rsm: an R package for Response Surface Methodology

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Introduction

rsm is an R package for Response Surface Methodology.
For 1st order response surfaces rsm provides

- Calculation of the Path of Steepest Ascent
- Precision of the Path

For 2nd order response surfaces rsm provides

- Ridge Analysis
- Maximum or Minimum plots
- Canonical Analysis
- Precision of canonical analysis based on Double Linear Regression

1st Order Response Surfaces

The model is

$$y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + \varepsilon_i$$

Path of Steepest Ascent

The path of steepest ascent is given by:

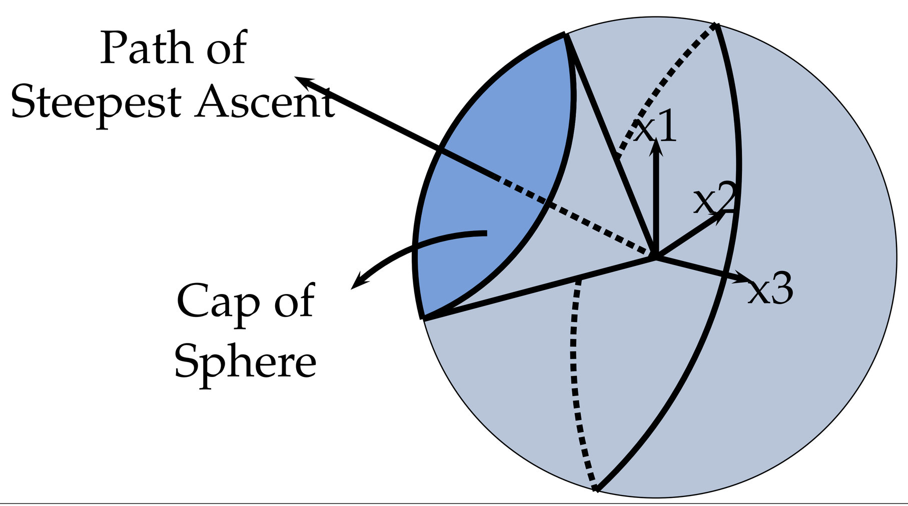
$$x_1 = \frac{rb_1}{\sqrt{\sum_{i=i}^{k} b_i^2}}, x_2 = \frac{rb_2}{\sqrt{\sum_{i=i}^{k} b_i^2}}, \ldots, x_k = \frac{rb_k}{\sqrt{\sum_{i=i}^{k} b_i^2}}$$

where $b_1, \ldots, b_k$ are the estimates of $\beta_1, \ldots, \beta_k$ and r is the Radius, the distance to the centre of the design region. The estimated response on the path is given by

$$\hat{y} = b_0 + r\sqrt{\sum_{i=i}^{k} b_i^2}$$

Precision of the Path of Steepest Ascent

Box (1955) and Box and Draper (1987, pp. 190-194) gave a method for computing a confidence cone for the direction of steepest ascent. The proportion of directions included in the confidence cone gives a measure of the precision of the path of steepest ascent, and is measured by taking the ratio of the surface area of the cap of the sphere within the confidence cone to the surface area of the sphere. See also Sztendur and Diamond (2002).



Implementation

rsm provides first order objects which include print, summary and plot methods:

`fit1 <- firstorder(X,y)` creates a firstorder fit object.

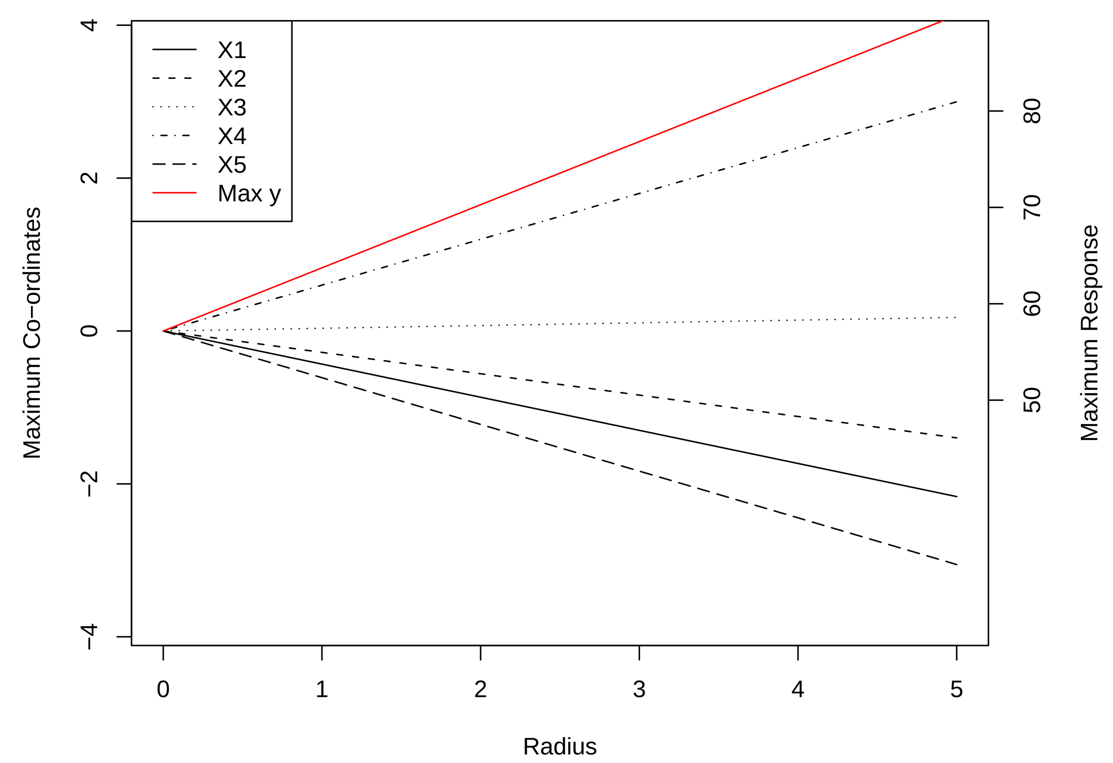
`print(fit1)` adds the path of steepest ascent:

```
(Intercept)     X1     X2    X3    X4     X5
     57.175 -3.350 -2.162 0.275 4.638 -4.725
The path of steepest ascent is:

                  X1 = -0.433r
                  X2 = -0.280r
                  X3 =  0.036r
                  X4 =  0.598r
                  X5 = -0.611r

The estimated response on the path is ycap = 57.175 + 7.734r
```

`summary(fit1)` gives, in addition, the percentage of directions excluded from the 95% confidence cone.

```
The 95% confidence cone for the path of steepest ascent
excludes 99.03% of possible directions.
```

`plot(fit1)` gives the co-ordinates of the path of steepest ascent and the predicted response on the path:



Second Degree Response Surfaces

The equation is

$$\hat{y} = b_0 + \mathbf{x}^\mathbf{T}\mathbf{b} + \mathbf{x}^\mathbf{T}\mathbf{B}\mathbf{x}$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} b_{11} & \frac{1}{2}b_{12} & \cdots & \frac{1}{2}b_{1k} \\ \frac{1}{2}b_{12} & b_{22} & \cdots & \frac{1}{2}b_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2}b_{1k} & \frac{1}{2}b_{2k} & \cdots & b_{kk} \end{bmatrix}$$

where $\mathbf{b}$ is the $(k \times 1)$ vector of the first-order regression coefficients and $\mathbf{B}$ is the $(k \times k)$ symmetric matrix whose diagonal elements are the pure quadratic coefficients and whose off-diagonal elements are one-half the mixed quadratic coefficients.

Ridge Analysis

Ridge analysis is equivalent to the path of steepest ascent applied to second order response surfaces and was developed by A.W. Hoerl (1959) and R.W. Hoerl(1985). In Ridge analysis, stationary points of the response surface subject to $\mathbf{x}^T\mathbf{x} = r^2$ are found, resulting in

$$\mathbf{x}_S = -\frac{1}{2}(\mathbf{B} - \mu\mathbf{I})^{-1}\mathbf{b}$$

for various values of μ. For maximisation of the response, only values of μ greater than the largest eigenvalue of $\mathbf{B}$ are used; while for minimisation of the response, only values of μ less then the smallest eigenvalue are used. A ridgeplot gives the dependence of the radius of the stationary values of the response against the value of the Lagrangian multipler, μ.

Canonical Analysis

Canonical analysis of the 2nd degree response surface allows the investigation of the underlying nature of the response surface and whether it is a maximum, minimum, saddle, rising ridge, or stationary ridge.

A Canonical Form

In the A Canonical Form, the axes are rotated so that the cross-product terms are removed, resulting in the model:

$$\hat{y} = b_0 + \mathbf{X}^\mathbf{T}\theta + \mathbf{X}^\mathbf{T}\mathbf{\Lambda}\mathbf{X}$$

where $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_k)$.

B Canonical Form

In the B Canonical Form, both cross-product and linear terms are removed by shifting the origin and rotating the axes, resulting in the model:

$$\hat{y} = \hat{y}_S + \tilde{\mathbf{X}}^T\mathbf{\Lambda}\tilde{\mathbf{X}}$$

The values of the λs show the nature of the surface. If all the λs are negative, the surface is a maximum; if all the λs are positive, the surface is a minimum; if the λs are of mixed sign, the surface is a saddle; while if some of the λs are zero, the surface is a stationary ridge. The latter is particularly important, as it indicates a linear or planar maximum or minimum, rather than a point maximum or minimum.

Double Linear Regression Method

In practice, because of experimental error and mild lack of fit, λs exactly equal to 0 will not occur. However, small λs indicate that the surface can be approximated by a ridge system. The standard errors of the λs are determined using the double linear regression method, due to Bisgaard and Ankenman (1996).

Implementation

rsm provides second order objects which include print, summary and plot methods:

`fit2 <- secondorder(X,y)` creates a secondorder fit object.

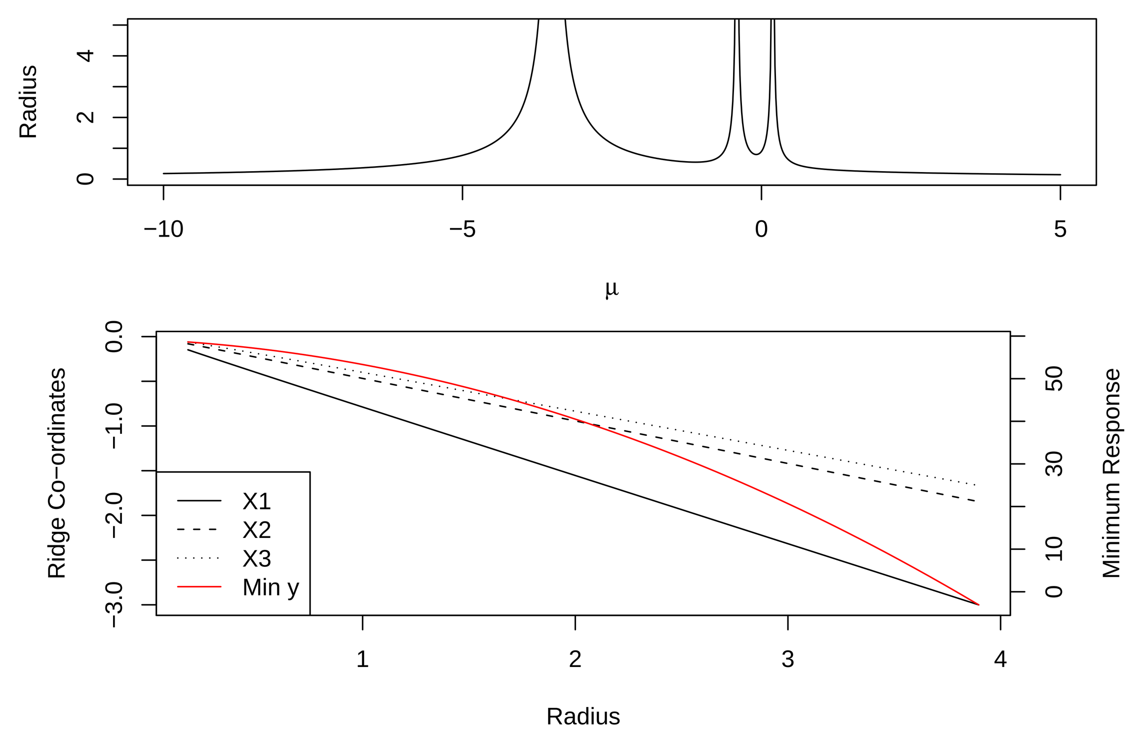
`print(fit2)` adds the A and B Canonical Forms:

```
(Intercept)     x1     x2    x3   x1sq   x2sq   x3sq
     59.140  2.006  1.004 0.670 -1.999 -0.731 -0.998
       x1x2   x1x2   x2x3
     -2.801 -2.179 -1.154

A Canonical Form:
y=59.140+0.273X1-0.341X2+2.300X3+0.188X1sq-0.411X2sq-3.505X3sq

          X1 =  0.585x1 -0.797x2 -0.149x3
          X2 = -0.280x1 -0.371x2 +0.885x3
          X3 =  0.761x1 +0.476x2 +0.440x3

Location of Stationary Point: (-0.058, 0.888, -0.114)
Distance of Stationary Point from Origin:  0.898
B Canonical Form:
y=59.490+0.188XX1sq-0.411XX2sq-3.505XX3sq

   XX1 =  0.585(x1+0.058) -0.797(x2-0.888) -0.149(x3+0.114)
   XX2 = -0.280(x1+0.058) -0.371(x2-0.888) +0.885(x3+0.114)
   XX3 =  0.761(x1+0.058) +0.476(x2-0.888) +0.440(x3+0.114)
```

`summary(fit2)` adds the standard errors of the λs based on the double linear regression method:

```
             Estimate Std.  Error t value Pr(>|t|)
(Intercept)  5.949e+01   8.307e-01  71.610 1.02e-13
      XX1sq  1.880e-01   1.188e-01   1.583    0.148
      XX2sq -4.114e-01   3.775e-01  -1.090    0.304
      XX3sq -3.505e+00   4.473e-01  -7.835 2.61e-05
```

`plot(fit2)` gives the ridge plot and the maximum or minimum plot.



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