USING PROC NLIN TO FIT SEGMENTED REGRESSION MODELS

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1. Introduction

Often a simple mathematical function cannot describe the underlying unknown model generating data. One may know some of the properties of the model or one may know very little about the underlying model. Often such data can be described by a series of segmented models, where the forms of the models being segmented are known but the points at which the functions join are unknown and need to be estimated. Segmented models can be applied in many diverse situations from tables of numbers without variation to data with substantial variation.

The numbers in Table 1 represent the cost to haul a ton of fertilizer the specified number of miles. The cost-mile relationship is shown in figure 1 where for short hauls the cost is almost constant (the cost of loading and unloading) and the cost of driving time gradually dominates the cost. This relationship can be adequately described by a model with a quadratic segment for the curvature part of the graph with a linear segment for the remainder.

The two models segmented together are linear models but when the point where the models join is unknown, the resulting model is a nonlinear model. The class of segmented models considered in this discussion must satisfy two conditions: (1) the pairs of models join together (they are equal) at the respective join points (sometimes called knots) providing a continuous model and (2) the derivatives of pairs of models are equal at the respective join points, providing a smooth model. The types of segmented functions which do not satisfy the second condition cannot be fit using a nonlinear estimation routine which is derivative based.

Segmented straight lines can be fit to data using the procedure described in Hudson (1965.)

II. Simple Segmented Models

The segmented model needed to describe the cost-mile data in Table 1 consists of a quadratic segment joined by a linear segment. The model can be expressed as

\[ C_i = \begin{cases} \beta_{01} + \beta_{11}m_i + \beta_{21}m_i^2 & \text{if } m_i \leq a \\ \beta_{02} + \beta_{12}m_i & \text{if } m_i > a \end{cases} \]

Substituting for the above two parameters in equation (1), the model becomes

\[ C_i = \begin{cases} \beta_{02} + \beta_{12}m_i + \beta_{21}(a-m_i)^2 & \text{if } m_i \leq a \\ \beta_{02} + \beta_{12}m_i & \text{if } m_i > a \end{cases} \]  

Define the indicator function

\[ I(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases} \]

The model in (2) can be expressed as

\[ C_i - \beta_{02} + \beta_{12}m_i + \beta_{21}(a - m_i)^2 I(a - m_i) \].

The model has four parameters which need to be estimated and the model is nonlinear since it is a nonlinear function of \( a \) and \( \beta_{21} \). If \( a \) is known, the model in (3) is a linear model and a linear regression program can be used to fit the segmented models.

The process is easily expanded to more complex models. The model in equation (4) is a quadratic model segmented to a quadratic model, i.e.,

\[ Y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \epsilon_i & \text{if } x_i \leq a \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \epsilon_i & \text{if } x_i > a \end{cases} \]

Here an error term has been added to the model to allow for the possibility of the \( Y_i \) being observed values of random variables and it is assumed that the \( \epsilon_i \) are independent, with mean 0 and variance \( \sigma^2 \). The condition restricting the models to be continuous at \( x = a \) is

\[ \beta_{01} + \beta_{11}a + \beta_{21}a^2 - \beta_{02} + \beta_{12}a + \beta_{22}a^2 \]

and the condition restricting the derivatives to be equal is

\[ \beta_{11} + 2\beta_{21}a = \beta_{12} + 2\beta_{22}a. \]

After a little algebra, the model in equation (4), subject to the two restrictions is

\[ Y_i = \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \epsilon_i \]

It is interesting to note that the models in equations (3) and (5) are expressed as the second model plus an additional term when the independent variable is less than the join point. The reparameterization could have been carried out such that the models consist of the first segment model plus an additional term when the independent variable is larger than the join point.

As a third example, an exponential decay function is segmented with a linear function. The segmented model is...
The two restrictions are
\[ y_1 = \begin{cases} \beta_{01} e^{-\beta_{11} x_1} + \epsilon_1 & \text{if } x_1 \leq \alpha \\ \beta_{02} + \beta_{12} x_1 + \epsilon_1 & \text{if } x_1 > \alpha \end{cases} \quad (6) \]

and the resulting single nonlinear models are displayed in Table 2.

To demonstrate the reparameterization process, the quadratic-quadratic model in equation (4) was reparameterized to the model in equation (5). Rewrite equation (5) as

\[ y_1 = \theta_1 e^{\theta_2 x_1^{1/2} x_1^{2/3} (\theta_2 - x_1)^{1/4} (\theta_3 - x_1)^{1/3}} \quad (7) \]

where
\[
\begin{align*}
\theta_1 &= \theta_{01} - \theta_{02}, \\
\theta_{01} &= -\theta_0^2, \\
\theta_{11} &= \theta_{12} = \theta_2, \\
\theta_{21} &= \theta_3, \\
\theta_{22} &= \theta_4.
\end{align*}
\]

As the form of the segmented functions become more complex, this reparameterization process becomes much more difficult.

### III. General Segmented Polynomial Models.

The general situation for polynomial models involves approximating an unknown function of \( x \) over the interval \([A, B]\) by a series of low order polynomial functions of \( x \) over the intervals \([A, a_1], [a_1, a_2], \ldots, [a_{r-1}, B]\). The approximating function is

\[
f(x) = \sum_{i=0}^{k_1} \beta_1^i x^i \quad \text{for } A \leq x \leq a_1
\]

\[
f(x) = \sum_{i=0}^{k_2} \beta_2^i x^i \quad \text{for } a_1 < x \leq a_2
\]

\[
\vdots
\]

\[
f(x) = \sum_{i=0}^{k_r} \beta_r^i x^i \quad \text{for } a_{r-1} < x \leq B.
\]

To ensure that the approximating function is continuous and has continuous first derivatives in \( x \) over \([A, B]\) (i.e., the approximating function is smooth), the functions must satisfy

\[
\begin{align*}
&k_1 + 1) \quad \sum_{j=0}^{k_1} \beta_{11}^j = \sum_{j=0}^{k_1} \beta_{12}^j, \quad j = 1, 2, \ldots, r-1 \quad \text{and} \\
&k_{j-1} + 1) \quad \sum_{j=0}^{k_{j-1}} \beta_{11}^j = \sum_{j=0}^{k_{j-1}} \beta_{12}^j, \quad j = 1, 2, \ldots, r-1.
\end{align*}
\]

Following the technique for reparameterization described by Gallant and Fuller (1973) and expanded upon in Perneski, McDonald and Milliken (1973), several different combinations of segmented models have been reparameterized to a single nonlinear model and are summarized in Table 2. The segmented functions expressed in terms of the \( \beta \)'s are reparameterized to a function in terms of \( \theta \)'s. The relationships between the \( \beta \)'s and the \( \theta \)'s become more complex, the reparameterization process becomes tedious.

### IV. Parameter Estimation and Example 1.

To demonstrate the process, start by examining the graph in Figure 1 of the data in Table 1, select \( a = 50 \) as the initial values of the join point. Then according to equation (2) construct the variable \( w_1 \) as

\[
w_1 = \begin{cases} 0 & \text{if } m > 50 \\ (50 - m_i)^2 & \text{if } m_i \leq 50
\end{cases}
\]

Finally, use a linear regression code to obtain estimates of \( \hat{\theta}_1, \hat{\theta}_2 \) and \( \hat{\theta}_3 \) by fitting the model

\[ \hat{c}_i = \theta_1 + \theta_2 m_i + \theta_3 w_i \quad (8) \]

Finally, use a linear regression code to obtain estimates of \( \hat{\theta}_1, \hat{\theta}_2 \) and \( \hat{\theta}_3 \) by fitting the model

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the nonlinear model to the data in Table 1 is in Table 5 and the resulting output is in Table 6. The derivative-free process took 22 iterations. The graph of the estimated model with the data is in Figure 3. The model describes that data very well. The $R^2$ value is computed as

$$R^2 = 1 - \frac{SS_{Residual}}{SS_{Total}}$$

Example 2: O/LIO

The data in Table 7, graphed in Figure 4, is modeled by three segments, quadratic-linear-quadratic. The three segment model is

$$y_i = \begin{cases} 
\beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \epsilon_i & \text{for } x_i \leq \alpha_1 \\
\beta_{02} + \beta_{12}x_i + \epsilon_i & \text{for } \alpha_1 < x_i \leq \alpha_2 \\
\beta_{03} + \beta_{13}x_i + \epsilon_i & \text{for } x_i > \alpha_2
\end{cases}$$

(9)

The continuity restrictions are

1) $\beta_{01} + \beta_{11}\alpha_1 + \beta_{21}\alpha_1^2 = \beta_{02} + \beta_{12}\alpha_1^2$

2) $\beta_{02} + \beta_{12}\alpha_2 = \beta_{03} + \beta_{13}\alpha_2^2 + \beta_{23}\alpha_2^2$

and the derivative restrictions are

3) $\beta_{11} + 2\beta_{21}\alpha_1 = \beta_{12}$

4) $\beta_{12} = \beta_{13} + 2\beta_{23}\alpha_2$

After some algebraic steps, the model can be expressed as

$$y_i - \beta_{01} - \beta_{11}\alpha_i + \beta_{21}\alpha_i^2 + \epsilon_i$$

$$+ \beta_3(\alpha_i - x_i)^2 + \epsilon_i$$

(10)

The model in equation 10 is linear when the joint points, $\alpha_1$ and $\alpha_2$, are known. From Figure 4, guess the joint points as $\alpha_1 = 6$ and $\alpha_2 = 9$. Define the variables $w_i$ and $v_i$ as

$$w_i = \begin{cases} 
(x_i - 6)^2 & \text{if } x_i \leq 6 \\
0 & \text{if } x_i > 6
\end{cases}$$

and

$$v_i = \begin{cases} 
(x_i - 9)^2 & \text{if } x_i \leq 9 \\
0 & \text{if } x_i > 9
\end{cases}$$

The initial estimates for $\beta_1$, $\beta_2$, $\beta_3$ and $\beta_4$ given $\alpha_1 = 6$ and $\alpha_2 = 9$ are obtained by fitting the linear regression model

$$y_i - \beta_{01} - \beta_{11}\alpha_i - \beta_{21}\alpha_i^2 + \epsilon_i$$

(11)

The SAS System code to read the data and fit the model (11) via PROC REG is in Table 8. The results of PROC REG are in Table 9 and the graph of the model with joint points $\alpha_1 = 6$ and $\alpha_2 = 9$ is in Figure 5. The PROC NLIN code is in Table 10 and the results are in Table 11. The procedure using derivatives required 9 iterations. Since derivatives were included, 95% confidence limits about the mean and about an individual (prediction) can be obtained. The graph of the data, the final model, 95% confidence intervals about the model and 95% prediction intervals are in Figure 6.

Example 3: Exponential Decay - Linear

An exponential decay function segmented with a linear function is used to describe the data in Table 12. The model is

$$y_i = \begin{cases} 
\beta_{01} + \beta_{11}x_i - \beta_{21}x_i^2 + \epsilon_i & \text{if } x_i \leq \alpha \\
\beta_{02} + \beta_{12}x_i + \epsilon_i & \text{if } x_i > \alpha
\end{cases}$$

(12)

The continuity restriction is

$$\beta_{01} + \beta_{11}\alpha - \beta_{02} + \beta_{12}$$

and the derivative restriction is

$$-\beta_{21}\alpha - \beta_{21}$$

By incorporating the two restrictions into the model, the intercept ($\beta_{02}$) and slope ($\beta_{12}$) of the linear segment can be expressed as functions of the parameters of the exponential decay function and the join point as

$$\beta_{02} = \beta_{01} - \beta_{11}\alpha$$

and

$$\beta_{12} = -\beta_{21}\alpha$$

Plot the data, see Figure 7, and guess that the join point is $\alpha = 8.1$. The set of data with $x_i \leq 8.1$ can be described by the model

$$y_i = \beta_{01} + \beta_{11}x_i - \beta_{12}x_i^2 + \epsilon_i$$

(13)

Let $\beta_{01} = \min y_i - \delta, \delta > 0$, then the mean of model (13) can be linearized as

$$\ln\{y_i - \beta_{01}\} = \ln(\beta_{11}) - \beta_{12}x_i$$

(14)

With $\beta_{01} = 6.3$, model (14) was fit to the observations with $x_i \leq 8.1$ to obtain initial values for $\beta_{11}$ and $\beta_{21}$ (where the initial values for $\beta_{02}$ and $\alpha$ are 6.3 and 8.1 respectively). The SAS System code to partition the data set and use PROC REG to obtain the initial values is in Table 14 where the initial values for $\beta_{11}$ and $\beta_{12}$ are $e = 1.5606$, $-4.759$ and $-.3505$.

The SAS System code, using the above initial values, to fit the segmented model is in Table 15 and the results are in Table 16. The graph of the data, the final model and 95% confidence limits are in Figure 8.

Example 4: Segmented Surface Model

The data in Table 17 represents the kinetics of a reaction rate which was studied for fixed temperature over time. The relationship between the reaction rate (RATE) and TIME for a fixed temperature (TEMP) can be described by a quadratic-linear segmented model. The values of the parameters of the segmented model change as TEMP changes, thus a segmented surface model is constructed by replacing the...
parameters of the quadratic-linear segmented model with functions of TEMP.

By using equation (8), the model to describe RATE as a function of TIME for a fixed level of TEMP is

\[ \text{RATE}_i = \theta_1 + \theta_2 \text{TIME}_i + \theta_3 (\text{TIME}_i - \theta_4)^2 + \varepsilon_i \]  

where \( \theta_4 \) is the join point.

The data was graphed for each TEMP and initial join points were selected. The initial estimates of \( \theta_1, \theta_2 \) and \( \theta_3 \) for each TEMP was obtained by fitting the linear model (when \( \theta_4 \) is known) of equation (8). The SAS System statements required to read the data, compute

\[ w_i = (\text{TIME}_i - \theta_4)^2 \text{TIME}_i, \]  

and use PROC REG for each TEMP to obtain the starting values, are in Table 18 and the results are in Table 19.

The next step is to express these starting values as function of TEMP. The SAS System code for fitting a linear function and a quadratic function of TEMP to each set of parameter estimates from model (8) is in Table 20 and the results are summarized in Table 21. From the graph of the relationship between \( \theta_i \) and TEMP and the results from Table 21, the following expressions for the \( \theta_i \) were selected:

\[ \theta_1 = a_0 + a_1 \text{TEMP}_i + a_2 \text{TEMP}_i^2 \]  

\[ \theta_2 = b_0 + b_1 \text{TEMP}_i + b_2 \text{TEMP}_i^2 \]  

\[ \theta_3 = c_0 + c_1 \text{TEMP}_i + c_2 \text{TEMP}_i^2 \]  

The resulting segmented surface is

\[ \text{RATE}_{ij} = d_0 + d_1 \text{TEMP}_i + d_2 \text{TEMP}_i^2 \]  

+ \( (d_0 + d_1 \text{TEMP}_i + d_2 \text{TEMP}_i^2) \text{TIME}_j \)  

+ \( (e_0 + e_1 \text{TEMP}_i + e_2 \text{TEMP}_i^2) \text{TIME}_j \)  

+ \( (f_0 + f_1 \text{TEMP}_i + f_2 \text{TEMP}_i^2) \text{TIME}_j \)  

where \( \theta_4 = d_0 + d_1 \text{TEMP}_i + d_2 \text{TEMP}_i^2 \).

Using the starting values from Table 21, the PROC NLIN code was constructed and is displayed in Table 22. Derivatives have been included so that confidence intervals can be computed. The final estimates of the parameters of the segmented surface are in Table 23. The graph of the estimated models with 95% confidence intervals about the mean for all TEMPS are in Figure 9. Figure 10 contains a three dimensional graph of the estimate of the segmented surface.

References


Table 1. Cost to haul a ton of fertilizer the given number of miles.

<table>
<thead>
<tr>
<th>MILES</th>
<th>COST</th>
<th>MILES</th>
<th>COST</th>
<th>MILES</th>
<th>COST</th>
</tr>
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<tbody>
<tr>
<td>5</td>
<td>1.28</td>
<td>15</td>
<td>1.29</td>
<td>25</td>
<td>1.31</td>
</tr>
<tr>
<td>15</td>
<td>1.29</td>
<td>85</td>
<td>1.87</td>
<td>155</td>
<td>3.25</td>
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<td>1.31</td>
<td>95</td>
<td>2.05</td>
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<td>175</td>
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<td>1.48</td>
<td>125</td>
<td>2.65</td>
<td>195</td>
<td>4.04</td>
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<td>1.59</td>
<td>135</td>
<td>2.84</td>
<td>205</td>
<td>4.24</td>
</tr>
</tbody>
</table>

Table 2. Reparameterized form for several segmented polynomial models.

MODEL L/O:

Initial Model

\[ f(x) = \beta_0 + \beta_1 x + \beta_2 x^2, \quad \alpha < x < \beta \]

Reparameterized Model

\[ f(x) = e_0 + e_1 x + e_2 x^2, \quad \alpha < x < \beta \]

Relationship of Parameters

\[ \beta_0 = e_0, \quad \beta_1 = e_1, \quad \beta_2 = e_2 \]

MODEL C/L:

Initial Model

\[ f(x) = \beta_0 + \beta_1 x + \beta_2 x^2, \quad \alpha < x < \beta \]

Reparameterized Model

\[ f(x) = e_0 + e_1 x + e_2 x^2, \quad \alpha < x < \beta \]

Relationship of Parameters

\[ \beta_0 = e_0, \quad \beta_1 = e_1, \quad \beta_2 = e_2 \]

MODEL G/G:

Initial Model

\[ f(x) = \beta_0 + \beta_1 x + \beta_2 x^2, \quad \alpha < x < \beta \]

Reparameterized Model

\[ f(x) = e_0 + e_1 x + e_2 x^2, \quad \alpha < x < \beta \]
f(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3

\theta_4 (\theta_6 - x)^2 I_4 (\theta_6 - x) + \theta_5 (2 \theta_6 - 3 \theta_6 x + 3 \theta_6 x^2) I_5 (\theta_6 - x)

Reparameterized Model

\beta_0 = \theta_0
\beta_1 = \theta_1
\beta_2 = \theta_2
\beta_3 = \theta_3
\alpha = \theta_6
\beta_4 = \theta_4
\beta_5 = \theta_5

MODEL 0/0/0

Initial Model

f(x) = \left\{ \begin{array}{ll}
\beta_0 x^2 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3, & \text{as} \ x < A \\
\beta_0 + \beta_1 x & \text{as} \ x \geq A
\end{array} \right.

Reparameterized Model

f(x) = \theta_4 (\theta_6 - x)^2 I_4 (\theta_6 - x) + \theta_5 (2 \theta_6 - 3 \theta_6 x + 3 \theta_6 x^2) I_5 (\theta_6 - x)

MODEL 0/0/0

Initial Model

f(x) = \left\{ \begin{array}{ll}
\beta_0 x^2 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3, & \text{as} \ x < A \\
\beta_0 + \beta_1 x & \text{as} \ x \geq A
\end{array} \right.

Reparameterized Model

f(x) = \theta_4 (\theta_6 - x)^2 I_4 (\theta_6 - x) + \theta_5 (2 \theta_6 - 3 \theta_6 x + 3 \theta_6 x^2) I_5 (\theta_6 - x)

Reparameterized Model

f(x) = \theta_4 (\theta_6 - x)^2 I_4 (\theta_6 - x) + \theta_5 (2 \theta_6 - 3 \theta_6 x + 3 \theta_6 x^2) I_5 (\theta_6 - x)

\beta_0 = \theta_0
\beta_1 = \theta_1
\beta_2 = \theta_2
\beta_3 = \theta_3
\alpha = \theta_6
\beta_4 = \theta_4
\beta_5 = \theta_5

Table 3. SAS System code to read data, compute w, and use PROC REG to obtain starting values.

DATA QUADLIN; *DATA SET TO FIT A;
INPUT MILES Q; *QUADRATIC SEGMENTED;
CARDS; *TO A LINEAR;
*DATA IS PRICE PER;
*TON TO HAUL FERTILIZER;
DATA INITIAL; SET QUADLIN; A=50;
W=(MILES-A)**2; IF MILES>A THEN W=W;
*LOOK AT DATA-STARTING JOIN POINT=50;
*GENERATE W TO BE USED BY PROC REG TO;
*GET STARTING VALUES;
PROC REG DATA=INITIAL ; MODEL Q=MILES W;

Table 4. The results of fitting the linear model (with join point of 50) to obtain starting values for example 1.

<table>
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<tr>
<th>VARIABLE</th>
<th>DF</th>
<th>PARAMETER Estimate</th>
</tr>
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<tr>
<td>INTERCEP</td>
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<td>0.4555</td>
</tr>
<tr>
<td>MILES</td>
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<td>0.01801</td>
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<tr>
<td>W</td>
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</tr>
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</table>

Table 5. PROC NLIN code to fit the Q/L model to the data of example 1.

PROC NLIN DATA=QUADLIN; PARGS T1=.45555 T2=.01801 T3=.00011 T4=50; IF MILES < T4 THEN DO;
MODEL Q=T1+T2*MILES+T3*(T4-MILES)**2; END;
ELSE DO;
*SECOND SEGMENT IS LINEAR;
MODEL Q=T1+T2*MILES;
END;

Table 6. Final results from NLIN from fitting the Q/L model to the data of example 1.

<table>
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<th>SOURCE</th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
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<td>RESIDUAL</td>
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<td>0.000032</td>
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<tr>
<td>UNCORR TOTAL</td>
<td>21</td>
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<td>20.402</td>
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<tr>
<td>RESQUARE = .99997</td>
<td></td>
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</table>

PARM ESTIM ASYMPT ASYMPTOTIC 95 %

| PARAMETER | ASYMPT | ASYMPTOTIC 95 | |
|-----------|--------|---------------|
| T1        | 0.00004 | 0.0198408     |
| T2        | 0.00004 | 0.0198408     |
| T3        | 0.00004 | 0.0198408     |
| T4        | 0.00004 | 0.0198408     |

Table 7. SAS System code to read data, compute w, and use PROC REG to obtain starting values.
Table 7. Data for example 2 for the Q/L/Q model.

<table>
<thead>
<tr>
<th>X</th>
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</tbody>
</table>

Table 8. Code using PROC REG to obtain initial estimates for fitting the Q/L/Q model of example 2.

DATA QLQ;
INPUT X Q;
CARDS;
*DATA SET TO FIT;
*QUAD-LINEAR-QUAD;
DATA INITIAL; SET QLQ; IF X>A THEN W=0;
V=(X·B)**2; IF X<B THEN V=0;
PROC REG DATA=INITIAL ; MODEL Q-X W V;
OUTPUT OUT=ONE P=PQ;

Table 9. Results from PROC REG to obtain initial estimates for Example 2.

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DF</th>
<th>ESTIMATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTERCEP</td>
<td>1</td>
<td>1.5696</td>
</tr>
<tr>
<td>X</td>
<td>1</td>
<td>0.1649</td>
</tr>
<tr>
<td>W</td>
<td>1</td>
<td>-0.0341</td>
</tr>
<tr>
<td>V</td>
<td>1</td>
<td>-0.0362</td>
</tr>
</tbody>
</table>

Table 10. PROC NLIN code to fit the Q/L/Q model to the data of example 2 using the initial estimates from PROC REG.

PROC NLIN DATA=QLQ; PARMS T1=1.5696 T2=.0341 T3=-.0362 T5=6 T6=9; *
* FIRST SEGMENT IS QUADRATIC; *
* IF X<=T5 THEN DO;
MODEL Q = T1 + T2*X + T3*(T5-X)**2;
DER.T1=1;
DER.T2=X;
DER.T3=(T5-X)**2;
DER.T4=0;
DER.T5=2*T3*(T5-X);
DER.T6=0;
END;
*
* SECOND SEGMENT IS LINEAR;
* IF X>T5 AND X<=T6 THEN DO;
MODEL Q=T1 + T2*X;
DER.T1=1;
DER.T2=X;
DER.T3=0;
DER.T4=0;
DER.T5=0;
DER.T6=0;
END;

Table 11. Final estimates from NLIN for the Q/L/Q model for example 2.

<table>
<thead>
<tr>
<th>SOURCE</th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>REGRESSION</td>
<td>6</td>
<td>119.3980</td>
<td>19.8967</td>
</tr>
<tr>
<td>RESIDUAL</td>
<td>15</td>
<td>0.2891</td>
<td>0.0192</td>
</tr>
<tr>
<td>UNCORR TOTAL</td>
<td>21</td>
<td>119.6871</td>
<td></td>
</tr>
</tbody>
</table>

Table 12. Data for Decay-linear model for example 3.

<table>
<thead>
<tr>
<th>X</th>
<th>Q</th>
<th>X</th>
<th>Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>10.23</td>
<td>7</td>
<td>7.33</td>
</tr>
<tr>
<td>1</td>
<td>10.21</td>
<td>8</td>
<td>6.40</td>
</tr>
<tr>
<td>2</td>
<td>8.45</td>
<td>9</td>
<td>6.51</td>
</tr>
<tr>
<td>3</td>
<td>7.88</td>
<td>10</td>
<td>6.68</td>
</tr>
<tr>
<td>4</td>
<td>7.24</td>
<td>11</td>
<td>5.73</td>
</tr>
<tr>
<td>5</td>
<td>7.27</td>
<td>12</td>
<td>7.12</td>
</tr>
<tr>
<td>6</td>
<td>7.15</td>
<td>13</td>
<td>6.34</td>
</tr>
</tbody>
</table>

Table 13. SAS code to partition data set and use PROC REG to obtain initial estimates for example 3.

DATA EXP LINE;
INPUT X Q;
CARDS;
DATA EXP;SET EXP LINE; IF X<8.1;
LOGQ=LOG(Q-6.3);
*GUESS JOIN AT A=8.1 SELECTION DATA WITH;
* X<8.1. TAKE LOG TO FIT LINEAR MODEL;
PROC REG DATA=EXP ; MODEL LOGQ-X;

Table 14. PROC REG results to obtain initial values for example 3.

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DF</th>
<th>ESTIMATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTERCEP</td>
<td>1</td>
<td>1.5606</td>
</tr>
<tr>
<td>T1</td>
<td>1</td>
<td>0.3505</td>
</tr>
</tbody>
</table>

Table 15. SAS code to partition data set and use PROC REG to obtain initial estimates for example 3.

DATA EXP LINE;
INPUT X Q;
CARDS;
DATA EXP:SET EXP LINE; IF X<8.1;
LOGQ=LOG(Q-6.3);
*GUESS JOIN AT A=8.1 SELECTION DATA WITH;
* X<8.1. TAKE LOG TO FIT LINEAR MODEL;
* TO GET STARTING VALUES FOR DECOY PART;
LOGQ=LOG(Q-6.3);
PROC REG DATA=EXP ; MODEL LOGQ-X;

Table 16. PROC REG results to obtain initial values for example 3.

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DF</th>
<th>ESTIMATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTERCEP</td>
<td>1</td>
<td>1.5606</td>
</tr>
<tr>
<td>X</td>
<td>1</td>
<td>-0.3505</td>
</tr>
</tbody>
</table>
Table 15. PROC NLIN code to fit decay-linear model to data of example 3.

```plaintext
PROC NLIN DATA=EXP LINE; PARMS B01=6.3 B11=0.759 B21=3.51 A=0;
IF X=A THEN DO; *DECAY FIRST;
MODEL Q=B01+B11*EXP(-B21*X);
DER.B01=1;
DER.B11=-B11*EXP(-B21*X);
DER.B21=-B11*X*EXP(-B21*X);
DER.A=0;
END;
ELSE DO; *LINEAR SECOND
XG=B01+B11*EXP(-B21*A)*(1+B21*A);
XR=B11*B21*EXP(-B21*A);
W=B11*EXP(-B21*A);
MODEL Q=B02+B12*X;
DER.B01=1;
DER.B11=EXP(-B21*A)*(1-B21*X+B21*A);
DER.B21=W*(X*B21*A-A*A*B21-X);
DER.XA=W*B21*B21*(X-A);
END;
```

Table 16. Final NLIN results from fitting the decay-linear model to example 3 data.

<table>
<thead>
<tr>
<th>SOURCE</th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>REGRESSION</td>
<td>4</td>
<td>1034.512</td>
<td>258.6280</td>
</tr>
<tr>
<td>RESIDUAL</td>
<td>17</td>
<td>3.712</td>
<td>0.2183</td>
</tr>
<tr>
<td>UNCORR TOTAL</td>
<td>21</td>
<td>1038.224</td>
<td></td>
</tr>
</tbody>
</table>

**COR TOTAL** 20 39.518

RSQUARE = .90607

<table>
<thead>
<tr>
<th>PARM ESTI</th>
<th>ASYMP</th>
<th>ASYMPTOTIC 95 %</th>
</tr>
</thead>
<tbody>
<tr>
<td>STD. ER CONFIN INTerval</td>
<td>LOWER</td>
<td>UPPER</td>
</tr>
<tr>
<td>B01</td>
<td>6.514</td>
<td>0.527</td>
</tr>
<tr>
<td>B11</td>
<td>4.053</td>
<td>0.541</td>
</tr>
<tr>
<td>B21</td>
<td>0.327</td>
<td>0.130</td>
</tr>
<tr>
<td>A</td>
<td>7.391</td>
<td>2.453</td>
</tr>
</tbody>
</table>

Table 17. TEMP, TIME and RATE for Q/L models of example 4.

<table>
<thead>
<tr>
<th>TEMPERATURE DEGREES C</th>
<th>TIME</th>
<th>20</th>
<th>30</th>
<th>35</th>
<th>40</th>
<th>45</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td>21.5</td>
<td>21.7</td>
<td>22.5</td>
<td>22.2</td>
<td>22.0</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>21.3</td>
<td>20.2</td>
<td>19.3</td>
<td>19.2</td>
<td>17.7</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>19.0</td>
<td>17.7</td>
<td>17.0</td>
<td>16.3</td>
<td>15.7</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>19.7</td>
<td>17.1</td>
<td>15.3</td>
<td>14.6</td>
<td>13.2</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>19.0</td>
<td>16.7</td>
<td>14.6</td>
<td>12.2</td>
<td>10.2</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>18.9</td>
<td>15.7</td>
<td>13.7</td>
<td>10.3</td>
<td>8.5</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>17.9</td>
<td>14.9</td>
<td>12.6</td>
<td>9.4</td>
<td>6.3</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>19.1</td>
<td>14.9</td>
<td>12.2</td>
<td>8.3</td>
<td>5.4</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>17.8</td>
<td>14.9</td>
<td>11.9</td>
<td>8.1</td>
<td>4.2</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>18.2</td>
<td>15.0</td>
<td>11.8</td>
<td>7.6</td>
<td>3.1</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>18.0</td>
<td>16.0</td>
<td>11.4</td>
<td>7.1</td>
<td>2.6</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>17.3</td>
<td>13.6</td>
<td>11.0</td>
<td>6.7</td>
<td>2.4</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>17.5</td>
<td>14.0</td>
<td>10.8</td>
<td>7.3</td>
<td>2.2</td>
</tr>
<tr>
<td></td>
<td>13</td>
<td>16.9</td>
<td>13.6</td>
<td>10.2</td>
<td>6.4</td>
<td>1.8</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>17.4</td>
<td>13.4</td>
<td>10.0</td>
<td>6.3</td>
<td>2.0</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>17.9</td>
<td>12.2</td>
<td>10.2</td>
<td>6.4</td>
<td>1.7</td>
</tr>
</tbody>
</table>

| TRT 1=TEMP 20, TRT2=TEMP 30, TRT 3=TEMP 35, TRT 4=TEMP 40, TRT 5=TEMP 45 |

Table 18. Code to obtain starting values for example 4.

```plaintext
DATA QL TRT;
INPUT TRT TEMP TIME RATE;
CARDS;
DATA JOIN; SET QL TRT; *AFTER PLOTTING;
A=3; *DATA. CHOOSE;
IF TRT=2 THEN A=5; *JOIN POINTS FOR;
IF TRT=3 THEN A=6; *EACH TREATMENT;
IF TRT=4 THEN A=8;
IF TRT=5 THEN A=10;
W= (TIME-A)**2; IF TIME<A THEN W=0;
PROC REG; BY TRT; MODEL RATE=TIME W;
```

Table 19. The results of fitting the linear model to get starting values for each TEMP of example 4.

<table>
<thead>
<tr>
<th>TEMPERATURE</th>
<th>VALUE</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>38.0</td>
</tr>
<tr>
<td>30</td>
<td>35.0</td>
</tr>
<tr>
<td>35</td>
<td>40.0</td>
</tr>
<tr>
<td>40</td>
<td>45.0</td>
</tr>
</tbody>
</table>

**MSRESI** 0.295 0.157 0.086 0.081 0.110

**RSQUAR** 0.857 0.979 0.994 0.997 0.997

**INTERC** 19.67 17.18 14.34 10.11 5.602

**TIME** -.17 -.09 -.31 -.07 -.27 -.275

**W** 0.237 0.183 0.212 0.190 0.162

**t_4** 3.0 5.0 6.0 8.0 10.0

Table 20. Code to express respective estimates as linear and as quadratic functions of TEMP.

```plaintext
DATA ESTIMATE; INPUT TEMP A B02 B12 B21;
TEMP2=TEMP**2;
CARDS;
20 3 19.67 -.1725 .2379
30 5 17.18 -.2949 .1838
35 6 14.54 -.3143 .2128
40 8 10.12 -.2702 .1908
45 10 5.60 -.2752 1.620
PROC REG; MODEL A B02 B12 TEMP TEMP2;
```

Table 21. Results of modeling the respective estimates as linear and quadratic functions of TEMP.

<table>
<thead>
<tr>
<th><em><strong>LINEAR FUNCTION OF TEMP</strong></em></th>
</tr>
</thead>
<tbody>
<tr>
<td>PARAMETER</td>
</tr>
<tr>
<td>MSRESI</td>
</tr>
<tr>
<td>RSQUAR</td>
</tr>
<tr>
<td>INTERC</td>
</tr>
<tr>
<td>TEMP</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><em><strong>QUADRATIC FUNCTION OF TEMP</strong></em></th>
</tr>
</thead>
<tbody>
<tr>
<td>PARAMETER</td>
</tr>
<tr>
<td>MSRESI</td>
</tr>
<tr>
<td>RSQUAR</td>
</tr>
<tr>
<td>INTERC</td>
</tr>
<tr>
<td>TEMP</td>
</tr>
<tr>
<td>TEMP2</td>
</tr>
</tbody>
</table>
Table 22. Code to fit the segmented surface for example 4.

```plaintext
PROC NLIN DATA=QL TRT; PARMS
 AO=-12.027997 Al=-.806215 A2=-.021152
 BO=-.352157 B1=-.03658033 B2=.000509
 CO=-.282570 C1=-.002503
 DO=3.402062 D1=-.150616 D2=-.006598;
 *; * EVALUATE PARAMETERS OF MODEL AS;
 * FUNCTIONS OF TEMP;
 T1=AO+Al*TEMP+A2*TEMP**2;
 T2=BO+B1*TEMP+B2*TEMP**2;
 T3=CO+C1*TEMP;
 T4=DO+D1*TEMP+D2*TEMP**2;
 M2=(TIME-T4)**2;
 M=(TIME-T4);
 *; * FIRST SEGMENT IS QUADRATIC;
 *;
 IF TIME < T4 THEN DO;
 MODEL RATE=T1+T2*TIME+T3*(TIME-T4)**2;
 DER.AO-1;
 DER.A1-TEMP;
 DER.A2-TEMP**2;
 DER.B0-TEMP;
 DER.B1-TEMP*TIME;
 DER.B2=TIME*TEMP**2;
 DER.C0-M2;
 DER.C1-TEMP*M2;
 DER.DO=-2*T3*M;
 DER.D1=-2*T3*M*TEMP;
 DER.D2=-2*T3*M*TEMP**2;
 END;
 *; * SECOND SEGMENT IS LINEAR;
 *;
 ELSE DO;
 MODEL RATE=T1+T2*TIME;
 DER.A0-1;
 DER.A1-TEMP;
 DER.A2-TEMP**2;
 DER.B0-TEMP;
 DER.B1-TEMP*TIME;
 DER.B2=TIME*TEMP**2;
 DER.C0-0;
 DER.C1-0;
 DER.D0-0;
 DER.D1-0;
 DER.D2-0;
 END;
```

Table 23. Final estimates for the segmented surface for example 4.

<table>
<thead>
<tr>
<th>SOURCE</th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>REGRESSION</td>
<td>11</td>
<td>16262.12</td>
<td>1478.375</td>
</tr>
<tr>
<td>RESIDUAL</td>
<td>69</td>
<td>9.88</td>
<td>0.143</td>
</tr>
<tr>
<td>UNCORR TOTAL</td>
<td>80</td>
<td>16272.01</td>
<td></td>
</tr>
</tbody>
</table>

(RSS) 79 2524.86
RSQ = .9961

<table>
<thead>
<tr>
<th>PARM</th>
<th>EST ASYMPT</th>
<th>STD. ERR</th>
<th>95 % CONFID INTERVAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>AO</td>
<td>10.6791</td>
<td>0.9225</td>
<td>(5.28086, 16.0773)</td>
</tr>
<tr>
<td>A1</td>
<td>-0.0235</td>
<td>0.00345</td>
<td>(-0.03032, 0.0067)</td>
</tr>
<tr>
<td>A2</td>
<td>-0.0441</td>
<td>0.00693</td>
<td>(-0.07824, 0.00009)</td>
</tr>
<tr>
<td>B0</td>
<td>0.19129</td>
<td>0.00289</td>
<td>(0.1673, 0.2152)</td>
</tr>
<tr>
<td>B1</td>
<td>0.46734</td>
<td>0.0124</td>
<td>(-0.00007, 0.0076)</td>
</tr>
<tr>
<td>B2</td>
<td>0.00066</td>
<td>0.00001</td>
<td>(0.00005, 0.00007)</td>
</tr>
<tr>
<td>C0</td>
<td>0.3655</td>
<td>0.00873</td>
<td>(0.19129, 0.5397)</td>
</tr>
<tr>
<td>C1</td>
<td>-0.0047</td>
<td>0.00023</td>
<td>(-0.00881, 0.0038)</td>
</tr>
<tr>
<td>D0</td>
<td>3.2699</td>
<td>0.0023</td>
<td>(1.9610, 4.5389)</td>
</tr>
<tr>
<td>D1</td>
<td>-0.1805</td>
<td>0.0013</td>
<td>(-0.3734, 0.0124)</td>
</tr>
<tr>
<td>D2</td>
<td>0.0076</td>
<td>0.00195</td>
<td>(0.0038, 0.0114)</td>
</tr>
</tbody>
</table>

Figure 1. Plot of Cost to Haul A Ton of Fertilizer the specified number of miles

Figure 2. Plot of Cost-Fertilizer model with join point at 50
Figure 3. D/L Function fit to the Cost-Fertilizer Data

Figure 4. Plot of raw data for Example 2.

Figure 5. Plot of data and initial model from PROC REG for Example 2.

Figure 6. Graph of final model with interval estimates for Example 2.

Figure 7. Graph of Data for Example 3.

Figure 8. Graph of data, model, and confidence limits for the Decay-Linear model of Ex 3.
Figure 9 Graph of models with 95% Confidence Intervals about the models with Confidence bands.

Figure 10 Segmented Surface for Example 4