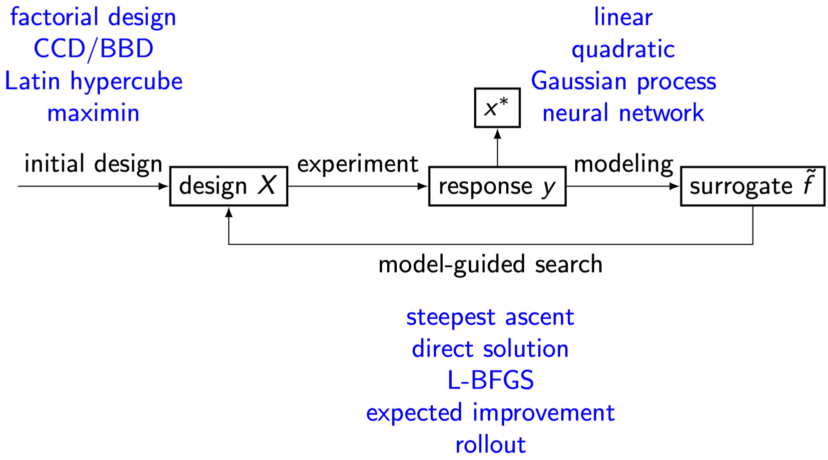
Response Surface Methodology: Central Composite Designs

BIOE 498/598 PJ

Spring 2022

Surrogate Optimization



Approximating f with a general quadratic

Let's find the second-order Taylor series of $f(x_1, x_2)$ centered at zero:

$$f(x_1, x_2) \approx \left. f\right|_0 + \left.\frac{\partial f}{\partial x_1}\right|_0 x_1 + \left.\frac{\partial f}{\partial x_2}\right|_0 x_2 + \frac{1}{2}\left.\frac{\partial^2 f}{\partial x_1^2}\right|_0 x_1^2 + \frac{1}{2}\left.\frac{\partial^2 f}{\partial x_2^2}\right|_0 x_2^2 + \frac{1}{2}\left.\frac{\partial^2 f}{\partial x_1 \partial x_2}\right|_0 x_1 x_2$$

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- In general we will have k factors and the quadratic approximation will be

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{j=1}^{k} \sum_{i=1}^{j-1} \beta_{ij} x_i x_j.$$

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- This model has $1 + 2k + k(k-1)/2$ parameters, so RSM designs must have at least this many runs.

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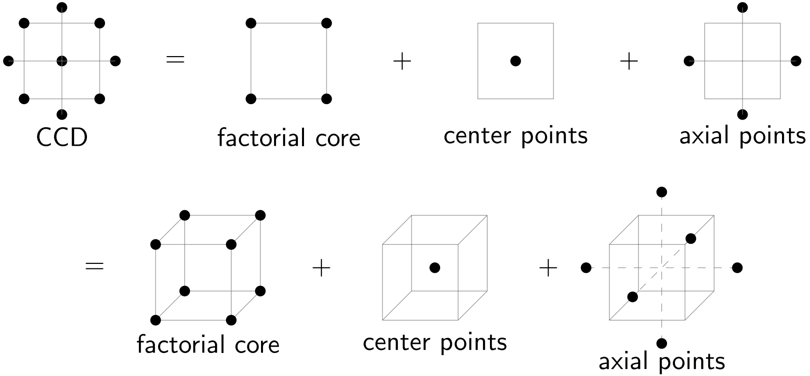
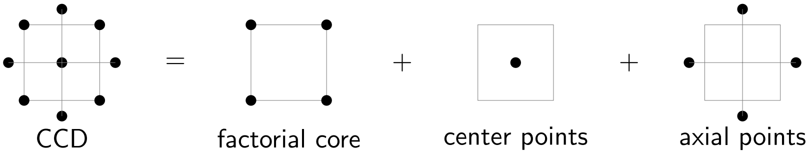


Parts of the CCD



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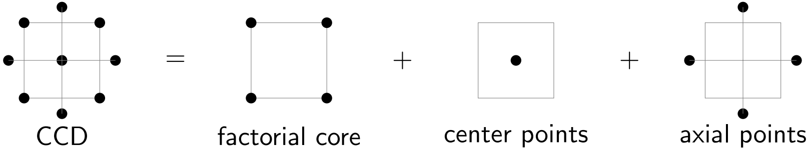

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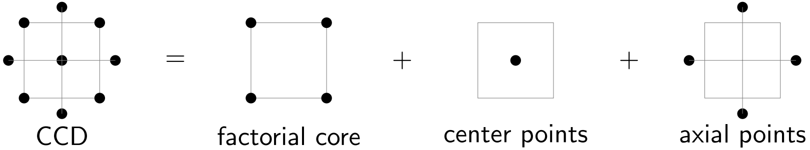

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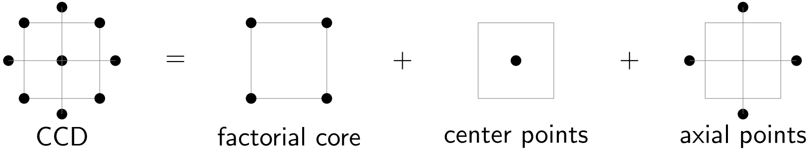

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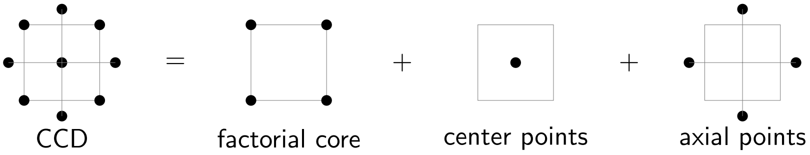

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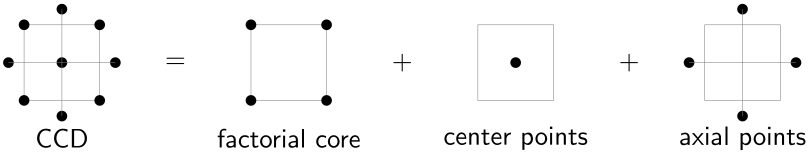

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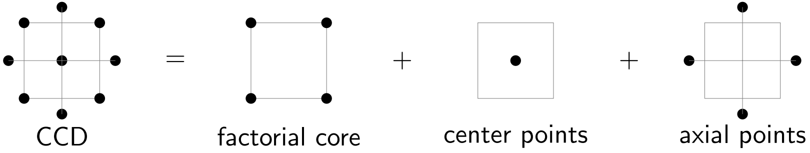

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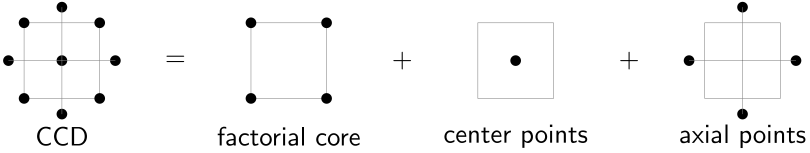

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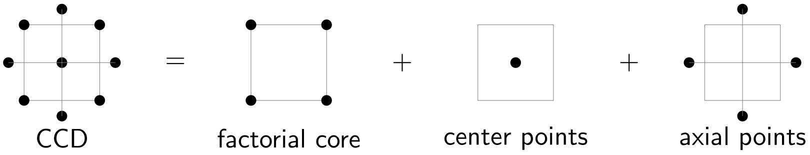

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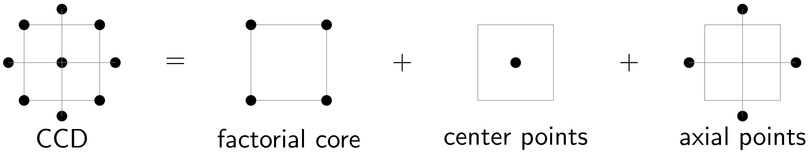

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  3. The value of α

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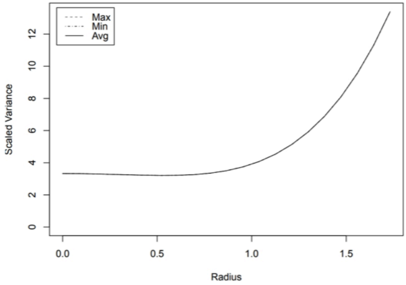

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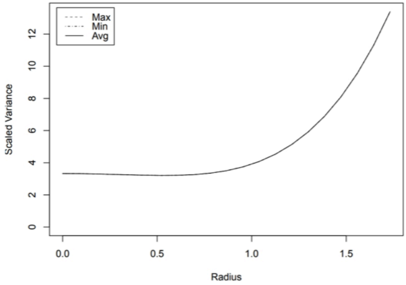

- Choosing the correct number of center points in a CCD ensures uniform precision.

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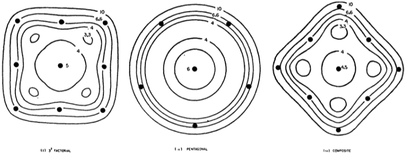

Fig. 2. Variance contours for some 2 dimensional designs

Image from Box and Hunter 1957.

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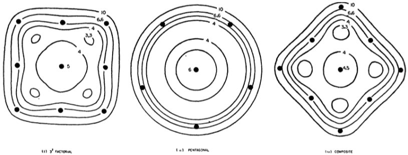

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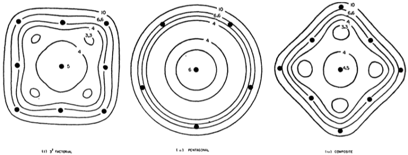

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- A CCD with F factorial points is rotatable when $\alpha = \sqrt[4]{F}$.

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

Factor levels in a CCD

Each factor in the CCD will be set at five levels:

$$-\alpha \quad -1 \quad 0 \quad 1 \quad \alpha$$

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Unlike a 2-level design, the coded units in a CCD have meaning!

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Let's say we're designing a combination screening of three drugs. The absolute widest concentration range we can use for drug A is $[-3.2, 1.0]$ on a $\log_{10}$-μM scale. What are the five levels assuming a full-factorial CCD?

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$$\begin{aligned} \mathsf{A} &= \text{center(A)} + \frac{\text{range(A)}}{2\alpha}[\text{code}] \\ &= -1.1 + \frac{1-(-3.2)}{2(1.68)}[\text{code}] \end{aligned}$$

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code:	$-\alpha$	-1	0	1	α
$\log_{10}$-μM:	-3.2	-2.4	-1.1	0.2	1.0