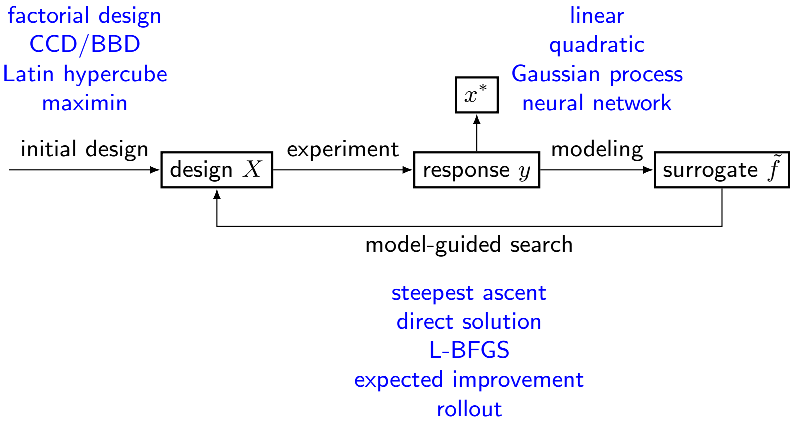
Response Surface Methodology: Alternative Designs

BIOE 498/598 PJ

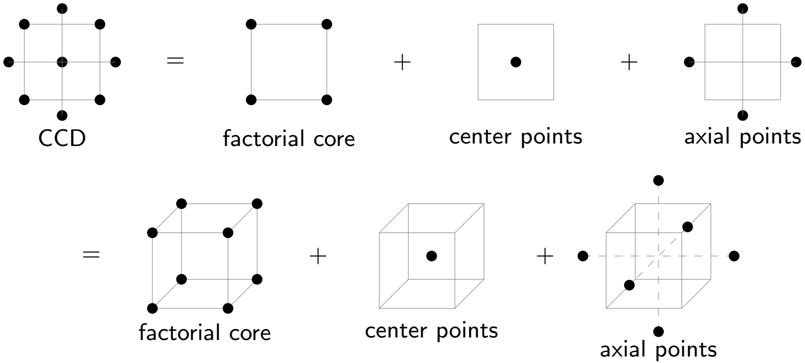
Spring 2022

Surrogate Optimization



The Central Composite Design (CCD)

- A factorial or FF design can estimate FO and TWI terms.
- Estimating curvature requires points beyond the factorial corners.
- One popular option is the **Central Composite Design**.



Why alternatives to the CCD?

- The CCD is excellent (and in many ways optimal) for RSM.
- Many alternatives have been developed to address one of two CCD shortcomings:
    1. CCDs require 5 levels for each factor.
    2. CCDs require a lot of runs.

Rotatable, uniform precision CCDs

factors (k)	2	3	4	5	$5-1$	6
factorial points	4	8	16	32	16	64
axial points	4	6	8	10	10	12
center points	5	6	7	10	6	15
axial distance (α)	1.414	1.682	2.000	2.378	2.000	2.828

factors (k)	$6-1$	7	$7-1$	8	$8-1$	$8-2$
factorial points	32	128	64	256	128	64
axial points	12	14	14	16	16	16
center points	9	21	14	28	20	13
axial distance (α)	2.378	3.364	2.828	4.000	3.364	2.828

Box-Behnken Designs (BBD)

- 3-level design with performance close to a CCD.
- Similar number of runs to a CCD.
- Built from 2^2 factorials for each pair of factors.

Box-Behnken Designs (BBD)

- 3-level design with performance close to a CCD.
- Similar number of runs to a CCD.
- Built from 2^2 factorials for each pair of factors.

x_1	x_2	x_3
-1	-1	0
-1	1	0
1	-1	0
1	1	0
-1	0	-1
-1	0	1
1	0	-1
1	0	1
0	-1	-1
0	-1	1
0	1	-1
0	1	1
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$

Note that in the bottom row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

Box-Behnken Designs (BBD)

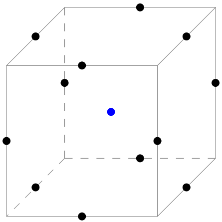
- 3-level design with performance close to a CCD.
- Similar number of runs to a CCD.
- Built from 2^2 factorials for each pair of factors.
- Nearly rotatable (rotatable for $k = 4$ or 7).
- 3–5 center runs are recommended. (At least one center run is required for $k = 4$ or 7).

x_1	x_2	x_3
-1	-1	0
-1	1	0
1	-1	0
1	1	0
-1	0	-1
-1	0	1
1	0	-1
1	0	1
0	-1	-1
0	-1	1
0	1	-1
0	1	1
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$

Note that in the bottom row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

The BBD is a spherical design

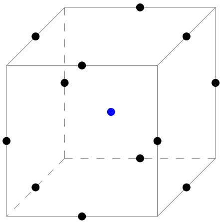
- All points in a BBD are on the edges, not the corners, of the design space.
- For $k = 3$, all points are $\sqrt{2}$ away from the design center.



BBD with $k = 3$.
Center point is in blue.

The BBD is a spherical design

- All points in a BBD are on the edges, not the corners, of the design space.
- For $k = 3$, all points are $\sqrt{2}$ away from the design center.
- The BBD is not good at predicting responses near the corners (*extremes*) of the design space.
- Since the BBD is spherical and rotatable, "ample" center points should be used (Myers 2009).



BBD with $k = 3$.
Center point is in blue.

Hoke Designs

- Hoke (1974) developed smaller, 3-level designs for $k = 3 - 6$ factors.
- For each k there are seven variants, $\mathbf{D}_1 \ldots \mathbf{D}_7$. Designs $\mathbf{D}_1$ – $\mathbf{D}_3$ are saturated, and the others are near-saturated.
- The most popular designs are $\mathbf{D}_2$ and $\mathbf{D}_6$. For $k = 3$ factors:

$\mathbf{D}_2 =$

x_1	x_2	x_3
-1	-1	-1
1	1	-1
1	-1	1
-1	1	1
1	-1	-1
-1	1	-1
-1	-1	1
-1	0	0
0	-1	0
0	0	-1

$\mathbf{D}_6 =$

x_1	x_2	x_3
-1	-1	-1
1	1	-1
1	-1	1
-1	1	1
1	-1	-1
-1	1	-1
-1	-1	1
-1	0	0
0	-1	0
0	0	-1
1	1	0
1	0	1
0	1	1

Koshal Designs

- Koshal (1933) developed saturated d-level designs for modeling a response surface of order d.
- Koshal designs are augmented OFAT designs. They should be reserved for small numbers of factors.

First-order design
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

x_1	x_2	x_3
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$
1	0	0
0	1	0
0	0	1

FO+TWI design
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$$

x_1	x_2	x_3
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$
1	0	0
0	1	0
0	0	1
1	1	0
1	0	1
0	1	1

Second-order design
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$$

x_1	x_2	x_3
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$
1	0	0
0	1	0
0	0	1
1	1	0
1	0	1
0	1	1
-1	0	0
0	-1	0
0	0	-1

Note that in the top row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

Roquemore Hybrid Designs

- Roquemore (1976) defined a series of **hybrid designs** for $k = 3$, 4, 6, & 7.
- The designs are near-rotatable and saturated or near-saturated.

$\mathbf{D}_{310}$ (saturated)

x_1	x_2	x_3
0	0	1.2906
0	0	-0.1360
-1	-1	0.6386
1	-1	0.6386
-1	1	0.6386
1	1	0.6386
1.736	0	-0.9273
-1.736	0	-0.9273
0	1.736	-0.9273
0	-1.736	-0.9273

$\mathbf{D}_{311\mathrm{A}}$ (near-saturated)

x_1	x_2	x_3
0	0	$\sqrt{2}$
0	0	$-\sqrt{2}$
-1	-1	$1/\sqrt{2}$
1	-1	$1/\sqrt{2}$
-1	1	$1/\sqrt{2}$
1	1	$1/\sqrt{2}$
$\sqrt{2}$	0	$-1/\sqrt{2}$
$-\sqrt{2}$	0	$-1/\sqrt{2}$
0	$\sqrt{2}$	$-1/\sqrt{2}$
0	$\sqrt{2}$	$-1/\sqrt{2}$
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$

Note that in $\mathbf{D}_{311\mathrm{A}}$ the bottom row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

Small Composite Design (SCD)

- A CCD uses a full or Resolution V factorial core.
- One alternative is to replace the core with a Resolution III* design — a Resolution III with no 4-letter word in the defining relation.

x_1	x_2	x_3
-1	-1	-1
1	1	-1
1	-1	1
-1	1	1
$-\alpha$	0	0
α	0	0
0	$-\alpha$	0
0	α	0
0	0	$-\alpha$
0	0	α
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$

Small Composite Design (SCD)

- A CCD uses a full or Resolution V factorial core.
- One alternative is to replace the core with a Resolution III* design — a Resolution III with no 4-letter word in the defining relation.
- Unfortunately, the SCD has high variance for main effects and TWI terms.
- However, a Resolution III* design from steepest ascent can be converted into an SCD by adding axial points and center points.

x_1	x_2	x_3
-1	-1	-1
1	1	-1
1	-1	1
-1	1	1
$-\alpha$	0	0
α	0	0
0	$-\alpha$	0
0	α	0
0	0	$-\alpha$
0	0	α
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$

Final recommendations

Many designs can be used for RSM. Here are our recommendations in descending order of preference.

1. The **CCD** is the best overall choice for RSM.
2. A **BBD** is a close second, but only preferable to a CCD when 3-level factors are more convenient than 5-level factors.
3. **Hoke** or **Hybrid** designs are the preferred designs when your run budget is too small for a CCD or BBD.
4. The **SCD** should only be used when a tight budget demands immediate follow-up from steepest ascent. In this case, you need to use a Resolution III* screening design for steepest ascent.
5. **Koshal** designs are obsolete; we include them only for a historical perspective.

Final recommendations

Many designs can be used for RSM. Here are our recommendations in descending order of preference.

1. The **CCD** is the best overall choice for RSM.
2. A **BBD** is a close second, but only preferable to a CCD when 3-level factors are more convenient than 5-level factors.
3. **Hoke** or **Hybrid** designs are the preferred designs when your run budget is too small for a CCD or BBD.
4. The **SCD** should only be used when a tight budget demands immediate follow-up from steepest ascent. In this case, you need to use a Resolution III* screening design for steepest ascent.
5. **Koshal** designs are obsolete; we include them only for a historical perspective.

...but wait, there's one more!

Definitive Screening Designs (DSD)

- The DSD combines features of FF screening, foldover, PB, and BB designs.
- For k factors a DSD requires only $2k+1$ runs.
- Continuous factors use 3 levels; some discrete 2-level factors can be added.
- Can estimate FO, TWI, and PQ terms (up to saturation).
  - Main effects are clear of TWI and PQ terms.
  - All PQ terms are estimable.
  - Complex aliasing of TWI and PQ terms.

6-factor, minimum run DSD

A	B	C	D	E	F
0	1	1	1	1	1
0	-1	-1	-1	-1	-1
1	0	-1	1	1	-1
-1	0	1	-1	-1	1
1	-1	0	-1	1	1
-1	1	0	1	-1	-1
1	1	-1	0	-1	1
-1	-1	1	0	1	-1
1	1	1	-1	0	-1
-1	-1	-1	1	0	1
1	-1	1	1	-1	0
-1	1	-1	-1	1	0
0	0	0	0	0	0

Constructing a DSD

- Jones and Nachtsheim (2011) discovered the DSD for 6 – 30 factors using a computer search.
- Xiao et al. (2012) showed that DSDs for even k can be built with *conference matrices*. Nguyen and Stylianou (2013) developed a new approach for even and odd k.

Constructing a DSD

- Jones and Nachtsheim (2011) discovered the DSD for 6 – 30 factors using a computer search.
- Xiao et al. (2012) showed that DSDs for even k can be built with *conference matrices*. Nguyen and Stylianou (2013) developed a new approach for even and odd k.
- Similar to a PB design, you can add "dummy factors" to increase the number of runs. The dummy columns for the unused factors are dropped. The original paper recommended adding at least two dummy factors.

Analyzing a DSD

There are many choices for analyzing the results of a DSD. For a standard DSD with k factors and $2k + 1$ runs you can

- Fit an intercept, clear FO terms, and up to k aliased TWI terms.
- Fit an intercept, FO, and PQ model. This model will be saturated.
- Perform subset selection to identify smaller models (like a PB design).
- If $k \geq 6$ you can fit a full SO model for any subset of 3 factors (or 4 factors if $k \geq 18$ or 5 factors if $k \geq 24$).

Analyzing a DSD

There are many choices for analyzing the results of a DSD. For a standard DSD with k factors and $2k + 1$ runs you can

- Fit an intercept, clear FO terms, and up to k aliased TWI terms.
- Fit an intercept, FO, and PQ model. This model will be saturated.
- Perform subset selection to identify smaller models (like a PB design).
- If $k \geq 6$ you can fit a full SO model for any subset of 3 factors (or 4 factors if $k \geq 18$ or 5 factors if $k \geq 24$).
  - A DSD can be used for both screening and RSM if the final number of factors is small!