Using the `rsm` package

Russell V. Lenth
The University of Iowa

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1 Overview

The `rsm` package provides several useful functions to facilitate response-surface analysis. The primary one is the `rsm` function itself, which is an extension of `lm` but with some enhancements. In specifying a model in `rsm`, the model formula is just like in `lm`, ut the response-surface portion of the model is specified using one or more of the special functions `FO` (first-order), `TWI` (two-way interactions), `PQ` (pure quadratic), or `SO` (second-order, and alias for all three of the previous functions, combined). The `summary` method for `rsm` results includes the usual regression summary (but with the coefficients compactly relabeled), an analysis of variance table with a lack-of-fit test, and additional information depending on the order of the model.

An important aspect of response-surface analysis is using an appropriate coding transformation of the data. The functions `coded.data`, `as.coded.data`, `decode.data`, `code2val`, and `val2code` facilitate these transformations; we simply provide formulas for the desired transformations. If a `coded.data` object is used in place of an ordinary `data.frame` in the call, to `rsm`, then appropriate additional output is provided in the `summary` and `steepest` outputs.

Auxiliary functions include `steepest` for finding a path of steepest ascent (for second-order models, this uses ridge analysis); and `contour` for obyaining a contour plot of the response surface.

2 Chemical reactor example

The provided dataset `ChemReact` comes from Table 7.7 of Myers and Montgomery (2002).

```
R> library(rsm)
R> ChemReact

    Time   Temp Block Yield
1  80.00 170.00    B1  80.5
2  80.00 180.00    B1  81.5
3  90.00 170.00    B1  82.0
4  90.00 180.00    B1  83.5
5  85.00 175.00    B1  83.9
6  85.00 175.00    B1  84.3
7  85.00 175.00    B1  84.0
8  85.00 175.00    B2  79.7
9  85.00 175.00    B2  79.8
10 85.00 175.00    B2  79.5
```

```
11 92.07 175.00    B2  78.4
12 77.93 175.00    B2  75.6
13 85.00 182.07    B2  78.5
14 85.00 167.93    B2  77.0
```

The context is that block `B1` of this data were collected first and analyzed, after which block `B2` was added and a new analysis was done. Accordingly, we woll illustrate the analysis in two stages.

First, though, we need to take care of coding issues. The data are provided in their original units, and the original experiment (block `B1`) used factor settings of Time $= 85 \pm 5$ and Temp $= 175 \pm 5$, with three center points. Thus, the coded variables are $x_1 = (\text{Time} - 85)/5$ and $x_1 = (\text{Temp} - 175)/5$. Let's create a coded dataset with the appropriate codings. We do this via formulas:

```
R> CR = coded.data (ChemReact,  x1 ~ (Time - 85)/5,  x2 ~ (Temp - 175)/5 )
R> CR[1:7, ]   ### Initial experiment only

  x1 x2 Block Yield
1 -1 -1    B1  80.5
2 -1  1    B1  81.5
3  1 -1    B1  82.0
4  1  1    B1  83.5
5  0  0    B1  83.9
6  0  0    B1  84.3
7  0  0    B1  84.0
Variable codings ...
x1 ~ (Time - 85)/5
x2 ~ (Temp - 175)/5
```

2.1 Analysis of initial block

The initial 7 runs are only good enough to estimate a first-order model. We will fit this by calling `rsm` just like we would `lm`, but use the special function `FO` (first-order response surface) in the model formula:

```
R> CR.rsm1 = rsm (Yield ~ FO(x1, x2), data = CR, subset = 1:7)
R> summary(CR.rsm1)

Call:
rsm(formula = Yield ~ FO(x1, x2), data = CR, subset = 1:7)
Residuals:
      1       2       3       4       5       6       7
-0.8143 -1.0643 -1.0643 -0.8143  1.0857  1.4857  1.1857
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  82.8143     0.5472 151.346 1.14e-08 ***
x1            0.8750     0.7239   1.209    0.293
x2            0.6250     0.7239   0.863    0.437
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Residual standard error: 1.448 on 4 degrees of freedom
Multiple R-squared: 0.3555,       Adjusted R-squared: 0.0333
F-statistic: 1.103 on 2 and 4 DF,  p-value: 0.4153
Analysis of Variance Table
Response: Yield
            Df Sum Sq Mean Sq F value  Pr(>F)
FO(x1, x2)   2 4.6250  2.3125  1.1033 0.41534
Residuals    4 8.3836  2.0959
Lack of fit  2 8.2969  4.1485 95.7335 0.01034
Pure error   2 0.0867  0.0433
Direction of steepest ascent (at radius 1):
       x1        x2
0.8137335 0.5812382
Corresponding increment in original units:
    Time     Temp
4.068667 2.906191
```

Note that the summary includes a lack-of-fit test, and it is significant. We can try adding two-way interactions to see if it helps:

```
R> CR.rsm1.5 = update(CR.rsm1, . ~ . + TWI(x1, x2))
R> summary(CR.rsm1.5)

Call:
rsm(formula = Yield ~ FO(x1, x2) + TWI(x1, x2), data = CR, subset = 1:7)
Residuals:
      1       2       3       4       5       6       7
-0.9393 -0.9393 -0.9393 -0.9393  1.0857  1.4857  1.1857
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  82.8143     0.6295 131.560 9.68e-07 ***
x1            0.8750     0.8327   1.051    0.371
x2            0.6250     0.8327   0.751    0.507
x1:x2         0.1250     0.8327   0.150    0.890
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 1.665 on 3 degrees of freedom
Multiple R-squared: 0.3603,       Adjusted R-squared: -0.2793
F-statistic: 0.5633 on 3 and 3 DF,  p-value: 0.6755
Analysis of Variance Table
Response: Yield
            Df Sum Sq Mean Sq  F value   Pr(>F)
FO(x1, x2)   2 4.6250  2.3125   0.8337 0.515302
TWI(x1, x2)  1 0.0625  0.0625   0.0225 0.890202
Residuals    3 8.3211  2.7737
Lack of fit  1 8.2344  8.2344 190.0247 0.005221
Pure error   2 0.0867  0.0433
Stationary point of response surface:
x1 x2
```

```
-5 -7
Stationary point in original units:
Time Temp
  60  140
Eigenanalysis:
$values
[1]  0.0625 -0.0625
$vectors
          [,1]       [,2]
[1,] 0.7071068 -0.7071068
[2,] 0.7071068  0.7071068
```

The lack of fit is still significant. Note that the `summary` output now shows a canonical analysis rather than the direction of steepest ascent, as the response surface now has second-order terms.

2.2 Analysis of combined blocks

The lack-of-fit results motivate us to collect additional runs at "star" points, plus some additional center points; these are the second block. In coded units, the data are

```
R> CR[8:14, ]

       x1     x2 Block Yield
8   0.000  0.000    B2  79.7
9   0.000  0.000    B2  79.8
10  0.000  0.000    B2  79.5
11  1.414  0.000    B2  78.4
12 -1.414  0.000    B2  75.6
13  0.000  1.414    B2  78.5
14  0.000 -1.414    B2  77.0
Variable codings ...
x1 ~ (Time - 85)/5
x2 ~ (Temp - 175)/5
```

The choice of $\alpha = \sqrt{2}$ provides for rotatability, and the blocks are orthogonal as well. To do the analysis of the combined data, we should account for the block effect. We could fit a full second-order model by including `FO`, `TWI`, and `PQ` terms, but this is more easily done using `SO` which generates all three sets of variables:

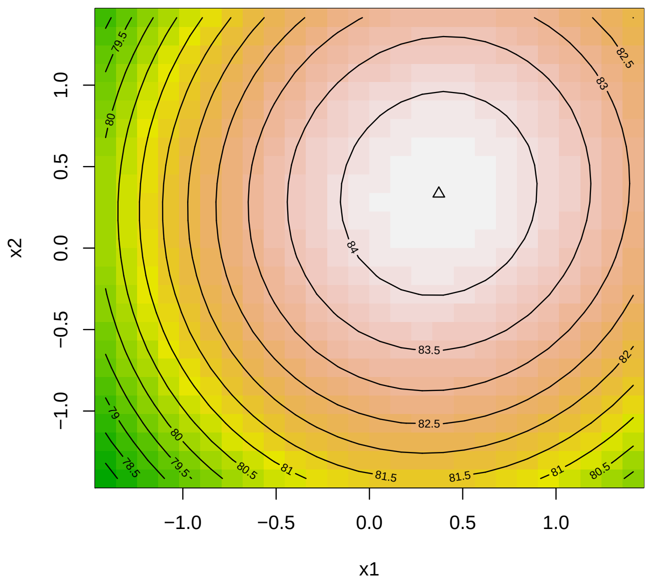
```
R> CR.rsm2 = rsm (Yield ~ Block + SO(x1, x2), data = CR)
R> summary(CR.rsm2)

Call:
rsm(formula = Yield ~ Block + SO(x1, x2), data = CR)
Residuals:
     Min       1Q   Median       3Q      Max
-0.19543 -0.09369  0.02157  0.06153  0.20457
Coefficients:
            Estimate Std. Error  t value Pr(>|t|)
```

```
(Intercept) 84.09543    0.07963 1056.067  < 2e-16 ***
BlockB2     -4.45753    0.08723  -51.103 2.88e-10 ***
x1           0.93254    0.05770   16.162 8.44e-07 ***
x2           0.57771    0.05770   10.013 2.12e-05 ***
x1:x2        0.12500    0.08159    1.532    0.169
x1^2        -1.30856    0.06006  -21.786 1.08e-07 ***
x2^2        -0.93344    0.06006  -15.541 1.10e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 0.1632 on 7 degrees of freedom
Multiple R-squared: 0.9981,        Adjusted R-squared: 0.9964
F-statistic: 607.2 on 6 and 7 DF,  p-value: 3.811e-09
Analysis of Variance Table
Response: Yield
            Df Sum Sq Mean Sq   F value    Pr(>F)
Block        1 69.531  69.531 2611.0950 2.879e-10
FO(x1, x2)   2  9.626   4.813  180.7341 9.450e-07
TWI(x1, x2)  1  0.063   0.063    2.3470    0.1694
PQ(x1, x2)   2 17.791   8.896  334.0539 1.135e-07
Residuals    7  0.186   0.027
Lack of fit  3  0.053   0.018    0.5307    0.6851
Pure error   4  0.133   0.033
Stationary point of response surface:
       x1        x2
0.3722954 0.3343802
Stationary point in original units:
     Time      Temp
 86.86148 176.67190
Eigenanalysis:
$values
[1] -0.9233027 -1.3186949
$vectors
           [,1]       [,2]
[1,] -0.1601375 -0.9870947
[2,] -0.9870947  0.1601375
```

This model fits well. The canonical analysis reveals that the stationary point is near the center of the experiment and that both eigenvalues are negative. This indicates that the fitted surface has a maximum at Time ≈ 86.9, Temp ≈ 176.7. We may visualize the response surface using the `lm` method for `contour`, provided with this package:

```
R> contour (CR.rsm2, list(x1=NULL, x2=NULL))
R> points (.372, .334, pch = 2)
```



3 Helicopter example

The provided dataset `heli` is presented in Table 12.5 of Box, Hunter, and Hunter (2005). It is also a central composite design in two blocks. There are four variables and 30 observations altogether. This is a `coded.data` object already; here are a few observations:

```
R> heli[1:4, ]

  block x1 x2 x3 x4 ave log100s
1     1 -1 -1 -1 -1 367      72
2     1  1 -1 -1 -1 369      72
3     1 -1  1 -1 -1 374      74
4     1  1  1 -1 -1 370      79
Variable codings ...
x1 ~ (A - 12.4)/0.6
x2 ~ (R - 2.52)/0.26
x3 ~ (W - 1.25)/0.25
x4 ~ (L - 2)/0.5
```

The response variable `ave` is the average flight time (in csec.) of four test runs each of paper helicopters made with different wing areas W, wing-length ratios R, body widths W, and body lengths L. The goal is to maximize flight time.

Like the Chemical Reaction data, the first block was analyzed first and then the star points were added. We'll skip the first part and go straight to the second-order analysis.

```
R> heli.rsm = rsm(ave ~ block + SO(x1, x2, x3, x4), data=heli)
R> summary(heli.rsm)
```

```
Call:
rsm(formula = ave ~ block + SO(x1, x2, x3, x4), data = heli)
Residuals:
   Min     1Q Median     3Q    Max
-3.850 -1.579 -0.175  1.925  4.200
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 372.80000    1.50638 247.481  < 2e-16 ***
block2       -2.95000    1.20779  -2.442 0.028452 *
x1           -0.08333    0.63656  -0.131 0.897707
x2            5.08333    0.63656   7.986 1.40e-06 ***
x3            0.25000    0.63656   0.393 0.700429
x4           -6.08333    0.63656  -9.557 1.63e-07 ***
x1:x2        -2.87500    0.77962  -3.688 0.002436 **
x1:x3        -3.75000    0.77962  -4.810 0.000277 ***
x1:x4         4.37500    0.77962   5.612 6.41e-05 ***
x2:x3         4.62500    0.77962   5.932 3.66e-05 ***
x2:x4        -1.50000    0.77962  -1.924 0.074926 .
x3:x4        -2.12500    0.77962  -2.726 0.016410 *
x1^2         -2.03750    0.60389  -3.374 0.004542 **
x2^2         -1.66250    0.60389  -2.753 0.015554 *
x3^2         -2.53750    0.60389  -4.202 0.000887 ***
x4^2         -0.16250    0.60389  -0.269 0.791788
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 3.118 on 14 degrees of freedom
Multiple R-squared: 0.9555,       Adjusted R-squared: 0.9078
F-statistic: 20.04 on 15 and 14 DF,  p-value: 6.54e-07
Analysis of Variance Table
Response: ave
                    Df  Sum Sq Mean Sq F value    Pr(>F)
block                1   16.81   16.81  1.7281  0.209786
FO(x1, x2, x3, x4)   4 1510.00  377.50 38.8175 1.965e-07
TWI(x1, x2, x3, x4)  6 1114.00  185.67 19.0917 5.355e-06
PQ(x1, x2, x3, x4)   4  282.54   70.64  7.2634  0.002201
Residuals           14  136.15    9.72
Lack of fit         10  125.40   12.54  4.6660  0.075500
Pure error           4   10.75    2.69
Stationary point of response surface:
        x1         x2         x3         x4
 0.8607107 -0.3307115 -0.8394866 -0.1161465
Stationary point in original units:
        A         R         W         L
12.916426  2.434015  1.040128  1.941927
Eigenanalysis:
$values
[1]  3.258222 -1.198324 -3.807935 -4.651963
$vectors
```

```
           [,1]       [,2]       [,3]        [,4]
[1,]  0.5177048 0.04099358  0.7608371 -0.38913772
[2,] -0.4504231 0.58176202  0.5056034  0.45059647
[3,] -0.4517232 0.37582195 -0.1219894 -0.79988915
[4,]  0.5701289 0.72015994 -0.3880860  0.07557783
```

This time, the situation is more complicated. Since the eigenvalues are of mixed sign, we have a saddle point. Here we obtain contour plots of each pair of variables, holding the other two fixed at their stationary values. The plots are shown in Figure 1.

```
R> par (mfrow = c(2, 3))
R> contour(heli.rsm, list(x1=NULL, x2=NULL, x3=-.84, x4=-.12))
R> points(.86, -.33, pch=2)
R> contour(heli.rsm, list(x1=NULL, x3=NULL, x2=-.33, x4=-.12))
R> points(.86, -.84, pch=2)
R> contour(heli.rsm, list(x1=NULL, x4=NULL, x2=-.33, x3=-.84))
R> points(.86, -.12, pch=2)
R> contour(heli.rsm, list(x2=NULL, x3=NULL, x1= .86, x4=-.12))
R> points(-.33, -.84, pch=2)
R> contour(heli.rsm, list(x2=NULL, x4=NULL, x1= .86, x3=-.84))
```

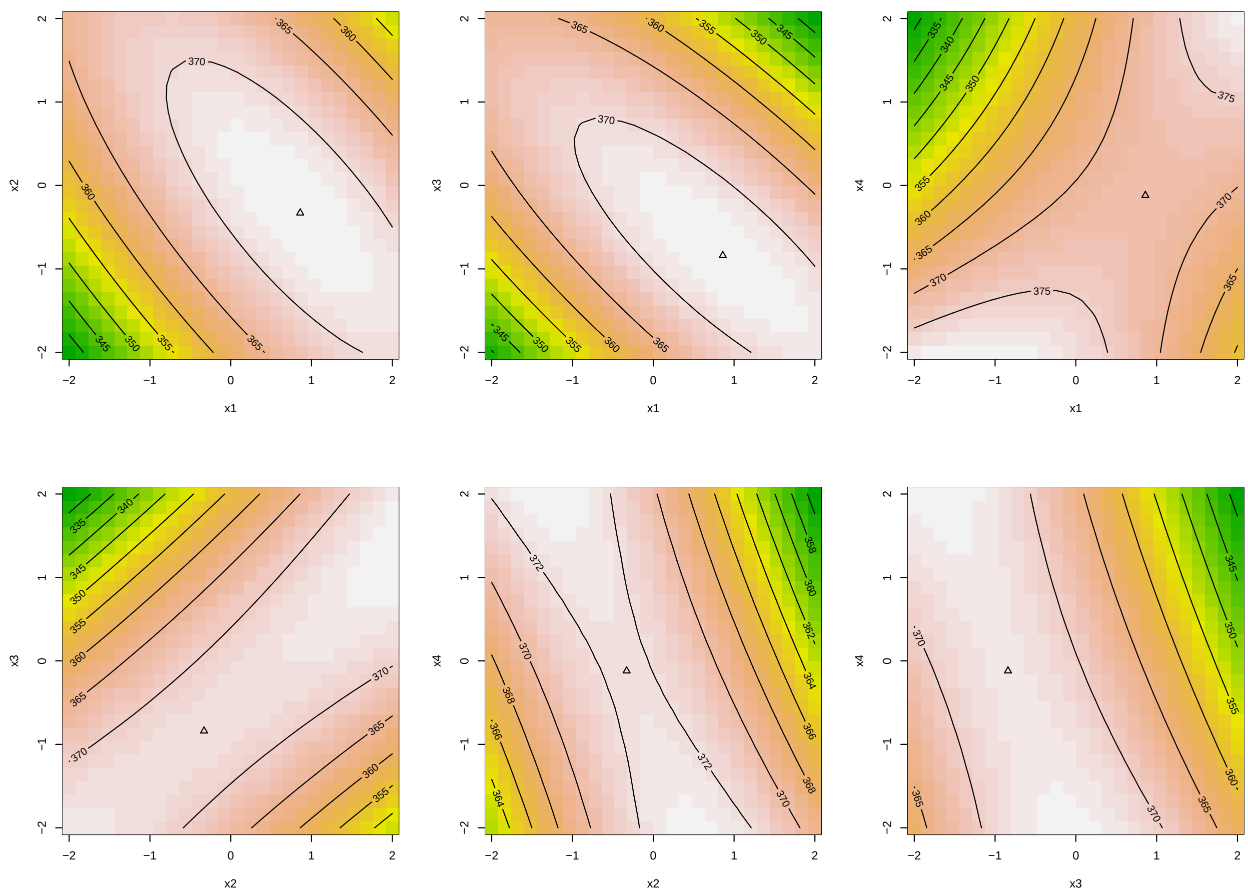


Figure 1: Contour plots for `heli` data.

```
R> points(-.33, -.12, pch=2)
R> contour(heli.rsm, list(x3=NULL, x4=NULL, x1= .86, x2=-.33))
R> points(-.84, -.12, pch=2)
```

Since we have not found a maximum, our next step might be to experiment in the direction of steepest ascent:

```
R> steepest (heli.rsm)

Path of steepest ascent from ridge analysis:
   dist     x1    x2    x3     x4 |       A       R       W      L |    yhat
1   0.0  0.000 0.000 0.000  0.000 | 12.4000 2.52000 1.25000 2.0000 | 372.800
2   0.5 -0.127 0.288 0.116 -0.371 | 12.3238 2.59488 1.27900 1.8145 | 377.106
3   1.0 -0.351 0.538 0.312 -0.700 | 12.1894 2.65988 1.32800 1.6500 | 382.675
4   1.5 -0.595 0.775 0.526 -1.009 | 12.0430 2.72150 1.38150 1.4955 | 389.783
5   2.0 -0.846 1.007 0.745 -1.309 | 11.8924 2.78182 1.43625 1.3455 | 398.485
6   2.5 -1.101 1.237 0.966 -1.605 | 11.7394 2.84162 1.49150 1.1975 | 408.819
7   3.0 -1.356 1.465 1.189 -1.897 | 11.5864 2.90090 1.54725 1.0515 | 420.740
8   3.5 -1.613 1.693 1.413 -2.188 | 11.4322 2.96018 1.60325 0.9060 | 434.322
9   4.0 -1.870 1.920 1.637 -2.477 | 11.2780 3.01920 1.65925 0.7615 | 449.497
10  4.5 -2.127 2.147 1.862 -2.766 | 11.1238 3.07822 1.71550 0.6170 | 466.323
11  5.0 -2.385 2.373 2.086 -3.054 | 10.9690 3.13698 1.77150 0.4730 | 484.750
```

This gives a path that starts at the *origin* in the coded variables. An alternative is to explore along a path through the *stationary point*. The function `canonical.path`, by default, returns the path of steepest ascent each direction from the stationary point. This path is linear.

```
R> canonical.path(heli.rsm)

   dist     x1     x2     x3     x4 |       A       R       W      L |    yhat
1  -5.0 -1.728  1.921  1.419 -2.967 | 11.3632 3.01946 1.60475 0.5165 | 453.627
2  -4.5 -1.469  1.696  1.193 -2.682 | 11.5186 2.96096 1.54825 0.6590 | 438.150
3  -4.0 -1.210  1.471  0.967 -2.397 | 11.6740 2.90246 1.49175 0.8015 | 424.302
4  -3.5 -0.951  1.246  0.742 -2.112 | 11.8294 2.84396 1.43550 0.9440 | 412.094
5  -3.0 -0.692  1.021  0.516 -1.827 | 11.9848 2.78546 1.37900 1.0865 | 401.504
6  -2.5 -0.434  0.795  0.290 -1.541 | 12.1396 2.72670 1.32250 1.2295 | 392.534
7  -2.0 -0.175  0.570  0.064 -1.256 | 12.2950 2.66820 1.26600 1.3720 | 385.203
8  -1.5  0.084  0.345 -0.162 -0.971 | 12.4504 2.60970 1.20950 1.5145 | 379.502
9  -1.0  0.343  0.120 -0.388 -0.686 | 12.6058 2.55120 1.15300 1.6570 | 375.429
10 -0.5  0.602 -0.105 -0.614 -0.401 | 12.7612 2.49270 1.09650 1.7995 | 372.986
11  0.0  0.861 -0.331 -0.839 -0.116 | 12.9166 2.43394 1.04025 1.9420 | 372.172
12  0.5  1.120 -0.556 -1.065  0.169 | 13.0720 2.37544 0.98375 2.0845 | 372.987
13  1.0  1.378 -0.781 -1.291  0.454 | 13.2268 2.31694 0.92725 2.2270 | 375.428
14  1.5  1.637 -1.006 -1.517  0.739 | 13.3822 2.25844 0.87075 2.3695 | 379.499
15  2.0  1.896 -1.232 -1.743  1.024 | 13.5376 2.19968 0.81425 2.5120 | 385.206
16  2.5  2.155 -1.457 -1.969  1.309 | 13.6930 2.14118 0.75775 2.6545 | 392.538
17  3.0  2.414 -1.682 -2.195  1.594 | 13.8484 2.08268 0.70125 2.7970 | 401.498
18  3.5  2.673 -1.907 -2.421  1.879 | 14.0038 2.02418 0.64475 2.9395 | 412.088
19  4.0  2.932 -2.132 -2.646  2.164 | 14.1592 1.96568 0.58850 3.0820 | 424.295
20  4.5  3.190 -2.358 -2.872  2.449 | 14.3140 1.90692 0.53200 3.2245 | 438.140
21  5.0  3.449 -2.583 -3.098  2.734 | 14.4694 1.84842 0.47550 3.3670 | 453.615
```

These paths match fairly closely in one direction as we proceed outward. For example, the point at distance -5 from `canonical.path` is similar to the one at distance 4 from `steepest`.

4 Miscellaneous notes and examples

4.1 Coded data

Use `coded.data` as shown in the Chemical reactor example to convert a dataset that has its predictors in raw units. If the dataset is already in coded units, you may embed the coding information using `as.coded.data`:

```
R> dat = expand.grid(t = c(-1,1), w = -1:1)
R> dat = as.coded.data(dat, t ~ (Thickness - 3.5) / .5,  w ~ (Width - 12)/2)
R> dat
```

```
   t  w
1 -1 -1
2  1 -1
3 -1  0
4  1  0
5 -1  1
6  1  1
Variable codings ...
t ~ (Thickness - 3.5)/0.5
w ~ (Width - 12)/2
```

```
R> decode.data(dat)
```

```
  Thickness Width
1         3    10
2         4    10
3         3    12
4         4    12
5         3    14
6         4    14
```

```
R> code2val(c(t = -.5, w = .25),  attr(dat, "codings"))
```

```
Thickness     Width
     3.25     12.50
```

4.2 Contour plots

The `contour` method provided by this package works for any `lm` object, not just response surfaces. By default, it overlays the contour plot on an image plot using terrain colors. Arguments provide for the image portion to be disabled or the colors changed if desired.

To make `contour` work, it was necessary to obtain the data used by a `lm` object. The standard function `get_all_vars` does not make it very easy, and `model.frame` incorporates transformations and expands polynomials and factors. The provided function `model.data` makes it very easy to obtain just the variables included in the model formula. For example, following the first-order model for the chemical reactor example,

```
R> model.data (CR.rsm1)

  Yield x1 x2
1  80.5 -1 -1
2  81.5 -1  1
3  82.0  1 -1
4  83.5  1  1
5  83.9  0  0
6  84.3  0  0
7  84.0  0  0
```

Note that only the observations in the `subset` argument are included.

References

Box, G.E.P., Hunter, J.S., and Hunter, W.G. (2005), *Statistics for Experimenters: Design, Innovation, and Discovery* (2nd ed.), New York: Wiley-Interscience.

Myers, R. H. and Montgomery, D. C. (2002), *Response Surface Mehodology: Process and Product Optimization Using Designed Experiments* (2nd ed.), New York: Wiley-Interscience.

Contact information

Russell V. Lenth
Department of Sttaistics
The University of Iowa
Iowa City, IA, USA 52242
`russell-lenth@uiowa.edu`