CATDAT
A Program For Parametric And Nonparametric Categorical Data Analysis

User's Manual, Version 1.0

Annual Report 1999

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CATDAT

a program for parametric and nonparametric categorical data analysis
User's manual, version 1.0
http://www.fs.fed.us/rm/boise/fish/catdat/catdat.html

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Natural resource professionals are increasingly required to develop rigorous statistical models that relate environmental data to categorical responses data (e.g., species presence or absence). Recent advances in the statistical and computing sciences have led to the development of sophisticated methods for parametric and nonparametric analysis of data with categorical responses. The statistical software package CATDAT was designed to make some of these relatively new and powerful techniques available to scientists. The CATDAT statistical package includes 4 analytical techniques: generalized logit modeling, binary classification tree, extended K-nearest neighbor classification, and modular neural network. CATDAT also has 2 methods for examining the classification error rates of each technique and a Monte Carlo hypothesis testing procedure for examining the statistical significance of predictors. We describe each technique provided in CATDAT, present advice on developing analytical strategies, and provide specific details on the CATDAT algorithms and discussions of model selection procedures.

Introduction

Natural resource professionals are increasingly required to predict the effect of environmental or anthropogenic impacts (e.g., climate or land-use change) on the distribution or status (e.g., strong/ depressed/ absent) of animal populations (see Example 1). These predictions depend, in part, on the development of rigorous statistical models that relate environmental data to categorical population responses (e.g., species presence or absence). Unfortunately, categorical responses cannot be modeled using the statistical techniques that are familiar to most biologists, such as linear regression. In addition, environmental data are often non-normal and/or consist of mixtures of continuos and discrete-valued variables, which cannot be analyzed using traditional categorical data analysis techniques (e.g., discriminant analysis). Recent advances in the statistical and computing sciences, however, have led to the development of sophisticated methods for parametric and nonparametric analysis of data with categorical responses. The statistical software package CATDAT, an acronym for CATegorical DATa analysis, was designed to make some of these relatively new and powerful techniques available to scientists.

CATDAT analyses are not restricted to the development of predictive models. Categorical data analysis can be used to find the variables (or combination thereof) that best characterize pre-defined classes (i.e., categories). For example, CATDAT has been used to determine which physical habitat features best characterize stream habitat types (see Example 2). Categorical data analysis can also be used to examine the efficacy of new classification systems or to determine if existing classification systems can be applied under new conditions (see Examples 1 and 2).

The CATDAT statistical package includes 4 analytical techniques: generalized logit modeling, binary classification tree, extended K-nearest neighbor classification, and modular neural network. CATDAT also has 2 methods for examining the classification error rates of each technique and a Monte Carlo hypothesis testing procedure for examining the statistical significance of predictors. In the following sections, a brief description of each technique is provided to introduce the user to CATDAT. For a thorough theoretical treatment of the CATDAT models and an assessment of the performance of each technique, see Haas et al. (In prep.). Specific details on the CATDAT algorithms and discussions of model selection procedures can be found in Details. Additionally, definitions for much of the terminology used throughout this manual can be found in Table 1.1. We also strongly encourage users to consult the references cited throughout this manual for a more thorough understanding of the uses and limitations of each technique.

Generalized logit model.- Generalized logit models include a suite of statistical models that are used to relate the probability of an event occurring to a set of predictor variables (Agresti 1990). A well-known form of the generalized logit model, logistic regression, is used when there are 2 response categories. When the probability of several mutually exclusive responses are estimated simultaneously based on several predictors, the form of the generalized logit model is known as the multinomial logit model. It is similar to other traditional linear classification methods, such as discriminant analysis, where classification rules are based on linear combinations of predictors. However, generalized logit models have been found to outperform discriminant analysis when the data are non-normal and when many of the predictors are qualitative (Press and Wilson 1978). For an excellent introduction to generalized logit models, see Agresti (1996) and for a more detailed discussion, see Agresti (1990).

***Classification tree*.-** Tree-based classification is one of a larger set of techniques recently developed for analyzing non-standard data (e.g., mixtures of quantitative and qualitative predictors; Brieman et al. 1984). Classification trees consist of a collection of decision rules (e.g., if A then "yes", otherwise "no"), which are created during a procedure known as recursive partitioning (see Details). Consequently, the structure of tree classification rules differ significantly from techniques, such as discriminant analysis and generalized logit models, where classification rules are based on linear combinations of predictors. For illustration, Figure 1.1 depicts a greatly simplified example of recursive partitioning for a data set containing two response categories, *A* and *B*. The tree growing process begins with all of the data contained in parent node, t_1. The initial partition, at X = 30, produced child nodes t_2, which contained of an equal number of members of both categories and t_3, a relatively homogeneous node (i.e., 8/9 = 89% *B*). The second partition of parent node t_2, at Y = 20, produced child nodes t_4, which contained a majority of category *A* and t_5, with a majority of *B*. Assuming that the partitioning was complete, the predicted response at each terminal node would be the category with the greatest representation (i.e., the mode of the distribution of the response categories). In this example, the predicted responses would be *B*, *A*, and *B* for nodes t_3, t_4, and t_5, respectively. The recursive partitioning technique also makes tree classifiers more flexible than traditional linear methods. For example, classification tree models can incorporate qualitative predictors with more than 2 levels, integrate complex mixtures of data types, and automatically incorporate complex interactions among predictors. One drawback however, is that the statistical theory for tree-based models remain in the early stages of development (Clark and Pregibon 1992). For a though description of tree-based methods, consult Brieman et al. (1984).

***Nearest neighbor classification*.-** *K*-nearest neighbor classification (KNN), also known as nearest neighbor discriminant analysis, is used to predict the response of an observation using a nonparametric estimate of the response distribution of its *K* nearest (i.e., in predictor space) neighbors. Consequently, KNN is relatively flexible and unlike traditional classifiers, such as discriminant analysis and generalized logit models, it does not require an assumption of multivariate normality or strong assumption implicit in specifying a link function (e.g., the logit link). KNN classification is based on the assumption that the characteristics of members of the same class should be similar and thus, observations located close together in covariate (statistical) space are members of the same class or at least have the same posterior distributions on their respective classes (Cover and Hart 1967). For example, Figure 1.2 depicts a simplified example of the classification of unknown observations, *U1*and *U2*. Using a 1-nearest neighbor rule (i.e. *K*=1) the unknown observations (*U1* and *U2*) are classified into the group associated with the 1 observation located nearest in predictor space (i.e., groups *B* and *A*, respectively). In addition to its flexibility, KNN classification has been found to be relatively accurate (Haas et al. In prep.). One drawback however, is that KNN classification rules are difficult to interpret because they are only based on the identity of the *K* nearest neighbors. Therefore, information for the remaining *n* - *K* classifications is ignored (Cover and Hart 1967). For an introduction to KNN and similar classification techniques, consult Hand 1982.

***Modular neural network*.-** Artificial neural networks are relatively new classification techniques that were originally developed to simulate the function of biological nervous systems (Hinton 1992). Consequently, much of the artificial neural network terminology parallels that of biological fields. For example, fitting (i.e., parameterizing) an artificial neural network is often referred to as "learning". Although they are computationally complex, artificial neural networks can be thought of as simply a collection of interconnected functions. These functions, however, do not include explicit error terms or model a response variable's probability distribution, which is in sharp contrast to traditional parametric methods (Haas et al. In prep.). However, artificial neural network classifiers are quite often extremely accurate (Anand et al. 1995). Unfortunately, they are generally considered black-box classifiers because of difficulties in interpreting the complex nature of their interconnected functions. An excellent introduction to artificial neural networks can be found in Hinton (1992). For a more thorough treatment, consult Hertz et al. (1991).

Manual format. - The *Data entry*, *Terminal dialogue*, and *Output* sections are the heart of the manual and should be read prior to running CATDAT. The *Data entry* section describes the structure of a CATDAT data file and should be thoroughly reviewed prior to creating a data file. The *Terminal dialogue* section describes how to specify an analysis and provides specific information on analytical options, while the *Output* section explains the CATDAT output. Thorough examples of analyses are provided in *Examples* and a description of commonly encountered error messages, with some potential solutions, are given in *Catdat info*. The catdat info section also contains the installation instructions, computer requirements, and troubleshooting options. Definitions of the much of the terminology used in the manual can be found in Table 1.1.

Table 1.1. Definitions of terms used throughout the CATDAT manual and their synonyms.

Term	Definition
Activation function	Maps the neural net output into the bounded range 0, 1
Categorical response	A response variable for which the measurement scale consists of a set of categories, e.g., alive, dead, good, bad
Classifier	A model created via categorical data analysis
Model training	Parameterizing or fitting a model, also referred to as learning for neural networks
Nonparametric data analysis	Procedures that do not require an assumption of the population distribution (e.g., the normal distribution) from which the sample has been selected.
Parametric data analysis	Procedures that require an assumption of the underlying population distribution. The appropriateness of these procedures depends, in part, upon the fulfillment of this assumption.
Predictor	An explanatory variable, an independent variable in the generalized logit model
Response	The class or category from which an observation was selected or predicted to be a member
Test data	Data with known responses that were not used to fit the classification model
Training data	Data that were used to fit (i.e., parameterize) the classification model
Unknown data	Data for which the true responses are unknown

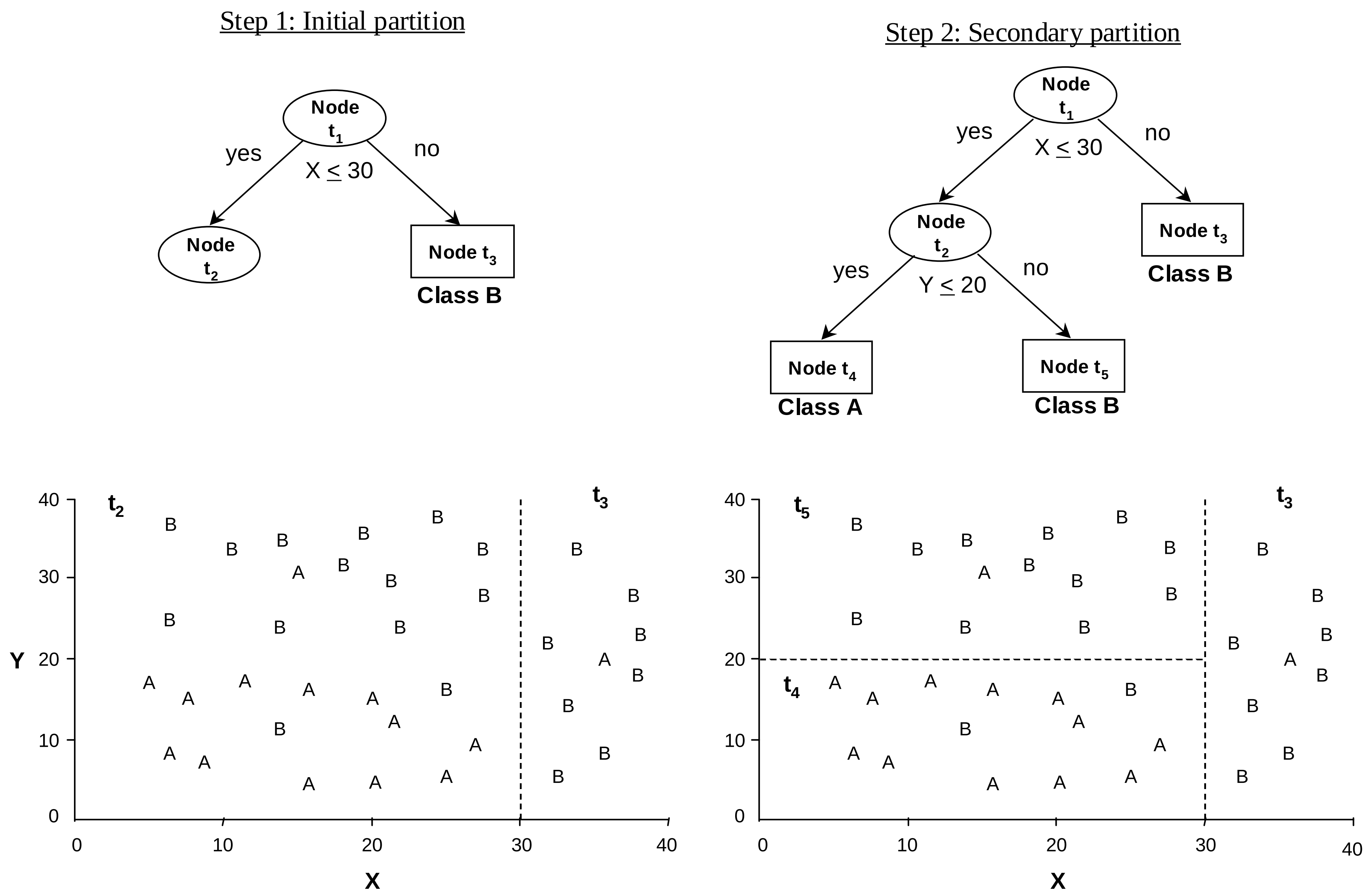


Figure 1.1. An example of recursive partitioning. The trees (top) correspond to their respective graphs (below). The initial partition (left) is at X=30 with the corresponding tree decision if X ≤ 30 go left.. The second partition is at Y = 20 with the corresponding tree decision if Y ≤ 20 go left. Partitions are separated by broken lines and are labeled with their corresponding tree node identifiers (t). Non-terminal nodes are represented by ovals and terminal nodes by boxes.

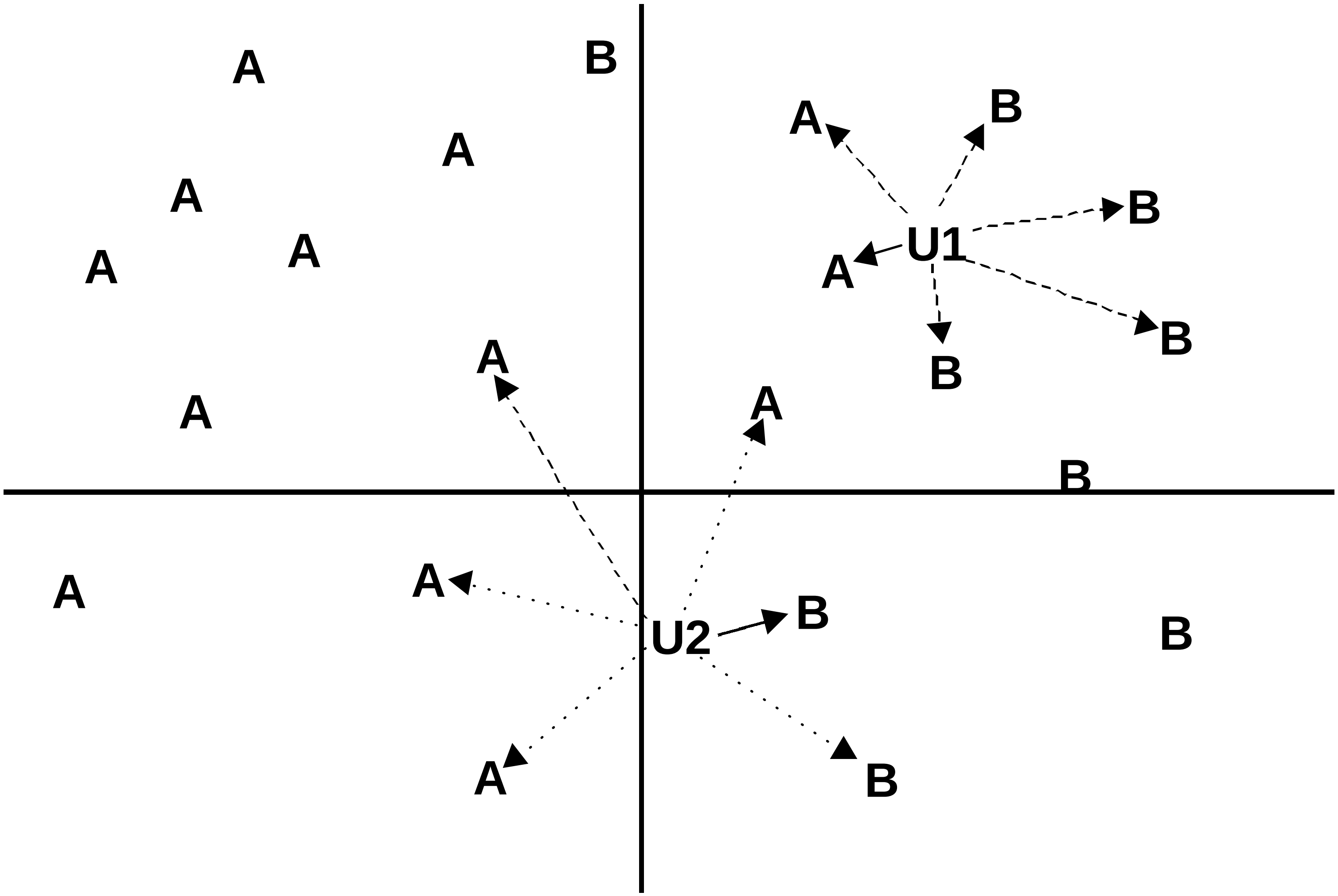


Figure 1.2. A simplified example of the classification of unknown observations, U1 and U2, as members of one of two groups, A or B. Arrows represent the distance from the unknown observations to their nearest neighbors. Using a *K* = 1 nearest neighbor classification rule (solid arrows), unknown observations U1 and U2 would be classified as members of groups A and B, respectively. A *K* =6 nearest neighbor rule (all arrows), however, would classify U1 and U2 as members of groups B and A, respectively.

Data Input

CATDAT data files can easily be created from ASCII files exported from spread sheets (e.g., Applix, Excel, Lotus 1,2, 3) and other database management software (e.g., Oracle, Dbase, Paradox). These data files can be used repeatedly, which allows one to perform several analyses with the same data. For example, a single data set can be used to compare the classification accuracy of the various techniques or to gain insight into the rule sets generated by the black-box classifiers.

All CATDAT data files must be single-space delimited and should consist of two corresponding sections, the heading and body. The data file heading can be created and attached to the exported ASCII file using a text editor. The heading always contains three lines that are used to identify the response categories and predictors. The first line is used to declare the number and names of the response categories, which should not exceed 10 characters in length. Their order in should correspond with the number used to identify each response category in the data file body. For example, the first line of the ocean-type chinook salmon data file heading (Table 2.1) identifies 4 response categories, *Strong*, *Depressed*, *Migrant*, and *Absent*, which are represented by the numbers 1, 2, 3, and 4 respectively, in the first column of the data file body. The second line of the heading is used to declare the number and name of the quantitative (i.e., continuous, ratio, interval) predictors. Their order in the heading should correspond with their order in the data file body. For example, the ocean-type chinook data file (Table 2.1) contains 11 quantitative predictors, *Hucorder*, *Elev*, *Slope*, *Drnden*, *Bank*, *Baseero*, *Hk*, *Ppt*, *Mntemp*, *Solar,* and, *Rdmean*. Consequently, column 2 in the data file body contains the *Hucorder* data, column 3 contains the *Elev* data, and so forth. The third line of the heading is used to declare the number and name of the qualitative (i.e., nominal, class) predictors. Similar to the quantitative predictors, their order in line 3 should correspond to their column order in the data file body. The third line of the heading must also be terminated with an asterisk (Table 2.1 and 2.2). If the data contains no quantitative or qualitative predictors, a zero must begin line 2 or 3, respectively. For example, the Ozark stream channel-unit data (Table 2.2) has 5 quantitative predictors, but zero qualitative predictors. Thus, the third line of the heading begins with a zero and ends with an asterisk (*).

The data file body contains the data to be analyzed with CATDAT. Each line of the data file body contains a single observation. The first column always contains the response category, which can only be represented by an integer greater than zero (i.e., zeros cannot be used to represent response categories). The quantitative and qualitative predictors then follow in the order listed in lines 2 and 3 of the heading, respectively, with a single space between each. Quantitative predictors should not exceed single precision limits (i.e., approximately 7 digits) and qualitative predictor categories can only be represented by an integer greater than zero. In addition, observations with missing values must be removed from the data file prior to all analyses.

Table 2.1. Ocean-type chinook salmon population status data in the correct format for input into CATDAT. This data file contains 4 response categories, 11 quantitative predictors, and 1 qualitative predictor. See *Data Input* for a complete description of format.

```
4 Strong Depressed Migrant Absent
11 Hucorder Elev Slope Drnden Bank Baseero Hk Ppt Mntemp Solar Rdmean
1 Mgntcls *
1 18 2193 9.67 0.6843 73.953 12.2004 0.37 979.612 7.746 273.381 2.0528 1
2 20 2793 19.794 1.3058 58.708 29.9312 0.3697 724.264 6.958 260.583 3.440 3
1 22 2421 23.339 1.231 44.845 36.3927 0.3697 661.677 7.6 254.733 2.364 2
3 23 3833 34.553 1.3661 19.092 52.7353 0.3692 714.559 6 252.889 1.489 1
4 36 1925 23.797 1.0873 28.026 36.3066 0.3695 544.183 8.5 252.857 2.336 2
4 38 1775 13.549 0.7118 67.898 19.0161 0.3699 757.989 8.533 276.156 1.311 3
2 47 1387 17.264 1.582 35.8019 25.6341 0.3696 326.714 9.688 249.938 2.372 2
3 168 732 7.69 1.3472 92.8437 6.6349 0.2477 183.966 11.652 262.913 0.4281 1
1 234 1606 9.209 1.2716 84.167 8.2979 0.3186 346.479 10.478 289.13 0.8019 1
4 247 1750 15.899 2.4221 86.722 21.3021 0.3462 341.379 11 290.875 1.1037 3
.
....remainder of data....
.
4 263 135 22.431 1.06 79.4377 23.1364 0.2601 304.631 10.111 275.037 0.946 1
1 1418 768 5.677 0.3317 99.1893 3.0148 0.2114 210.137 11.21 262.01 0.293 1
2 0 2992 17.831 1.5458 68.8551 26.3373 0.3695 411.158 6.929 258.071 1.866 2
```

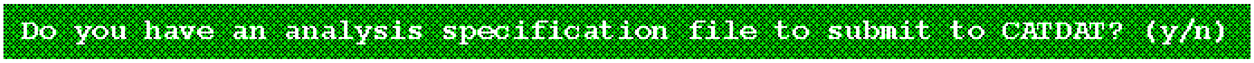
Table 2.2. Ozark stream channel unit data in the correct format for input into CATDAT. This data file contains 5 response categories, 5 quantitative predictors, and no qualitative predictors. See *Data Input* for a complete description of format.

```
5 Riffle Glide Edgwatr Sidchanl Pool

5 Depth Current Veget Wood Cobb

0 *

1 1.95 1.004 0 0 4.394

1 2.08 1.075 1.386 0 4.111

1 1.79 1.224 1.792 1.099 4.19

2 1.61 .863 0 0 4.025

2 1.61 1.109 0 0 4.19

4 2.20 1.157 0 1.099 4.19

.

....remainder of data....

.

4 2.49 0 1.386 2.197 0

5 1.61 .095 0 0 2.398

3 1.95 0 4.111 3.258 0

4 3.14 .166 0 3.258 3.714

4 2.89 .231 0 3.045 3.932

1 1.89 .174 0 0 3.714

4 1.79 .207 3.045 1.386 3.434

5 1.61 .3 1.792 0 4.331
```

Terminal dialogue

Activation. - CATDAT is designed as an interactive computer program. It asks the user a series of questions about the specifications of the analysis. The answers to these questions are written to an "analysis specification file", which is in ACSII (i.e., text) format. Analysis specification files can also be manually created or modified, which is very useful when investigating the optimal classification tree size, or the optimal number of K nearest neighbors or hidden nodes for the modular neural network. After installation, CATDAT is activated by typing "catdat" at the prompt.

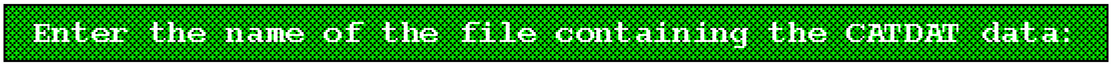
Specifying the type of analysis.- The CATDAT analysis specification subroutines are case sensitive. Consequently, all questions must be answered with lower-case letters. In addition, the names of input and output files should consist no more than 12 alphanumeric characters. After activation, CATDAT begins with the question:



```
Do you have an analysis specification file to submit to CATDAT? (y/n)
```

If the answer is no, type "n" and press RETURN or ENTER. The user will then be asked several questions about the name of the input file and the type of analysis to be performed (see the following sections). If the answer is yes, type "y" and press RETURN or ENTER. CATDAT will then ask for the name of the analysis specification file. Type in the name of the file and the analysis will proceed automatically. Although analysis specification files can be created with most word processing software, we recommend only editing those created by CATDAT. The format of the CATDAT analysis specification files is precise (Table 3.1 and 3.2)and analysis specification file may cause CATDAT to perform the wrong analysis or crash. Consequently, mistakes in an

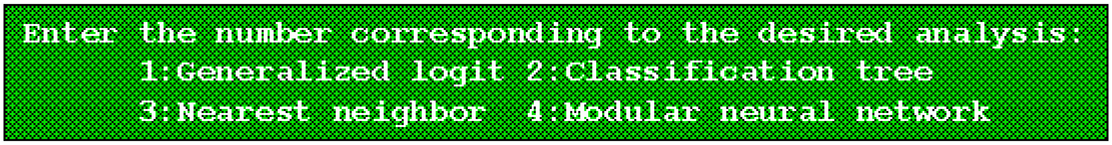
If an analysis specification file is not submitted, CATDAT then asks:



```
Enter the name of the file containing the CATDAT data:
```

This file must be in the correct format and should contain the data for analysis or the training data when classifying unknown or test data sets. If CATDAT cannot find the data file, it will ask for the name of the file again. Make sure that the file name is spelled correctly (CATDAT is case sensitive) and that the path (i.e., the location of the file) is also correct. If CATDAT cannot locate the file after several attempts, the program must be terminated manually by holding down the CONTROL ("Ctrl") button and hitting the "c".

Once the data file has been correctly specified, CATDAT will ask:

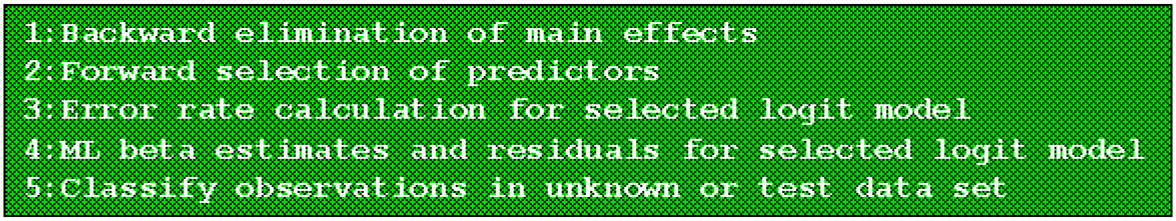


```
Enter the number corresponding to the desired analysis:
      1:Generalized logit 2:Classification tree
      3:Nearest neighbor  4:Modular neural network
```

After selecting the desired analysis, CATDAT will provide an analysis-specific list of options, outlined below.

Generalized logit model options. -CATDAT constructs *J*-1 baseline category logits, where *J* is the number of response categories (see Details). The response category coded with the largest number (i.e., the last category in the data file heading) is always used as the baseline (*J*) category during model parameterization. For example, the *Absent* response category would be used as the baseline for the ocean-type chinook salmon population status data (Table 2.1). For the most robust model, the most frequent response (i.e., the category with the greatest number of observations) should be used as the baseline (Agresti 1990). Consequently, we recommend that users code their response categories accordingly. In addition, the generalized logit model cannot directly incorporate qualitative predictors. Thus, qualitative predictors should be recoded into dummy regression variables (i.e., 0 or 1, see Example 1). We also recommend using only the qualitative predictors that occur in at least 10% of observations, because rarely occurring predictor categories may cause unstable maximum likelihood estimates (Agresti 1990).

After choosing the generalized logit model, CATDAT will provide the following list of options:



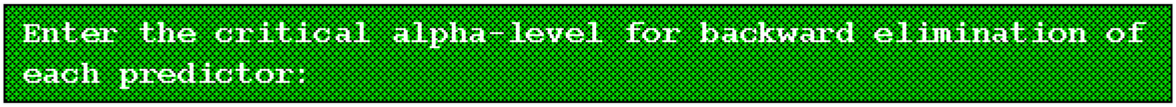
```
1:Backward elimination of main effects
2:Forward selection of predictors
3:Error rate calculation for selected logit model
4:ML beta estimates and residuals for selected logit model
5:Classify observations in unknown or test data set
```

The first two choices are mechanized model selection procedures that use hypothesis tests. Option 1 is used to select statistically significant main effects with the Wald test, whereas option 2 is for forward selection of statistically significant predictor and two-way interactions using the

Score statistic (see Details). Option 3 is used to estimate the model prediction error rates and option 4 will provide maximum likelihood β_j estimates, goodness-of-fit statistics, and studentized Pearson residuals for selected logit models. Option 5 is used to classify unknown or test data using the generalized logit model parameterized with a training data set, specified earlier.

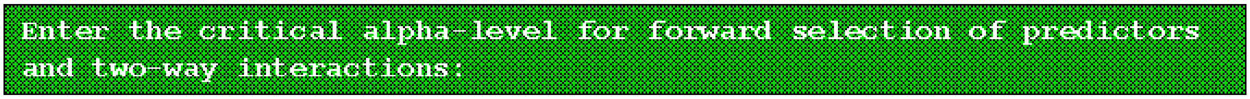
If option 2 is selected, the user will be asked to specify the forward selection of predictors and two-way interactions or two-way interactions only. In addition, CATDAT will prompt the user to select the critical alpha-level for the hypothesis tests.

(if option = 1)



```
Enter the critical alpha-level for backward elimination of
each predictor:
```

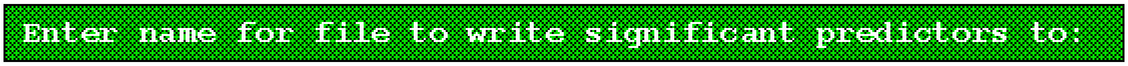
(or option = 2)



```
Enter the critical alpha-level for forward selection of predictors
and two-way interactions:
```

This alpha is used to calculate the critical value for the Wald test or Score statistic. Predictors or interactions that exceed the critical value for their respective hypothesis test will be output and written to a file, below. To maintain a relatively consistent experiment-wise error rate, we suggest users adjust the alpha-level (a) with a Bonferroni correction (i.e., a/k, where k= number of predictors or interactions to be tested).

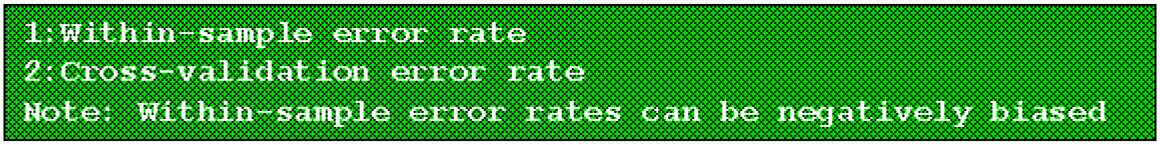
CATDAT will then ask for the name of a file to output the significant predictors or interactions.



```
Enter name for file to write significant predictors to:
```

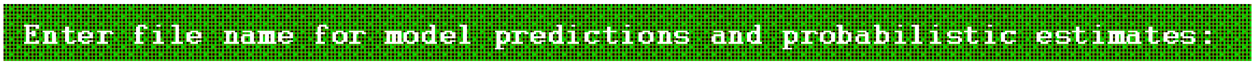
This significant predictor file can be then submitted to CATDAT later for error rate estimation or to estimate the maximum likelihood β_j and output the residuals. If a filename is not entered, the significant predictors will be written to the default file "output.dat".

If the error rate option is selected, CATDAT will ask for the type of error rate estimate.



```
1:Within-sample error rate
2:Cross-validation error rate
Note: Within-sample error rates can be negatively biased
```

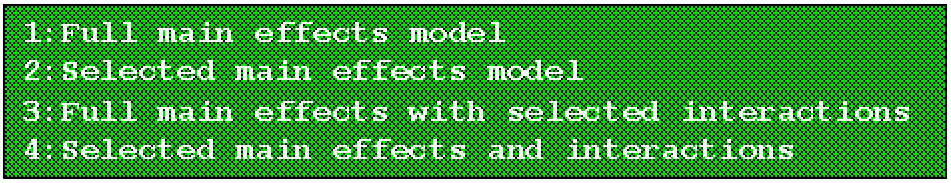
The within-sample error rate, also known as the apparent error rate, is the classification error rate for the data that was used to fit the logit model. It is usually optimistic (i.e., negatively biased), whereas the cross-validation error rate should provide a much better estimate of the expected classification error rate of the logit model. To obtain a V-fold cross-validation rate, a test data set must be submitted (see Details, expected error rate estimation). CATDAT will then ask for the name of the file to output the predicted response, response probabilities, and predictor values for each observation.



```
Enter file name for model predictions and probabilistic estimates:
```

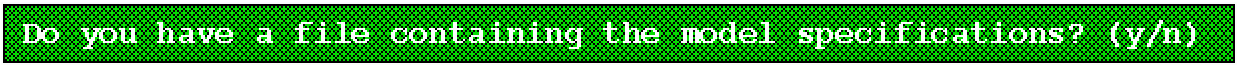
Selection of the maximum likelihood $\boldsymbol{\beta}_j$ estimates option (above) will prompt CATDAT to ask if the quantitative predictors should be normalized to the interval [0,1]. If the answer is yes, the maximum likelihood $\boldsymbol{\beta}_j$ will be estimated using the normalized data. Otherwise, they will be estimated with the untransformed (i.e., raw) data.

CATDAT will also ask for the structure of the logit model.



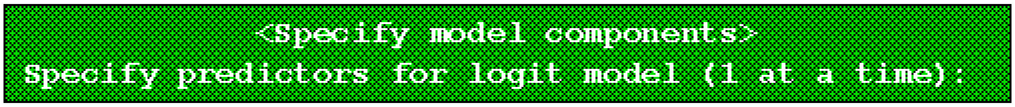
```
1:Full main effects model
2:Selected main effects model
3:Full main effects with selected interactions
4:Selected main effects and interactions
```

If the full main effects model is selected, the analysis will proceed with all of the predictors in the logit model. Selection of one the remaining three options will cause CATDAT to ask:



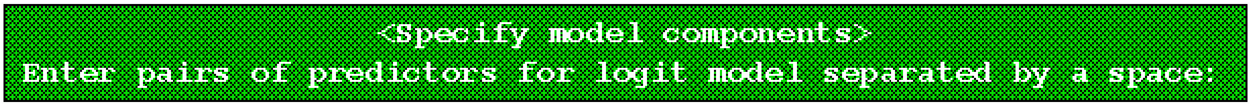
```
Do you have a file containing the model specifications? (y/n)
```

If you have a model specification file from a previous analysis or the significant predictor file from the hypothesis testing procedure, enter "y" and CATDAT will ask for the file name. Enter the file name and the analysis will proceed. If there isn’t a model specification file, answer "n" and CATDAT will ask:



```
            <Specify model components>
Specify predictors for logit model (1 at a time):
```

or for interactions

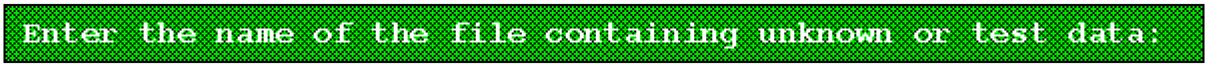


```
                  <Specify model components>
Enter pairs of predictors for logit model separated by a space:
```

Enter the name of a predictor, or a pair of predictors (i.e., interactions) separated by a space, and press ENTER or RETURN. CATDAT will then ask if more predictors or interactions are to be included in the model. Continue adding predictors or interactions in this manner until the desired model is achieved. Note that quadratic responses (i.e., x^2) can be modeled by entering the interaction of a quantitative predictor with itself in the logit model.

If the maximum likelihood $\boldsymbol{\beta}_j$ estimates and residuals option was previously selected, CATDAT will ask for the name of the residual file. Enter the name of the residual file and the analysis will proceed.

If classification of an unknown or test data set was selected, CATDAT will ask:

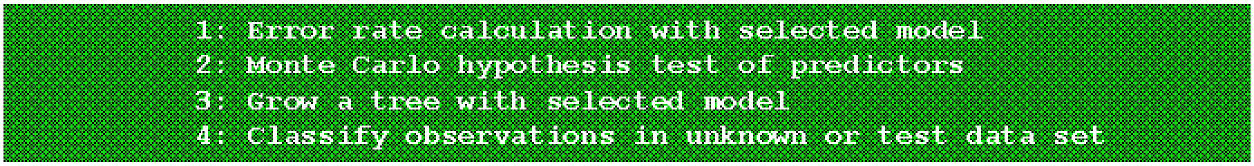


```
Enter the name of the file containing unknown or test data:
```

The file should have the identical format (i.e., same number of predictors) as the data set that was used to fit the logit model (i.e., the training data set, specified earlier) with **NO** data file heading. The unknown or test data file should also contain a response category, which in the case of an unknown observation, must simply be a nonzero integer less than or equal to the number of response categories in the training data set. CATDAT will also ask for the name of a file to output the classification predictions. After the fitting the logit model, this file will contain the original response category codes of the unknown or test data, predicted responses, the estimated probabilities for each response, and the original predictor values.

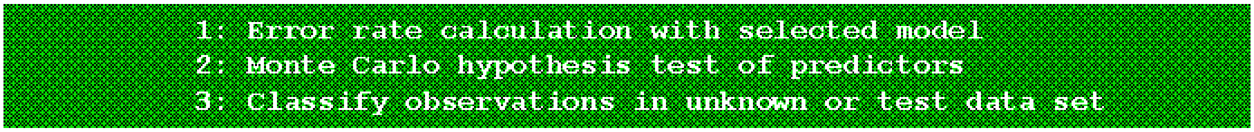
Classification tree, nearest neighbor, and modular neural network options.- When either of these three techniques are selected, CATDAT will ask for the "best" classification tree parameter and minimum partition size, the number of *K* nearest neighbors, or the number of modular neural network hidden nodes. These parameters are used to limit the number of K nearest neighbors or size of the classification tree and modular neural network and are necessary for model selection (see Details). Once the optimum value of these parameters is found, the same value should be used for the Monte Carlo hypothesis tests, to build the final classification tree, and for classifying an unknown or test data set.

For the classification tree, CATDAT has the following options:



```
1: Error rate calculation with selected model
2: Monte Carlo hypothesis test of predictors
3: Grow a tree with selected model
4: Classify observations in unknown or test data set
```

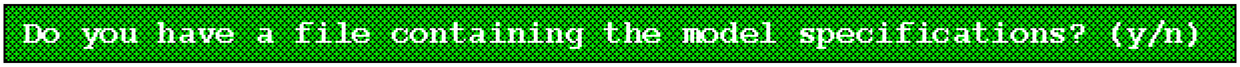
The options for *K*-nearest neighbor and the modular neural network include:



```
1: Error rate calculation with selected model
2: Monte Carlo hypothesis test of predictors
3: Classify observations in unknown or test data set
```

The error rate calculation option is used to estimate the expected error rate of the respective classifier and to select the best sized tree and the optimal number nearest neighbors (*K)* or modular neural network hidden nodes. Similar to the logit model, the user has the option of calculating the within-sample or cross-validation error rate. However, only the cross-validation error rate should be used for finding the optimum tree size, number of neighbors, or number of modular neural network hidden nodes (see Details, expected error rate estimation). In addition, the output files from the error rate estimation of the k-nearest neighbor include the average distance between each observation and its *k* neighbors and the modular neural network output contains the values of $\underline{Z}^*$.

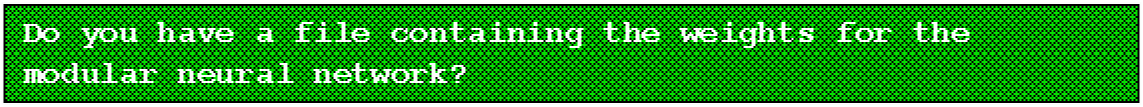
If the error rate or grow a tree options are specified, CATDAT will ask for the structure of the model (i.e., the full effects or selected effects). If a pre-selected model is desired, CATDAT will ask:



```
Do you have a file containing the model specifications? (y/n)
```

If you have a model specification file from a previous analysis, enter "y" and CATDAT will ask for the file name. Enter the file name and the analysis will proceed. If there isn’t a model specification file, answer "n" and CATDAT will ask for the names of the predictors to be included in the model. Similar to the generalixed logit model specification, enter the name of a predictor and press ENTER or RETURN. CATDAT will then ask if more predictors are to be included in the model. Continue adding predictors or interactions in this manner until the desired model is achieve.

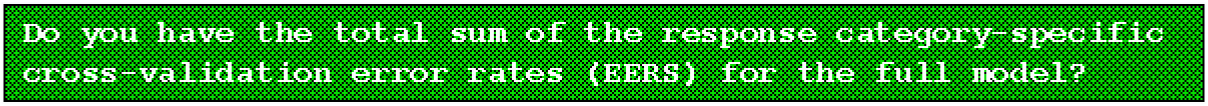
When using a modular neural network, CATDAT will also ask:



```
Do you have a file containing the weights for the
modular neural network?
```

These weights are analogous to the parameters of a generalized linear model, such as the logit model β_j. During the initial fit of the neural network, the answer to the above question will be "n" and initial weights will be randomly assigned and iteratively fit to the data (see Details). If the answer is yes, CATDAT will then ask for the name of the file. In addition, CATDAT will ask for the name of the file to write the final (i.e., fitted) weights of the neural network during error rate estimation.

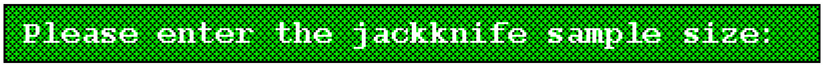
If a Monte Carlo hypothesis test is specified, CATDAT will ask:



```
Do you have the total sum of the response category-specific
cross-validation error rates (EERS) for the full model?
```

The sum of the category-specific cross-validation error rates for the full (i.e. all predictors) model (EER_F) is used to calculate the test statistic, T_s, for the Monte Carlo hypothesis test (see Details). If error estimates were calculated during a previous analysis (e.g., while determining the best classification tree size), answer "y" and CATDAT will ask for the value. If not, answer "n" and the value will be calculated by CATDAT. The Monte Carlo hypothesis test is time intensive. Thus, providing the full model error rates prior to the test can significantly shorten this time.

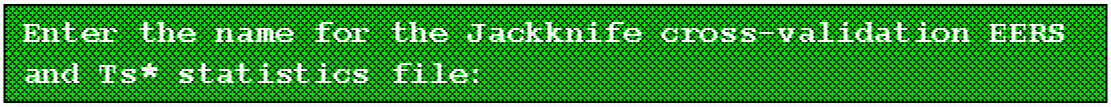
CATDAT will then ask:



```
Please enter the jackknife sample size:
```

The jackknife sample will be used to calculate the jackknife T_s^* for the hypothesis test (see Details). Because the T_s^* is potentially sensitive to the jackknife sample size, we recommend setting the sample size to 20-30% of the size of the entire data set. For example, the jackknife sample size for a data set with 1000 observations should be between 200 - 300. In addition, the user will be asked for the number of jackknife samples. These samples will be used to determine the distribution of the T_s^* statistic and thus, the p-value of the hypothesis test. For example, if the jackknife T_s^* exceeded the observed T_s in 1 of 100 jackknife samples, the p-value = 1/100 or 0.01. Consequently, hypothesis test requires a minimum of 50 samples for a reliable test statistic (Shao and Tu 1995). For the most robust test, we recommend using at least 300 samples.

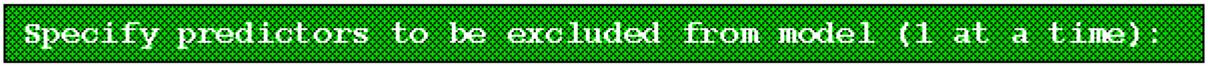
CATDAT will then ask:



```
Enter the name for the Jackknife cross-validation EERS
and Ts* statistics file:
```

This file will contain the full and reduced model cross-validation error rates and the T_s^* statistic for each jackknife sample.

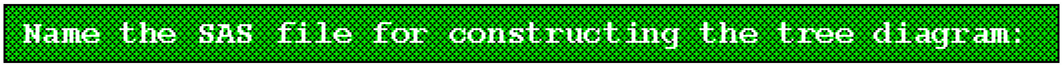
For the Monte Carlo hypothesis test, CATDAT will also ask for a file with the model specifications (i.e., predictors to be tested). This file should contain the predictors that are to be *excluded* (i.e., tested) from the respective classifier (see Details). If there is no model specification file, CATDAT will ask:



```
Specify predictors to be excluded from model (1 at a time):
```

Enter the name of a predictor and press ENTER or RETURN. CATDAT will then ask if more predictors are to be excluded. Continue adding predictors in this manner until the desired model is achieved.

When growing a classification tree with a selected model, CATDAT will ask:

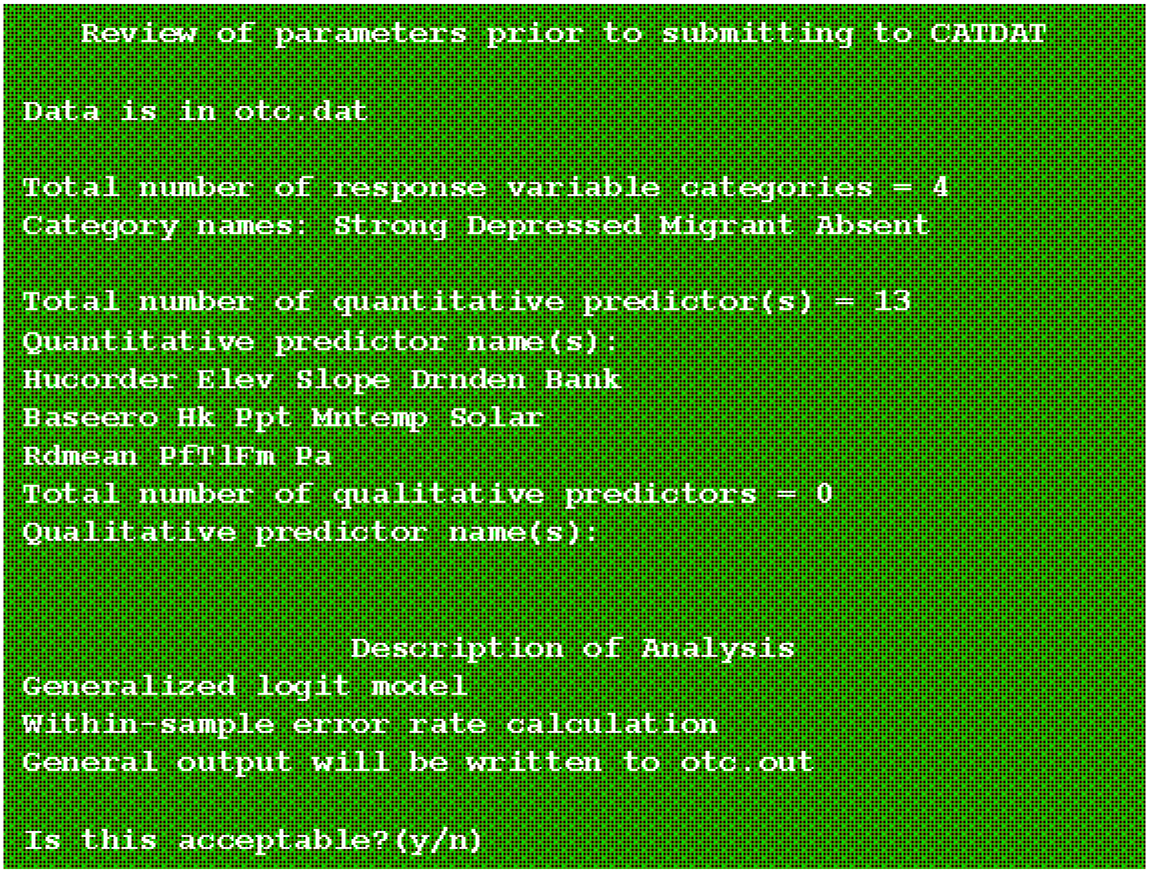


```
Name the SAS file for constructing the tree diagram:
```

The file name should end with the extension ".sas". After the tree is fit, this file can be submitted to SAS (1989) and the classification tree will be automatically drawn and written to gsasfile ‘tree.ps’. Trees can also be drawn manually using the CATDAT general output (see Output, classification tree blueprints).

CATDAT can also be used to classify an unknown or test data set with these three techniques. The directions for submitting an unknown or test data set are identical to those for the generalized logit model, outlined above.

***Naming the input-output files and review of the analysis.*-** After specifying the desired classification technique and options, CATDAT will ask for the names of the analysis specification and output files. The output file will contain the all of the program output not written to pre-specified files, such as the residual file. After naming the files, CATDAT will review the data file parameters and the options selected for the analysis, e.g.,



```
    Review of parameters prior to submitting to CATDAT

Data is in otc.dat

Total number of response variable categories = 4
Category names: Strong Depressed Migrant Absent

Total number of quantitative predictor(s) = 13
Quantitative predictor name(s):
Hucorder Elev Slope Drnden Bank
Baseero Hk Ppt Mntemp Solar
Rdmean PfT1Fm Pa
Total number of qualitative predictors = 0
Qualitative predictor name(s):


                 Description of Analysis
Generalized logit model
Within-sample error rate calculation
General output will be written to otc.out

Is this acceptable?(y/n)
```

If all of the parameters are correct, answer "y" and the analysis will begin. Otherwise, the user will be returned to the analysis specification subroutines.

Table 3.1. An analysis specification file written by CATDAT. The corresponding CATDAT data file can be found in Table 2.1. Note that field descriptors (in parenthesis) are shown for illustration. See Appendix A for a list of variable identifiers.

```
flenme    otc.dat (CATDAT data file)
nmquan    11      (the number of quantitative predictors)
esttyp    2       (specifies classification tree)
calc      2       (error rate calculation)
besttre   19      (BEST parameter)
selerr    2       (cross-validation, for within-sample error selerr = 1)
genout    otc.out (general output file)
nmcat     4       (the number of response categories)
Strong            (response category names)
Depressed
Migrant
Absent
nmprd     12      (the total number of predictors)
Hucorder          (quantitative predictor names)
Elev
Slope
Drnden
Bank
Baseero
Hk
Ppt
Mntemp
Solar
Rdmean
Mgnclus           (qualitative predictor name)
```

Table 3.2. An analysis specification file written by CATDAT. The corresponding CATDAT data file can be found in Table 2.2. Note that field descriptors (in parenthesis) are shown for illustration. See Appendix for a list of variable identifiers.

flenme	bccu.dat	(CATDAT data file)
nmquan	5	(the number of quantitative predictors)
sigp	0.0100000	(critical alpha-level)
esttyp	1	(specifies generalized logit model)
calc	7	(forward selection of main effects predictors)
fleout	bccu.mod	(output file with significant predictors)
genout	bccu.out	(general output file)
nmcat	5	(the number of response categories)
Riffle		(response category names)
Glide		
Edgwatr		
Sidchanl		
Pool		
nmprd	5	(the total number of predictors)
Depth		(quantitative predictor names)
Current		
Veget		
Wood		
Cobb		

Output

General output.- Prior to each analysis, CATDAT outputs a summary of the data that includes the total number of observations, number of observations for each response category, and the name and number of predictors (Table 4.1). If the data contains qualitative predictors, CATDAT outputs the frequency of each category. The summary data is useful for confirming that the data file heading and body are properly specified. For example, when the general output reports an incorrect number of observations per response category, it's usually an indication that the number of predictors was incorrectly specified in the data file heading. The summary is also useful for confirming that the last response category has the greatest number of observations for the generalized logit model. When all analyses are completed, CATDAT reports "Analysis completed".

Generalized logit model-specific output.- The output of the generalized logit model hypothesis tests includes the critical alpha-level and a summary table with the results of the backward elimination of main effects or forward selection of main effects and/or interactions. The summary table contains the statistically significant predictors or interactions, their associated Wald test or Score statistics, and the p-values (Table 4.2). When no main effects or interactions exceed the critical value, CATDAT outputs "*None found*" in the significant predictor table (Table 4.2).

The individual predictors or pairs of predictors that exceed their respective critical values are also written to the model specification file, with one predictor or interaction per line. The predictors are represented by numbers that correspond to their order in the data file heading. For example, numbers 1 and 2 would represent the first two predictors listed in the ocean-type chinook salmon status data file heading, *Hucorder* and *Elev* (Table 2.1). The main effects are always listed first followed by each pair of predictors (i.e., interaction), separated by a space. An asterisk is used to separate the main effects from the interactions.

The names of the generalized logit model predictors (i.e., main effects and/or interactions) are output prior to estimating the maximum likelihood $\boldsymbol{\beta}_j$. CATDAT then outputs the AIC$_c$, QAIC$_c$, and -2 log likelihood of the intercept-only and specified models and the log likelihood test statistic and its p-value. The $\boldsymbol{\beta}_j$ of the specified model are then output for each response category *j*, except the baseline (Table 4.3). Finally, the goodness-of-fit statistics are output and "studentized" Pearson residuals (Fahrmeir and Tutz 1994) are written to the specified file. Residual files are ASCII formatted, space-delimited, and contain the residuals and their associated chi-squared scores (see Details). Thus, they can be imported into most spreadsheets or statistical software packages for further analysis.

Classification tree blueprints.- The classification tree blueprints are output only when the "Grow a tree with selected model" option is selected during analysis specification. CATDAT outputs the BEST parameter, the number of nodes in the final "pruned" tree, the residual deviance, and the non-terminal and terminal node characteristics necessary for tree construction (Table 4.4). The non-terminal node characteristics include the parent node number, sub-tree deviance, the node numbers of its children, the covariate at the parent node and associated split-value, and the number of observations (i.e., the size) at the node. The terminal node characteristics consist of the node number, the residual deviance, the predicted response at the node, and the terminal node size. The classification tree can be draw manually or automatically by SAS when the tree SAS file is used. However, the node size and split values need to be added manually to the SAS graphics output, if desired (Figure 4.1).

An example of the interpretation of tree blueprints is shown for the chinook salmon population status data (Table 4.4 and Figure 4.1), the first parent node begins with all of the observations (n=477) and the initial split on the predictor *Elev*. The split-value of *Elev* is 2075 and thus, observations with *Elev* less than or equal to 2075 (n=136) go to the left-child node (i.e., down in the SAS graphics output) and observations that exceed 2075 (n=341) go to the right-child node. The next predictor at parent nodes 2 and 3 is *Hucorder* and the split-values are 1051 and 1823, respectively. This process continues until the tree is completed (Figure 4.1). For an explanation of tree terminology, see Details, classification tree.

Classification error rate output.- The format of the expected error rate output is similar for all classification techniques. CATDAT lists the type of classifier and error estimate (i.e., within-sample or cross-validation), and the model specifications (Table 4.5). For example, the model specifications for the generalized logit model include the main effects and/or interactions, whereas the BEST parameter and number of hidden nodes are listed for the classification tree and modular neural networks, respectively. The modular neural network output also includes the name of the source of the initial network weights (e.g., the file name or random number generator seed). In addition, the pairwise mean Mahalanobis distances between response groups is output prior to error rate estimation of the *K*-nearest neighbor classifier (see Details, nearest neighbor).

The remainder of the classification error output includes the overall (i.e., across response categories) number and proportion of misclassification errors (EER). Category-wise error rates include the number and proportion (EER) of misclassified observations per response category. CATDAT also reports the number of times a response category was predicted and the proportion (Perr) of those that were incorrect. For example, 50 observations were misclassified during cross-validation of the ocean-type chinook salmon status classification tree (Table 4.5, top). Of these, 11 observations from the *Strong* category, 23 from the *Depressed* category, 10 from the *Absent* category, and 6 from the *Migrant* category were misclassfied. Observations were most often classified as *Absen*t (359 observations), whereas only 16 observations were classified as *Strong*. However, 37.5% of the observations of the *Strong* predictions were incorrect (Table 4.5). The cross-validation subroutines used for estimating the expected error rates and the Monte Carlo hypothesis tests (below) are very computer and time intensive. Consequently, CATDAT periodically reports the degree of completion for these procedures to allow the user to estimate the amount of time needed to complete the analysis.

Monte Carlo hypothesis test output.- Similar to the classification error rate, output for the Monte Carlo hypothesis test is alike for all the classification techniques. CATDAT initially outputs the type of classifier, the classifier specifications (e.g., the number of *K* neighbors), and a list of the excluded predictor(s). The expected error rate for the full model, $\mathrm{EERS}_{\mathrm{F}}$, (i.e., all predictors) and reduced model $\mathrm{EERS}_{\mathrm{R}}$ (i.e., without the excluded predictors) are then estimated and reported (Table 4.6). The EERS that is estimated for the Monte Carlo hypothesis test is the sum of the category-wise EER. Therefore, it will differ from the overall EER estimated during cross-validation (outlined above). For example, the classification tree in Table 4.5 would have an $\mathrm{EERS}_{\mathrm{F}} = 0.5238 + 0.4035 + 0.0294 + 0.1017 = 1.0584$, which is also the $\mathrm{EERS}_{\mathrm{F}}$ shown in Table 4.6. This is to ensure that the hypothesis test is not sensitive to sharply unequal sample sizes among response categories (see Details). CATDAT then reports the jackknife sample size and number of jackknife samples. Finally, CATDAT outputs a summary of the jackknife T_{s}^{*} statistics and reports the estimated p-value. The p-value is the number of jackknife samples in which the jackknife T_{s}^{*} exceeded observed T_{s}. The jackknife cross-validation and T_{s}^{*} statistics file contains the EERS_F^*, EERS_R^*, and T_s^* for each jackknife sample and can be used to examine the distribution of the T_s^* statistic and verify the estimated p-value.

Output from the classification of unknown or test data.- When classifying unknown or test data sets, CATDAT outputs a general summary of the training data set including the names and number of predictors and response categories and the total number of observations. CATDAT also reports the type of classifier and relevant specifications (e.g., the number of hidden nodes). The training data summary ends with an "--END--" statement. The remainder of the output is a summary of the test or unknown data set including the total number of observations, the number and percentage (EER) of overall misclassification errors, and the residual tree deviance for test data, if applicable. The prediction files are ASCII formatted, single-space delimited and can therefore, be imported into a spread sheet or statistical software package for additional analyses. These files contain the original response category codes for the unknown or test data, the predicted responses, and the original raw data (Table 4.7).

Table 4.1. An example of CATDAT general output for data with (otc.dat, top) and without (bccu.dat, bottom) qualitative predictors. The corresponding data files are in Tables 2.1 and 2.2, respectively. The analysis-specific output would immediately follow this general output during program execution.

```
                 ---- CATDAT analysis of data in otc.dat ----

Qualitative predictor(s):

                   Mgnclus category           Frequency
                          1                     0.3061
                          2                     0.3187
                          3                     0.3690

Quantitative predictors:

Hucorder     Elev         Slope        Drnden       Bank         Baseero
Hk           Ppt          Mntemp       Solar        Rdmean

Observed frequencies of response variable categories

                                               Marginal
                           Response Count     frequency
                             Strong     21       0.0440
                          Depressed     57       0.1195
                            Migrant     59       0.1237
                             Absent    340       0.7128


Number of observations in otc.dat, 477
and number of predictors, 13
```

--- CATDAT analysis of data in bccu.dat ----

```
Quantitative predictors:

Depth        Current      Veget        Wood         Cobb

Observed frequencies of response variable categories

                  Marginal
Response  Count  frequency
    Riffle    53      0.1661
     Glide    65      0.2038
  Edgewatr    60      0.1881
  Sidchanl    64      0.2006
      Pool    77      0.2414


Number of observations in bccu.dat, 319
and number of predictors, 5
```

Table 4.2. CATDAT backward elimination of generalized logit model main effects (top) and forward selection of predictors and two-way interactions (bottom) for the Ozark stream channel-unit data in Table 2.1.

```
Full main effects model initially fit.
Backward elimination of generalized logit model main effects
Predictors accepted at P < 0.010000


            Wald Chi-
 Predictor             p-value
             square
     Depth   59.5209    0.000001
   Current   30.0978    0.000005
```

```
Forward selection of generalized logit model main effects and interactions
Main effects and interactions accepted at P < 0.010000


           Score Chi-
 Predictor             p-value
             square
     Depth  260.5298   0.000001
   Current  208.5219   0.000001


           Interaction  Score Chi-
   Predictor                          p-value
            Predictor     square
None found.
```

Table 4.3. CATDAT output for maximum likelihood β_j estimates of the full main effects model of Ozark stream channel-unit physical characteristics in Table 2.1.

```
Generalized logit model- Full main effects
Note: maximum likelihood estimation ended at iteration 10 because
log likelihood decreased by less than 0.00001


              Model fit and global hypothesis test H0: BETA = 0

               Intercept    Intercept &
 Statistic       only       predictors   Chi-square  DF   p-value
      AICc     1024.0662     208.2199
     QAICc     1020.8622     208.2199
   -2 LOG L    1022.0662     198.2199    823.8463   16  0.000001


                      Maximum likelihood Beta estimates
Predictor          Parameter estimate     Standard error
Riffle
Intercept                  37.5567647          7.2843923
Depth                     -19.0793739          3.0448025
Current                    12.2224038          3.4525225
Veget                      -0.2762036          1.4883817
Wood                       -0.1670234          2.1025782
Cobb                        0.7878549          0.7707288
Glide
Intercept                  19.6055404          5.5615438
Depth                      -7.3922776          1.6523091
Current                     4.0508781          2.0663587
Veget                      -0.7411187          0.7782046
Wood                       -0.0873240          1.4366273
Cobb                        0.6955888          0.5004676
Edgwatr
Intercept                  36.8944958          7.1234382
Depth                     -12.3203028          2.2069905
Current                   -17.5510358          7.2972258
Veget                       0.6827152          0.7303764
Wood                        0.0736687          0.9712411
Cobb                        1.4765257          0.7298189
Sidchanl
Intercept                  31.7236748          7.0901073
Depth                      -9.5399044          2.1677537
Current                   -25.0343513          7.4302069
Veget                       0.4216387          0.7205377
Wood                        0.3719920          1.4017324
Cobb                        1.4786542          0.7233326
```

Table 4.3. (continued)

```
                           Goodness-of-Fit tests
Note: 178 estimated probabilities for Riffle were less than 10e-5
Note: 23 estimated probabilities for Glide were less than 10e-5
Note: 139 estimated probabilities for Edgwatr were less than 10e-5
Note: 150 estimated probabilities for Sidchanl were less than 10e-5
                 Osius and Rojek increasing-cells asymptotics
 Pearson chi-
    square         Mu          Sigma^2        Tau        p-value
   300.9296    1276.0000   6.292127e+19   -0.000001   1.000000


Andrews omnibus chi-square goodness-of-fit
              Number of
 Chi-square    clusters        DF        p-value
   25.4008        2            8        0.004858
Residuals have been saved in Bccu.rsd
```

Table 4.4. CATDAT classification tree output for the ocean-type chinook salmon population status data in Table 2.1. The corresponding classification tree can be found in Figure 4.1.

```
Classification tree BEST specification = 19
and minimum partition size = 19
Pruned Tree: Number of nodes = 19
Residual deviance = 114.109


Nonterminal Nodes:


                Sub-tree Left-Right-                               Split-
            Node Deviance Child  Child    Size    Predictor         Value
               1  425.100     2      3     477         Elev    2075.0000
               2  171.078     4      5     136     Hucorder    1051.0000
               3  151.181     6      7     341     Hucorder    1823.0000
               4  113.775     8      9      90     Hucorder       9.0000
               5    4.818    10     11      46       Rdmean       0.2934
               8   19.715    14     15      30          Ppt     233.7170
               9   71.276    16     17      60     Hucorder     263.0000
              16   44.443    22     23      41     Hucorder     228.0000
              22   30.575    30     31      32          Ppt     363.3410


Terminal Nodes:


                                                  Predicted
                    Node     Deviance      Size    response
                       6      114.109       326      Absent
                       7        0.000        15   Depressed
                      10        0.000         1      Strong
                      11        0.000        45     Migrant
                      14        0.000        16      Absent
                      15        0.000        14     Migrant
                      17        0.000        19      Absent
                      23        0.000         9      Strong
                      30        0.000        26   Depressed
                      31        0.000         7      Strong
```

Table 4.5. An example of CATDAT output for classification tree cross-validation (top) and generalized logit model within-sample (bottom) error rate estimation. EER and Perr are the expected error rate and prediction error rates, respectively.

```
Classification Tree with BEST fit specification = 21
and minimum partition size = 19
Cross-validation error rate calculation


                   Overall number of errors          EER
                                  50               0.1048

     Category   Number of errors      EER          No. of Predictions   Perr
       Strong          11             0.5238                       16    ---
    Depressed          23             0.4035                       43   0.3750
      Migrant          10             0.0294                      359   0.0808
       Absent           6             0.1017                       59   0.1017

                    -------------------------------------


Generalized Logit Model
Within-sample error rate calculation
Full main effects model
After model selection the number of predictors = 5


                   Overall number of errors          EER
                                  33                0.1034


      Category Number of errors    EER        No. of Predictions   Perr
        Riffle        2           0.0377                      55   0.0727
         Glide        5           0.0769                      63   0.0476
       Edgwatr       10           0.1667                      66   0.2424
      Sidchanl       16           0.2500                      57   0.1579
          Pool        0           0.0000                      78   0.0128
```

Table 4.6. CATDAT output for the Monte Carlo hypothesis test. The predictor tested is *Hucorder* and the type of classifier is the classification tree. The data is the ocean-type chinook salmon population status data in Table 2.1.

```
Monte Carlo hypothesis test of classification tree
BEST fit specification = 21
and minimum partition size = 19
Excluded covariate(s): Hucorder

              ***** Full model cross validation results *****
                  Full sample error rate, EER(f)= 1.058425
             ***** Reduced model cross-validation results *****
                 Reduced model error rate, EER(r)= 1.583001
           ***** Jackknife sample cross-Validation Results *****
         Jackknife sample size=250, Number of jackknife samples=100


                           Monte Carlo Test Results
  Jackknife  Observed Ts   Jackknife
 Ts* minimum  statistic   Ts* minimum    p-value
   -0.7858      0.5245       0.1527      0.0001
```

Table 4.7. An example of a classification prediction or cross validation file. The first column contains the original response category (class) and the second is the response category predicted by the CATDAT classifier. The next 5 columns contain the probabilities for each response and the remaining columns contain the original raw data. In this example, the original response category was unknown, so all observations were originally coded as response category one. Note that k- nearest neighbor output would include the average distance in the third column and modular neural network output would contain Z scores rather than probabilities.

```
orig predict

class class P(1) P(2) P(3) P(4) P(5) Depth Current Veget Cobb

1 1 0.3546 0.0676 0.1461 0.0948 0.3369 1.790 0.718 0.000 0.000 3.045

1 2 0.2513 0.4487 0.2461 0.0230 0.0308 1.790 0.673 0.000 0.000 3.045

1 1 0.2971 0.2544 0.1627 0.2650 0.0209 1.790 1.058 0.000 0.000 3.258

1 3 0.1207 0.1107 0.3966 0.2801 0.0920 1.710 1.012 0.000 0.000 2.398

1 4 0.1704 0.2306 0.1186 0.2841 0.1964 1.610 0.811 0.000 0.000 3.045

1 1 0.2789 0.2095 0.1949 0.1923 0.1244 1.610 1.125 0.000 0.000 0.000

1 1 0.2527 0.1977 0.1375 0.2521 0.1600 1.610 1.092 0.000 0.000 3.045

.

. remainder of output ...

.

1 2 0.0525 0.2947 0.2747 0.0942 0.2839 2.640 0.982 1.386 0.000 4.331

1 4 0.0292 0.0798 0.3011 0.3349 0.2551 2.890 1.289 0.000 0.000 3.932

1 2 0.0965 0.3646 0.2219 0.0683 0.2486 2.890 1.115 0.000 1.792 4.025

1 5 0.0997 0.2871 0.2197 0.0247 0.3689 2.940 1.037 3.045 0.000 4.111

1 2 0.2058 0.3692 0.1353 0.0089 0.2808 3.090 1.241 0.000 0.000 4.025

1 3 0.1871 0.2990 0.3972 0.0433 0.0735 2.890 1.138 0.000 0.000 3.932

1 2 0.1550 0.3544 0.2425 0.0414 0.2067 2.710 1.085 0.000 0.000 4.025
```

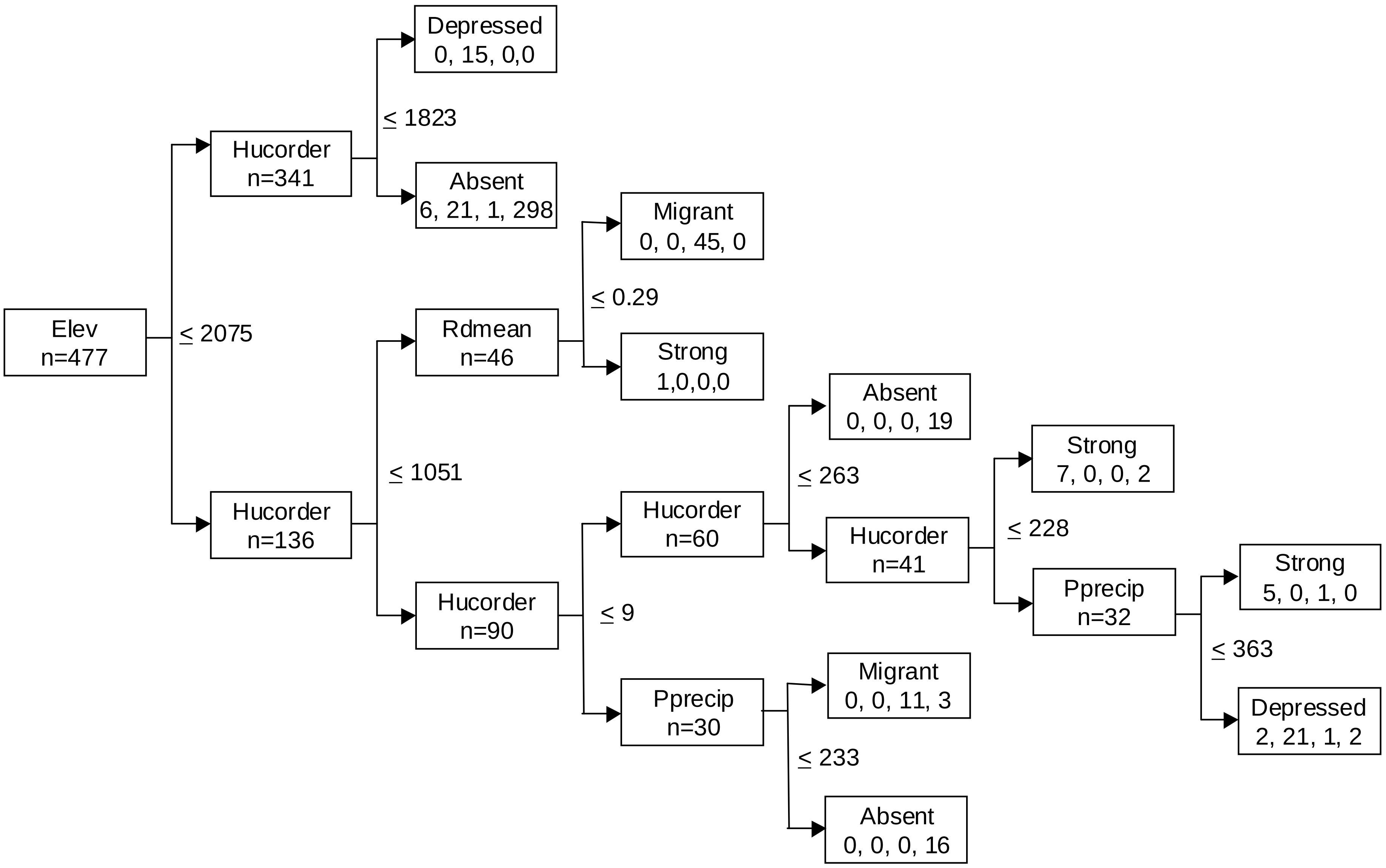


Figure 4.1. Classification tree for ocean-type chinook salmon population status. Non-terminal nodes are labeled with predictor and number of observations (n) and terminal nodes with predicted status and the distribution of responses in the order: strong, depressed, migrant, and absent. Split-values are to the right of the predictors with node decision: if yes, then down.

Examples

Ocean-type chinook salmon population status

The ocean-type chinook salmon status data were collected by the USDA Forest Service to (1) investigate the influence of landscape characteristics on the known status of ocean-type chinook salmon populations and (2) develop models to predict the status of the populations in unmonitored areas (Lee et al. 1997). These data are contained in the example data file otc.dat. The file heading and a partial list of the data can also be found in Table 2.1. It contained 4 response categories (i.e., population status): strong, depressed, migrant and absent; 11 quantitative predictors: *Hucorder* (a surrogate index of stream order), mean elevation (*Elev*), slope, drainage density (*Drnden*), bank (*Bank*) and base erosion (*Baseero*) scores, soil texture (*Hk*), average annual precipitation (*Ppt*), temperature (*Mntemp*), solar radiation (*Solar*), and mean road density (*Rdmean*); and 1 qualitative predictor: land management cluster (*Mgntcls*) with 3 levels.

Generalized logit model.- The qualitative covariate *Mgntcls* was recoded into 2 dummy predictors prior to fitting the generalized logit model (Table 5.1 and example data set otc2.dat). Absent was the most frequent response in the data (Table 4.1, top) and was used as the baseline for the logit model. Backward elimination of the main effects indicated that mean elevation, slope, and mean annual temperature were statistically significant at the Bonferroni adjusted alpha-level ($\underline{P} < 0.0038$, Table 5.2). Forward selection of two-way interactions for the full main effects model indicated 1 statistically significant ($\underline{P} < 0.0001$) interaction between *Hucorder* and mean elevation.

An examination of the within-sample error rates indicated that the full main effects and *Hucorder* by mean elevation interaction had the lowest overall within-sample error rate of 13.0% (Table 5.3 and 5.4). The full, main effects model had the next lowest error rate (14.7%), while the reduced main effects model was the least accurate with a 20.6% overall within-sample error rate. Although these error rates seem relatively low, a comparison of the within-sample errors for the best logit model (i.e., full main effects and interaction) with its cross-validation counterparts illustrate the optimism of the within-sample estimator. For example, the cross-validation error rate suggested that the overall within-sample error rate may have underestimated the logit model EER by 21.8% (Table 5.4). Similarly, the response category cross-validation error rates indicated that the best generalized logit model would have been very poor at estimating strong, depressed, and migrant population status (Table 5.4).

The best logit model for ocean-type chinook salmon population status, full main effects and *Hucorder* by mean elevation interaction, was statistically significant ($\underline{P} < 0.0001$; Table 5.5). In addition, the QAIC$_c$ suggested that the data may be overdispersed (i.e., $\hat{c} > 1$; Details, generalized logit model) and an examination of the residuals suggested that the logit model was not appropriate for modeling salmon population status (Figure 5.1). Similarly, the Andrews omnibus chi-square test detected significant ($\underline{P} < 0.0001$) lack-of-fit, whereas the Osius and Rojeck increasing cell asymptotics failed to reject the null hypothesis that the logit model fit ($\underline{P} =$ 1.000). The failure of the Osius and Rojeck test was probably due to the large proportion of extremely small estimated probabilities, 238 of which were less than 10^{-5}(Table 5.5), and their affect on the estimate of the asymptotic variance, σ^2. This large variance, 10^{13}, caused the Osius and Rojeck test to have almost no power for detecting lack-of-fit (Haas et al. In prep.).

If the generalized logit model had fit the population status data better, the interpretation of coefficients would have been straightforward. For example, Table 5.5 contains the maximum likelihood β_j of the full main effects with interaction logit model for each response category except the baseline, absent. Thus, the equation for the *strong* response probability, π_S, is

$$\log(\pi_S/\pi_A) = -26.2348 + 0.0068Hu - 0.0047El + 0.4395Sl + 2.0798Dr - 0.0901Bk - 0.1276Bs + 27.9306Hk + 0.0030Pp + 0.3595Mt + 0.0728So - 0.6856Rd + 1.58351Pf + 1.2088Pa - 0.000004Hu*El$$

where Hu = *Hucorder*, El = *Elev*, Sl = slope, Dr = *Drnden*, Bk = *Bank*, Bs = *Baseero*, Hk= *Hk*, Pp = *Ppt* , Mt = *Mntemp*, So = *Solar*, Rd = *Rdmean*, and Pf= *PfTlFm* and Pa = *Pa* (i.e., *Mgntcls* dummy variable categories 1 and 2, respectively). The estimated odds that the ocean-type chinook salmon population is strong rather than absent in a particular watershed is exp(0.0068) = 1.0068 times higher for each unit increase in *Hucorder*, 1.0047 times lower per 1 foot increase in average elevation, 1.5519 times higher for each degree increase in average slope, and so forth.

Classification tree.- An examination of the cross-validation error rates for various sized classification trees suggested that the optimum tree for classifying salmon population status contained 21 nodes (Figure 5.2). The Monte Carlo hypothesis test of the predictors, individually and in various combinations, indicated that *Hucorder* and mean elevation, annual precipitation, and road density significantly (P > 0.05) influenced the classification accuracy of salmon population status (Table 5.6). An examination of the initial plot of the classification tree, with the 4 significant predictors, suggested that population status could be modeled with a 19 node tree (Figure 4.1). To confirm this, cross-validation error rates were calculated for BEST parameter values 19 and 21. The error rates were identical with an overall cross-validation rate of 10.1% (Table 5.7). The final 19 node classification tree was best a predicting absent (EER= 2.9%, Perr =8.1%) and migrant status (EER= 10.2%, Perr =10.2%) and poorest at predicting depressed (EER=38.6%) and strong (EER= 47.6%) population status.

Nearest neighbor.- Cross-validation error rates for different numbers of nearest neighbors, *K*, indicated that the optimum classifier had 3 nearest neighbors (Figure 5.3). The Monte Carlo hypothesis test of predictors for the 3-nearest neighbor classifier indicated that mean slope, drainage density, bank and base erosion scores, soil texture, mean annual precipitation, temperature, and solar radiation, mean road density, and land management type did not significantly (P > 0.05) influence classification accuracy (Table 5.8). Cross-validation rates of the 3-nearest neighbor classifier with 2 statistically significant predictors, *Hucorder* and mean elevation, were higher than those for the classification tree with an overall rate of 17.2% (Table 5.9).

Ocean-type chinook salmon generally migrate to the ocean before the end of their first year of life, whereas the stream-type migrates after their first year (Lee et al. 1997). Fishes exhibiting these two life histories vary in their migratory patterns and habitat requirements. Consequently, each may be affected differently by the landscape features that influence critical requirements, such as instream habitat characteristics or streamflow patterns. To examine whether selected landscape characteristics influence the status of populations exhibiting the two life history strategies similarly, a 3-nearest neighbor classifier with *Hucorder* and mean elevation was trained using the ocean-type chinook salmon population status data. This model was then used to predict the status of stream-type populations for which the actual status was known (i.e., it was a "test" data set). Overall, the classifier created with the ocean-type data predicted the status of the stream-type chinook with a 23.3% overall EER (Table 5.10). However, after importing the prediction file into a spreadsheet, an examination of the category-specific errors indicated that the ocean-type model was very poor at predicting strong (EER = 100%), depressed

(EER=98.9%) and migrant status (EER=82.7%), whereas absent was correctly predicted in 99% of the observations.

The above example illustrates the influence that sharply unequal sample sizes among response categories can have on the overall EER. Strong and depressed responses comprised 0.3% and 15.5% of the stream-type chinook salmon status data, respectively. Consequently, their very high category-wise errors represented only 15.6% all observations, which resulted in a relatively low overall EER of 23.3%.

Modular neural network.- An examination of the cross-validation error rates for different numbers hidden nodes indicated that the optimum modular network for predicting ocean-type salmon status had a 10 hidden nodes (Figure 5.4). The MNN had the lowest overall EER, 2.1%, and the lowest category specific EER of any of the classifiers considered (Table 5.11).

Ozark stream channel-units

To evaluate the utility of a channel-unit classification system for Ozark streams, Peterson and Rabeni (In review) measured selected physical habitat characteristics of channel-unit types. The goals of the study were to (1) identify the differences in physical characteristics among channel units and (2) determine if the channel unit classification system was applicable to different sized streams. The format of the data for large streams has already been presented in Table 2.2. It consisted of 5 response categories (i.e., channel unit types): riffle, glide, edgewater (*Edgwatr*), side-channel (*Sidchanl*), and pool; and 5 quantitative predictors: average depth and current velocity, percent of the channel unit covered with vegetation (*Veget*) or woody debris (*Wood*), and percent of the channel unit bottom composed of cobble substrate (*Cobb*).

Generalized logit model.- Pool was the most frequent response in the data (Table 4.1, bottom) and was therefore, used as the baseline for the generalized logit model. Backward elimination of the logit model main effects indicated that depth and current velocity were statistically significant ($\underline{P} < 0.0001$). Similarly, forward selection of logit model main effects and two-way interactions indicated that that depth and current velocity were the only statistically significant ($\underline{P} < 0.0001$) predictors.

A comparison of the within-sample error rates indicated that the full, main effects model had the lowest overall EER of 10.3%, whereas the statistically significant main effects model had a much greater EER of 26.6% (Table 5.12). Cross-validation of the best logit model (i.e., full main effects) however, indicated a very high EER with 56.1% of the observations misclassified (Table 5.12).

The full main effects logit model was statistically significant ($\underline{P} < 0.0001$; Table 4.3). In contrast to the ocean-type chinook logit model, the $QAIC_c$ suggested that the channel unit data were not overdispersed (i.e., $\hat{c} = 1$; Details, generalized logit model). Nonetheless, an examination of the residuals (Figure 5.1) and the Andrews omnibus chi-square test ($\underline{P} = 0.0048$) suggested that the logit model was not appropriate for modeling the physical characteristics of channel units (Table 4.3). Similar to the ocean-type chinook salmon logit model, the Osius and Rojek test failed to detect lack-of-fit.

Classification tree.- An examination of the cross-validation error rates for various sized trees suggested that the optimum tree for classifying channel-units contained 13 nodes (Figure 5.2). The Monte Carlo hypothesis test of the predictors, individually and in various combinations, indicated that percent vegetation, woody debris, and cobble substrate did not significantly ($\underline{P} > 0.05$) influence the tree classification accuracy for channel-unit types (Table 5.13).

The overall cross-validation EER of the classification tree with 13 nodes and 2 predictors, depth and current velocity, was much lower than that of the best fitting logit model (Tables 5.12 and 5.14). In general, the classification tree was best a classifying pool (EER= 9.1%, Perr = 6.7%) and riffle channel units (EER= 11.3%, Perr = 7.8%) and poorest at classifying side-channels (EER = 34.4%) and edgewaters (Perr = 28.6%). The relatively poor classification of the latter two was probably due to their highly variable physical habitat characteristics (Peterson and Rabeni In review).

An examination of the final classification tree indicated that pools were the deepest channel-units with average depths greater than 0.56 m and variable current velocities (Figure 5.5). In contrast, riffles were generally less than 0.20 m deep with current velocities greater than 0.20 m/s. Glides were moderately deep (0.2 - 0.6 m) with current velocities greater than 0.12 m/s. Side-channels had similar depths (0.29- 0.56m), but lower current velocities.

Nearest neighbor.- Cross-validation of various numbers of *K* nearest neighbors suggested that the most parsimonious classifier had 2 neighbors (Figure 5.3). Similar to the classification tree, the Monte Carlo hypothesis test of predictors for the 2-nearest neighbor classifier indicated that percent vegetation, woody debris, and cobble substrate did not significantly ($\underline{P} > 0.05$) influence classification accuracy (Table 5.15). In addition, the cross-validation rates of the 2-nearest neighbor classifier with statistically significant predictors, depth and current velocity, were slightly lower than the classification tree with an overall rate of 11.9% (Table 5.16). In addition, the mean Mahalanobis distance between channel-unit types indicated that riffles and glides were physically similar, as were edgewaters and side-channels (Table 5.16). The physical characteristics of pools however, differed substantially from all other channel unit types.

Modular neural network.- An examination of the cross-validation error rates for different numbers hidden nodes indicated that the optimum modular neural network for classifying channel units had a 7 hidden nodes (Figure 5.4). Similar to the ocean-type chinook salmon status, the channel-unit modular neural network had the lowest overall EER, 3.1%, and the lowest category specific EER of any of the classifiers considered (Table 5.17).

Stream habitat characteristics are largely controlled by the local and watershed-level features that control sediment supply, erosion, and deposition (e.g., valley physiography, land-use). Thus, the physical characteristics of channel units may vary from reach to reach. To assess the relative accuracy of the channel-unit habitat classification system for different sized stream reaches, measurements from channel units in a small (i.e. 3rd order) Ozark stream were classified with the 7 node modular neural network trained with the data from the larger (6th order) Ozark stream. The influence of possible site-specific differences were minimized by standardizing the site-specific data, across CUs, into z-scores (i.e., mean=0, SD=1). In general, the modular neural network trained with large stream data was surprisingly good at classifying the channel units in the small stream with an overall misclassification rate of 4.4% (Table 5.18).

Table 5.1. Ocean-type chinook salmon population status data with 2 dummy coded predictors *PfTlFm* and *Pa* representing 3 levels of the qualitative covariate *Mgntcls* in Table 2.1. Note that the third *Mgntcls* level receives a zero coding for dummy predictors *PfTlFm* and *Pa*.

```
4 Strong Depressed Migrant Absent

13 Hucorder Elev Slope Drnden Bank Baseero Hk Ppt Mntemp Solar Rdmean PfTlFm Pa

0 *

1 18 2193 9.67 0.6843 73.953 12.2004 0.37 979.612 7.746 273.381 2.0528 1 0

2 20 2793 19.794 1.3058 58.708 29.9312 0.3697 724.264 6.958 260.583 3.440 0 0

1 22 2421 23.339 1.231 44.845 36.3927 0.3697 661.677 7.6 254.733 2.364 0 1

3 23 3833 34.553 1.3661 19.092 52.7353 0.3692 714.559 6 252.889 1.489 1 0

4 36 1925 23.797 1.0873 28.026 36.3066 0.3695 544.183 8.5 252.857 2.336 0 1

4 38 1775 13.549 0.7118 67.898 19.0161 0.3699 757.989 8.533 276.156 1.311 0 0

2 47 1387 17.264 1.582 35.8019 25.6341 0.3696 326.714 9.688 249.938 2.372 0 1

3 168 732 7.69 1.3472 92.8437 6.6349 0.2477 183.966 11.652 262.913 0.4281 1 0

.

...remainder of data...

.

4 263 135 22.431 1.06 79.4377 23.1364 0.2601 304.631 10.111 275.037 0.946 1 0

1 1418 768 5.677 0.3317 99.1893 3.0148 0.2114 210.137 11.21 262.01 0.293 1 0

2 0 2992 17.831 1.5458 68.8551 26.3373 0.3695 411.158 6.929 258.071 1.866 0 1
```

Table 5.2. CATDAT output of backward elimination of generalized logit model main effects (top) and forward selection of two-way interactions (bottom) for ocean-type chinook salmon population status. Two-way interactions were tested for the full main effects model.

```
Full main effects model initially fit.
Backward elimination of generalized logit model main effects
Predictors accepted at P < 0.003846


Predicto   Wald Chi-
       r     square   p-value
 Hucorder   28.1736   0.000003
     Elev   26.8128   0.000006
      Ppt   19.8359   0.000184

            ------------------------------------------------------
```

```
Full main effects generalized logit model
with forward selection of interactions
Interactions accepted at P < 0.000320


Predicto  Interaction  Score Chi-
       r    predictor     square   p-value
 Hucorder        Elev    20.4180   0.000139
```

Table 5.3. CATDAT output of within-sample classification error rates for chinook salmon population status generalized logit models. The model predictors include full main effects (top) and statistically significant main effects (bottom).

```
Generalized Logit Model
Within-sample error rate calculation
Full main effects model
After model selection the number of predictors = 13

                   Overall number of errors          EER
                                  70             0.1468

     Category   Number of errors     EER         No. of Predictions   Perr
       Strong          15            0.7143                       9  0.3333
    Depressed          30            0.5263                      47  0.4255
      Migrant           8            0.1356                      58  0.1207
       Absent          17            0.0500                     363  0.1102

      ------------------------------------------------------------------


Generalized Logit Model
Within-sample error rate calculation
Reduced model with 3 main effects:
Elev Slope Mntemp
After model selection the number of predictors = 3


                   Overall number of errors          EER
                                  98             0.2055

      Category   Number of errors     EER         No. of Predictions  Perr
        Strong          21            1.0000                       0  ---
     Depressed          38            0.6667                      38  0.4412
       Migrant          18            0.3051                      67  0.3881
        Absent          21            0.0618                     376  0.1516
```

Table 5.4. CATDAT output of within-sample (top) and cross-validation (bottom) classification error rates for the best generalized logit model, full main effects and significant interaction, of ocean-type chinook salmon population status.

```
Generalized Logit Model
Within-sample error rate calculation
Full main effects model
and the following 1 interaction(s):
                           Hucorder & Elev
After model selection the number of predictors = 14


                   Overall number of errors          EER
                                  60               0.1300

     Category   Number of errors      EER         No. of Predictions   Perr
       Strong          9              0.4286                      20  0.4000
    Depressed         28              0.4912                      42  0.3095
      Migrant          8              0.1356                      57  0.1053
       Absent         17              0.0500                     358  0.0978

      ------------------------------------------------------------------

Generalized Logit Model
Cross-validation error rate calculation
Full main effects model
and the following 1 interaction(s):
                          Hucorder & Elev
After model selection the number of predictors = 14


                   Overall number of errors          EER
                                 166               0.3480

     Category  Number of errors     EER       No. of Predictions     Perr
       Strong         21            1.0000                      36      1.0000
    Depressed         51            0.8947                      25      0.7600
      Migrant         59            1.0000                       6      1.0000
       Absent         35            0.1029                     410      0.2561
```

Table 5.5. CATDAT output of maximum likelihood beta estimates for the best, generalized logit model of ocean-type chinook salmon population status. Model predictors include all main effects and a *Hucorder* by mean elevation interaction.

```
Generalized logit model- Full main effects
and the following 1 interaction(s):
                                Horder & Elev
Note: maximum likelihood estimation ended at iteration 9 because
log likelihood decreased by less than 0.00001


              Model fit and global hypothesis test H0: BETA = 0

             Intercept    Intercept &
   Statistic             Chi-square       DF   p-value
               only        predictors
        AICc     852.2005     354.5266
       QAICc     850.4181     346.8581
    -2 LOG L     850.2005     323.5266   526.6739     42   0.000001


                       Maximum likelihood Beta estimates
     Predictor                     Parameter estimate     Standard error
Strong
     Intercept                            -26.2347681         11.0243112
      Hucorder                              0.0067506          0.0026071
          Elev                             -0.0046858          0.0014341
         Slope                              0.4394876          0.2110173
        Drnden                              2.0797678          1.0274691
          Bank                             -0.0901087          0.0363842
       Baseero                             -0.1276053          0.1284560
            Hk                             27.9306370         14.0247187
           Ppt                              0.0029755          0.0012508
        Mntemp                              0.3595229          0.6826518
         Solar                              0.0727642          0.0276365
        Rdmean                             -0.6855937          0.6197469
        PfTlFm                              1.5835155          0.9379961
            Pa                              1.2088449          1.0003054
   Horder*Elev                             -0.0000039          0.0000015
Depressed
     Intercept                             -6.1864855          6.9518825
      Hucorder                             -0.0036728          0.0012492
```

(remainder of ML betas)

Table 5.5 (continued)

```
                            Goodness-of-Fit tests
Note: 54 estimated probabilities for Strong were less than 10e-5
Note: 36 estimated probabilities for Depressed were less than 10e-5
Note: 148 estimated probabilities for Migrant were less than 10e-5
                 Osius and Rojek increasing-cells asymptotics
Pearson chi-
   square         Mu         Sigma^2         Tau        p-value
 1419.6494    1431.0000   1.106656e+13   -0.000003    0.999997
                  Andrews omnibus chi-square goodness-of-fit
    Chi-square        Number of clusters       DF   p-value
     70.7831                  8                24   0.000002
Residuals have been saved in otc.rsd
```

Table 5.6. CATDAT output of the classification tree Monte Carlo hypothesis test for chinook salmon population status. The 8 predictors tested, mean slope, drainage density, bank and base erosion scores, soil texture, mean annual temperature and solar radiation, and land management type, were not statistically significant at the $\alpha = 0.05$ level. The remaining variables, *Hucorder*, mean elevation, mean annual precipitation, and mean road density, were statistically significant at $\alpha = 0.05$.

```
Monte Carlo hypothesis test of classification tree
BEST fit specification = 21
Excluded covariate(s):
Slope Drnden Bank Baseero Hk Mntemp Solar Mgnclus

              ***** Full model cross validation results *****
                 Full sample error rate, EER(f)= 1.058425
            ***** Reduced model cross-validation results *****
                Reduced model error rate, EER(r)= 0.993262
           ***** Jackknife sample cross-Validation Results *****
        Jackknife sample size=350, Number of jackknife samples=100


                           Monte Carlo Test Results


Jackknife Ts*  Observed Ts  Jackknife Ts*
   minimum      statistic      maximum      p-value
   -0.3628       -0.0651       0.5869       0.8200
```

Table 5.7. CATDAT output of cross-validation error rates for 19 (top) and 21 (bottom) node classification trees with 4 statistically significant (P<0.05) predictors *Hucorder*, mean elevation, mean annual precipitation, and mean road density.

```
Classification Tree with BEST fit specification = 19

Cross-validation error rate calculation
                  Overall number of errors            EER
                                  48                0.1006


     Category   Number of errors      EER         No. of Predictions   Perr
       Strong          10             0.4762                      18    0.3889
    Depressed          22             0.3860                      41    0.1463
       Absent          10             0.0294                     359    0.0808
      Migrant           6             0.1017                      59    0.1017
               ------------------------------------------------
Classification Tree with BEST fit specification = 21

Cross-validation error rate calculation
                   Overall number of errors           EER
                                  50               0.1048

     Category   Number of errors      EER         No. of Predictions   Perr
       Strong          11             0.5238                      16    0.3750
    Depressed          23             0.4035                      43    0.2093
       Absent          10             0.0294                     359    0.0808
      Migrant           6             0.1017                      59    0.1017
```

Table 5.8. CATDAT output of the Monte Carlo hypothesis test for the 3-nearest neighbor classifier of chinook salmon status. The 8 predictors tested, mean slope, drainage density, bank and base erosion scores, soil texture, mean annual precipitation, temperature, and solar radiation, mean road density, and land management type, were not statistically significant at the $\alpha = 0.05$ level.

```
Monte Carlo hypothesis test of nearest neighbor classification
Excluded covariate(s):
Slope Drnden Bank Baseero Hk Ppt Mntemp Solar Rdmean Mgnclus

              ***** Full model cross-validation results *****
                  Full sample error rate, EER(f)= 1.420199
             ***** Reduced model cross-validation results *****
                 Reduced model error rate, EER(r)= 1.474307
            ***** Jackknife sample cross-Validation Results *****
        Jackknife sample size=350, Number of jackknife samples=100


                           Monte Carlo Test Results


  Jackknife   Observed Ts   Jackknife
 Ts* minimum   statistic   Ts* maximum   p-value
   -0.5585      0.0541       0.7015      0.5100
```

Table 5.9. CATDAT output of cross-validation error rates for the 3-nearest neighbor classifier with 2 statistically significant (P<0.05) predictors *Hucorder* and mean elevation.

```
Nearest neighbor classification with 3 neighbor(s)

Cross-validation error rate calculation
             Pairwise mean distances, d(xi,xj), between responses
                                 Distance to response group
 From response
     group                Strong        Depressed         Absent         Migrant
         Strong           0.0000           0.8343         1.0826          2.6317
      Depressed           0.8343           0.0000         0.9723          2.1561
         Absent           1.0826           0.9723         0.0000          3.1112
        Migrant           2.6317           2.1561         3.1112          0.0000


                   Overall number of errors          EER
                                 81               0.1698



      Category   Number of errors     EER        No. of Predictions   Perr
        Strong          13           0.6190                      19    0.5789
     Depressed          28           0.4912                      53    0.4528
        Absent          25           0.0735                     352    0.1051
       Migrant          15           0.2542                      53    0.1698
```

Table 5.10. CATDAT output of the classification of stream-type chinook population status using the 2-predictor, 3-nearest neighbor classifier trained with the ocean-type chinook population status data.

```
                      ----Training data in otc5.dat ----
Quantitative predictors:

Hucorder Elev
             Observed frequencies of response variable categories
    Response  Count   Marginal frequency
      Strong     21         0.0440
   Depressed     57         0.1195
      Absent    340         0.7128
     Migrant     59         0.1237


Number of observations = 477
Number of predictors = 2
Computing covariate space distance with training data
for nearest neighbor classification with 3 neighbor(s)
                    ----------------END---------------


Number of observations in stctst.dat = 3025
Classification error summary for data in stctst.dat

 Overall number of errors    Err
           705            0.2331

Predictions written to stctst.out
```

Table 5.11. CATDAT output of cross-validation error rates of 10-node modular neural network fit to the ocean-type chinook salmon status data..

```
Modular Neural Network classification with 10 hidden nodes
Cross-validation error rate calculation
384 records read from otcwts9.sed

Network weights written to otcwts10.out


                   Overall number of errors          EER
                                  10               0.0210

     Category   Number of errors     EER         No. of Predictions   Perr
       Strong          0             0.0000                      24    0.1250
    Depressed          1             0.0175                      61    0.0820
      Migrant          0             0.0000                      60    0.0167
       Absent          9             0.0265                     332    0.0030
```

Table 5.12. CATDAT output of within-sample classification error rates for the full main effects (top) and statistically significant main effects (middle) generalized logit model of channel-unit physical characteristics. Cross-validation error rates for the full main effects model shown at the bottom.

```
Generalized Logit Model
Within-sample error rate calculation
Full main effects model
After model selection the number of predictors = 5
                   Overall number of errors           EER
                                  33                0.1034

      Category Number of errors    EER         No. of Predictions   Perr
        Riffle         2           0.0377                      55   0.0727
         Glide         5           0.0769                      63   0.0476
       Edgwatr        10           0.1667                      66   0.2424
      Sidchanl        16           0.2500                      57   0.1579
          Pool         0           0.0000                      78   0.0128

          -----------------------------------------------------------

Generalized Logit Model
Within-sample error rate calculation
Reduced model with 2 main effects:
                            Depth Current
After model selection the number of predictors = 2
                   Overall number of errors           EER
                                  85                0.2665

      Category Number of errors    EER         No. of Predictions   Perr
        Riffle        12           0.2264                      65   0.3692
         Glide        13           0.2000                      70   0.2571
       Edgwatr        27           0.4500                      50   0.3400
      Sidchanl        30           0.4688                      56   0.3929
          Pool         3           0.0390                      78   0.0513

          -----------------------------------------------------------

Generalized Logit Model
Cross-validation error rate calculation
Full main effects model
After model selection the number of predictors = 5
                   Overall number of errors           EER
                                 179                0.5611

      Category Number of errors    EER         No. of Predictions   Perr
        Riffle        22           0.4151                      99   0.7634
         Glide        65           1.0000                      38   1.0000
       Edgwatr        58           0.9667                      28   0.5000
      Sidchanl        57           0.8906                      38   0.3636
          Pool        35           0.4545                     116   0.7308
```

Table 5.13. CATDAT output of the classification tree Monte Carlo hypothesis test for channel-unit physical habitat characteristics. The predictors tested, percent vegetation, woody debris, and cobble substrate, were not statistically significant at the $\alpha = 0.05$ level.

```
Monte Carlo hypothesis test of classification tree with
BEST fit specification = 13
Excluded covariate(s):
Veget Wood Cobb

              ***** Full model cross-validation results *****
                 Full sample error rate, EER(f)= 0.725238
             ***** Reduced model cross-validation results *****
                Reduced model error rate, EER(r)= 0.723524
           ***** Jackknife sample cross-Validation Results *****
        Jackknife sample size=225, Number of jackknife samples=100


Monte Carlo Test Results


  Jackknife   Observed Ts  Jackknife
 Ts* minimum   statistic  Ts* maximum   p-value
   -0.0616      0.0017      0.1505      0.1900
```

Table 5.14. CATDAT output of cross-validation error rates for a classification tree with a BEST fit specification of 13 and statistically significant (P<0.05) predictors, depth and current velocity.

```
Classification Tree with BEST fit specification = 13
Cross-validation error rate calculation
                  Overall number of errors          EER
                               46                 0.1442



      Category Number of errors    EER        No. of Predictions   Perr
        Riffle        6           0.1132                      51   0.0784
         Glide        6           0.0923                      68   0.1324
       Edgwatr        5           0.0833                      77   0.2857
      Sidchanl       22           0.3438                      48   0.1250
          Pool        7           0.0909                      75   0.0667
```

Table 5.15. CATDAT output of the Monte Carlo hypothesis test for the 2-nearest neighbor classification of stream channel-units. The predictors tested, percent vegetation, woody debris, and cobble substrate, were not statistically significant at the $\alpha = 0.05$ level.

```
Monte Carlo hypothesis test of nearest neighbor classification
Excluded covariate(s):
Veget Wood Cobb

              ***** Full model cross-validation results *****
                 Full sample error rate, EER(f)= 0.430172
             ***** Reduced model cross-validation results *****
                Reduced model error rate, EER(r)= 0.614473
            ***** Jackknife sample cross-Validation Results *****
        Jackknife sample size=225, Number of jackknife samples=100


Monte Carlo Test Results
  Jackknife   Observed Ts   Jackknife
 Ts* minimum   statistic   Ts* maximum    p-value
   -0.2641      0.1843       0.2467       0.0900
```

Table 5.16. CATDAT output of cross-validation error rates for nearest neighbor classification of channel units with statistically significant (P<0.05) predictors, depth and current velocity.

```
Nearest neighbor classification with 2 neighbor(s)

Cross-validation error rate calculation
                          Pairwise mean distances, d(xi,xj), between responses
                                         Distance to response group
 From response
     group          Riffle       Glide  Edgwatr Sidchanl     Pool
       Riffle       0.0000      1.2216   3.7593   3.9925   5.3719
        Glide       1.2216      0.0000   3.3025   3.4757   4.1549
      Edgwatr       3.7593      3.0325   0.0000   0.6030   4.8538
     Sidchanl       3.9925      3.4757   0.6030   0.0000   4.3323
         Pool       5.3719      4.1549   4.8538   4.3323   0.0000
                    Overall number of errors          EER
                                  38               0.1191



     Category   Number of errors     EER         No. of Predictions   Perr
       Riffle          5            0.0943                       52    0.1346
        Glide          7            0.1077                       68    0.1618
      Edgwatr         11            0.1833                       62    0.2258
     Sidchanl         13            0.2031                       62    0.2097
         Pool          2            0.0260                       75    0.0133
```

Table 5.17. CATDAT output of cross-validation error rates of the 7-node modular neural network fit to the stream channel-unit physical habitat data.

```
Modular Neural Network classification with 7 hidden nodes
Cross-validation error rate calculation
180 records read from bcwts6.sed

Network weights written to bcwts7.out


                    Overall number of errors          EER
                                  10               0.0313

      Category Number of errors    EER         No. of Predictions   Perr
        Riffle        3           0.0566                       50   0.0000
         Glide        0           0.0000                       68   0.0441
       Edgwatr        4           0.0667                       59   0.0508
      Sidchanl        3           0.0469                       65   0.0615
          Pool        0           0.0000                       77   0.0000
```

Table 5.18. CATDAT output of the classification of small-stream channel-unit physical habitat characteristics the 7-node modular neural network trained with large-stream channel-unit data .

```
                    ----Training data in bccu.dat ----

Quantitative predictors:

Depth Current Veget Wood Cobb

Observed frequencies of response variable categories

                  Marginal
Response  Count   frequency
    Riffle    53       0.1661
     Glide    65       0.2038
  Edgewatr    60       0.1881
  Sidchanl    64       0.2006
      Pool    77       0.2414


Number of observations in training data set, 319
and number of predictors, 5
Constructing modular neural network with training data
and 7 hidden nodes
                  ----------------END--------------


Number of observations in smlcu.dat = 319

Classification error summary for data in smlcu.dat



 Overall number of errors    Err
           14             0.0439

Predictions written to cupred.out
```

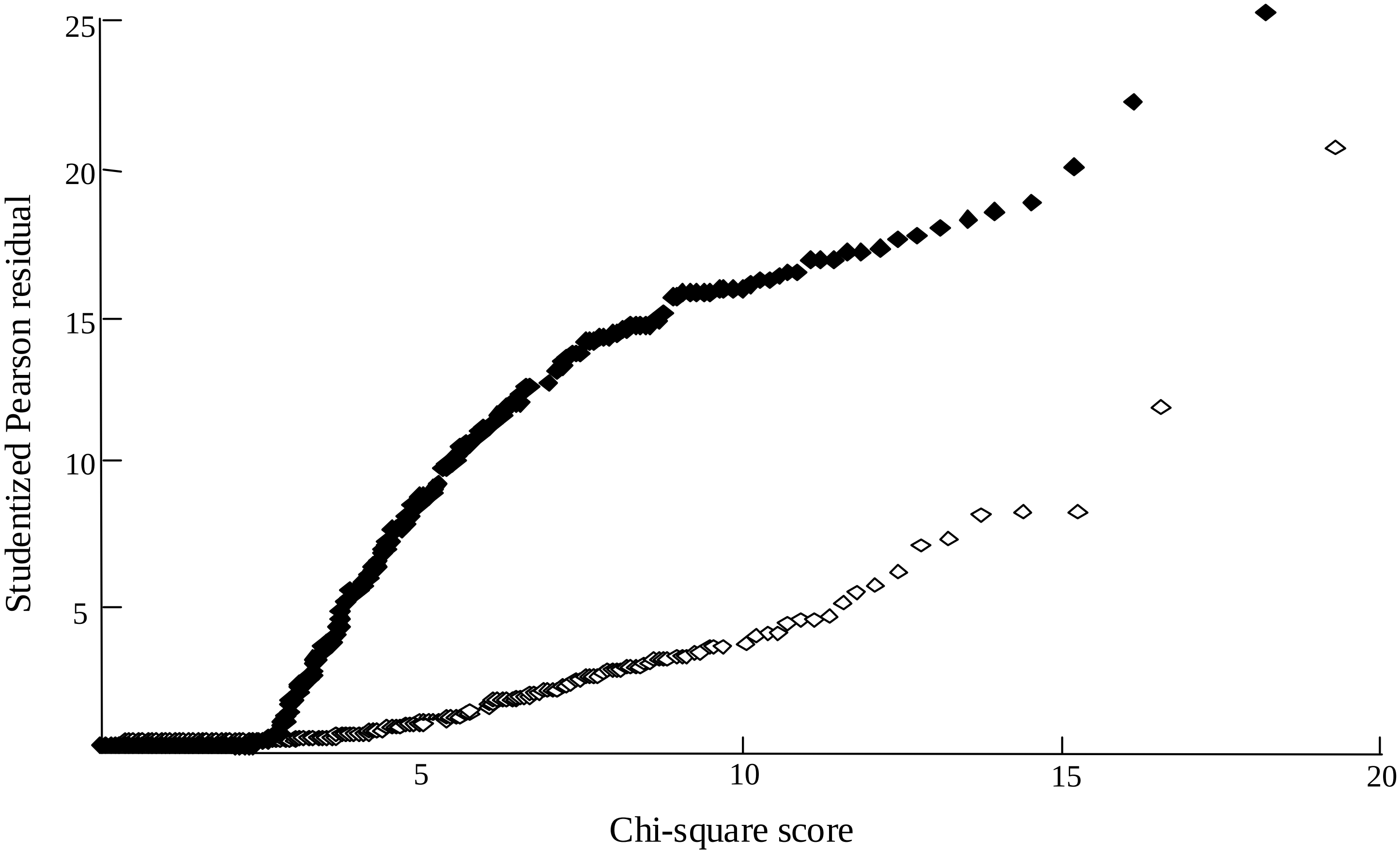


Figure 5.1 A Q-Q plot of the studentized Pearson residuals for the best salmon status (open) and channel unit (filled) generalized logit models. Note :the residuals were log transformed and thus, if the relationships were linear the residual plots should be logarithmically shaped.

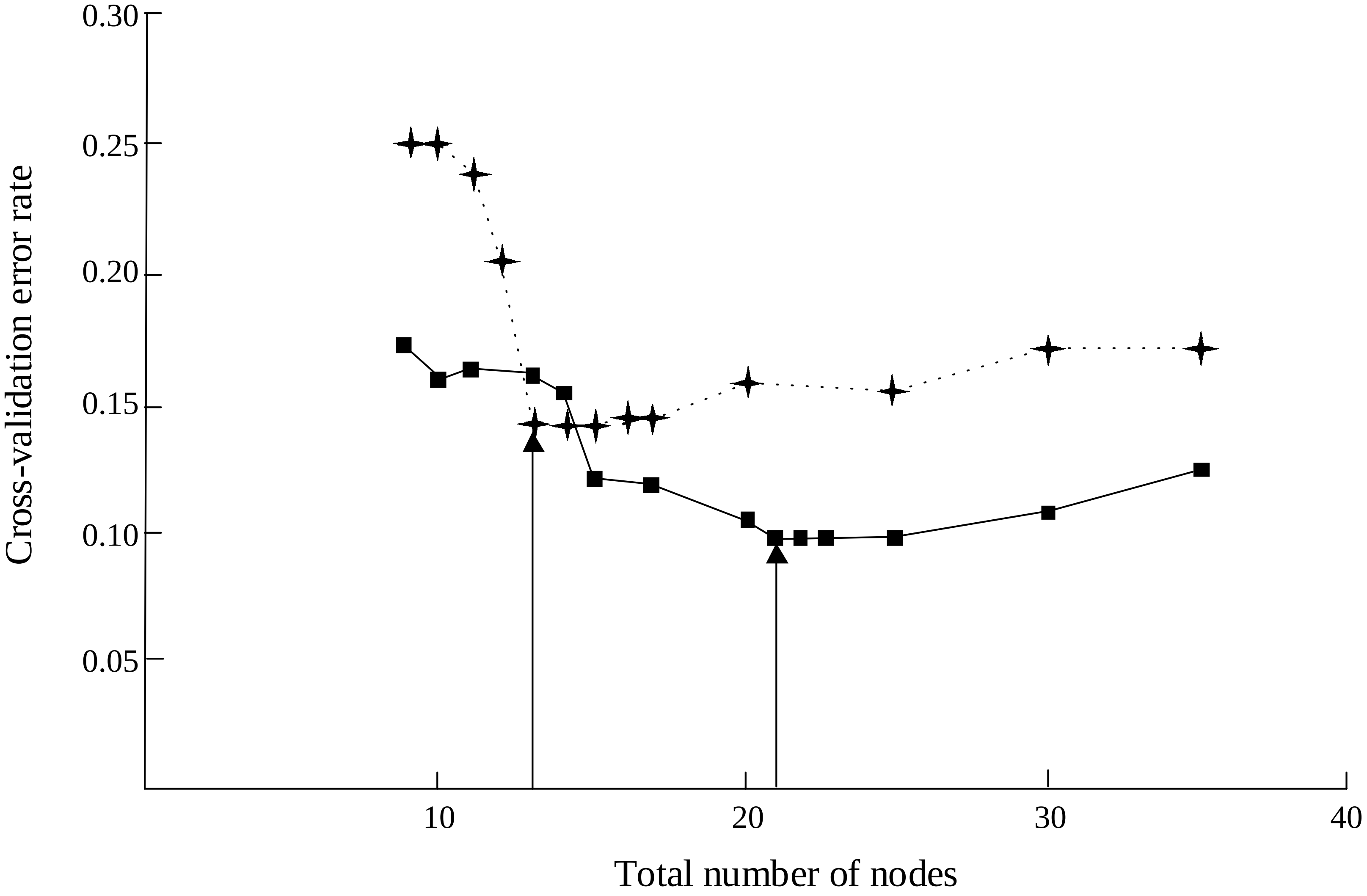


Figure 5.2. Overall cross-validation error rate of various sized classification trees for ocean-type chinook salmon population status (solid line and boxes) and Ozark stream channel-unit physical habitat characteristics (broken line and stars). The most parsimonious tree for the chinook salmon and channel-unit models (indicated by the arrow) contained 13 and 21 nodes, respectively.

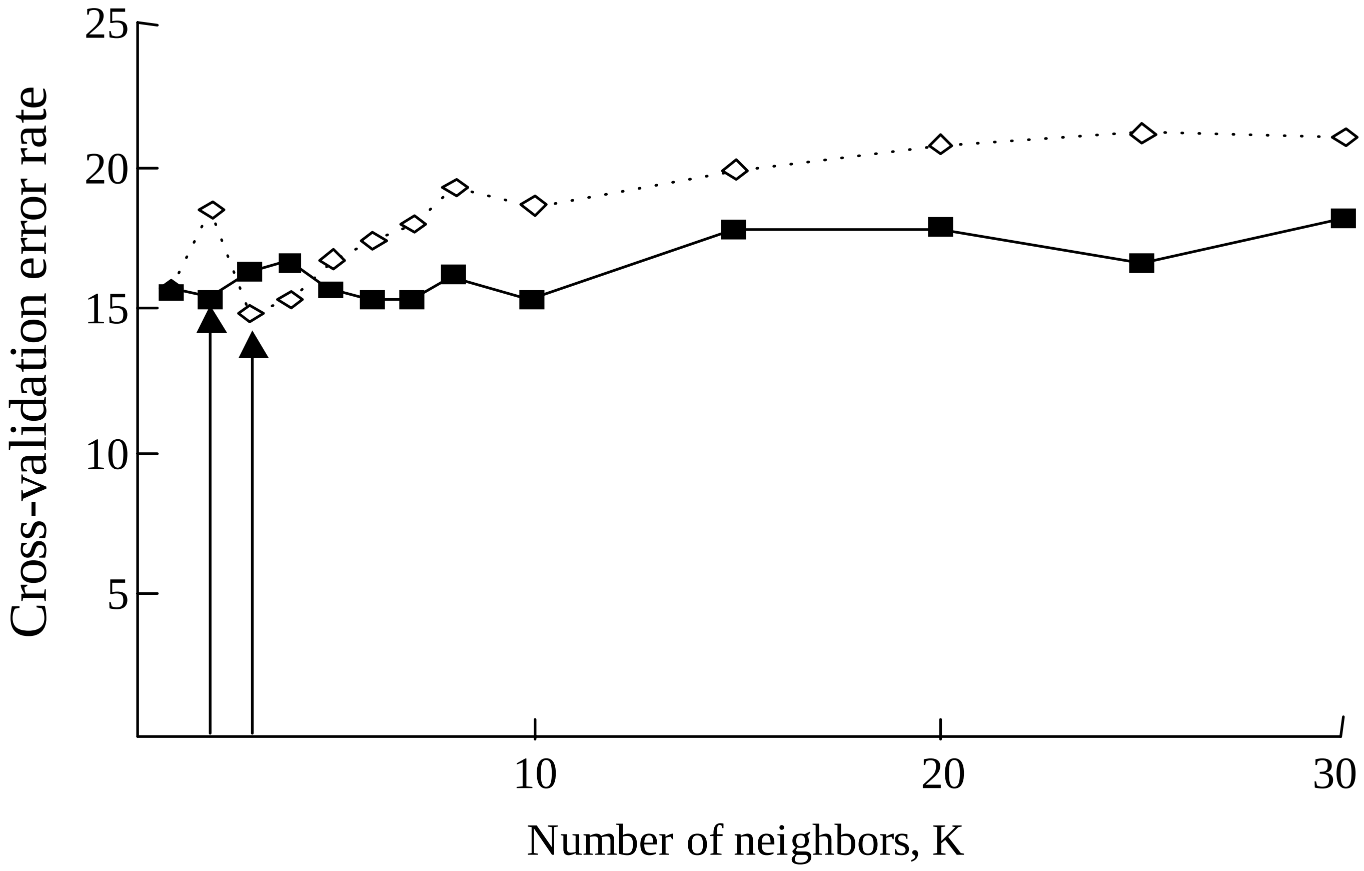


Figure 5.3. Overall cross-validation error rate of various numbers of nearest neighbors, *K*, for ocean-type chinook salmon population status (broken line and open symbols) and physical characteristics of stream channel units (solid lines and symbols). Arrows indicate the optimal *K* values. A complete description of the data can be found in Examples 1 and 2.

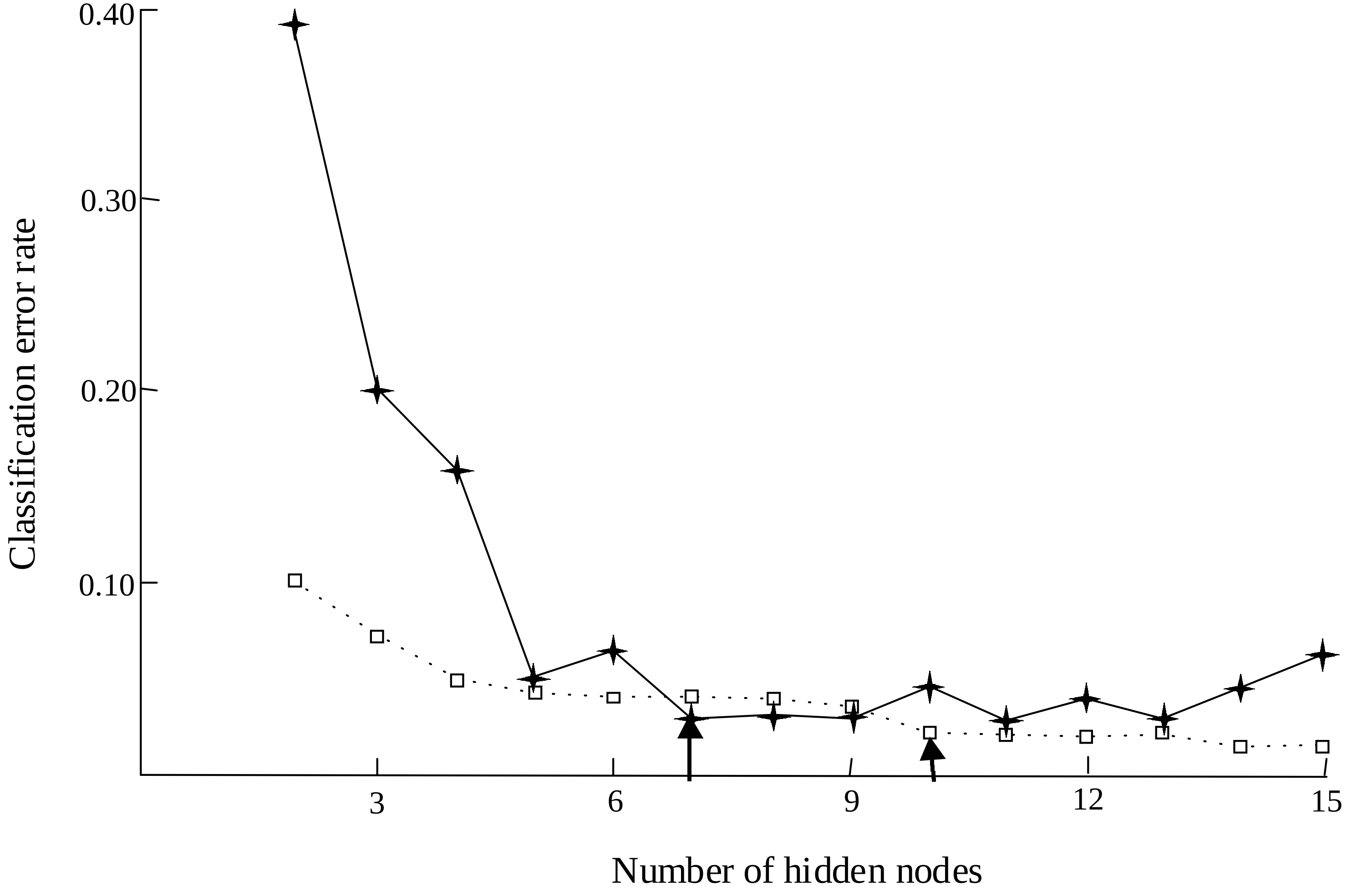


Figure 5.4. Overall cross-validation error rate of various numbers of hidden nodes for ocean-type chinook salmon population status (broken line and open symbols) and physical characteristics of stream channel units (solid lines and symbols). Arrows indicate the optimal number of hidden nodes. A complete description of the data can be found in Examples 1 and 2.

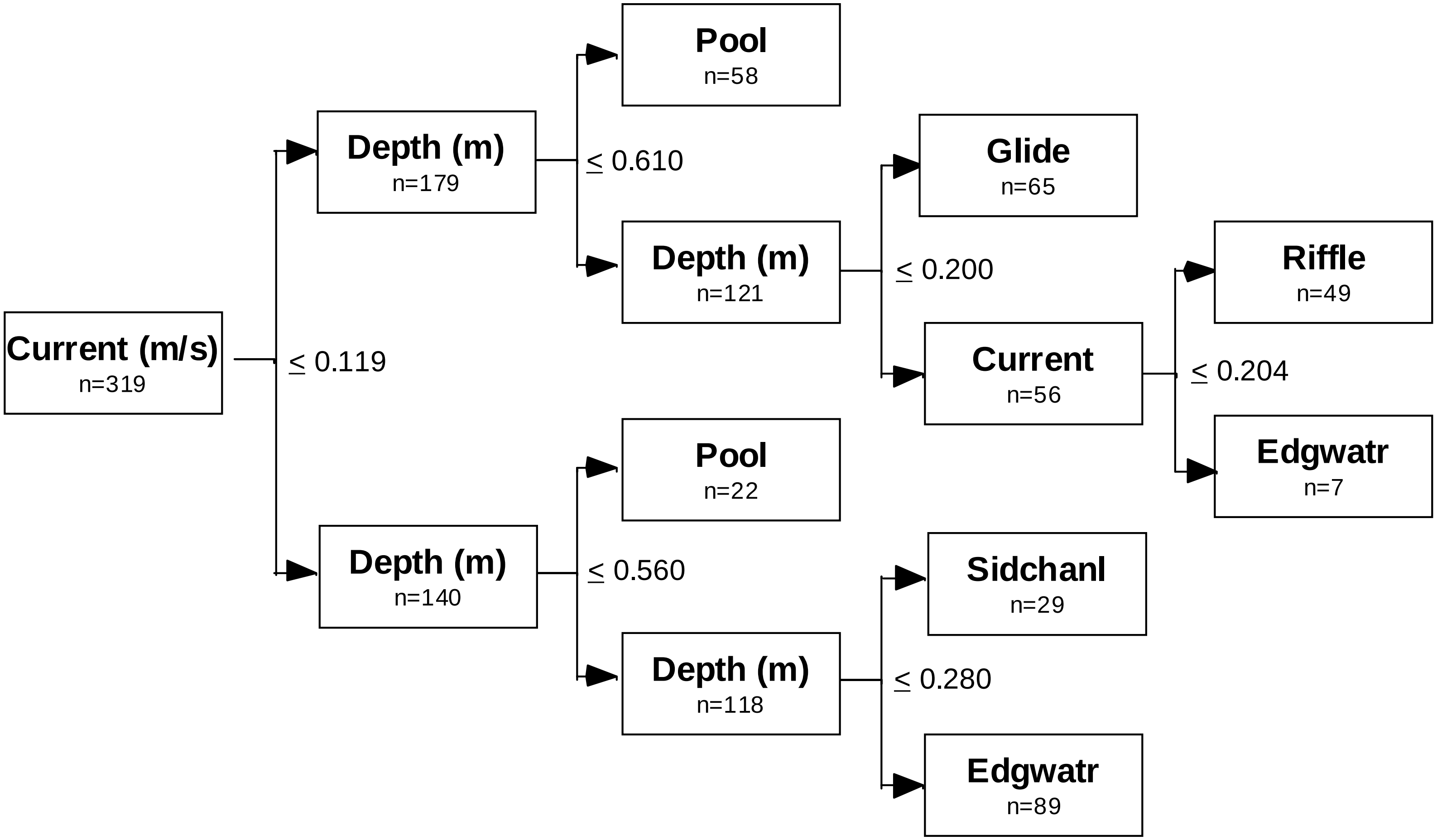


Figure 5.5. Classification tree with significant (P<0.05) predictors, depth and current velocity, for channel units in large Ozark streams.

DETAILS

Generalized logit models.- The CATDAT logit model classifier is based on the generalized logit model:

$$\log\left[\frac{\pi_{ij}}{\pi_{iJ}}\right] = x_i \beta_j , \qquad 6.1$$

where π_{ij} is the probability of response *j* at the *i*th setting of the *k* predictor values, $\boldsymbol{x}_i = (1, x_{i1}, x_{i2},\ldots.x_{ik})$, $\boldsymbol{\beta}_j$ is a separate parameter vector for *j*= 1, 2, … *J*-1 nonredundant baseline category logits, and *J* is the number of response categories (Agresti 1990). The $J^{\underline{th}}$ response category, also known as the baseline category, forms the basis of the *J*-1 logit pairs.

The j^{th} response category probability for predictor variables $\boldsymbol{x}_i$ is estimated as a nonlinear function of the parameter vector, $\boldsymbol{\beta}_j$:

$$\pi_j x_i = \frac{\exp\left(x_i \beta_j\right)}{\sum_{k=1}^{J-1} \exp\left(x_i \beta_k\right)}. \qquad 6.2$$

CATDAT iteratively estimates the maximum likelihood $\boldsymbol{\beta}_j$ parameters using the Fisher scoring method until the proportional decrease in the log likelihood between successive iterations (i.e., the convergence) is less than 5.0e-5. If this criterion is not reached after 20 iterations, CATDAT assumes convergence, outputs a warning message, and reports the decrease in the log likelihood during final the iteration.

To obtain category-specific probability estimates for unknown or test data or during expected error rate estimation, the maximum likelihood $\boldsymbol{\beta}_j$ estimates from a logit model fit to training data and the predictor values, $\boldsymbol{x}_i$, for the unknown or test data are substituted into equation 6.2. For illustration, assume that a logit model, fit to training data with hypothetical responses *A*, *B*, and *C*, have the maximum likelihood $\boldsymbol{\beta}_j$ shown in Table 6.1. An unknown observation with predictor values $\boldsymbol{x}_{unk}$= (1, 10, 100) would have the following response, $\boldsymbol{\beta}_j\,\boldsymbol{x}_i$.

$$\begin{aligned}
\boldsymbol{\beta}_A\,\boldsymbol{x}_{unk} &= 0.565 + (-0.0004 * 1) + (-0.0018 * 10) + (0.0027 * 100) = 0.8166\\
\boldsymbol{\beta}_B\,\boldsymbol{x}_{unk} &= 0.037 + (0.0009 * 1) + (-0.0008 * 10) + (-0.0007 * 100) = -0.0401\\
\boldsymbol{\beta}_C\,\boldsymbol{x}_{unk} &= 0 + (0 * 1) + (0 * 10) + (0 * 100) = 0
\end{aligned}$$

Note that for probability estimation category C, the baseline (J^{th}) category, has a $\boldsymbol{\beta}$ vector containing all zeros. Therefore, the denominator of the generalized logit model formula (6.2) would be exp(0.8166) + exp(-0.0401) + exp(0) = 4.2235 and the probability that the unknown observation belonged to each response category would be

$$\begin{aligned}
p(A) &= \exp(0.8166) / 4.2235 = 0.536\\
p(B) &= \exp(-0.0401) / 4.2235 = 0.227\\
p(C) &= \exp(0) / 4.2235 = 0.237.
\end{aligned}$$

Based on these estimated probabilities, CATDAT would have classified the unknown response as *A*. In the unlikely event that two categories had exactly the same probability, CATDAT would assign the observation to the first response category listed in the data file heading (i.e., the category with the smallest identification number, see Data Input).

Two mechanistic model selection procedures, forward selection and backward elimination, are available on CATDAT. Forward selection begins by computing the Score statistic (Fahrmeier and Tutz 1994) for each predictor or two-way interaction not already in the model. The predictor (or interaction) with the largest Score statistic that is also greater than the user-specified critical alpha-level is retained in the model. The process is then repeated until every covariate or interaction has been examined. Note that interactions are only examined for pairs of predictors already in the model.

In contrast to forward selection, the backward elimination procedure first fits the full model (i.e., all predictors). A Wald statistic (Fahrmeier and Tutz 1994) is then computed for each predictor and those predictors with Wald statistics exceeding the user-specified critical alpha-level are retained. This model selection procedure can only be used to examine main effects because fitting a full model with all predictors and two-way interactions would likely fail due to a very large number of parameters (Haas et al. In prep.).

CATDAT outputs 3 criteria for assessing model fit. The -2 log likelihood, also known as the Deviance, is estimated as

$$-2\log L = \sum_{i=1}^{g} n_i \sum_{j-1}^{J} \bar{y}_{ij} \log\left(\bar{y}_{ij} \Big/ \hat{\pi}_{ij} \right), \qquad 6.3$$

where $\bar{y}_{ij} \equiv y_{ij} \big/ n_i$ (Fahrmeir and Tutz 1994). The log likelihood test statistic output by CATDAT is the difference between the log likelihood of intercept-only logit model and the model specified. It's asymptotically distributed as a chi-square under the null hypothesis that there is no effect of the predictors. CATDAT outputs this statistic and its p-value during the estimation of the maximum likelihood $\boldsymbol{\beta}_j$.

The other two criteria are versions of Akaike's information criteria (AIC, Akaike 1973). The first is the AIC with the small-sample bias adjustment (AIC$_c$; Hurvich and Tsai 1989) which is calculated as

$$AIC_c = -2\log L + 2M + \left[\frac{2M(M+1)}{n-M-1} \right], \qquad 6.4$$

where M is the number of parameters. The second is the quasi-likelihood AIC with small-sample adjustment (QAIC$_c$, Burnham and Anderson 1998),

$$QAIC_c = -[2\log L/\hat{c}] + 2M + \left[\frac{2M(M+1)}{n-M-1} \right], \qquad 6.5$$

where $\hat{c} = \chi^2 / df$ is the variance inflation factor estimated using the goodness-of-fit chi-square statistic (χ^2) and its degrees of freedom (Cox and Snell 1989). Both the AIC and QAIC are used to compare candidate models for the same data. In general, the model with the lowest AIC$_c$ or QAIC$_c$ is considered the most parsimonious. For a through discussion of the use of AIC, model selection, and statistical inference, see Burnham and Anderson (1998).

Following estimation of the maximum likelihood $\boldsymbol{\beta}_{j,}$ CATDAT writes studentized Pearson residuals to a file and outputs two goodness-of-fit statistics, the Osius and Rojek increasing cell asymptotics and Andrews omnibus chi-square test. The studentized Pearson residuals should be distributed as a chi-square if the generalized logit model were appropriate for modeling the given data (Fahrmeir and Tutz 1994). Consequently, a plot of the studentized

Pearson residuals by their corresponding chi-square scores, which are also written to the residual file, should resemble a logarithmic shape.

The CATDAT implementation of the Osius and Rojek increasing cell asymptotics test is based on the relationship (χ^2 - μ_1)/σ_1, where μ_1 and σ_1^2 the asymptotic mean and variance, respectively. Under certain conditions (Osius and Rojek 1992), this relationship is approximately normally distributed under the null hypothesis that the generalized logit model is appropriate. It is important to note that the power of this test can be significantly lowered by small cell counts. Consequently, CATDAT reports the number of extreme predicted probabilities (i.e., > 10e-5) for each response category.

The Andrews omnibus chi-square test is a generalization of the more familiar Hosmer-Lemeshow test that can be used when a generalized logit model contains any number of response categories (Andrews 1988). This test is also more robust test than the Osius and Rojek increasing-cell-count asymptotics, above. The test begins by partitioning the data with a *K*-means clustering algorithm (Johnson and Winchern 1992) into *K* groups. These groups form the basis for a comparison of the distribution of observed and predicted responses, which is distributed as a chi-square under the null hypothesis that the generalized logit model is appropriate for modeling the responses.

Classification trees.- CATDAT classification trees are more precisely called binary tree classifiers because they are created by repeatedly splitting the data set into 2 smaller subsets using binary rule-sets. The tree growing process begins with the all the data at a single location known as a node (e.g., t_1 in Figure 1.1). This parent node is split into two child nodes (e.g., t_2 and t_3 in Figure 1.1) using a rule generated during a recursive partitioning. Note that this rule is always presented in tree form as: if yes then left, else right (Figure 1.1). During recursive partitioning, CATDAT searches for a predictor and its cutoff value that results in the greatest within-partition homogeneity for the response categories' distribution. In other words, the data is split into two subsets, each containing greater proportions of one response category. CATDAT uses deviance as a measure of within-partition homogeneity with the reduction in deviance for a particular split-value at parent node *t* estimated as

$$2\sum_{k=1}^{all\ categories}\left[n_{lk}\ \log\left\{\frac{n_{lk}n_{t}}{n_{tk}n_{l}}\right\}+n_{rk}\ \log\left\{\frac{n_{rk}n_{t}}{n_{tk}n_{r}}\right\}\right], \qquad 6.6$$

where n is the number of observations assigned to the left, l, or right-child, r, for each response category, k (Haas et al. In prep.). Note that deviance is zero when a node contains observations from only one category. This process is continued recursively down each branch of the classification tree until the size of a partition at any node is smaller than n, where n is the number of observations (i.e., the **minimum partition size**). After the partitioning is complete, the nodes at the end of the classification tree branches, defined as terminal nodes, are where responses are predicted (e.g., t3, t4, and t5 in Figure 1.1).

The classification trees resulting from recursive partitioning are generally too large and tend to overfit the data (i.e., the model becomes data set-specific; Figure 6.1). To reduce tree size, CATDAT recursively evaluates the effect of removing different terminal nodes (i.e., pruning the tree) on tree deviance, which is the sum of the deviance at each terminal node. The routine stops pruning when the tree reaches the size (i.e., maximum number of nodes) specified by the user with the best variable option. This tree will have the lowest deviance of any tree of its size (Chou et al. 1989). To improve the predictive ability of tree models (i.e., reduce overfitting), the expected error rate is evaluated for various sized trees using split-sample or leave-one-out cross-validation (see Expected error rate estimation, below). Optimum tree sizes are usually determined by examining plots of the cross-validation error rate by tree size (Brieman et al. 1984). These plots generally show an initially rapid decrease in error rate with increasing tree size, followed by relatively stable error rates, and then gradual increases in error as the larger trees begin overfitting the data (Figure 6.1). The most parsimonious tree model is generally considered the one in which size and expected error are minimized (e.g., the 21 node tree in Figure 6.1).

To obtain predicted responses for unknown or test data or during expected error rate estimation, an observation is dropped-down a classification tree that was fit with training data and the terminal node where it falls to is the predicted response. This technique can also be used to estimate the probability distribution of responses at each terminal node using a test data set and a classification tree fit with (other) training data. The response category probability distribution at a node is then estimated as the empirical distribution of the responses of the test data observations ending up at that node (Brieman et al. 1984).

Nearest neighbor classification.- The CATDAT implementation of nearest neighbor classification uses an extension of a nonparametric categorical regression smoother (Tutz 1990), referred to here as the *extended K*-nearest neighbor classifier (Haas et al. In prep.), to estimate the distance between observations. For instance, $\mathbf{x}_i$ is defined as an observation with predictor vector $\mathbf{x}_i = (z_1, z_2,..z_q, w_1, w_2,..w_r)$, which consists of q quantitative and r qualitative predictors. The vector of generalized differences between $\mathbf{x}_0$ and $\mathbf{x}_i$ is $s \equiv D^{-1/2}\left(x_0 - x_i\right)$, where $D_{ii} = \begin{cases} \sqrt{Var[z_i]}, & i \le q \\ 1, & i > q \end{cases}$ and

$$s = (x_0 - x_i) \equiv \begin{bmatrix} \left|z_{01} - z_{i1}\right| \\ \vdots \\ \left|z_{0q} - z_{iq}\right| \\ d_w\left(w_{01}, w_{i1}\right) \\ \vdots \\ d_w\left(w_{0r}, w_{ir}\right) \end{bmatrix}. \qquad 6.7$$

The distance between qualitative predictors, which are assumed to be uncorrelated among themselves and with the quantitative predictors, is defined following Tutz (1990) as

$$d_w\left(w_{0r}, w_{ij}\right) \equiv \begin{cases} 0, & w_{0j} = w_{ij} \\ 1, & w_{0j} \ne w_{ij} \end{cases}. \qquad 6.8$$

Let V be the correlation matrix of the covariates:

$$V \equiv D^{-1/2} \begin{bmatrix} C_{qq} & 0 \\ 0 & I \end{bmatrix} D^{-1/2} \qquad 6.9$$

where C_{pp} is the within-category pooled variance-covariance matrix of the quantative covariates. Then $d(x_0, x_i) = \sqrt{s'V^{-1}s}$ is the generalized Mahalanobis distance between x_0 and x_1 (Johnson and Wichern 1992). Note that the Mahalanobis distance may not accurately represent the true distance when the assumption of the independence of the qualitative predictors is not met.

The classification of an observation, $\mathbf{x}_0$, depends upon the response distribution of its *K* nearest neighbors (i.e., those with the *K* smallest Mahalanobis distances), which is estimated as $f_j(\mathbf{x}_0) = k_j / K$, where k_j is the number of *K* nearest neighbors belonging to category *j*. The observation is then predicted using the mode (i.e., greatest frequency) of this distribution. For example in Figure 1.2, the response distribution of the 6 nearest neighbors of observation *U1* is group *B*, 4/6 = 0.67 and group *A*, 2/6 = 0.33. Conversely, the response distribution of the 6 nearest neighbors of observation *U1* is group *B*, 2/6 = 0.33 and group *A*, 4/6 = 0.67. Based on these estimates, CATDAT would have classified observation *U1* and *U2* as belonging to groups *B* and *A*, respectively (Figure 1.2). Observations with 2 or more modal categories are classified as belonging to the first response category listed in the data file heading (i.e., the category with the smallest identification number, see Data Input).

Similar to the classification tree, the optimal number of neighbors (*K*) is determined by examining a plot of the cross-validation error rate by *K*, with the best *K* considered to be the one in which *K* and error are minimized (e.g., *K*= 2 and 3 in Figure 6.2). Although *K* can vary from 1 to *n*–1, we have found that the optimal values for *K* tend to be small in most practical applications (i.e., < 10, Haas et al. In prep.).

Modular neural networks.- Artificial neural networks generally consist of four linked components: the input, hidden, and output layers, and the target (Figure 6.3). The input layer is made up of predictor variable nodes (a.k.a. neurons) and a bias node used during neural network training. The hidden layer is the location where the neural network is trained (i.e., parameterized). It's composed of hidden nodes, each containing a set of weights (one for each predictor and the bias term), that are analogous to parameter estimates in a generalized linear model. During neural network construction (described below), these hidden nodes are added in a stepwise manner to increase the accuracy and complexity of the neural network. The output layer is comprised of output nodes, each containing a set of link weights from the hidden layer, which are used to calculate the activation function and output the model prediction to the target (described below). One additional feature of CATDAT neural networks that differs from classical designs is their modularity. Modular neural networks differ from classical neural networks in that there is a hidden layer module for each response category (Figure 6.3). Thus, each module becomes specialized at predicting its category, resulting in more accurate classifiers (Anand et al. 1995).

Although some components of neural network models have analogs in traditional parametric models (e.g., weights ~ parameters), both differ substantially in their algorithms. CATDAT uses quasi-Newton minimization (Press et al. 1986) with the Broyden-Fletcher-

Goldfarb-Shanno (BFGS) update to train the modular neural network. Training begins with 2 hidden nodes per module. Node weights are randomly assigned and the quasi-Newton routine searches for a minimum. Although this routine is relatively fast and efficient, it can converge to a local minimum where classification accuracy is very low (Setiono and Hui 1995). To break free of potential local minima, CATDAT artificially sets one observation in the data set to 'missing' (only) during the initial modular neural network training. After the neural net is trained, the fitted weights for the two hidden nodes are written to a file.

Modular neural network construction is a process by which additional hidden nodes are added to the model to increase its predictive ability. Construction begins by assigning random initial weights for the new hidden nodes. Initial weights for the other (L-1) hidden nodes are read from a file (above), and the modular neural network is retrained. By adding hidden nodes in this stepwise manner, a modular neural network can approximate almost any function. This attractive feature also makes MNN prone to overfitting (i.e., the model becomes data set-specific). Thus, constructing an optimal modular neural network in similar to the selection of the best sized classification tree, with the optimal modular neural network considered the one in which size (i.e., number of hidden nodes) and cross-validation error are minimized (e.g., the 6 and 10 hidden node modular neural network in Figure 6.4).

MNN predictions of unknown or test data responses are estimated using activation functions in both the hidden and output layers. CATDAT uses a sigmoidal mashing function (i.e., logistic function bounded by 0-1) to compute the hidden layer output vector $\boldsymbol{y}_l$ as

$$y_l = \frac{\exp(x'\omega_l)}{1+\exp(x'\omega_l)}, \qquad 6.9$$

where **x** is the vector of predictor variables and $\boldsymbol{\omega}_l$ is the vector of weights for hidden node, l= 1,..., L+1. Note that the $\boldsymbol{\omega}_{L+1}$ is the hidden layer bias and $\mathbf{x}_{p+1}$ and $\mathbf{y}_{p+1}$ are set to 1 prior to computing the function. The output vectors, $\boldsymbol{y}_l$, are then passed to the output layer and used to compute the output layer node values as

$$z^*_j = \frac{\exp(y'v'_j)}{1+\exp(y'v'_j)}, \qquad 6.10$$

where $\boldsymbol{v}_j$ is the vector of link weights and z^*_j is the output value for module j = 1,.., J. The values of z^* are used to predict an observation's response, which is identified as the response with the largest z^*. Similar to other CATDAT techniques, observations with identical z^* for 2 or more responses are classified as belonging to the first response category listed in the data file heading (i.e., the category with the smallest identification number, see Data Input).

Expected error rate estimation.- The most relevant measure of a classifier is its expected error rate (EER), which is defined as the error rate averaged over all possible combinations of predictors, including those not observed in the training data (Lachenbruch 1975). CATDAT automatically computes two EER estimators, within-sample and leave-one-out cross-validation. The within-sample EER estimator is calculated by applying a classification model to the observations in its training data set and summing the number of misclassified observations. This type of EER estimate tends to be negatively biased (Johnson and Wichern 1992) and should never be used during model selection (e.g., determining the optimal tree size; Brieman et al. 1984). However, the time required to compute a within-sample EER is generally much shorter than required for the cross-validation procedure. Thus, the within-sample EER can provide a quick, rough estimate of model performance when examining several complex models with large data sets.

CATDAT also automatically computes a leave-one-out cross-validation EER estimate. During this procedure, one observation is left out of the data, a model is fit with the remaining *n*-1 observations, and the left out observation is classified using the fitted model. This procedure is repeated for all observations and the proportion of misclassifications is used as an estimate of the EER. The leave-one-out cross-validation was found to be a nearly unbiased EER estimator for nonparametric classifiers (Funkunaga and Kessel 1971). Consequently, we recommend its use when evaluating model performance.

A third type of EER estimate can also be obtained with CATDAT using a *V*-fold cross-validation (Brieman et al 1984). During this procedure, observations are randomly placed into *V* groups, one group's observations are excluded and a model is fit with the data in the remaining *V*-1 groups (i.e., the training data). The excluded group's observations (i.e., the test data) are then classified using the model. This procedure is repeated for each group, and the proportion of misclassifications, across groups, is used to estimate the EER.

Although EER estimates are generally used to evaluate a classifier's performance or to compare different classifiers, it is important to note that EER is also influenced the magnitude of the difference between response categories. For example, a classifier created to distinguish between 2 groups that don't differ or that differ very little based on the predictors used in the model, will likely have high EER. Consequently, consistently high EER, across classification techniques, may be an indication that there are few differences among groups or that the predictors used are poor at characterizing the groups.

***Monte Carlo Hypothesis tests*.-** The Monte Carlo hypothesis test in CATDAT can be used, in part, to find the best performing nonparametric model and to examine the importance of one or more predictors on model performance (Haas et al. In prep.). The test is based on resampling statistics (Hall and Titterington 1989) and uses the index of most practical relevance, the cross-validation EER, as the basis for the test. One drawback to the use of an overall (average) EER is that sharply unequal response category sample sizes could significantly affect the results of the Mote Carlo test (Haas et al In prep.). To eliminate this potential source of bias, CATDAT uses the sum of the category-wise cross-validation errors, EERS, to give equal weight to each category.

The null hypotheses of the Monte Carlo test, H_0, is that there is no difference in EERS between the full model with all predictors and the reduced model with the predictor or set of predictors excluded (i.e., the predictor(s) being tested). Thus, the test statistic, T_s, is calculated using $\delta_s = EERS_R - EERS_F$, where F and R are the true error rates for the full and reduced models, respectively. The test statistic T_s is then defined as $T_s = \hat{\delta}_s - \delta$, with $T_s = \hat{\delta}_s$ under the null hypothesis.

The Monte Carlo hypothesis test procedure is as follows, following Haas et al. (In prep).

Step 1: Compute the full and reduced error rates EERSF and EERSR, respectively, from the actual data set. Compute $T_s = \delta_s$, the observed value of the test statistic assuming H0 is true.

Step 2: Sample without replacement r (< n) observations from the full sample.

Step 3: Compute the full and reduced error rates, EERS*F and EERS*R, respectively, using this m jackknife sample. Compute and store $T_s{}^* = \hat{\delta}_s - \delta$, the jackknife sample's test statistic value. Note that the true (but unknown) error rates have been replaced with those estimated from the full sample, which gives the Monte Carlo test good statistical power (Hall and Titterington 1989).

Step 4: Repeat steps 2 and 3 m times always with a new randomly selected jackknife sample.
Step 5: Compute the p-value of the test to be the fraction of T_s* values greater than T_s.

Note that when r < n-1, the histogram of the m T_s* values is a deleted-d jackknife statistic (Shao and Tu 1995) where d = n - r. Therefore, both d and m need to be large for a conststant hypothesis test (Shao and Tu 1995).

Table 6.1. Hypothetical maximum likelihood estimates for generalized logit model with 3 response categories and 3 predictors.

	-------------------Maximum likelihood betas------------------			
Response	intercept	predictor-1	predictor-2	predictor-3
A	0.5650	-0.0004	-0.0018	0.0027
B	0.0370	0.0009	-0.0008	-0.0007
C	---------------	--(baseline)-	---------------	---------------

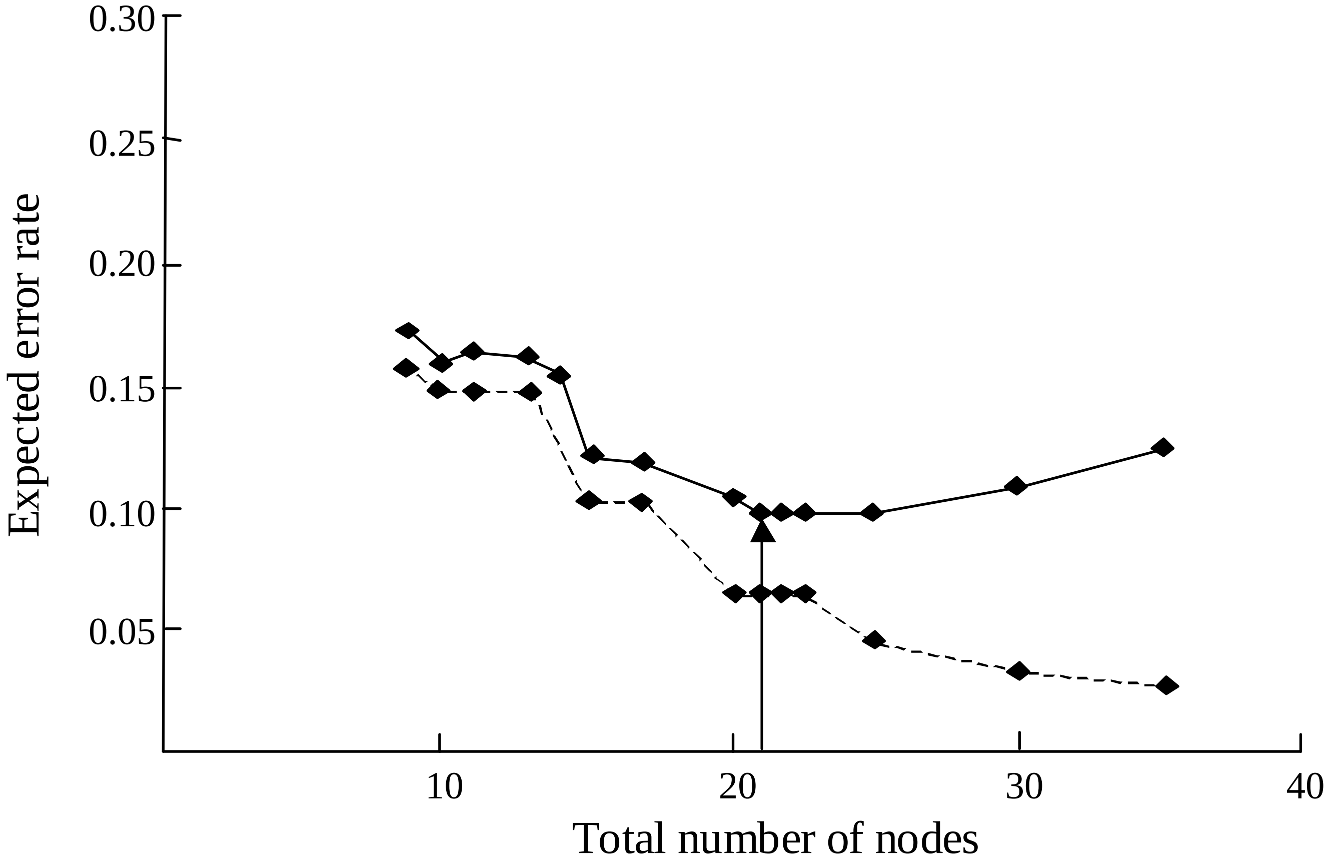


Figure 6.1. Overall cross-validation (solid line) and within-sample (broken line) error rate of various sized classification trees for ocean-type chinook salmon population status (Example 1). The most parsimonious tree model, shown by the arrow, consisted of 21 nodes. The continued decrease in the within-sample error with increasing tree size, in contrast to the gradual increase in the cross-validation error after 21 nodes, is due to model overfitting. Consequently, within-sample error should never be used to determine optimal tree size.

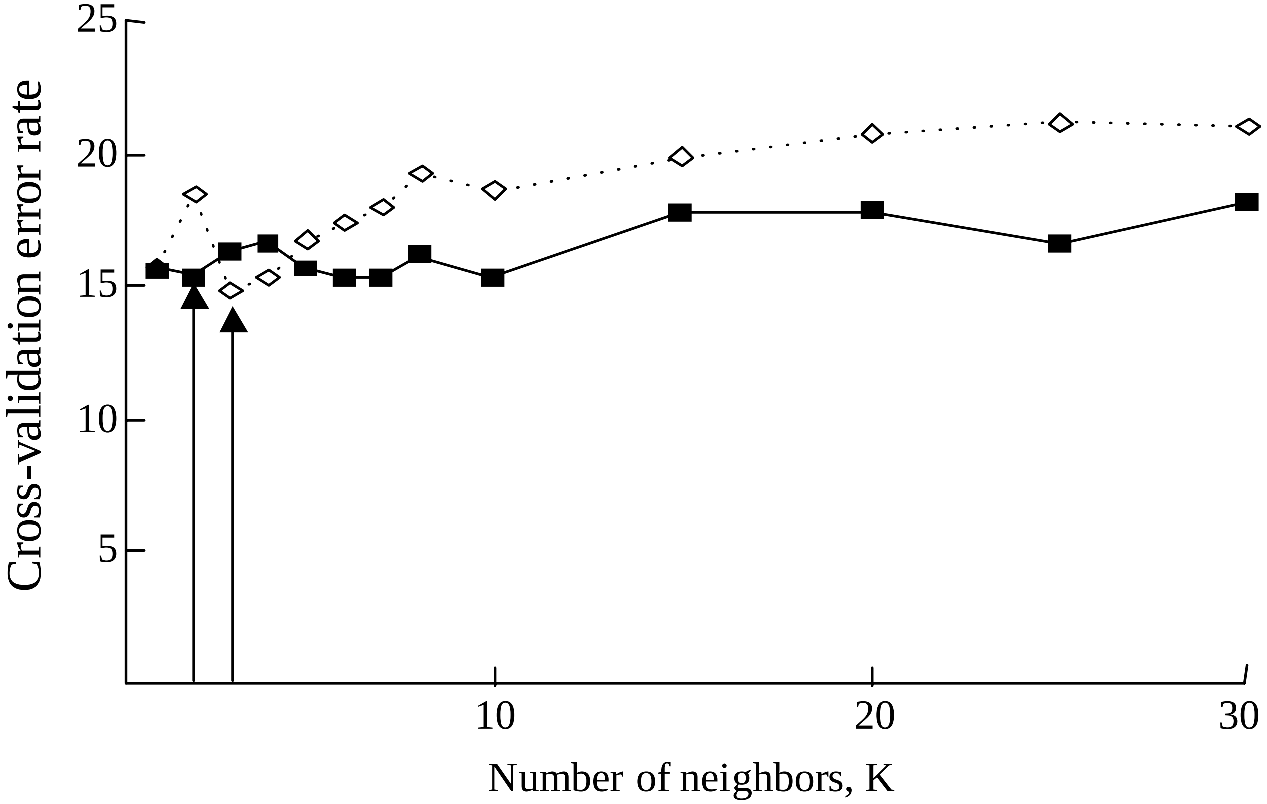


Figure 6.2. Overall cross-validation error rate for various numbers of nearest neighbors, K, for ocean-type chinook salmon population status (broken line and open symbols) and physical habitat characteristics of stream channel-units (solid lines and symbols). Arrows indicate the optimal K values. A complete description of the data can be found in Examples 1 and 2.

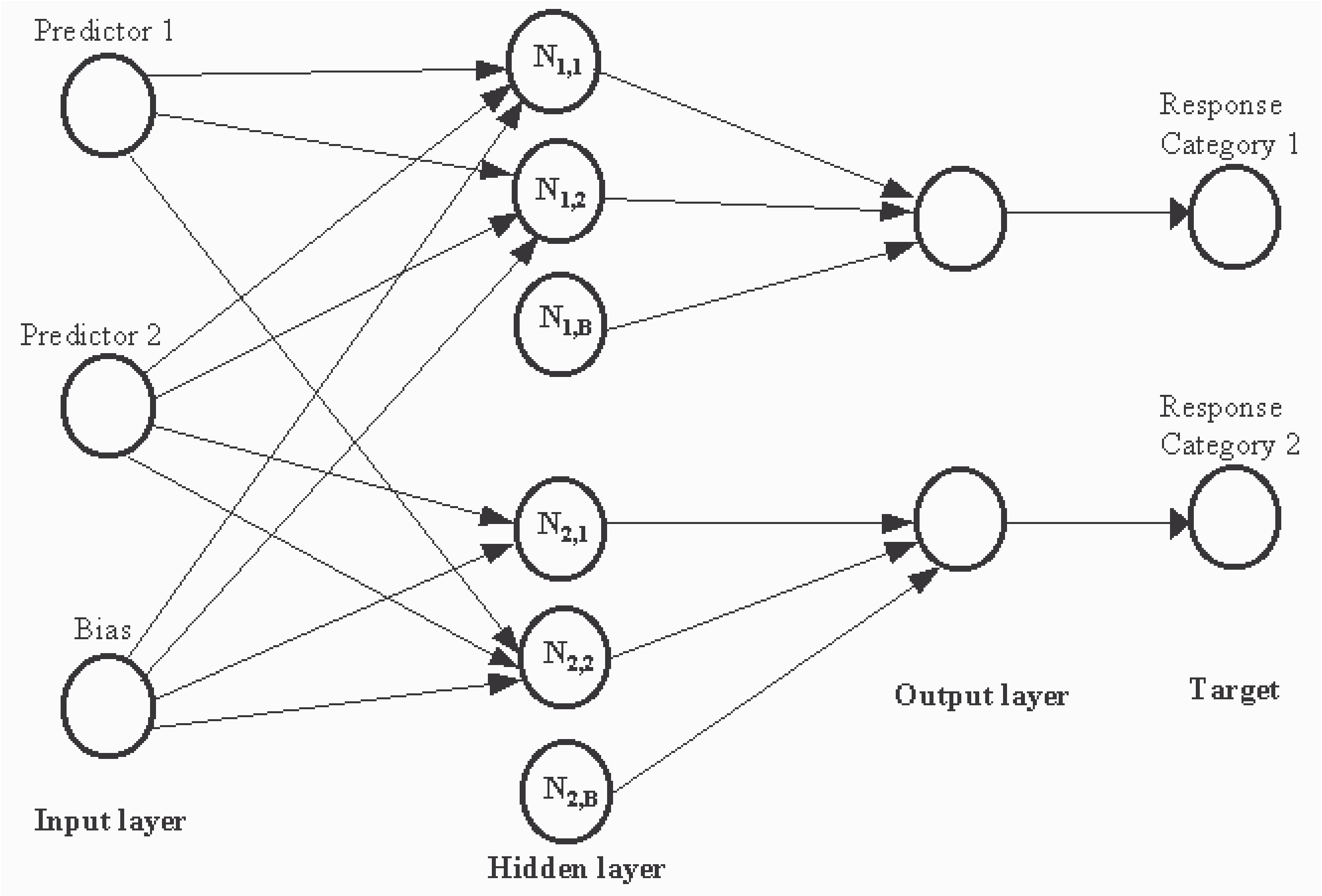


Figure 6.3. The schematics for a modular neural network with 2 predictor variables, 2 responses, and 2 hidden nodes per module labeled as N_{jk} with j = module and k = hidden node number, respectively. Nodes with B subscripts represent the bias term for the output layer, which is analogous to an intercept in generalized linear models.

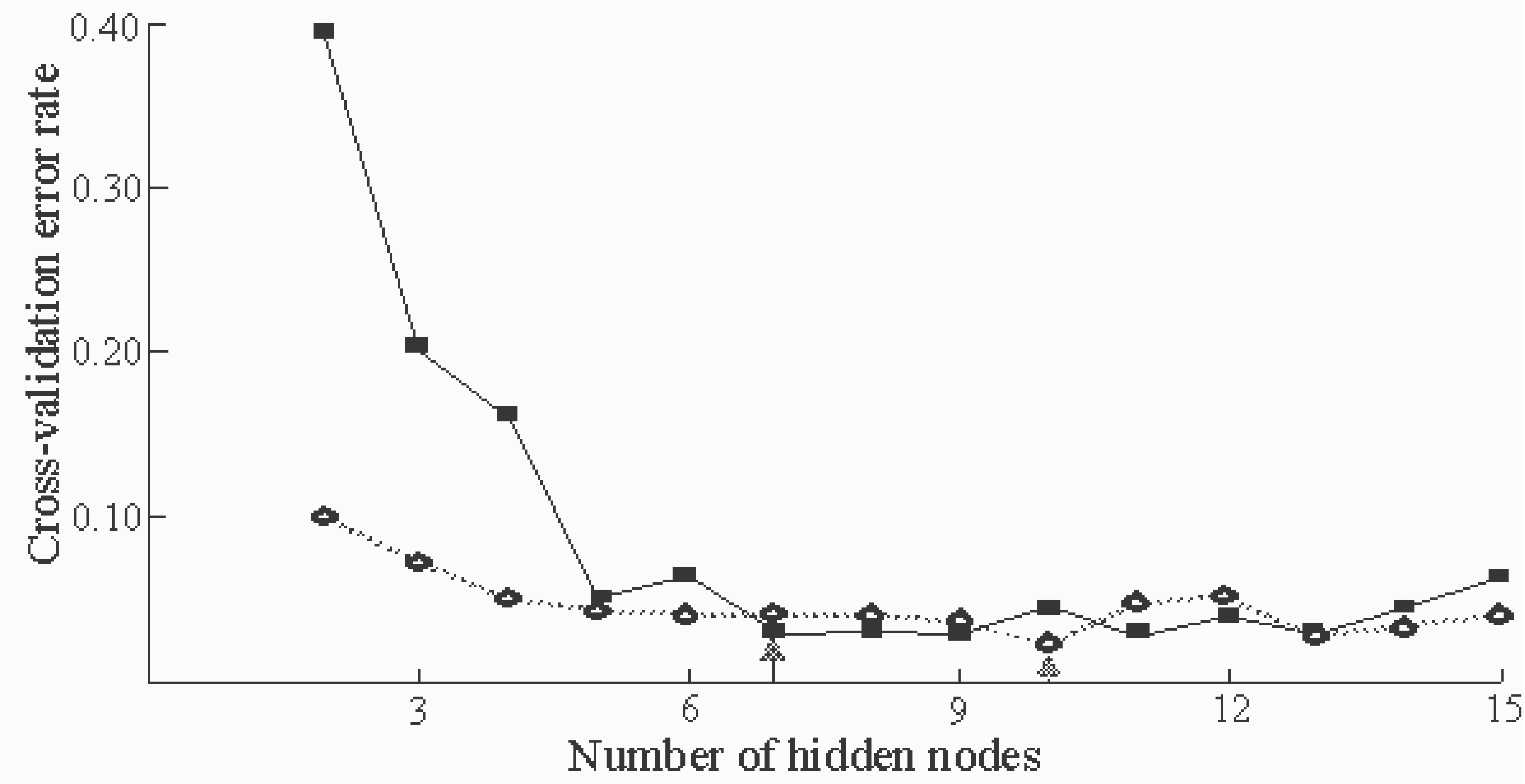


Figure 6.4. Cross-validation classification error rate of various sized modular neural network for chinook salmon population status (broken line and open symbols) and physical habitat characteristics of stream channel-units (solid line and symbols). Arrows indicate optimal number of hidden nodes. A complete description of the data can be found in Examples 1 and 2.

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Installation

CATDAT consists of a set of C programs for analyzing parametric and nonparametric categorical data. To use CATDAT, the entire set of programs must be installed and compiled in a single location. Knowledge of the C programming language is not necessary to install or run CATDAT.

Requirements.- CATDAT will run under most variants of Unix and has been tested under AIX 4.2 and DEC Alpha. It also has an option for running under Borland C++ (Table 7.1), but has yet to be tested under this environment. The program requires an ANSI-compliant C compiler with standard C libraries and approximately 1 MB of free disk-space.

***Installation*.-** For convenience, all of the CATDAT program and two data files, otc.dat and otc2.data, from Example 1 are compressed in a single file, catprgm.zip, and require pkunzip to unzip them. To install CATDAT, complete the following steps.

1. Download catprgm.zip and copy to the desired directory. We recommend setting-up a separate directory for CATDAT.

2. Unzip the program files within the CATDAT directory,

3. Configure the make file, "catdat.mk", for the current operating system by adding or removing the pound signs (#) at the beginning of the respective statements with a text editor (Table 7.1). Note that the default is AIX. Also, make sure that the two statements below catdat.time or catdat.tme begin with a single tab. If these two statements are not led by tabs, the following (or similar) error message will be displayed during compiling.

"catdat.mk" line [line number] *Dependency needs colon or double colon operator*

4. To compile the program, enter the following at the prompt:

```
make -f catdat.mk
```

The program will then be complied and written to the current directory. CATDAT is now ready to run.

***Error messages*.-** CATDAT has several error-catching routines within the program, most of which output relatively self-explanatory messages. Listed below are all of error messages that are likely to be encountered during program execution with a brief description of each.

***General error messages*.**- The following error messages are the most common and are usually displayed immediately following input of the data file.

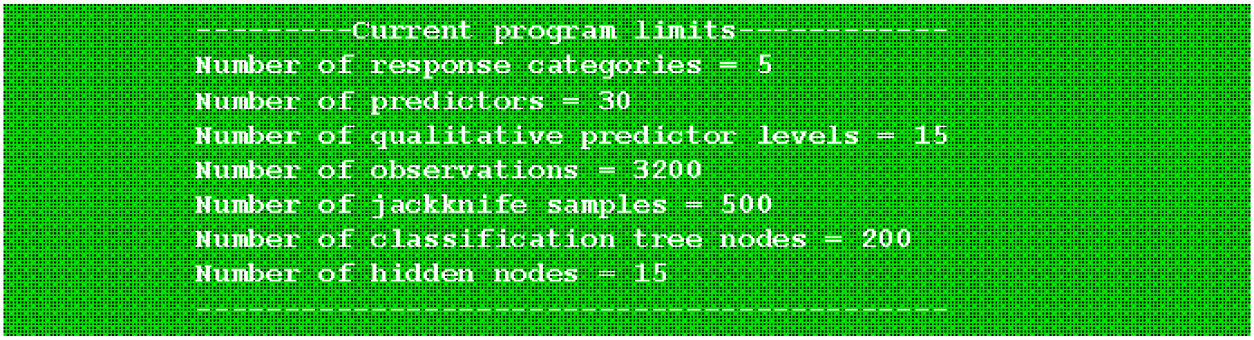
Number of predictors exceeds maximum

Number of obs. exceeds maximum

Design matrix exceeds maximum

No. of qualitative predictor categories exceeds max

The most obvious source of these errors is that the variables have exceeded the program limits defined in the catdat header file, "catdat.h". These limits are displayed just below the heading at start-up, e.g.,



```
           ---------Current program limits------------
           Number of response categories = 5
           Number of predictors = 30
           Number of qualitative predictor levels = 15
           Number of observations = 3200
           Number of jackknife samples = 500
           Number of classification tree nodes = 200
           Number of hidden nodes = 15
           -------------------------------------------
```

and can be changed by redefining the appropriate symbolic constant in the header file (Table 7.2). Note that the CATDAT object files (i.e., those ending with the extension ".o" or ".obj") should be deleted and catdat recompiled following changes to the header file.

Another likely source for these error messages is an incorrect match between the data file heading and body. For example, if the specified number of predictors (p) is less than the actual number in the data file body, CATDAT will treat the p+1 predictor for the first observation as the response category for the second observation. The actual response variable for the second observation will then be treated as the value of its first predictor variable and so forth.

The following message is displayed when CATDAT cannot locate the specified file.

File open failure for [filename] *status* = [r = read, a = append]

The following error message is generally due to an incorrectly formatted analysis specification file and/or the name of a file, predictor, or response category that exceeds 10 characters in the analysis specification file.

Fatal error encountered while reading analysis specification file

Generalized logit model.- The most common error encountered while fitting the generalized logit model is the use of qualitative predictors, which will result in the following message.

Warning [file name] *contains qualitative predictors. Recode using*
dummy variables (i.e., 0 or 1) before constructing logit model.

The following error message is displayed when a logit model specification file contains too many predictors or when the logit model is incorrectly specified (e.g., the predictor identification numbers are incorrect).

Number of predictors = [value], *p*= [value], *Max p* = [value]
exceeded maximum during logit model parameterization

The following messages are displayed when the data cannot be fit with the generalized logit model (e.g., when predictors are perfectly linearly correlated, resulting in a singular matrix).

F matrix ill-conditioned, giving up

Matrix ill-conditioned

Cholesky decomposition failed

Singular matrix detected

Error detected while calculating Sigma^2, exiting

Rarely occurring predictors (i.e., dummy coded) can also prevent the logit model-fitting algorithm from converging resulting in the errors listed above. Possible remedies include combining rarely occurring dummy predictors, data transformation, eliminating highly correlated predictors, and combining related response categories (e.g., ocean-type chinook salmon strong + depressed population status = ocean-type chinook salmon present).

The following errors are encountered during hypothesis testing and computing goodness of fit tests for logit model main effects and interactions.

Fatal error, critical score statistic < 0

Bad values for estimating incomplete gamma function

Failure during estimation of incomplete gamma function

Unable to partition data with k-means clustering

Too many response categories for goodness of fit test

Maximum number of iterations exceeded during k-means clustering

Number of clusters exceeds maximum during k-means clustering

In many instances, these error messages may result from incorrectly specifying the critical alpha-level (e.g., a negative number or alpha > 1). Other potential sources include poor model fit, which may be remedied by one or more the above suggestions.

Classification tree.- The most common error message for the classification tree is given when the BEST parameter exceeds the maximum number of nodes.

Maximum number of nodes possible = [value] < *best* = [value],

BEST specification too large

The following errors are rare, but may be encountered when none of the predictors are useful for classifying responses with the classification tree. For example, these errors might occur during a Monte Carlo hypothesis test in which the all of the significant predictors were excluded (i.e., tested).

Maximum number of classification tree nodes exceeded

Terminal node reached while searching for delta_min

Singleton tree obtained while pruning tree

Number of classification tree partitions exceeds maximum

Fatal error detected during tree growing

***Nearest neighbor*.-** The following message is usually output when one or more of the response categories has too few observations to calculate the kernel distance (see Details).

Insufficient no. of obs. in [response category name] *for kernel smoothing*

When this error occurs, the response category should be dropped from the analysis or its observations combined with a similar category. For example, if there were an insufficient number of observations for the "strong" ocean-type chinook salmon status (Example 1), they could have been combined with observations from the "depressed" category and redefined as ocean-type chinook salmon "present".

Similar to the logit model, the following messages are displayed when the kernel distance cannot be computed with the data (e.g., when qualitative predictors are perfectly linearly dependent).

Warning covariance matrix has zero variances-

variances

[list of variances]

Generalized correlation matrix ill conditioned

Modular neural network.- The following error message is the most common for the modular neural network.

Number of hidden nodes exceeds maximum

This limit is displayed along with others (above) just below the heading at start-up and can be changed by redefining the appropriate symbolic constant in the header file (Table 7.2).
The following error message would be output in the extremely rare occasion when more than 500 iterations were needed to locate minima while fitting the neural network.

Maximum number of iterations exceeded

Although the maximum number of iterations (ITMAX) can be re-specified in dfpmin.c, exceeding ITMAX suggests that the predictors may not be useful for constructing a neural network.

Another problem that is may be encountered when fitting a modular neural network is an insufficient amount of stack memory. CATDAT uses a quasi-Newton method to locate minima while fitting the neural network (see Details). Consequently, the stack memory requirements are fairly large when compared to neural networks that employ conjugate gradient methods. The greatest local memory requirement for the neural network is the pseudo Hessian matrix (hessin[][]) whose requirements are roughly the product of MAXP, MAXHID, and MAXK located in the catdat header file (Table 7.2).

Before fitting a neural network, CATDAT automatically checks for the amount of memory available and, if insufficient, the program is immediately stopped. If this happens, there are two possible solutions.

1. Find out the maximum stack size and reduce the size of MAXP, MAXHID, and/or MAXK in the CATDAT header file as necessary.

2. For many systems, the stack size can be changed to "unlimited" (i.e., up to the virtual space limit, which is typically 100's of megabytes). This can usually be changed by the system administrator where the user limits are stored (e.g., /etc/security/limits).

Monte Carlo hypothesis test.- The following error message is displayed when the model specification file contains too many predictors or when the predictors are incorrectly specified (i.e., the predictor identification numbers are incorrect).

Number of predictors in mod. specific. file exceeds number in data file

The following message is displayed when the specified jackknife sample size exceeds the number of samples in the data file.

Jackknife sample size greater than maximum allowed

The following message is displayed when the number of jackknife sample size exceeds the maximum, which can be changed by redefining the appropriate symbolic constant in the header file (Table 7.2).

Number of jackknife samples [value] > *maximum allowed* [value]

Additional error messages.- The most frequently encountered non-CATDAT error messages are the following.

NaN (not-a-number)

NaNQ

INF

These messages are usually output when: (1) the exponent of a value is too large to be represented, (2) a nonzero value is so small that it cannot be represented as anything other than zero, (3) a nonzero value is divided by zero, (4) operations are performed on values for which the results are not defined, such as infinity-infinity, 0.0/0.0, or the square root of a negative number or (5) a computed value cannot be represented exactly, so a rounding error is introduced.

Troubleshooting.- Although most errors should be detected and reported by CATDAT, there may be some situations where the program will crash without identifying and reporting the problem. In these situations, CATDAT should be run under a debugger to determine the source of the problem. Below is an outline for debugging CATDAT with AIX 4.2. Consult the user's manual for specific information on debugging options for other systems.

To run a C debugger with AIX 4.2, the optimization flag "**`-O2`**" should be replaced with "**`-g`**" in the catdat make file "catdat.mk". For example, the declarations in the original CATDAT make file should read:

```
# For the SUN or AIX
CFLAGS = -O2 -I/usr/openwin/share/include
PFLAGS = -lm -lc -L/usr/openwin/lib -lX11
.c.o: ; cc -c $(CFLAGS) $*.c
```

After replacing the optimization flag, the declarations should read:

```
# For the SUN or AIX
CFLAGS = -g -I/usr/openwin/share/include
PFLAGS = -lm -lc -L/usr/openwin/lib -lX11
.c.o: ; cc -c $(CFLAGS) $*.c
```

After recompiling CATDAT, enter " dbx -r catdat " at the AIX prompt and run the same analysis that caused the problem. The debugger will run the program and output the problem statement and its location (i.e., the CATDAT program file). Note that the optimization flag should be changed back and CATDAT recompiled after debugging.

Table 7.1. The CATDAT make file "catdat.mk". This make file is set-up to compile CATDAT on an AIX or SUN operating system. To configure the file for DEC Alpha or Borland 4.5 C++, remove the pound signs (#) in front of the respective compiler statements and place them in front of the SUN/AIX statements. Note that the two statements below the *catdat.time* or *catdat.tme* begin with a single tab.

```
# For the ALPHA
#CFLAGS = -O2 -ieee_with_no_inexact -Olimit 1000
#PFLAGS = -lm -lc -lX11
#.c.o: ; cc -c $(CFLAGS) $*.c
# For the SUN or AIX
CFLAGS = -O2 -I/usr/openwin/share/include
PFLAGS = -lm -lc -L/usr/openwin/lib -lX11
.c.o: ; cc -c $(CFLAGS) $*.c
# For Borland 4.5 C++
#.AUTODEPEND
#CC = -c -p- -vi -W -X- -P -O2
#CD = -D_OWLPCH;
#INC = -Ic:\bc4\include
#LIB = -Lc:\bc4\lib
#.c.obj:
# bcc32 $(CC) $(CD) $(INC) $*.c
OBJ = catdat.o \
bslct.o \
.
(remainder of object files)
.
zscores.o
#Unix
catdat.time: $(OBJ)
cc $(OBJ) -o catdat ${PFLAGS} (this line begins with a tab)
touch catdat.time (this line begins with a tab)
#
#For Borland 4.5 C++
# Note that tlink32 will fail if array dimensions in catdat.h are too
big.
# Also, shut down Windows to run Borland make and create a swapfile
first
# with makeswap 20000. tlink32 and rlink32 take
# alot of time. Finally, runtime linking only shaves 3 megabytes off of
# the 25 megabyte Borland executable file -- it's not worth doing.
#
#catdat.tme: $(OBJ:.o=.obj) catdat.exe
# tlink32 -aa -c -Tpe $(LIB) @catdat.lnk (when used, this line begins
with a tab)
# touch catdat.tme (when used, this line begins with a tab)
```

Table 7.2. The variables used to define CATDAT memory limits in header file *catdat.h*.

Symbolic constant name	Description
MAXQ	Maximum number of response variable categories
MAXP	Maximum number of predictors
MAXLVLS	Maximum number of qualitative predictor levels
MAXN	Maximum number of observations
MAXNIN	Maximum size of the design (i.e., model) matrix
MAXNDES	Maximum number of classification tree nodes
MAXSIM	Maximum number of jackknife samples
MAXNMR	Maximum number of partitions in classification trees
MAXHID	Maximum number of hidden nodes

Appendix A. The name and description of the variables used to identify the desired criteria in CATDAT analysis specification files. Asterisk identifies the variables that must be in all analysis specification files. See Tables 3.1 and 3.2 for examples of the structure of analysis specification files.

Variable name	**Type**	**Description**
flenme*	string	The name of the CATDAT data file.
genout*	string	The name of the general output file.
flein	string	The name of an input files that depends on the type of analysis. For the logit model error and maximum likelihood (ML) beta estimation and the Monte Carlo hypothesis test, it is the name of the model specification file. It is also the name of the file containing unknown or test data.
fleout	string	The name of an output file that depends on the type of analysis. For the logit model hypothesis tests, it is the name of the file for recording the significant predictors or interactions. Fleout is also the name of the logit model residual file, the classification tree SAS file, Monte Carlo hypothesis test T_s^* statistics file, and the file containing the predictions for the unknown or test data.
omegfil	string	The name of the file containing previously estimated neural network weights.
omegfil2	string	The name of the file to output fitted neural network weights.
nmcat*	integer	The number of response variables which must be followed by the response variable names (1 per line).
nmprd*	integer	The total number of predictors.
nmquan*	integer	The number of quantitative predictors which must be followed by the quantitative predictor names and the qualitative predictor names (1 per line).
esttyp*	integer	Identifier used to declare the type of classifier with values of: 1 = generalized logit model, 2 = classification tree, 3 = nearest neighbor, and 4 = MNN.

Variable name	**Type**	**Description**
calc*	integer	Identifier used to declare the type of analysis with values of: 1 = forward selection of generalized logit model interactions, 2 = error rate calculation with the full *esttyp* model, 3 = Monte Carlo hypothesis test, 4 = estimation of ML betas and residua analysis of full main effects logit model, 6 = fit the *esttyp* model to the full dataset, 7 = Wald test of each predictor in generalized logit model, 8 = error rate calculation or ML beta estimation with selected main effects logit model, 9 = error rate calculation or ML beta estimation with full main effects and selected interactions logit model, 10 = error rate calculation or ML beta estimation with selected main effects and interactions logit model, and 11= classification of unknown or test data.
selerr	integer	The type of classification error rate calculation with values of: 1 = within-sample and 2 = cross-validation.
xtrparm	integer	The value of this parameter depends on the type of analysis. It takes a value of "1" when estimating the ML betas of selected main effects or interactions logit models with untransformed data and 2 when the data are normalized, whereas it is the number of jackknife samples for Monte Carlo hypothesis tests.
sigp	real	The critical alpha-level for logit model hypothesis tests.
besttre	integer	The classification tree BEST parameter.
nmhid	integer	The number of MNN hidden nodes or the number of nearest neighbors (K).
omegseed	integer	Identifier used to declare that MNN weights are to be read from a file (i.e., omegseed = 1).
jackno	integer	The jackknife sample size.
cverfull	real	The full model cross-validation error rate used during the Monte Carlo hypothesis tests.