SAS Macro for checking the rotatability of Response Surface Design

Eldho Varghese[1*], Hemavathi M., Ashutosh Dalal, Arpan Bhowmik and Seema Jaggi
ICAR-Indian Agricultural Statistics Research Institute, New Delhi
[1]ICAR-Central Marine Fisheries Research Institute, Kochi
Email: eldho.varghese@icar.gov.in

Response Surface Designs (RSDs) are widely used in process or product optimization studies to explore the input-response relationship. A response surface design is said to be rotatable if it has constant prediction variance, $Var[\hat{y}(x)]$ for all points which are at equal distance from the design centre. To ensure the orthogonality among the parameter estimates and constancy in the variance of the estimated responses at points which are equidistant from the design centre, x_{iu}'s (designs variables) must satisfy certain Orthogonality-Rotatability conditions (Hemavathi et al., 2022) depending on the order of the polynomial used for the approximation of input-response relationship. When rotatability is obtained, the expression of variance of the estimated response is a function of $\sum_{i=1}^{v} x_{i0}^2 = d^2$. Hence, the variance of estimated response at all points which are equidistant from the centre of the design will be the same.

Here, a macro has been developed for assessing the rotatbility of a given response surface design under three different model set up viz., first order model, second order model and third order model. User need to enter the order of the polynomial model and the design to check the rotatability with respect to a given polynomial model.

```
%let order=2; /* User need to enter the order of the model: 1=
FIRST order, 2=SECOND order and 3=THIRD order*/
proc iml;
/* Enter design without the coefficient for the intercept term*/
*a={-1    -1   -1   ,
-1   -1   1    ,
-1   1    -1   ,
-1   1    1    ,
1    -1   -1   ,
1    -1   1    ,
1    1    -1   ,
1    1    1
}; /*Entered design is an example for First order design for
v=3*/

a={-1     -1   -1   -1   ,
1    -1   -1   -1   ,
-1   1    -1   -1   ,
```

```
1    1    -1   -1   ,
-1   -1   1    -1   ,
1    -1   1    -1   ,
-1   1    1    -1   ,
1    1    1    -1   ,
-1   -1   -1   1    ,
1    -1   -1   1    ,
-1   1    -1   1    ,
1    1    -1   1    ,
-1   -1   1    1    ,
1    -1   1    1    ,
-1   1    1    1    ,
1    1    1    1    ,
2    0    0    0    ,
-2   0    0    0    ,
0    2    0    0    ,
0    -2   0    0    ,
0    0    2    0    ,
0    0    -2   0    ,
0    0    0    2    ,
0    0    0    -2   ,
0   0   0   0,
0   0   0   0,
0   0   0   0,
0   0   0   0
}; /*Entered design is an example for Second order design for
v=4 (few centre points added to the design to ensure non-
singularity)*/

*a={-1    -1   -1   -1   ,
1    -1   -1   -1   ,
-1   1    -1   -1   ,
1    1    -1   -1   ,
-1   -1   1    -1   ,
1    -1   1    -1   ,
-1   1    1    -1   ,
1    1    1    -1   ,
-1   -1   -1   1    ,
1    -1   -1   1    ,
-1   1    -1   1    ,
1    1    -1   1    ,
```

```
-1   -1   1    1    ,
1    -1   1    1    ,
-1   1    1    1    ,
1    1    1    1    ,
2    0    0    0    ,
-2   0    0    0    ,
0    2    0    0    ,
0    -2   0    0    ,
0    0    2    0    ,
0    0    -2   0    ,
0    0    0    2    ,
0    0    0    -2   ,
1.200919009    1.200919009    0.256303  -0.256303 ,
1.200919009    1.200919009    0.256303  0.256303  ,
1.200919009    1.200919009    -0.256303 -0.25630363    ,
1.200919009    1.200919009    -0.25630363    0.25630363     ,
1.200919009    -1.200919009   0.256303  -0.256303 ,
1.200919009    -1.200919009   0.256303  0.256303  ,
1.200919  -1.200919 -0.256303 -0.256303 ,
1.200919  -1.200919 -0.256303 0.256303  ,
-1.200919 1.200919  0.256303  -0.256303 ,
-1.200919 1.200919  0.256303  0.256303  ,
-1.200919 1.200919  -0.256303 -0.256303 ,
-1.200919 1.200919  -0.256303 0.256303  ,
-1.200919 -1.200919 0.256303  -0.256303 ,
-1.200919 -1.200919 0.256303  0.256303  ,
-1.200919 -1.200919 -0.256303 -0.256303 ,
-1.200919 -1.200919 -0.256303 0.256303  ,
0.256303  1.200919  1.200919  -0.256303 ,
0.256303  1.200919  1.200919  0.256303  ,
-0.256303 1.200919  1.200919  -0.256303 ,
-0.256303 1.200919  1.200919  0.256303  ,
0.256303  1.200919  -1.200919 -0.256303 ,
0.256303  1.200919  -1.200919 0.256303  ,
-0.256303 1.200919  -1.200919 -0.256303 ,
-0.256303 1.200919  -1.200919 0.256303  ,
0.256303  -1.200919 1.200919  -0.256303 ,
0.256303  -1.200919 1.200919  0.256303  ,
-0.256303 -1.200919 1.200919  -0.256303 ,
-0.256303 -1.200919 1.200919  0.256303  ,
0.256303  -1.200919 -1.200919 -0.256303 ,
```

```
0.256303  -1.200919 -1.200919 0.256303  ,
-0.256303 -1.200919 -1.200919 -0.256303 ,
-0.256303 -1.200919 -1.200919 0.256303  ,
0.256303  -0.256303 1.200919  1.200919  ,
0.256303  0.256303  1.200919  1.200919  ,
-0.256303 -0.256303 1.200919  1.200919  ,
-0.256303 0.256303  1.200919  1.200919  ,
0.256303  -0.256303 1.200919  -1.200919 ,
0.256303  0.256303  1.200919  -1.200919 ,
-0.256303 -0.256303 1.200919  -1.200919 ,
-0.256303 0.256303  1.200919  -1.200919 ,
0.256303  -0.256303 -1.200919 1.200919  ,
0.256303  0.256303  -1.200919 1.200919  ,
-0.256303 -0.256303 -1.200919 1.200919  ,
-0.256303 0.256303  -1.200919 1.200919  ,
0.256303  -0.256303 -1.200919 -1.200919 ,
0.256303  0.256303  -1.200919 -1.200919 ,
-0.256303 -0.256303 -1.200919 -1.200919 ,
-0.256303 0.256303  -1.200919 -1.200919 ,
1.200919  0.256303  -0.256303 1.200919  ,
1.200919  0.256303  0.256303  1.200919  ,
1.200919  -0.256303 -0.256303 1.200919  ,
1.200919  -0.256303 0.256303  1.200919  ,
-1.200919 0.256303  -0.256303 1.200919  ,
-1.200919 0.256303  0.256303  1.200919  ,
-1.200919 -0.256303 -0.256303 1.200919  ,
-1.200919 -0.256303 0.256303  1.200919  ,
1.200919  0.256303  -0.256303 -1.200919 ,
1.200919  0.256303  0.256303  -1.200919 ,
1.200919  -0.256303 -0.256303 -1.200919 ,
1.200919  -0.256303 0.256303  -1.200919 ,
-1.200919 0.256303  -0.256303 -1.200919 ,
-1.200919 0.256303  0.256303  -1.200919 ,
-1.200919 -0.256303 -0.256303 -1.200919 ,
-1.200919 -0.256303 0.256303  -1.200919 ,
1.200919  0.256303  1.200919  -0.256303 ,
1.200919  0.256303  1.200919  0.256303  ,
1.200919  -0.256303 1.200919  -0.256303 ,
1.200919  -0.256303 1.200919  0.256303  ,
1.200919  0.256303  -1.200919 -0.256303 ,
1.200919  0.256303  -1.200919 0.256303  ,
```

```
1.200919  -0.256303 -1.200919 -0.256303 ,
1.200919  -0.256303 -1.200919 0.256303  ,
-1.200919 0.256303  1.200919  -0.256303 ,
-1.200919 0.256303  1.200919  0.256303  ,
-1.200919 -0.256303 1.200919  -0.256303 ,
-1.200919 -0.256303 1.200919  0.256303  ,
-1.200919 0.256303  -1.200919 -0.256303 ,
-1.200919 0.256303  -1.200919 0.256303  ,
-1.200919 -0.256303 -1.200919 -0.256303 ,
-1.200919 -0.256303 -1.200919 0.256303  ,
0.256303  1.200919  -0.256303 1.200919  ,
0.256303  1.200919  0.256303  1.200919  ,
-0.256303 1.200919  -0.256303 1.200919  ,
-0.256303 1.200919  0.256303  1.200919  ,
0.256303  1.200919  -0.256303 -1.200919 ,
0.256303  1.200919  0.256303  -1.200919 ,
-0.256303 1.200919  -0.256303 -1.200919 ,
-0.256303 1.200919  0.256303  -1.200919 ,
0.256303  -1.200919 -0.256303 1.200919  ,
0.256303  -1.200919 0.256303  1.200919  ,
-0.256303 -1.200919 -0.256303 1.200919  ,
-0.256303 -1.200919 0.256303  1.200919  ,
0.256303  -1.200919 -0.256303 -1.200919 ,
0.256303  -1.200919 0.256303  -1.200919 ,
-0.256303 -1.200919 -0.256303 -1.200919 ,
-0.256303 -1.200919 0.256303  -1.200919 ,
-1.736604 0    0    0    ,
1.736604  0    0    0    ,
0    -1.736604 0    0    ,
0    1.736604  0    0    ,
0    0    -1.736604 0    ,
0    0    1.736604  0    ,
0    0    0    -1.736604 ,
0    0    0    1.736604

}; /*Entered design is an example for third order design for v=4
(Gardiner, 1958)*/
one=j(nrow(a),1,1);
aa=a#a;
*print aa;
kkk=allcomb(ncol(a),2);
```

```
dd=j(nrow(a),comb(ncol(a),2),1);
do l = 1 to  comb(ncol(a),2);
do j = 1 to nrow(a);
do m=1 to ncol(kkk);
dd[j,l]=dd[j,l]*a[j,kkk[l,m]];
end;
end;
end;
*print dd; /*2 term cross product*/

kkk1=allcomb(ncol(a),3);
dd1=j(nrow(a),comb(ncol(a),3),1);
do l = 1 to  comb(ncol(a),3);
do j = 1 to nrow(a);
do m=1 to ncol(kkk1);
dd1[j,l]=dd1[j,l]*a[j,kkk1[l,m]];
end;
end;
end;
*print dd1; /*3 term cross product*/
sec=one||aa; /*As per the ordering given by Gardiner (1958)*/
do i=1 to ncol(a);
do j=1 to ncol(sec);
sec1=a[ ,i]#sec[ ,j]; /*As per the ordering given by Gardiner
(1958)*/
sec2=sec2||sec1;
end;
end;
*print sec2; /*multiplication of each variable with sec */
If &order=1 then do;
/*******FIRST ORDER ROTATABILITY*********/
design_first=one||a;
*print design_first;
xx_first=design_first`*design_first;
*print xx_fisrt;
xx_inv_first=inv(xx_first);
*print xx_inv_first;
print "Moment Matrix for first order model";
MomentMatrix_first=xx_first/nrow(a);
print MomentMatrix_first;
var_pred_first=design_first*xx_inv_first*design_first`;
```

```
pred_var_first=vecdiag(var_pred_first);
print "Prediction variance for first order model";
print pred_var_first;
unique_pred_first=unique(round(pred_var_first, 0.0000001));
print "Unique prediction variance for first order model";
print unique_pred_first;
/*****************************************/
end;
if &order=2 then do;
/*******SECOND ORDER ROTATABILITY*********/
design_second=one||a||aa||dd; /*As per the ordering given by
Gardiner (1958)*/
*print design_second;
xx_second=design_second`*design_second;
*print xx_second;
xx_inv_second=inv(xx_second);
*print xx_inv_second;
MomentMatrix_second=xx_second/nrow(a);
print "Moment Matrix for second order model";
print MomentMatrix_second;
var_pred_second=design_second*xx_inv_second*design_second`;
pred_var_second=vecdiag(var_pred_second);
print "Prediction variance for second order model";
print pred_var_second;
unique_pred_second=unique(round(pred_var_second, 0.0000001));
print "Unique prediction variance for second order model";
print unique_pred_second;
/*****************************************/
end;
if &order=3 then do;
/*******THIRD ORDER ROTATABILITY******************/
design_third=sec||dd||sec2||dd1; /*As per the ordering given by
Gardiner (1958)*/
*print design_third;
xx_third=design_third`*design_third;
*print xx_third;
xx_inv_third=inv(xx_third);
*print xx_inv_third;
MomentMatrix_third=xx_third/nrow(a);
print "Moment Matrix for third order model";
print MomentMatrix_third;
```

```
var_pred_third=design_third*xx_inv_third*design_third`;
pred_var_third=vecdiag(var_pred_third);
print "Prediction variance for third order model";
print pred_var_third;
unique_pred_third=unique(round(pred_var_third, 0.00001));
print "Unique prediction variance for third order model";
print unique_pred_third;
/*******************************/
end;
quit;
```

SAS Output

The SAS System

Moment Matrix for second order model

MomentMatrix_second

	COL1	COL2	COL3	COL4	COL5	COL6	COL7	COL8	COL9	COL10	COL11	COL12	COL13	COL14	COL15
ROW1	1	0	0	0	0	0.8571429	0.8571429	0.8571429	0.8571429	0	0	0	0	0	0
ROW2	0	0.8571429	0	0	0	0	0	0	0	0	0	0	0	0	0
ROW3	0	0	0.8571429	0	0	0	0	0	0	0	0	0	0	0	0
ROW4	0	0	0	0.8571429	0	0	0	0	0	0	0	0	0	0	0
ROW5	0	0	0	0	0.8571429	0	0	0	0	0	0	0	0	0	0
ROW6	0.8571429	0	0	0	0	1.7142857	0.5714286	0.5714286	0.5714286	0	0	0	0	0	0
ROW7	0.8571429	0	0	0	0	0.5714286	1.7142857	0.5714286	0.5714286	0	0	0	0	0	0
ROW8	0.8571429	0	0	0	0	0.5714286	0.5714286	1.7142857	0.5714286	0	0	0	0	0	0
ROW9	0.8571429	0	0	0	0	0.5714286	0.5714286	0.5714286	1.7142857	0	0	0	0	0	0
ROW10	0	0	0	0	0	0	0	0	0	0.5714286	0	0	0	0	0
ROW11	0	0	0	0	0	0	0	0	0	0	0.5714286	0	0	0	0
ROW12	0	0	0	0	0	0	0	0	0	0	0	0.5714286	0	0	0
ROW13	0	0	0	0	0	0	0	0	0	0	0	0	0.5714286	0	0
ROW14	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5714286	0
ROW15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5714286

Prediction variance for second order model

pred_var_second
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333
0.5833333

Unique prediction variance for second order model

unique_pred_second	
0.25	0.5833333

Research Paper:

M. Hemavathi, Shashi Shekhar, Eldho Varghese*, Seema Jaggi, Bikas Sinha & Nripes Kumar Mandal (2022) Theoretical developments in response surface designs: an informative review and further thoughts, *Communications in Statistics - Theory and Methods*, 51:7, 2009-2033, DOI: 10.1080/03610926.2021.1944213