Application of a radial basis function neural network for diagnosis of diabetes mellitus

P. Venkatesan* and S. Anitha

Tuberculosis Research Centre, ICMR, Chennai 600 031, India

In this article an attempt is made to study the applicability of a general purpose, supervised feed forward neural network with one hidden layer, namely. Radial Basis Function (RBF) neural network. It uses relatively smaller number of locally tuned units and is adaptive in nature. RBFs are suitable for pattern recognition and classification. Performance of the RBF neural network was also compared with the most commonly used multilayer perceptron network model and the classical logistic regression. Diabetes database was used for empirical comparisons and the results show that RBF network performs better than other models.

Keywords: Artificial neural network, logistic regression, multilayer perceptron, radial basis function, supervised learning.

MULTILAYER Perceptron (MLP) network models are the popular network architectures used in most of the research applications in medicine, engineering, mathematical modelling, etc.[1]. In MLP, the weighted sum of the inputs and bias term are passed to activation level through a transfer function to produce the output, and the units are arranged in a layered feed-forward topology called Feed Forward Neural Network (FFNN). The schematic representation of FFNN with n inputs, m hidden units and one output unit along with the bias term of the input unit and hidden unit is given in Figure 1. An artificial neural network (ANN) has three layers: input layer, hidden layer and output layer. The hidden layer vastly increases the learning power of the MLP. The transfer or activation function of the network modifies the input to give a desired output. The transfer function is chosen such that the algorithm requires a response function with a continuous, single-valued with first derivative existence. Choice of the number of the hidden layers, hidden nodes and type of activation function plays an important role in model constructions[2–4].

Radial basis function (RBF) neural network is based on supervised learning. RBF networks were independently proposed by many researchers[5–9] and are a popular alternative to the MLP. RBF networks are also good at modelling nonlinear data and can be trained in one stage rather than using an iterative process as in MLP and also learn the given application quickly. They are useful in solving problems where the input data are corrupted with additive noise. The transformation functions used are based on a Gaussian distribution. If the error of the network is minimized appropriately, it will produce outputs that sum to unity, which will represent a probability for the outputs. The objective of this article is to study the applicability of RBF to diabetes data and compare the results with MLP and logistic regression.

RBF network model

The RBF network has a feed forward structure consisting of a single hidden layer of J locally tuned units, which are fully interconnected to an output layer of L linear units. All hidden units simultaneously receive the n-dimensional real-valued input vector X (Figure 2). The main difference from that of MLP is the absence of hidden-layer weights. The hidden-unit outputs are not calculated using the weighted-sum mechanism/sigmoid activation; rather each hidden-unit output Z_j is obtained by closeness of the input X to an n-dimensional parameter vector m_j associated with the jth hidden unit[10,11].

The response characteristics of the jth hidden unit ($j = 1, 2, \ldots, J$) is assumed as,

$$Z_j = K\left(\frac{\| X - m_j \|}{s_j^2}\right), \tag{1}$$

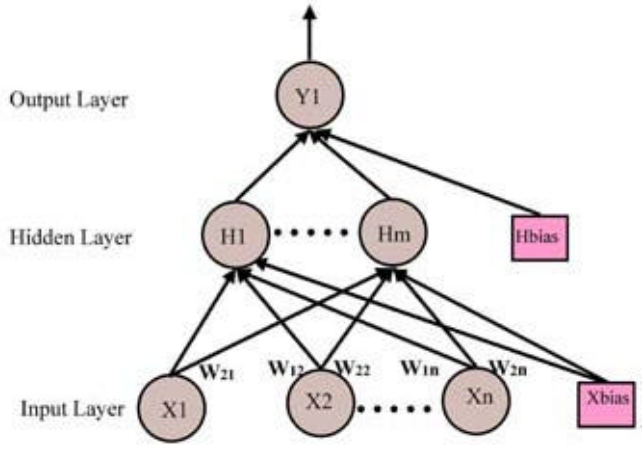

Figure 1. Feed forward neural network.

*For correspondence. (e-mail: perumal_venkatesan@hotmail.com)

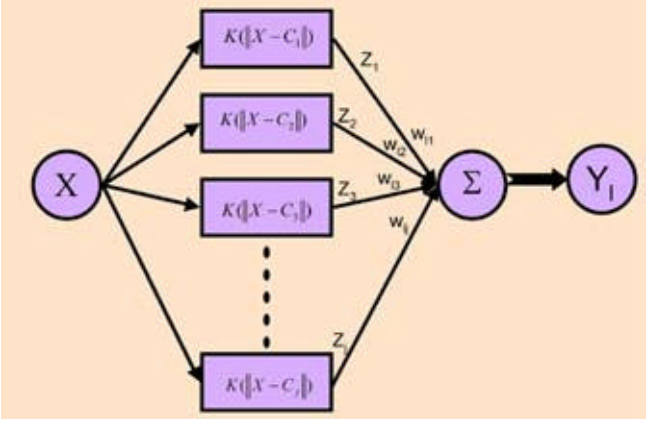

Figure 2. Radial basis function neural network.

where K is a strictly positive radially symmetric function (kernel) with a unique maximum at its 'centre' m_j and which drops off rapidly to zero away from the centre. The parameter s_j is the width of the receptive field in the input space from unit j. This implies that Z_j has an appreciable value only when the distance $\| X - m_j \|$ is smaller than the width s_j. Given an input vector X, the output of the RBF network is the L-dimensional activity vector Y, whose lth component ($l = 1, 2 \ldots L$) is given by,

$$Y_l(X) = \sum_{j=1}^{J} w_{lj} Z_j(X) . \tag{2}$$

For $l = 1$, mapping of eq. (1) is similar to a polynomial threshold gate. However, in the RBF network, a choice is made to use radially symmetric kernels as 'hidden units'.

RBF networks are best suited for approximating continuous or piecewise continuous real-valued mapping $f: R^n \to R^L$, where n is sufficiently small. These approximation problems include classification problems as a special case. From eqs (1) and (2), the RBF network can be viewed as approximating a desired function $f(X)$ by superposition of non-orthogonal, bell-shaped basis functions. The degree of accuracy of these RBF networks can be controlled by three parameters: the number of basis functions used, their location and their width[10–13].

In the present work we have assumed a Gaussian basis function for the hidden units given as Z_j for $j = 1, 2, \ldots J$, where

$$Z_j = \exp\left(-\frac{\| X - m_j \|^2}{2 s_j^2} \right), \tag{3}$$

and m_j and s_j are mean and the standard deviation respectively, of the jth unit receptive field and the norm is the Euclidean.

Training of RBF neural networks

A training set is an m labelled pair $\{X_i, d_i\}$ that represents associations of a given mapping or samples of a continuous multivariate function. The sum of squared error criterion function can be considered as an error function E to be minimized over the given training set. That is, to develop a training method that minimizes E by adaptively updating the free parameters of the RBF network. These parameters are the receptive field centres m_j of the hidden layer Gaussian units, the receptive field widths s_j, and the output layer weights (w_{ij}). Because of the differentiable nature of the RBF network transfer characteristics, one of the training methods considered here was a fully supervized gradient-descent method over E[7,9]. In particular, m_j, s_j and w_{ij} are updated as follows:

$$\Delta m_j = -r_m \nabla_{m_j} E , \tag{4}$$

$$\Delta s_j = -r_s \frac{\partial E}{\partial s_j} , \tag{5}$$

$$\Delta w_{ij} = -r_w \frac{\partial E}{\partial w_{lj}} , \tag{6}$$

where r_m, r_s, and r_w are small positive constants. This method is capable of matching or exceeding the performance of neural networks with back-propagation algorithm, but gives training comparable with those of sigmoidal type of FFNN[14].

The training of the RBF network is radically different from the classical training of standard FFNNs. In this case, there is no changing of weights with the use of the gradient method aimed at function minimization. In RBF networks with the chosen type of radial basis function, training resolves itself into selecting the centres and dimensions of the functions and calculating the weights of the output neuron. The centre, distance scale and precise shape of the radial function are parameters of the model, all fixed if it is linear. Selection of the centres can be understood as defining the optimal number of basis functions and choosing the elements of the training set used in the solution. It was done according to the method of forward selection[15]. Heuristic operation on a given defined training set starts from an empty subset of the basis functions. Then the empty subset is filled with succeeding basis functions with their centres marked by the location of elements of the training set; which generally decreases the sum-squared error or the cost function. In this way, a model of the network constructed each time is being completed by the best element. Construction of the network is continued till the criterion demonstrating the quality of the model is fulfilled. The most commonly used method for estimating generalization error is the cross-validation error.

Formulation of network models for diabetes data

Data collected from 1200 individuals (600 diabetic, 600 non-diabetic) attending a private hospital during the period 1996–98 were used in this work for empirical comparison of the network models. The WHO criteria for classifying a patient as diabetic namely fasting plasma glucose (FPG) greater than 126 mg/dl or 2 h post glucose value greater than 200 mg/dl was used in selection of diabetic patients[16]. The risk factors considered for analysis are age, gender, family history of diabetes, body mass index (BMI), total cholesterol level (TC), triglycerides (TG), low density lipids (LDL) and high-density lipids (HDL). A dataset of 600 individuals (400 diabetics and 200 non-diabetics) from another specialty hospital during the same period was used to validate the model externally.

The RBF neural network architecture considered for this application was a single hidden layer with Gaussian RBF. The basis function f is a real function of the distance (radius) r from the origin, and the centre is c. The most common choice of f includes thin-plate spline, Gaussian and multiquadric. Gaussian-type RBF was chosen here due to its similarity with the Euclidean distance and also since it gives better smoothing and interpolation properties[17]. The choice of nonlinear function is not usually a major factor in network performance, unless there is an inherent special symmetry in the problem.

Training of the RBF neural network involved two critical processes. First, the centres of each of the J Gaussian basis functions were fixed to represent the density function of the input space using a dynamic 'k means clustering algorithm'. This was accomplished by first initializing the set of Gaussian centres m_j to random values. Then, for any arbitrary input vector $X^{(t)}$ in the training set, the closest Gaussian centre, m_j, is modified as:

$$m_j^{\text{new}} = m_j^{\text{old}} + a\,(X^{(t)} - m_j^{\text{old}}), \tag{7}$$

where a is a learning rate that decreases over time. This phase of RBF network training places the weights of the radial basis function units in only those regions of the input space where significant data are present. The parameter s_j is set for each Gaussian unit to equal the average distance to the two closest neighbouring Gaussian basis units. If m_1 and m_2 represent the two closest weight centres to Gaussian unit j, the intention was to size this parameter so that there were no gaps between basis functions and only minimal overlap between adjacent basis functions were allowed. After the Gaussian basis centres were fixed, the second step of the RBF network training process was to determine the weight vector W which would best approximate the limited sample data X, thus leading to a linear optimization problem that could be solved by ordinary least squares method. This avoids the problem of gradient descent methods and local minima characteristic of back propagation algorithm[18].

For MLP network architecture, a single hidden layer with sigmoid activation function, which is optimal for the dichotomous outcome, is chosen. A back propagation algorithm based on conjugate gradient optimization technique was used to model MLP for the above data[19–21].

A logistic regression model[22] was fitted using the same input vectors as in the neural networks and diabetic status as the binary dependent variable. The efficiency of the constructed models was evaluated by comparing the sensitivity, specificity and overall correct predictions for both datasets. Logistic regression was performed using logistic regression in SPSS package[23] and MLP and RBF were constructed using Neural Connections Software[24].

Results

Of the 1200 cases, a random sample of 600 cases (50%) was used as training, 300 (25%) for validation, 300 (25%) for testing. Training data were used to train the application; validation data were used to monitor the neural network performance during training and the test data were used to measure the performance of the trained application. Of the 1200 cases, two-third were males (62.4%) and 38.4% had family history of diabetes. Gender composition and family history of diabetes were similar in both the diabetic and non-diabetic groups. The mean of the covariates: TC, HDL, TG significantly differs between the groups ($P < 0.001$). The mean of other covariates like age, BMI and LDL are similar in both groups. The logistic regression fitted to the total cases ($n = 1200$) gave a sensitivity of 74.8%, specificity of 71.8% and overall correct prediction of 73.3%.

Of the 300 samples of test data, 110 (36.6%) were diabetic cases and the remaining 190 (63.4%) were non-diabetic cases. Gender composition and family history of diabetes were similar in both diabetic and non-diabetic groups. The mean of the covariates: TC, LDL, HDL, TG significantly differs between the groups ($P < 0.001$). The mean of other covariates like age and BMI is similar in both groups. Logistic regression was performed on the test set of 300 cases and it showed sensitivity of 75.5%, specificity of 72.6% and percentage correct prediction was 73.7%, giving almost similar results to that of total cases. The MLP architecture had five input variables, one hidden layer with four hidden nodes and one output node. Total number of weights present in the model was 29. The best MLP was obtained at lowest root mean square of 0.2126. Sensitivity of the MLP model was 92.1%, specificity was 91.1% and percentage correct prediction was 91.3%. RBF neural networks performed best at ten centres and maximum number of centres tried was 18. Root mean square error using the best centres was 0.3213. Sensitivity of the RBF neural network model was 97.3%, specificity was 96.8% and the percentage correct prediction was 97%. Execution time of RBF network is lesser than MLP and when compared

Table 1. Comparative predictions of three models

Database	Model	Sensitivity (%)	Specificity (%)	Correct prediction (%)
Test	LOGISTIC	75.5	72.6	73.7
	MLP (4)*	92.1	91.1	91.3
	RBFNN (10)**	97.3	96.8	97.0
External	LOGISTIC	77.8	75.5	77.0
	MLP (3)	94.5	94.0	94.3
	RBFNN (8)	98.5	97.0	98.0

*Number of hidden node in MLP, **Number of centres in RBFNN.

with logistic regression, neural networks take slightly higher time.

The external data of 600 cases (diabetic – 400 and non-diabetic – 200) were used to test the networks' learning ability of a given problem. Out of these, 38.7% of the external data were females and 39.1% of them had a family history of diabetes. The gender proportion and family history proportion were similar in both the diabetic and non-diabetic groups. The mean of the covariates: TC, LDL, HDL, TG significantly differs between the groups ($P < 0.0001$). The mean of other covariates like age and BMI are similar in both the groups. Logistic regression performed on the external data gave sensitivity of 77.8%, specificity of 75.5% and the overall correct prediction of 77.0%. The MLP architecture had five input variable, three hidden nodes and one output variable. Total number of weights present in the model was 22 and the best MLP was obtained at lowest root mean square of 0.1346. Sensitivity of the MLP model was 94.5%, specificity was 94.0% and percentage correct prediction was 94.3%. The RBF neural network performed best at eight centres and maximum number of centres tried was 13. Root mean square error using the best centres was 0.1125. Sensitivity of the RBF neural network model was 98.5%, specificity was 97.0% and percentage correct prediction was 98.0%. The comparative results of all the models are presented in Table 1. The results indicate that the RBF network has a better performance than other models.

Conclusion

The sensitivity and specificity of both neural network models had a better predictive power compared to logistic regression. Even when compared on an external dataset, the neural network models performed better than the logistic regression. When comparing, RBF and MLP network models, we find that the former outperforms the latter model both in test set and an external set. This study indicates the good predictive capabilities of RBF neural network. Also the time taken by RBF is less than that of MLP in our application. Though application of RBF network is limited in biomedicine, many comparative studies of MLP and statistical methods are illustrated using a wide range of databases[25–32]. The limitation of the RBF neural network is that it is more sensitive to dimensionality and has greater difficulties if the number of units is large.

Generally, neural network results presented are mostly based only on the same dataset and that there were no results presented based on the external/similar independent dataset[33]. Here an independent evaluation is done using external validation data and both the neural network models performed well, with the RBF model having better prediction. The predicting capabilities of RBF neural network had showed good results and more applications would bring out the efficiency of this model over other models. ANN may be particularly useful when the primary goal is classification and is important when interactions or complex nonlinearities exists in the dataset. Logistic regression remains the clear choice when the primary goal of model development is to look for possible causal relationships between independent and dependent variables, and one wishes to easily understand the effect of predictor variables on the outcome.

There have been ingenious modifications and restrictions to the neural network model to broaden its range of applications. The bottleneck networks for nonlinear principle components and networks with duplicated weights to mimic autoregressive models are recent examples. When classification is the goal, the neural network model will often deliver close to the best fit. The present work was motivated in this direction.

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