Soft-Computing based Methods in Analysing Nanometric Scaled Topographic Patterns

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Abstract:
In this paper we discuss the application of the Difference-Autopower-Spectra (DAS) for topographic pattern recognition. By experimental results we will show that this adaptive signal-processing method is not restricted to the use as spectral oriented pre-processing step in the frequency domain but can also be used as feature-extracting operator for topographic pattern recognition. This result takes by surprise in so far as the same feature extraction calculation to optimise the classification/identification behaviour of neural net holds for 1-dimension spectra and 3 dimensional pattern. On the other hand the physiological oriented formulation of the DAS recommends such results that have been proved now. As we will show furthermore the DAS-representation of topographic pictures enables SOMs and backpropagation neural networks to detect the dynamics of ultra-fast energy transfers between semiconductor surfaces and adsorbed chromophores in a very easy way.

Keywords: DAS, nanometric scaled topographic pattern recognition

Introduction

As the mathematical theory of DAS calculation was discussed in several papers [Reuter 1989-1998], we will summarise only some basic assumptions to verify what pattern recognition and feature extraction done by the DAS-representation means.

The charge of the signal processing is to extract the source-specific information out of any scenario, so ideally it eliminates all information that do not describe the analysed system. Analysing technological and biological systems it is obvious, that the sufficient feature representations are mostly covered by noisy contributions or cannot by elaborated as the resolution of experimental data are not sensitive enough. That leads to the fact that a problem-specific extraction of features has to be done. So this aim is the reason to calculate the Difference-Autopower-Spectra (DLS).

The basic-idea of the DAS is to divide the x-and y-axis of measured data spectrum into classes, calculate the mean-value of these classes and use the class-related mean-value as the new zero-line of the DAS. As many technological applications show, this kind of fitting curve is extremely robust and flexible for all kinds of noisy contributions and is an extremely useful preprocessing algorithm for all kinds of neural classifiers. For a DAS algorithm the following parameters must be chosen:

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- Beginning of the spectrum to be analyzed	(m)
- End of the spectrum to be analyzed	(f)
- class-width of the first DAS-Fitting	(H)
- class-width of the second DAS-Fitting	(Z)

The DAS-operator itself is characterized by the symbol whereas the DAS parameters are given in the bracket that follows. The spectra on which the DAS-operation will act are characterized by the expression: Ampl (f_i):

$$\text{DAS Ampl } (f_i) = \Delta\,(m,f,H,Z)\ \text{Ampl}(f_i)$$

So the DAS results from a fitting procedure, which is composed of two successive class-oriented average calculations, shown in Figure 1, while the effort of this operation depends on the choice of adequate class-widths.

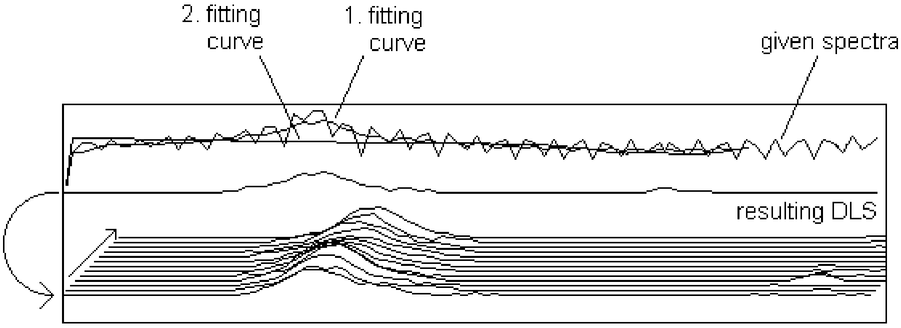

Fig.1: 2-step adaptive fitting procedure of an artificial 50 Hz signal

While choosing suitable feature extractions we have to be conscious of another aspect of problem-oriented representations:
For neural classifiers supervising a time-continuous signal, a discontinuous changing in the course of spectra is an insufficient basis for evaluation because the trajectories of the time-dependent amplitudes seem to skip over the time. If that behaviour had corresponded with the signature-producing source, it would have acted as a non-deterministic system.

Actually dynamic, non-linear processes in biological and technological systems often occur as sudden changes because the "system-parameters", which could be any combination of measured parameters, are not really known. In absence of that knowledge complex systems are often regarded in wrong state-continua.

Especially problem-related representations demand linear time-trajectories. In particular biological systems for example, if they will be deeply determined, reveal a linear behaviour in crossover their status. This fact is shown in Figure 2a that shows a non-adequate EEG-signal-representation and Figure 2b that shows a non-adequate EEG-signal-representation [Zemke, Reuter 1997].

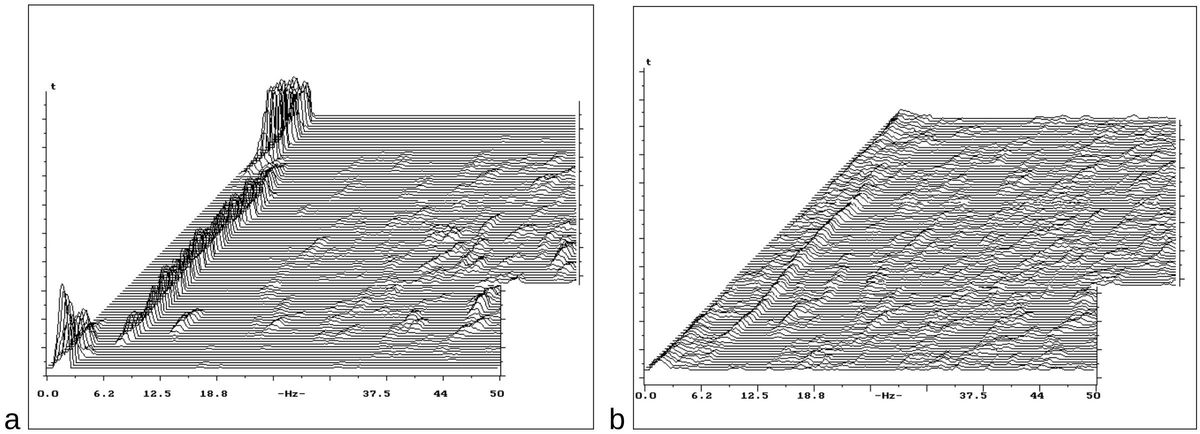

Abb.2: Example of an adequate pre-processing of time dependent amplitudes

a: Apparent sudden crossover (classic EEG of an epileptic event)

b: Detection of the linear development of the patient status (pre-processed EEG)

Indeed the use of adequate pre-processing algorithms as a part of neural classifier chains in topographic pattern recognition is even more important. The charge is to detect non-linear crossovers not only time-dependent but also in space. Actually we have to despite those signatures that are corresponding in space, from those that act individually and lead to separate the feature representation.

Experimental results

Our recent investigations discussed in this paper deal with ultra-fast energy transfer dynamics between semiconductor surfaces and adsorbed chromophores. The technique of near-field scanning optical microscopy (NSOM) offers the possibility of high spatial (Äx < 50 nm) and temporal (Ät < 100 fs) resolution while retaining the advantages of optical spectroscopy. By a pump-probe laser operation we get 3D (x, y, Ät) images as a result from changes in the probe beam transmittance or reflectance which is a function of pump-probe delay (Ät). NSOM is a scanned probe microscopy in which light from a tapered fibre optic held close to a surface allows illumination on sub-wavelength dimension. Experiments demonstrating femtosecond time-contrast NSOM have not yet been accomplished. Silicon-based devices in common electronics (e.g., the Pentium chip) already rely on features in the 350-nm size range. As the evolution towards smaller, faster devices continues, measurement techniques must be developed which probe the chemistry and physics of interfaces on shorter spatial and temporal scales simultaneously.

Figure 3a-d shows two examples of a feature extraction which is done by a two-step successive class-oriented average DAS calculation[2]. Irrelevant portions of information that would have been part of the neural classifier's decision-basis (shown on the left-hand side) are eliminated, and the system-relevant information is thrown into relief (shown on the right hand side).

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[2] All pictures and calculations done with the ‘zz-2 software-tool’ from: Ingenieurbüro RT&S

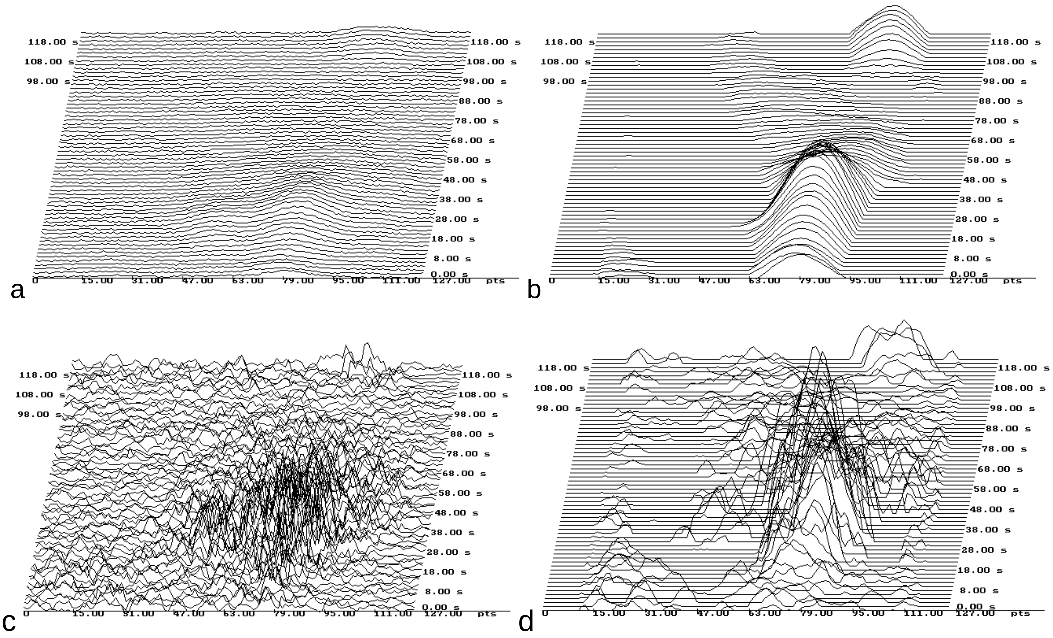

Fig.3: Spectra of emission on a semiconductor surface
a: Defect on surface without pre-processing
b: Defect on surface pre-processed by DLS
c: Pump-impulse without pre-processing
d: Pump-impulse pre-processed by DLS

Due to the high temporal and spatial resolution of this pre-processed pattern it becomes possible to investigate dynamic processes in semiconductor materials, e.g. the energy transfer between adsorbed molecules and their topologic relations, the affect of the binding condition of single molecules and the effects of defects on the semiconductors surface by soft-computing based classifiers in detail. While the knowledge of those interacting and non-interacting sub-processes is incomplete, first their correlation is analysed by self-organising maps (SOM) as this method of a non-supervised learning strategy of neural nets will allow to detect the correlation between contributed sub-systems, even if the knowledge of them is incomplete.

Due to the characteristics of the SOM we also expected that it should be recommended to detect structures and dependencies of dynamic process data which are encoded in input vectors as especially in vast and muddled data sets SOM are an outstanding tool to verify inner relationships.

As a first interim result in context to the present problem of analysing ultra-fast energy transfer processes between single molecules and a semiconductor surface, defects on the surface are identified as a permanent background noise contribution that masked the emission spectra of the pump-probe experiment.

Figure 4 presents a temporary extract of snapshots of the semiconductor surface as input vectors (spectra below) and their representation as areas of activity (light coloured) on the SOM. The topographic patterns are each presented to a SOM (with 40*40 neurons) as single vectors that consist of all successive rows of the emission spectra-scan.

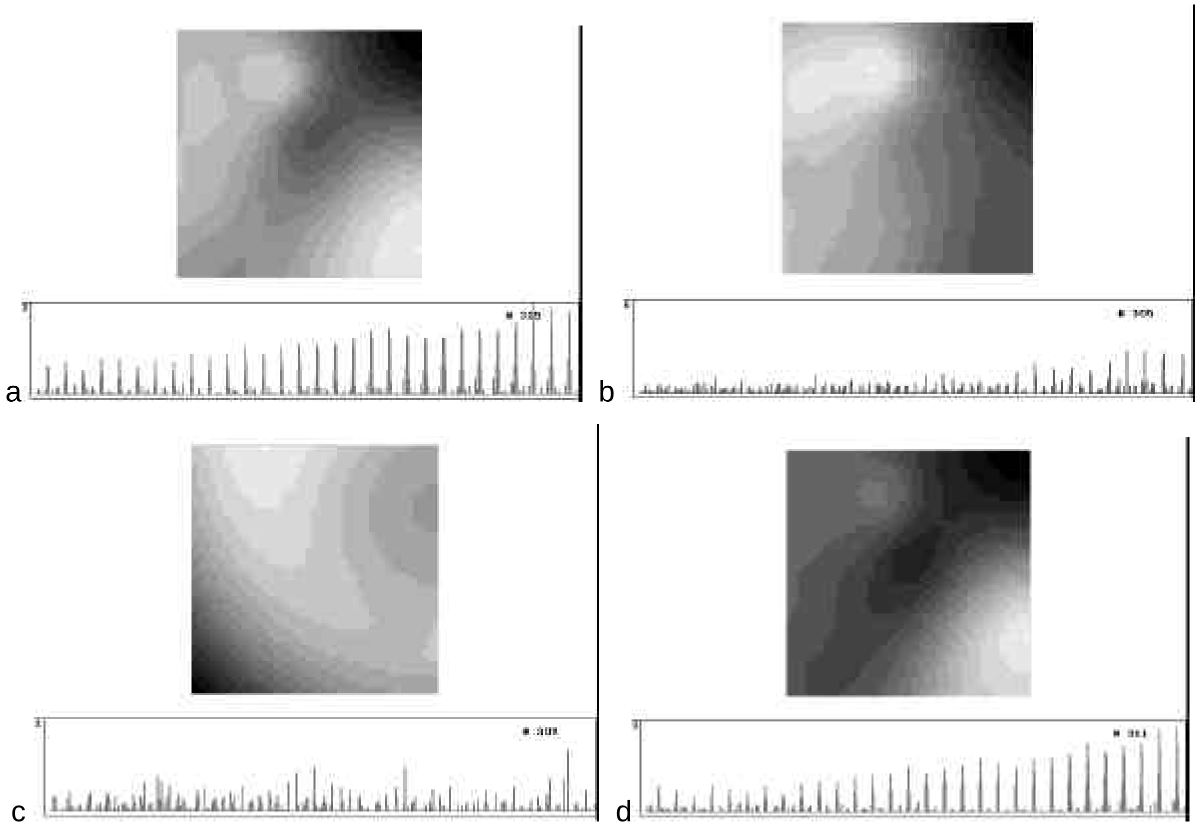

Abb.4: representation of the NSOM experiment on a self-organising map (SOM)

a: Initial sequence b: Pump-impulse occurs c: Sequence of restoration d: Final sequence

As the initial reps. final sequence of the measured time interval Fig. 4a and 4d show similar structures of the areas of activity due to the fact that the emission spectra are restored completely. Fig 4b depicts the emission spectra when the pump impulse occurred. Though a new centre of activity has been established on the SOM, the activity-area of the initial sequence has not been destroyed completely and is participate at the actual spectra as an independent system-parameter. The decrease of influence of the pump impulse as a consequence of the increasing time gap between pump and probe impulse is distinctly expressed by the smoothly migration of the centre of activity towards its initial structure.

To detect the exact moment when the pump impulse influences the emitted spectra, a Backpropagation net was trained with the same pre-processed data, while the optimal choice of the learning vectors are derived by the results of the SOM analysis. In Figure 5a the learning period of this neural net is shown. The gap between the two curves marks the degree of probability of identification while the upper border of the gaps represent a probability of ‘1’ and the lower border a probability of ‘0’. The first surprising result is, that after a period of less than 100 learning steps the classification behaviour of the net satisfies and the net was ready for action.

The temporary identification of the pump pulse in an infinite slope done by this net is shown in Figure 5b while the time of its influence is also a matter of interest.

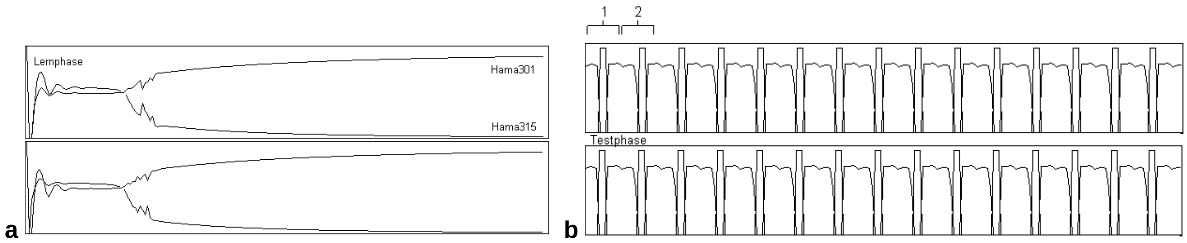

Fig. 5a,b: Classification of the emission spectra by a backpropagation net

Clearly the pump impulses can be identified as columns which occur periodical.

Conclusions

The effective use of the DAS pre-processing calculation as an feature extracting strategy for 3-dimensional pictures can be shown by the design of SOM and Backpropagation networks analysing ultra-fast dynamic processes on a semiconductor. The further investigations will show how the relation between the dimension of input vectors and SOM matrix affects the learning behaviour and the classification result of the SOM. The reduction of the input vectors by pre-processing strategies without a loss of system-relevant data will lead to embedded classificator/identificator systems that supports the analysis of pump-probe NSOM data-sets.

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