```
> data <- read.csv("Conversion.csv");data
```

These are data taken from the examples in the Design-Expert manual. We are making a product that should have an activity of 63; we could accept the range 60 to 66, but 63 is more desirable. There are three process variables: time (minutes), temperature (degrees C), and catalyst (percent). When we do our experiment, we have two responses: the conversion factor (essentially the percent yield) and the activity.

Our goal is to get process variables so that we hit an activity of 63 (or very close) and maximize the conversion. In addition, we want to operate within the "cube" part of the experimental region.

```
    Time Temperature Catalyst Conversion Activity
1  45.00       85.00     2.50         75     60.4
2  45.00       85.00     2.50         83     60.6
3  45.00       85.00     2.50         76     59.1
4  45.00       85.00     2.50         81     59.2
5  45.00       85.00     2.50         91     58.9
6  45.00       85.00     2.50         80     60.8
7  53.41       85.00     2.50         79     65.9
8  36.59       85.00     2.50         76     53.6
9  45.00       85.00     1.66         55     57.4
10 45.00       85.00     3.34         81     63.2
11 45.00       93.41     2.50         97     60.7
12 45.00       76.59     2.50         85     60.0
13 40.00       80.00     2.00         74     53.2
14 40.00       90.00     3.00         66     59.8
15 50.00       90.00     2.00         70     62.6
16 40.00       90.00     2.00         88     53.4
17 50.00       90.00     3.00         97     67.8
18 50.00       80.00     3.00         90     67.9
19 40.00       80.00     3.00         71     57.3
20 50.00       80.00     2.00         51     62.9
```

```
> CD <- coded.data(data,cTime~(Time-45)/5,cTemp~(Temperature-85)/5,
  cCat~(Catalyst-2.5)/.5);CD
```

This was a central composite design with center at (45, 85, 2.5) and steps of (5, 5, and .5). So let's recode the variables.

```
    cTime  cTemp  cCat Conversion Activity
1   0.000  0.000  0.00         75     60.4
2   0.000  0.000  0.00         83     60.6
3   0.000  0.000  0.00         76     59.1
4   0.000  0.000  0.00         81     59.2
5   0.000  0.000  0.00         91     58.9
6   0.000  0.000  0.00         80     60.8
7   1.682  0.000  0.00         79     65.9
8  -1.682  0.000  0.00         76     53.6
9   0.000  0.000 -1.68         55     57.4
10  0.000  0.000  1.68         81     63.2
11  0.000  1.682  0.00         97     60.7
12  0.000 -1.682  0.00         85     60.0
13 -1.000 -1.000 -1.00         74     53.2
14 -1.000  1.000  1.00         66     59.8
15  1.000  1.000 -1.00         70     62.6
16 -1.000  1.000 -1.00         88     53.4
```

```
17  1.000  1.000  1.00         97     67.8
18  1.000 -1.000  1.00         90     67.9
19 -1.000 -1.000  1.00         71     57.3
20  1.000 -1.000 -1.00         51     62.9

Variable codings ...
cTime ~ (Time - 45)/5
cTemp ~ (Temperature - 85)/5
cCat ~ (Catalyst - 2.5)/0.5
```

> **fit1<-rsm(Conversion~SO(cTime,cTemp,cCat),data=CD)**

Let's fit a second order model to the conversion (yield) variable.

> **plot(fit1);boxCox(fit1)**

Not shown, but things look OK with the residuals, etc.

> **summary(fit1)**

Looking things over, there is no (significant) lack of fit for this model, and we see that there are highly significant effects at all orders. Temperature and catalyst seem to behave in a second order fashion. Time does not seem to do much by itself, but it interacts (a lot) with catalyst.

The stationary point is more or less within the region of experimentation, but the eigen analysis shows that it is a saddle point, not a maximum or minimum.

```
Call:
rsm(formula = Conversion ~ SO(cTime, cTemp, cCat), data = CD)

Residuals:
   Min     1Q Median     3Q    Max
-6.092 -1.452 -0.289  1.474  9.908

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   81.092      1.923  42.163 1.35e-12 ***
cTime          1.028      1.276   0.806  0.43902
cTemp          4.040      1.276   3.166  0.01005 *
cCat           6.206      1.277   4.861  0.00066 ***
cTime:cTemp    2.125      1.667   1.275  0.23129
cTime:cCat    11.375      1.667   6.823 4.61e-05 ***
cTemp:cCat    -3.875      1.667  -2.324  0.04247 *
cTime^2       -1.831      1.242  -1.474  0.17115
cTemp^2        2.941      1.242   2.368  0.03942 *
cCat^2        -5.203      1.244  -4.181  0.00188 **
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 4.716 on 10 degrees of freedom
Multiple R-squared:  0.92,Adjusted R-squared: 0.8479
F-statistic: 12.77 on 9 and 10 DF,  p-value: 0.0002207

Analysis of Variance Table
```

```
Response: Conversion
                        Df  Sum Sq Mean Sq F value   Pr(>F)
FO(cTime, cTemp, cCat)   3  762.93  254.31 11.4357 0.001428
TWI(cTime, cTemp, cCat)  3 1191.37  397.12 17.8576 0.000243
PQ(cTime, cTemp, cCat)   3  601.51  200.50  9.0160 0.003414
Residuals               10  222.38   22.24
Lack of fit              5   56.38   11.28  0.3397 0.869479
Pure error               5  166.00   33.20

Stationary point of response surface:
     cTime      cTemp       cCat
-1.0179845 -0.5294920 -0.3192329

Stationary point in original units:
       Time Temperature    Catalyst
  39.910077   82.352540    2.340384

Eigenanalysis:
$values
[1]  3.408437  2.322758 -9.824322

$vectors
           [,1]      [,2]       [,3]
[1,]  0.1380685 0.7982920  0.5862312
[2,] -0.9428308 0.2872127 -0.1690534
[3,]  0.3033270 0.5293758 -0.7923093
```

> **fit2<-rsm(Activity~SO(cTime,cTemp,cCat),data=CD)**

Now let's try fitting activity.

> **plot(fit2);boxCox(fit2)**

Not shown, but things are OK with this model too.

> **summary(fit2)**

The main thing we see is that the first order terms are highly significant, but the mixed and quadratic terms are not.

```
Call:
rsm(formula = Activity ~ SO(cTime, cTemp, cCat), data = CD)

Residuals:
    Min      1Q  Median      3Q     Max
-1.2757 -0.6433 -0.1112  0.6254  1.1969

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 59.81833    0.42544 140.603  < 2e-16 ***
cTime        4.26033    0.28226  15.094 3.29e-08 ***
cTemp        0.25460    0.28226   0.902    0.388
cCat         2.23118    0.28240   7.901 1.31e-05 ***
cTime:cTemp -0.38750    0.36881  -1.051    0.318
cTime:cCat  -0.03750    0.36881  -0.102    0.921
```

```
cTemp:cCat   0.31250    0.36881   0.847    0.417
cTime^2      0.06769    0.27472   0.246    0.810
cTemp^2      0.27977    0.27472   1.018    0.333
cCat^2       0.26294    0.27525   0.955    0.362
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 1.043 on 10 degrees of freedom
Multiple R-squared: 0.9672,Adjusted R-squared: 0.9376
F-statistic: 32.74 on 9 and 10 DF,  p-value: 2.955e-06

Analysis of Variance Table

Response: Activity
                       Df Sum Sq Mean Sq F value    Pr(>F)
FO(cTime, cTemp, cCat)  3 316.71 105.571 97.0169 1.079e-07
TWI(cTime, cTemp, cCat) 3   1.99   0.665  0.6107    0.6232
PQ(cTime, cTemp, cCat)  3   1.94   0.645  0.5931    0.6336
Residuals              10  10.88   1.088
Lack of fit             5   7.23   1.446  1.9786    0.2359
Pure error              5   3.65   0.731

Stationary point of response surface:
    cTime     cTemp      cCat
 15.05168  17.57008 -13.61031

Stationary point in original units:
       Time Temperature    Catalyst
 120.258424  172.850398   -4.305155

Eigenanalysis:
$values
[1]  0.48931661  0.18268588 -0.06160297

$vectors
           [,1]       [,2]       [,3]
[1,]  0.3691679  0.4710760  0.8011258
[2,] -0.7502855 -0.3576299  0.5560328
[3,] -0.5484402  0.8063425 -0.2214160
```

> **fit2b<-rsm(Activity~FO(cTime,cTemp,cCat),data=CD)**

Refit with just first order terms.

> **summary(fit2b)**

Still no lack of fit. Coefficients are the same as what we had before (except for intercept).

```
Call:
rsm(formula = Activity ~ FO(cTime, cTemp, cCat), data = CD)

Residuals:
    Min      1Q  Median      3Q     Max
```

```
-1.5009 -0.6843  0.1231  0.6285  1.4281

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  60.2350     0.2151 279.977  < 2e-16 ***
cTime         4.2603     0.2603  16.364 2.06e-11 ***
cTemp         0.2546     0.2603   0.978    0.343
cCat          2.2312     0.2605   8.566 2.26e-07 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.9621 on 16 degrees of freedom
Multiple R-squared: 0.9553,Adjusted R-squared: 0.9469
F-statistic:   114 on 3 and 16 DF,  p-value: 5.193e-11

Analysis of Variance Table

Response: Activity
                       Df Sum Sq Mean Sq  F value    Pr(>F)
FO(cTime, cTemp, cCat)  3 316.71 105.571 114.0412 5.193e-11
Residuals              16  14.81   0.926
Lack of fit            11  11.16   1.014   1.3883    0.3782
Pure error              5   3.65   0.731

Direction of steepest ascent (at radius 1):
     cTime      cTemp       cCat
0.88462865 0.05286616 0.46328968

Corresponding increment in original units:
       Time Temperature    Catalyst
  4.4231432   0.2643308   0.2316448
```

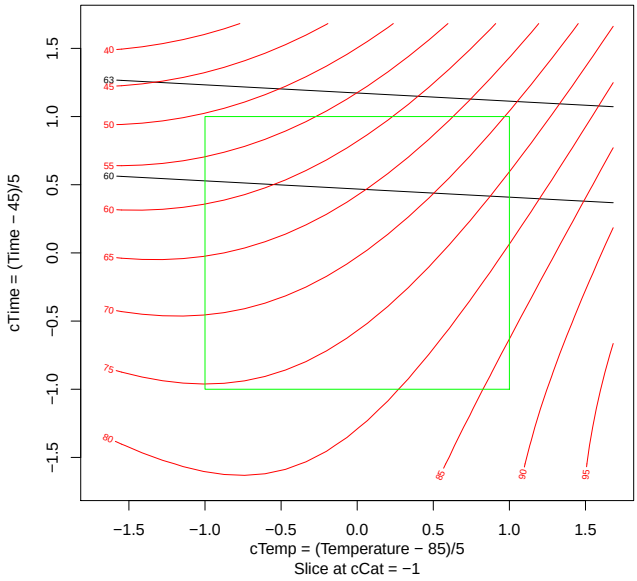
```
> #
```

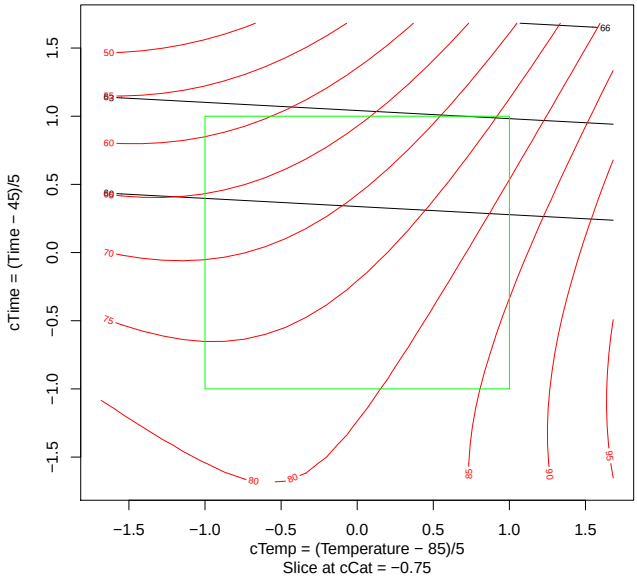
We have our models, now we work on the experimental goal. We are going to approach this graphically. For each level of cCat from -1 to 1 by increments of .25 we will:

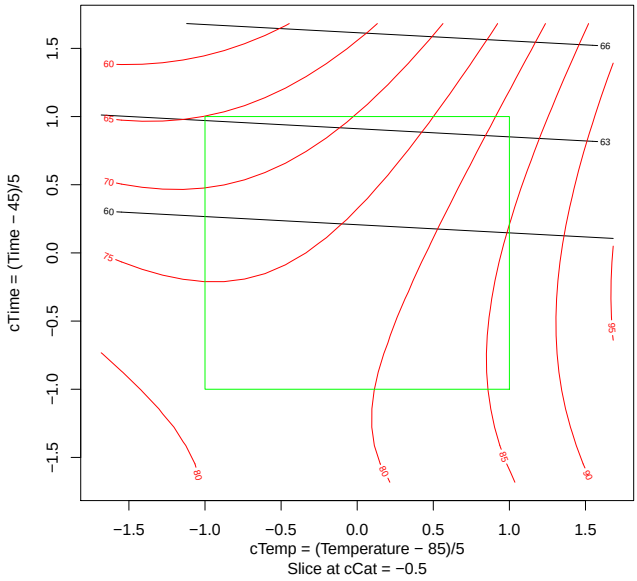
1. Make a contour plot of activity with contours at levels 60, 63, and 66 (the minimum, desired, and maximum levels);
2. Overlay a contour plot of conversion (red, to make it visible);
3. Overlay a box (in green) to show the experimental area.

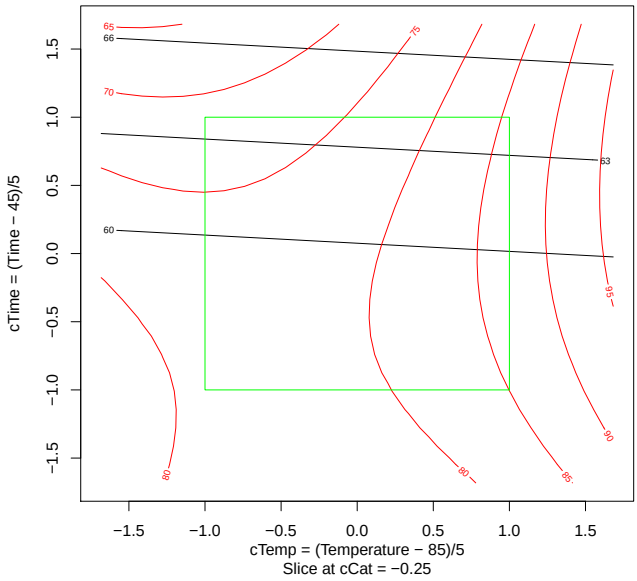
The goal is to walk through the images and find where we want to operate the system. This will involve some tradeoff between being as close as possible to 63 for activity and having the highest conversion.

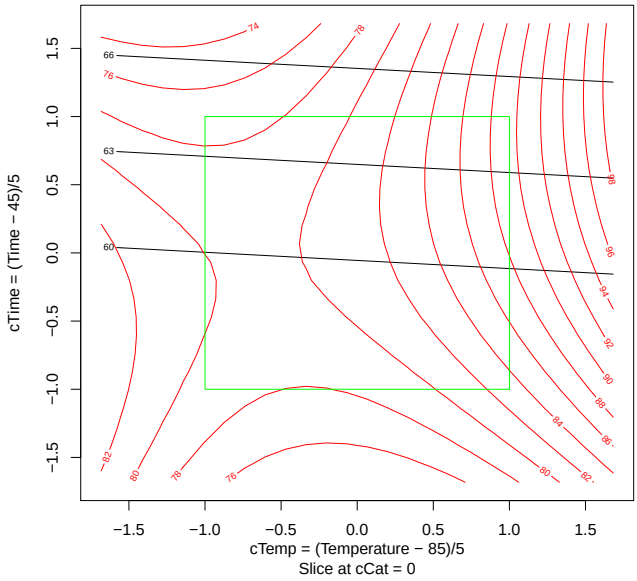
```
> for(cc in seq(-1,1,.25)) {
    contour(fit2b,cTime~cTemp,at=list(cCat=cc),levels=c(60,63,66))
    contour(fit1,cTime~cTemp,at=list(cCat=cc),add=TRUE,col="red")
    lines(c(1,1,-1,-1,1),c(-1,1,1,-1,-1),col="green")
}
```

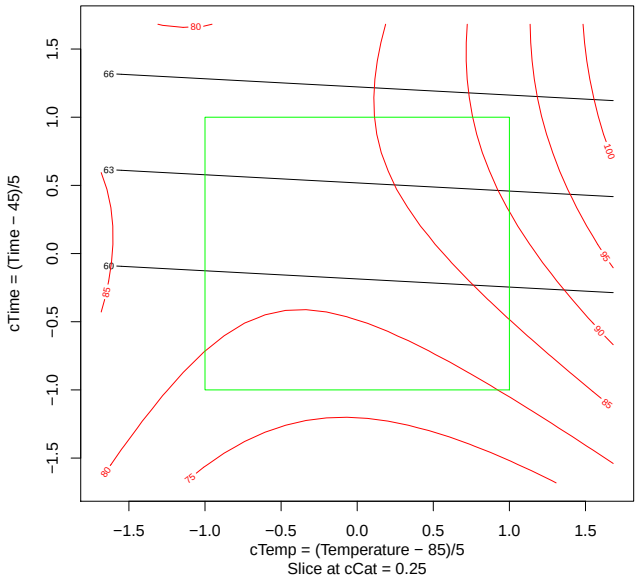

cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = −1

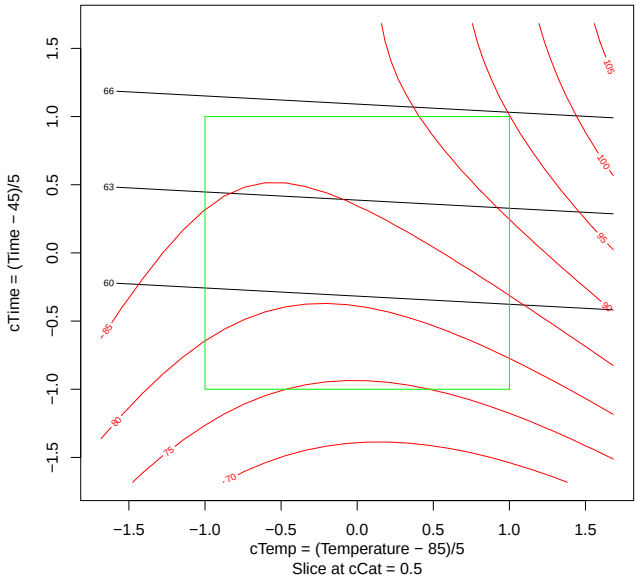

cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = −0.75

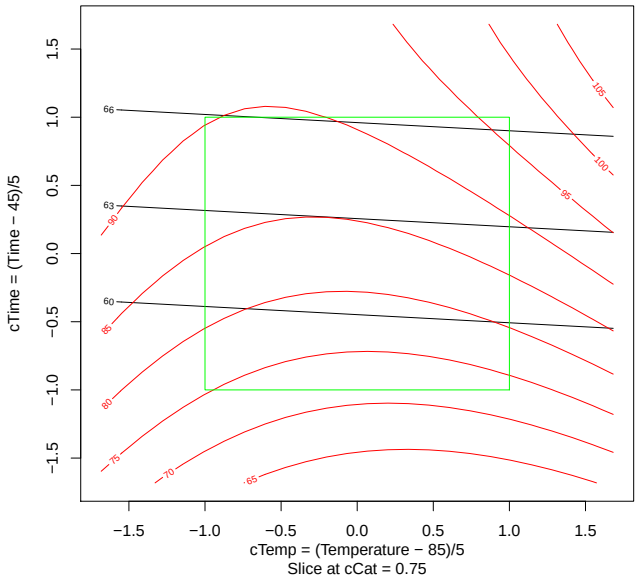

cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = −0.5
66
63
60
60
65
70
75
80
85
90
95

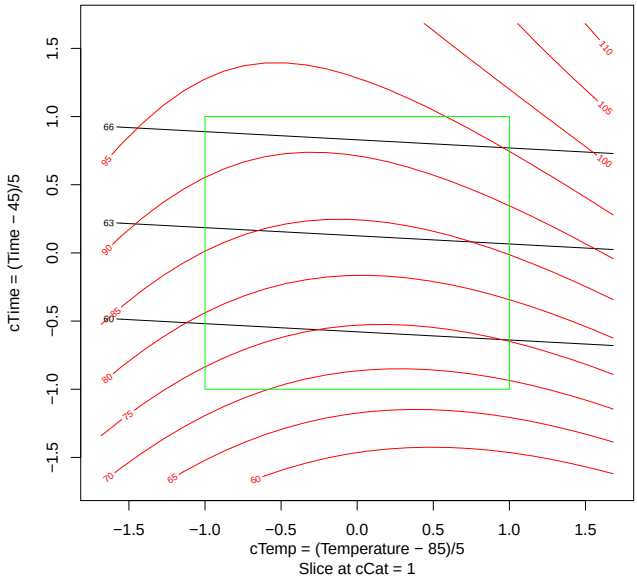

cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = −0.25
65
66
70
63
60
75
80
85
90
95


cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = 0


cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = 0.25


cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = 0.5
66
63
60
105
100
95
90
85
80
75
70


cTime = (Time − 45)/5
cTemp = (Temperature − 85)/5
Slice at cCat = 0.75
66
63
60
105
100
95
90
85
80
75
70
65




```
> #
```

We can get 63 activity and conversion of 90% or better when cCat is about .25 to .5. However, we are right on the border for Temperature. Alternatively, if we want a high conversion with any activity from 60 to 66, then we can get just a bit over 95% with cCat at .75; again, we're on the border for temperature.