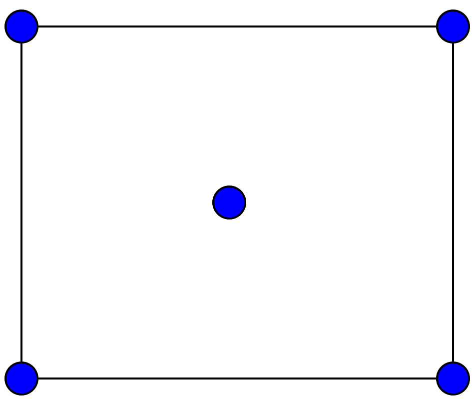
Choices for Alpha in a Split-Plot CCD

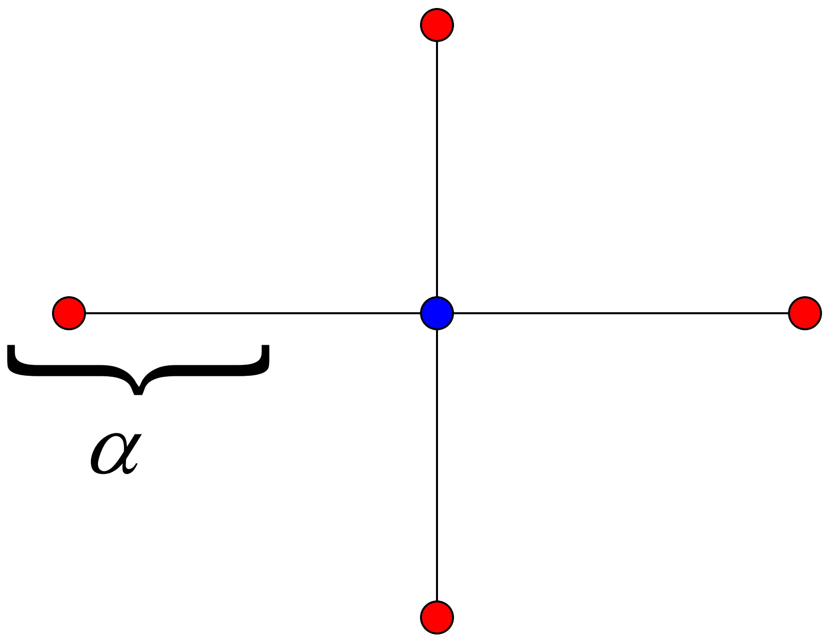
Scott Kowalski, *Minitab Inc.*

Li Wang, *Bristol-Myers Squibb*

Geoff Vining, *Virginia Tech*

Central Composite Design





Common Choices for Alpha

- Cuboidal Region (Face Centered Cube)

$$\alpha = 1$$

- Rotatable (Prediction Variance)

$$\alpha = \sqrt[4]{F}$$

- Orthogonal Blocking (Sequential Design)

$$\alpha = \sqrt{\frac{F(2k + n_{0A})}{2(F + n_{0F})}}$$

Split-Plot CCD

- There are two types of factors
  - Hard-to-change factors
  - Easy-to-change factors

- There is now alpha and beta axial distances

WP	w_1	w_2	s_1	s_2	WP	w_1	w_2	s_1	s_2
	-1	-1	-1	-1		α	0	0	0
1	-1	-1	1	-1	6	α	0	0	0
	-1	-1	-1	1		α	0	0	0
	-1	-1	-1	1		α	0	0	0
	1	-1	-1	-1		0	-α	0	0
2	1	-1	1	-1	7	0	-α	0	0
	1	-1	-1	1		0	-α	0	0
	1	-1	-1	1		0	-α	0	0
	-1	1	-1	-1		0	α	0	0
3	-1	1	1	-1	8	0	α	0	0
	-1	1	-1	1		0	α	0	0
	-1	1	-1	1		0	α	0	0
	1	1	-1	-1		0	0	-β	0
4	1	1	1	-1	9	0	0	β	0
	1	1	-1	1		0	0	-β	0
	1	1	-1	1		0	0	β	0
	-α	0	0	0		0	0	0	-β
5	-α	0	0	0	10	0	0	0	β
	-α	0	0	0		0	0	0	-β
	-α	0	0	0		0	0	0	β

Cuboidal WP Design

- Using alpha=1 makes less settings for the hard-to-change factors
- Can be used to create minimum whole plot designs
- Beta is not constrained here

Rotatability

- Consider the model $\mathbf{y} = \mathbf{X}\beta + \mathbf{M}\gamma + \varepsilon$

- Consider partitioning the design matrix as

$$\mathbf{X} = \begin{bmatrix} \mathbf{1}_1 & \mathbf{W}_{Q_1} & \mathbf{S}_{Q_1} & \mathbf{W}_{F_1} & \mathbf{S}_{F_1} \\ \mathbf{1}_2 & \mathbf{W}_{Q_2} & \mathbf{S}_{Q_2} & \mathbf{W}_{F_2} & \mathbf{S}_{F_2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{1}_m & \mathbf{W}_{Q_m} & \mathbf{S}_{Q_m} & \mathbf{W}_{F_m} & \mathbf{S}_{F_m} \end{bmatrix} = \begin{bmatrix} \mathbf{W}^* & \mathbf{S}_F \end{bmatrix}$$

- Then:

$$\mathbf{X}'\Sigma^{-1}\mathbf{X} = \begin{bmatrix} \dfrac{1}{\sigma^2 + n\sigma_\delta^2}\left(\mathbf{W}'^*\mathbf{W}^*\right) & \mathbf{0} \\ \mathbf{0} & \dfrac{1}{\sigma^2}\left(\mathbf{S}_F'\mathbf{S}_F\right) \end{bmatrix}$$

Rotatability

- Let's look at the pure second-order moment for the i[th] subplot factor. A rotatable design would require

$$[ii]_{sp}^{S_F} = [ii]_{sp}^{W^*}$$

However, there is a multiplier of $\frac{1}{\sigma^2}$ in S_F and $\frac{1}{\sigma^2 + n\sigma_\delta^2}$ in W*.

Unless $\sigma_\delta^2 = 0$, we cannot achieve exact rotatability.

Partial Rotatability

- We propose a concept of partial rotatability. It has similar properties, and it is more logical in the split-plot case.

- In a two-strata rotatable design, there are two axial distances instead of one. The whole plot axial distance, ρ_W^2 and the second is the subplot axial distance, ρ_S^2

- A two-strata rotatable design will allow all the points with same ρ_W^2 and ρ_S^2 to have same prediction variance.

Partial Rotatability

- In a rotatable design, $Var[\hat{y}(\mathbf{x}_0)] = f\left(\rho_W^2 + \rho_S^2\right)$ which is a function of the overall distance.

- In a two-strata rotatable design, $Var[\hat{y}(\mathbf{x}_0)] = f\left(\rho_W^2, \rho_S^2\right)$ a function of the two separate distances.

- Therefore, the stronger assumption in rotatable designs is being relaxed to accommodate the split-plot structure.

Partial Rotatability

We define the two-strata rotatable designs as:

In a k-factor split-plot design with k_1 WP factors and k_2 SP factors, let z_i be the i^{th} WP factor and x_j be the j^{th} SP factor. If for any two design runs

$t_0=(z_{10},z_{20},\ldots,z_{k1,0},x_{10},\ldots,x_{k2,0})$ and $t_1=(z_{\_11},z_{21},\ldots,z_{k1,1},x_{11},\ldots,x_{k2,1})$ *satisfying*

$$\sum_{i=1}^{k_1} z_{i0}^2 = \sum_{i=1}^{k_1} z_{i1}^2 = \rho_W^2 \quad \textit{and} \quad \sum_{j=1}^{k_2} x_{j0}^2 = \sum_{j=1}^{k_2} x_{j1}^2 = \rho_S^2$$

the corresponding prediction variances $Var\left[\hat{y}(t_0)\right] = Var\left[\hat{y}(t_1)\right]$ *are equal, the design is called a two-strata rotatable split-plot design.*

Partial Rotatability

- The values of alpha and beta are

WP	w_1	w_2	s_1	s_2
9	0	0	-β	0
	0	0	β	0
	0	0	-β	0
	0	0	β	0
10	0	0	0	-β
	0	0	0	β
	0	0	0	-β
	0	0	0	β

$$\alpha = \sqrt[4]{\frac{F}{n}} \quad \text{and} \quad \beta = \sqrt[4]{\frac{2(1+nd)F}{n}}$$

WP	w_1	w_2	s_1	s_2
9	0	0	-β	0
	0	0	β	0
	0	0	0	-β
	0	0	0	β

$$\alpha = \sqrt[4]{\frac{F}{n}} \quad \text{and} \quad \beta = \sqrt[4]{\frac{4F}{n}}$$

Partial Rotatability

- General conditions for these designs

WP	w_1	w_2	s_1	s_2
9	0	0	-β	0
	0	0	β	0
	0	0	-β	0
	0	0	β	0
10	0	0	0	-β
	0	0	0	β
	0	0	0	-β
	0	0	0	β

$$r = 8$$

$$a = 4$$

$$\alpha = \sqrt[4]{\frac{2F}{r}} \quad \text{and} \quad \beta = \sqrt[4]{\frac{2(1+nd)F}{a}}$$

WP	w_1	w_2	s_1	s_2
9	0	0	-β	0
	0	0	β	0
	0	0	0	-β
	0	0	0	β

$$r = 8$$

$$a = 2$$

$$\alpha = \sqrt[4]{\frac{2F}{r}} \quad \text{and} \quad \beta = \sqrt[4]{\frac{2F}{a}}$$

- where r = # alphas in a column and a = # betas

Partial Rotatability

- What if we had a CRD?
- Then d=0, n=1, r=2, a=2

$$\alpha = \sqrt[4]{\frac{2F}{r}} = \sqrt[4]{\mathrm{F}} \text{ and } \beta = \sqrt[4]{\frac{2(1+nd)F}{a}} = \sqrt[4]{\mathrm{F}}$$

$$\alpha = \sqrt[4]{\frac{2F}{r}} = \sqrt[4]{\mathrm{F}} \text{ and } \beta = \sqrt[4]{\frac{2F}{a}} = \sqrt[4]{\mathrm{F}}$$

- So they all reduce to the CRD rotatable value

Partial Rotatability

- Conditions can be generalized to other combinations of HTC and ETC factors
- Unbalance in the WPs with axial runs can be handled, then there are subscripts on the *n*
- Only condition is $\mathbf{1}'\mathbf{S}_{D_i} = \mathbf{0}'$

Orthogonal Blocking

- Condition for Orthogonal Blocking:

  For any column of X, the average in block i is the equal to the average in block j is equal to the overall average

- Khuri (1992) and Goos (2002) show that for an OB design, OLS=GLS for a balanced fixed block design

Orthogonal Blocking

- Extend this concept to SP-CCD
- Not going to show proof
- Block sizes do not have to be equal, but the whole plot sizes need to be equal

WP	w_1	w_2	s_1	s_2	WP	w_1	w_2	s_1	s_2
1	-1	-1	-1	-1	6	α	0	0	0
	-1	-1	1	-1		α	0	0	0
	-1	-1	-1	1		α	0	0	0
	-1	-1	-1	1		α	0	0	0
2	1	-1	-1	-1	7	0	-α	0	0
	1	-1	1	-1		0	-α	0	0
	1	-1	-1	1		0	-α	0	0
	1	-1	-1	1		0	-α	0	0
3	-1	1	-1	-1	8	0	α	0	0
	-1	1	1	-1		0	α	0	0
	-1	1	-1	1		0	α	0	0
	-1	1	-1	1		0	α	0	0
4	1	1	-1	-1	9	0	0	-β	0
	1	1	1	-1		0	0	β	0
	1	1	-1	1		0	0	0	-β
	1	1	-1	1		0	0	0	β
5	-α	0	0	0	10	0	0	0	0
	-α	0	0	0		0	0	0	0
	-α	0	0	0		0	0	0	0
	-α	0	0	0		0	0	0	0

Orthogonal Blocking

- Sequential Design will have WPs 1-4 in Block 1 and WPs 5-9 in Block 2
- For OB, trying to solve for the number of WP 10s to add into Blocks 1 & 2 as well as find the values for alpha and beta
- Only need to focus on quadratics

Orthogonal Blocking

- F = # factorial points
- k_1 = # WP factors
- k_2 = # SP factors
- n_{c1} = # overall center runs added to B1
- n_{c2} = # overall center runs added to B2
- r = # alphas in a column
- a = number of betas in a column

Orthogonal Blocking

$$\frac{F}{F+n_{c1}} = \frac{r\alpha^2}{k_1 r + k_2 a + n_{c2}} = \frac{r\alpha^2 + F}{k_1 r + k_2 a + n_{c2} + F + n_{c1}}$$

$$\frac{F}{F+n_{c1}} = \frac{a\beta^2}{k_1 r + k_2 a + n_{c2}} = \frac{a\beta^2 + F}{k_1 r + k_2 a + n_{c2} + F + n_{c1}}$$

$$\alpha^2 = \frac{(k_1 r + k_2 a + n_{c2})F}{r(F + n_{c1})}$$

$$\beta^2 = \frac{(k_1 r + k_2 a + n_{c2})F}{a(F + n_{c1})}$$

Orthogonal Blocking

- There is a tradeoff between the size of the overall design, size of the blocks and reasonable values for alpha and beta

- With n_{c1}=8 and n_{c2}=4, our example yields:

$$\alpha = 1.414, \beta = 2.828$$

- With one replicate of the beta WP, gives

$$\alpha = 1.53, \beta = 2.16$$

Summary

- When conducting a CCD, the axial distance must be chosen
- In a SP-CCD, there are now two distances
- Simple solution is to use a distance of 1
- Cannot achieve the general definition of rotatability but can use partial rotatability
- OLS-GLS designs can be OB