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Theory and Applications of Neural Maps

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Abstract. In this tutorial paper about neural maps we review the current state in theoretical aspects like mathematical treatment of convergence, ordering and topography, magnification and others. Therby we concentrate on two well-known examples: Self-Organizing Maps and Neural Gas. Moreover we briefly reflect outstanding applications showing the power of neural maps.

1 Introduction

Fundamentals and basic notations Neural maps occur in real brains in all sensory modalities as well as motor areas being an important step in information processing. From these biological fundamentals models have been derived, which today constitute an important neural network paradigm comprising a broad variety of methods ranging from statistical approaches to strong biologically realistic models [2, 56, 81, 113, 149]. In this paper we restrict ourselves to those models which are designed for data processing. In this technical context, neural maps are utilized in the fashion of topographic vector quantizers. More formally, in neural mapping we consider a set $\mathbf{W} \subseteq \mathbb{R}^{D_V}$ of reference vectors $\mathbf{w_r}$ (codebook vectors) to represent a large data set $V \subseteq \mathbb{R}^{D_V}$. Each vector is uniquely assigned to a certain $\mathbf{r} \in A$ whereby A is an arbitrary index set. Reflecting the biological roots, the elements of A are called neurons. Then, a data vector $\mathbf{v} \in V$ is projected onto that neuron $\mathbf{s} \in A$, of which the reference vector $\mathbf{w_{s(v)}}$ has a minimum distance d to $\mathbf{v}$, compared to all elements of $\mathbf{W}$:

$$\Psi_{V\to A} : \mathbf{v} \mapsto \mathbf{s} = \operatorname*{argmin}_{\mathbf{r}\in A} \left(d\left(\mathbf{v}, \mathbf{w_r}\right)\right). \tag{1}$$

The distance $d(\mathbf{v}, \mathbf{w_r}) = \|\mathbf{v} - \mathbf{w_r}\|$ is based on an appropriate norm, usually the Euclidean. The reverse mapping is $\Psi_{A\to V} : \mathbf{r} \mapsto \mathbf{w_r}$. Both functions together determine the (neural) map $\mathcal{M} = \left(\Psi_{V\to A}, \Psi_{A\to V}\right)$. All data points $\mathbf{v} \in \mathbf{V}$ that are projected onto the neuron $\mathbf{r}$ make up its (masked) receptive field $\Omega_{\mathbf{r}}$.

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Generally, neural maps can be taken as stochastic realizations of the Linde-Buzo-Gray-algorithm (LBG or *k-means,* [91]) with the additional feature of topographic mapping [71]. The convergence of these approaches is based on the theorems from Kushner&Clark or Ljung [93, 86].

The main task of neural map approaches is to describe given data in a faithful way, such that the main properties are preserved as good as possible. These properties may be the usual reconstruction error, the probability density [133], the shape of data in the sense of possibly non-linear principle component analysis (PCA) [105, 116] or visualization like multi-dimensional scaling (MDS) [110], topology preserving (topographic) mapping [144], the classification error etc. For the different goals several approaches exist, whereby we further have to differentiate between supervised and unsupervised learning schemes.

Types of neural maps A very popular algorithm is the Self-Organizing Map (SOM) introduced by Kohonen in [80]. Beside a huge amount of models derived from the original one (for an overview see [81]), the SOM also inspired other (neighborhood oriented) VQ schemes. Historically earlier but closely related to SOM is the Elastic Net (EN) with well defined mathematical properties (convergence) and biological motivation [149]. The Topology Representing Network (TRN) has a structurally similar learning scheme compared to SOM but a dynamically adapted topology between the neurons in A [97].

A further topographic mapping scheme is the Generative Topographic Mapping [14], based on a constraint Gaussian mixture model, the parameters of which are determined by a maximum likelihood procedure using a simplified Expection-Maximum-principle (EM) procedure which is more complicate than SOM learning. Linsker proposed a topographic VQ network with optimal information transfer [92] based on information theoretic learning [109]. Equiprobabilistic topographic map formation based on kernel methods is extensively studied by van Hulle [133] also under the constraint of maximum entropy [134]. Vector quantization based on potential dynamics is of great interest because of its clear mathematical treatment, for instance based on the EM [20]. Beside the above mentioned TRN such topographic approaches are the stochastic topographic mapping and its variants [56, 71, 134]. Thereby, the basic mathematical trick is the mean field approximation to derive the EM-steps. Other related neural maps to be mentioned here are the counterpropagation network [67] which includes a SOM-layer or the ART-map family based on adaptive resonance theory [22].

As mentioned above, the topographic mapping as well as the neighborhood cooperativeness during learning are the essentials in neural vector quantization. In the following we will focus on the SOM and TRN as well-known and widely ranged examples for static and dynamic neighborhood handling in neural maps. Thereby, in SOM the apriori given lattice A is usually a possibly high-dimensional rectangular lattice or a grid based on hexagonal structures.

2 SOM and TRN

2.1 Convergence properties

Although the adaptation process in SOM is simple, the mathematical treatment is difficult [28, 30]. Most results are valid only for the one-dimensional case.

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For the continuous case (continuous inputs as well as continuous lattice A) the stationary state and convergence properties are investigated by means of the spectral density of fluctuations in the equilibrium [114]. These considerations were extended by several authors to analyze the dynamic behavior in convergence and ordering [35, 39]. Further, it has been shown that it is impossible to associate a global potential function to SOM for continuous inputs and studied the role of the neighborhood function [42, 43]. A straightforward definition of an energy function leads to slightly different winner determination in Eq.(1) [71]. Before convergence, an ordering process takes place. The ordering conditions and time behavior of ordering were studied in [19, 38].

The discrete cases are more complicate than the continuum case. For discrete lattices, the first convergence proof was given in [118] based on the observation that SOM can be taken as a Robbins-Monro-algorithm [115]. The respective differential equations for weight adaptation are shown to be absorbing. Further convergence and ordering theorems for several, more general, parameter settings are studied by several authors, verifying the almost sure convergence in dependence on the concrete choice of the neighborhood shape and range, learning rate etc. [10, 11, 16, 17, 44, 47]. Meta stable states may occur for certain configurations (non-vanishing learning rate) [48]. Sufficient conditions for convergence are given in [45]. Lebesque continuous inputs are studied in [46], discrete inputs are considered in [27, 90]. Discrete inputs but high-dimensional lattices A are investigated in [119]. More higher-dimensional cases results can be found in [49, 89, 30]. Depending, for instance, on grid configurations [94, 95] instabilities may occur [29]. For short range neighborhoods, instabilities may be observed, too, although starting from an ordered configuration [36].

The TRN weight adaptation process is based on the Neural Gas (NG) algorithm [98]. The adaptation process is equivalent to the dynamic of a diffunding gas. Hence, it follows a gradient descent of an energy function which is the usual mean squared error.

2.2 Density estimation, magnification and magnification control

The SOM as well as NG/TRN distribute the weight vectors according to the input probability density P: $\rho(\mathbf{w}) \sim P(\mathbf{w})^{\alpha}$. The exponent α is called magnification. Using this property both models can be used to estimate the usually unknown data distribution P [88]. A magnification $\alpha = 1$ implies an information optimal coding of data by the network [152]. The deviations from this optimal values for SOM and NG are due to the incorporation of neighborhood learning and topology preservation [30, 98, 144]. Depending on the shape of neighborhood different magnifications are achieved [40, 111, 146]. Therefore, several modifications exist to control magnification by control of the winning frequency [41], local learning rates [5, 69, 140] or winner relaxing terms [24, 26], the latter one also available for EN [25]. A review of these methods is given in [143]. SOM and maximum mutual information with respect to additional knowledge (auxiliary data) is discussed in [79, 125].

The theoretical magnification law for SOM is only valid for the one-dimensional case whereas for NG the result holds for higher-dimensional cases,

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too. In [76, 99], both in this book, numerical properties for higher-dimensional cases for SOM are investigated.

2.3 Topographic mapping and growing variants of SOM and NG

One main idea of neural maps is topographic (or topology preserving) mapping by means of Eq.(1) which is closely related to the above mentioned ordered states in SOM. Generally, neural maps project data from a possibly high-dimensional input space $V \subseteq \mathbb{R}^{D_V}$ onto a position in a topologically ordered output space A using a set of associated (to A) reference vectors such that, roughly speaking, a continuous change of a parameter of the input data should lead to a continuous change of the position of a localized excitation in the output space. The mathematically exact definition is based on the receptive field of the neurons [97, 144] including all aspects of earlier approaches [7, 12, 33, 55, 153]. For TRN topographic mapping can be achieved if the weight vectors are lying *dense* in the data space whereas for SOM one has to proof topology preservation for a given map. Several measures were established to judge the degree of preservation. Although not based on the mathematical exact definition, the topographic product [7] and its derivatives [139] seem to be the best tools [6].

Two aspects may lead to violations of topology preservation: beside the convergence problems, violoations of topology preservation may be observed due to the topological mismatch between the chosen lattice structure and data shape. For instance in case of rectangular typed lattices with dimension D_A: if D_A differs from the effective data dimension $D_{eff} \neq D_V$ topological mismatches generally may occur. The respective theory of meta- and instable states is initially based on Fokker-Planck approaches [113]. Thereby the learning is taken as Markov process [70, 96]. Further studies also use the Ginzburg-Landau-theory to describe the phenomena in more detail [37, 35]. The high-dimensional analysis was pointed out in [8] using phase diagrams.

To overcome the topological mismatch problem, growing variants of SOM were developed [50, 123, 9] or input pruning was tried [15]. The structure adaptation is closely related to the problem of SOM and PCA [34] and its non-linear extension of principal curves [66]. A growing approach for NG was proposed in [52] and for EN in [51].

3 Further variants

Non-standard metrics and general lattice structures Usually the similarity measure in input space is the Euclidean metric or the scalar product. However, non-standard metrics were investigated to extend the possibilities of neural maps for different environments. Scaled input dimensions are used in the above mentioned methods using auxiliary information to be information optimal [79, 125]. Related to scaled input dimensions are such SOM and NG approaches, which are dedicated to input pruning for determination of relevant input dimensions in dependence on different optimization goals [64, 15]. An approach for *clustering functions* by SOM according to a respective similarity measure can be found in this book [1]. Another variant is the extension of

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SOM for exploration of subspaces [83]. Structured data as trees, for instance, are considered in [108]. A general frame work for unsupervised structured data processing is provided in [57, 59]. The context learning approach [129] presented in this book can be seen as matching this topic, too. Otherwise, in SOM also non-standard metrics also may occur between the neurons in the output space A. In particular, hyperbolic structures are of interest [112] which can be related to recursive variants [127]. Tree-structured SOMs were established in [21, 84].

Supervised learning The combination of neighborhood cooperativeness with methods of supervised learning in Learning Vector Quantization (LVQ) has gained an increasing importance during last years. After the initial work about supervised SOM and LVQ mentioned in [81] and the generalization of LVQ by an energy function [120], neighborhood learning in NG was proposed [145]. Further, neighborhood cooperativeness in NG was combined with non-standard metrics approaches in LVQ [65] for better classification performance [60, 63]. Thereby, it can be shown that the generalization ability is the same as for Support Vector Machines (SVM) [61, 62].

Recursive and recurrent maps Recursive variants of SOM [138] and NG may be used in sequence processing [128, 127]. Recurrent SOMs and temporal SOMs are studied in [23, 135] which can be applied in time series and sequence processing [85]. These investigations are closely related to the above mentioned studies about neural maps for structured data processing.

Links to other Soft Computing paradigms Vector quantization and neural maps have strong links to other soft computing paradigms. Naturally, there is a great overlap to Fuzzy methods. Fuzzy clustering and neural maps are widely discussed [13, 54, 107, 132, 77]. The Fuzzy approaches can also be interpreted by the stochastic neural map variants as suggested in [56, 73].

New trends in hybrid systems also combine evolutionary approaches and neural maps. Examples for evolving neural maps are in [82, 102, 131]. Vice versa, neighborhood cooperativeness known from neural maps are incorporated in strategies in evolutionary approaches, too. Examples are migration strategies [141] or neighborhood attraction in genetic operators [75, 74]. A review can be found in [148]

4 Implementation on computer hardware

Sequential processing In the field of neural maps there is a big variety of software, ranging from rather independent modules on source code level (e.g. C/C++ or Java functions) to partly pre-compiled objects (e.g. SOM-PAK [158]) of general purpose simulation systems (e.g. MatLab [154]) up to integrated parts of stand-alone neural network simulators (e.g. SNNS [159], NeuroSolutions [156], PDP++ [157], NeuralWorks [155]). Almost all of them provide a more or less extensive library of neural network paradigms, among them neural maps, to be run on popular combinations of mainly single processor hardware and operating systems. This way, at least neural maps in standard type can be easily trained and simulated. More specialized neural designs or more recent developments [112] are often not yet included in universal SOM repositories.

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Parallel processing From the scientific point of view parallel implementations of neural maps seem to be much more promising. In general, there is a dualism between artificial neural networks and parallel hardware, which is mainly based on the inherent parallelism of neural networks themselves [4, 72, 117] and on the request or even the necessity to speed-up training and simulation of larger complex networks. While the first aspect makes a parallel implementation of artificial neural networks suggestive at all, the second one represents its motivation. The properties of this dualism depend on topology, learning strategy and control parameters of considered neural networks on the one hand and on the hardware and software architecture on the other. For a survey refer to [121].

Keeping this in mind it is rather obvious, that different neural networks perform[1] variably on different hardware. Independent of a particular hardware *Amdahl*'s law reflects the possible speed-up only depending on the fraction of instructions inherently sequential (β) and the number of available parallel processors p.

$$s = \frac{p}{\beta p + (1 - \beta)} \tag{2}$$

If, for example, $\beta = 0.2$, the equation shows that as p increases, the speedup s goes asymptotically to 5.

However, *Amdahl*'s law is only one issue to judge a particular parallel implementation. For parallel processes it is a basic necessity to exchange data between each other. Thus, the performance also is affected by the amount of data to be exchanged at each step (e.g. learning step) in relation to the mathematical (numerical) complexity from the algorithmic point of view and the computational power of each node in conjunction with data transmission properties between them as hardware system characteristic. In addition to these issues, a number of further properties of the utilized hardware, such as processor registers, processor cache and system memory sizes and structure, computation speed and inter-node bandwidth and latency as well as some software features influence the benefit from a parallel implementation.

Neural maps, especially the in this paper more detailed considered Self-Organizing Maps, are characterized by a rather close relationship to parallel hardware. There are many successful implementations on different platforms, such as shared memory systems, computer clusters and special purpose processors [104, 130, 58, 124]. In relation to the above mentioned issues, neural maps are very interesting and especially promising neural network paradigms:

- Often rather large maps consisting of a big number of neurons are required to feature the desired projection resolution.
- Since all neurons are located within the same layer (in contrast to layered networks with a hierarchical data processing), SOMs offer a high degree of independent computation and consequently a high level of parallelism.

[1] Here we refer to instruction parallel processing. In contrast to data parallel processing, which only requires a partitioning of the data set and not a decomposition of the algorithm into independent and thus parallelizable parts.

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- The favorable balance between computational complexity and data transmission leads to a good scaling of parallel implementations.

A comparison of parallel implementations of different hardware by means of some SOM benchmark applications can be found in [121].

5 Outline on possible real world applications

There exist a lot of interesting and outstanding applications of SOMs, NG and other types of neural maps. The main features required are clustering and topology preserving mapping for visualization of high-dimensional data [136, 137]. The range of applications is very broad. One of the largest project is WEBSOM [78], a SOM-based document exploration tool whereby the topology preservation property helps finding related documents, once any interesting document is found. Other innovative topics are economic and financial applications [32, 31] which may be combined with classical statistical features [126]. Another wide application area is image processing [3, 87]. In this light one also can see the task of visual person tracking using a supervised SOM as presented in [68]. A special fascinating topic in image processing is satellite remote sensing image analysis [147]. Thereby, huge-dimensional spectral data called hyperspectral images are to be processed and visualized. Neural Maps are convenient tools for extensive explorative analysis [18, 53, 103, 100]. Especially, we here have particular interest in magnification control to detect rare features as pointed out in [99] in this book.

Another application area is medical data processing and analysis. Here one can find classical applications of image processing and standard data analysis. But also interesting new developments in algorithm design can be found which are motivated by ideas in medical applications, for example the deformable feature map [150]. Further medical applications can be found in [142]. A very recent research area is bioinformatics. Yet, neural maps can valuably contribute to knowledge discovery and data processing also in this topic as demonstrated in an increasing number of publications [101, 122, 106, 151].

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