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Mathematical Neural Network (MaNN) Models Part II: Self Organizing Maps (SOMs) in chemical sciences

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(Dedicated to Dr. K V Ramana, former professor of bioinorganic chemistry, Andhra University, on completion of seventy five years of life on the lap of Mother Nature)

ABSTRACT

Vector quantization (VQ) determines representative set of vectors, each of them called a quantizer/code vector/template/centroid for unsupervised multi-dimensional data sets (i.e. without teaching signal or response). The limitation is that it does not have the concept of neighborhood and topology. The geometric proximity of pre-synaptic biological neurons in the brain was the source of inspiration for Kohonen-self-organizing-map (Kohonen-SOM) with a grid of 1D-, 2D- or 3D- frame of a vector-, matrix- and tensor- of equi-distant neurons which are not connected to each other. The shapes of the neighborhood structures which are in wide use are diamond, square and hexagonal. Winner takes all (WTA) and winner takes most (WTM) mechanisms are used to determine winning neurons or quantizers. It belongs to a class of unsupervised-NN model for numeric data employing competitive learning with neighborhood lateral interaction. The end result is arriving at a topological structure hidden in the data set. In the visual display of Kohonen map, clusters of different classes are clearly distinguished and two patterns close in input space are nearer in output space. SOM is equivalent as a special case to the popular multi-dimensional-scaling (MDS) and regularized mixture models. U-, U*, P-, U*F procedures are used in the display of average distances of winning neurons from neighbors. ViSOM, generative topographic mapping, consensus tree etc., are recent visualization methods. The noteworthy advances in architectures are evident in tree-, evolving-tree, self-evolving-tree-, hierarchical-, hybrid-hierarchical-, grey-, spherical-, geo-, parallel-, kernel-, granular-, greedy-granular-, median- and self-organizing-relationship- SOMs. The scope of chemical science in this century is broad encompassing not only bio-, environmental-, geo-, marine-, drug-/ material-, clinical-, dietary- pharmaceutical- tasks but also atomic to macro-molecular systems at very-high-/very-low temperatures/pressures/sizes. The future thrust area of fundamental prime research is around chemical transformations to the present day universe since the formation of hydrogen, helium and lighter chemical-elements with the knowledge of particle physics mind blowing research. The references are sorted journal wise for ease of down loading from print/ online-or-offline electronic resources.

Keywords: Neural network models, Self-organising-map, Unsupervised multi dimensional data, 2D-/3D-visualization, Chemical-engineering-medical applications, Hybrid SOM, Hierarchical-growing-SOM..
