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# Fault Prediction Modeling for Software Quality Estimation: Comparing Commonly Used Techniques

TAGHI M. KHOSHGOFTAAR taghi@cse.fau.edu
*Florida Atlantic University, Boca Raton, Florida*

NAEEM SELIYA nseliya@cse.fau.edu
*Florida Atlantic University, Boca Raton, Florida*

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**Abstract.** High-assurance and complex mission-critical software systems are heavily dependent on reliability of their underlying software applications. An early software fault prediction is a proven technique in achieving high software reliability. Prediction models based on software metrics can predict number of faults in software modules. Timely predictions of such models can be used to direct cost-effective quality enhancement efforts to modules that are likely to have a high number of faults.

We evaluate the predictive performance of six commonly used fault prediction techniques: CART-LS (least squares), CART-LAD (least absolute deviation), S-PLUS, multiple linear regression, artificial neural networks, and case-based reasoning. The case study consists of software metrics collected over four releases of a very large telecommunications system. Performance metrics, average absolute and average relative errors, are utilized to gauge the accuracy of different prediction models. Models were built using both, original software metrics (RAW) and their principle components (PCA). Two-way ANOVA randomized-complete block design models with two blocking variables are designed with average absolute and average relative errors as response variables. System release and the model type (RAW or PCA) form the blocking variables and the prediction technique is treated as a factor. Using multiple-pairwise comparisons, the performance order of prediction models is determined. We observe that for both average absolute and average relative errors, the CART-LAD model performs the best while the S-PLUS model is ranked sixth.

**Keywords:** Software quality prediction, software metrics, fault prediction, CART, S-PLUS, multiple linear regression, neural networks, case-based reasoning.

## 1. Introduction

Software reliability is an important attribute of high-assurance and mission-critical systems. Such complex systems are heavily dependent on reliability and stability of their underlying software applications. The challenges involved in achieving high software reliability increases the importance in developing and quantifying measures for software quality. Early fault prediction is a proven technique in achieving high software reliability, and can be used to direct cost-effective quality enhancement efforts to modules that are likely to have a high number of faults. A software fault is a defect that causes software failure in an executable product.

Previous research (Khoshgoftaar et al., 2000b) has shown that software quality models based on software metrics (Schneidewind, 1995; Schneidewind, 1997) can yield predictions with useful accuracy. Such models can be used to predict the response variable which can either be the class of a module (e.g. fault-prone or not fault-prone) or a quality factor (e.g. number of faults) for a module. The former is usually referred to as classification models (Khoshgoftaar and Allen, 2001; Ohlsson and Runeson, 2002) while the latter is usually referred to as prediction models (Gokhale and Lyu, 1997; Khoshgoftaar and Seliya, 2002; Troster and Tian, 1995). The focus of this paper is on the latter, i.e., prediction models. Software quality prediction models can predict quantities like number of faults and software development effort. Software metrics used by the model and the response variable are referred to as the independent variables and dependent variable respectively.

Over the last few decades many software quality modeling techniques have been developed and used in real life software quality predictions. A few commonly used modeling techniques for software quality estimation include, regression trees (Gokhale and Lyu, 1997; Khoshgoftaar and Allen, 2001; Khoshgoftaar and Seliya, 2002; Takahashi et al., 1997; Troster and Tian, 1995), artificial neural networks (ANN) (Finnie et al., 1997; Khoshgoftaar and Lanning, 1995), case-based reasoning (CBR) (Ganesan et al., 2000; Kolodner, 1993), and multiple linear regression (MLR) (Berenson et al., 1983). Other recently developed techniques that have also been used include, fuzzy logic (Xu, 2001) and optimal set reduction (Briand et al., 1993). Many of these techniques facilitate software quality estimation modeling using both classification and prediction models.

Despite the fact that currently many techniques are used to build and apply prediction models for real life software quality estimations, not many extensive studies have been done that compare the performance of commonly used prediction modeling techniques. Very few studies have performed comparative evaluations of a few of the available techniques and methods, for example, Finnie et al. (1997) and Gray and MacDonell (1999).

Gray and MacDonell (1999), use three small-scale case studies to evaluate software development effort (or maintenance changes) estimation accuracy of prediction models built using MLR and ANN. The importance of factors other than predictive accuracy such as data characteristics, expertize, and interpretability have been demonstrated, however, the comparative study lacks statistical verification. The overall conclusion was that no single modeling technique can be used as a panacea for software effort estimation problems. Finnie et al. (1997) compare models built using ANN, CBR, and MLR. Similar to Gray and MacDonell, (1999), this study compares software effort estimation accuracy of different modeling methods. It was concluded that both ANN and CBR gave similar accuracy, however, both of them yielded better results than MLR. Statistical verification using *t*-test was performed to determine the significance of their conclusions. In both of the comparative studies mentioned above, the case studies used were relatively small-scale and the research did not include other available prediction techniques, such as regression trees.

This study presents a comparative evaluation of predictive accuracy of six commonly used software quality prediction modeling techniques or algorithms. These are,[1] CART-least squares (CART-LS), CART-least absolute deviation (CART-

LAD), S-PLUS, MLR, ANN, and CBR. Software quality models that predict the number of faults in software modules, were built using all of the six techniques. Performance metrics, average absolute error (AAE) and average relative error (ARE), are used to gauge the fault prediction accuracy of modeling techniques. To our knowledge this is the first extensive study that compares the fault prediction capabilities of commonly used modeling techniques in the context of a large-scale case study.

The case study used to build models consists of software metrics collected over four historical releases of a very large legacy telecommunications system, abbreviated as LLTS. Software metrics collected included 24 product and four execution metrics, i.e., a total of 28 independent variables. Each system release has over 3500 updated modules or observations. A common model building and validation methodology was adopted for all six techniques. Release 1 was used to build the models while Releases 2, 3 and 4 were used to validate the final models. For each of the modeling techniques considered, models were built using both RAW and domain (reduced by principle components analysis) metrics, and the models built are denoted as LLTS-RAW and LLTS-PCA models, respectively.

CART-LS, CART-LAD, and S-PLUS (it's regression tree algorithm) are tree-based prediction techniques (Khoshgoftaar and Seliya, 2002; Seliya, 2001) that provide simple white-box models which are attractive to analysts (Breiman et al., 1984; Clark and Pregibon, 1992). To our knowledge, these are the only tree-based prediction techniques currently available. CBR is a problem-solving technique which solves new problems by adapting solutions that were used to solve similar problems (Kolodner, 1993). ANN (Khoshgoftaar and Lanning, 1995) adopt a learning approach to deriving a predictive model. MLR (Berenson et al., 1983) is a traditional statistical means of predicting a dependent variable as a function of known independent variables. A more elaborate description of each of these methods is presented in the later sections.

Software metrics extracted (usually referred to as RAW metrics) from configuration and problem reporting systems are often heavily correlated to each other (Fenton and Pfleeger, 1997). This is usually because they often represent measurements of related attributes of the given software system. The correlation among the independent variables can often lead to poor robustness and prediction accuracy of models built based on them. Principle components analysis (PCA) is a statistical technique that is used to alleviate the problems due to correlation of independent variables. As we will see shortly, we use domain (PCA) metrics in addition to RAW metrics to build and evaluate our prediction models.

The use of AAE and ARE for comparing different prediction techniques can sometimes be difficult and may lead to erroneous results. The problem is increased when comparing models based on multiple releases (Khoshgoftaar et al., 2000b). A scenario with two releases that illustrates the possible difficulties is presented next. For Release 2, method A may have better AAE than method B, but for Release 3, method B may have better AAE than method A. The problem arises as to which release to use to compare methods A and B. The issue is further complicated with the use of over two releases to compare modeling methods.

The comparative approach adopted by Finnie et al. (1997) is not suited for comparing models based on multiple releases. It is geared more towards case studies involving data collected from only one project release, i.e. *fit* and *test* data sets are extracted from the same release. A unique approach is adopted in our study to compare software quality estimation models. The approach compares the models over all system releases, which alleviates the problem addressed above.

Two-way ANOVA (analysis of variance) randomized-complete block design models with two blocking variables are built. These ANOVA models use AAE and ARE as the response variables. System release (Releases 2, 3, and 4) and the model type (LLTS-RAW or LLTS-PCA model) form the two blocking variables, while the modeling technique or algorithm is treated as a factor. Release 1 is not used as a block since it was used to build or train the fault prediction models. Model type was used as a blocking variable (in ANOVA models) to observe if models built using RAW metrics were significantly apart from those built using domain metrics. It was observed that both models types performed similar, however, it should be noted that models based on principle components are generally more robust than the corresponding models based on RAW metrics. ANOVA models indicated that both system releases and modeling techniques were significantly different from their respective counterparts. Multiple-pairwise comparisons (Berenson et al., 1983) were performed to evaluate a performance or rank order of the six modeling techniques considered.

Comparisons of fault prediction accuracy (based on AAE and ARE) of the different modeling techniques considered in our study revealed the following performance order (decreasing accuracy): CART-LAD, CBR, MLR, ANN, CART-LS, and S-PLUS. It is indicated that CART-LAD and CBR models have better fault prediction than the MLR, ANN, CART-LS, and S-PLUS models. The superior performance of CART-LAD and CBR as well as the inferior performance of S-PLUS is verified in a similar study that used data from other case studies (Khoshgoftaar and Seliya, 2002; Seliya, 2001). The comparative technique presented in our study is not limited to only six modeling methods. It can be extended to compare fewer or more prediction modeling methods. However, data from multiple releases or multiple projects is needed to effectively utilize ANOVA design models (one-way or two-way) for performance comparisons of fault prediction models for software quality estimation.

The layout of the of rest the paper is as follows. Description of the different modeling methods is presented in Section 2. In Section 3, the adopted modeling methodology, comparative techniques used, and related technical concepts are presented. Section 4 describes the case study used in our study. Sections 5 and 6, present the results and conclusions of our comparative study.

## 2. Fault Prediction Techniques

### *2.1. Classification and Regression Trees*

Classification and regression trees (CART) is a statistical tool for tree structured data analysis (Breiman et al., 1984). CART uses a regression tree to show how data may be predicted by a series of decisions at each internal node of the tree. In regression, a case consists of data ($\mathbf{x}_i$, $y_i$) where, $\mathbf{x}_i$ is the $i$th measurement vector of independent variables and $y_i$ is the $i$th response variable. The CART algorithm partitions the input data set into terminal nodes by a sequence of recursive binary splits. Binary splits are generated by CART, based on the significant independent variables. At each binary partition, the two subsets are as homogeneous as possible with respect to the dependent variable, which in our case is the number of faults in a software module.

The CART algorithms initially build a large tree (Breiman et al., 1984; Briand et al., 2000), and then prune it back using *cross validation* to avoid overfitted trees (Khoshgoftaar et al., 2001). Starting with the *fit* data set (learning sample $L$), three elements are necessary to determine a regression tree predictor: (1) A way to select a split at every internal node; (2) A rule for determining when a node is terminal, and (3) A rule for assigning a value $\hat{y}(t)$ to every terminal node, where $\hat{y}(t)$ is the predicted value of the response variable for terminal node $t$.

CART provides three ways to estimate the accuracy of regression trees: resubstitution estimate, test sample estimate and *v-fold* cross validation estimate. Empirical studies in this paper use the *v-fold* cross validation estimate to evaluate regression tree models. In a *v-fold* cross validation estimate, the learning sample $L$ (fit data set) is divided into $v$ subsets of approximately equal size. ($v$-1) subsets are used as *fit* data sets while one remaining subset is used as a *test* data set. $v$ such trials are performed such that each subset of the learning sample is used once as a *test* data set. The average error over these $v$ trials, gives the cross validation error estimate. In our empirical studies we have used the 10-*fold* cross validation approach.

Certain parameters can be controlled when building regression trees with CART. These include number of terminal nodes, depth or level of regression tree, and node size before splitting. The first two parameters by default are automatically forecasted by the algorithm depending on the case study. The third parameter, node size, is set to 10 by default. In our experiments in regression tree modeling for the LLTS case study (Seliya, 2001) we have used default values for these parameters.

In the following two sections we present the essential differences between the CART-LS (least squares) and CART-LAD (least absolute deviation) methods of CART. Further in-depth mathematical details including tree pruning methods and standard error estimates of the CART regression tree algorithms can be found in Breiman et al. (1984). The final tree models are selected based on their cross validation[2] (mean square or average absolute deviation) relative errors, described in the following subsections.

### *2.1.1. Least Squares Method*

This method generates regression trees using the within node mean value observed in each terminal node as its predicted value. Ranking of regression trees of different sizes is evaluated based on the mean square error estimate. Given a learning sample $L$ consisting of $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$, $L$ is used to construct regression trees and also to estimate their accuracy. The resubstitution error estimate for the CART-LS method, as a measure of accuracy for a regression tree $T$ is given by,

$$R(T) = \frac{1}{N} \sum_{t \in T} \sum_{(\mathbf{x}_n, y_n) \in t} (y_n - \bar{y}(t))^2 \tag{1}$$

where, $N$ is the total number of cases in the learning sample, $t$ is a terminal node in the regression tree $T$, and $\bar{y}(t)$ is the mean value of response variables in $t$.

Given any set of possible splits $\mathbf{S}$ of a current terminal node $t$, the best split $\check{s}$ of $t$ is that split in $\mathbf{S}$ which most decreases $R(T)$. For any split $s$ of $t$ into $t_L$ and $t_R$, let $\Delta R(s, t) = R(t) - R(t_L) - R(t_R)$. Then the best split $\check{s}$ is given by,

$$\Delta R(\check{s}, t) = \max\{\Delta R(s, t)\} \tag{2}$$

Thus, a regression tree is formed by iteratively splitting nodes so as to maximize the decrease in $R(T)$. The best split at a node is that split which most successfully separates the high response values from the low ones.

When using the test sample estimate, a *fit* data set is used to build regression trees, while a *test* data set is used to evaluate the accuracy of the tree models. The test sample error estimate for the CART-LS method is given by,

$$R^{ts}(T) = \frac{1}{N_2} \sum_{(\mathbf{x}_n, y_n) \in L_2} (y_n - d(\mathbf{x}_n))^2 \tag{3}$$

where, $L_2$ is the test data set with $N_2$ cases and $d(\mathbf{x}_n)$ denotes the predictor corresponding to the $\mathbf{x}_n$ measurement vector of independent variables. The learning sample $L_1$ is used to build regression trees, while the test sample $L_2$ is used to evaluate the accuracy of trees.

The *v-fold* cross validation error estimate for the CART-LS method is given by,

$$R^{cv}(T) = \frac{1}{N} \sum_{v} \sum_{(\mathbf{x}_n, y_n) \in L_v} (y_n - d_v(\mathbf{x}_n))^2 \tag{4}$$

where, $d_v(\mathbf{x}_n)$ denotes the predictor for the $v$th trial of the cross validation and $L_v$ is the $v$th subset of the learning sample $L$.

Let $\bar{y}$ be a sample mean of $y_1, \ldots, y_N$, and set $R(\bar{y})$ as,

$$R(\bar{y}) = \frac{1}{N} \sum_{n} (y_n - \bar{y})^2 \tag{5}$$

Then the mean square relative error estimates for resubstitution, test sample and *v-fold* cross validation are given by, $R(T)/R(\bar{y}), R^{ts}(T)/R(\bar{y})$ and $R^{cv}(T)/R(\bar{y})$, respectively.

### *2.1.2. Least Absolute Deviation Method*

This method generates regression trees using the within node median value observed in each terminal node as its predicted value. Ranking of regression trees of different sizes is evaluated based on the mean absolute deviation estimate.

The resubstitution error estimate $R(T)$ for the CART-LAD method is given by,

$$R(T) = \frac{1}{N} \sum_{t \in T} \sum_{(\mathbf{x}_n, y_n) \in t} |y_n - \tilde{y}(t)| \tag{6}$$

where, $N$ is the total number of cases in the learning sample, $t$ is a terminal node in the regression tree $T$ and $\tilde{y}(t)$ is the median value of the $y$ values in node $t$. The splitting criteria is analogous to that mentioned for the CART-LS method.

The test sample error estimate for the CART-LAD method is given by,

$$R^{ts}(T) = \frac{1}{N_2} \sum_{(\mathbf{x}_n, y_n) \in L_2} |y_n - d(\mathbf{x}_n)| \tag{7}$$

The *v-fold* cross validation error estimate for the CART-LAD method is given by,

$$R^{cv}(T) = \frac{1}{N} \sum_{v} \sum_{(\mathbf{x}_n, y_n) \in L_v} |y_n - d_v(\mathbf{x}_n)| \tag{8}$$

Let $\tilde{y}$ be a sample median of $y_1, \ldots, y_N$, and set $R(\tilde{y})$ as,

$$R(\tilde{y}) = \frac{1}{N} \sum_{n} |y_n - \tilde{y}| \tag{9}$$

Then the absolute relative error estimates for resubstitution, test sample and *v-fold* cross validation are given by, $R(T)/R(\tilde{y})$, $R^{ts}(T)/R(\tilde{y})$ and $R^{cv}(T)/R(\tilde{y})$ respectively.

## ***2.2. S-plus Regression Trees***

S-PLUS is a solution for advanced data analysis, data mining, and statistical modeling. It combines an intuitive graphical user interface with an extensive data analysis environment to offer ease of use and flexibility. Statistics in S-PLUS include regression tree models among other data mining functions. At the core of the S-PLUS system is *S*, the only language designed specifically for data visualization and exploration, statistical modeling and programming with data. *S* provides a rich, object-oriented environment designed for interactive data discovery. With a huge library of functions for all aspects of computing with data, *S* offers good extensibility.

In-depth mathematical details of the S-PLUS regression tree algorithm are presented in Clark and Pregibon (1992). The predictors are software metrics treated by S-PLUS as ordinal measures, which are used to build regression trees to predict the response variable. The S-PLUS tree algorithm that can process only numerical data, constructs a regression tree which is a collection of decision rules determined by recursive binary partitioning of the training data set. These decision rules can be controlled by specifying certain parameters, which limit the growth of the tree model. These parameters are *minsize*, the size threshold which limits the number of observations in a leaf node and *mindev*, the uniformity threshold which limits the allowable deviance in the leaf nodes. By controlling these parameters, the analyst can prune the tree model to the desired level. However, S-PLUS provides a function that can be used to prune the tree after it has been constructed by the algorithm, without sacrificing the goodness-of-fit of the tree model. In the course of the S-PLUS regression tree algorithm, modules in the *fit* data set are assigned to tree nodes. A software module is considered as an *object*.

Predictors are derived from software metrics as explained below. Let $x_{ij}$ be the $j$th predictor's value for module $i$, $\mathbf{x}_i$ be the vector of predictors for module $i$, and $y_i$ be the response variable, i.e., number of faults. The algorithm initially assigns all the modules in the *fit* data set to the root node. The algorithm then recursively partitions each node's modules into two subsets that are assigned to its child nodes, until a stopping criterion halts further partitioning.

The deviance of module $i$ is minus twice the log-likelihood, scaled by the variance, which reduces to the following (Clark and Pregibon, 1992).

$$D(\mu_i, y_i) = (y_i - \mu_i)^2 \tag{10}$$

where, $\mu_i$ is estimated by the mean value of $y$ over all training modules that fall in the same leaf as module $i$. The deviance of a node $l$ is the sum of the deviances of all the training modules in the node (Clark and Pregibon, 1992).

$$D(\mu_l; y) = \sum_{i \in l} (y_i - \mu_i)^2 \tag{11}$$

The tree-building algorithm chooses the predictor whose best split maximizes the change in deviance between the deviance of the current node and the sum of the deviances of the prospective child nodes. The "best split" of a predictor partitions the current node's set of modules into two subsets choosing the cut-point that minimizes the sum of the deviances of the left and right prospective child nodes. Partitioning stops when the node deviance is less than a small fraction of the root node deviance.

$$\frac{D(\mu_l; y)}{D(\mu_{\text{root}}; y)} < mindev \tag{12}$$

or the number of modules in the current node is less than a threshold,

$$n_l < minsize \tag{13}$$

where, *mindev* and *minsize* are model parameters.

Let $L(\mathbf{x}_i)$ be the leaf that the $i$th module falls into according to the structure of the tree. The predicted value of the response variable for module $i$ is the mean of training modules in the leaf it falls into.

$$\hat{y}_i = \mu_{L(\mathbf{x}_i)} \tag{14}$$

Empirical studies using regression tree modeling with S-PLUS were performed by our research team in Seliya (2001). Regression trees were built for the LLTS case study, by varying parameters *mindev* and *minsize*. For each of the models, performance metrics AAE and ARE was computed and the final model was selected based on quality of fit values.

### 2.3. Case-based Reasoning

A CBR system arrives at a solution by retrieving past instances of the same or a similar problem (Kolodner, 1993). The past instances are in a library of cases containing all known data. Each case in the library contains information about the program module it describes, which will include predictors and the response variable. A CBR system can take advantage of availability of new or revised information, by adding new cases or by removing obsolete cases from the case library. Good scalability of CBR provides fast retrieval even as the size of the case library goes up. CBR systems can be designed to alert users when a new case is outside the bounds of current experience.

The first step is to determine a good software quality model that can predict the dependent variable with minimal error. This is done by varying the parameter which in this case is the value of *nearest neighbors*. Let $N$ be the complete set of *nearest neighbors*, which are cases in the *fit* data set that are most similar to the present case in the target (*test*) data set. The number of *nearest neighbors*, $n_N$ (number of cases), is empirically determined by the user.

A CBR model is the training data with associated parameters like similarity functions, i.e., *Euclidean Distance, Absolute Difference*, or *Mahalanobis Distance*, and solution algorithms, i.e., *Unweighted Average* or *Inverse Distance Weighted Average*. The case library is also known as the *fit* data set and the new cases, whose number of faults is to be predicted, is known as the *test* data set. The problem is to estimate the value of the dependent variable for a future or currently under development program module, relatively early in its life cycle. The closer the predicted value is to the actual value, the better the accuracy of prediction.

The model selection is done by using the case library as both *fit* and target (*test*) data sets. Cross-validation is used to build the model. If the *fit* data set (case library) has $n$ observations, at each iteration one case or observation is removed from the case library and the dependent variable (i.e., number of faults) is predicted using the remaining $n - 1$ cases, i.e., the case library will have $n - 1$ observations and the target (*test*) data set will have one observation. The one isolated observation acts as the test case to evaluate the prediction made by the $n - 1$ cases. The prediction error (i.e., AAE and ARE) of the $n$ iterations is computed and the CBR model with the least error is finally selected. The algorithms described below are used in the retrieval of the cases from the *fit* data set that are most similar to the target module and to estimate the dependent variable.

The RAW metrics in a software system module usually have vastly differing measurement units and highly varied ranges. Often, each metric has a unit of its own. Standardization is a technique that converts all the metrics to a uniform system of co-ordinates so that they will all have the same unit of measure. For each metric, $x_i$, the standardized metric is given by,

$$Z_i = \frac{x_i - \bar{x}_i}{s_i}$$

where $\bar{x}_i$ is the mean and $s_i$ is the standard deviation of the $i$th metric, $x_i$. All independent variables in the data set are standardized to a mean of zero and a variance of one. While other studies used normalization technique (Briand et al., 2000), we used standardization (except for *Mahalanobis Distance* function, in which neither is required (Sundaresh, 2001)).

A similarity function is used to compute the distance $d_{ij}$ between the current module $i$ and each of the modules $j$ in the case library. Let $c_{jk}$ be the value of the $k$th independent variable of case $j$, and let $\mathbf{c}_j$ be the vector of independent variable values for case $j$. Let $x_{ik}$ be the value of the $k$th independent variable for target module $i$, and $\mathbf{x}_i$ be the vector of independent variable values for module $i$. The *Euclidean Distance* is given by,

$$d_{ij} = \left( \sum_{k=1}^{m} (w_k (c_{jk} - x_{ik}))^2 \right)^{1/2} \tag{15}$$

where $m$ is the number of independent variables and $w_k$ is the weight of the $k$th independent variable. The *Absolute Difference* or *City Block Distance* is given by,

$$d_{ij} = \sum_{k=1}^{m} w_k \left| c_{jk} - x_{ik} \right| \tag{16}$$

The *Mahalanobis Distance* is given by,

$$d_{ij} = (\mathbf{c}_j - \mathbf{x}_i)' \mathbf{S}^{-1} (\mathbf{c}_j - \mathbf{x}_i) \tag{17}$$

where ($'$) means transpose, and $\mathbf{S}^{-1}$ is the inverse of the variance-covariance matrix of the independent variables for all the modules in the case library. $\mathbf{S}$ becomes an identity (unit) matrix and *Mahalanobis* becomes the *Euclidean* distance squared when the independent variables are orthogonal and have unit variance. When the independent variables are highly correlated and/or vary on vastly differing scales, the *Mahalanobis* distance is a very good alternative to other distance measures. Whenever the *Mahalanobis* measure is used, the independent variables do not need to be standardized or normalized.

The solution algorithm finally predicts the value of the dependent variable, $y_i$. The *Unweighted Average* solution algorithm is given by,

$$\hat{y}_i = \frac{1}{n_N} \sum_{j \in N} y_j \tag{18}$$

where, $\hat{y}_i$ is the mean value of the dependent variable of the most similar $n_N$ modules from the case library.

The *Inverse Distance Weighted Average* solution algorithm is given by,

$$\delta_{ij} = \frac{1/d_{ij}}{\sum_{j \in N} 1/d_{ij}} \tag{19}$$

$$\hat{y}_i = \sum_{j \in N} \delta_{ij} y_j \tag{20}$$

where, $y_i$ is estimated using the distance measures for the $n_N$ closest cases as weights in a weighted average. Since smaller distances indicate a closer match and each case is weighted by a normalized inverse distance. The case most similar to the target module has the largest weight, thus playing a major role in prediction.

Fault prediction models were built by our research group (Khoshgoftaar et al., 2000a; Sundaresh, 2001) for the LLTS case study. All three similarity functions mentioned above were considered. The number of similar cases, $n_N$, selected from the fit data set is a significant parameter during model building process. The model whose $n_N$ results in the least value of AAE with cross validation is selected as the final model (Sundaresh, 2001). Experiments were therefore conducted by varying $n_N$ to find the optimum value. It was observed that the *Mahalanobis Distance* function gave better prediction results as compared to prediction obtained with *Euclidean Distance* and *Absolute Difference* functions. It was also observed that the *Inverse Distance Weighted Average* solution algorithm yielded better prediction than the *Unweighted Average* solution algorithm. Thus, *Inverse Weighted Distance Average* together with *Mahalanobis Distance* gave the best prediction results.

### *2.4. Artificial Neural Networks*

Artificial neural networks (ANN)[3] are systems that are deliberately constructed to make use of some organizational principles resembling those of the human brain. ANN have been studied since Rosenblatt (1962) first introduced single layer perceptrons. Because of the limitations of single-layer systems pointed out by Minsky and Papert (1969), interest in ANN has been dwindling. Recent resurgence in the field of ANN was encouraged by the new learning algorithms (Nielsen, 1987), analog VLSI techniques, and parallel processing (Lippmann, 1987).

According to learning rules, ANN can be classified into two categories, supervised-learning networks and unsupervised-learning networks (Lin and Lee, 1996). The ANN we studied are supervised learning networks, in which at each

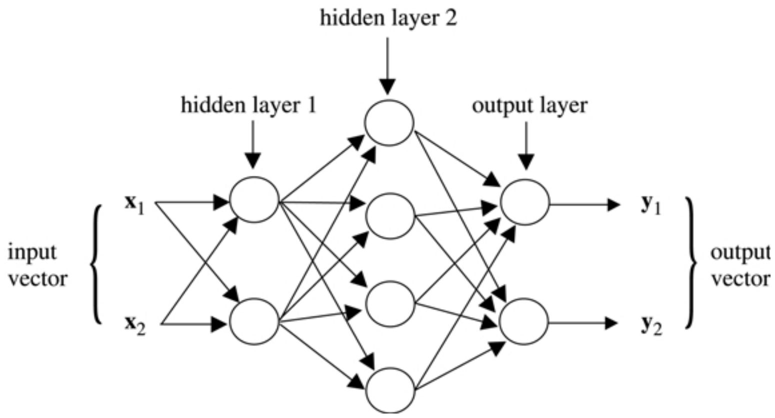


*Figure 1.* A feedforward neural network.

instant of time when input is applied to an ANN, the corresponding desired response of the system is given. The network is thus told precisely what it should be emitting as output. In summary, we confine our study to feedforward supervised-learning neural networks, in particular backpropagation (Lippmann, 1987; Nielsen, 1987) neural networks. Figure 1 illustrates the structure of a feedforward supervised-learning neural network.

Neural networks consist of neurons. Figure 2 shows the structure of a neuron. In this model, the $k$th processing element computes a weighted sum of its inputs $x_j$ (independent variable) and basis $b_k$ as the input to the activation function, the output of the activation function is the output of the neuron $o_k$ (dependent variable). Suppose there are $m$ inputs, $x_1, x_2, \ldots, x_m$, to the neurons and the weights associated with these inputs are $w_{1k}, w_{2k}, \ldots, w_{mk}$. So the operation of the neuron can be described as following.

$$net_k = w_{1k}x_1 + w_{2k}x_2 + \cdots + w_{mk}x_m + b_k \tag{21}$$

$$o_k = f(net_k) \tag{22}$$

where $f(\cdot)$ is the activation function of this neuron.

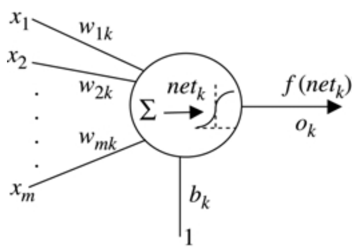


*Figure 2.* Anatomy of a neuron.

*Backpropagation* (Rumelhart et al., 1962) is the most popular training algorithm for multilayer neural networks. The algorithm initializes the network with a random set of weights and basis, and the network trains from a set of input-output pairs. Each pair requires a two stage learning algorithm: forward pass and backward pass. The forward pass propagates the input vector through the network until it reaches the output layer. First the input vector propagates to the hidden units. Each hidden unit calculates the weighted sum of the input vector and its interconnection weights. Each hidden unit uses the weighted sum to calculate its activation. Next, hidden unit activations propagate to the output layer. Each node in the output layer calculates its weighted sum and activation. The output of the network is compared to the expected output of the input-output pair, and their difference (error vector) is used to train the network to minimize the error, this is called backward pass. First the error passes from the output layer to the hidden layer updating output weights. Next each hidden unit calculates an error based on the error from each output unit, the error from the hidden units updates input weight. The training stops only when the sum of squared error satisfies the requirement or the number of epochs passes the set point, where an epoch means that all the training data go through the forward pass and backward pass once.

The least mean square algorithm computes the weight updates for each input sample and the weights are modified after each sample. This procedure is called sample-by-sample learning. An alternative solution is to compute the weight update for each input sample and store these values (without changing the weights) during one pass through the training set (epoch). At the end of the epoch, all the weight updates are added together, and only then will the weights be updated with the composite value. This is called batch training and is what we used in our case studies.

A neural network model was built for the LLTS case study (both RAW and PCA data sets) in Sundaresh, (2001). Since the neural networks use the unipolar sigmoid function as their activation function for all the nodes, the dependent variable, number of faults, was scaled to the range [0,1]. After the training process, the result was converted back to the original scale. The training data set was normalized to avoid a slow network training process, and it was found that the training speed increased after normalization. The overall architecture of the final neural network model was determined empirically, and further details of our study is presented in Khoshgoftaar and Lanning (1995) and Sundaresh (2001).

### *2.5. Multiple Linear Regression*

This technique provides a statistical means of estimating or predicting a dependent variable as a function of known independent variables. The model is in the form of an equation where the response variable is expressed in terms of predictors. The general form of a multiple linear regression (MLR) model can be given by,

$$\hat{y}_i = a_0 + a_1 x_{i1} + \cdots + a_p x_{ip} \tag{23}$$

$$y_i = a_0 + a_1 x_{i1} + \cdots + a_p x_{ip} + e_i \tag{24}$$

where, $x_{i1}, \ldots, x_{ip}$ are the independent variables' values, $a_0, \ldots, a_p$ are the parameters to be estimated, $\hat{y}_i$ is the dependent variable to be predicted, $y_i$ is the actual value of the dependent variable, and $e_i = y_i - \hat{y}_i$ is the error in prediction for the $i$th case.

The data available is initially subject to statistical analysis, with the aim to remove any correlation existing between independent variables and to remove insignificant independent variables, not accounting for the dependent variable. The process of determining the variables which are significant is known as model selection. Several methods of model selection exist. They are forward elimination, stepwise selection and backward elimination. Here, stepwise regression is used.

Stepwise regression (Berenson et al., 1983) selects an optimal set of independent variables for the model. In this process, variables are either added or deleted from the regression model at each step of the model building process. Once the model is selected, the parameters $a_0, \ldots, a_p$ are then estimated using the least squares method. The values of the parameters are selected such that they minimize $\sum_{i=1}^{N} e_i^2$, where, $N$ is the number of observations in the *fit* data set.

## 3. Modeling Methodology

In this section, we present a discussion of the approach adopted in comparing the different fault prediction modeling techniques discussed earlier. Theory and related principles of our comparative technique is also presented in this section.

### *3.1. Building Fault Prediction Models*

The general model building and validation approach adopted in fault prediction modeling with CART-LS, CART-LAD, S-PLUS, CBR, ANN, and MLR is summarized by the following steps.

1. *Preprocessing Data:* A few modeling tools demand preprocessing of data before analysis. Some preprocessing may include, logarithmic transformation, standardization, and grouping of data.

2. *Formatting Data:* The *fit* and *test* data sets may have to be converted to a format acceptable by the tool. For example, when using CART, data sets have to be converted to the SYSTAT file format.

3. *Building Prediction Models:* Release 1, the *fit* data set is used to build different models. Certain parameters specific to the modeling technique (Section 2), are varied. Average absolute (AAE) and average relative errors (ARE) of models built are computed (for Release 1).

4. *Selecting Prediction Models:* Models with the lowest AAE and ARE values are selected as our final fault prediction models. In the case of CART-LS and CART-

LAD the models were selected based on the lowest cross-validation relative error[4] value (Seliya, 2001). S-PLUS, ANN, and MLR models were selected based on their quality-of-fit values. A cross-validation (with lowest AAE) model selection approach (Sundaresh, 2001) was adopted for CBR.

5. *Validating Prediction Models*: Releases 2, 3, and 4 are used as *test* data sets to evaluate the prediction accuracy of the models selected. Performance metrics, AAE and ARE are computed. These are used to observe the estimation accuracy of models.

### 3.2. Performance Metrics

Fault prediction accuracy of the models selected is determined by estimating performance metrics. Two common statistics for evaluating predictions, AAE and ARE are computed as,

$$AAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \tag{25}$$

$$ARE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i + 1}\right| \tag{26}$$

where, $n$ is the number of modules in the target data set. The denominator in ARE has a one added to avoid division by zero (Khoshgoftaar et al., 1992). Our study compares fault prediction models using both AAE and ARE, since the effectiveness of one over the other is out of scope for this paper.

### 3.3. Analysis of Variance Models

ANOVA, abbreviated for analysis of variance, is a commonly used statistical technique when comparing differences between the means of three or more independent groups or populations. In our study, we employ the two-way ANOVA: randomized complete block design modeling approach (Berenson et al., 1983; Neter et al., 1996), in which $n$ heterogeneous subjects are classified into $b$ homogeneous groups, called blocks so that the subjects in each block can then be randomly assigned, one each, to the levels of the factor of interest prior to the performance of a two-tailed $F$ test, to determine the existence of significant factor effects.

Selecting the appropriate experimental design approach depends on the level of reduction in experimental error required. Since the primary objective for selecting a particular experimental design is to reduce experimental error (variability within data), a better design could be obtained if subject variability is separated from the experimental error (Neter et al., 1996). A two-way ANOVA randomized complete block design, is a restricted randomization design in which the experimental units are first sorted into homogeneous groups, i.e., blocks, and the treatments are then assigned randomly within the blocks.

We are interested in observing if different prediction techniques are different from each other and if the system releases are different from each other. We are also interested in observing if principle components analysis (Khoshgoftaar et al., 2000c) of the independent variables, results in better fault prediction accuracy of models. Substantial reduction in experimental errors can be obtained if more than one variable is used for determining blocks (Berenson et al., 1983). We designed two-way ANOVA models using two blocking variables, namely, system release and model type, i.e. models build based on RAW metrics and their principle components.

AAE and ARE values predicted by models for different releases and data sets (RAW and PCA) are the response variables in our experimental design models (ANOVA), which involve six factor treatments (six fault prediction techniques) and two blocking variables. The first one has three blocks (system releases 2, 3, and 4) while the second one has two blocks (RAW and PCA models). The $p$-values obtained from the ANOVA design models (Table 5, p. 276), indicate the significance of the difference between the different modeling methods, between the different system releases, and between the models built using RAW and PCA metrics.

To develop the ANOVA procedure for a randomized complete block design, $Y_{ijk}$, the observation in the $i$th block $(i = 1, 2, \ldots, b)$ of $B$ and the $k$th block $(k = 1, 2, \ldots, c)$ of $C$ under the $j$th level $(j = 1, 2, \ldots, a)$ of factor $A$, can be represented by the model,

$$Y_{ijk} = \mu + A_j + B_i + C_k + \varepsilon_{ijk} \tag{27}$$

where,

$\mu$ is the overall effect or mean common to all observations; $A_j = \mu_{\bullet j \bullet} - \mu$, a treatment effect peculiar to the $j$th level of factor $A$ (method); $B_i = \mu_{i \bullet \bullet} - \mu$, a block effect (system release) peculiar to the $i$th block of $B$; $C_k = \mu_{\bullet \bullet k} - \mu$, a block effect (model type, RAW or PCA) peculiar to the $k$th block of $C$; $\varepsilon_{ijk}$ is the random variation or experimental error associated with the observation in the $i$th block of $B$ and $k$th block of $C$ under the $j$th level of factor $A$; $\mu_{\bullet j \bullet}$ is the true mean for the $j$th level of factor $A$; $\mu_{i \bullet \bullet}$ is the true mean for the $i$th block of $B$; $\mu_{\bullet \bullet k}$ is the true mean for the $k$th block of $C$.

### *3.4. Hypothesis Testing: a p-value Approach*

Hypothesis testing is concerned with the testing of certain specified (i.e., hypothesized) values for those population parameters. Statisticians and software analysts alike, often perform hypothesis tests (Berenson et al., 1983) when comparing different models. A null hypothesis, $H_0$, is tested against its compliment, the alternative hypothesis, $H_A$. Hypotheses are usually set up to determine if the data supports a belief as specified by $H_A$. These tests indicate the significance ($\alpha$) of difference between two methods or populations.

The selection of the pre-determined significance level, $\alpha$, may depend on the analyst and the project involved. In some cases the selection of $\alpha$ may be too ambiguous or difficult (Beaumont, 1996). In such situations, it may be preferred to perform hypothesis testing without setting a value for $\alpha$. This may be achieved by employing the $p$-value approach to hypothesis testing (Beaumont, 1996; Berenson et al., 1983). This approach involves finding a value $p$ such that a given $H_0$ will not be accepted for any $\alpha \geq p$. Otherwise, $H_0$ will not be rejected, i.e., $\alpha < p$. If this probability ($p$-value) is very high, $H_0$ is not rejected, while if this likelihood is very small (traditionally $\leq 0.05$), $H_0$ is rejected. Hypotheses tests may be one-tailed or two-tailed, depending on the alternative hypothesis of interest to the researcher.

In this study, we use the *Minitab* software tool (Beaumont, 1996), which has provision for statistical comparative analysis. We compute the $p$-values to determine if a prediction method is significantly better than another method. These $p$-values are used in deciding on the performance order of the different fault prediction methods. In making decisions regarding the rejection or non-rejection of $H_0$, the appropriate test statistic would be compared against the critical values for the particular sampling distribution of interest. For our comparative study, we use the $F$ statistic (Berenson et al., 1983). If the test statistic, $F$, is distributed as $F(v_1, v_2)$, then the $p$-value is given by,

$$p = Pr\{F(p; v_1, v_2) \leq F(v_1, v_2)\} \tag{28}$$

where, $v_1$ and $v_2$ are the degrees of freedom for the $F$ distribution, $F(p; v_1, v_2)$ is the entry in the $F$-table (Beaumont, 1996), and $F(v_1, v_2)$ is the computed statistic for the hypothesis test.

### 3.5. Multiple-Pairwise Comparison

The ANOVA block design models do not specify or indicate which means differ from which of the other means. Multiple comparison methods provide more detailed information about the differences of these means. Specifically they provide a statistical technique to compare two methods (e.g. method A and method B) at a time. A variety of multiple comparison methods are available, and for our study we employ Bonferroni's multiple comparison equation (Beaumont, 1996). Hypothesis testing using the $p$-value approach is performed as discussed in Section 3.4. The null and alternative hypotheses used for the multiple-pairwise comparisons, using AAE are given by Equations (29) and (30). Comparisons for ARE, are done by substituting ARE for AAE in the below stated equations.

$$H_0 : \text{AAE}_A \geq \text{AAE}_B \tag{29}$$

$$H_A : \text{AAE}_A < \text{AAE}_B \tag{30}$$

## 4. System Description

The data for the case study used in this paper was collected over four releases, from a very large legacy telecommunications system (abbreviated as LLTS). Each release has approximately 3500 to 4000 updated software modules. The software system is an embedded-computer application that included finite-state machines. The software was written in PROTEL, a high-level language, using the procedural development paradigm and was maintained by professional programmers in a large organization.

A software module was considered as a set of related source-code files. Fault data, collected at the module-level by the problem reporting system, comprised of faults discovered during post unit testing phases. Post unit testing phases recorded faults that were discovered before and after the product was released to customers. Faults that were discovered by customers were recorded only if the discovery resulted in changes to the source code of the module.

Configuration management data analysis, identified software modules that were unchanged from the prior release. Fault data collected from the problem reporting system were tabulated into problem reports and anomalies were resolved. The number of modules that had faults was too few to facilitate effective software quality modeling. As a result, we considered only the updated modules, i.e., those modules that were new or had at least one update to its source code since its prior release. For modeling, we selected updated modules with no missing data in relevant variables. These updated modules had several million lines of code, and there were a few thousands of these modules in each system release.

The set of available software metrics is usually determined by pragmatic considerations. A data mining approach is preferred in exploiting software metrics data (Fenton and Pfleeger, 1997), by which a broad set of metrics are analyzed rather than limiting data collection according to predetermined research questions. Data collection for LLTS involved extracting source code from the configuration management system. Measurements were recorded using the EMERALD software metrics analysis tool (Hudepohl et al., 1996). Preliminary data analysis selected metrics that were appropriate for our modeling purposes.

Software metrics for this system was collected over four different releases. We label these releases as Release 1, Release 2, Release 3, and Release 4. The number of observations in Release 1, Release 2, Release 3, and Release 4 were 3649, 3981, 3541, and 3978 respectively. The software metrics collected included 24 product metrics, 14 process metrics and four execution metrics. The 14 process metrics were not used in our empirical study, because our research study is focussed on early fault prediction of modules for software quality modeling. Only the software metrics used in our empirical study, are presented in this paper (Tables 1 and 2). The data sets consist of 28 independent variables that were used to predict the number of faults in a software module during the post unit testing phases. We shall refer to this case study as LLTS-RAW.

The software product metrics in Table 1 are based on call graph, control flow graph, and statement metrics. An example of call graph metrics is number of distinct procedure calls. A module's control flow graph, consists of nodes and arcs depicting

*Table 1.* Software product metrics.

| Symbol | Description |
|---|---|
| *Call graph metrics* | |
| *CALUNQ* | Number of distinct procedure calls to others. |
| *CAL2* | Number of second and following calls to others. $CAL2 = CAL - CALUNQ$ where $CAL$ is the total number of calls. |
| *Control flow graph metrics* | |
| *CNDNOT* | Number of arcs that are not conditional arcs. |
| *IFTH* | Number of non-loop conditional arcs, i.e., if-then constructs. |
| *LOP* | Number of loop constructs. |
| *CNDSPNSM* | Total span of branches of conditional arcs. The unit of measure is arcs. |
| *CNDSPNMX* | Maximum span of branches of conditional arcs. |
| *CTRNSTMX* | Maximum control structure nesting. |
| *KNT* | Number of knots. A "knot" in a control flow graph is where arcs cross due to a violation of structured programming principles. |
| *NDSINT* | Number of internal nodes (i.e., not an entry, exit, or pending node). |
| *NDSENT* | Number of entry nodes. |
| *NDSEXT* | Number of exit nodes. |
| *NDSPND* | Number of pending nodes, i.e., dead code segments. |
| *LGPATH* | Base 2 logarithm of the number of independent paths. |
| *Statement metrics* | |
| *FILINCUQ* | Number of distinct include files. |
| *LOC* | Number of lines of code. |
| *STMCTL* | Number of control statements. |
| *STMDEC* | Number of declarative statements. |
| *STMEXE* | Number of executable statements. |
| *VARGLBUS* | Number of global variables used. |
| *VARSPNSM* | Total span of variables. |
| *VARSPNMX* | Maximum span of variables. |
| *VARUSDUQ* | Number of distinct variables used. |
| *VARUSD2* | Number of second and following uses of variables. $VARUSD2 = VARUSD - VARUSDUQ$ where $VARUSD$ is the total number of variable uses. |

the flow of control of the program. Statement metrics are measurements of the program statements without implying the meaning or logistics of the statements. The problem reporting system maintained records on past problems. The proportion of installations that had a module, *USAGE*, was approximated by deployment data on a prior release (Jones et al., 1999). Execution times in Table 2 were measured in a laboratory setting with different simulated workloads.

Software metrics extracted (usually referred to as RAW metrics) from configuration and problem reporting systems are often highly correlated to each other (Khoshgoftaar et al., 2000c). This is usually because they often represent measurements of related attributes of the given software system. The correlation among the independent variables can often lead to poor robustness and prediction accuracy of models built based on them. Principle components analysis (PCA) is a statistical technique that is used to alleviate the problems due to correlation of

*Table 2.* Software execution metrics.

| Symbol | Description |
|---|---|
| *USAGE* | Deployment percentage of the module. |
| *RESCPU* | Execution time of an average transaction on a system serving consumers. |
| *BUSCPU* | Execution time of an average transaction on a system serving businesses. |
| *TANCPU* | Execution time of an average transaction on a tandem system. |

independent variables. The appendix describes the details of principle components analysis.

The dimensionality of the 28 RAW metrics was reduced using PCA. Earlier research (Khoshgoftaar et al., 2000b) indicated that the product and execution metrics groups of the RAW data were not correlated with each other. Hence, PCA was performed only on the 24 product metrics. Table 3 shows the six principle components extracted from the 24 product metrics of the LLTS-RAW data set. This table contains a $24 \times 6$ matrix, in which the 24 rows represent the product metrics

*Table 3.* Factor pattern of product metrics for LLTS-RAW.

| Metric | PROD1 | PROD2 | PROD3 | PROD4 | PROD5 | PROD6 |
|---|---|---|---|---|---|---|
| *CALUNQ* | **0.9024** | 0.0518 | 0.1044 | 0.2323 | 0.1739 | 0.0616 |
| *VARUSDUQ* | **0.8950** | 0.1889 | 0.1527 | 0.1770 | 0.1468 | 0.1938 |
| *LOC* | **0.8861** | 0.2807 | 0.1816 | 0.1693 | 0.1643 | 0.1445 |
| *NDSENT* | **0.8797** | −0.1114 | 0.0177 | 0.1839 | 0.1099 | 0.1720 |
| *STMEXE* | **0.8687** | 0.2587 | 0.1761 | 0.1732 | 0.2688 | 0.0717 |
| *STMCTL* | **0.8670** | 0.2607 | 0.2741 | 0.1726 | 0.0851 | 0.1743 |
| *NDSEXT* | **0.8467** | 0.0197 | 0.1086 | 0.2010 | 0.0857 | 0.3529 |
| *STMDEC* | **0.8460** | 0.2013 | 0.1415 | 0.1492 | 0.0712 | 0.1490 |
| *IFTH* | **0.8457** | 0.3416 | 0.2788 | 0.1816 | 0.1040 | 0.1066 |
| *NDSINT* | **0.8419** | 0.3436 | 0.2761 | 0.1525 | 0.1849 | 0.1092 |
| *CNDNOT* | **0.8348** | 0.3117 | 0.2623 | 0.1522 | 0.2370 | 0.1750 |
| *LOP* | **0.8282** | 0.1082 | 0.2084 | 0.0171 | 0.0213 | −0.0959 |
| *VARGLBUS* | **0.8019** | 0.3596 | 0.2012 | 0.1437 | 0.2120 | 0.2045 |
| *VARUSD2* | **0.7909** | 0.4410 | 0.2711 | 0.1119 | 0.1808 | 0.1293 |
| *CAL2* | **0.5972** | 0.2042 | 0.0728 | 0.1932 | 0.5690 | −0.0526 |
| *VARSPNSM* | 0.3917 | **0.8602** | 0.1772 | 0.1043 | 0.0675 | 0.0842 |
| *VARSPNMX* | 0.1404 | **0.8349** | 0.1772 | 0.3515 | 0.1036 | 0.0914 |
| *CNDSPNMX* | 0.1212 | 0.2763 | **0.7566** | 0.1429 | 0.2565 | 0.3060 |
| *CTRNSTMX* | 0.3223 | 0.0960 | **0.7092** | 0.4210 | −0.0073 | −0.0157 |
| *CNDSPNSM* | 0.6097 | 0.2155 | **0.6424** | 0.0070 | 0.2201 | 0.1309 |
| *FILINCUQ* | 0.3956 | 0.2579 | 0.1554 | **0.7265** | −0.0357 | 0.1696 |
| *LGPATH* | 0.2102 | 0.3796 | 0.3579 | **0.6396** | 0.1699 | −0.0415 |
| *KNT* | 0.2136 | 0.0691 | 0.1746 | −0.0064 | **0.8890** | 0.0972 |
| *NDSPND* | 0.4021 | 0.1489 | 0.2169 | 0.0751 | 0.0841 | **0.8156** |
| Variance | 11.6164 | 2.8209 | 2.3717 | 1.6952 | 1.6428 | 1.2300 |
| % Variance | 48.40% | 11.75% | 9.88% | 7.06% | 6.85% | 5.13% |
| Cum. % | 48.40% | 60.15% | 70.03% | 77.09% | 83.94% | 89.07% |

Stopping rule: at least 89% of variance

while the 6 columns represent the principle components, *PROD1, PROD2, PROD3, PROD4, PROD5* and *PROD6*. Each element in the matrix indicates the correlation between a principle component and a raw metric. These six principle components and the four execution metrics in Table 2 form the second set of data sets. We refer to this case study as LLTS-PCA.

## 5. Empirical Results

Two models were built for the LLTS case study using each of the six prediction techniques, namely, CART-LS, CART-LAD, S-PLUS, CBR, ANN, and MLR. The first model was built using the LLTS-RAW data set while second model was built using the LLTS-PCA data set. Performance metrics AAE and ARE are computed for the both models, and are shown in Table 4. The values shown in Table 4 are for Releases 2, 3, and 4 only since Release 1 was used as the *fit* data set.

The two-way ANOVA randomized complete block design models built using AAE and ARE as response variables, consisted of two blocking variables, i.e., system release and model type (RAW and PCA) and one factor, i.e., prediction technique. ANOVA models were built over all the test data sets, i.e., Releases 2, 3, and 4. The results of the ANOVA models are presented in Table 5. Notations of Table 5 are, DF—degrees of freedom, SS—sums of squares, MS—mean squares, and

*Table 4.* LLTS-RAW: AAE and ARE values.

| Model based on LLTS-RAW case study | | | | | | |
|---|---|---|---|---|---|---|
| Modeling method | Release 2 | | Release 3 | | Release 4 | |
| | AAE | ARE | AAE | ARE | AAE | ARE |
| CART-LS | 0.948 | 0.618 | 0.942 | 0.602 | 1.407 | 0.838 |
| CART-LAD | 0.705 | 0.324 | 0.803 | 0.391 | 0.867 | 0.418 |
| S-PLUS | 0.909 | 0.577 | 0.954 | 0.602 | 1.267 | 0.774 |
| CBR | 0.884 | 0.585 | 0.861 | 0.499 | 0.831 | 0.492 |
| ANN | 0.946 | 0.584 | 1.016 | 0.620 | 1.249 | 0.749 |
| MLR | 0.890 | 0.571 | 0.960 | 0.602 | 0.926 | 0.584 |
| **Model based on LLTS-PCA case study** | | | | | | |
| Modeling method | Release 2 | | Release 3 | | Release 4 | |
| | AAE | ARE | AAE | ARE | AAE | ARE |
| CART-LS | 0.972 | 0.647 | 0.975 | 0.633 | 1.113 | 0.682 |
| CART-LAD | 0.727 | 0.344 | 0.823 | 0.407 | 0.860 | 0.456 |
| S-PLUS | 0.925 | 0.602 | 0.973 | 0.621 | 1.568 | 0.948 |
| CBR | 0.835 | 0.523 | 0.871 | 0.519 | 0.810 | 0.477 |
| ANN | 0.887 | 0.555 | 0.948 | 0.576 | 0.989 | 0.615 |
| MLR | 0.875 | 0.567 | 0.976 | 0.626 | 0.954 | 0.637 |

*Table 5.* ANOVA models for LLTS case study.

| Source | DF | SS | MS | F | *p*-value |
|---|---|---|---|---|---|
| Average absolute error | | | | | |
| Technique | 5 | 0.4262 | 0.0852 | 5.99 | 0.001 |
| Model Type | 1 | 0.0022 | 0.0022 | 0.16 | 0.695 |
| Release | 2 | 0.2460 | 0.1230 | 8.64 | 0.001 |
| Error | 27 | 0.3842 | 0.0142 | | |
| Total | 35 | 1.0586 | | | |
| Average relative error | | | | | |
| Technique | 5 | 0.3688 | 0.0738 | 15.8 | 0.000 |
| Model Type | 1 | 0.0000 | 0.0000 | 0.00 | 0.989 |
| Release | 2 | 0.0657 | 0.0329 | 7.02 | 0.004 |
| Error | 27 | 0.1264 | 0.0047 | | |
| Total | 35 | 0.5609 | | | |

F—the *F* statistic (Berenson et al., 1983). In the ANOVA models we have six (treatments) modeling methods, three (first blocking variable) system releases, and two (second blocking variable) types of data sets. Consequently, we have (36–1) degrees of freedom.

It is observed from Table 5, for both AAE and ARE the system releases are significantly apart from each other ($p$-value $= 0.001$ and 0.004, respectively). It is also seen that the prediction techniques are also significantly apart from each other, i.e., $p$-value $= 0.001$ (AAE) and 0.000 (ARE). However, the LLTS-RAW and LLTS-PCA models interestingly performed similar, i.e., have similar prediction accuracies. Since the AAE and ARE values of the prediction techniques are significantly different from each other, we proceeded with multiple-pairwise comparisons of the different techniques.

Each of the six modeling methods is compared with the other five methods using a one-tailed pairwise comparison. For example, CART-LAD is compared with CART-LS, S-PLUS, CBR, ANN, and MLR individually. Thus, for each pair of techniques we have two comparisons, for example, is CART-LAD better than CBR? and is CBR better than CART-LAD? The *p*-value of the comparison is computed, and is used to observe whether a method is better than the one it is compared with.

Table 6 presents the *p*-values obtained from multiple pairwise comparisons. Comparisons are shown for both AAE and ARE performance metrics. The table can be viewed as a matrix, i.e., each pair of two methods forms a comparison. This implies each method listed in the first column is compared with (except itself) methods listed as headings of subsequent columns. For example, CART-LAD vs. CART-LS, CART-LAD vs. S-PLUS, and so on. Methods are not compared to themselves, and this is indicated by a * in the two tables. Since we compared six prediction techniques, there are 30 comparisons for each of the performance metrics. The *p*-values indicate the significance level of the difference in AAE or ARE values

*Table 6*. Multiple pairwise comparisons: *p*-values.

| Average absolute error | | | | | | |
|---|---|---|---|---|---|---|
| | CART-LAD | CART-LS | S-PLUS | ANN | MLR | CBR |
| CART-LAD | * | 0.0019 | 0.0004 | 0.0134 | 0.1515 | 0.7328 |
| CART-LS | 1.0000 | * | 0.8092 | 0.9995 | 1.0000 | 1.0000 |
| S-PLUS | 1.0000 | 0.9982 | * | 1.0000 | 1.0000 | 1.0000 |
| ANN | 1.0000 | 0.7158 | 0.3850 | * | 0.9999 | 1.0000 |
| MLR | 1.0000 | 0.1670 | 0.0506 | 0.5318 | * | 1.0000 |
| CBR | 0.9993 | 0.0124 | 0.0028 | 0.0742 | 0.4826 | * |
| Average relative error | | | | | | |
| | CART-LAD | CART-LS | S-PLUS | ANN | MLR | CBR |
| CART-LAD | * | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0090 |
| CART-LS | 1.0000 | * | 0.8682 | 1.0000 | 1.0000 | 1.0000 |
| S-PLUS | 1.0000 | 0.9959 | * | 1.0000 | 1.0000 | 1.0000 |
| ANN | 1.0000 | 0.3877 | 0.1945 | * | 0.9966 | 1.0000 |
| MLR | 1.0000 | 0.1821 | 0.0773 | 0.8548 | * | 1.0000 |
| CBR | 1.0000 | 0.0014 | 0.0004 | 0.0414 | 0.1134 | * |

*Table 7*. Performance order: LLTS case study.

| Average absolute error | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CART-LAD | < | CBR | < | MLR | < | ANN | < | CART-LS | < | S-PLUS |
| Average relative error | | | | | | | | | | |
| CART-LAD | < | CBR | < | MLR | < | ANN | < | CART-LS | < | S-PLUS |

between two prediction techniques, and are used to conclude the final performance or rank order.

To indicate how we inferred the final performance order of the prediction methods, we present details for ARE in the next few paragraphs. A similar approach was followed in computing the performance order for AAE. Let's look at the ARE section of Table 6. Comparisons CART-LAD vs. CART-LS, CART-LAD vs. S-PLUS, CART-LAD vs. ANN, CART-LAD vs. MLR, and CART-LAD vs. CBR have very low *p*-values, therefore indicate that CART-LAD has better predictive accuracy than the other five techniques. Hence, CART-LAD will be ranked first in the final order. Let's denote this deduction as **Da**.

From comparisons CBR vs. CART-LAD ($p = 1.0000$), CBR vs. CART-LS ($p = 0.0014$), CBR vs. S-PLUS ($p = 0.0004$), CBR vs. ANN ($p = 0.0414$), and CBR vs. MLR ($p = 0.1134$) it is observed that CBR is better than all techniques except CART-LAD (verified by **Da**). Hence, CBR will be ranked second in the final order. Let's denote this deduction as **Db**.

Comparisons MLR vs. CART-LS ($p = 0.1821$), MLR vs. S-PLUS ($p = 0.0773$), MLR vs. ANN ($p = 0.8548$), and ANN vs. MLR ($p = 0.9966$) indicate that MLR is significantly better than both CART-LS and S-PLUS, but is only slightly better than ANN. Using this observation together with **Da** and **Db**, we conclude that MLR will be ranked third in the final order.

From comparisons ANN vs. CART-LS ($p = 0.3877$) and ANN vs. S-PLUS ($p = 0.1945$) we observe that ANN is better than both CART-LS and S-PLUS, and will be placed fourth in the rank order since we already have the first three. CART-LS will be placed before S-PLUS because comparisons CART-LS vs. S-PLUS ($p = 0.8682$) and S-PLUS vs. CART-LS ($p = 0.9959$) demonstrate that CART-LS performs slightly better than S-PLUS. Hence, CART-LS and S-PLUS will be placed fifth and sixth in the final rank order.

Performance orders for both AAE and ARE are shown in Table 7. The modeling techniques are ordered from left to right with decreasing prediction accuracy. The symbol $<$ in the table indicates that the left hand side method has better fault prediction than the method on the right hand side. Thus, it is observed that CART-LAD and CBR yield better fault prediction as compared to MLR and ANN, which in turn are better predictors than CART-LS and S-PLUS.

## 6. Conclusion

Software reliability is an important attribute of high-assurance and mission-critical systems. Such complex systems are heavily dependent on the reliability and stability of their underlying software applications. The challenges involved in achieving high software reliability increases the importance of developing and quantifying measures for software quality. Early software fault prediction, a proven technique for achieving high software reliability, can be used to direct cost-effective software quality enhancement efforts to modules that are likely to have a high number of faults. Software quality models based on software metrics can yield predictions with useful accuracy. Such models can be used for early fault predictions in software quality estimation applications.

In this paper we compare the fault prediction accuracies of six commonly used prediction modeling techniques, CART-LS, CART-LAD, S-PLUS, CBR, ANN, and MLR. The large-scale case study used in this comparative study, consisted of data collected over four successive system releases of a very large legacy telecommunications system. Models were built using RAW metrics as well as domain metrics (PCA). Two-way ANOVA models, with two blocking variables (system release and model type) were designed (over all releases) to investigate: if the releases were different from each other; if the techniques were different from each other, and if the RAW models were different from the corresponding PCA models. The ANOVA models were designed with average absolute error and average relative error as the response variables.

From the ANOVA models, it was observed that the releases and the modeling methods were significantly different than their respective counterparts, while the RAW models and PCA models gave similar results. Therefore, it is indicated that

PCA may not necessarily improve fault prediction accuracy of software quality models. However, it should be noted that PCA removes correlation among the RAW metrics and the resulting models are more robust. Multiple-pairwise comparisons for the six modeling techniques were performed, and a performance or rank order was determined based on the *p*-values obtained. The comparisons were performed for both AAE and ARE. The rank order of the six modeling methods suggest that CART-LAD and CBR have superior fault prediction accuracy than MLR, ANN, CART-LS, and S-PLUS. In the final rank order for both AAE and ARE, CART-LAD was ranked first while S-PLUS was ranked sixth.

Future work in related research areas may include investigating a similar comparative study, with software metrics from a software system other than a telecommunications system.

## Appendix

### *Principle Components Analysis*

Software metrics extracted (RAW metrics) from configuration and problem reporting systems are often heavily correlated to each other (Khoshgoftaar et al., 2000c). This is usually because they often represent measurements of related attributes of the given software system. The correlation among the independent variables, can often lead to poor robustness and prediction accuracy of models built based on them. (PCA) is a statistical technique that is used to alleviate the problems due to correlation of independent variables.

The RAW metrics are transformed into a smaller set of linear combinations that account for, most if not all the variance of the RAW data set. PCA also reduces the number of independent variables used in building models. The principle component variables are called domain metrics as compared to original independent variables which form the RAW metrics. The first principle component, accounts for the largest fraction of the total variance in the original data. Let's denote the first component by $PC_1$. Thus $PC_1$ is the linear combination of the observed independent variables $x_j$, where $j = 1, 2, \ldots, m$.

$$PC_1 = w_{(1)1}x_1 + w_{(1)2}x_2 + \cdots + w_{(1)m}x_m \tag{31}$$

In the above equation, the weights $w_{(1)1}, w_{(1)2}, \ldots, w_{(1)m}$ have been chosen to maximize the ratio of the variance of $PC_1$ to the total variance, subject to the constraint that $\sum_{j=1}^{m} w_{(1)j}^2 = 1$. The second principle component, $PC_2$, is the weighted linear combination of the observed variables that are not correlated with the first linear combination (i.e., $PC_1$), and accounts for the maximum amount of the remaining total variance. Let's denote the second component by $PC_2$. In general, the $i$th principle component is the weighted linear combination of the $x$'s and is given by,

$$PC_i = w_{(i)1}x_1 + w_{(i)2}x_2 + \cdots + w_{(i)m}x_m \tag{32}$$

It is possible to extract the same number of principle components as the number of the original variables. The goal, however, is to account for most of the total variance with as few principle components as possible. Therefore, a stopping rule is introduced to choose as few domain metrics as possible. Hence, given $m$ software metrics, a stopping rule chooses $p \ll m$ domain metrics and ignores the remaining domain metrics because they have insignificant variation across the data set. The stopping rule, terminates principle components analysis, once a particular variance is accounted for during analysis.

Suppose we have $m$ product measurements on each of the $n$ modules. PCA performs the following calculations, given an $n \times m$ matrix of standardized metric data, $\mathbf{Z}$.

1. Compute the covariance matrix, $\mathbf{\Sigma}$, of $\mathbf{Z}$.

2. Compute the eigenvalues, $\lambda_j$, and the eigenvectors, $\mathbf{e}_j$, of $\mathbf{\Sigma}$, $j = 1, \ldots, m$.

3. Minimize the dimensionality of the data. If we choose to explain at least 90% of the total variance of the original standardized metrics, we then choose the minimum $p$ such that $\sum_{j=1}^{p} \lambda_j / m \geq 0.90$.

4. Compute a standardized transformation matrix $T$, where each column is defined as,

$$\mathbf{t}_j = \frac{\mathbf{e}_j}{\sqrt{\lambda_j}} \quad \text{for } j = 1, \ldots \tag{33}$$

5. Compute the domain metrics for each module, where

$$D_j = \mathbf{Z}\mathbf{t}_j \tag{34}$$

$$\mathbf{D} = \mathbf{Z}\mathbf{T} \tag{35}$$

The final result, of a principle components analysis of a given raw metrics, is an $n \times p$ matrix of domain metrics data $\mathbf{D}$, where each domain metric, $D_j$, has a mean of zero and a unit variance.

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## Notes

1. CART stands for the Classification and Regression Trees tool, while S-PLUS is a S language-based statistical modeling tool.
2. Not to be confused with ARE (Section 3.2).
3. Notations in this Section are independent to those of other sections. They are used exclusively for illustrating the theory of neural networks.
4. Not to be confused with ARE. Please refer to Section 2.1 for details.

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**Taghi M. Khoshgoftaar** is a professor of the Department of Computer Science and Engineering, Florida Atlantic University and the Director of the Empirical Software Engineering Laboratory. His research interests are in software engineering, software metrics, software reliability and quality engineering, computational intelligence, computer performance evaluation, data mining, and statistical modeling. He has published more than 200 refereed papers in these areas. He has been a principal investigator and project leader in a number of projects with industry, government, and other research-sponsoring agencies. He is a member of the Association for Computing Machinery, the IEEE Computer Society, and IEEE Reliability Society. He served as the general chair of the 1999 International Symposium on Software Reliability Engineering (ISSRE'99), and the general chair of the 2001 International Conference on Engineering of Computer Based Systems. Also, he has served on technical program committees of various international conferences, symposia, and workshops. He has served as North American editor of the *Software Quality Journal*, and is on the editorial boards of the journals *Empirical Software Engineering, Software Quality, and Fuzzy Systems.*

**Naeem Seliya** received the MS degree in Computer Science from Florida Atlantic University, Boca Raton, FL, USA, in 2001. He is currently a PhD student in the Department of Computer Science and Engineering at Florida Atlantic University. His research interests include software engineering with computational intelligence, software metrics, software architecture, computer data security, and software quality and reliability modeling.