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Selecting Neural Network Architectures via the Prediction Risk: Application to Corporate Bond Rating Prediction

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Abstract

The notion of generalization can be defined precisely as the prediction risk, *the expected performance of an estimator on new observations. In this paper, we propose the prediction risk as a measure of the generalization ability of multi–layer perceptron networks and use it to select the optimal network architecture. The prediction risk must be estimated from the available data; here we approximate the prediction risk by* v–fold cross–validation *and asymtotic estimates of* generalized cross–validation *or Akaike's* final prediction error. *We apply the technique to the problem of predicting corporate bond ratings. This problem is very attractive as a case study, since it is characterized by the limited availability of the data and by the lack of complete* a priori *information that could be used to impose a structure to the network architecture.*

1 Generalization and Prediction Risk

The notion of generalization can be defined precisely as the *prediction risk*, the expected performance of an estimator on new observations.

Consider a set of observations $D = \{(\vec{x}_j, t_j); j = 1 \ldots N\}$ that are assumed to be generated as

$$t_j = \mu(x_j) + \epsilon_j \tag{1}$$

where $\mu(x)$ is an unknown function, the inputs x_j are drawn independently with an unknown stationary probability density function $p(x)$, the ϵ_j are independent random variables with zero mean ($\bar{\epsilon} = 0$) and variance σ_ϵ^2, and t_j are the observed target values.

The learning or regression problem is to find an estimate $\hat{\mu}_\lambda(x; D)$ of $\mu(x)$ given the data set D from a class of predictors or models $\mu_\lambda(x)$ indexed by λ.

In general, $\lambda \in \Lambda = (S, A, W)$, where $S \subset X$ denotes a chosen subset of the set of available input variables X, A is a selected architecture within a class of model architectures $\mathcal{A}$, and W are the adjustable parameters (weights) of architecture A.

The *prediction risk* $P(\lambda)$ is defined as the expected performance on future data:

$$P(\lambda) = \int dx\, p(x)[\mu(x) - \hat{\mu}(x)]^2 + \sigma_\epsilon^2 \; . \tag{2}$$

This is approximated by the expected performance on a finite test set:

$$P(\lambda) \approx E\{\frac{1}{N}\sum_{j=1}^{N}(t_j^* - \hat{\mu}_\lambda(x_j^*))^2\} \tag{3}$$

where (x_j^*, t_j^*) are new observations that were not used in constructing $\hat{\mu}_\lambda(x)$. In what follows, we shall use $P(\lambda)$ as a measure of the generalization ability of a model. See [4] and [6] for more detailed presentations.

Our strategy is to choose an architecture λ in the model space Λ which minimizes an estimate of the prediction risk $P(\lambda)$. In this paper, we use a systematic although not exhaustive search over the model space Λ of two layer perceptron models. This search varies the number of internal units, the set of input variables, and the set of non-zero weights of the perceptron architecture.

2 Estimates of Prediction Risk

Since we cannot directly calculate the prediction risk P_λ, we have to estimate it from the available data D. The standard method based on test–set validation is not advisable when the data set is small. In this paper we consider such a case; the prediction of corporate bond ratings from a database of only 196 firms.

Cross-validation (CV) is a sample re–use method for estimating prediction risk; it makes maximally efficient use of the available data. Other methods are the generalized cross–validation (GCV) and the final prediction error (FPE) criteria, which combine the *MSE* with a measure of the model complexity. Here, we shall use CV, GCV and FPE to estimate P_λ. These will be discussed in the next sections.

2.1 Cross Validation

Cross–Validation is a method that makes minimal assumptions on the statistics of the data. The idea of cross validation can be traced back to Mosteller and Tukey [7]. For reviews, see Stone [8, 9], Geisser [5] and Eubank [4].

Let $\hat{\mu}_{\lambda(j)}(x)$ be a predictor trained using all observations except (x_j, t_j) such that $\hat{\mu}_{\lambda(j)}(x)$ minimizes

$$MSE_j = \frac{1}{(N-1)} \sum_{k \neq j} \left(t_k - \hat{\mu}_{\lambda(j)}(x_k)\right)^2$$

Then, an estimator for the prediction risk $P(\lambda)$ is the *cross validation mean squared error*

$$CV(\lambda) = \frac{1}{N} \sum_{j=1}^{N} \left(t_j - \hat{\mu}_{\lambda(j)}(x_j)\right)^2 \tag{4}$$

This form of $CV(\lambda)$ is known as *leave–one–out* cross–validation.

However, $CV(\lambda)$ in (4) is expensive to compute for neural network models; it involves constructing N networks, each trained with $N-1$ patterns.

For the work described in this paper we therefore use a variation of the method, called *v-fold cross–validation*, that was introduced by Geisser [5] and Wahba *et al* [11]. Instead of leaving out only one observation for the computation of the sum in (4) we delete larger subsets of D.

Let the data D be divided into v randomly selected disjoint subsets P of roughly equal size: $\cup_{j=1}^{v} P_j = D$ and $\forall i \neq j,\ P_i \cap P_j = \emptyset$. Let N_j denote the number of observations in subset P_j. Let $\hat{\mu}_{\lambda(P_j)}(x)$ be an estimator trained on all data except for $(x,t) \in P_j$. Then, the cross-validation mean square error for subset j is defined as

$$CV_{P_j}(\lambda) = \frac{1}{N_j} \sum_{(x_k,t_k) \in P_j} \left(t_k - \hat{\mu}_{\lambda(P_j)}(x_k)\right)^2, \tag{5}$$

and

$$CV_P(\lambda) = \frac{1}{v} \sum_j CV_{P_j}(\lambda). \tag{6}$$

Typical choices for v are 5 and 10. Note that leave–one–out CV is obtained in the limit $v = N$. Note that CV_P is an estimate of the prediction risk that relies only on the available data.

2.2 Generalized Cross-Validation and Final Prediction Error

For linear models, two useful criteria for selecting a model architecture are *generalized cross–validation (GCV)* (Wahba [10]) and Akaike's *final prediction error (FPE)* ([1]). See [4] for a tutorial treatment. The forms of GCV and FPE are:

$$GCV(\lambda) = MSE(\lambda) \frac{1}{\left(1 - \frac{S(\lambda)}{N}\right)^2} \tag{7}$$

$$FPE(\lambda) = MSE(\lambda) \left(\frac{1 + \frac{S(\lambda)}{N}}{1 - \frac{S(\lambda)}{N}}\right), \tag{8}$$

where $S(\lambda)$ denotes the number of weights of model λ. Note that although they are slightly different for small sample sizes, they are asymptotically equivalent for large N:

$$\hat{P}(\lambda) \equiv MSE(\lambda)\left(1 + 2\frac{S(\lambda)}{N}\right) \approx GCV(\lambda) \approx FPE(\lambda) \tag{9}$$

We shall use this asymptotic estimate for the prediction risk in our analysis of the bond rating models.

It has been shown by Moody [6] that FPE and therefore $\hat{P}(\lambda)$ is an unbiased estimate of the prediction risk for the neural network models considered here provided that the noise ϵ_j in the observed targets t_j is independent and identically distributed and provided that weight decay is not used and that the resulting model is unbiased. FPE is a special case of Barron's PSE [2] and Moody's GPE [6]. Although FPE and $\hat{P}(\lambda)$ are unbiased only under the above assumptions, they are much cheaper to compute than CV_P since no retraining is required.

3 A Case Study: Prediction of Corporate Bond Ratings

A bond is a debt security which constitutes a promise by the issuing firm to pay a given rate of interest on the original issue price and to redeem the bond at face value at maturity. Bonds are rated according to the default risk of the issuing firm by independent rating agencies such as Standard & Poors (S&P) and

Representation of S&P Bond Ratings												
CCC	B-	B	...	BBB+	A-	A	A+	AA-	AA	AA+	AAA-	AAA
2	3	4	...	11	12	13	14	15	16	17	18	19
high default risk						....						low default risk

Table 1: Key to S&P bond ratings. We only used the range from 'AAA' or 'very low default risk' to 'CCC' meaning 'very high default risk'. (Note that AAA- is a not a standard category; its inclusion was suggested to us by a Wall Street analyst.) Bonds with rating BBB- or better are "investment grade" while "junk bonds" have ratings BB+ or below. For our output representation, we assigned an integer number to each rating as shown.

Moody's Investor Service. The firm is in default if it is not able make the promised interest payments.

S&P and Moody's determine the rating from various financial variables and possibly other information, but the exact set of variables is unknown. It is commonly believed that the rating is at least to some degree judged on the basis of subjective factors and on variables not directly related to a particular firm. In addition, the method used for assigning the rating based on the input variables is unknown.

The problem we are considering here is to predict the S&P rating of a bond based on fundamental financial information about the issuer which is publicly available. Since the rating agencies update their bond ratings infrequently, there is considerable value to being able to anticipate rating changes before they are announced. A predictive model which maps fundamental financial factors onto an estimated rating can accomplish this.

The input data for our model consists of 10 financial ratios reflecting the fundamental characteristics of the firms. The database was prepared for us by analysts at a major financial institution. Since we did not attempt to include all information in the input variables that could possibly be related to a firms bond rating (e.g. all fundamental or technical financial factors, or qualitative information such as quality of management), we can only attempt to approximate the S&P rating.

3.1 A Linear Bond Rating Predictor

For comparison with the neural network models, we computed a standard linear regression model. All input variables were used to predict the rating which is represented by a number in $[0, 1]$. The rating varies continuously from one category to the next higher or next lower one and this "smoothness" is captured in the single output representation and should make the task easier. To interpret the network response, the output was rescaled from $[0, 1]$ to $[2, 19]$ and rounded to the nearest integer; 19 corresponds to a rating of 'AAA' and 2 to 'CCC' and below (see Table 1). (Note: An alternative, but more expensive, output representation would use a separate output for each of the rating categories.) The input variables were normalized to the interval $[0, 1]$ since the original financial ratios differed widely in magnitude.

Table 2 summarizes the results obtained with the linear regression model.

Training Error, Linear Regression Model using all inputs			
Error	no. of firms	% of firms	cumulative
0	42	21.4	21.4
1	73	37.2	58.6
2	43	21.9	80.5
> 2	38	19.5	100.0
number of weights			11
standard deviation			1.665
mean absolute deviation			1.311
training error			1.930

Table 2: Results for the linear regression model using all input variables. The standard deviation and the mean absolute deviation are computed after rescaling the output of the network to [2,19] and rounding to the nearest integer (notches). The RMS training error is computed using the rescaled output of the network before rounding. The table also describes the predictive ability of the network by a histogram; the error column gives the number of rating categories the network was off from the correct target.

3.2 Beyond Linear Regression: Prediction by Two Layer Perceptrons

Learning networks, particularly multilayer perceptrons, have been found to be capable of solving many practical classification and regression problems. Among the many examples of real world applications are automobile control systems, speech synthesis, credit risk analysis, autonomous vehicle guidance and control, and handprinted zipcode recognition.

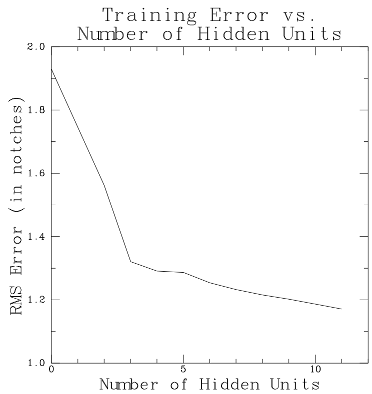


Figure 1: Training error versus number of hidden units H_λ.

The class of models we are considering as predictors are two-layer perceptron networks with I_λ input variables, H_λ internal units and a single output unit having the form

$$\hat{\mu}_\lambda(x) = f(\, v_0 + \sum_{\alpha=1}^{H_\lambda} v_\alpha \, g(w_{\alpha 0} + \sum_{\beta=1}^{I_\lambda} w_{\alpha\beta} \, x_\beta)) \; . \quad (10)$$

The hidden units have a sigmoidal transfer function

$$g(x) = \frac{1}{1+e^{-x}}$$

while the single outputs unit uses a piecewise linear function

$$f(x) = \begin{cases} 1 & x > 16 \\ x/32 + 0.5 & -16 < x < 16 \\ 0 & x < -16 \end{cases} .$$

3.3 Selecting the Number of Hidden Units

We initially trained fully connected networks with all 10 available inputs but with the number of hidden units H_λ varying from 2 to 11.

Figure 1 shows the training error for networks of increasing size as measured by H_λ; as expected it is decreasing as the number of hidden units increases.

Five–fold cross–validation and $\hat{P}(\lambda)$ were used to select the number of hidden units. We compute $CV_P(\lambda)$ according to equation (6); the data set was partitioned into $v = 5$ subsets. We also computed $\hat{P}(\lambda)$ according to equation (9). The results of the two methods are consistent in having a common minimum for $H_\lambda = 3$ internal units (see figure 2).

Table 3(A) shows the results for the network with $H_\lambda = 3$ trained on the entire data set. A more accurate description of the performance of the model is shown in table 3(B) were the predictive ability is calculated from the hold–out sets of the cross–validation procedure.

3.4 Pruning of Input Variables via Sensitivity Analysis

Next, we attempted to further reduce the number of weights of the network by eliminating some of the input variables. To test which inputs are most significant for determining the network output, we perform a sensitivity analysis. We define the "Sensitivity" averaged over all observations in the training data as:

$$S_i = \frac{1}{N} \sum_p \frac{\partial \hat{\mu}_p}{\partial x_{pi}} \; .$$

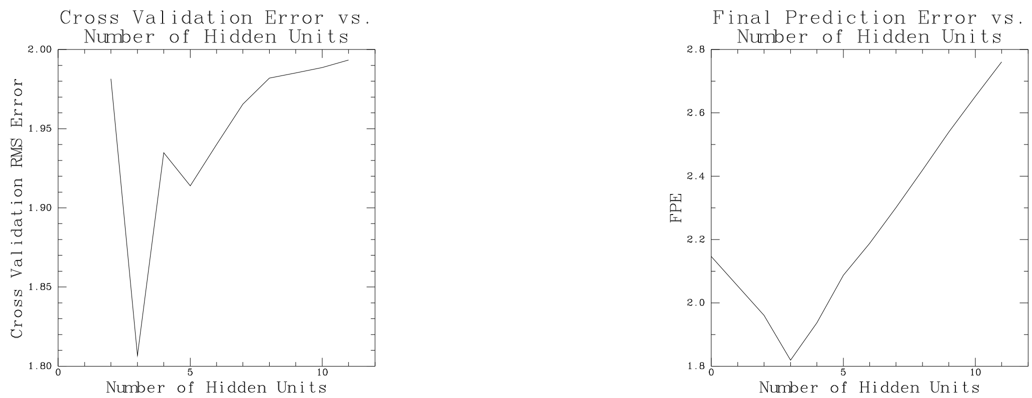
Again we use 5-fold cross–validation and $\hat{P}$ to estimate the prediction risk P_λ. We constructed a sequence of models by deleting an increasing number of input variables according to the ranking of $|S_j|$. For each model, CV_P and $\hat{P}$ was computed, figure 3 shows the results. A minimum was attained for the model with $I_\lambda = 8$ input variables (2 inputs were removed). This reduces the number of weights by $2H_\lambda = 6$.

Table 4 shows the performance of this network. The cross-validation error CV_P as well as the standard and mean absolute deviation have decreased and the predictive ability of the model has improved when compared to the network using all input variables (table 3).

3.5 Weight Pruning via "Optimal Brain Damage"

Optimal Brain Damage (OBD) was introduced by Le Cun *at al* [3] as a method to reduce the number of weights in a neural network to avoid overfitting. OBD is designed to select those weights in the network whose removal will have a small effect on the training error *MSE*. Assuming that the original network was too large, removing these weights and retraining the now smaller network should improve the generalization performance. The method approximates *MSE* at a minimum in weight space by a diagonal quadratic expansion. The saliency

$$s_i = \frac{1}{2} \frac{\partial^2 MSE}{\partial w_i^2} w_i^2 \quad (11)$$



(A) (B)

Figure 2: A: Cross validation error $CV_P(\lambda)$ versus number of hidden units. B: $\hat{P}(\lambda)$ versus number of hidden units.

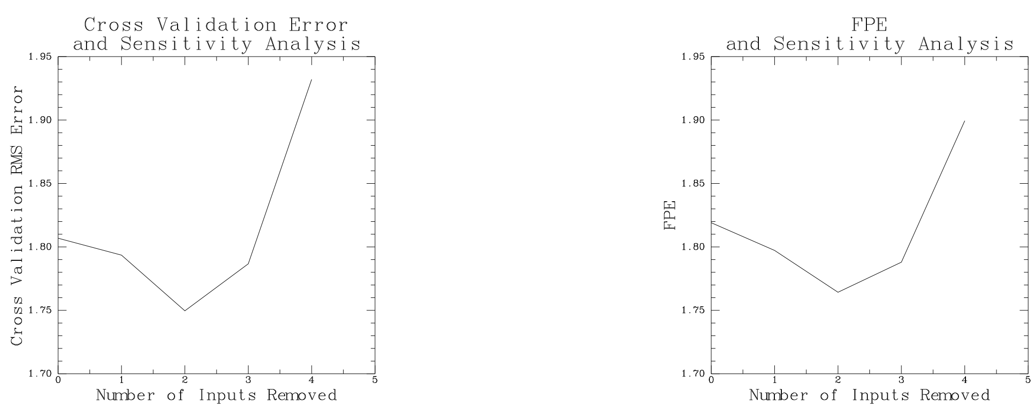
Training Error 3 Hidden Units			
Error	no. of firms	% of firms	cumulative
0	67	34.2	34.2
1	84	42.9	77.1
2	34	17.3	94.4
> 2	11	5.6	100.0
number of weights			37
standard deviation			1.206
mean absolute deviation			0.898
training error			1.320

(A)

Cross Validation Error 3 Hidden Units			
Error	no. of firms	% of firms	cumulative
0	54	28.6	28.6
1	77	38.8	67.3
2	35	17.3	84.7
> 2	30	15.3	100.0
number of weights			37
standard deviation			1.630
mean absolute deviation			1.148
cross validation error			1.807

(B)

Table 3: A: Results for the network with 3 hidden units (trained using the entire data set). See the caption for Table 2 for explanatory description. The network with 3 hidden units significantly outperformed the linear regression model described in Table 2. B: Cross Validation results for the network with 3 hidden units. In order to predict the rating for a firm, we choose among the networks trained for the cross-validation procedure the one that was not trained using the subsets the firm belongs to. Thus the results concerning the predictive ability of the model reflect the expected performance of the model trained on all the data (described in (A)) with new data in the cross–validation–sense.



(A) (B)

Figure 3: A: Cross validation error $CV_P(\lambda)$ for the sensitivity analysis. B: $\hat{P}(\lambda)$ for the sensitivity analysis.

Cross Validation Error 3 Hidden Units, 2 Inputs Removed			
Error	no. of firms	% of firms	cumulative
0	61	31.1	31.1
1	77	39.3	70.4
2	31	15.8	86.2
> 2	27	13.8	100.0
number of weights			31
standard deviation			1.605
mean absolute deviation			1.129
cross validation error			1.750

(A)

Cross Validation Error 3 Hidden Units, 9 Connections Removed			
Error	no. of firms	% of firms	cumulative
0	57	29.1	29.1
1	77	39.3	68.4
2	35	17.9	86.2
> 2	27	13.8	100.0
number of weights			28
standard deviation			1.539
mean absolute deviation			1.111
cross validation error			1.707

(B)

Table 4: A: Cross Validation results for the network with 3 hidden units with 2 inputs removed. B: Cross Validation results for the network with 3 hidden units with 9 connections removed.

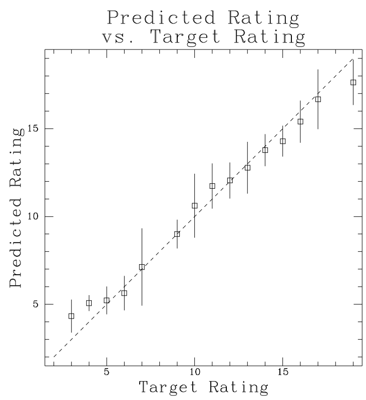


Figure 5: Predicted rating vs. target rating for the final model (trained on all data). For each rating category the "square" denotes the predicted rating averaged over all firms in that category, the vertical bars denote the standard deviation.

computed after training has stopped is a measure (in the diagonal approximation) for the change of *MSE* when weight w_i is removed from the network.

CV_P and $\hat{P}$ were computed to select the optimal model. We find that CV_P and $\hat{P}$ are minimized when 9 weights are deleted from the network using all input variables. However, some overlap exists when compared to the sensitivity analysis described above: 5 of the deleted weights would also have been removed by the sensitivity method. This result confirms the usefulness of the sensitivity analysis. Table 4 shows the results for this case.

Table 5 and Figure 5 show the overall performance of our model when the two techniques were combined. Note the improvement in estimated prediction performance (CV error) in table 5(B) relative to 3(B).

4 Discussion

Our example shows that (1) nonlinear network models can out–perform linear regression models (compare tables 2 and 5(A)), and (2) there is both a need and a benefit to developing structured neural networks. Structured networks are optimized with respect to the task at hand, even though it may not be possible to design them based on *a priori* knowledge.

Estimates of the prediction risk offer a sound basis for assessing the performance of the model on new data and can be used as a tool for architecture selection. Cross–validation, GCV and FPE provide computationally feasible means of estimating the prediction risk. These estimates of prediction risk provide principled criteria for selecting the number of internal units and performing sensitivity analysis and OBD. Any network modification should be followed by retraining and the modifications should be accepted only if the modified network performs better as measured by the prediction risk.

The model developed for rating bonds should not be interpreted as a complete production model, since a number of aspects of the problem were not represented by the available input variables. However, the problem is very attractive as a case study of the procedures proposed here, since it is characterized by the limited availability of the data and by the lack of complete *a priori* information that could be used to impose a structure to the network architecture.

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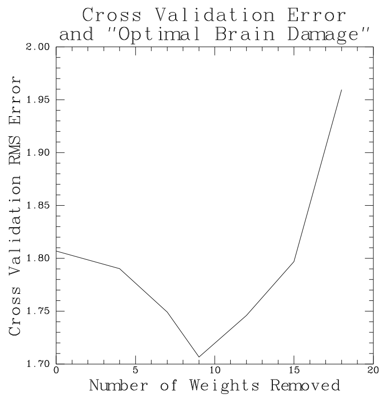
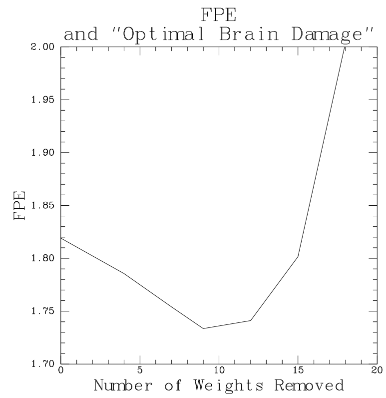


(A)



(B)

Figure 4: A: Cross validation error $CV_P(\lambda)$ for "Optimal Brain Damage". B: $\hat{P}(\lambda)$ for "Optimal Brain Damage".

Training Error, 3 Hidden Units 2 Inputs and 9 Connections Removed			
Error	no. of firms	% of firms	cumulative
0	69	35.2	35.2
1	81	41.3	76.5
2	32	16.3	92.8
> 2	14	7.2	100.0
number of weights			27
standard deviation			1.208
mean absolute deviation			0.882
training error			1.356

(A)

Cross Validation Error, 3 Hidden Units 2 Inputs and 9 Connections Removed			
Error	no. of firms	% of firms	cumulative
0	58	29.6	29.6
1	76	38.8	68.4
2	37	18.9	87.2
> 2	26	12.8	100.0
number of weights			27
standard deviation			1.546
mean absolute deviation			1.117
cross validation error			1.697

(B)

Table 5: Results for the network with 3 hidden units with both, sensitivity analysis and OBD applied. A: Training error results. B: Cross validation results. Note the improvement in CV error performance of relative to Table 3.

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