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Performing response surface analysis using the SAS RSREG procedure

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ABSTRACT

Response surface methodology is a set of technology to present the cause and/or effect relationship between factor variables and response variable. The standard procedure of response surface contains four steps: (a) design the experiment, (b) estimate the coefficient of response surface, (c) do the lack-of fit test, and (d) investigate the region of interest. This paper described the RSREG procedure, which was designed for standard response surface analysis. Application of the RSREG procedure includes estimating the coefficient of response surface, lack of fit test and canonical structure analysis and predicting the new response values.

INTRODUCTION

Response surface methodology is a useful tool in modeling curvature effects in many scientific areas. The general scenario requires that the response is a quantitative continuous variable; the most important function is to identify the combination of levels of factors in experimental design that leads to determine optimum conditions and save resources. The RSREG procedure is specialized for analyzing the response surface analysis. GLM procedure also can estimate the coefficient of response surface and carry out lack of fit test. The fundamental function of response surface analysis is to examine the characteristics of the fitted surface with first or second order of quantitative predictors. Give that, response surface analysis is like a regression issue. However, response surface analysis is quite different from routine regression analysis in using very unique experimental design, coded predictor variables, etc. Therefore, RSREG procedure is superior to GLM and/or REG procedure with response surface analysis because: (1) RSGRE contains canonical analysis and ridge of optimum response; (2) it requires comparably shorter model statement.

The primary goal of this paper is to present an overview of RSREG procedure and how its commands used in design and analyzing response surface experiments. The second goal is to provide illustrative SAS codes in producing visual graphs to help the researcher deeply understand the design and the properties of dataset.

EXAMPLE ONE

The following example uses a two factor quadratic model and the data set is from Table 16.9 of Dean and Voss (1999). The experiment studied the relation between the standard deviation of a copper-plating thickness (Y) and anode-cathode separation (x1) and cathodic current density (x2) of the product.

```
x1      x2        Y
9.5     31      5.6
9.5     41      6.45
11.5    31      4.84
11.5    41      5.19
10.5    36      4.32
10.5    36      4.25
9       36      5.76
12      36      4.42
10.5    29      5.46
10.5    43      5.81
```

The quadratic model for this example is written as

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{1i}^2 + \beta_4 x_{2i}^2 + \beta_5 x_{1i} x_{2i} + \varepsilon_i$$

We will take the following steps to analyze this data:

1. fit the model and estimate the parameter
2. use canonical analysis to examine the shape of response surface
3. use ridge analysis to look for the optimum region.

MODEL FITTING AND PARAMTER ESTIMATION

The following statement invokes the RRREG procedure on data a. We require a lack of fit test on the fitted model with LACKFIT option. We will orderly illustrate the output tables from the following statement.

```
proc rsreg data=a;
model y=x1 x2/lackfit;
   run;
```

Using an appropriate coding transformation of the data is one important aspect of response-surface analysis. The coding way on predictors will affect the results of canonical analysis. The coding approach makes all coded variables vary over the same range and fall between -1 and 1. Therefore, each predictor has an equal share in potentially determining the dominant predictor in response surface analysis. The coded variable x1=(factor A-10.5)/1.5 and X2=(Factor B-36)/7 (Table1).

Table 1.1: Summary statistics for example one

```
                 The RSREG Procedure

 Coding Coefficients for the Independent Variables
  Factor     Subtracted off       Divided by

  x1              10.500000         1.500000
  x2              36.000000         7.000000

  Response Surface for Variable y
  Response Mean                     5.210000
  Root MSE                          0.189920
  R-Square                            0.9705
  Coefficient of Variation            3.6453
```

Simple statistics of response of y is also showed in Table 1. R square is 0.9705, which indicates 97% of variability explained by the fitted model. Hypothesis test on linear, quadratic and crossproduct in ANOVA table indicates the linear and quadratic terms are significantly important, and interaction between x1 and x2 is not significant (Table2).

Regression	DF	Type I Sum of Squares	R-Square	F Value	Pr > F
Linear	2	2.271313	0.4645	31.49	0.0036
Quadratic	2	2.411708	0.4932	33.43	0.0032
Crossproduct	1	0.062500	0.0128	1.73	0.2584
Total Model	5	4.745521	0.9705	26.31	0.0037

Parameter	DF	Estimate	Error	t Value	Pr > |t|	Parameter Estimate Standard from Coded Data
Intercept	1	79.689773	13.747965	5.80	0.0044	4.293903
x1	1	-7.818717	1.831147	-4.27	0.0130	-0.711176
x2	1	-1.812593	0.330244	-5.49	0.0054	0.298737
x1*x1	1	0.392600	0.080832	4.86	0.0083	0.883350
x2*x1	1	-0.025000	0.018992	-1.32	0.2584	-0.262500
x2*x2	1	0.029413	0.003651	8.06	0.0013	1.441260
Total Model	5	4.745521	0.9705	26.31	0.0037	

Table 1.2: Analysis of Variance

Residual	DF	Sum of Squares	Mean Square	F Value	Pr > F
Lack of Fit	3	0.1418	0.0473	19.30	0.1654
Pure Error	1	0.00245	0.00245		
Total Error	4	0.144279	0.036070		

Table1.3: Lack of fit test

The table 3 includes a breakdown of lack of fit and pure error. The test indicates the second-order model is adequate for the data (p-value=0.1654).

CANONICAL ANALYSIS

Canonical analysis is used to investigate the overall shape of the curvature and determine the stationary point is a maximal, minimal or saddle point. The eigenvalues and eigenvectors indicate the shape of the response surface. Positive eigenvalues direct an upwards curvature, and negative eigenvalues direct a downward curvature. Therefore, all positive eigenvalue indicate an estimate stationary is a minimum, and all positive eigenvalue indicate a maximum and mixture of positive and negative eigenvalues indicate a saddle point. The larger absolute eigenvalues indicate the more importance in the curvature of response surface.

```
The RSREG Procedure
 Canonical Analysis of Response Surface Based on Coded Data

                Critical Value
Factor           Coded         Uncoded
 x1            0.392457       11.088685
 x2           -0.067898       35.524714

   Predicted value at stationary point: 4.144209

Eigenvectors             Eigenvalues
                   x1             x2
1.470594       -0.218120        0.975922
 0.854015       0.975922        0.218120

     Stationary point is a minimum.
```

A canonical analysis of the surface on example one indicates that the stationary point of the fitted surface is at (11.09, 35.52) in raw data and (0.39, -0.07) (Table 4) in coded units. Both eigenvalues are positive, indicating that the stationary point is a minimum. The eigenvalue of x1(anode-cathode separation) is larger than that of x2 (cathodic current density), indicates x1 is relatively more important than x2 (Table 4). This is an ideal situation in response surface design. The previous two steps may be sufficient, since optimum point is within a range of the experimental design. If the optimum is out of the range of experiment, ridge analysis will be applied to further search for the optimum region. Example two will illustrate how to use ridge analysis.

Table 1.4: Canonical Analysis for Example one

EXAMPLE TWO: A SADDLE SURFACE USING RIDGE ANALYSIS

This data is from problem 6.15 of Kutner et al. (2004) to study the relation between patient satisfaction (Y) and three factors x1(patient age), x2(severity of illness) and x3 (anxiety level) in a hospital. There are 46 patients were collected and data set are available in the following address: http://br312.math.tntech.edu/6080/cd/KutnerData/Chapter%20%206%20Data%20Sets/CH06PR15.txt .

The following statement invokes RSREG procedure containing LACKFIT option and ridge analysis. The statements produce Output table 2.1 through table 2.3.

```
proc rsreg data=patient;
model y=x1 x2 x3/lackfit;
ridge max;
run;
```

Table2.1 summary statistics for example two

```
                The RSREG Procedure

     Coding Coefficients for the Independent
Variables

 Factor     Subtracted off      Divided by

 x1              38.500000       16.500000
 x2              51.500000       10.500000
 x3               2.350000        0.550000

 Response Surface for Variable y: satisfaction

Response Mean                   61.565217
Root MSE                         9.252264
R-Square                           0.7695
```

Table2.2 shows that the model is adequate for data with p-value=0.8510. The linear regression and corssproduct showed significant contrition to the model. Note that the X1(patient's age is not significant in the analysis of variance for the model.

The canonical analysis (Table 2.3) indicates that the shape of predicted response surface like a saddle. The eigenvlue of -33.21 shows that the hill orientation of the saddle is more curved than valley orientation, with eigenvalues of 30.05 and 0.63, respectively. The coefficients of the associated eigenvectors show that the valley is more aligned with X3(anxiety level) and hill with X2(severity of illness). There is no a unique optimum, since a saddle point in the canonical analysis.

Table2.2 Lack of fit test and analysis of variance

Regression	DF	Type I Sum of Squares	R-Square	F Value	Pr > F
Linear	3	9120.463666	0.6822	35.51	<.0001
Quadratic	3	215.590388	0.0161	0.84	0.4812
Crossproduct	3	951.492601	0.0712	3.70	0.0202
Total Model	9	10288	0.7695	13.35	<.0001

Residual	DF	Sum of Squares	Mean Square	F Value	Pr > F
Lack of Fit	35	2901.257693	82.893077	0.46	0.8510
Pure Error	1	180.500000	180.500000		
Total Error	36	3081.757693	85.604380		

Parameter	DF	Estimate	Standard Error	t Value	Pr > |t|	Parameter Estimate from Coded Data
Intercept	1	22.435576	143.810689	0.16	0.8769	58.697270
x1	1	-1.308107	3.304523	-0.40	0.6945	-22.494445
x2	1	14.158692	7.850701	1.80	0.0797	-4.121989
x3	1	-218.700531	89.903816	-2.43	0.0201	-4.595765
x1*x1	1	0.039910	0.024817	1.61	0.1165	10.865365
x2*x1	1	0.115937	0.085696	1.35	0.1845	20.086024
x2*x2	1	-0.247873	0.129187	-1.92	0.0630	-27.327950
x3*x1	1	-3.871899	1.162199	-3.33	0.0020	-35.137482
x3*x2	1	2.772787	2.628167	1.06	0.2984	16.012847
x3*x3	1	46.088116	26.486581	1.74	0.0904	13.941655

The RSREG Procedure

Factor	DF	Sum of Squares	Mean Square	F Value	Pr > F	Label
x1	4	3754.898605	938.724651	10.97	<.0001	patient age
x2	4	357.235231	89.308808	1.04	0.3985	severity of illness
x3	4	1422.924474	355.731118	4.16	0.0072	anxiety level

Table 2.3 Canonical analysis for example two

The RSREG Procedure
Canonical Analysis of Response Surface Based on Coded Data

Factor	Critical Value Coded	Critical Value Uncoded	Label
x1	10.279168	208.106267	patient age
x2	6.458802	119.317420	severity of illness
x3	9.409070	7.524989	anxiety level

Predicted value at stationary point: -91.847309

Eigenvalues	Eigenvectors x1	x2	x3
30.054195	-0.679937	-0.016717	0.733080
0.633872	0.661899	0.416236	0.623407
-33.208997	-0.315556	0.909103	-0.271949

Stationary point is a saddle point.

The ridge analysis in Table 2.4 indicates that the maximum satisfaction will result from relatively young age, relatively lighter severity of illness and higher anxiety level.

Table2.4 Ridge analysis for example two

The RSREG Procedure

Estimated Ridge of Maximum Response for Variable y: satisfaction

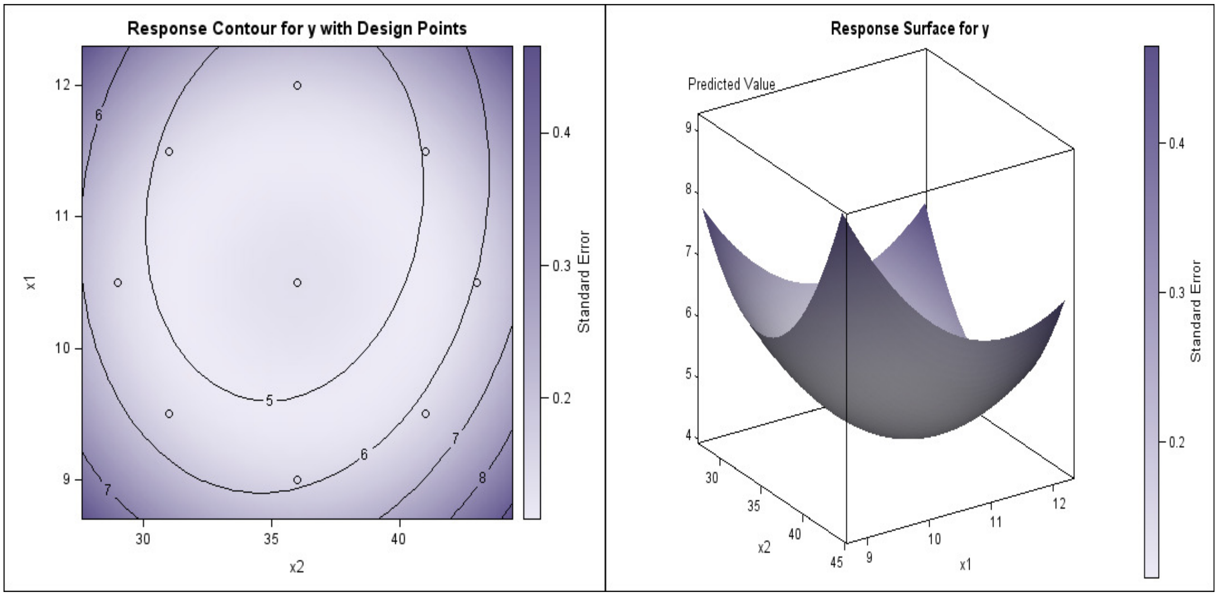
Coded Radius	Estimated Response	Standard Error	Uncoded Factor Values x1	x2	x3
0.0	58.697270	2.658718	38.500000	51.500000	2.350000
0.1	61.121258	2.639690	36.887244	51.289162	2.346387
0.2	63.812896	2.635607	35.273517	51.085272	2.357823
0.3	66.892226	2.715762	33.724997	50.925388	2.381385
0.4	70.446485	2.978678	32.264079	50.806620	2.412237
0.5	74.527045	3.505900	30.878784	50.716552	2.446976
0.6	79.162288	4.325171	29.550451	50.645359	2.483799
0.7	84.368246	5.423290	28.263794	50.586758	2.521798
0.8	90.154432	6.775988	27.007848	50.536846	2.560501
0.9	96.526790	8.362759	25.774946	50.493141	2.599649
1.0	103.489208	10.169313	24.559691	50.454014	2.639091

GRAPHS FOR RESPONSE SURFACE

The canonical analysis provided the shape of a second-order response surface, the effective graphs will make the explanation easier and help the researcher understand deeply on the data. In RSREG procedure, plot option can produce appropriate plots through ODS graphics. For example, plot =all will produce all plots in some output panels.

You may choose some plots, such as, plot=surface option allows you to print out contour plot(s) of all pairs of predictors, and plot=surface(3D) option will provide a three-dimension plot. The following code was used to generate plot in RSREG procedure with Example one.

```
ods graphics on;
proc rsreg data=a plots=(surface);
model y=x1 x2/lackfit;
run;
ods graphics off;
```



CREATING YOUR OWN PLOT

Beyond the SAS default contour and surface graphs, you can make your own 3D graphs with GCONTOUR, G3D or G3DGRID procedures. In GCONTOUR the response to two independent variables is displayed as different contour lines. G3D is a 3-dimensional perspective representation, either as a 'sheet' of joined points or a scatter plot. In this section, we will demonstrate how to produce the various shapes of a plot. Data step allows you to create potential data points used in graphs step. The example is showed with data=grid. The predicted response would be stored in the data predict using the OUT=predict.

```
data grid;
do y=.;
do x1=9 to 13 by 0.02;
do x2 = 29 to 43 by 0.02;
output;
end;
end;
end;
run;

data new;
set a grid;
run;

proc rsreg data=new out=predict noprint;
```

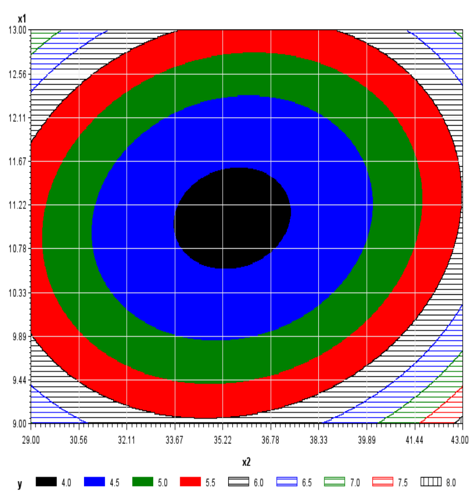
```
model y=x1 x2/lackfit predict;
run;
```

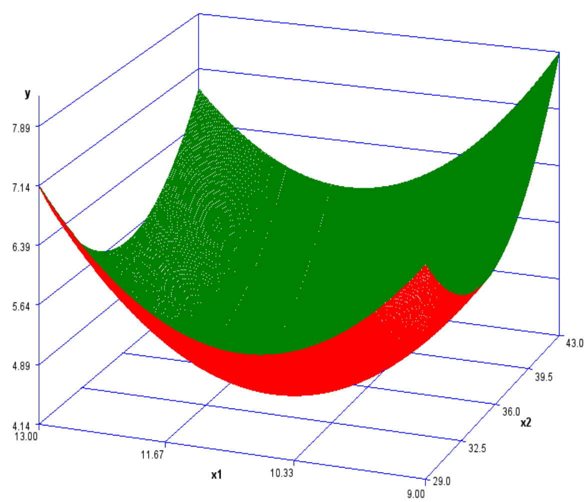
The plots from GCONTOUR procedure represent three-dimensional relationships in two dimensions. Lines or areas in a contour plot represent levels of magnitude (**z**) corresponding to a position (**x**, **y**) on a plane. By default, the GCONTOUR procedure automatically use seven contour levels of the contour variable, representing those levels with default colors and line types, you also can create more or less levels according to the need with levels option (see example below), meanwhile, it generates a legend that is labeled with the contour variable's name. The G3D procedure allows you to view the surface plot from different angles by rotating the X-Y plane around the Z axis, or tilting the X-Y plane.

```
goptions /*reset=global*/ gunit=pct border cback =white
colors=(black blue green red);

proc gcontour data=predict;
plot x1*x2=y/grid xticknum=10 yticknum=10 levels=4 to 8 by 0.5 pattern join;
run;

proc g3d data=predict;
plot x1*x2=y/plot x1*x2=y/grid caxis=blue xticknum=5 yticknum=4 zticknum=6
rotate=0 to 180 by 60 tilt=0 to 90 by 15;
run;
```





CONCLUSION

The RSREG procedure is another method to execute response surface analysis. It is easier to understand and use in graphing and canonical analysis. We would recommend learning this useful procedure when you need response surface analysis. GCONTOUR, G3D and G3dGRID are useful procedures to obtain nicer graphs.

REFERENCES

Dean A M and Voss D (1999). Design and Analysis of Experiments. Springer.

Kutner M, Nachtsheim C, Meter J and Li W (2004) Applied Linear Statistical Methods. McGraw -Hill/Irwin.

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