



State-of-Art-Review (SAR-Invited)

**Mathematical Neural Network (MaNN) Models
Part V: Radial basis function (RBF) neural networks (NNs) in Chemometrics,
Envirometrics and Medicinometrics (ChEM)**

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(Dedicated with reverence to Sri S Somayajulu, former Head of chemistry Dept., S R R & C V R Govt. College, Vijayawada on his birth centenary celebrations)

ABSTRACT

Radial basis function (RBF)-neural network (NN) has a single hidden (radial) layer of neurons with Gaussian kernel transfer function (TF). The names of many RBF_NNs correspond to the type TF viz. raised cosine-, generalised-binary, q-, Hunt- etc. The product type functions are Lowe, thin-plate and AuPar. The individual neurons in hidden layer of NN operated by TF (RBF, sigmoid) perform non-linear operation and layer as a whole maps input space into higher dimensions. A two phase training involving determination of centers of RBFs by clustering procedures followed by estimation of WRLO (weight vector of connections between neurons of radial and output layers) is the simplest protocol adapted. Although pseudo-inverse and orthogonal procedures are sought after optimization methods in weights refinement, Bayesian Ying-Yang (BYY-), incremental-, reinforced-, rival-penalized-continuous- (RPCL) and life-long-learning are used with success. Universal function approximation theorem, convergence proofs and error bounds imparted a strong theoretical support.

The evolution in architecture leads to recurrent-, self-organizing-, growing- and shrinking categories. Clifford/complex-RBF_NNs accept imaginary values for input unlike other RBF category. The trained network is pruned by temporary dynamic decay algorithm. The resource-allocating- (RA-), minimum-RA-, dynamic-decay-adjustment- belong to growing architecture category. The off-spring of RBF_NN are generalized regression- and probabilistic- NNs with statistical flavor. The power of RBF_NN increases with evolution of structure of network and weights of connections. The addition/deletion of RB neurons, connection making/breaking are implementable through mutation operators. Novelty detection, popularized by Grossberg in ART type NNs, is implemented in RBF_NN. Binary hybridization of RBF_NN with wavelets, support vector machines (SVM), self-organizing maps (SOM), logistic regression etc. increased the functional value of this NN. Nature inspired algorithms viz. evolutionary strategy, genetic algorithm, particle swarm optimization (PSO),

mimetic approach, honey bee algorithm are instrumental in arriving at viable solution of intractable hard task of simultaneous optimization of number of clusters, their centers/ widths and weights. SOM-Generalised_RBF emulates finite automata. The imbibing capability of RBF_NN, novelty detection, robust character brought it to the forefront in modeling phase of interdisciplinary research tasks. The ensembles, voting methods and Pareto-front brought renaissance to multiple alternate decisions instead of single best one of yesteryears. The applications of RBF_NN and its clones encompass science, engineering, industry, commerce and forex. The noteworthy results in chemometrics, envirometrics, piscimetrics, pharmacometrics and medicinometrics are briefly discussed pertaining to multi-variate-multi-response calibration, function approximation, interpolation, classification with non-linear boundaries, time-series data, pattern recognition and parameterization.

Keywords:Radial basis function, Neural network, Chemometrics, Medicine, Pharmacometrics, Environment, Interpolation, Function approximation, Classification.
