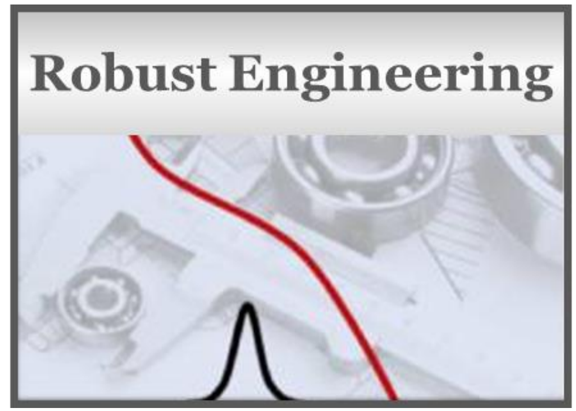
UNIVERSITY of BRADFORD

Statistiques Appliquées Formation Industrielle



Session 8: Three Level Designs

In This Session We Will…

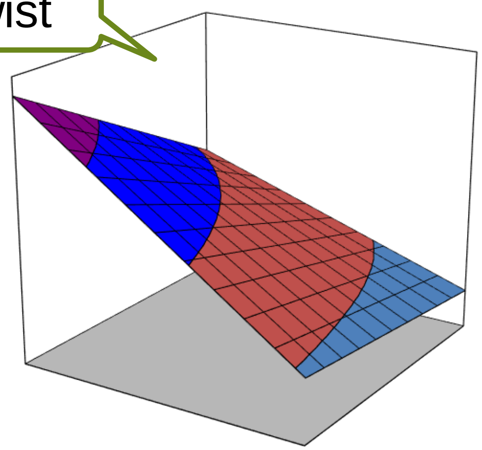
- Define the face-centred Central Composite design, which allows us to fit a complete 2nd order response surface.
- Plot the design as a pattern in factor space.
- Introduce Custom designs, generated by maximizing or minimizing a mathematical optimality criterion.
  - this allows us to choose the number of runs , the terms to be fitted and the design region.
  - define D optimality, which is the most commonly used criterion.

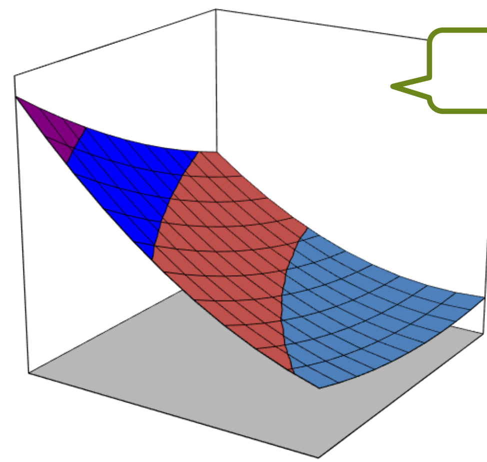
In This Session We Will…

- Discuss some measures of design ‘quality’:
  - relative standard errors of regression coefficients,
  - relative prediction standard deviation (PSD),
  - orthogonality measures,
  - Leverages.

Why Run A Three-level Design?

- If we use a sequential experimentation strategy, the second stage is often to design an experiment to fit a **2nd order** surface





To fit this surface requires at least three levels of each factor

Terminology

- In books and software a ‘response surface design’ usually means a design with at least three levels of each factor.
  - but we have seen that all designs can be used to fit a response surface.
- To get a 2nd order surface we add quadratic terms to the equation, e.g.

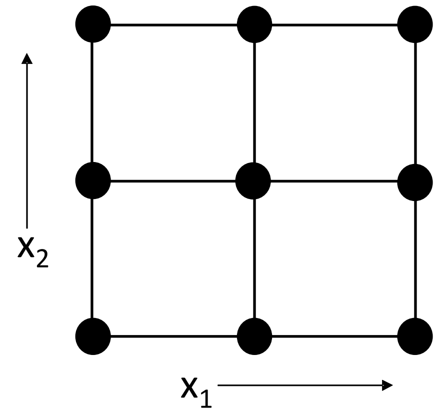
$$y = b_0 + b_1x_1 + b_2x_2 + b_{12}x_1x_2 + b_{11}{x_1}^2 + b_{22}{x_2}^2$$

Think of this as ‘b 2,2’ not ‘b twenty-two’

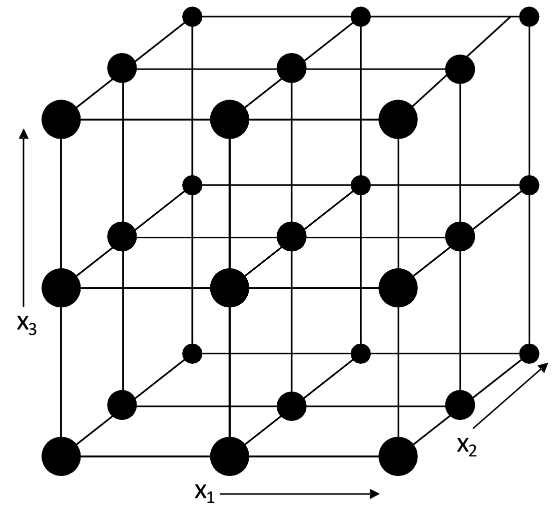
- Technically, the right-hand side is a complete 2nd order polynomial (there are no missing 2nd order terms)
- Historically, most of the theory and practice of response surface methods has focussed on fitting complete 2nd order polynomials.

What Design Should We Use?

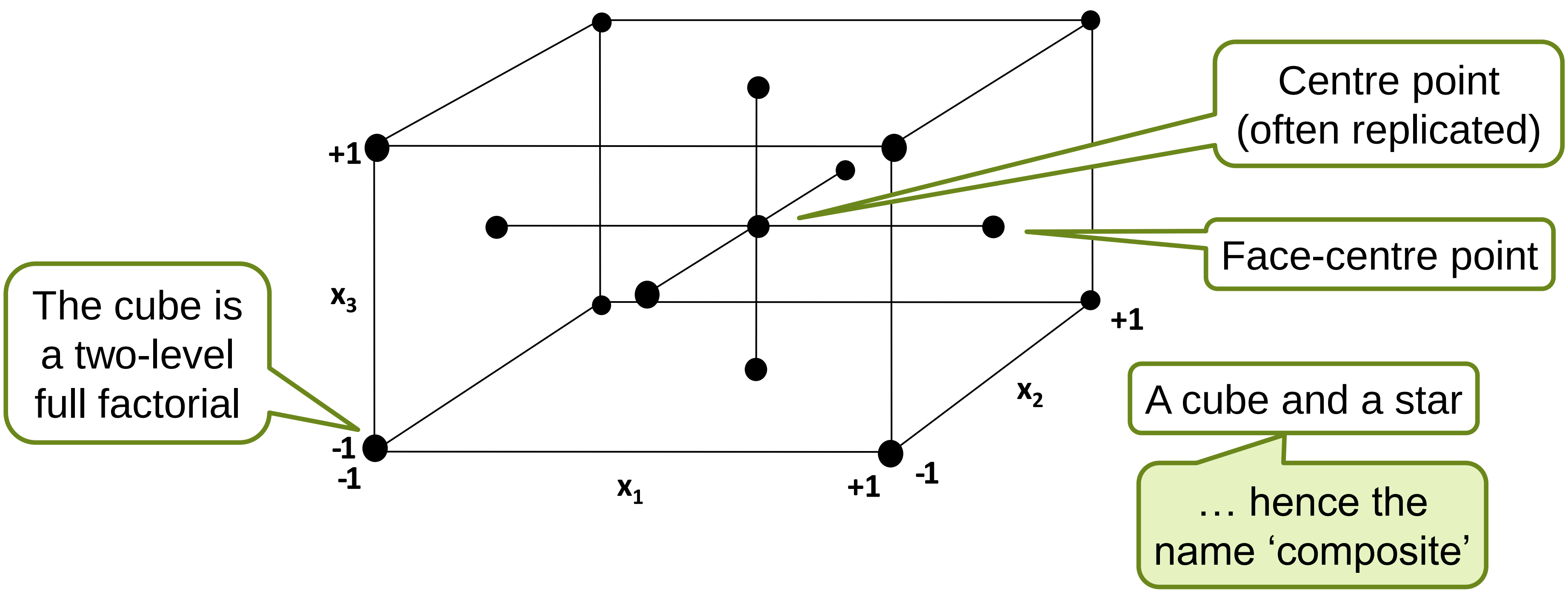
- With only two factors, we can use the 3^2 full factorial:



- But with three or more factors, the full factorials are usually too big:



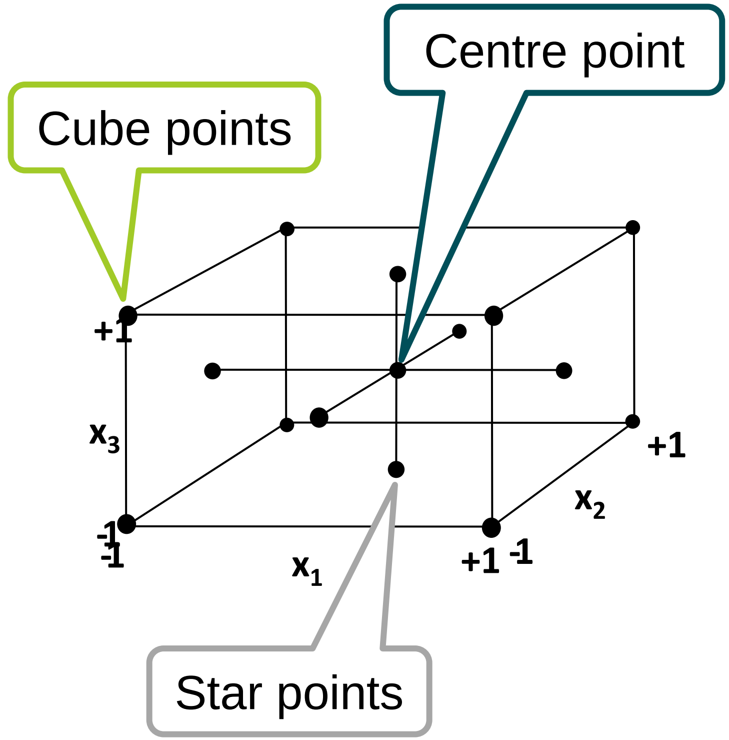
- This is a type of fractional three-level factorial, specially chosen for fitting a complete 2nd order polynomial.



Face-Centred Central Composite Design

- Here are the coded factor combinations, listed in a standard order:

Row	x_1	x_2	x_3
1	–1	–1	–1
2	+1	–1	–1
3	–1	+1	–1
4	+1	+1	–1
5	–1	–1	+1
6	+1	–1	+1
7	–1	+1	+1
8	+1	+1	+1
9	–1	0	0
10	+1	0	0
11	0	–1	0
12	0	+1	0
13	0	0	–1
14	0	0	+1
15	0	0	0



Custom Design

- A custom design is generated by a computer search algorithm.
- The software looks for a set of points that maximize or minimize some mathematical optimality criterion.

Custom designs are also known as Optimal designs

Specifying A Custom Design

- Custom designs are ‘tailor-made’ for a specific project; we can specify:
  - the number of runs,
  - the terms to be fitted,
  - the design region (not necessarily a regular shape),
  - an optimality criterion.
- The criterion most commonly used is D optimality.
- Let M be the model matrix defined by the specified polynomial and a given set of n points in the design space.
- Choose the levels to maximize D, where $D = \det(M'M)$.

In practice we work with $ln(D)$

Maximizing $ln(D)$ is equivalent to maximizing D

In the next Tutorial you will be able to evaluate $\ln(D)$ for different designs

Some Applications of A Custom Design Algorithm

Constrained design region

- Often there are parts of the design space that we do not want to explore, because of
  - safety considerations,
  - prior knowledge that the response will be poor.

We should not take a standard design and leave points out!

Design repair

- If the operating envelope is only known approximately, try to run the potentially difficult points early on.
- If points cannot be run, use Custom design to choose replacements.

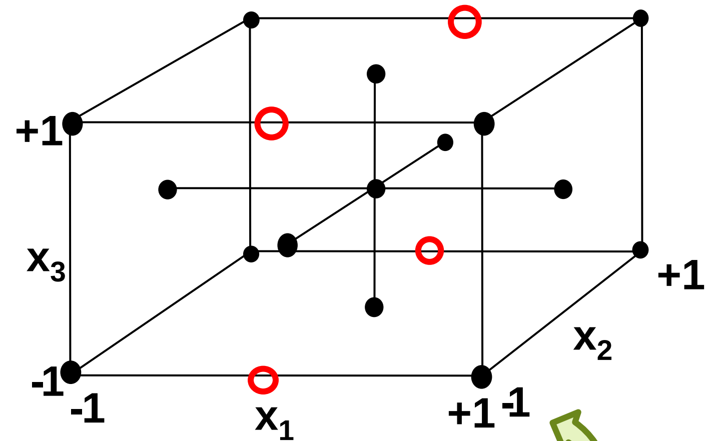
Some Applications of A Custom Design Algorithm

Augmentation 1

- Decide on a sensible set of runs (say m of them) that will be forced into the design
- Select another n–m runs to optimise the properties of the set of n points

This can save a lot of time in complicated problems

Augmentation 2



- Having analysed our results, we want to put extra terms into the prediction equation.
- For example, we run a face-centred CC in three factors, and x_1 seems to be very important
  - we want to fit a cubic term in x_1.
  - we can afford 4 extra runs.

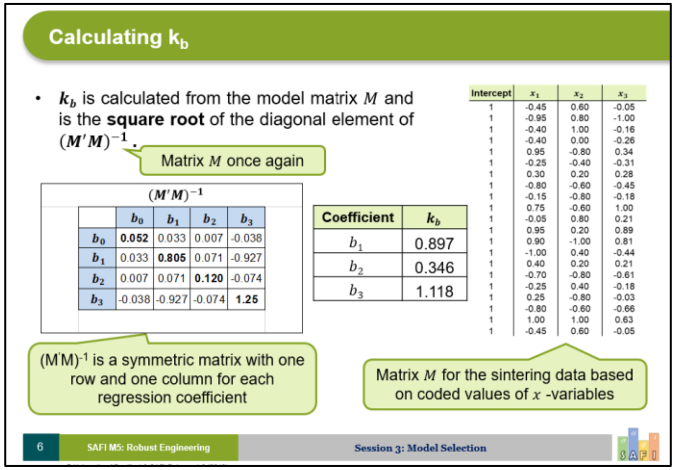
x_1	x_2	x_3
-0.5	-1	1
0.5	-1	1
-0.5	1	-1
0.5	1	-1

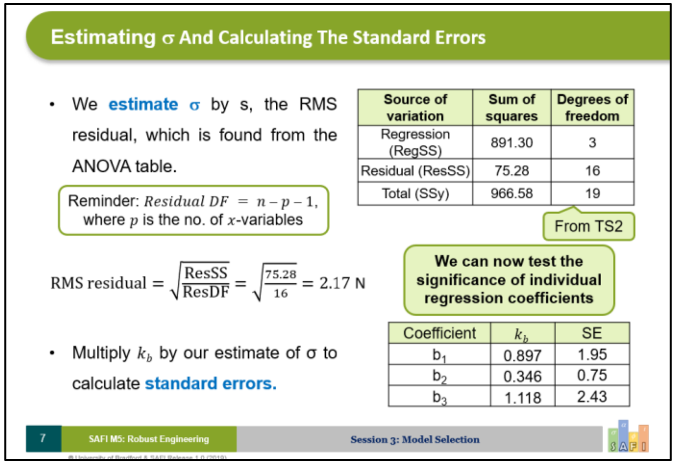
Design Evaluation

- Whether we use a standard design or generate a custom design, we should check the following measures of design 'quality':
  - Relative standard errors of regression coefficients;
  - Prediction Standard Deviation (PSD) map, maximum relative PSD and average relative PSD if available;
  - Orthogonality measures;
  - Leverages and robustness to loss of data.

Relative Standard Errors

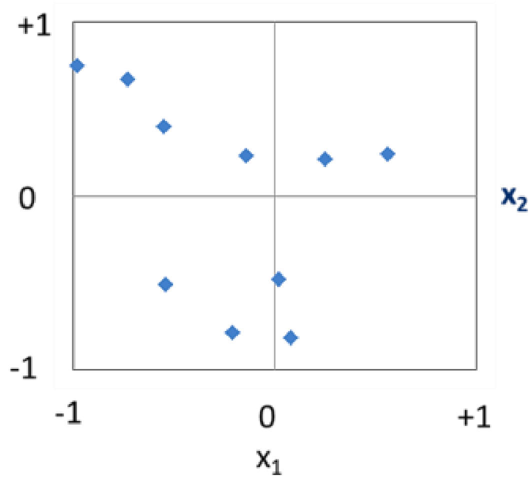
- We saw in Session 3 that for a typical regression coefficient b, the SE takes the form $k_b \cdot \sigma$.
  - k_b depends only on the factor levels in the design.
  - σ is the standard deviation of the random part of y.
- Before the experiment, we won't usually have an estimate of σ, but this doesn't matter because we can use k_b to compare two designs at the planning stage (in effect we set $\sigma = 1$).
  - we call this the relative standard error of the coefficient.





Relative Standard Errors

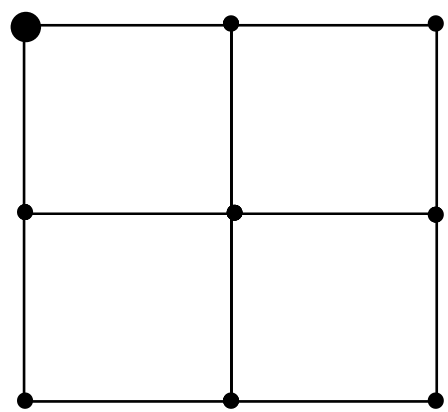
Random design



Random design

Term	Relative SE
x_1	1.09
x_2	2.02
x_1x_2	3.17
${x_1}^2$	2.37
${x_2}^2$	3.47

D-opt design



D-opt design

Term	Relative SE
x_1	0.39
x_2	0.39
x_1x_2	0.70
${x_1}^2$	0.70
${x_2}^2$	0.46

Prediction Standard Deviation (PSD)

- Suppose we predict the response y at a set of factor levels $\underline{x}$, based on fitting a 2nd order polynomial to our data.
  - how precise is this prediction?
  - how much uncertainty is there?
- PSD is a measure of the potential for random variation in a response prediction.
  - like the standard error of a regression coefficient but relating to a response prediction.
- Specialist DoE software such as MATLAB / MBC, JMP or Design Expert will plot the PSD as a function of $\underline{x}$.

Formula For The PSD

- For example, for a given 2-Factor design, the 2nd order response surface equation is:

$$y = b_0 + b_1x_1 + b_2x_2 + b_{12}x_1x_2 + b_{11}{x_1}^2 + b_{22}{x_2}^2$$

- Let $\underline{m}$ be a row vector with an entry for every term in the equation, i.e. like a row of the model matrix M, but based on a new point $(x_1\,, x_2)$ where we want to predict the response, y

$$\underline{m} = [1 \quad x_1 \quad x_2 \quad x_1x_2 \quad {x_1}^2 \quad {x_2}^2]$$

$$PSD = \sigma \times \underline{m}\,(M'M)^{-1}\underline{m}'$$

As before, we compare designs in terms of relative PSDs, not absolute

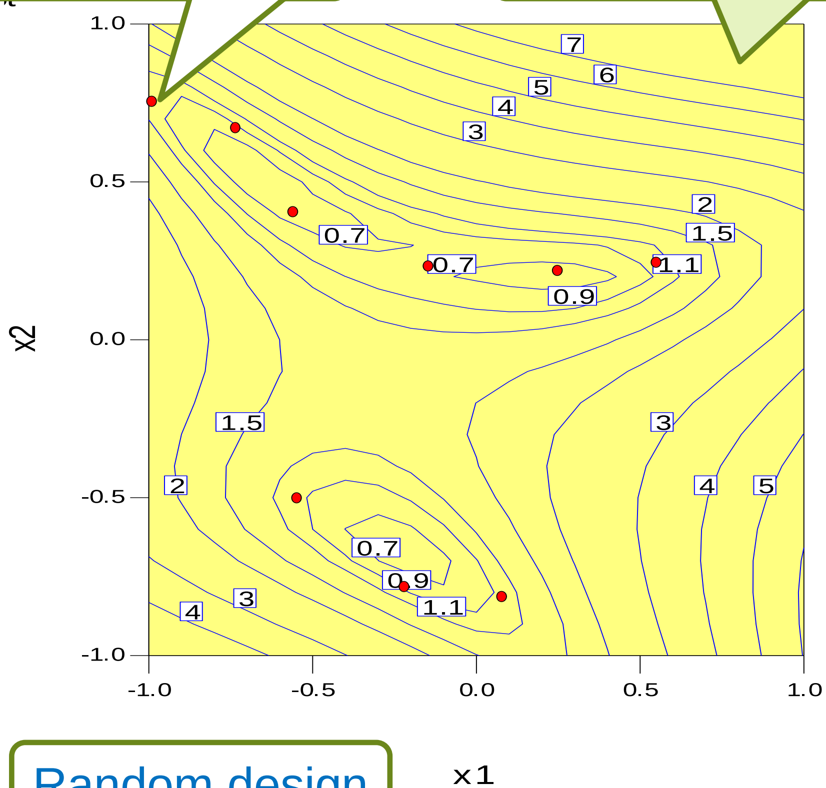
In effect we take $\sigma = 1$

The PSD is the product of two terms, like the standard error of a regression coefficient

Contour Plots of Relative PSD

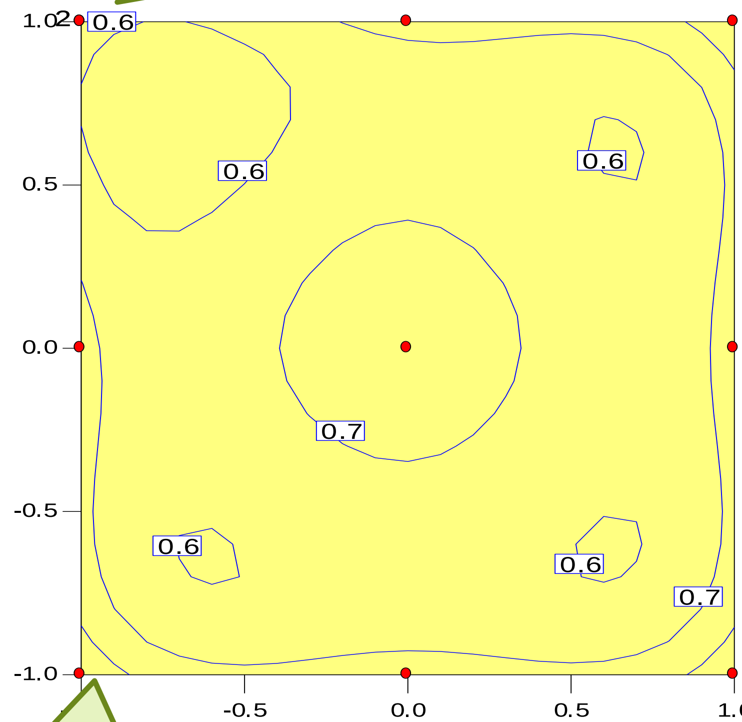
Design point

Max PSD ≈ 10



Random design

Replicated Design point



Max PSD ≈ 0.9

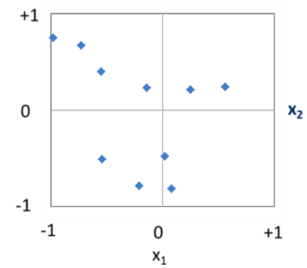
D-opt design

Orthogonality Measures

- In Session 3 we introduced a Variance Inflation Factor (VIF) for the variable x_j, defined as:

$$\left\{\frac{\text{SE of } \mathrm{b_j} \text{ if the full model is fitted}}{\text{SE of } \mathrm{b_j} \text{ if all other x's are removed}}\right\}^2$$

This is defined for each pair of terms in the equation



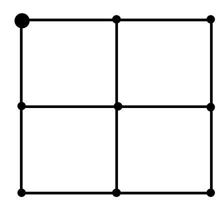
Random design

	b_1	b_2	b_{11}	b_{22}
b_2	1.03			
b_{11}	1.21	1.58		
b_{22}	1.00	5.10	1.31	
b_{12}	1.07	3.08	1.06	2.58

i.e. the SE of b_2 changes a lot if the ${x_2}^2$ term is removed

- In designed experiments a more useful measure is:

$$\left\{\frac{\text{SE of } \mathrm{b_j} \text{ if the full model is fitted}}{\text{SE of } \mathrm{b_j} \text{ if just term k is removed}}\right\}^2$$



D-opt design

	b_1	b_2	b_{11}	b_{22}
b_2	1.01			
b_{11}	1.00	1.00		
b_{22}	1.00	1.00	1.00	
b_{12}	1.02	1.02	1.01	1.01

Leverages

- If a run cannot be completed, or the response value is set aside during the analysis (because it is flagged as an outlier), there may be major changes in the PSD map.
  - these changes are most severe if a high leverage point is lost.
- If a point with leverage h is lost, the relative PSD at that point in the design space increases from $\sqrt{h}$ to $\sqrt{\frac{h}{(1-h)}}$.
  - e.g. if h = 0.8, the relative PSD increases from 0.89 to 2.0.
- For our random design, the maximum leverage is 0.84; for the D-optimal design it is 0.81, so there is little to choose between them
- Note: for any design with n runs, the average leverage is:

$$\frac{\#\ terms\ in\ equation}{n}$$

$= \frac{6}{10}$ *or* 0.6 in our examples

Other Optimality Criteria

- Some custom design algorithms offer other criteria in addition to D-optimality; these include:
  - A optimality: minimize the average variance of the regression coefficients.
  - V or I optimality: minimize the average prediction variance over the design region.

The prediction variance is the square of the prediction standard deviation (PSD)

- G optimality: minimize the maximum PSD over the design region

In This Session We Have…

- Defined the Central Composite design, which allows us to fit a complete 2nd order response surface.
- Plotted the design in factor space.
- Introduced Custom designs, generated by maximizing or minimizing a mathematical optimality criterion.
  - this allows us to choose the number of runs , the terms to be fitted and the design region.
  - defined D optimality, which is the most commonly used criterion.
- Discussed some measures of design ‘quality’:
  - relative standard errors of regression coefficients,
  - relative prediction standard deviation (PSD),
  - orthogonality measures,
  - Leverages.

Session 8: Three Level Designs

Tutorial and Exercise

Tutorial

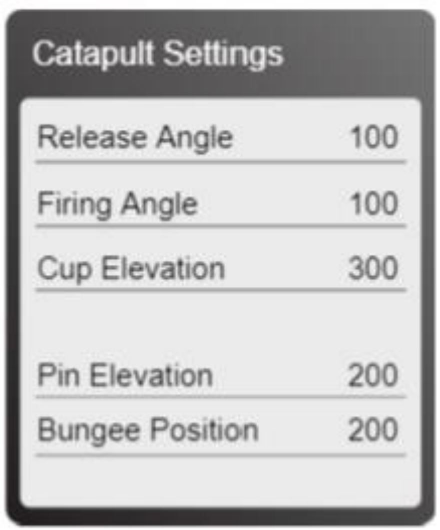
- **Session TS08+09: Three Level Designs**
- **Objective:**
  - Develop skills for generating and evaluating three-level designs.
  - This tutorial is based on the Technical Sessions TS08 and TS09 - see the Technical Session slides for details.
- **Python Environment**

  A self-guided tutorial has been created as a Colab notebook with pre-designed Python code and notes. For this tutorial, follow the instructions in the notes, upload data files and run the code. No modification of code is required. Interpret the results in accordance with the Technical session.
- **Tutorial Tasks**
  1. Generate a face-centred Central Composite design for three factors.
  2. Make a 3D scatter plot of the design in factor space.
  3. Generate a D-optimal design in 15 runs for fitting a 2nd order response surface in three factors.
  4. Compare the CC and D-optimal designs.

Exercise

- **Sessions TS08+09 & 10: Three Level Experiment**
- **Objective**
- To design, analyse and discuss the results of a follow up three level experiment for the Virtual Catapult.

https://sigmazone.com/catapult/



Exercise

- **Sessions TS08+09 & 10: Three Level Experiment**
- **Python Environment**

  The exercise has been created as a Colab notebook with notes. Follow the instructions in the notes, and create your own code using tutorials 08 to 11 as a guide. Interpret the results in accordance with the Technical Sessions.
- **Objectives:**
  - To plan, run and analyse a three-level experiment on the catapult, using **three** factors selected on the basis of your screening results
  - To make predictions for factor combinations that you have not already tested
  - To test your predictions by firing the catapult.
- **Guidelines**

  For this session you should stop when you have completed the experimental design.
  - Decide which design to use; which three factors to use; which levels to use for each factor; how many runs to make.
  - If you decide to run a CC design you need to decide how many runs to make at the centre point. If you choose a D-optimal design you should consider whether to add one or more runs at the centre.