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Introducing the New ADAPTIVEREG Procedure for Adaptive Regression

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ABSTRACT

Predicting the future is one of the most basic human desires. In previous centuries, prediction methods included studying the stars, reading tea leaves, and even examining the entrails of animals. Statistical methodology brought more scientific techniques such as linear and generalized linear models, discriminant analysis, logistic regression, and so on. In this paper, you will learn about multivariate adaptive regression splines (Friedman 1991), a nonparametric technique that combines regression splines and model selection methods. It extends linear models to analyze nonlinear dependencies and to produce parsimonious models that do not overfit the data and thus have good predictive power. This paper shows you how to use PROC ADAPTIVEREG (a new SAS/STAT® procedure for multivariate adaptive regression spline models) by presenting a series of examples that show the relationship between adaptive regression models and other statistical modeling techniques.

INTRODUCTION

The ADAPTIVEREG procedure fits multivariate adaptive regression splines, which were proposed by Friedman (1991). Multivariate adaptive regression splines extend linear models to analyze nonlinear dependencies and produce parsimonious models that do not overfit the data and thus have good predictive power. This method is a nonparametric regression technique that combines both regression splines and model selection. It constructs spline basis functions in an adaptive way by automatically selecting appropriate knot values for different variables, and it obtains reduced models by applying model selection techniques. The method does not assume parametric model forms and does not require specification of knot values.

This paper explains the basics of PROC ADAPTIVEREG by using a series of examples that include linear, logistic, and Poisson models. The first three examples demonstrate some basic capabilities of PROC ADAPTIVEREG and show how it constructs the basis functions. These examples explain the algorithms that are used by PROC ADAPTIVEREG by showing you ways in which they correspond to more familiar multiple regression models. The logistic regression junk e-mail example is the most comprehensive example and illustrates the most important capability of PROC ADAPTIVEREG, namely prediction. That example shows you how to build a model and use it to score observations that were not used in the initial model. When the correct classification is known, the scored observations are used to evaluate the goodness of the predictions. The final example illustrates a nonparametric Poisson regression model.

PROC ADAPTIVEREG is available as an experimental procedure in SAS/STAT 12.1, which was released in 2012. The examples in this paper were run in SAS/STAT 13.1, which will be available in 2013. All example code also works in the SAS/STAT 12.1, but the results might differ in some cases.

PROC ADAPTIVEREG FEATURES

The ADAPTIVEREG procedure provides the following features:

- fits nonparametric regression models (linear, logistic, and Poisson)
- supports quantitative and classification variables
- can run using multiple threads
- enables you to force effects in the final model or restrict variables in linear forms
- supports options for fast forward-selection
- supports data that have response variables that are distributed in the exponential family (Buja et al. 1991)
- supports partitioning of data into training, validation, and testing roles
- provides leave-one-out and k-fold cross validation
- produces a graphical representation of the selection process, model fit, functional components, and fit diagnostics
- produces an output data set that contains predicted values and residuals
- produces an output data set that contains the design matrix of basis functions
- can score multiple data sets

NONLINEAR FIT FUNCTION EXAMPLE

The following DATA step creates artificial data, and the PROC SGPLOT step shows loess and penalized B-spline fit functions (see Figure 1). The final step uses PROC ADAPTIVEREG to find a nonparametric fit function (see Figure 2):

```
data x;
   do i = 1 to 500;
      x = 1 + uniform(121) * 4;
      y = sin(x) + 0.2 * normal(121);
      output;
   end;
run;

proc sgplot;
   loess y=y x=x;
   pbspline y=y x=x / nomarkers;
run;

ods graphics on;
proc adaptivereg plots=all details=bases;
   model y = x;
run;
```

The ODS GRAPHICS ON statement enables ODS Graphics so that PROC ADAPTIVEREG will produce graphs.[1] The PROC ADAPTIVEREG fit function in Figure 2 shows that the relationship between y and x in these data is nonlinear. PROC ADAPTIVEREG finds a piecewise linear fit function that tracks the continuous nonlinear function. In contrast, the loess and penalized B-spline fit functions in Figure 1 are continuous, smooth, and virtually indistinguishable from each other for these data. All three methods show that the underlying function is a section of a sine curve. If your goal is to find a nonlinear fit function with two continuous variables, then you might prefer the loess or penalized B-spline model. However, PROC ADAPTIVEREG can handle models that are much more general than the model that this example uses. This example uses the simple nonlinear fit function as a convenient way to introduce some basic properties of the method.

Figure 1: Artificial Data Nonlinear Fit Functions

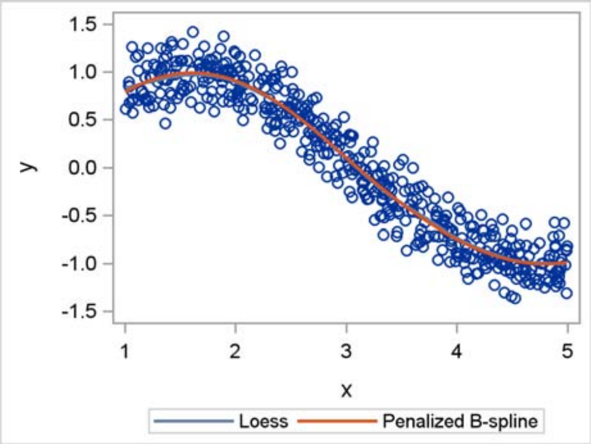
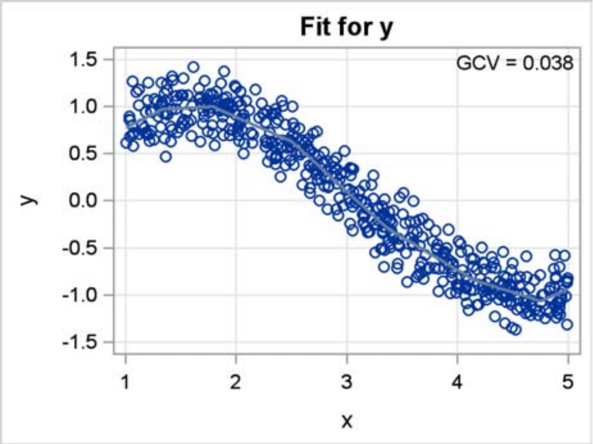


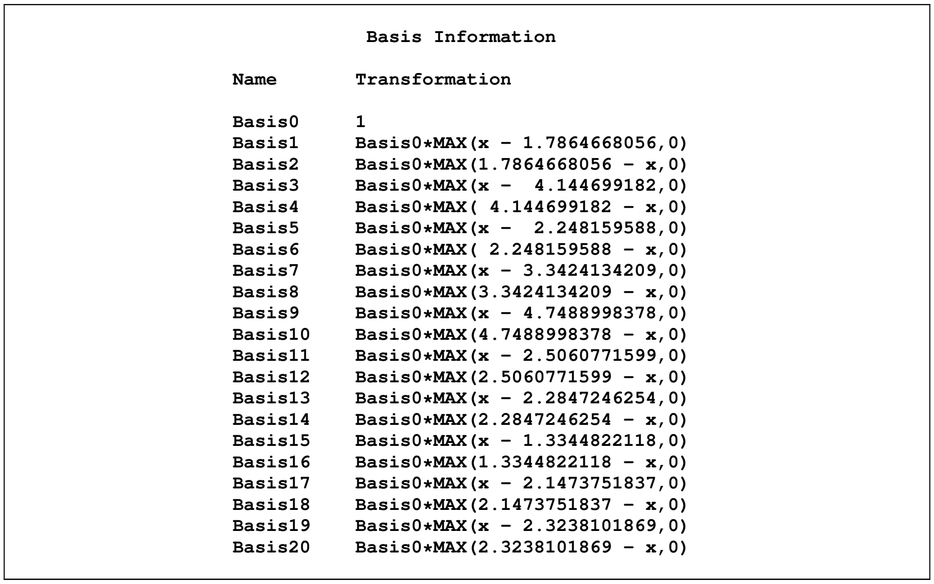
Figure 2: Adaptive Regression Fit Function



[1] ODS Graphics is enabled and not subsequently disabled, so ODS Graphics remains enabled for the duration of this paper.

PROC ADAPTIVEREG first constructs a set of basis functions and then uses variable selection to find a model. Figure 3 displays the transformations that are used to generate the basis matrix for the piecewise linear fit.

Figure 3 Basis Information



```
                         Basis Information

             Name        Transformation

             Basis0      1
             Basis1      Basis0*MAX(x - 1.7864668056,0)
             Basis2      Basis0*MAX(1.7864668056 - x,0)
             Basis3      Basis0*MAX(x -  4.144699182,0)
             Basis4      Basis0*MAX( 4.144699182 - x,0)
             Basis5      Basis0*MAX(x -  2.248159588,0)
             Basis6      Basis0*MAX( 2.248159588 - x,0)
             Basis7      Basis0*MAX(x - 3.3424134209,0)
             Basis8      Basis0*MAX(3.3424134209 - x,0)
             Basis9      Basis0*MAX(x - 4.7488998378,0)
             Basis10     Basis0*MAX(4.7488998378 - x,0)
             Basis11     Basis0*MAX(x - 2.5060771599,0)
             Basis12     Basis0*MAX(2.5060771599 - x,0)
             Basis13     Basis0*MAX(x - 2.2847246254,0)
             Basis14     Basis0*MAX(2.2847246254 - x,0)
             Basis15     Basis0*MAX(x - 1.3344822118,0)
             Basis16     Basis0*MAX(1.3344822118 - x,0)
             Basis17     Basis0*MAX(x - 2.1473751837,0)
             Basis18     Basis0*MAX(2.1473751837 - x,0)
             Basis19     Basis0*MAX(x - 2.3238101869,0)
             Basis20     Basis0*MAX(2.3238101869 - x,0)
```

The first basis function, Basis0 = 1, is the intercept. The second basis function, Basis1, is x – 1.7864668056 when x > 1.7864668056 and 0 otherwise (where k = 1.7864668056 is a knot). The third basis function, Basis2, is 1.7864668056 – x when x < 1.7864668056 and 0 otherwise. Other basis functions are constructed in a similar manner by using other knot values. The knots are automatically chosen. These bases are constructed by using truncated power functions.

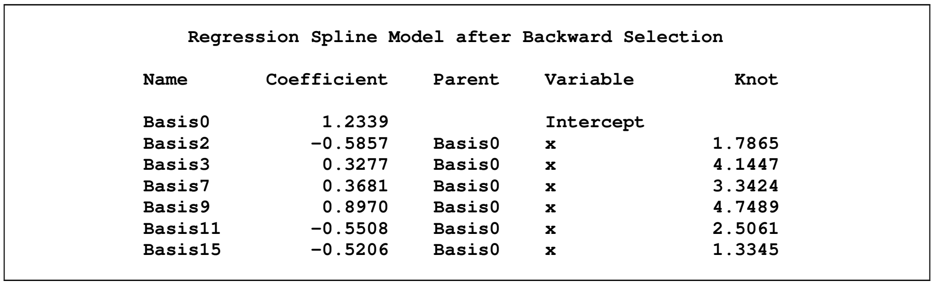
$$x_+^n = \begin{cases} x^n & : \quad x > 0 \\ 0 & : \quad x \le 0 \end{cases}$$

$$(x-k)_+ = \max(x-k, 0)$$

The exponent, n, is 1 for the piecewise linear splines that PROC ADAPTIVEREG uses.

Figure 4 displays the parameter estimates and the selected basis variables.

Figure 4 Parameter Estimates



```
              Regression Spline Model after Backward Selection

         Name          Coefficient      Parent     Variable          Knot

         Basis0             1.2339                 Intercept
         Basis2            -0.5857      Basis0     x               1.7865
         Basis3             0.3277      Basis0     x               4.1447
         Basis7             0.3681      Basis0     x               3.3424
         Basis9             0.8970      Basis0     x               4.7489
         Basis11           -0.5508      Basis0     x               2.5061
         Basis15           -0.5206      Basis0     x               1.3345
```

The following steps create and display the basis functions as a function of x. The coding details of these steps are not important. Briefly, PROC ADAPTIVEREG creates an output data set that contains the basis information from Figure 3 (which provides the information needed to write the statements that construct the basis functions), the DATA _NULL_ step writes assignment statements and a LABEL statement to the file *code.sas* to create the basis functions, the next DATA step creates those basis functions from the SAS® data set x and the generated code, and the PROC SGPLOT steps display in Figure 5 and Figure 6 the basis functions as a functions of x.

```
proc adaptivereg data=x details=bases;
   ods output bases=b;
   model y = x;
run;

data _null_;
   set b end=eof;
   file 'code.sas';
   put name '= ' transformation ';';      /* Basis functions */
   if eof then do;                        /* LABEL statement */
      put 'label';
      do i = 1 to 20;
         put +6 'Basis' i 2. -L ' = "' i 2. '"';
      end;
      put +6 ';';
   end;
run;

data bases;
   set x;
   %inc 'code.sas';
run;

proc sort data=bases; by x; run;

proc sgplot data=bases;
   %macro s; %do i = 1 %to 19 %by 2; series y=basis&i x=x; %end; %mend; %s
   yaxis label='Bases';
run;

proc sgplot data=bases;
   %macro s; %do i = 2 %to 20 %by 2; series y=basis&i x=x; %end; %mend; %s
   yaxis label='Bases';
run;
```

Figure 5: Odd-Numbered Basis Variables

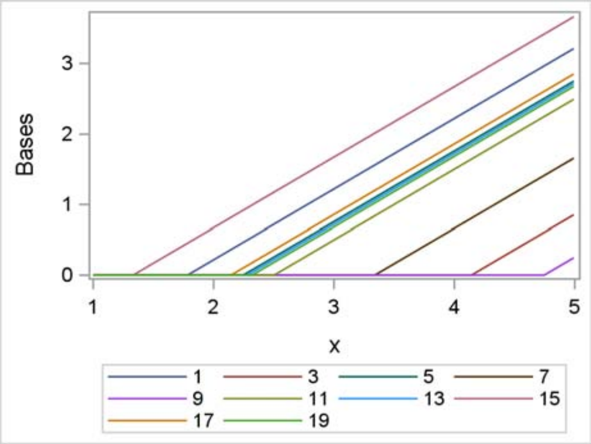
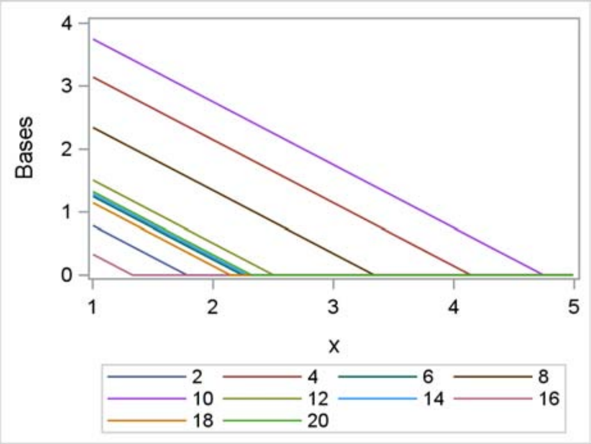


Figure 6: Even-Numbered Basis Variables



The odd-numbered basis functions in Figure 5 capture the change in the fit function as x progresses beyond each knot value and make no contribution to the predicted values when x is less than the knot. The even-numbered basis functions in Figure 6 capture the change in the fit function as x decreases from each knot value and make no contribution to the predicted values when x is greater than the knot. Basis function j is redundant given variable x and basis function $j - 1$ for every even j (2 is redundant given 1, and so on). Similarly, basis function j is redundant given variable x and basis function $j + 1$ for every odd j (1 is redundant given 2, and so on). Piecewise linear splines (such as those used in the TRANSREG procedure) are traditionally defined based on the variable x and the odd-numbered basis functions. Since the variable x is not part of the model, at least one odd-numbered basis function and one even-numbered basis function are required. In this case, there is one even-numbered basis function and the rest are odd.

Model selection in PROC ADAPTIVEREG consists of two phases:

1. The first phase is forward selection, in which pairs of corresponding basis functions are selected and added to the model (basis functions j and $j + 1$ for odd j). The pair that results in the largest reduction in the lack of fit (LOF) criterion (which is a function of the residual sum of squares) is added. Selection stops when the LOF criterion change is minimal or the maximum number of basis functions has been selected. This intermediate model overfits the data and probably does not have good power to predict new observations.
2. The next phase is backward elimination of a single basis function in each step. PROC ADAPTIVEREG chooses the basis function whose elimination minimizes the generalized cross validation criterion (GCV), which is a function of the residual sum of squares. Backward elimination progresses until all terms except the intercept are eliminated, and then the model with the minimum GCV is chosen.

The progression of the backward elimination phase is displayed in Figure 7. The GCV criterion provides an estimate of how well the model will perform with new data. The final model should have good predictive properties. The table in Figure 4 and the graph in Figure 7 show that the final model consists of bases 2, 3, 7, 9, 11, and 15 in addition to the intercept. Figure 7 shows that the backward elimination step eliminates basis functions 1, 19, 17, 13, and 5. Fit diagnostics are displayed in Figure 8.

Figure 7: Selection Plot

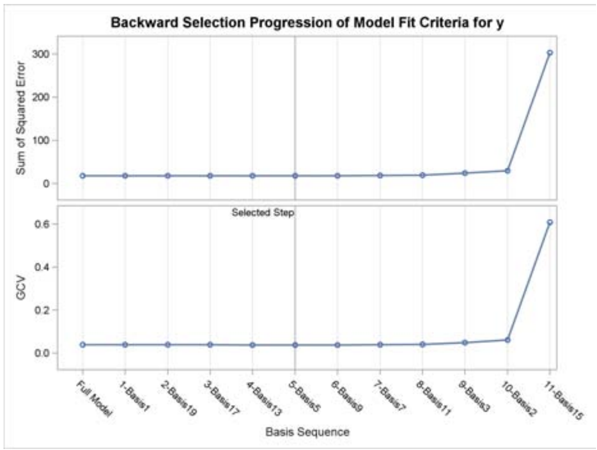
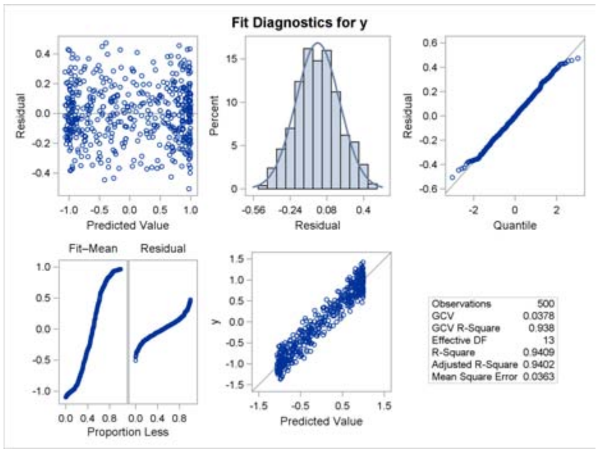


Figure 8: Diagnostics Panel



Observations	500
GCV	0.0378
GCV R-Square	0.938
Effective DF	13
R-Square	0.9409
Adjusted R-Square	0.9402
Mean Square Error	0.0363

The following steps use the information in Figure 3 and just the selected basis functions to regenerate the chosen model:

```
data FinalModel;
   set x;
   Basis2  = max(1.7864668056 - x, 0);
   Basis3  = max(x -  4.144699182, 0);
   Basis7  = max(x - 3.3424134209, 0);
   Basis9  = max(x - 4.7488998378, 0);
   Basis11 = max(x - 2.5060771599, 0);
   Basis15 = max(x - 1.3344822118, 0);
run;

proc reg;
   model y = basis:;
run; quit;
```

The parameter estimates and R square (not shown) that are produced by the REG procedure in the preceding step match those produced by PROC ADAPTIVEREG. However, you cannot easily duplicate the selection method that is used by PROC ADAPTIVEREG. For example, the following step uses the GLMSELECT procedure to find a model that is similar to the PROC ADAPTIVEREG model, but PROC GLMSELECT does not select Basis9.

```
proc glmselect data=bases(drop=basis0);
   model y = basis: / selection=backward;
run;
```

The PROC ADAPTIVEREG R square (0.9409) and the PROC GLMSELECT R square (0.9402) are almost identical.

You can score new data most easily by using a SCORE statement in PROC ADAPTIVEREG. For example:

```
data NewData;
   do x = 1 to 5 by 0.1;
      output;
   end;
run;

proc adaptivereg data=x details=bases;
   model y = x;
   score data=newdata out=scores;
run;
```

The following step displays the resulting scores in Figure 9:

```
proc sgplot data=scores;
   series x=x y=Pred;
run;
```

Figure 9: Scores Created by Using the SCORE Statement

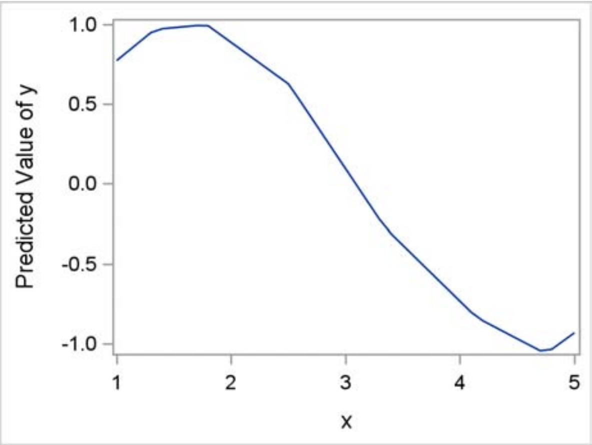
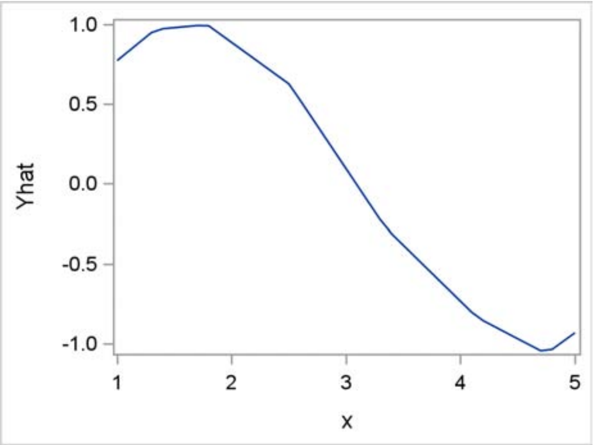


Figure 10: Scores Created Manually



These steps show the principles that are involved in scoring by creating ODS output data sets from the basis information and the parameter estimates tables and then combining them to generate scoring code:

```
proc adaptivereg data=x details=bases;
   ods output bases=b bwdparams=p;
   model y = x;
run;

proc sort data=b; by name; run;
proc sort data=p; by name; run;

data _null_;
   merge b p(in=p); by name; if p;
   file 'score.sas';
   if _n_ = 1 then put 'Yhat = 0;';
   put 'yhat + ' coefficient best16. ' * ' transformation +(-1) ';';
run;
```

```
data Scores(drop=basis:);
   set NewData;
   %inc 'score.sas';
run;
```

The basis information and parameter estimates tables are merged, and only the basis functions that are selected (those that appear in the parameter estimates table) are used to create the scoring code. The DATA _NULL_ step generates the following scoring code:

```
Yhat = 0;
yhat + 1.23385787751513 * 1;
yhat +  -0.550771231335 * Basis0*MAX(x - 2.5060771599,0);
yhat + -0.5206207092575 * Basis0*MAX(x - 1.3344822118,0);
yhat + -0.5856576485722 * Basis0*MAX(1.7864668056 - x,0);
yhat + 0.32765205975946 * Basis0*MAX(x -  4.144699182,0);
yhat + 0.36810578081331 * Basis0*MAX(x - 3.3424134209,0);
yhat + 0.89695230303698 * Basis0*MAX(x - 4.7488998378,0);
```

The DATA SCORES step uses these statements to score new data. Most statements are SAS sum statements.[2] The following step displays the results in Figure 10:

```
proc sgplot data=scores;
   series x=x y=yhat;
run;
```

The graphs in Figure 9 and Figure 10 are identical.

AUTOMOBILE MILES PER GALLON EXAMPLE

The preceding example shows how you can use PROC ADAPTIVEREG to find a nonlinear fit function by fitting a simple (nonparametric) regression model. This example shows how to fit a model with a quantitative dependent variable (automobile miles per gallon or MPG) and multiple independent variables (attributes of the automobile and its engine). The independent variables include both quantitative and categorical variables. This example also shows how PROC ADAPTIVEREG creates the basis functions when some data are missing. The following steps read the MPG data set from the University of California at Irvine (UCI) Machine Learning Data Repository (Asuncion and Newman 2007):

```
title 'Automobile MPG Study';
%let base = http://archive.ics.uci.edu/ml/machine-learning-databases;
proc format;
   invalue q '?' = .;
run;

data AutoMPG;
   infile "&base/auto-mpg/auto-mpg.data" device=url expandtabs lrecl=120 pad;
   input MPG Cylinders Displacement HorsePower :q. Weight Acceleration Year Origin Name $50.;
   name = propcase(left(tranwrd(name, '"', '')));
run;
```

The macro variable base enables you to construct a long URL from components that can be easily displayed on a printed page. The Q informat enables SAS to read data in which missing values are indicated by a question mark.

[2] "yhat +" is equivalent to "yhat = yhat +" and also retains yhat (which is not important in this example).

The following step fits an adaptive regression model for MPG:

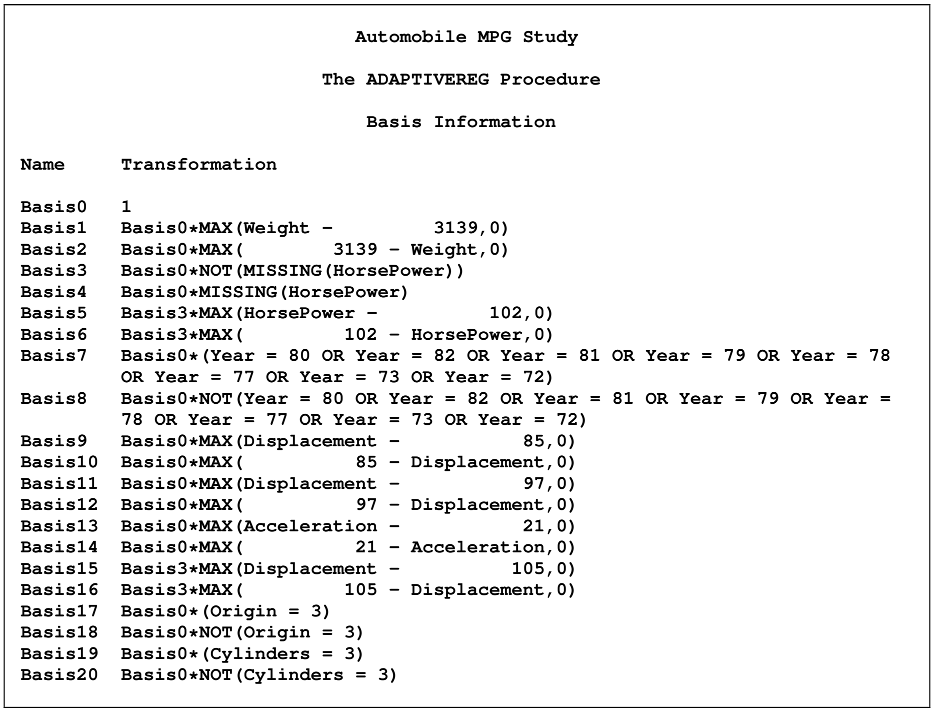
```
   proc adaptivereg data=autompg plots=all details=bases;
      class cylinders year origin;
      model mpg = cylinders displacement horsepower
                  weight acceleration year origin / additive;
   run;
```

The variables Cylinders, Year, and Origin are classification variables; the other variables are continuous. You can use the ADDITIVE option in the MODEL statement to request an additive model. The basis information is displayed in Figure 11. As in the previous example, there is an intercept (Basis0). For continuous variables, there are terms of the form $\max(v - k, 0)$ and $\max(k - v, 0)$ for variable v and knot k. The variable HorsePower has missing values, which are accounted for in Basis3 and Basis4. Basis3 is 1 when HorsePower is not missing and 0 otherwise. Basis4 is the reverse of Basis3 and enables the model to estimate the missing value. Basis5 and Basis6 can have an effect when HorsePower is not missing. This is illustrated for three observations in the following table:

HorsePower	Basis3	Basis4	Basis5	Basis6
95	1	0	$(95 - 158)_+$	$(158 - 95)_+$
.	0	1	0	0
100	1	0	$(100 - 158)_+$	$(158 - 100)_+$

If the variable Year is treated as a classification variable in an ordinary linear model with a less-than-full-rank binary coding, then 13 binary variables are created, one for each of the 13 values of the variable Year. Basis7 is the sum of those binary variables for the values of the variable Year: 80, 82, 81, 79, 78, 77, 73, and 72. PROC ADAPTIVEREG automatically determines how to combine the categories. Basis6 is nonzero only when HorsePower is not missing. In the adaptive regression model, this dependence is part of handling missing values and is not considered to be a departure from the main-effects-only model that is specified by the ADDITIVE option. Basis19 and Basis20 are binary variables for describing three-cylinder engines (Basis19) or not (Basis20). The final model is built from the 21 basis functions that are displayed in Figure 11.

Figure 11 Basis Information



```
                        Automobile MPG Study

                     The ADAPTIVEREG Procedure

                         Basis Information

Name      Transformation

Basis0    1
Basis1    Basis0*MAX(Weight -         3139,0)
Basis2    Basis0*MAX(        3139 - Weight,0)
Basis3    Basis0*NOT(MISSING(HorsePower))
Basis4    Basis0*MISSING(HorsePower)
Basis5    Basis3*MAX(HorsePower -          102,0)
Basis6    Basis3*MAX(         102 - HorsePower,0)
Basis7    Basis0*(Year = 80 OR Year = 82 OR Year = 81 OR Year = 79 OR Year = 78
          OR Year = 77 OR Year = 73 OR Year = 72)
Basis8    Basis0*NOT(Year = 80 OR Year = 82 OR Year = 81 OR Year = 79 OR Year =
          78 OR Year = 77 OR Year = 73 OR Year = 72)
Basis9    Basis0*MAX(Displacement -            85,0)
Basis10   Basis0*MAX(           85 - Displacement,0)
Basis11   Basis0*MAX(Displacement -            97,0)
Basis12   Basis0*MAX(           97 - Displacement,0)
Basis13   Basis0*MAX(Acceleration -            21,0)
Basis14   Basis0*MAX(           21 - Acceleration,0)
Basis15   Basis3*MAX(Displacement -           105,0)
Basis16   Basis3*MAX(          105 - Displacement,0)
Basis17   Basis0*(Origin = 3)
Basis18   Basis0*NOT(Origin = 3)
Basis19   Basis0*(Cylinders = 3)
Basis20   Basis0*NOT(Cylinders = 3)
```

The final parameter estimates, chosen basis functions, and levels for basis functions that are constructed from categorical variables are displayed in Figure 12.

Figure 12 Parameter Estimates

```
                 Regression Spline Model after Backward Selection

Name       Coefficient    Parent    Variable           Knot    Levels

Basis0         29.3788              Intercept
Basis2        0.003577    Basis0    Weight          3139.00
Basis3         -4.0349    Basis0    HorsePower            .
Basis5        -0.05079    Basis3    HorsePower       102.00
Basis6          0.1925    Basis3    HorsePower       102.00
Basis7          2.6665    Basis0    Year                       10 12 11 9 8 7 3 2
Basis9         -0.6600    Basis0    Displacement    85.0000
Basis11         0.6394    Basis0    Displacement    97.0000
Basis13         1.6047    Basis0    Acceleration    21.0000
Basis14         0.5071    Basis0    Acceleration    21.0000
Basis16        -0.2960    Basis3    Displacement     105.00
Basis17         1.7761    Basis0    Origin                     2
Basis19        -7.0066    Basis0    Cylinders                  0
```

The component panels are displayed in Figure 13 and Figure 14. These panels show the transformations of the variables that are used in model fitting. The function of the variable Cylinders is binary (3 cylinders versus 4, 5, 6, and 8 cylinders). The function of the variable Displacement is nonlinear, and the majority of the nonlinearity is in the smaller values. The function of the variable HorsePower has two linear components with a knot at 100. The function of the variable Weight is linear over the range 0 to 3139 and 0 outside that range. (This transformation is based on one of the two basis functions for the variable Weight and knot 3139.) The function of the variable Acceleration has two linear components with a knot at 21. The functions of the variables Year and Origin are binary.

Figure 13: Component Panel 1

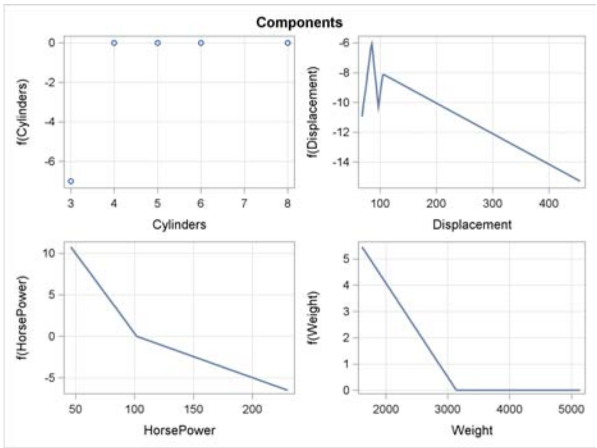


Figure 14: Component Panel 2

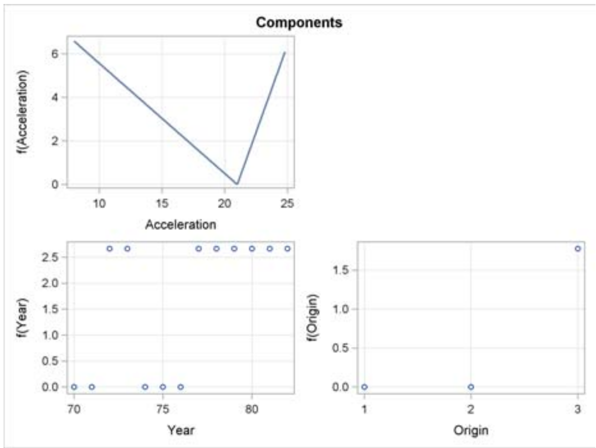


Figure 15 displays the variable importance information. The importance of each variable is the square root of the GCV value from a submodel from which all basis functions that involve that variable have been removed, minus the square root of the GCV value for the selected model, then scaled so that the largest importance value is 100. The variables HorsePower and Year are the most important in predicting MPG.

Figure 15 Variable Importance Table

```
                     Variable Importance

                            Number of
           Variable             Bases    Importance

           HorsePower               2        100.00
           Year                     1         89.34
           Displacement             3         49.44
           Acceleration             2         34.17
           Origin                   1         13.75
           Weight                   1         12.05
           Cylinders                1         10.73
```

MEDIAN HOME VALUES EXAMPLE

This example shows you how to fit a nonadditive model. When you do not specify the ADDITIVE option, PROC ADAPTIVEREG automatically builds two-way interactions into the model. All variables in this example are quantitative. The following step reads the median home values data set from the UCI Machine Learning Data Repository (Asuncion and Newman 2007):

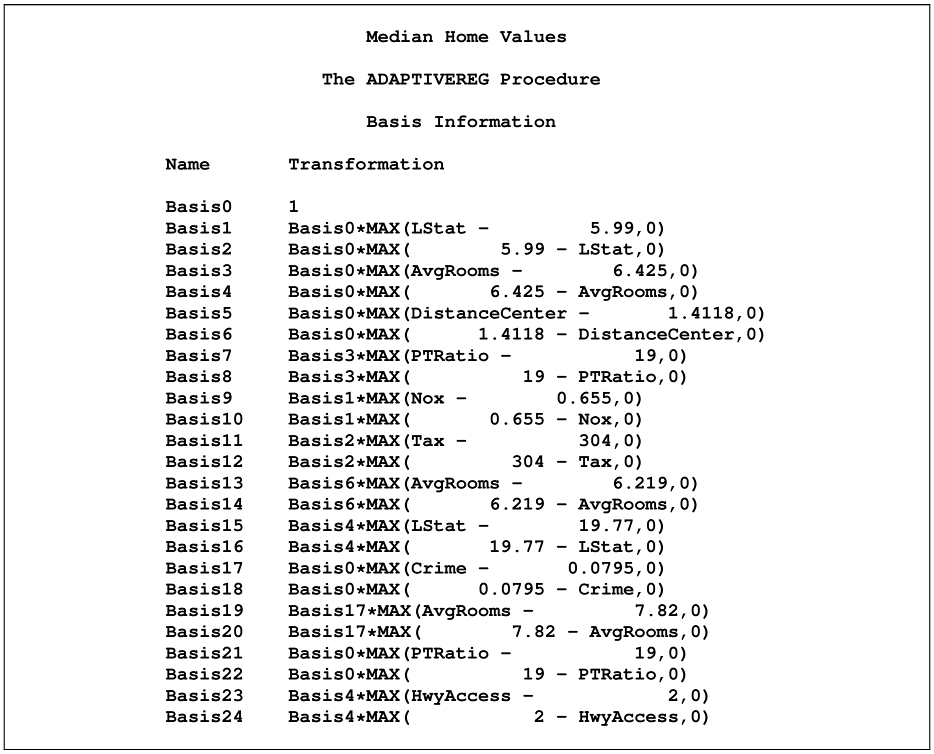
```
title 'Median Home Values';
%let base = http://archive.ics.uci.edu/ml/machine-learning-databases;
data Housing(drop=_);
   infile "&base/housing/housing.data" device=url expandtabs lrecl=120 pad;
   input Crime Zone Industrial Charles Nox AvgRooms Age DistanceCenter HwyAccess
         Tax PTRatio _ LStat MedianValue;
   label Crime          = 'Per capita crime rate by town'
         Zone           = 'Proportion of residential land zoned for lots over 25,000 sq.ft.'
         Industrial     = 'Proportion of nonretail business acres per town'
         Charles        = 'Charles River (1 if tract bounds river; 0 otherwise)'
         Nox            = 'Nitric oxides concentration (parts per 10 million)'
         AvgRooms       = 'Average number of rooms per dwelling'
         Age            = 'Proportion of owner-occupied units built prior to 1940'
         DistanceCenter = 'Weighted distances to five Boston employment centers'
         HwyAccess      = 'Index of accessibility to radial highways'
         Tax            = 'Full-value property-tax rate per $10,000'
         PTRatio        = 'Pupil-teacher ratio by town'
         LStat          = 'Percent lower status of the population'
         MedianValue    = 'Median value of owner-occupied homes in $1000''s';
run;
```

The following step fits the adaptive regression model:

```
proc adaptivereg data=housing details=bases plots=all;
   model medianvalue = crime -- lstat;
run;
```

The basis information is displayed in Figure 16.

Figure 16 Basis Information



```
                               Median Home Values

                            The ADAPTIVEREG Procedure

                               Basis Information

           Name       Transformation

           Basis0     1
           Basis1     Basis0*MAX(LStat -         5.99,0)
           Basis2     Basis0*MAX(        5.99 - LStat,0)
           Basis3     Basis0*MAX(AvgRooms -        6.425,0)
           Basis4     Basis0*MAX(       6.425 - AvgRooms,0)
           Basis5     Basis0*MAX(DistanceCenter -       1.4118,0)
           Basis6     Basis0*MAX(      1.4118 - DistanceCenter,0)
           Basis7     Basis3*MAX(PTRatio -           19,0)
           Basis8     Basis3*MAX(          19 - PTRatio,0)
           Basis9     Basis1*MAX(Nox -        0.655,0)
           Basis10    Basis1*MAX(       0.655 - Nox,0)
           Basis11    Basis2*MAX(Tax -          304,0)
           Basis12    Basis2*MAX(         304 - Tax,0)
           Basis13    Basis6*MAX(AvgRooms -        6.219,0)
           Basis14    Basis6*MAX(       6.219 - AvgRooms,0)
           Basis15    Basis4*MAX(LStat -        19.77,0)
           Basis16    Basis4*MAX(       19.77 - LStat,0)
           Basis17    Basis0*MAX(Crime -       0.0795,0)
           Basis18    Basis0*MAX(      0.0795 - Crime,0)
           Basis19    Basis17*MAX(AvgRooms -         7.82,0)
           Basis20    Basis17*MAX(        7.82 - AvgRooms,0)
           Basis21    Basis0*MAX(PTRatio -           19,0)
           Basis22    Basis0*MAX(          19 - PTRatio,0)
           Basis23    Basis4*MAX(HwyAccess -            2,0)
           Basis24    Basis4*MAX(           2 - HwyAccess,0)
```

Bases consist of the intercept ($\mathrm{Basis0}$), truncated power functions ($\mathrm{Basis1}$ through $\mathrm{Basis6}$, $\mathrm{Basis17}$, $\mathrm{Basis18}$, $\mathrm{Basis21}$, and $\mathrm{Basis22}$), and additional terms. These additional terms consist of two-way interactions between a previously defined truncated power function and a newly defined truncated power function. Examples include $\mathrm{Basis7} = \mathrm{Basis3} \times (\mathrm{PTRatio} - 19)_+$ and $\mathrm{Basis24} = \mathrm{Basis4} \times (2 - \mathrm{HwyAccess})_+$. This model is not additive. Some predictors are interactions of truncated power functions. By default, with m predictor variables, there are a maximum of $2 \times m = 25$ basis functions. You can change the number of basis functions by specifying the MAXBASIS= option. By default, the maximum order of interactions is 2. You can change the maximum order by specifying the MAXORDER= option. The following step illustrates the MAXORDER= option:

```
proc adaptivereg data=housing details=bases;
   model medianvalue = crime -- lstat / maxbasis=100 maxorder=3;
run;
```

The results of this step are not shown. However, the basis functions consist of an intercept, truncated power functions (for example, $\mathrm{Basis19} = (0.0795 - \mathrm{Crime})_+$), two-way products of truncated power functions (for example, $\mathrm{Basis23} = \mathrm{Basis19} \times (\mathrm{AvgRooms} - 8.04)_+$), and three-way products of truncated power functions (for example, $\mathrm{Basis51} = \mathrm{Basis23} \times (\mathrm{Nox} - 0.55)_+$). Compared to the additive model (not shown), the nonadditive model has a smaller GCV value. For highly structured data, increasing model complexity by adding interactions might help improve predictive power.

LOGISTIC REGRESSION JUNK E-MAIL EXAMPLE

The preceding examples result in a final linear model after basis creation and selection. This example shows how you can use PROC ADAPTIVEREG to fit nonlinear models by specifying a nonnormal distribution. This example fits a logistic regression model by specifying a binomial distribution.

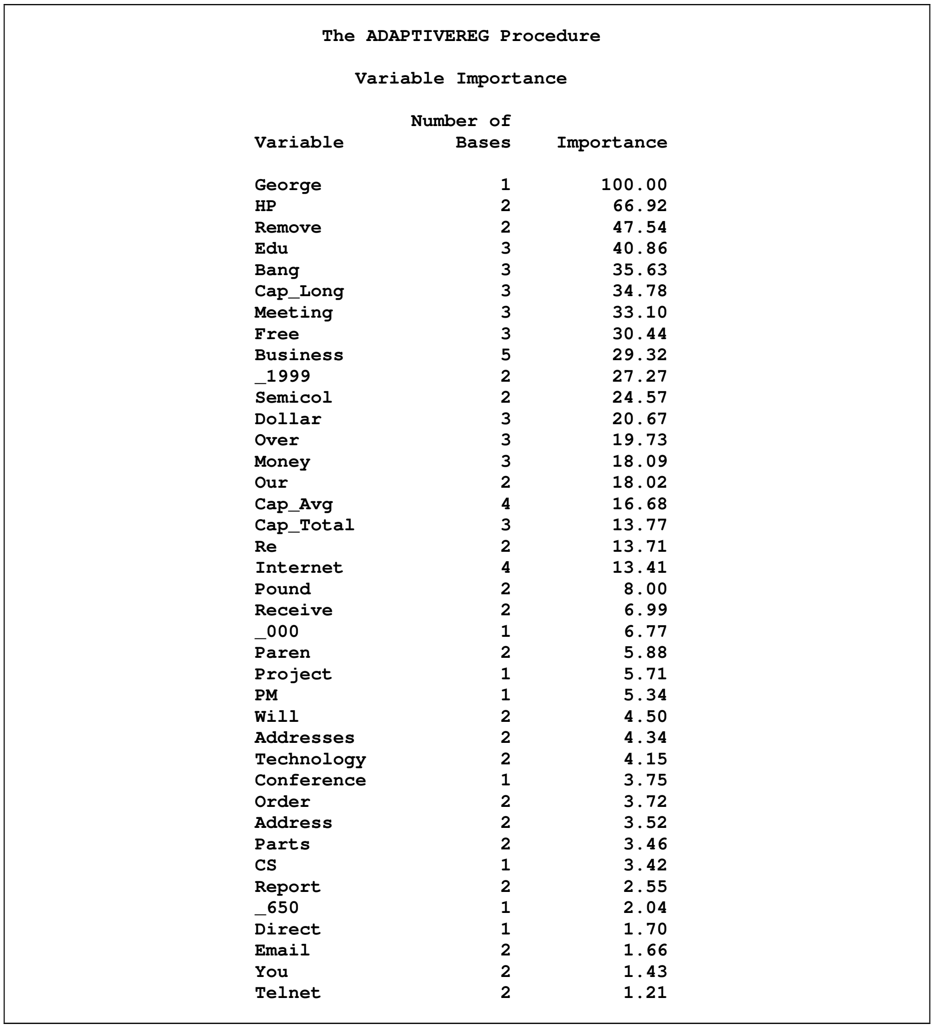
This example models whether an e-mail is junk or not. The quantitative predictor variables record the frequencies of some common words and characters in e-mails, and they record lengths of uninterrupted sequences of capital letters. The data are available at the UCI Machine Learning repository (Asuncion and Newman 2007). The following steps read and analyze the data:

```
title 'Junk Email Classification';

proc format; value junk 1 = 'Junk' 0 = 'Good'; run;

%let base = http://archive.ics.uci.edu/ml/machine-learning-databases;
data junkemail;
   infile "&base/spambase/spambase.data" device=url dsd dlm=',';
   input Make Address All _3d Our Over Remove Internet Order Mail Receive
         Will People Report Addresses Free Business Email You Credit Your Font
         _000 Money HP HPL George _650 Lab Labs Telnet _857 Data _415 _85
         Technology _1999 Parts PM Direct CS Meeting Original Project Re Edu
         Table Conference Semicol Paren Bracket Bang Dollar Pound Cap_Avg
         Cap_Long Cap_Total Class;
   format class junk.;
run;

proc adaptivereg data=junkemail seed=10359 details=bases;
   class class;
   model class = make -- cap_total / additive distribution=binomial;
   partition fraction(test=0.333);
   output out=JunkOut p(ilink);
run;
```

The dependent variable is a binary classification variable that indicates junk e-mail (1) or not (0). Most of the 115 basis variables (not displayed) are pairs that are constructed from a predictor variable and a single knot. A few have two knots. The final model has 90 basis functions and involves most of the predictor variables.

The variable importances are displayed in Figure 17. The variables George and HP (which contain the number of times 'George' and 'HP' appear in the e-mail, respectively) are important because the e-mail recipient is George Forman from HP.

Figure 17 Variable Importance Table



```
                The ADAPTIVEREG Procedure

                   Variable Importance

                           Number of
           Variable            Bases    Importance

           George                  1        100.00
           HP                      2         66.92
           Remove                  2         47.54
           Edu                     3         40.86
           Bang                    3         35.63
           Cap_Long                3         34.78
           Meeting                 3         33.10
           Free                    3         30.44
           Business                5         29.32
           _1999                   2         27.27
           Semicol                 2         24.57
           Dollar                  3         20.67
           Over                    3         19.73
           Money                   3         18.09
           Our                     2         18.02
           Cap_Avg                 4         16.68
           Cap_Total               3         13.77
           Re                      2         13.71
           Internet                4         13.41
           Pound                   2          8.00
           Receive                 2          6.99
           _000                    1          6.77
           Paren                   2          5.88
           Project                 1          5.71
           PM                      1          5.34
           Will                    2          4.50
           Addresses               2          4.34
           Technology              2          4.15
           Conference              1          3.75
           Order                   2          3.72
           Address                 2          3.52
           Parts                   2          3.46
           CS                      1          3.42
           Report                  2          2.55
           _650                    1          2.04
           Direct                  1          1.70
           Email                   2          1.66
           You                     2          1.43
           Telnet                  2          1.21
```

In this example, the PARTITION statement randomly selects two-thirds of the observations to fit the model and uses the remaining one-third to test the model. The explicit random number seed that is specified in the PROC ADAPTIVEREG statement ensures that you can reproduce the same results in subsequent runs. The P(ILINK) option outputs the predicted probabilities from the logistic model to the SAS data set JunkOut.

An e-mail is classified as junk if the predicted modeled probability of event (Class = '0', which classifies the e-mail as not junk) is less than 0.5. The following statements evaluate the classification results and create Figure 18:

```
data test;
   set junkout(where=(_ROLE_ = 'TEST'));
   Prediction = (pred < 0.5);
   format class prediction junk.;
run;

proc freq data=test;
   tables class * prediction / norow nocol;
run;
```

Figure 18 Test Data Set Classification Errors, Full Model

The FREQ Procedure

Frequency Percent

Table of Class by Prediction			
	Prediction		
Class	Good	Junk	Total
Good	885 56.26	59 3.75	944 60.01
Junk	37 2.35	592 37.64	629 39.99
Total	922 58.61	651 41.39	1573 100.00

Compared to results from other statistical learning algorithms (Hastie, Tibshirani, and Friedman 2001), the PROC ADAPTIVEREG results are competitive. Exact comparisons of the error rates between the two sources are not meaningful with different random samples of the data. Also, if you specify different random number seeds, you will get different results. However, you can compare the results if you have the same sample. Hastie, Tibshirani, and Friedman (2001) provide a binary variable that shows which observations they used for training (Test = 0) and which they used for testing (Test = 1). The following steps read the Hastie, Tibshirani, and Friedman (2001) Test variable and merge it with the JunkEmail data set:

```
%let base = http://www-stat.stanford.edu/~tibs/ElemStatLearn/datasets;
data Test;
   infile "&base/spam.traintest" device=url dsd;
   input Test;
run;

data junkemail2;
   merge test junkemail;
run;
```

The following step fits the model by using the same training and test set that Hastie, Tibshirani, and Friedman (2001) used:

```
proc adaptivereg data=junkemail2 details=bases;
   class class;
   model class = make -- cap_total / additive distribution=binomial;
   partition rolevar=test(test='1' train='0');
   output out=JunkOut p(ilink);
run;
```

The option ROLEVAR=TEST(TEST='1' TRAIN='0') names the Test variable as the variable that contains testing and training information, and it specifies the values for each role. The results of this step are not shown; just the output data set is used. The JunkOut data set is processed as before to evaluate the prediction of the test observations. The following steps produce Figure 19:

```
data test;
   set junkout(where=(_ROLE_ = 'TEST'));
   Prediction = (pred < 0.5);
   format class prediction junk.;
run;

proc freq data=test;
   tables class * prediction / norow nocol;
run;
```

Figure 19 Test Data Set Classification Errors, Full Model

The FREQ Procedure

Frequency Percent

Table of Class by Prediction			
	Prediction		
Class	Good	Junk	Total
Good	898 58.46	43 2.80	941 61.26
Junk	35 2.28	560 36.46	595 38.74
Total	933 60.74	603 39.26	1536 100.00

Hastie, Tibshirani, and Friedman (2001) report the following results:

	Prediction	
Class	Good	Junk
Good	58.5%	2.5%
Junk	2.7%	36.2%

The two sets of results are quite similar.

PROC ADAPTIVEREG uses 115 as the maximum number of basis functions in this example. You can specify a smaller number in the MODEL statement. For example, the following step specifies MAXBASIS=61:

```
proc adaptivereg data=junkemail seed=10359 details=bases;
   class class;
   model class = make -- cap_total / additive distribution=binomial maxbasis=61;
   partition fraction(test=0.333);
   output out=JunkOut2 p(ilink);
run;

data test;
   set junkout2(where=(_ROLE_ = 'TEST'));
   Prediction = (pred < 0.5);
   format class prediction junk.;
run;

proc freq data=test;
   tables class * prediction / norow nocol;
run;
```

Figure 20 displays the classification results.

Figure 20 Test Data Set Classification Errors, Reduced Model

The FREQ Procedure

Frequency Percent

Table of Class by Prediction			
	Prediction		
Class	Good	Junk	Total
Good	898 57.09	46 2.92	944 60.01
Junk	37 2.35	592 37.64	629 39.99
Total	935 59.44	638 40.56	1573 100.00

When you specify a smaller number of basis functions, you might get a simpler model that runs more quickly and has fewer opportunities for overfitting. In this case, the prediction results for the reduced model are in the range of results that are reported previously.

MACKEREL EGG DENSITY EXAMPLE

This example demonstrates how you can use PROC ADAPTIVEREG to fit a nonparametric Poisson regression model. The data are a subset of the 1992 mackerel egg survey that was conducted over the Porcupine Bank west of Ireland (Bowman and Azzalini 1997). Scientists took samples by hauling a net up from the deep sea. They counted the number of spawned mackerel eggs and used other geographic information to estimate the sizes and distributions of spawning stocks. The following steps read the data from the SAS sample library entry for the fourth PROC ADAPTIVEREG example and create the SAS data set Mackerel:

```
data _null_;
   infile 'http://support.sas.com/documentation/onlinedoc/stat/ex_code/121/adptex4.html'
          device=url;
   file 'junk.junk';
   retain pre 0;
   input;
   if pre then put _infile_;
   if _infile_ eq ';' then pre = 0;
   if index(_infile_, '<pre>')  then pre = 1;
run;

%inc 'junk.junk' / nosource;
```

The SAS statements that create the SAS data set are embedded in a Web page. The statements begin after the HTML preformatted tag (“<pre>”) and extend through a line that consists of a single semicolon. This data set contains 634 observations and five variables. The response variable Egg_Count is the number of mackerel eggs that are collected from each sampling net. The variables Longitude and Latitude provide the location of each sample station. The variable Net_Area is the area of the sampling net in square meters. The variable Depth records the sea bed depth in meters at the sampling location. The variable Distance is the distance in geographic degrees from the sample location to the continental shelf edge. You can use the CONTENTS and PRINT procedures to learn more about this data set.

Mackerel egg density is defined as

$$\text{density} = \mathsf{E}(\text{count}) / \text{net\_area}$$

This equation is equivalent to a Poisson regression with the response variable Egg_Count, an offset variable log(net_area), and other covariates.

The following statements produce a plot of the mackerel egg density with respect to the sampling station locations:

```
data plotdata;
   set mackerel;
   density = egg_count / net_area;
run;

%let off0 = offsetmin=0 offsetmax=0 linearopts=(thresholdmin=0 thresholdmax=0);
proc template;
   define statgraph surface;
      dynamic _title _z;
      begingraph / designwidth=defaultDesignHeight;
         entrytitle _title;
         layout overlay / xaxisopts=(&off0) yaxisopts=(&off0);
            contourplotparm z=_z y=latitude x=longitude / gridded=FALSE;
         endlayout;
      endgraph;
   end;
run;

proc sgrender data=plotdata template=surface;
   dynamic _title='Mackerel Egg Density' _z='density';
run;
```

Figure 21 displays the mackerel egg density in the sampling area. The black hole in the upper right corner is caused by missing data in that area.

Figure 21: Mackerel Egg Density

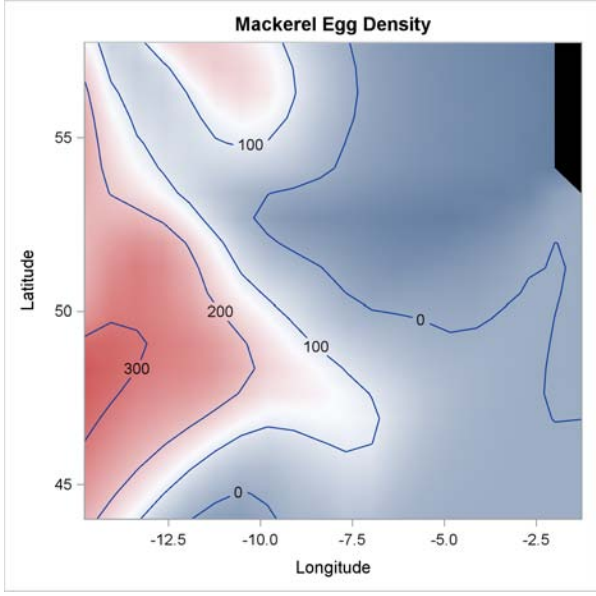
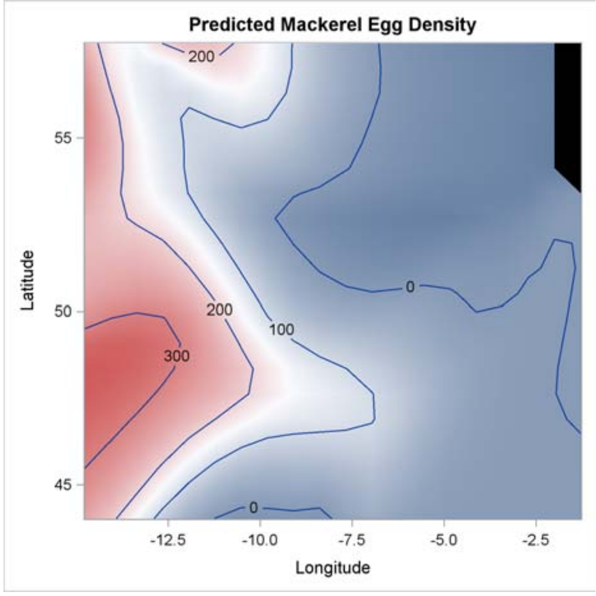


Figure 22: Predicted Mackerel Egg Density



In this example, the dependent variable is mackerel egg count, the independent variables are the geographical information about each of the sampling stations, and the logarithm of the sampling area is the offset variable. The following statements use the DIST=POISSON option to fit the nonparametric Poisson regression model:

```
data mack2;
   set mackerel;
   log_net_area = log(net_area);
run;

proc adaptivereg data=mack2;
   model egg_count = longitude latitude depth distance
                   / offset=log_net_area dist=poisson;
   output out=mackerelout p(ilink);
run;
```

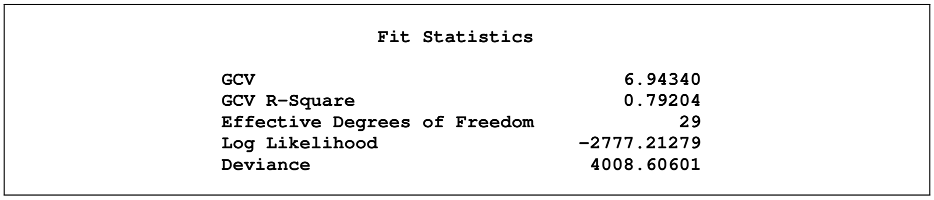
Figure 23 lists basic model information such as the offset variable, distribution, and link function.

Figure 23 Model Information

```
                      Mackerel Egg Density Study

                      The ADAPTIVEREG Procedure

                          Model Information

                  Data Set                 WORK.MACK2
                  Response Variable        Egg_Count
                  Offset Variable          log_net_area
                  Distribution             Poisson
                  Link Function            Log
```

Figure 24 lists fit statistics for the final model.

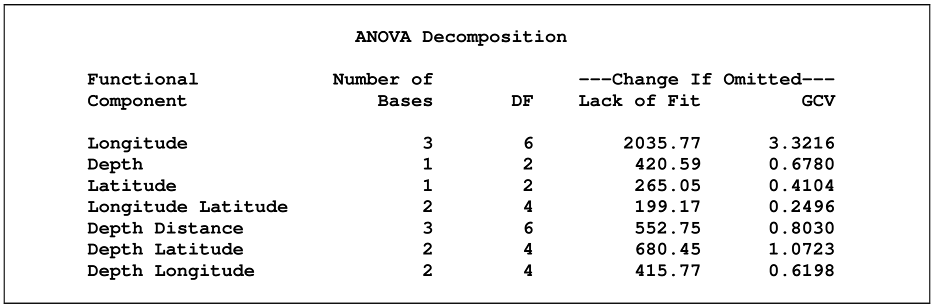
Figure 24 Fit Statistics



```
                         Fit Statistics

              GCV                                   6.94340
              GCV R-Square                          0.79204
              Effective Degrees of Freedom               29
              Log Likelihood                    -2777.21279
              Deviance                           4008.60601
```

The final model consists of basis functions and interactions between basis functions for three geographic variables. Figure 25 lists seven functional components of the final model, including three one-way spline transformations and four two-way spline interactions.

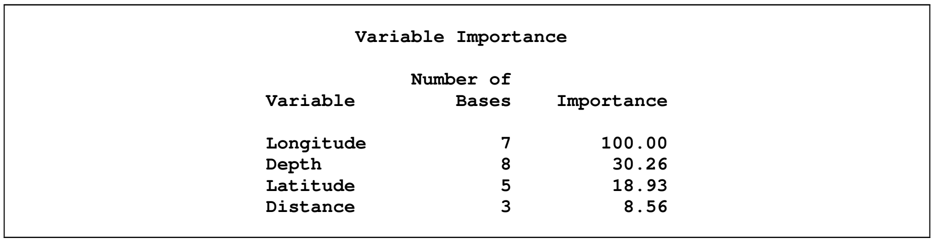
Figure 25 ANOVA Decomposition



```
                         ANOVA Decomposition

      Functional             Number of                ---Change If Omitted---
      Component                  Bases         DF     Lack of Fit         GCV

      Longitude                      3          6         2035.77      3.3216
      Depth                          1          2          420.59      0.6780
      Latitude                       1          2          265.05      0.4104
      Longitude Latitude             2          4          199.17      0.2496
      Depth Distance                 3          6          552.75      0.8030
      Depth Latitude                 2          4          680.45      1.0723
      Depth Longitude                2          4          415.77      0.6198
```

The “Variable Importance” table in Figure 26 displays the relative variable importance among the four variables. Longitude is the most important variable.

Figure 26 Variable Importance



```
                         Variable Importance

                                  Number of
                      Variable        Bases    Importance

                      Longitude           7        100.00
                      Depth               8         30.26
                      Latitude            5         18.93
                      Distance            3          8.56
```

The following steps create and display in Figure 22 the predicted mackerel egg density over the spawning area:

```
data mackplot;
   set mackerelout;
   pred = pred / net_area;
run;

proc sgrender data=mackplot template=surface;
   dynamic _title='Predicted Mackerel Egg Density'
           _z='pred';
run;
```

The graphs in Figure 21 and Figure 22 are quite similar.

CONCLUSIONS

The multivariate adaptive regression spline method of Friedman (1991), which is implemented in PROC ADAPTIVEREG, produces parsimonious models that do not overfit the data and thus have good predictive power. PROC ADAPTIVEREG can fit both linear and nonlinear nonparametric regression models. SAS/STAT software offers various tools for nonparametric regression, including the GAM, LOESS, and TPSPLINE procedures. Typical nonparametric regression methods involve a large number of parameters in order to capture nonlinear trends in data. Thus, the nonparametric model space is much larger than the parametric model space. The LOESS and TPSPLINE procedures are limited to problems in low dimensions. PROC GAM fits generalized additive models and can handle larger data sets than PROC LOESS and PROC TPSPLINE can handle. However, the additivity assumption ignores variable interactions in high-dimensional space, and convergence for nonnormal distributions is not guaranteed. PROC ADAPTIVEREG can fit models that these other procedures cannot fit. PROC ADAPTIVEREG is easy to use because it automatically selects the knots, creates the basis functions, performs the initial forward selection, and the final backward selection to generate the final model. Simple options enable you to train, test, validate, score, and predict new data.

SOFTWARE CREDITS

The ADAPTIVEREG procedure was designed and programmed by Weijie Cai, Principal Research Statistician at SAS.

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