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Mathematical Neural Network (MaNN) Models
Part VI: Single-layer perceptron [SLP] and Multi-layer perceptron [MLP] Neural networks in ChEM- Lab

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(Dedicated with profound respects to V Surya Prakasam, M.Sc. (Hons), A.E.S, former lecturer and Head of Dept. of physics, S R R & C V R Govt. College, Vijayawada during his birth centenary celebrations)

ABSTRACT

Multi-layer perceptron (MLP) NN deals with fully connected feed-forward-supervised NNs in which the flow of data is in the forward direction i.e. from input layer to output layer through hidden ones (IL → HL ... → OL). Each neuron in a layer is connected to all the other neurons in the succeeding layer. But, the neurons within the layer are not connected. The data comprises of explanatory variables(x) and response (y). In general $LP_NN (with $:0-, 1-, 2- and >2-hidden layers) represents I/O (or 0-LP), S(ingle)LP or 1-LP, 2-LP and M(ulti)LP. Starting with a single neuron, the popular ADALINE and MEDALINE-NNs with illustrative examples like copying, 'AND' 'OR' Boolean gates are described in I/O category. SLP_NN, the life of today's data driven NN paradigm with extensive applications in industry, research and defense has its origin in mid 1980s. It is the start of a new era of NN research, 25 years after the death blow to linear-ANNs for their inability to explain even a simple XOR problem.

The imbibing character of SLP and its superiority are demonstrated with numerical and literature reports in classification, function approximation, pattern recognition etc. The new NNs emerged (based on input type, TFs, accumulation operators) are complex-, quaternion-, fuzzy-, higher-order SLPs, retaining the basic philosophy of SLP architecture. RBF is also a SLP with Kernel TFs in the hidden layer and recurrent NNs are with partial/complete backward connections. The output of hidden layer of SLP is a transformed form of input into a new space generated through TFs. The applications of SLP and MLP are multifold covering nook and corner of every discipline. Only typical select case studies are briefed engulfing chemistry/chemical engineering, medicine/pharmacy/biosciences, electrical/ mechanical/ computer engineering, robotics, forecast of forex and weather prediction/environment/pollution. Multi-sensor hyphenated instruments generate tensorial data in chemical, environmental, pharmaceutical and

*clinical laboratory tasks. Mostly, the same sets of algorithms are used in **ch**emometrics, **e**nviromentrics and **m**edicinometrics (**Chem**) for **tensor** data sets (**Chem_Tensor** abbreviated as **CT**). The computational activity is now accepted as laboratory experiments (**thus CT-Lab)**, just the same way of wet and dry labs of last century.*

SLP mimics PCA, non-linear PCA, ARMA and polynomials when suitable object function and architecture are used. The posterior probability and Bayesian estimation are also derived from the output. The evolution in architecture gave birth to dynamic architectures, Ito/Funahashi model, centroid based/adaptive/self-feed-back/cascade correlation MLPs. The selection/sub-sets of patterns, layer-wise learning/pseudo-inverse/mixture-of-experts, dynamic learning, AdaBoost, batch-wise training are a few noteworthy advances in training Ws. The incorporation of a priori-knowledge into MLP is a new dimension. The modifications of basic back propagation (BP) algorithm used to train MLP_NN are extensive. The first-/second- order optimization methods and nature inspired algorithms like SAA, GA, PSO, ABC, ACO and differential evolution increased quality of Ws. Inverse NNs based on SLP/MLP for XOR and function approximation tasks are successfully dealt with. The cognitron, neocognitron, neural gas, spiking nets, complicated NNs mimicking (partial) biological functions, recent intelligent integration of statistics and NNs (NeuralWorks® Predict) and hybrids with nature-inspired algorithms find a niche in the annals of data driven information extraction.

Keywords: Multi-Layer Perceptron (MLP), Neural networks, Function approximation, Interpolation, Pattern recognition, Chemistry, Medicinometrics, Pharmaceutics, Technology, Pollution, multiple-classes.
