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CLINICAL/MEDICAL OUTCOME PREDICTION BY NEURAL NETWORKS WITH STATISTICAL ENHANCEMENT

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Abstract

Neural networks offer a powerful new approach to information processing through their ability to generalize from a specific training data set. The success of this approach has raised interesting new possibilities of incorporating statistical methodology in order to enhance their predictive ability. This paper reports on two complementary methods of prediction. one using neural networks and the other using traditional statistical methods. The two methods are compared on the basis of their prediction applied to standardized developmental infant outcome measures using preselected infant and maternal variables measured at birth. Three neural network algorithms were employed. In our study, no one network outperformed the other two consistently. The neural networks provided significantly better results than the regression model in terms of variation and prediction of extreme outcomes. Finally we demonstrated that selection of relevant input variables through statistical means can produce a reduced network structure with no loss in predictive ability.

Keywords

feed forward MLP; functional link net (FLN); flat net; regression

1. Introduction

Neural network computation [14] continues to gain popularity as an information processing tool and has been applied to several problems in medical decision-making that traditionally have been attacked using statistical methods [1,4,10,11,14,23-26]. When neural network methodology is compared to statistical approaches to solve these problems, it is seen to have both advantages and disadvantages. On the positive side, neural networks are "model free" in that no *a priori* mathematical model must be assumed. Thus, expert knowledge about the process being modeled is not needed. Neural networks are also self-training and amenable to incremental training after being put into use. On the negative side, neural networks operate as "black boxes" in that they fail to elucidate any "deep" knowledge about the process being modeled. Further, since neural networks learn by example, training data must be available for use by the learning process.

We report on our experience in combining both statistical and neural network techniques in constructing predictive models in the context of a pediatric psychological study. In particular, we compare the predictive modeling capabilities of a linear regression model, three different neural network models, and a neural network model with statistical enhancement. The objective of this study was to identify ways in which statistical techniques can be incorporated into neural processing, thereby taking advantage of the strengths of each.

1.1. Neural Network Architectures

Among the many different neural network architectures that have been proposed, the most commonly used neural network structure for supervised learning is the multi-layer perceptron (MLP) [8,14]. An MLP is a network of simple processing nodes ("neurons") arranged into an input layer, zero or more hidden layers, and an output layer. The layers are fully interconnected in that the output from each node of one layer is linked to the inputs of all of the nodes of the next layer. A second commonly-used neural network architecture is the flat net [14]. The flat net is a simplified version of the MLP in which there is no hidden layer. A third neural network architecture in use is the functional-link net (FLN) [14-16]. The FLN is a recent modification of the flat net in which functional enhancements of the original inputs are used as additional inputs to the network. These functional enhancements typically take the form of sinusoidal functions, power series, or random vectors. The enhancements provide the nonlinear dynamics that the additional layers in an MLP provide, but at a significantly lower algorithmic overhead. The three types of net work models are shown in Figure [1].

1.2. Statistical Techniques

Several regression methodologies are available for statistical predictive modeling. Multiple logistic regression [9], discriminant analysis [13] and classification and regression trees [2]

have been used for binary outcomes. For continuous outcomes, multiple linear regression, nonparametric regression, and generalized additive models [7] have been employed. The choice of any of these models is dependent on the dimensionality of the input variables. In low dimensional settings, piecewise polynomial fitting procedures based on splines [22] and locally weighted straight-line smoothers [3] are very popular non-parametric procedures. However, due to problems with surface smoothers in higher dimensional settings, several multivariate nonparametric regression techniques have been devised. Both recursive-partitioning regression [5] and projection-pursuit regression [12] methodologies attempt to approximate general functions in higher dimensions by adaptive computation. Friedman [6] presented the multivariate adaptive regression splines as a tool for flexible modeling of high dimensional data. Statistical pattern recognition based on Bayes' decision rules has also been used. Here, classification techniques like discriminant analysis and nearest-neighbor methods are employed [17].

1.3. Objectives

Our overall goal in this work as well as in previous efforts and in ongoing parallel efforts is to construct a high quality predictive model in the context of an ongoing study of the medical, social, and developmental correlates of chronic lung disease during the ftrst three years of life [18-21]. Specifically, we want to predict developmental outcome at twelve months of age from data gathered at and immediately following birth. In this particular investigation, our goal was to determine the comparative advantages and disadvantages of several predictive models in this context, including models that combine statistical and neural network methodologies.

2. Methods

2.1. Data Collection

Data were obtained from an ongoing five-year prospective investigation of the medical, social, and developmental correlates of chronic lung disease during the first three years of life [18-21]. Twenty-eight variables capturing demographic factors and neonatal medical history believed to affect infant development during early childhood and two variables measuring developmental outcome at twelve months of age were selected for 331 study subjects. The outcome variables, chosen to be measurements of infant development, were the 12-month Bayley Mental Development Index (MDI) and the 12-month Bayley Psychomotor Development Index. (POI). The twenty-eight input variables are listed in Table [1].

Only subjects with complete data for all of the 30 selected variables were included in the final data set. This data set was randomly divided three times into a 200-record set for training and a 131 -record set for evaluation. This allowed for the performance of three independent trials for the fit of each predictive model that we investigated. The same data sets were used for construction of both statistical and neural network models. The neural network programmer and biostatistician were blinded to each other's efforts at this point in our work.

2.2. Baseline Statistical Model

For the statistical regression models, we used fourteen explanatory variables believed to play a role in early infant development to help predict the developmental outcome variables. Several approaches to construction of a statistical model for this data were investigated, including non-linear regression and logistic regression. We settled on a multiple regression model and did not pursue other candidate models further. The fourteen variables this linear regression model are those listed in Table [2].

2.3. Baseline Neural Network Models

For each of the three neural network architectures under consideration, a network was trained using the 28 input variables and two output variables. In the case of the MLP, a hidden layer of fifteen nodes was used. In the case of the FLN, fifteen enhanced features of random vector type were used to supplement the 28 original features. In all cases, each neuron's activation function was sigmoidal with the momentum set to 0.001 and the learning parameter set to 0.005. Each network was trained for 200 iterations. We used neural network simulation software developed in-house by one of the authors (S.M. Hosseini-Nezhad).

2.4. Neural Network Models with Statistical Preprocessing

Beginning with the fourteen variables used in the linear regression described earlier, a stepwise linear regression was fit to the data. A variable was considered significant for entry into the stepwise model if the p-value associated with that variable was less than 0.4, and it was allowed to leave the model if the p-value was over 0.4.

The variables identified in the stepwise models were deemed to be more relevant to prediction of the outcomes than the variables omitted from the models. We used this reduced subset of "relevant" variables in the training of new neural network models of the same three architectures as described earlier. Once again, each network was trained for 200 iterations.

2.5. Comparison of Models

In all, we constructed seven predictive models: three baseline neural network models, one baseline regression model, and three statistically enhanced neural network models. We compared these models on the bases of both goodness of fit to training data and the ability to predict outcomes from previously unseen input data.

3. Results

All of the models fit well to the data used in their construction. The mean-squared error (MSE) was computed by averaging the squares of the differences between actual outcome and predicted outcome for all inputs in the training data set. Among the neural network models, the flat net fit slightly better for both MDI and PDI prediction on the basis of a comparison of mean square error at 200 iterations. Among the three neural network models, the flat net required the least training time and the MLP the greatest time to achieve an acceptable training error. The flat net model for predicting MDI achieved a training error of 0.01 within only 50 iterations while neither of the other networks had achieved that training error by the 200 iteration maximum. The flat net model for predicting POI achieved a

training error of 0.0125 within only five iterations while the FLN required ten and the MLP over 50 iterations to achieve that training error. Figures [2] and [3] graphically display the results of the training experiments.

3.1. Prediction Error

Prediction error for each of the various models was determined by computing a percent error using the target outcome and the predicted outcome within each of the trial sets. Comparisons of models were made by using pairwise t-test. In order to reduce the effects of sampling, we performed this test in each of three trials in which 200 data records of the 331 were used for training and the remaining records used for testing. For each trial and for each of PDI and MDI prediction data records missing any values required for the trial were eliminated, resulting in slightly different data set size among the six experiments.

Among the baseline neural network models, the MLP generally provided the lowest prediction error and the flat net the highest (Table [3]). The flat net performed at least as well as the other network models in two of the three trial sets for PDI. The MLP outperformed the other network models in the other PDT trial. In the MDI trials, the MLP was better for two of the trial data sets, and there was no significant difference in performance in the other trial.

The stepwise multiple linear regression model identified different sets of significant variables in each of the tree trials for each of PDI and MDI outcomes (Table [2]). Using these sets of regression-selected variables, "statistically" enhanced flat net models were constructed. Although there was no significant difference in prediction error between the multiple linear regression model and the statistically enhanced flat net model, the tlat net produced significantly lower variance predictions ($p < 0.0001$) in all three MDI trials and two of the three PDI trials ($p < 0.05$) (Table [4]). The flat net also performed better for the prediction of extreme outcomes.

When we compared the prediction performance of the baseline (28 variable) flat net model and the statistically enhanced flat net model, the statistically enhanced flat net model performed significantly better than the baseline flat net model for two of the three MDI trials ($p < 0.002$) with no significant difference in performance in the other trial. There was no significant difference in performance in any of the three PDI trials. Again, the statistically enhanced flat net model generally produced lower variance predictions than the baseline flat net model. See Table [5].

3.2 Importance of Predictor Variables

There was substantial agreement on included and excluded variables among the three stepwise multiple linear regression models (Table [2]). However, attempts to relate the contribution of a variable to the predictive ability of a neural network model via the magnitude of its associated link weights were inconclusive. Although a precise interpretation of the relevance of link weight magnitudes in neural networks has yet to be given, it seems reasonable that link weights of relatively small magnitudes (approaching zero) in a flat net architecture imply that the connecting input has very little bearing on the process outcome. Our results neither support nor reject this conclusion.

4. Discussion

The flat neural network model performed well as compared to the regression model (Table [4]). In addition to less variation in prediction error, the flat net also displayed robust learning in the presence of extraneous inputs. This characteristic is advantageous when there is not much knowledge about the influential factors on a process outcome.

Perhaps the most interesting finding in our work was the consistency with which both the statistical modeling approach and the neural network modeling approach rejected the introduction of nonlinear elements in this particular setting. The flat network with no enhancements generally performed as well as both the FLN and the MLP. This might be considered unexpected because the flat network is a special case of both the FLN and the MLP in which the nonlinear elements, enhanced inputs and hidden layers, respectively, are removed. The lack of improvement of performance that results from the inclusion of nonlinear model elements strongly suggests that there is a simple linear relationship between the input data and output data of the test data sets.

The results of the comparison of the baseline flat network model and the statistically enhanced flat net model were inconsistent in that in half of the trials the enhanced network was superior and in the other half there was no significant difference (Table [5]). Although the baseline flat network fits the data slightly better in training (Figures [4] and [5]) , training of the enhanced flat net required 50% less computational overhead due to of the fewer number of variables involved. Equally importantly, the enhanced flat net requires less neural computation in post-training work. In conventional neural computation, relevant inputs are selected by trial and error through a process of training a network and then analyzing the results to determine which inputs can be eliminated. This process is tedious and limited because redundancies among inputs cannot be isolated by this technique. As we have shown, regression can be used to select relevant inputs in a less tedious way .

Examination of the relative magnitudes of the link weights in the trained networks does not reveal a strong consistency in selection of the same variables as significant to the predicted outcome. The results of the linear regression model in this regard are more consistent. This is disappointing because it casts doubt on the possibility that direct analysis of link weights could supplant regression as a method for selecting relevant input variables.

With the advent of improved medical care for very low birth weight infants and those with BPD, more such infants are surviving and it is anticipated that most will probably enter childhood and early adulthood with significant medical and developmental problems. Because BPD is a relatively new disease, the long term outcome remains unknown. Thus, any technology that can help accurately predict the clinical outcome for such infants will improve overall clinical management. As we progress with our study we hope to continue to combine the strengths of statistical and neural network methods to predict second and third year outcomes of these children using demographic, medical and historical behavioral variables.

Acknowledgements

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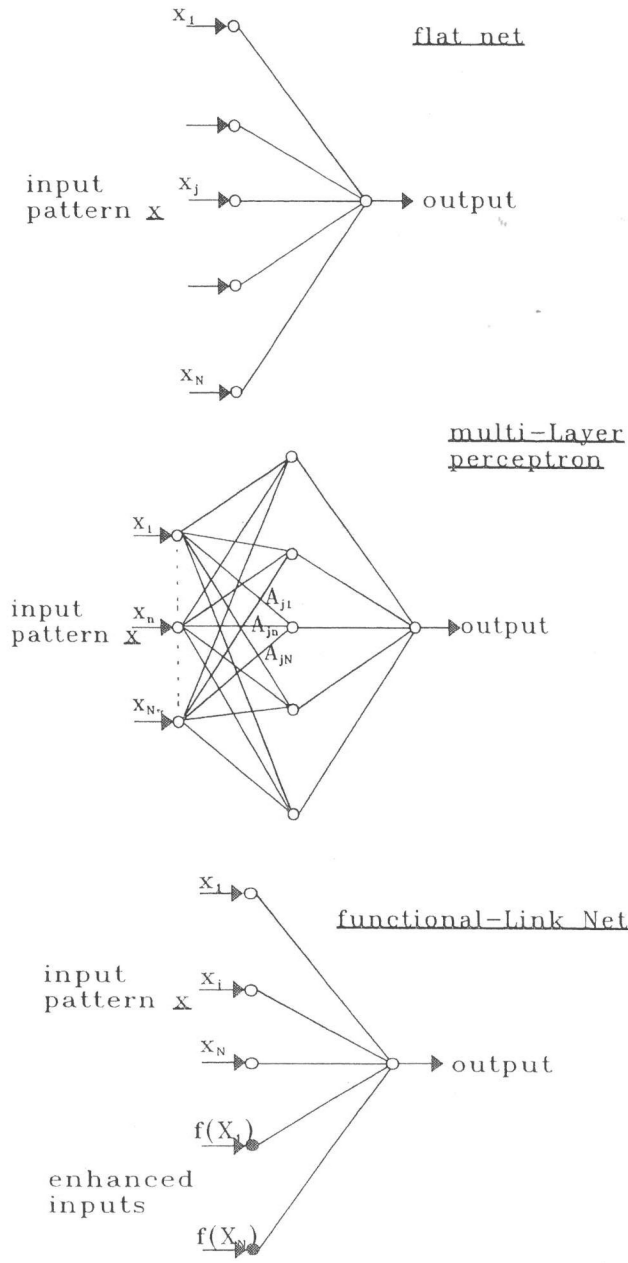
Figure I.
Three types of Neural Network Models: flat net, feed forward MLP and functional-link net.
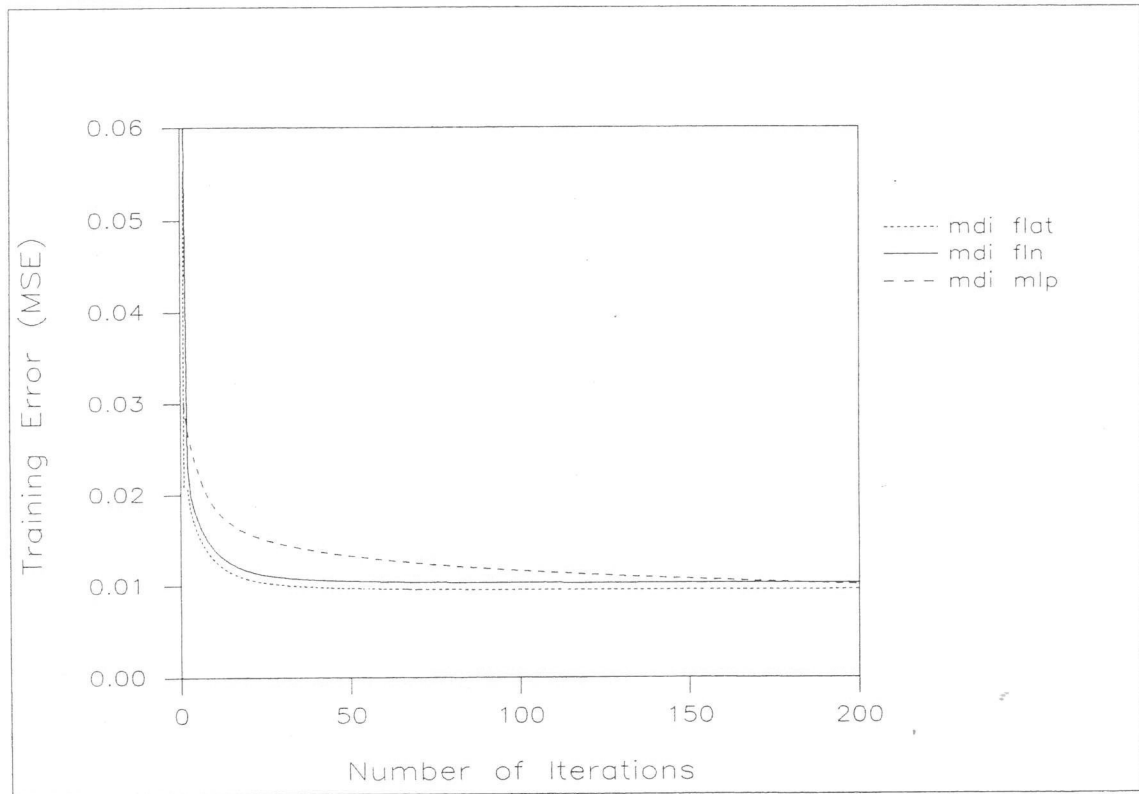
Figure 2.
A comparison of MDI training error (MSE) and the number of iterations for flat net (mdi flat), functional-link net (mdi fln) and feed forward MLP (mdi mlp) .
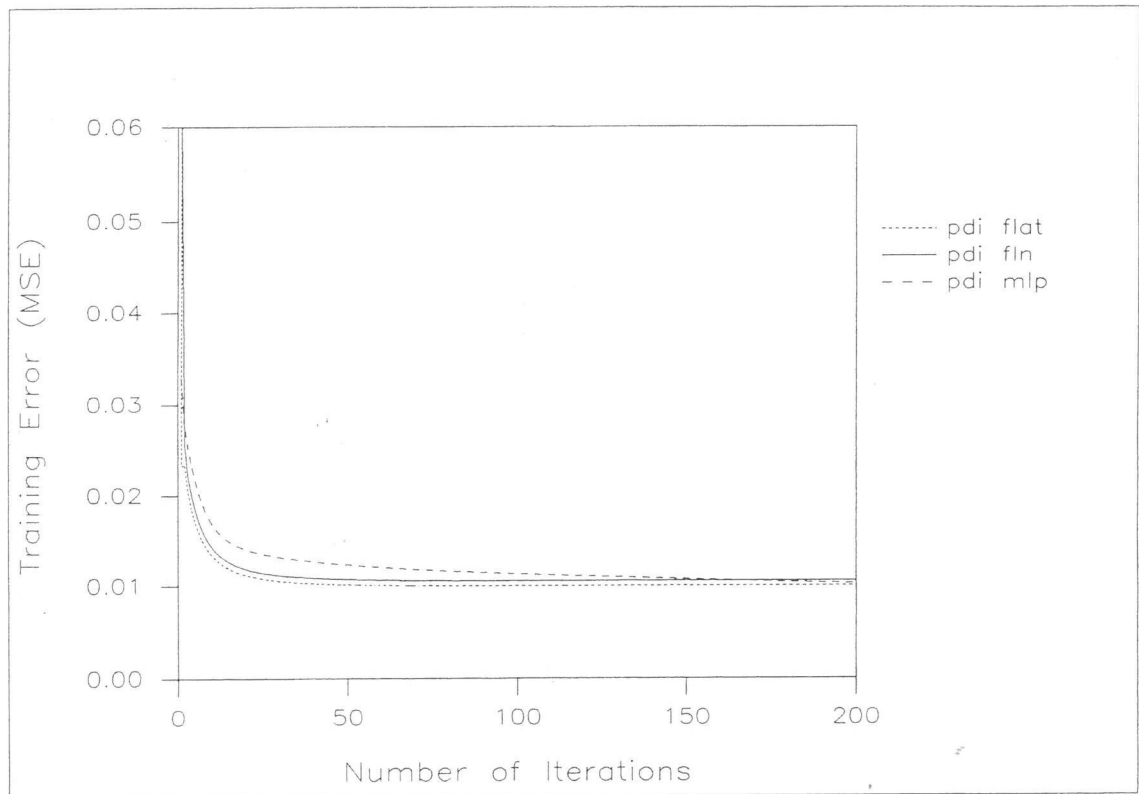
Figure 3.
A comparison of PDI training error (MSE) and the number of iterations for flat net (pdi flat), functional-link net (pdi fln) and feed forward MLP (pdi mlp).

Figure 4.
A comparison of MDI training error (MSE) and the number of iterations for flat net with stepwise regression selected variables (mdi sr) and all 28 variables (mdi 28).

Figure 5.
A comparison of PDI training error (MSE) and the number of iterations for flat net with stepwise regression selected variables (pdi sr) and all 28 variables (pdi 28).
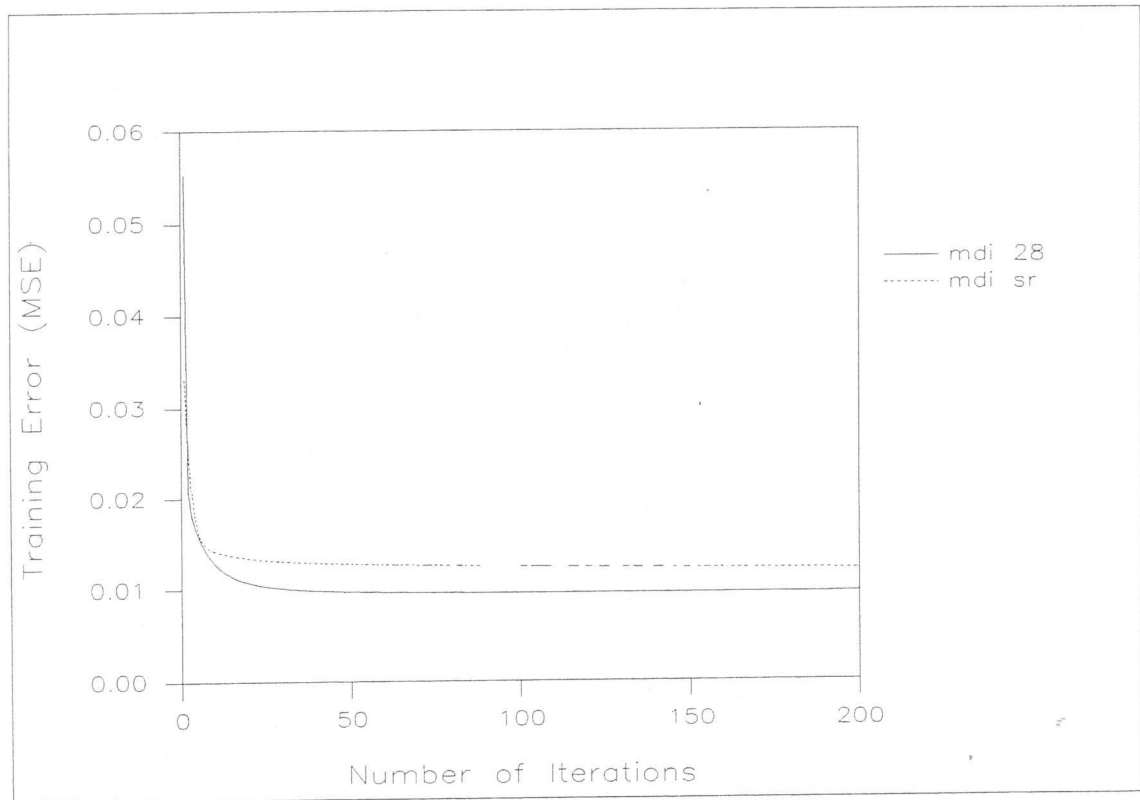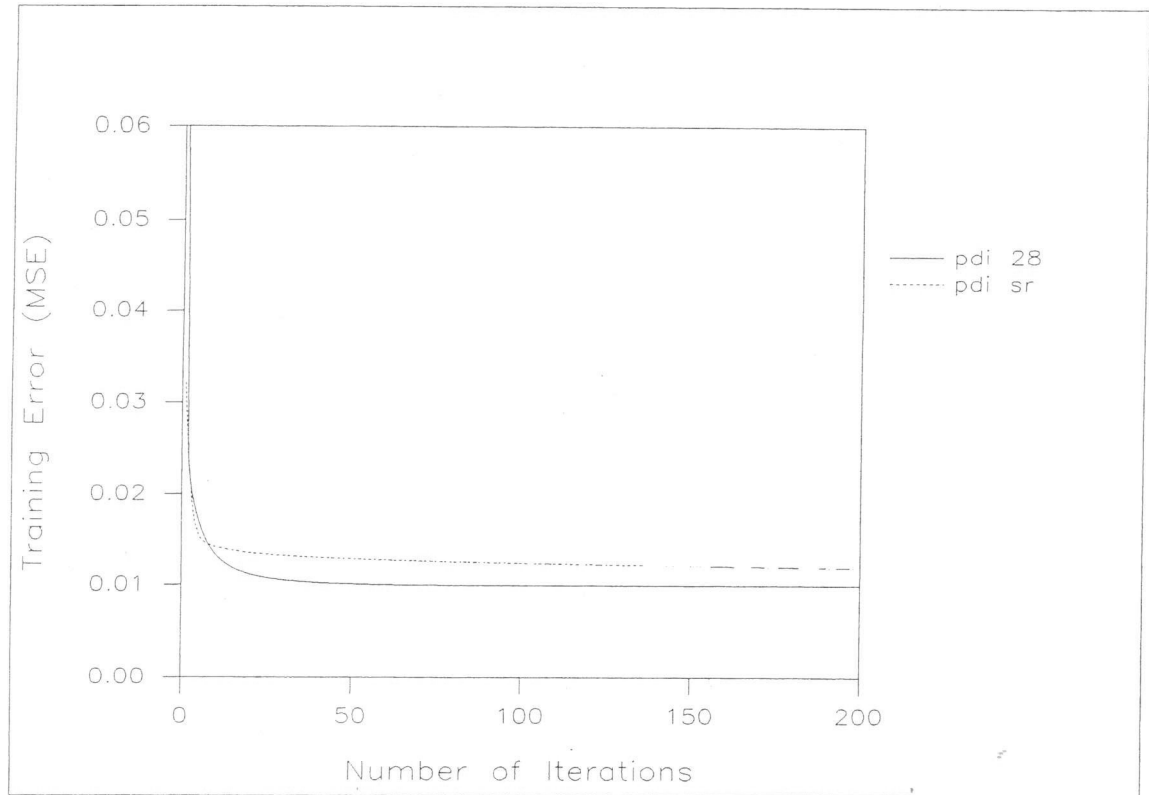
Table 1

Study Variables (N=272 to 331)

Variable Name	N	Mean(SD)	Note
Bayley (Outcome Variables)			
Mental Development Index 12 month (MDI)	272	104(23)	continuous
Psychomotor Development 12 month (PDI)	272	96(21)	continuous
Medical Risk (Input Variables)			
Total Days on Supplemental Oxygen [*]	303	29.2(44.1)	continuous
Intra-Ventricular Hemorrhaging (IVH)	303	0.44(0.94)	continuous
Intra-Ventricular hemorrhaging (IVH) [*]	303	0.23(0.42)	0/1
Neurological Malformation (NEURAL)	303	0.003(0.057)	0/1
Seizures	303	0.023(0.150)	0/1
Echodense Lesion	303	0.116(0.320)	0/1
Cystic Periventricular Leukomalacia	303	0.050(0.217)	0/1
Porencephaly on follow-up Sonogram	303	0.026(0.161)	0/1
Post-Hemorrhaging	303	0.056(0.231)	0/1
Ventriculo Peritoneal Shunt	303	0.017(0.128)	0/1
Meninges (MENING)	303	0.007(0.081)	0/1
Sum of IVH to MENING (MED_ACUM)	303	0.528(1.088)	continuous
Sum of NEURAL to MENING (MED_ACUM2) [*]	303	0.297(0.816)	continuous
MED_ACUM >0	303	0.281(0.450)	0/1
MED_ACUM2 >0	303	0.182(0.386)	0/1
Social/Demographic (Input Variables)			
Maternal Cocaine Use [*]	331	0.13(0.34)	0/1
Multiple Birth [*]	331	0.24(0.43)	0/1
Bronchopulmonary Dysplasia [*]	331	0.38(0.49)	0/1
Very Low Birthweight without BPD [*]	331	0.24(0.43)	0/1
Very Low Birthweight with or without BPD	331	0.62(0.49)	0/1
Healthy Term Control	331	0.38(0.49)	0/1
Gestational Age in weeks [*]	331	32.7(5.9)	continuous
Social Economic Status [*]	321	3.67(1.06)	continuous
White Race [*]	331	0.46(0.5)	0/1
Birthweight [*]	330	1950(1192)	continuous
Primary Caregiver is Biological Mother [*]	297	0.96(0.19)	0/1
Mother's Age at Birth [*]	318	27.7(5.8)	continuous
Mother's Education [*]	318	13.2(2.3)	continuous

0/1: 0=NO, l=YES

[*] = regression variables

Table 2

Stepwise Regression; Predictive Model Variables

Variable Name	MDI (set1)	MDI (set2)	MDI (set3)	PDI (set 1)	PDI (set 2)	PDI (set 3)
Total Days on Supplemental Oxygen	x	x	x	x	x	x
Intra-Ventricular hemorrhaging		x	x		x	x
Sum of NEURAL to MENING	x	x	x	x	x	x
Maternal Cocaine		x	x		x	x
Multiple Birth	x	x	x	x	x	x
Bronchopulmonary Dysplasia			x	x	x	
Very Low Birthweight without BPD	x					x
Gestational Age in weeks						x
Social Economic Status	x	x	x		x	
Race	x	x	x			
Birthweight	x					
Primary Caregiver is Biological Mother		x		x	x	x
Mother's Age at Birth						x
Mother's Education	x	x	x	x	x	
Coefficient of Determination (R²)	0.34	0.34	0.33	0.36	0.38	0.36
Total Degrees of Freedom (DF)	138	132	139	139	133	139

x = Stepwise Regression Selected Variables

Table 3

PERCENT PREDICTION ERROR: Flat Net, Feed Forward MLP and Functional-link Net (FLN) (28 input variables)

		N	Flat Net				FLN				Feed Forward MLP			
			Mean[1]	SD	Min	Max	Mean[1]	SD	Min	Max	Mean[1]	SD	Min	Max
MDI	Set1	82	−1.8	39.3	−268.6	52.5	−2.3	43.6	−262	53.8	3.9	20.4	−41.2	72.5
	Set2	88	6.6	14.7	−26.0	54.1	−4.0	17.1	−45.9	49.3	−.7	16.0	−48.8	49.8
	Set3	81	5.0	18.1	−34.8	66.7	6.3	16.8	−28.1	59.1	−1.3	20.2	−78.8	50.7
	MEAN		3.3	24.0			0.0	25.8			.63	18.87		
PDI	Set1	82	−1.6	24.3	−131.0	36.7	−9.1	36.1	−193.1	35.8	1.4	19.9	−55.3	70.0
	Set2	88	5.4	15.2	−26.6	37.8	1.9	16.4	−29.2	35.9	1.7	15.9	−41.2	32.2
	Set3	81	−1.2	21.9	−67.5	65.1	4.0	20.3	−63.7	50.6	−3.4	22.5	−105.2	42.4
	MEAN		0.9	20.5			−1.1	24.3			−0.1	19.4		

[1] Mean % error

Table 4

PERCENT PREDICTION ERROR: Stepwise Regression and Flat Net (using the Stepwise Regression Selected Variables)

		Stepwise Regression						Flat Net					
		Mean[1]	SD	Mean[2]	SD	Min	Max	Mean[1]	SD	Mean[2]	SD	Min	Max
MDI	Set1	−12.6	50.4	23.4	46.3	−338.8	28.9	0.3	19.5	14.8	12.6	−48.8	65.7
	Set2	−4.7	22.4	15.8	16.5	−126.6	29.5	0.6	18.0	14.1	11.1	−3.9	52.6
	Set3	−8.2	39.9	20.2	35.4	−283.5	32.2	0.9	20.9	15.5	13.8	−55.8	70.6
	MEAN	−8.5	37.6	19.8	32.7			0.6	19.5	14.8	12.5		
PDI	Set1	−8.4	46.5	22.0	41.8	−343.6	37.0	−2.9	21.7	16.3	14.5	−58.9	73.6
	Set2	−5.3	20.1	15.7	13.4	−74.9	34.7	1.1	19.0	15.1	11.5	−57.1	39.1
	Set3	−3.6	31.7	19.2	25.4	−175.5	37.9	−2.2	21.4	16.0	14.3	−49.5	60.8
	MEAN	−5.8	32.8	15.7	41.8			−1.3	20.7	15.8	14.5		

[1] Mean % error

[2] Mean % absolute error

Table 5

PERCENT PREDICTION ERROR: Flat Net with All 28 Variables and with Stepwise Regression Selected Variables

		Stepwise Regression Selected Variables						All Variables (28)					
		Mean[1]	SD	Mean[2]	SD	Min	Max	Mean[1]	SD	Mean[2]	SD	Min	Max
MDI	Set1	0.3	19.5	14.8	12.6	−48.8	65.7	−1.8	39.3	20.5	33.6	−268.6	52.5
	Set2	0.6	18.0	14.1	11.1	−43.9	52.6	6.6	14.7	12.6	9.9	−26.0	54.1
	Set3	0.9	20.9	15.5	13.8	−55.8	70.6	5.0	18.1	13.6	12.8	−34.8	66.7
	MEAN	0.6	19.5	14.8	12.5			3.3	24.0	15.6	18.8		
PDI	Set1	−2.9	21.7	16.3	14.5	−58.9	73.6	−1.6	24.3	16.6	17.8	−131.0	36.7
	Set2	1.1	19.0	15.1	11.5	−57.1	39.1	5.4	15.2	13.1	9.2	−26.6	37.8
	Set3	−2.2	21.4	16.0	14.3	−49.5	60.8	−1.2	21.9	15.8	15.0	−67.5	65.1
	MEAN	−1.3	20.7	15.8	13.4			0.9	20.5	15.2	14.0		

[1] Mean % error

[2] Mean % absolute error