GROWING COUNTER-PROPAGATION ARTIFICIAL NEURAL NETWORKS

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Teuvo Kohonen developed the original self-organizing maps (SOM) neural network algorithm in the 1980s. Even in those early years, Kohonen proposed SOMs with dynamically changing topology. The idea at the time, according to Kohonen, was to use standard rectangular SOM and if the distance between two neighbouring neurons is too large, the corresponding connection between them is *turned off*. This could be considered as *top-down* approach in changing of the network topology. Another interesting variant of SOMs with changing topology, this time using *bottom-up* approach, was developed in the 2000s. This algorithm, which is almost unknown for chemists, is called growing self-organizing maps (GSOM). In cases like this the network grows faster (adds new neurons and connections between them) in a direction of larger probability distribution of the data.

Here a supervised version of GSOM algorithm called *growing counter-propagation artificial neural network* (GCPANN) is presented. This algorithm, as its analogue with fix topology, is used for modelling purposed. Due to the variable size, GCPANN converges faster toward models with good performances. An additional advantage of the algorithm, because of its dynamically changing topology and network size, is that it usually solves the same modelling problem with smaller number of neurons.

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