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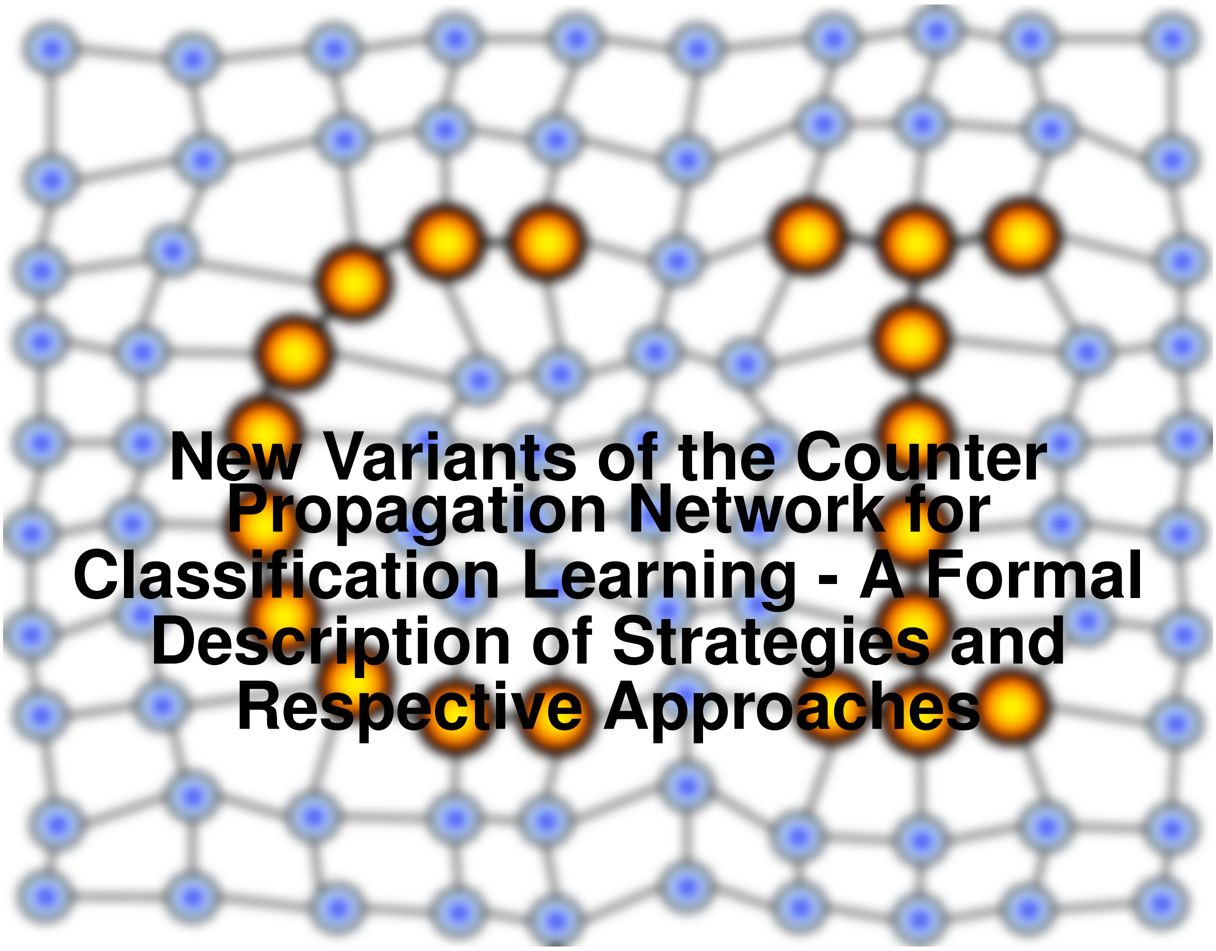

# New Variants of the Counter Propagation Network for Classification Learning - A Formal Description of Strategies and Respective Approaches

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# New Variants of the Counter Propagation Network fo Classification Learning

## – *A Formal Description of Strategies and Respective Approaches* –

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**Abstract**

In this paper we present new variants of the counter propagation network introduced already in 1987 by Robert Hecht-Nielsen, which is a network consisting of a vector quantization layer and a subsequent classification layer. In particular, we discuss several vector quantization layers and how to transmit the information to the classification layer. This is discussed in relation to the information-bottleneck-paradigm and regarding perspectives for network training are provided. Thereby, both layers are not longer handled independently during training as in the original approach. More precisely, we explain how the vector quantization layer can be optimized in dependence on the following classification layer. The mathematical formulations of the models are described in detail.

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# 1 Introduction and Motivation

The idea of a counter propagation network (CPN), as proposed by R. Hecht-Nielsen [15, 17] in 1987, is to combine a self-organizing map vector quantizer with a perceptron layer for supervised learning. The perceptron layer is also denoted as Grossberg-layer (defined in [13]) in this context and was later also used in ART networks [5]. Recently, the idea of this vector quantization combination with perceptron layers was renewed by C. Rudin for deep multi-layer perceptrons to achieve better robustness [6]. Further, if the vector quantization layer is interpreted as an data compressing tool, we can take a CPN as realization of the information bottleneck method proposed by N. Tishby and N. Zaslavsky in [48, 47]. Furthermore, it can be seen as an approach to the dilemma of representation versus classification as addressed in [34, 36].

The paper first briefly review original CPN. This approach trains the vector quantizer independently from the later Grossberg-layer, which is responsible for the supervised learning task. The main part of the paper deals with several approaches to overcome precisely the information gap. In particular, we investigate how to train the vector quantization layer in dependence of the classification/regression layer. Moreover, we discuss different vector quatizer models instead of the self-organizing map, which is mathematically inconsistent [10, 7]. This includes the neural gas approach from T. Martinetz [31], the Heskes-variant of SOM [19], as well as fuzzy variants of c-means proposed by J. Bezdek [3, 23]. Further, we propose to replace the perceptron layer by variants of learning vector quantizers for classification learning. In fact, we concentrate on classification learning. However, an extension to regression learning is straight-forward.

In this article, we suppose a vector quantizer with reference vectors $W = \{\mathbf{w}_1, \ldots, \mathbf{w}_K\} \subset \mathbb{R}^n$ for data representation and data $X \subseteq \mathbb{R}^n$. These vectors act as local sensors in the data space to detect signals $\mathbf{x} \in \mathbb{R}^n$ usually by means of a dissimilarity measure $d(\mathbf{x}, \mathbf{w}_k)$. We denote them as *sensoric prototypes* and $W$ is the respective the sensor array (set). Further, we assume data classes $\mathscr{C} = \{1, \ldots, C\}$ and training data labels $c(\mathbf{x}) \in \mathscr{C}$.

# 2 The Original Counter Propagation Network

As already mentioned, the original CPNs consists of two layers. The first one is a self-organizing map (SOM,[26]) layer denoted as in-star layer in this context. The second layer is a perceptron layer called here a Grossberg-outstar-layer [15]. We will denote the first layer as the *vector quantization layer* and the second layer as the *classification layer* to emphasize the more general context later in this paper.

For the SOM we assume that the sensoric prototype set $W$ is related to an external *sensoric grid* $\mathscr{S} \subset \mathbb{R}^p$ according to the feature map model for sensoric data processing introduced by T. Kohonen [24]. More specific, we assume $W$ to be consisting of $K$ prototypes $\mathbf{w}_\mathbf{r} \in W$ where the index $\mathbf{r} \in \mathscr{S}$ refers to a location in the external grid and $k(\mathbf{r}) \in \{1, \ldots, K\}$ returns the respective index in $W$. Usually, the projection dimension $p$ is chosen as $p = 2$ in agreement to cortical areas in human brain [40]. For a given input $\mathbf{x}$ the most appropriate prototype is determined by the winner-takes-all (WTA) rule

$$\mathbf{s}(\mathbf{x}) = \mathrm{argmin}_{\mathbf{r} \in \mathscr{S}} d_E(\mathbf{x}, \mathbf{w}_\mathbf{r}) \tag{1}$$

with $d_E(\mathbf{x}, \mathbf{w}_\mathbf{r})$ being the (squared) Euclidean distance. This WTA-rule is equivalent to the maximum Hebbian excitation principle

$$\mathbf{s}(\mathbf{x}) = \mathrm{argmax}_{\mathbf{r} \in A} \mathbf{w}_\mathbf{r}^T \cdot \mathbf{x}$$

for normalized data and prototypes. We suppose a response vector $\boldsymbol{\xi}(\mathbf{x}, W)$ with $\boldsymbol{\xi}(\mathbf{x}) = (\xi_1, \ldots, \xi_K)^T \in \Xi$ such that the WTA-rule delivers

$$\xi_{k(\mathbf{r})}(\mathbf{x}, W) = \begin{cases} 1 & \mathbf{r} = \mathbf{s}(\mathbf{x}) \\ \\ 0 & \mathbf{r} \neq \mathbf{s}(\mathbf{x}) \end{cases} \tag{2}$$

as stimulus response. We can interpret this mapping $\mathbf{x} \mapsto \boldsymbol{\xi}(\mathbf{x}, W)$ as an information compressing mapping realized by a vector quantizer.

The perceptron layer in CPN consists of a single linear perceptron realized as

$$y(\mathbf{x}) = \boldsymbol{\omega}^T \cdot \boldsymbol{\xi}(\mathbf{x}, W) \tag{3}$$

with an adjustable perceptron weight vector $\boldsymbol{\omega}$. The aim is to adapt this weight vector to predict the class label $c(\mathbf{x})$ as best as possible. In fact, due to the WTA-rule realization (2) the prediction value $y(\mathbf{x})$ is simply obtained according to the weighting $y(\mathbf{x}) = \omega_{k(\mathbf{s}(\mathbf{x}))} \cdot \xi_{k(\mathbf{s}(\mathbf{x}))}(\mathbf{x}, W)$ by means of the respective weight $\omega_{k(\mathbf{s})}$. We can summarize the CPN scheme as

$$X \underset{\text{SOM}}{\longrightarrow} W \underset{\text{crisp}}{\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\longrightarrow}} \Xi \underset{\text{perceptron}}{\overset{y(\mathbf{x})}{\longrightarrow}} \mathscr{C} \tag{4}$$

with the *vector quantization layer (VQ-layer)* $X \underset{\text{SOM}}{\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\longrightarrow}} \Xi$ and the *classification layer (C-layer)* $\Xi \underset{\text{perceptron}}{\overset{y(\mathbf{x})}{\longrightarrow}} \mathscr{C}$.

Training in CPN takes place as in two phases. First, the VQ-layer (SOM) is trained in an unsupervised manner. Second, for the C-layer, the perceptron weight vector $\boldsymbol{\omega}$ is adapted by supervised learning. Thus, the SOM layer yields a grouping of data whereas the perceptron learns to interpret this grouping for classification learning.

Two inprovements are discussed in the community so far:

1. Instead of only one perceptron, class-wise perceptrons are taken [12, p. 186], i.e.

$$y_k(\mathbf{x}) = f\left(\boldsymbol{\omega}_k^T \cdot \boldsymbol{\xi}(\mathbf{x}, W) - \beta_k\right) \tag{5}$$

   with biases $\beta_k$ and an activation function $f$ frequently taken as sigmoid or, currently, promising alternatives like ReLU, swish or others [9, 38, 51].

2. Several authors suggested to relax the WTA-rule taking more than a single winning unit [18, p. 248], [12, p. 189]. For this purpose, $N$ units of the SOM layer surrounding the winning unit $\mathbf{s}$ in $A$ are taken with $\xi_{k(\mathbf{r})}(\mathbf{x}, W) = \frac{1}{N}$ for all these including the winning neuron $\mathbf{s}$.

The CPN approach frequently works very successful although being simple [12, 17, 16, 55, 53, 54, 46, 20, 1]. One can see this also as a historic of incorporation of prototype layers in multi-layer perceptrons as recently discussed in [6]. Yet, the SOM-training takes place independently from the subsequent classification task and, hence, might be suboptimal for the later classification learning. Further, original SOM does not optimize any cost function such that mathematicl guarantees for data grouping behavior are given [10].

In the following we propose new variants and extension of the basic CPN.

# 3 New Variants of the Basic CPN

## 3.1 Modifications for the Vector Quantization Layer and the Response Vector $\boldsymbol{\xi}(\mathbf{x}, W)$

### 3.1.1 Alternatives for the Kohonen-SOM Layer

**3.1.1.1 The Heskes-SOM Layer** The vector quantization layer in original CPN is realized by standard SOM according to T. Kohonen [26]. As already mentioned, the optimization of SOM does not follow a gradient descent scheme of any cost function such that mathematical guarantees cannot be given. Modifying the original winner determination (1) to

$$\mathbf{s}_{\text{Heskes}} = \operatorname{argmin}_{\mathbf{r}} \left( \sum_{\mathbf{r}'} h_\lambda^{\mathscr{S}}(\mathbf{r}', \mathbf{r}) \cdot d(\mathbf{x}, \mathbf{w}_{\mathbf{r}}) \right) \tag{6}$$

yields the Heskes-variant of SOM following a well-defined stochastic gradient descent learning [19], where $\|\mathbf{r}'-\mathbf{r}\|^2_{\mathscr{S}}$ denotes the squared Euclidean distance in the external SOM grid $\mathscr{S}$ and

$$h^{\mathscr{S}}_{\lambda}\left(\mathbf{r}',\mathbf{r}\right)=\exp\left(-\frac{\|\mathbf{r}'-\mathbf{r}\|^2_{\mathscr{S}}}{\lambda}\right) \tag{7}$$

is the SOM *neighborhood function* evaluated for the external sensoric grid $\mathscr{S}$. The prototype update for given input $\mathbf{x}$ is obtained as

$$\Delta\mathbf{w}_{\mathbf{r}}\propto -h^{\mathscr{S}}_{\lambda}\left(\mathbf{s}\left(\mathbf{x}\right),\mathbf{r}\right)\cdot\frac{\partial d\left(\mathbf{x},\mathbf{w}_{\mathbf{r}}\right)}{\partial\mathbf{w}_{\mathbf{r}}} \tag{8}$$

as for the original SOM with $d\left(\mathbf{x},\mathbf{w}_{\mathbf{r}}\right)$ usually being the squared Euclidean distance.

The approach is summarized as

$$X\underset{\text{Heskes-SOM}}{\longrightarrow}W\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\underset{\text{crisp}}{\longrightarrow}}\Xi\overset{y(\mathbf{x})}{\underset{\text{perceptron}}{\longrightarrow}}\mathscr{C} \tag{9}$$

in relation to (4).

**3.1.1.2 The Neural Gas layer** Another alternative to standard SOM is to keep the winner determination but replace the neighborhood function: dropping the external grid $A$ we can define a distance based neighborhood of the prototypes regarding a given input implicitly by the exponential *winning-rank-function*

$$h^{NG}_{\lambda}\left(k,\mathbf{x},W\right)=\exp\left(-\frac{\mathrm{rk}\left(k,\mathbf{x},W\right)}{\lambda}\right) \tag{10}$$

of the prototype $\mathbf{w}_k$. The *rank function* $\mathrm{rk}\left(k,\mathbf{x},W\right)$ is defined in terms of a sum

$$\mathrm{rk}\left(k,\mathbf{x},W\right)=\sum_j H\left(d\left(\mathbf{x},\mathbf{w}_k\right)-d\left(\mathbf{x},\mathbf{w}_j\right)\right) \tag{11}$$

of Haeviside functions

$$H\left(z\right)=\begin{cases}1 & \text{for } z>0\\ \\ 0 & \text{eleswere}\end{cases}$$

such that $\mathrm{rk}\left(s\left(\mathbf{x}\right),\mathbf{x},W\right)=0$ is obtained for the best matching prototype $\mathbf{w}_{s(\mathbf{x})}$. Here, the WTA-rule simply is realized via

$$s\left(\mathbf{x}\right)=\mathrm{argmin}_k d\left(\mathbf{x},\mathbf{w}_k\right) \tag{12}$$

in analogy to the winner determination (1) for SOMs. The prototype dynamic is, similarly as for SOM, obtained as

$$\Delta\mathbf{w}_k\propto -h^{NG}_{\lambda}\left(k,\mathbf{x},W\right)\cdot\frac{\partial d\left(\mathbf{x},\mathbf{w}_k\right)}{\partial\mathbf{w}_k} \tag{13}$$

performing a stochastic gradient descent on the cost function

$$E^{NG}\left(X,W\right)=\frac{1}{C\left(\lambda\right)}\int\sum_k P\left(\mathbf{x}\right)\cdot h^{NG}_{\lambda}\left(k,\mathbf{x},W\right)\cdot d\left(\mathbf{x},\mathbf{w}_k\right)d\mathbf{x} \tag{14}$$

with $C\left(\lambda\right)$ being a normalization constant [31]. In fact, considering the prototypes as gas particles, the dynamic describe the diffusion of the gas according to the data density $P\left(\mathbf{x}\right)$ such that the cost function can be interpreted as the potential function of this gas [31, 30].

The approach can be summarized as

$$X\underset{\text{NG}}{\longrightarrow}W\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\underset{\text{crisp}}{\longrightarrow}}\Xi\overset{y(\mathbf{x})}{\underset{\text{perceptron}}{\longrightarrow}}\mathscr{C} \tag{15}$$

in relation to (4).

#### 3.1.2 Modification of the Response Vector $\boldsymbol{\xi}(\mathbf{x}, W)$

**3.1.2.1 Modifications According to the Vector Quantization Layer** In original CPN, the sensoric response vector $\boldsymbol{\xi}(\mathbf{x}, W)$ contains zeros for all entries except that one for the best matching prototype according to (1) or (12). As already mentioned, this strict rule was suggested to relax that also those entries $\xi_{k(\mathbf{r})}(\mathbf{x}, W)$ are considered to be non-zero, which are neighbored to the winner unit $\mathbf{s}$ in the external grid $A$. This could be taken over to the NG-approach considering the first winning ranks.

A simple generalization of this concept would be to take *gradual responses*

$$\xi_{k(\mathbf{r})}^{\mathscr{S}}(\mathbf{x}, W) = h_{\lambda}^{\mathscr{S}}(\mathbf{s}(\mathbf{x}), \mathbf{r}) \tag{16}$$

for the SOM-layer or

$$\xi_{k}^{G}(\mathbf{x}, W) = h_{\lambda}^{NG}(k, \mathbf{x}, W) \tag{17}$$

in case of a NG-layer. For $\lambda \searrow 0$, the gradual responses (16) and (17) realize a winner-takes-all (WTA) rule, i.e. $\xi_k(\mathbf{x}, W) \neq 0 \Longleftrightarrow k = s$ for NG or $k = k(\mathbf{s}(\mathbf{x}))$ in case of SOM. The derivative of the gradual responses are

$$\begin{aligned}
\frac{\partial \xi_{k(\mathbf{r})}^{\mathscr{S}}(\mathbf{x}, W)}{\partial \mathbf{w}_l} &= \frac{\partial h_{\lambda}^{\mathscr{S}}(\mathbf{s}(\mathbf{x}), \mathbf{r})}{\partial \mathbf{w}_l} \\
&= \frac{\partial}{\partial \mathbf{w}_l} \exp\left(-\frac{(\mathbf{s}(\mathbf{x}) - \mathbf{r})^2}{\lambda}\right) \\
&= -2 \cdot \exp\left(-\frac{(\mathbf{s}(\mathbf{x}) - \mathbf{r})^2}{\lambda}\right) \cdot (\mathbf{s}(\mathbf{x}) - \mathbf{r}) \cdot \frac{\partial \mathbf{s}(\mathbf{x})}{\partial \mathbf{w}_l}
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial \xi_{k}^{G}(\mathbf{x}, W)}{\partial \mathbf{w}_l} &= \frac{\partial h_{\lambda}^{NG}(k, \mathbf{x}, W)}{\partial \mathbf{w}_l} \\
&= \frac{\partial}{\partial \mathbf{w}_l} \exp\left(-\frac{\mathrm{rk}(k, \mathbf{x}, W)}{\lambda}\right) \\
&= -\exp\left(-\frac{\mathrm{rk}(k, \mathbf{x}, W)}{\lambda}\right) \cdot \frac{\partial \mathrm{rk}(k, \mathbf{x}, W)}{\partial \mathbf{w}_l}
\end{aligned}$$

with remaining derivatives $\frac{\partial \mathbf{s}(\mathbf{x})}{\partial \mathbf{w}_l}$ and $\frac{\partial \mathrm{rk}(k, \mathbf{x}, W)}{\partial \mathbf{w}_l}$, respectively. The first one is not feasible whereas the second one yields

$$\begin{aligned}
\frac{\partial \mathrm{rk}(k, \mathbf{x}, W)}{\partial \mathbf{w}_l} &= \frac{\partial \sum_j H(d(\mathbf{x}, \mathbf{w}_k) - d(\mathbf{x}, \mathbf{w}_j))}{\partial \mathbf{w}_l} \\
&= \sum_j \frac{\partial H(d(\mathbf{x}, \mathbf{w}_k) - d(\mathbf{x}, \mathbf{w}_j))}{\partial \mathbf{w}_k} \\
&= \sum_j \frac{\partial H(d(\mathbf{x}, \mathbf{w}_k) - d(\mathbf{x}, \mathbf{w}_j))}{d(\mathbf{x}, \mathbf{w}_k)} \cdot \frac{\partial d(\mathbf{x}, \mathbf{w}_k)}{\partial \mathbf{w}_l} \\
&= \delta_{k,l} \cdot \frac{\partial d(\mathbf{x}, \mathbf{w}_k)}{\partial \mathbf{w}_k} \cdot \sum_j \frac{\partial H(d(\mathbf{x}, \mathbf{w}_k) - d(\mathbf{x}, \mathbf{w}_j))}{d(\mathbf{x}, \mathbf{w}_k)} \\
&= \delta_{k,l} \cdot \frac{\partial d(\mathbf{x}, \mathbf{w}_k)}{\partial \mathbf{w}_k} \cdot \sum_j \delta_{\mathrm{Dirac}}(d(\mathbf{x}, \mathbf{w}_k) - d(\mathbf{x}, \mathbf{w}_j))
\end{aligned} \tag{18}$$

where $\delta_{k,l}$ denotes the Kronecker symbol, i.e. $\delta_{k,l} = 1 \Longleftrightarrow k = l$ and it is zero else.

However, these gradual responses ignore the the distance values. Therefore, we suggest to consider the *local responses*

$$\xi_{k(\mathbf{r})}^{SOM}(\mathbf{x},W)=h_{\lambda}^{\mathscr{S}}(\mathbf{s}(\mathbf{x}),\mathbf{r})\cdot d(\mathbf{x},\mathbf{w_r}) \tag{19}$$

and

$$\xi_{k}^{NG}(\mathbf{x},W)=h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot d(\mathbf{x},\mathbf{w}_k) \tag{20}$$

for SOM- and NG-layer, respectively. These local responses reflect both the winning rank as well as the dissimilarity. This is consistent to the winner determination (6) of the Heskes-SOM.

Moreover, the expected NG-response is

$$\left\langle\xi_{k}^{NG}(\mathbf{x},W)\right\rangle_{\mathbf{x}}=\int P(\mathbf{x})\cdot h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot d(\mathbf{x},\mathbf{w}_k)\,d\mathbf{x} \tag{21}$$

such that the sum $\sum_k\langle\xi_k(\mathbf{x},W)\rangle_{\mathbf{x}}$ is equivalent to the energy function (14) of the neural gas vector quantizer [31], if we swap integration and summation.

Yet, for the (non-averaged) gradient we have

$$\begin{aligned}
\frac{\partial\xi_{k}^{NG}(\mathbf{x},W)}{\partial\mathbf{w}_l} &= \frac{\partial}{\partial\mathbf{w}_l}\left(h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot d(\mathbf{x},\mathbf{w}_k)\right)\\
&= \frac{\partial}{\partial\mathbf{w}_l}\left(h_{\lambda}^{NG}(k,\mathbf{x},W)\right)\cdot d(\mathbf{x},\mathbf{w}_k)+\delta_{k,l}\cdot h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\\
&\overset{(10)}{=} -h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot\frac{1}{\lambda}\cdot\frac{\partial\mathrm{rk}(k,\mathbf{x},W)}{\partial\mathbf{w}_l}\cdot d(\mathbf{x},\mathbf{w}_k)+\delta_{k,l}\cdot h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\\
&= -h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\lambda}\cdot\frac{\partial\mathrm{rk}(k,\mathbf{x},W)}{\partial\mathbf{w}_l}+\delta_{k,l}\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\right)\\
&\overset{(18)}{=} -h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\lambda}\cdot\delta_{k,l}\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\cdot\sum_j\delta_{\mathrm{Dirac}}\left(d(\mathbf{x},\mathbf{w}_k)-d(\mathbf{x},\mathbf{w}_j)\right)+\delta_{k,l}\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\right) && (22)\\
&= -h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot\delta_{k,l}\cdot\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\lambda}\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\cdot\sum_j\delta_{\mathrm{Dirac}}\left(d(\mathbf{x},\mathbf{w}_k)-d(\mathbf{x},\mathbf{w}_j)\right)+\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\right) && (23)\\
& && (24)\\
&\overset{\text{in prob.}}{=} -h_{\lambda}^{NG}(k,\mathbf{x},W)\cdot\delta_{k,l}\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k}\cdot\frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial\mathbf{w}_k} && (25)
\end{aligned}$$

supposing a data density $P(\mathbf{x})$ with $\forall\mathbf{x}:P(\mathbf{x})<\infty$ to be valid.

The approach is summarized as

$$X\underset{\text{NG/SOM}}{\longrightarrow}W\underset{\text{NG/SOM-like}}{\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\longrightarrow}}\Xi\underset{\text{perceptron}}{\overset{y(\mathbf{x})}{\longrightarrow}}\mathscr{C} \tag{26}$$

in relation to (4).

#### 3.1.2.2 Modifications According to a Fuzzy Vector Quantization Interpretation

Another choice for gradual sensoric responses for a given prototype set $W$ is to evaluate fuzzy assignments of the data. According to [2, 3], the fuzzy assignment

$$u_k(\mathbf{x})=\frac{1}{\sum_{j=1}^{K}\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)^{\frac{2}{m-1}}} \tag{27}$$

gives the probability that data point $\mathbf{x}$ is assigned to prototype $\mathbf{w}_k$ taken as a local cluster center according to the fuzzy-c-means approach (FCM,[22]). The parameter $m>1$ is the fuzzyfier usually chosen as $m=2$. Explicitly note that $\sum_{j=1}^{K} u_j(\mathbf{x}) = 1$ is valid for the fuzzy assignments. Yet, the fuzzy assignments do not reflect all aspects of cluster assignments, in particular, if the distance $d(\mathbf{x}, \mathbf{w}_k)$ is large. Therefore, the typicality assignments

$$t_k(\mathbf{x}) = \frac{1}{1 + \left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\gamma_k}\right)^{\frac{1}{m-1}}} \tag{28}$$

were proposed [27] with the normalization

$$\gamma_k = \gamma \cdot \frac{E_{\mathbf{x}}[u_k(\mathbf{x}) \cdot d(\mathbf{x}, \mathbf{w}_k)]}{E_{\mathbf{x}}[u_k(\mathbf{x})]}$$

and the usual choice $\gamma = 1$ [28, 35]. Here, $E_{\mathbf{x}}[\cdot]$ denotes the expectation operator with respect to $\mathbf{x}$.

Both quantities, the fuzzy and the typicality assignments, can be combined by a convex sum

$$\xi_k^F(\mathbf{x}, W) = \alpha \cdot u_k(\mathbf{x}) + (1 - \alpha) \cdot t_k(\mathbf{x}) \tag{29}$$

with $\alpha \in (0, 1)$ to obtain fuzzy-based sensoric responses.

The gradient $\frac{\partial u_k(\mathbf{x})}{\partial \mathbf{w}_l}$ of the fuzzy assignments is calculated as

$$\begin{aligned}
\frac{\partial u_k(\mathbf{x})}{\partial \mathbf{w}_l} &= \frac{-1}{\left(\sum_{j=1}^{K}\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)^{\frac{2}{m-1}}\right)^2} \cdot \frac{\partial \sum_{j=1}^{K}\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)^{\frac{2}{m-1}}}{\partial \mathbf{w}_l} \\
&= \frac{-1}{\left(\sum_{j=1}^{K}\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)^{\frac{2}{m-1}}\right)^2} \cdot \sum_{j=1}^{K} \frac{\partial \left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)^{\frac{2}{m-1}}}{\partial \mathbf{w}_l} \\
&= \frac{-1}{\left(\sum_{j=1}^{K}\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)^{\frac{2}{m-1}}\right)^2} \cdot \sum_{j=1}^{K} \left(\frac{2}{m-1} \cdot \left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)^{\frac{1-m}{m-1}} \cdot \frac{\partial}{\partial \mathbf{w}_l}\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right)\right)
\end{aligned}$$

with

$$\frac{\partial}{\partial \mathbf{w}_l}\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{d(\mathbf{x},\mathbf{w}_j)}\right) = \begin{cases} \frac{1}{d(\mathbf{x},\mathbf{w}_j)} \cdot \frac{\partial d(\mathbf{x},\mathbf{w}_l)}{\partial \mathbf{w}_l} & l = k \neq j \\ \frac{-d(\mathbf{x},\mathbf{w}_k)}{(d(\mathbf{x},\mathbf{w}_l))^2} \cdot \frac{\partial d(\mathbf{x},\mathbf{w}_l)}{\partial \mathbf{w}_l} & l = j \neq k \\ 0 & else \end{cases}$$

whereas

$$\begin{aligned}
\frac{\partial t_k(\mathbf{x})}{\partial \mathbf{w}_l} &= \frac{-1}{\left(1 + \left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\gamma_k}\right)^{\frac{1}{m-1}}\right)^2} \cdot \frac{\partial}{\partial \mathbf{w}_l}\left(\left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\gamma_k}\right)^{\frac{1}{m-1}}\right) \\
&= \frac{-1}{\left(1 + \left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\gamma_k}\right)^{\frac{1}{m-1}}\right)^2} \cdot \frac{1}{m-1} \cdot \left(\frac{d(\mathbf{x},\mathbf{w}_k)}{\gamma_k}\right)^{\frac{2-m}{m-1}} \cdot \frac{1}{\gamma_k} \cdot \frac{\partial d(\mathbf{x},\mathbf{w}_k)}{\partial \mathbf{w}_l}
\end{aligned}$$

is obtained for the typicalities. Thus, the derivative

$$\frac{\partial \xi_k^F(\mathbf{x}, W)}{\partial \mathbf{w}_l} = \alpha \cdot \frac{\partial u_k(\mathbf{x})}{\partial \mathbf{w}_l} + (1 - \alpha) \cdot \frac{\partial t_k(\mathbf{x})}{\partial \mathbf{w}_l} \tag{30}$$

describes gradient of this fuzzy response. Yet, other fuzzy approaches like the application of general t-norms could also be of interest [11].

The approach is summarized as

$$X \underset{\text{FCM}}{\longrightarrow} W \underset{\text{fuzzy}}{\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\longrightarrow}} \Xi \underset{\text{perceptron}}{\overset{y(\mathbf{x})}{\longrightarrow}} \mathscr{C} \tag{31}$$

in relation to (4).

## 3.2 Modifications of the Classification Layer

As mentioned in the beginning, in original CPN, the classification layer consists of one or several perceptrons taking the sensoric reponse vector $\boldsymbol{\xi}(\mathbf{x}, W)$ as input. It is optimized after vector quantization training and does not fine-tune the vector quantization layer. Hence, no backward information is considered. In the following we propose several modifications of that scheme. To keep in mind that the sensoric response vector $\boldsymbol{\xi}(\mathbf{x}, W)$ depends on the

### 3.2.1 Multilayer Perceptron Layer

An obvious way to generalize the CPN is to replace the perceptron(s) in the classification layer by a (deep) multi-layer perceptron architecture with cross-entropy loss as cost function. This would realize the idea to incorporate vector quantization layers into deep networks as suggested in [6]. Considering the response determination as a mapping $\mathbf{x} \mapsto \boldsymbol{\xi}(\mathbf{x}, W)$ realized by a vector quantizer (SOM/NG/FCM), one can think to fine-tune the response mapping $\boldsymbol{\xi}(\mathbf{x}, W)$ by means of the gradients $\frac{\partial \boldsymbol{\xi}(\mathbf{x},W)}{\partial \mathbf{w}_l}$ for stochastic gradient learning with respect to the cross entropy. However, because of the deep architecture, the problem of vanishing gradients becomes apparent for this approach and has to be tackled carefully. Further, the interpretability of the vector quantization layer is destroyed by the subsequent deep network, which counter-acts to one of the central paradigms of vector quantization models.

The approach can be summarized as

$$X \underset{\text{NG/FCM}}{\longrightarrow} W \underset{\text{NG-like/fuzzy}}{\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\longrightarrow}} \Xi \underset{\text{deep network}}{\overset{y(\mathbf{x})}{\longrightarrow}} \mathscr{C} \tag{32}$$

in relation to (4).

### 3.2.2 LVQ Layers

**3.2.2.1 Non-probabilistic LVQ classifier** We suggest to replace the perceptron layer of CPN by a generalized learning vector quantization classifier (GLVQ, [44]) as cost function based variant of the heuristic learning vector quantizer (LVQ) introduced by T. Kohonen [25]. LVQ-models are interpretable prototype-based classifiers relying on an attraction-repulsing scheme for the prototypes [52]. Originally, LVQ was established to approximate Bayesian learning in supervised vector quantization learning for classification [26]. GLVQ is known to be interpretable [4, 50, 21], robust [42, ?] and implicitly optimizes the hypothesis margin during classification learning [8, 43].

Taking the sensoric responses $\boldsymbol{\xi}$ as input, the GLVQ assumes prototypes $\boldsymbol{\omega}_j \in \mathbb{R}^{\mathbb{K}}$ with class labels $c(\boldsymbol{\omega}_j)$. We denote the set $\mathcal{W} = \{\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_M\}$ as GLVQ-prototypes to distinguish them from the sensoric prototype set $W$. The cost function optimized by GLVQ-training in our setting is

$$E_{GLVQ}(\mathcal{W}) = \sum_{\mathbf{x}} f(\mu(\boldsymbol{\xi}(\mathbf{x}, W)))$$

where $f$ is a differentiable sigmoid function with range $[0, 1]$ and and the classifier function $\mathcal{W}$-dependent

$$\mu(\boldsymbol{\xi}(\mathbf{x}, W), \mathcal{W}) = \frac{\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^+) - \delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^-)}{\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^+) + \delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^-)} \tag{33}$$

with the dissimilarity measure

$$\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}) = (\boldsymbol{\Omega}(\boldsymbol{\xi}(\mathbf{x}, W) - \boldsymbol{\omega}))^2 \tag{34}$$

known from the matrix GLVQ (GMLVQ) [45] anf relevance GLVQ (GRLVQ) [14]. Thereby, $\boldsymbol{\omega}^+$ is the best matching prototype $\boldsymbol{\omega}_j$ according to the WTA-rule (1) known from SOM with the constraint of class label agreement $c(\boldsymbol{\omega}_j) = c(\boldsymbol{\xi}(\mathbf{x}, W))$. Analogously, $\boldsymbol{\omega}^-$ is the best matching prototype among all prototypes responsible for other classes than $c(\boldsymbol{\xi}(\mathbf{x}, W))$. Thus, the classifier function $\mu(\boldsymbol{\xi}(\mathbf{x}, W), \mathcal{W}) \in [-1, 1]$ becomes negative for correct classification. After training the network response is the label $c(\boldsymbol{\omega}_s)$ of the overall best matching prototype $\boldsymbol{\omega}_s$ according to the WTA-rule (1).

Stochastic gradient descent learning on the cost function $E_{GLVQ}(\mathcal{W})$ takes place as prototype updates according to the derivative of the local errors

$$E_{GLVQ}(\mathbf{x}, \mathcal{W}, W) = f(\mu(\boldsymbol{\xi}(\mathbf{x}, W), \mathcal{W}))$$

i.e.

$$\Delta\boldsymbol{\omega}^{\pm} \propto -\frac{\partial E_{GLVQ}(\mathbf{x}, \mathcal{W}, W)}{\partial\boldsymbol{\omega}^{\pm}}$$

has to be considered. In the following, we omit for $\boldsymbol{\xi}(\mathbf{x}, W)$ the dependencies on $\mathbf{x}$ and $W$ for simplicity if it is not necessary to refer explicitly to the dependencies. Thus, the gradient formally read as

$$\frac{\partial E_{GLVQ}(\mathbf{x}, \mathcal{W}, W)}{\partial\boldsymbol{\omega}^{\pm}} = \frac{\partial f(\mu)}{\partial\mu(\boldsymbol{\xi})} \cdot \frac{\partial\mu(\boldsymbol{\xi})}{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{\pm})} \cdot \frac{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{\mp})}{\partial\boldsymbol{\omega}^{\pm}} \tag{35}$$

with

$$\frac{\partial\mu(\boldsymbol{\xi})}{\partial\boldsymbol{\xi}} = \frac{\partial\mu(\boldsymbol{\xi})}{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{+})} \cdot \frac{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{+})}{\partial\boldsymbol{\xi}} + \frac{\partial\mu(\boldsymbol{\xi})}{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{-})} \cdot \frac{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{-})}{\partial\boldsymbol{\xi}} \tag{36}$$

for $\boldsymbol{\omega}^+, \boldsymbol{\omega}^-$. Further, we get

$$\frac{\partial\mu(\boldsymbol{\xi})}{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{\pm})} = \frac{\mp 2 \cdot \delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{\mp})}{(\delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{+}) + \delta(\boldsymbol{\xi}, \boldsymbol{\omega}^{-}))^2}$$

as derivatives for $\mu(\boldsymbol{\xi})$ depending on $\boldsymbol{\omega}^+$ and $\boldsymbol{\omega}^-$. The gradients

$$\nabla_{\boldsymbol{\xi}}\delta(\boldsymbol{\xi}, \boldsymbol{\omega}) = \frac{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega})}{\partial\boldsymbol{\xi}} = 2 \cdot \boldsymbol{\Omega}^T\boldsymbol{\Omega}(\boldsymbol{\xi} - \boldsymbol{\omega})$$

and

$$\nabla_{\boldsymbol{\omega}}\delta(\boldsymbol{\xi}, \boldsymbol{\omega}) = \frac{\partial\delta(\boldsymbol{\xi}, \boldsymbol{\omega})}{\partial\boldsymbol{\omega}} = -2 \cdot \boldsymbol{\Omega}^T\boldsymbol{\Omega}(\boldsymbol{\xi} - \boldsymbol{\omega})$$

reflect the contribution of the dissimilarity measure $\delta(\boldsymbol{\xi}, \boldsymbol{\omega})$.

Because the sensoric inputs $\boldsymbol{\xi}(\mathbf{x}, W)$ depend on the sensoric prototypes $\mathbf{w}_k$, we can optimize the classification performance of the GLVQ model also with respect to these quantities. Thus we have to consider the derivative

$$\begin{aligned}\frac{\partial\mu(\boldsymbol{\xi}(\mathbf{x}, W))}{\partial\mathbf{w}_k} &= \frac{\partial\mu(\boldsymbol{\xi}(\mathbf{x}, W))}{\partial\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^{+})} \cdot \frac{\partial\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^{+})}{\partial\boldsymbol{\xi}(\mathbf{x}, W)} \cdot \frac{\partial\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^{+})}{\partial\mathbf{w}_k} + \\ &\quad + \frac{\partial\mu(\boldsymbol{\xi})}{\partial\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^{-})} \cdot \frac{\partial\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^{-})}{\partial\boldsymbol{\xi}} \cdot \frac{\partial\delta(\boldsymbol{\xi}(\mathbf{x}, W), \boldsymbol{\omega}^{-})}{\partial\mathbf{w}_k}\end{aligned} \tag{37}$$

using (36). For the NG-like responses we calculate

$$\begin{aligned}
\frac{\partial\delta\left(\boldsymbol{\xi}^{NG}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)}{\partial\mathbf{w}_k} &= \left(\nabla_{\boldsymbol{\xi}}\delta\left(\mathbf{x},\boldsymbol{\omega}\right)\right)^T\cdot\frac{\partial\boldsymbol{\xi}^{NG}}{\partial\mathbf{w}_k} \\
&= \sum_{l=1}^{K}\left(\nabla_{\boldsymbol{\xi}}\delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)\right)_l\cdot\frac{\partial\xi_l^{NG}\left(\mathbf{x},W\right)}{\partial\mathbf{w}_k} \\
&\overset{(22)}{=} -\sum_{l=1}^{K}\left(\nabla_{\boldsymbol{\xi}}\delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)\right)_l\cdot\exp\left(-\frac{\mathrm{rk}\left(k,\mathbf{x},W\right)}{\lambda}\right) \\
&\quad\cdot\delta_{k,l}\cdot\left(\frac{d\left(\mathbf{x},\mathbf{w}_k\right)}{\lambda}\cdot\frac{\partial d\left(\mathbf{x},\mathbf{w}_k\right)}{\partial\mathbf{w}_k}\cdot\sum_j\delta_{\mathrm{Dirac}}\left(d\left(\mathbf{x},\mathbf{w}_k\right)-d\left(\mathbf{x},\mathbf{w}_j\right)\right)+\frac{\partial d\left(\mathbf{x},\mathbf{w}_k\right)}{\partial\mathbf{w}_k}\right) && (38) \\
& && (39) \\
&= -\left(\nabla_{\boldsymbol{\xi}}\delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)\right)_k\cdot\exp\left(-\frac{\mathrm{rk}\left(k,\mathbf{x},W\right)}{\lambda}\right) \\
& && (40) \\
&\quad\cdot\left(\frac{d\left(\mathbf{x},\mathbf{w}_k\right)}{\lambda}\cdot\frac{\partial d\left(\mathbf{x},\mathbf{w}_k\right)}{\partial\mathbf{w}_k}\cdot\sum_j\delta_{\mathrm{Dirac}}\left(d\left(\mathbf{x},\mathbf{w}_k\right)-d\left(\mathbf{x},\mathbf{w}_j\right)\right)+\frac{\partial d\left(\mathbf{x},\mathbf{w}_k\right)}{\partial\mathbf{w}_k}\right) && (41) \\
&\overset{\text{in prob. (25)}}{=} -\left(\nabla_{\boldsymbol{\xi}}\delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)\right)_k\cdot\exp\left(-\frac{\mathrm{rk}\left(k,\mathbf{x},W\right)}{\lambda}\right)\cdot\frac{\partial d\left(\mathbf{x},\mathbf{w}_k\right)}{\partial\mathbf{w}_k} && (42)
\end{aligned}$$

to be used in (37).

For the fuzzy responses $\xi_k^F\left(\mathbf{x},W\right)$ from (29) we similarly get (30)

$$\begin{aligned}
\frac{\partial\delta\left(\boldsymbol{\xi}^{F}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)}{\partial\mathbf{w}_k} &= \left(\nabla_{\boldsymbol{\xi}}\delta\left(\mathbf{x},\boldsymbol{\omega}\right)\right)^T\cdot\frac{\partial\boldsymbol{\xi}^{F}}{\partial\mathbf{w}_k} \\
&= \sum_{l=1}^{K}\left(\nabla_{\boldsymbol{\xi}}\delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)\right)_l\cdot\frac{\partial\xi_l^{F}\left(\mathbf{x},W\right)}{\partial\mathbf{w}_k} \\
&\overset{(30)}{=} \sum_{l=1}^{K}\left(\nabla_{\boldsymbol{\xi}}\delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}\right)\right)_l\cdot\left(\alpha\cdot\frac{\partial u_l\left(\mathbf{x}\right)}{\partial\mathbf{w}_k}+\left(1-\alpha\right)\cdot\frac{\partial t_l\left(\mathbf{x}\right)}{\partial\mathbf{w}_k}\right) && (43)
\end{aligned}$$

This GMLVQ-approach (and its variants) can be summarized as

$$X \underset{\text{NG/FCM}}{\leftrightarrows} W \underset{\text{NG-like/fuzzy}}{\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\leftrightarrows}} \Xi \underset{\text{GMLVQ}}{\overset{c(\boldsymbol{\omega}_s)}{\longrightarrow}} \mathscr{C} \tag{44}$$

in relation to (4).

**3.2.2.2 Probabilistic LVQ classifier** Probabilistic LVQ (PLVQ,[49]) uses information theoretic concepts to estimate the model probabilities $p_{\mathcal{W}}\left(c|\boldsymbol{\xi}\right)$. Let $\mathbf{p}\left(\boldsymbol{\xi}\right)=\left(p_1\left(\boldsymbol{\xi}\right),\ldots,p_C\left(\boldsymbol{\xi}\right)\right)$ be the class probability vector for sample $\boldsymbol{\xi}$ and

$$\mathbf{p}_{\mathcal{W}}\left(\boldsymbol{\xi}\right)=\left(p_{\mathcal{W}}\left(1|\boldsymbol{\xi}\right),\ldots,p_{\mathcal{W}}\left(C|\boldsymbol{\xi}\right)\right) \tag{45}$$

the respective *predicted class probability vector* provided by the probabilistic classifier model depending on PLVQ-prototype set $\mathcal{W}=\left\{\boldsymbol{\omega}_1,\ldots,\boldsymbol{\omega}_M\right\}$ as before. The target labels for trainng data are denoted by $\mathbf{t}\left(\boldsymbol{\xi}\right)\in\left[0,1\right]^C$ describing a probabilistic class assignment according to $t_c\left(\boldsymbol{\xi}\right)\in\left[0,1\right]$, i.e. $\sum_c t_c\left(\boldsymbol{\xi}\right)=1$. For a possibilistic assignment, the latter constraint has to be dropped.

The mutual information between $\mathbf{t}(\boldsymbol{\xi})$ and $\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi})$ has to be maximized, and, hence, the corresponding KLD $D_{KL}(\mathbf{p}(\boldsymbol{\xi})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}))$ has to be minimized for the probabilistic setting, which is equivalent to maximize the cross-entropy

$$Cr(\mathbf{t}(\boldsymbol{\xi})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi})) = \sum_c t_c(\boldsymbol{\xi})\cdot\log\left(p_{\mathcal{W}}(c|\boldsymbol{\xi})\right) \tag{46}$$

as shown in [37, p. 221ff]. For PLVQ, the cross-entropy $Cr(\mathbf{t}(\boldsymbol{\xi})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}))$ plays the role of a local cost such that

$$L_{PLVQ}(X,\mathcal{W}) = -\sum_k Cr(\mathbf{t}(\boldsymbol{\xi}_k)\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}_k)) \tag{47}$$

has to be minimzed [49]. Alternatively, the loss

$$L^{\alpha}_{PLVQ}(X,\mathcal{W}) = \sum_k D_{\alpha}(\mathbf{t}(\boldsymbol{\xi}_k)\,||p_{\mathcal{W}}(\boldsymbol{\xi}_k)) \tag{48}$$

based on the Rényi divergence [39]

$$D_{\alpha}((\boldsymbol{\xi}_k)\,||p_{\mathcal{W}}(\boldsymbol{\xi}_k)) = \frac{1}{1-\alpha}\log\left(\sum_c (t_c(\boldsymbol{\xi}_k))^{\alpha}\cdot(p_{\mathcal{W}}(c|\boldsymbol{\xi}_k))^{1-\alpha}\right) \tag{49}$$

could be taken as cost function. For the cross-entropy $Cr(\mathbf{t}(\boldsymbol{\xi})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}))$, the conditional class probability $p_{\mathcal{W}}(c|\boldsymbol{\xi}_k)$ depends on $p(\boldsymbol{\xi}|\mathbf{w}_j)$ via the class prediction probabilities

$$\begin{aligned}
p_{\mathcal{W}}(c|\boldsymbol{\xi}) &= \frac{P_{\mathcal{W}}(\boldsymbol{\xi},c)}{P_{\mathcal{W}}(\boldsymbol{\xi})}\\
&= \frac{\sum_{j:c(\boldsymbol{\omega}_j)=c} p(\boldsymbol{\xi}|\boldsymbol{\omega}_j)\cdot p(\boldsymbol{\omega}_j)}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)}\\
&= \sum_{j:c(\boldsymbol{\omega}_j)=c} S_{\mathcal{W}}(j,\boldsymbol{\xi})
\end{aligned} \tag{50}$$

with

$$S_{\mathcal{W}}(j,\boldsymbol{\xi}) = \frac{p(\boldsymbol{\xi}|\boldsymbol{\omega}_j)\cdot p(\boldsymbol{\omega}_j)}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)} \tag{51}$$

as so-called local quantities. For the possibilistic setting we refer to [32].

The gradient of the cross-entropy $Cr(\mathbf{t}(\mathbf{x})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}))$ from (46) with respect to the PLVQ-prototypes $\boldsymbol{\omega}_l$ reads as

$$\begin{aligned}
\frac{\partial Cr(\mathbf{t}(\boldsymbol{\xi})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}))}{\partial\boldsymbol{\omega}_l} &= \frac{\partial}{\partial\boldsymbol{\omega}_l}\left(\sum_c t_c(\boldsymbol{\xi})\cdot\log\left(p_{\mathcal{W}}(c|\boldsymbol{\xi})\right)\right)\\
&= \sum_c \frac{t_c(\boldsymbol{\xi})}{p_{\mathcal{W}}(c|\boldsymbol{\xi})}\cdot\frac{\partial p_{\mathcal{W}}(c|\boldsymbol{\xi})}{\partial\boldsymbol{\omega}_l}\\
&\overset{(50)}{=} \sum_c \frac{t_c(\boldsymbol{\xi})}{p_{\mathcal{W}}(c|\boldsymbol{\xi})}\cdot\frac{\partial}{\partial\boldsymbol{\omega}_l}\left(\sum_{j:c(\mathbf{w}_j)=c} S_{\mathcal{W}}(j,\boldsymbol{\xi})\right)\\
&= \sum_c \frac{t_c(\boldsymbol{\xi})}{p_{\mathcal{W}}(c|\boldsymbol{\xi})}\cdot\left(\sum_{j:c(\mathbf{w}_j)=c}\frac{\partial S_{\mathcal{W}}(j,\boldsymbol{\xi})}{\partial\boldsymbol{\omega}_l}\right)
\end{aligned}$$

with

$$
\begin{aligned}
\frac{\partial S_{\mathcal{W}}(j,\boldsymbol{\xi})}{\partial \boldsymbol{\omega}_l} &= \frac{\partial}{\partial \boldsymbol{\omega}_l}\left(\frac{p(\boldsymbol{\xi}|\boldsymbol{\omega}_j)\cdot p(\boldsymbol{\omega}_j)}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)}\right) \\
&= \frac{\delta_{kl}}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)} - p(\boldsymbol{\xi}|\boldsymbol{\omega}_j)\, p(\boldsymbol{\omega}_j)\left(\frac{\frac{\partial p(\boldsymbol{\xi}|\boldsymbol{\omega}_l)\cdot p(\boldsymbol{\omega}_l)}{\partial \boldsymbol{\omega}_l}}{\left(\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)\right)^2}\right) \\
&= \frac{\delta_{kl}}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)} - S_{\mathcal{W}}(j,\boldsymbol{\xi})\cdot\left(\frac{\frac{\partial p(\boldsymbol{\xi}|\boldsymbol{\omega}_l) p(\boldsymbol{\omega}_l)}{\partial \boldsymbol{\omega}_l}}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)}\right) \\
&= \frac{\delta_{kl} - S_{\mathcal{W}}(j,\boldsymbol{\xi})\cdot \frac{\partial p(\boldsymbol{\xi}|\boldsymbol{\omega}_l) p(\boldsymbol{\omega}_l)}{\partial \boldsymbol{\omega}_l}}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)} \\
&= \frac{\delta_{kl} - S_{\mathcal{W}}(j,\boldsymbol{\xi})\cdot \left(p(\boldsymbol{\omega}_l)\cdot\frac{\partial p(\boldsymbol{\xi}|\boldsymbol{\omega}_l)}{\partial \boldsymbol{\omega}_l} + p(\boldsymbol{\xi}|\boldsymbol{\omega}_l)\cdot\frac{\partial p(\boldsymbol{\omega}_l)}{\partial \boldsymbol{\omega}_l}\right)}{\sum_{k=1}^{N} p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)\cdot p(\boldsymbol{\omega}_k)}
\end{aligned}
$$

according to (51).

Now, we assume an arbitrary non-negative dissimilarity measure $\delta(\boldsymbol{\xi},\boldsymbol{\omega})$ according to [33] such that $\delta : \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathscr{D} \subseteq \mathbb{R}_+$, where $\mathscr{D}$ is the *data dissimilarity space*. Further, let the conditional probability $p(\boldsymbol{\xi}|\boldsymbol{\omega})$ be only depending on the measure $\delta(\boldsymbol{\xi},\boldsymbol{\omega})$, i.e.

$$
p(\boldsymbol{\xi}|\boldsymbol{\omega}_j) = \pi_{\mathscr{D}}(\delta(\boldsymbol{\xi},\boldsymbol{\omega}_j))\ . \tag{52}
$$

is an one-dimensional differentiable density function representing $P_{\mathscr{D}}$. We denote $P_{\mathscr{D}}(\delta(\boldsymbol{\xi}_i,\boldsymbol{\omega}_k))$ as a *dissimilarity density model*. Then we get

$$
\frac{\partial p(\boldsymbol{\xi}|\boldsymbol{\omega}_k)}{\partial \boldsymbol{\omega}_l} = \frac{\partial \pi_{\mathscr{D}}(\delta(\boldsymbol{\xi},\boldsymbol{\omega}_k))}{\partial \delta(\boldsymbol{\xi},\boldsymbol{\omega}_k)}\cdot\frac{\partial \delta(\boldsymbol{\xi},\boldsymbol{\omega}_k)}{\partial \boldsymbol{\omega}_l} \tag{53}
$$

as the derivative with respect to $\boldsymbol{\omega}_l$.

To combine the PLVQ with the CPN approach, we again assume $\boldsymbol{\xi}(\mathbf{x},W)$ to pe the sensoric response from the vector quantizer layer where the label is simply obtained $\mathbf{t}(\boldsymbol{\xi}) = \mathbf{t}(\mathbf{x})$ from the original data $\mathbf{x}$. Now, the cross-entropy (46) reads as

$$
Cr(\mathbf{t}(\mathbf{x})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}(\mathbf{x},W))) = \sum_c t_c(\mathbf{x})\cdot\log(p_{\mathcal{W}}(c|\boldsymbol{\xi}(\mathbf{x},W))) \tag{54}
$$

and we obtain

$$
\begin{aligned}
\frac{\partial Cr(\mathbf{t}(\mathbf{x})\,||\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi}(\mathbf{x},W)))}{\partial \mathbf{w}_l} &= \frac{\partial}{\partial \mathbf{w}_l}\left(\sum_c t_c(\mathbf{x})\cdot\log(p_{\mathcal{W}}(c|\boldsymbol{\xi}(\mathbf{x},W)))\right) \\
&= \sum_c \frac{t_c(\mathbf{x})}{p_{\mathcal{W}}(c|\boldsymbol{\xi}(\mathbf{x},W))}\cdot\frac{\partial p_{\mathcal{W}}(c|\boldsymbol{\xi}(\mathbf{x},W))}{\partial \mathbf{w}_l} \\
&\overset{(50)}{=} \sum_c \frac{t_c(\mathbf{x})}{p_{\mathcal{W}}(c|\boldsymbol{\xi}(\mathbf{x},W))}\cdot\frac{\partial}{\partial \mathbf{w}_l}\left(\sum_{j:c(\boldsymbol{\omega}_j)=c} S_{\mathcal{W}}(j,\boldsymbol{\xi}(\mathbf{x},W))\right) \\
&= \sum_c \frac{t_c(\mathbf{x})}{p_{\mathcal{W}}(c|\boldsymbol{\xi}(\mathbf{x},W))}\cdot\left(\sum_{j:c(\boldsymbol{\omega}_j)=c} \frac{\partial S_{\mathcal{W}}(j,\boldsymbol{\xi}(\mathbf{x},W))}{\partial \mathbf{w}_l}\right)
\end{aligned}
$$

as derivative of the cross-entropy with respect to the sensoric prototype $\mathbf{w}_l$. For the derivative $\frac{\partial S_{\mathcal{W}}(j,\boldsymbol{\xi}(\mathbf{x},W))}{\partial \mathbf{w}_l}$

we calulate

$$
\begin{aligned}
\frac{\partial S_{\mathcal{W}}\left(j,\boldsymbol{\xi}\left(\mathbf{x},W\right)\right)}{\partial \mathbf{w}_l} &= \frac{\partial}{\partial \mathbf{w}_l}\left(\frac{p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_j\right)\cdot p\left(\boldsymbol{\omega}_j\right)}{\sum_{k=1}^{N} p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)\cdot p\left(\boldsymbol{\omega}_k\right)}\right) \\
&= \frac{p\left(\boldsymbol{\omega}_j\right)\cdot\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_j\right)}{\partial \mathbf{w}_l}}{\sum_{k=1}^{N} p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)\cdot p\left(\boldsymbol{\omega}_k\right)} - p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_j\right)\cdot p\left(\boldsymbol{\omega}_j\right)\cdot\left(\frac{\sum_{k=1}^{N} p\left(\boldsymbol{\omega}_k\right)\cdot\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)}{\partial \mathbf{w}_l}}{\left(\sum_{k=1}^{N} p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)\cdot p\left(\boldsymbol{\omega}_k\right)\right)^2}\right) \\
&= \frac{p\left(\boldsymbol{\omega}_j\right)\cdot\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_j\right)}{\partial \mathbf{w}_l}}{\sum_{k=1}^{N} p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)\cdot p\left(\boldsymbol{\omega}_k\right)} - S_{\mathcal{W}}\left(j,\boldsymbol{\xi}\left(\mathbf{x},W\right)\right)\cdot\left(\frac{\sum_{k=1}^{N} p\left(\boldsymbol{\omega}_k\right)\cdot\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)}{\partial \mathbf{w}_l}}{\sum_{k=1}^{N} p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)\cdot p\left(\boldsymbol{\omega}_k\right)}\right) \\
&= \frac{p\left(\boldsymbol{\omega}_j\right)\cdot\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_j\right)}{\partial \mathbf{w}_l} - S_{\mathcal{W}}\left(j,\boldsymbol{\xi}\left(\mathbf{x},W\right)\right)\cdot\sum_{k=1}^{N} p\left(\boldsymbol{\omega}_k\right)\cdot\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)}{\partial \mathbf{w}_l}}{\sum_{k=1}^{N} p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)\cdot p\left(\boldsymbol{\omega}_k\right)}
\end{aligned}
$$

which includes the derivatives $\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_j\right)}{\partial \mathbf{w}_l}$. Using the dissimilarity density model (52) we have

$$
\frac{\partial p\left(\boldsymbol{\xi}\left(\mathbf{x},W\right)|\boldsymbol{\omega}_k\right)}{\partial \mathbf{w}_l} = \frac{\partial \pi_{\mathscr{D}}\left(\delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}_k\right)\right)}{\partial \delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}_k\right)}\cdot\frac{\partial \delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}_k\right)}{\partial \mathbf{w}_l} \tag{55}
$$

with the derivative $\frac{\partial \delta\left(\boldsymbol{\xi}\left(\mathbf{x},W\right),\boldsymbol{\omega}_k\right)}{\partial \mathbf{w}_l}$ according to (42) or to (43) for NG-based responses or fuzzy responses, respectively.

This PLVQ-approach (and its variants) can be summarized as

$$
X \underset{\text{NG/FCM}}{\leftrightarrows} W \underset{\text{NG-like/fuzzy}}{\overset{\boldsymbol{\xi}(\mathbf{x},W)}{\leftrightarrows}} \Xi \underset{\text{PLVQ}}{\overset{\mathbf{p}_{\mathcal{W}}(\boldsymbol{\xi})}{\longrightarrow}} \mathscr{C} \tag{56}
$$

in relation to (4).

# 4 Discussion

In this paper we describe formal extensions of counter propagation networks, which should make the original approach more flexible. In particular, we discussed several possibilities to transfer the data knowledge acquired by the vector quantization layer to the classification layer. Moreover, we considered several possibilities to replace the perceptron layer by alternative classification approaches. In the context of this we also studied how to realize a vector quantizer adaptation depending on the subsequent classification process realized in the second layer. Although this increases the complexity of the model, it could beneficial for certain applications.

At this point we did not discuss so far regularization aspects to achive model stability during learning and to control the flexibility. This should be done also in the context of the information bottleneck paradigm [47, 48] as well as reflecting the dilemma between information optimum data representation in the vector quantization layer and the demanded classification or regression performance [34, 36, 29].

An extension of the approach to the recently developed classification-by-components network (CbC, [41]) as alternative for LVQ variants should be investigated next.

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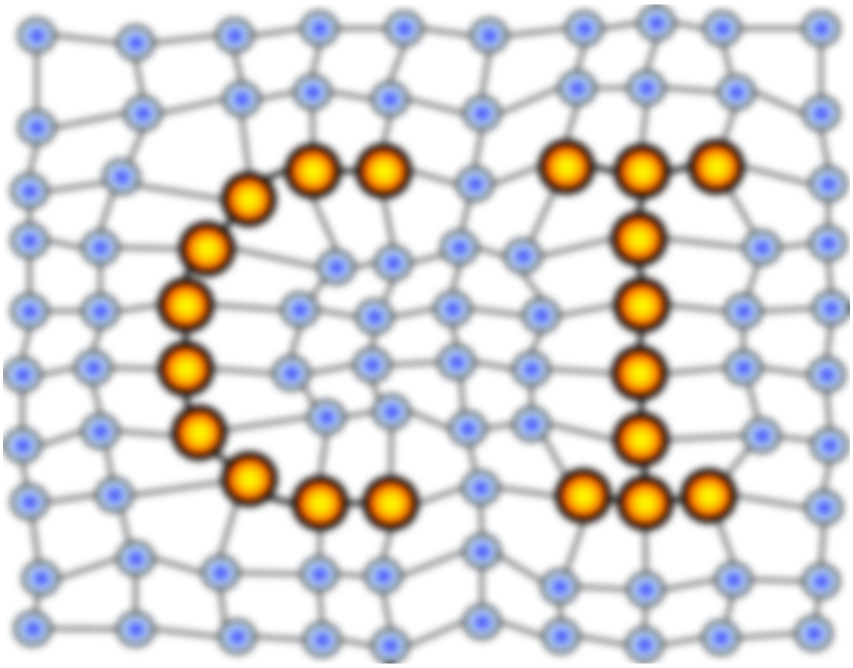

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