning wrong classes or a matrix  $S(C_i|C_i)$  measuring similarity of output classes. In some models the number of reference vectors k taken into account in the neighborhood of **X** is specified. An adaptive system may include several such models  $M_l$  and an interpolation procedure to select between different models or average results of a committee of models.

In RBF networks Euclidean distance functions  $D(\mathbf{X}, \mathbf{R}^j) = ||\mathbf{X} - \mathbf{R}^j||$  are assumed and radial, for example Gaussian  $G(D) = \exp(-D^2)$ , or  $G(D) = 1/(1+D^2)$  weighting functions are used. Essentially RBF is a minimal distance soft weighted method with no restrictions on the number of neighbors – reference vectors  $\mathbf{R}^j$  that are close to  $\mathbf{X}$  influence probabilities of classification more than those that are far. The SBM framework suggests that there is nothing special about this choice of distance function and the weighting function. Any distance function  $D(\mathbf{X}, \mathbf{R})$  and the weighting function G(D) may be used to create neural network. In the

Gaussian classifier [9] or in the original RBF network only one parameter, dispersion, was optimized [10]. Optimization of the positions of the reference centers  $\mathbf{R}^{j}$  leads to the LVQ method [11] in which the training set vectors are used to define the initial prototypes and the minimal distance rule is used to assign the classes. The Restricted Coulomb Energy (RCE) classifier [12] uses a hard-sphere weighting functions. The Feature Space Mapping model (FSM) is based on separable, rather than radial weighting functions [13]. Recently a method to create oblique probability distributions in *N*-dimensional space using only *N* parameters has been described [1].

MLPs and other networks using discriminant functions are also special cases of general SBM framework. Threshold neurons compute distances in a natural way. If the input signals **X** and the weights **W** are  $(\pm 1... \pm 1)$  vectors, neuron with *N* inputs and the threshold  $\theta$  realizes the following function:

$$\Theta(\sum_{i}^{N} W_{i}X_{i} - \theta) = \begin{cases} 0 & \text{if } ||\mathbf{W} - \mathbf{X}|| > (N - \theta)/2 \\ 1 & \text{if } ||\mathbf{W} - \mathbf{X}|| \le (N - \theta)/2 \end{cases}$$
(1)

where  $||\cdot||$  norm is defined by the Hamming distance. One can interpret the weights of neurons in the first hidden layer as addresses of the reference vectors in the input space and the activity of threshold neuron as activation by inputs falling into a hard sphere of radius  $\theta$  centered at **W**. The Hamming neural network [14] is actually a neural realization of the nearest neighbor method for a single neighbor and binary inputs. Changing binary into real values and threshold into sigmoidal neurons for inputs normalized to  $||\mathbf{X}|| = ||\mathbf{W}|| = 1$  leads to soft activation of neurons by input vectors close to **W** on a unit sphere. In general the activation of a neuron is written as:

$$\mathbf{W} \cdot \mathbf{X} = \frac{1}{2} \left( ||\mathbf{W}||^2 + ||\mathbf{X}||^2 - ||\mathbf{W} - \mathbf{X}||^2 \right)$$
(2)

For normalized input vectors sigmoidal functions (or any other monotonically growing transfer functions) may therefore be written in the form:

$$\sigma(\mathbf{W} \cdot \mathbf{X} + \theta) = \sigma(d_0 - D(\mathbf{W}, \mathbf{X}))$$
(3)

where  $D(\mathbf{W}, \mathbf{X})$  is the square of Euclidean distance between  $\mathbf{W}$  and  $\mathbf{X}$  and the 1/2 factor is absorbed in the sigmoid's slope. This function evaluates the influence of the reference vectors  $\mathbf{W}$  on the classification probability  $p(C_i|\mathbf{X}; \mathbf{W})$ . To avoid loss of information during normalization of input vectors an additional component  $X_r$  is added, a new feature measuring the difference between largest norm and the norm of the original input vectors.

Transfer function  $f(D(\mathbf{W}, \mathbf{X})) = \sigma(d_0 - D(\mathbf{W}, \mathbf{X}))$  decreases monotonically as a function of distance, with flat plateau for small distances D, reaching the value of 0.5 for  $D(\mathbf{W}, \mathbf{X}) = d_0$  and approaching zero for larger distances. For normalized  $\mathbf{X}$  but arbitrary  $\mathbf{W}$  the sigmoid arguments belong to the  $[\theta - |\mathbf{W}|, \theta + |\mathbf{W}|]$  interval. A unipolar sigmoid has its maximum curvature around  $\pm 2.4$ , therefore smaller thresholds and norms of the weights mean that the network operates in an almost linear regime, smoothing the network approximation to the training data. This is one of the reasons why regularization methods, adding penalty terms to the error function to reduce the weights, improve generalization [3].

From the similarity-based point of view MLP networks use sigmoidal functions to estimate the influence of weight vectors according to distance between these vectors and the training vectors, combining many such estimations to compute the final output. Changing the distance function in equation (3) from the square of the Euclidean distance to some other distance measures, new types of neural networks, called D-MLP networks [8], are defined. Another possibility is to write the weighted product in the form:

$$\sigma(\mathbf{W} \cdot \mathbf{X}) = \sigma\left(\frac{1}{4}(||\mathbf{W} + \mathbf{X}||^2 - ||\mathbf{W} - \mathbf{X}||^2)\right) \quad (4)$$

Euclidean norms may be replaced by Minkovsky or other type of norms. Backpropagation procedure requires derivatives of the distance functions, but for Minkovsky and several functions they are easily provided. Generalized Minkovsky's distance with the scaling factors is given by:

$$D(\mathbf{A}, \mathbf{B}; s)^{\beta} = \sum_{i}^{N} s_{i} d(\mathbf{A}_{i}, \mathbf{B}_{i})^{\alpha}$$
(5)

where  $\beta = \alpha$  is usually taken. The  $d(\cdot)$  function is used to estimate similarity at the feature level and in the simplest case  $d(\mathbf{A}_i, \mathbf{B}_i) = |\mathbf{A}_i - \mathbf{B}_i|$ . For  $\alpha = \beta = 2$  the vectors  $||\mathbf{A}|| = 1$  are on the unit sphere, for large  $\alpha$  the sphere is changed into a soft cuboid, for  $\alpha = 1$  it has pyramidal and for  $\alpha < 1$  hypocycloidal shape.

Thus using non-Euclidean distance activation functions changes the shape of decision borders completely, from the usual hyperplanes ( $\beta = 1$ ,  $\alpha = 2$  and  $W_r = 0$  for the weight corresponding to the  $X_r$  component) to spherical, cuboidal or hypocycloidal. Derivation of the backpropagation equations for  $\sigma(d_0 - D(\mathbf{X}, \mathbf{W}))$  functions with generalized Minkovsky distances is straightforward but requires extensive modification of standard MLP software. Instead of changing the activation function nonlinear transformation of input features may also change decision borders.

## III. NORMALIZATION OF INPUT VECTORS IN NON-EUCLIDEAN SPACES

The parameter  $d_0$  in Eq. (3) should be treated as an adaptive parameter only if **X** is normalized. This may always be

done without loss of information if one or more additional components are added to the vector, extending the feature space by at least one dimension. Taking  $X_r = \sqrt{R^2 - ||\mathbf{X}||^2}$ , where  $R \ge \max_X ||\mathbf{X}||$ , amounts to a projection of the data on a unit hemisphere with radius *R*. Vectors  $(\mathbf{X}, X_r)$  may be renormalized  $||(\mathbf{X}, X_r)||_D = 1$  using the metric defined by the distance function  $D(\mathbf{X}, \mathbf{R})$ .

The distance function may be heterogeneous, using Minkovsky's metric for numerical features and probabilistic metric functions for symbolic features. In memory-based reasoning the Modified Value Difference Metric (MVDM) has gained popularity [15]. The distance between two *N*-dimensional vectors  $\mathbf{A}$ ,  $\mathbf{B}$  with discrete (nominal, symbolic) elements, in a *K* class problem, is computed using conditional probabilities:

$$D_V^{\alpha}(A,B) = \sum_j^N \sum_i^K \left| p(C_i|A_j) - p(C_i|B_j) \right|^{\alpha} = \sum_j^N d_V^{\alpha}(A_j,B_j)$$
(6)

where  $p(C_i|A_j)$  is estimated by calculating the number  $N_i(A_j)$  of times the value  $A_j$  of the feature j occurred in vectors belonging to class  $C_i$ , and dividing it by the number of times  $A_j$  occurred for any class. A "value difference"  $d_V^{\alpha}(A_j, B_j)$  for each feature j allows to compute  $D_V(\mathbf{A}, \mathbf{B})$  as a sum of additive factors for all features. Distance is defined here via a data-dependent matrix with the number of rows equal to the number of classes and the number of columns equal to the number of all attribute values. Generalization for continuos values requires a set of probability density functions  $p_{ij}(x)$ , with i = 1..K, j = 1..N. Additional scaling factors may be introduced, as in Eq. (5).

Using VDM type of metrics leads to problems with calculation of gradients, but replacing symbolic features by vectors of  $p(C_i|A_j)$  probabilities (with dimension equal to the number of classes times the number of different symbolic values the feature takes) allows to reproduce MVDM distances using numerical values of vector components. Many other types of metric functions exist [15] and their performance should be empirically verified. Several alternative extensions of the input space may be considered, for example adding one or more features  $X_r = D(\mathbf{X}, \mathbf{R})$  equal to the distance of a given vector  $\mathbf{X}$  to some fixed vector  $\mathbf{R}$  a parabolic projection is made.

It may be of some advantage to increase the separation of the clusters projected on the hypersphere. It is impossible to make such a projection on the whole hypersphere without violating topological constraints. In the one-dimensional case with  $X \in [-1,+1]$  the  $(X,X_r)$  vector should not make a full circle when *X* is changed from -1 to +1 because the two extreme vectors  $X = \pm 1$  will then be identical. An optimal separation for 3 vectors with the length  $||X||, ||X|| + \Delta, ||X|| + 2\Delta$  is to place them in corners of equilateral triangle, for example at angles  $0, \pm 120^{\circ}$ . One can search for the best input preprocessing treating it as a rigorous optimization problem, or just use polar coordinates to shift some upper hemisphere vectors to the part of the lower hemisphere. Much simpler approach is to rescale all vectors to get their Euclidean norms  $\leq 1$ , and use the norm ||X|| mapping it to points on a circle:  $(\sin \frac{\pi}{3}(4-5||X||), \cos \frac{\pi}{3}(4-5||X||))$ . These points for  $0 \leq ||X|| \leq 1$  are within the angle  $-\pi/3$  and  $4\pi/3$ . The first factor,  $\sin \frac{\pi}{3}(4-5||X||)$  is used to rescale all components of the vector **X**, while the second factor is taken as an extra  $X_r$  component. Extended vectors  $||(\mathbf{X}^j, X_r^j)||_D$  are renormalized using the metric function  $D(\cdot)$ , placing them on a unit sphere defined by this metric.

#### IV. INITIALIZATION OF THE NETWORK

The network should be initialized taking the centers of clusters in the extended space as **W** and taking  $d_0 = D(\mathbf{W}, \mathbf{X}^b)$ , where  $\mathbf{X}^{b}$  is a vector at the border of the given cluster (we have tried [16] dendrograms and decision trees but other clusterization methods may also be used for initialization [9]). Using weighted activation the contribution of a center of an input data cluster C laying on the unit sphere is  $W \cdot C$ . The largest activation is obtained when the weights W point in the same direction as the center C. The logistic function  $\sigma(\mathbf{C} \cdot \mathbf{X} - \theta) = (1 + \exp((-\mathbf{C} \cdot \mathbf{X} + \theta)/T))^{-1}$ , where T determines the slope, has the largest gradient in the direction of W = C. The value  $\sigma(0) = 0.5$  is obtained at a  $\theta$  distance from the origin of the coordinate system. Since the C vector is normalized  $\theta = 1$  places the contours for 0.5 value tangentially to the unit hypersphere. Contours for lower values  $\sigma(\mathbf{C} \cdot \mathbf{X} - \theta) < 0.5$  cut segments of the hypersphere in which the value of  $\sigma(\mathbf{C} \cdot \mathbf{X} - \theta)$  is constant.

A parameter which is rarely changed in MLPs is the slope of sigmoidal functions. It defines the area which has an influence on performance of each node. If the slope is too high the area in which the sigmoidal function is not approximately constant is small and only a few training vectors have a chance to influence the gradient-based learning procedures. If it is too low then all functions strongly overlap and there is no possibility to create sharp decision borders. Normalization of the weights **W** is equivalent to a local change of the slope:

$$(\mathbf{W} \cdot \mathbf{X} + \mathbf{\theta})/T = (\frac{\mathbf{W}}{||\mathbf{W}||} \cdot \mathbf{X} + \frac{\mathbf{\theta}}{||\mathbf{W}||})||\mathbf{W}||/T = (\mathbf{W}' \cdot \mathbf{X} + \mathbf{\theta}')/T' = (d_0' - D(\mathbf{W}', \mathbf{X}))/T'$$
(7)

Thus without loss of generality both **X** and **W'** may be normalized. No special learning for slopes is required since they are computed from norms of weights. A useful variability range of the sigmoid is between its maximum curvature points, which for T = 1 are between  $\Delta(T) = \pm 2.4$ . If the variability range is assumed to be 1/10 of the size of the cluster, i.e.  $\Delta(T) = \pm d_0/10$  then setting  $T \approx d_0/24$  will be appropriate. After such initialization training of the network is usually quite short.

In the XOR case the input vectors for class = T are (0,1),(1,0) and for the class = F are (0,0),(1,1). The mean for each feature is 0.5 and after shifting and renormalizing the vectors are  $C_1 = (-1, +1)/\sqrt{2}$ ,  $C_2 = (+1, -1)/\sqrt{2}$  for class T and  $(-1,-1)/\sqrt{2}$ ,  $(+1,+1)/\sqrt{2}$  for class F. Selecting one of the classes for output, for example class T, initial weights for the first neuron are given by  $C_1$  and for the second neuron by  $C_2$ , while the hidden to output layer weights are all +1. This is the correct and the simplest solution for the XOR problem found without any optimization of the network! For more complex examples of this type of initialization see [16]. Since the architecture of the MLP network in the extended space is completely determined by the initialization procedure (clusterization method used determines all parameters), and the training should be rapid due to a good starting point, many distance functions may be tried on a given problem.

#### V. PEDAGOGICAL ILLUSTRATION

The influence of input renormalization (using non-Euclidean distance functions) on the shapes of decision borders is illustrated below on the classical Iris flowers dataset, containing 150 cases divided into 3 classes [17]. The flowers are described by 4 measurements (petal and sepal width and length). Two classes, Iris virginica and Iris versicolor, overlap, and therefore a perfect partition of the input space into separate classes is not possible. An optimal solution (from the point of view of generalization) contains 3 errors [18] and may be obtained using only two of the four input features ( $x_3$  and  $x_4$ ), therefore results are easy to display and only those two features have been left in simulations described below. The data has been standardized and rescaled to fit inside a square with  $\pm 1$  corners.

A standard MLP solution is obtained with 2 input, 4 hidden and 3 output neurons, with a total of 27 adaptive parameters. One discriminating plane per class for the smallest and the largest flowers (setosa and virginica) is needed and two planes are needed to separate the vectors of the versicolor class. To increase accuracy and speed up learning, in the final phase of learning only the vectors near the class borders were presented to the network. The selection algorithm loops over all vectors and for a given vector **X** finds *k* (for example k = 10) nearest vectors belonging to a different class than **X**. These vectors are written to a new training file providing a description of the border region. This method of training leads to sharper and more accurate decision borders, as seen in the first drawing of Fig. 2.

An additional input feature has been added and the 3-



Fig. 1. Shapes of decision borders in the Iris case for the network without the hidden layer (3 output neurons, 3 inputs), with growing  $W_3$  weight.

dimensional vectors normalized using various Minkovsky distance measures. The network has been initialized taking the normalized weights that are equal to the centers of the three clusters. In the extended feature space the same accuracy is achieved using only 3 input and 3 output neurons without the hidden layer, for a total of 12 adaptive parameters. Using such network architecture with squared Euclidean metric and the weight  $W_3 = 0$  for the third  $X_3$  component, only two classes are separated. The transition process from the planar to circular decision borders is shown in Fig. 1 (clockwise, from top left). In the learning process  $W_3$  grows, curving the borders for vectors near the center of the drawing.

In Fig. 2 dramatic changes in the final shapes of decision borders for Minkovsky metric are shown. Euclidean case corresponds to circular decision borders, the city block metric  $\alpha = 1$  gives sharp, romboidal shapes, for large  $\alpha$  almost rectangular decision borders are obtained (an approximation using logical rules is in this case quite accurate) while for small  $\alpha$  hypocycloidal shapes are created. For the Iris data the optimal solution (3 errors) has been recovered for all values of  $\alpha \ge 0.8$ . Smooth transition between these cases is made by changing  $\alpha$  and retraining the network.

For other datasets we have found significant improvements of accuracy for optimized  $\alpha$ .

#### VI. DISCUSSION

Distance-based neural networks increase flexibility of decision borders by modifying transfer functions, either in a global way (if the same distance function is used for each node), or locally (if distance function are different at each node). Non-Euclidean transformations of input vectors also lead to very flexible shapes of neural network decision bor-



Fig. 2. Shapes of decision borders in the Iris case for standard MLP (2 inputs, 3 hidden and 3 output neurons, first drawing) and using additional input dimension to renormalize data vectors with Minkovsky metric,  $\alpha$ =2.0, 0.5, and 7.0.

ders without any change in the standard computer programs. The training times are short since a good initialization procedure based on clusterization techniques determines weights, thresholds and slopes of all neurons. The complexity of network architecture defined in extended space is usually smaller comparing to the standard MLPs needed to obtain similar accuracy on a given dataset, as has been observed in the Iris example. Since the training is fast many different metric functions may be tried before selecting (using cross-validation tests) the best model. Networks with activation given by Eq.(3) or (4) have not yet been implemented but such models seem to be quite promising.

The change of the shapes of decision borders has been accomplished before by adding new type of units to neural networks (see the forthcoming review [2]). For example, Ridella et al. [19] used circular units in their Circular Backpropagation Networks. Different type of circular units have been used by Kirby and Miranda [20] – in their implementation two sigmoidal units are coupled together and their output is restricted to lie on a unit circle. Dorffner [21] proposed conic section transfer functions as a unified framework for MLP and RBF networks. Straight lines and ellipses are special cases of conic sections. Non-Euclidean metrics have been used to characterize the manifold of all Boltzman machines and EM algorithms by Amari [22], but not for increasing the flexibility of neural network decision borders. The input renormalization method may be treated as a generalization of the circular or conical unit method. It is not restricted to MLP neural networks, but can be used with any neural network and any classifier. An additional advantage of our approach is the understanding of what the network has really learned in terms of the prototypes (weights) and sigmoidally weighted distances (similarities) to these prototypes.

### Acknowledgments

Support by the KBN, grant 8 T11F 014 14, is gratefully acknowledged.

#### REFERENCES

- W. Duch, N. Jankowski, *New neural transfer functions*, Applied Mathematics and Computer Science 7 (1997) 639-658
- [2] W. Duch, N. Jankowski, *Survey of Neural Transfer Functions*. Neural Computing Surveys (submitted, 1999)
- [3] Bishop C, Neural networks for pattern recognition. Clarendon Press, Oxford, 1995
- W. Schiffman, M. Joost, R. Werner, Comparison of optimized backpropagation algorithms, Proc. of ESANN'93, Brussels 1993, pp. 97-104
- [5] D. Michie, D.J. Spiegelhalter and C.C. Taylor, *Machine learning, neu*ral and statistical classification. Elis Horwood, London 1994
- [6] W. Duch, Neural minimal distance methods, Proc. 3-rd Conf. on Neural Networks and Their Applications, Kule, Poland, Oct. 14-18, 1997, pp. 183-188
- [7] W. Duch, K. Grudzinski, G.H.F. Diercksen, *Minimal distance neural methods*. World Congress of Computational Intelligence, May 1998, Anchorage, Alaska, IJCNN'98 Proceedings, pp. 1299-1304
- [8] W. Duch, R. Adamczak, G.H.F. Diercksen, *Distance-based multilayer perceptrons*, In: Computational Intelligence for Modelling Control and Automation. Neural Networks and Advanced Control Strategies. Ed. M. Mohammadian, IOS Press, Amsterdam, pp. 75-80
- [9] P.R. Krishnaiah, L.N. Kanal, eds, *Handbook of statistics 2: classification, pattern recognition and reduction of dimensionality.* (North Holland, Amsterdam 1982)
- [10] P.D. Wasserman, Advanced methods in neural networks. (van Nostrand Reinhold 1993)
- [11] T. Kohonen, Self-organizing maps. (Berlin, Springer-Verlag 1995).
- [12] D.L. Reilly, L.N. Cooper, C. Elbaum, A neural model for category learning, Biological Cybernetics 45 (1982) 35–41
- [13] W. Duch, G.H.F. Diercksen, Feature Space Mapping as a universal adaptive system, Comp. Phys. Communic. 87 (1995) 341-371
- [14] R.P. Lippmann, An introduction to computing with neural nets, IEEE Magazine on Acoustics, Signal and Speech Processing 4 (1987) 4-22;
  P. Floreen, The convergence of Hamming memory networks, Trans. Neural Networks 2 (1991) 449-457
- [15] D.R. Wilson, T.R. Martinez, Improved heterogenous distance functions. J. Artificial Intelligence Research 6 (1997) 1-34
- [16] W. Duch, R. Adamczak, N. Jankowski, *Initialization and optimization of multilayered perceptrons*, 3rd Conf. on Neural Networks and Their Applications, Kule, Poland, October 1997, pp. 105-110
- [17] C.J. Mertz, P.M. Murphy, UCI repository, http://www.ics.uci.edu/pub/machine-learning-databases.
- [18] Duch W, Adamczak R, Grąbczewski K, Żal G, Hybrid neural-global minimization method of logical rule extraction, Journal of Advanced Computational Intelligence (in print, 1999)
- [19] S. Ridella, S. Rovetta, R. Zunino, Circular Backpropagation Networks for Classification, IEEE Trans. Neural Networks 8 (1997) 84–97
- [20] M.J. Kirby, R. Miranda, Circular Nodes in Neural Networks, Neural Computations 8 (1996) 390-402
- [21] G. Dorffner, A Unified Framework for of MLPs and RBFNs: Introducing Conic Section Function Networks, Cybernetics & Systems 25 (1994) 511-554
- [22] S-i. Amari, Information geometry of the EM and em algorithms for neural networks, Neural Networks 8 (1995) 1379-1408