Design of Experiments: Part 1

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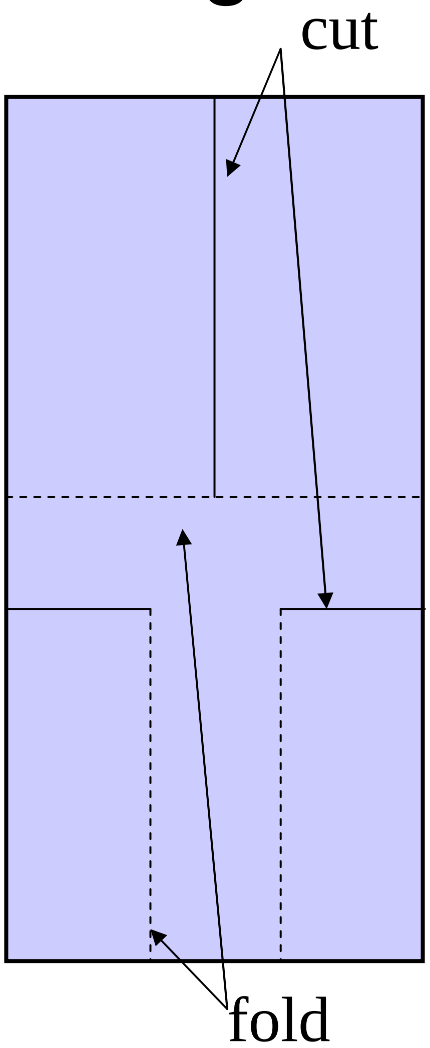
Plan for Today

- Discussion of the reading assignment
- History of DOE
- Full factorial designs
  - The design
  - The model
  - Analysis of the sum of squares
  - Hypothesis testing
- Other designs
  - Fractional factorial designs
  - Central composite designs

Statistics as a Catalyst to Learning

- Concerned improvement of a paper helicopter
- Screening experiment (16) 2_{IV}^{8-4}
- Steepest ascent (5)
- Full factorial (16) 2^4
- Sequentially assembled CCD (16+14=30)
- Ridge exploration (16)
- (16+5+30+16)*4 > 250 experiments
- Resulted in a 2X increase in flight time vs the starting point design



Box, G. E. P. and P. T. Y. Liu, 1999, "Statistics as a Catalyst to Learning by Scientific Method: Part 1", *Journal of Quality Technology*, **31** (1): 1-15.

Factors Considered Initially

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TABLE 1: Factor Levels Used in Design I: An Initial 2^{S-4}_{IV} Screening Experiment.
and FIGURE 1: The Initial Helicopter Design in Box and Liu, 1999.

Screening Design

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TABLE 2: Design I: Layout and Data for 2_{IV}^{8-4} Screening Design in Box and Liu, 1999.

- What is the objective of screening?
- What is special about this matrix of 1s and -1s?

Effect Estimates

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TABLE 3: Design I: Estimates for a 2_{IV}^{8-4} Screening Design in Box and Liu, 1999.

Normal Probability Plots

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FIGURE 2: Design I - Normal Plots for: (a) Location effects from y and (b) Dispersion Effects from 100 log(s) . in Box and Liu, 1999.

- What's the purpose of these graphs?

"Steepest" Ascent

- What does "steep" mean in this context?

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FIGURE 4: Data for 5 Helicopters on the path of Steepest Ascent Calculated from Design 1 in Box and Liu, 1999.

Factors Re-Considered

~~Wing width w~~
~~Wing length l~~

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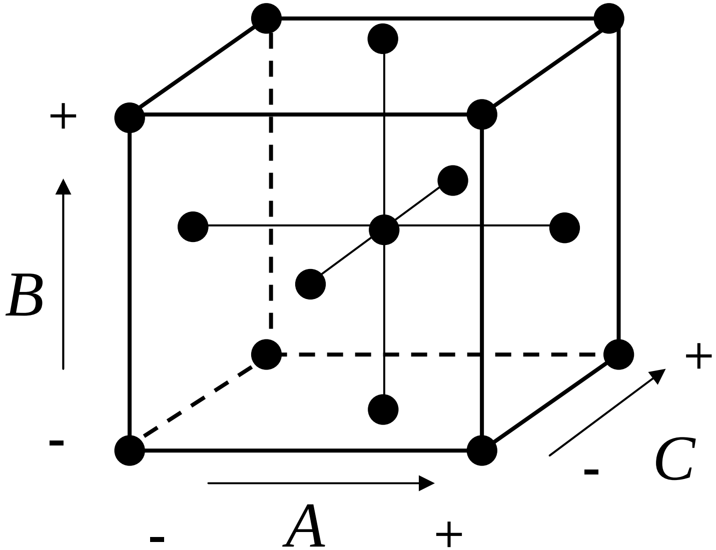
FIGURE 1: The Initial Helicopter Design in Box and Liu, 1999.

Wing area $A=lw$
Wing aspect ratio $Q=l/w$

Central Composite Design



2^n with center points

and axial runs

Enables a model to be fit with all second order polynomial terms included (i.e. A^2, AB, etc.)

2^3 shown here

2^4 run by Box

Analysis of Variance

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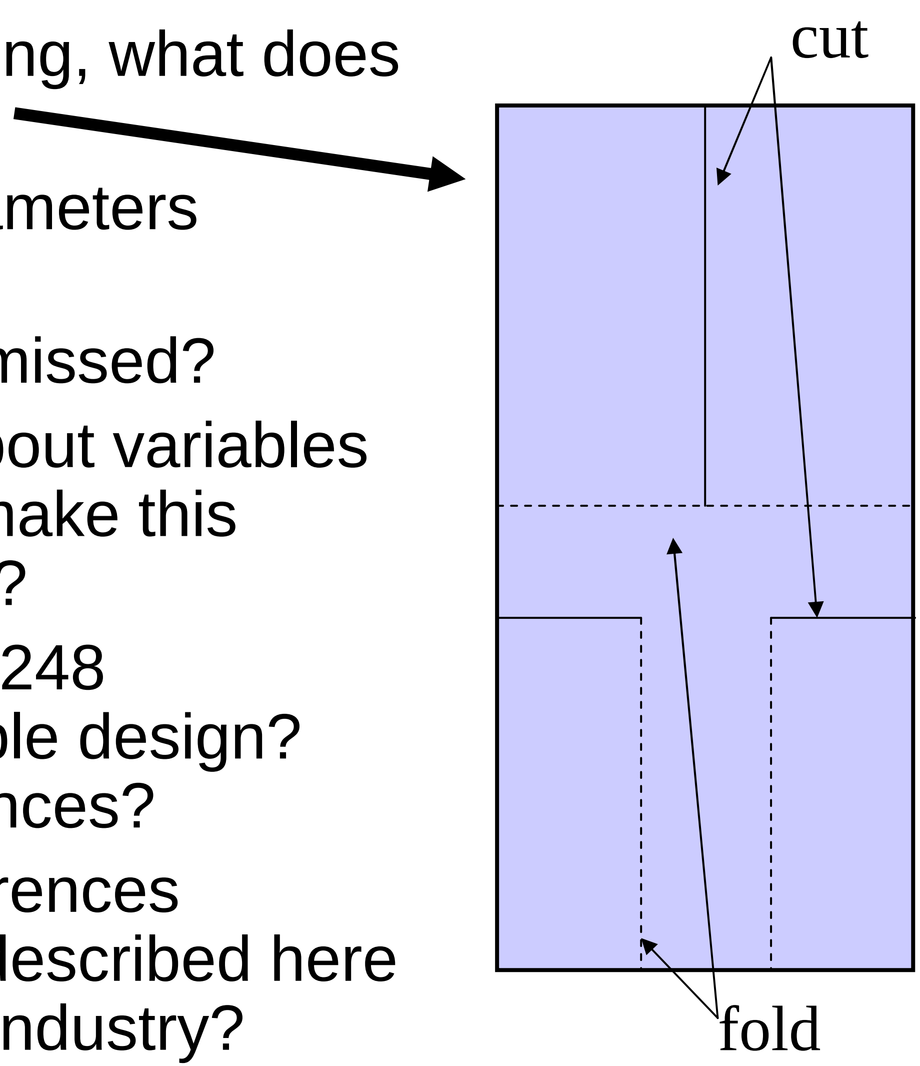
TABLE 10: Design III: Analysis of Variance for Completed Composite Design in Box and Liu, 1999.

- What would you conclude about lack of fit?
- What is being used as the denominator of F?

Thought Questions

- If we "optimize" this thing, what does that mean?
- How were design parameters chosen?
- Were important ones missed?
- What does Box say about variables being recombined to make this process more efficient?
- Is it reasonable to run 248 experiments on a simple design? Under what circumstances?
- What are the key differences between the process described here and system design in industry?



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"An experiment is simply a question put to nature … The chief requirement is simplicity: only one question should be asked at a time."

Russell, E. J., 1926, "Field experiments: How they are made and what they are," *Journal of the Ministry of Agriculture* **32**:989-1001.

Table III.

Plot	Mean yield (Bushels per acre)	Mean annual decrement (Bushels per acre)	Mean annual decrement %
5, no ammonia	14·18 ± ·44	·090	·63 ± ·16
6, single ammonia	22·58 ± ·71	·141	·62 ± ·19
7, double ,,	31·37 ± ·90	·144	·46 ± ·15
8, treble ,,	35·69 ± ·93	·092	·26 ± ·14

Fisher, R.A., 1921, "Studies in Crop Variation. I. An Examination of the Yield of Dressed Grain from Broadbalk," *Journal of Agricultural Science* **11**:107-135.

“To call in the statistician after the experiment is done may be no more than asking him to perform a post-mortem examination: he may be able to say what the experiment died of.”

- Fisher, R. A., Indian Statistical Congress, Sankhya, 1938.

	2M EARLY	2S LATE		2S LATE			1S EARLY
1S EARLY	1M EARLY	1M LATE	1S LATE	2M EARLY	2M LATE	1M EARLY	1M LATE
	2M LATE		2S EARLY		1S LATE		2S EARLY
2S EARLY	2M EARLY		1M LATE		2S EARLY	2S LATE	2M LATE
	1S LATE	1S EARLY	1M EARLY	1M LATE			1S LATE
2M LATE		2S LATE		2M EARLY		1M EARLY	1S EARLY
2S EARLY	2M LATE	1S EARLY	2M EARLY	2S LATE	2S EARLY	2M EARLY	
		1M LATE		1M EARLY	2M LATE		1M LATE
2S LATE	1M EARLY		1S LATE			1S EARLY	1S LATE
2M EARLY	1M EARLY	2M LATE	2S LATE	1S EARLY			1S LATE
1S LATE			1M LATE	1M EARLY	2S EARLY	2M LATE	
1S EARLY		2S EARLY			2M EARLY	2S LATE	1M LATE

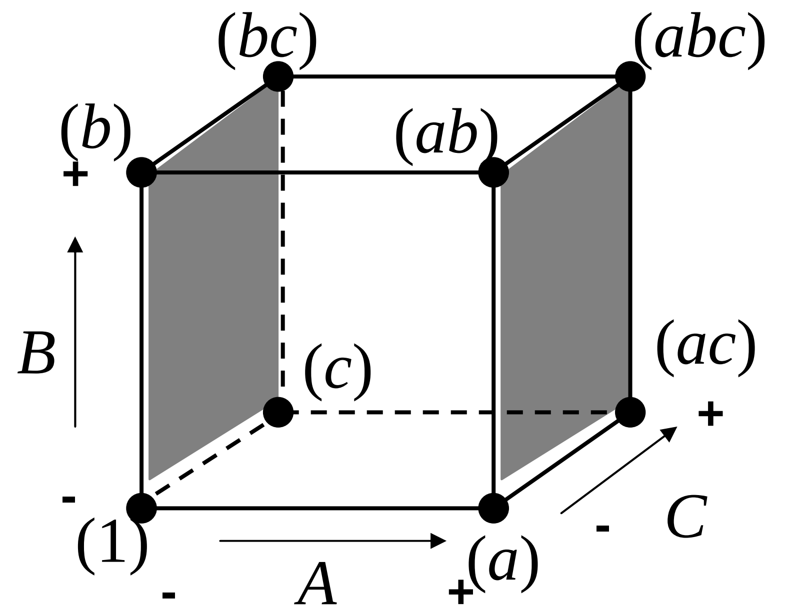
FIG. 1.—A COMPLEX EXPERIMENT WITH WINTER OATS.

Fisher, R. A., 1926, "The Arrangement of Field Experiments,"
Journal of the Ministry of Agriculture of Great Britain, 33: 503-513.

Concept Question

Say the independent experimental error of observations (a), (ab), et cetera is σ_{ε}.

We define the main effect estimate A to be



$$A \equiv \frac{1}{4}\left[(abc)+(ab)+(ac)+(a)-(b)-(c)-(bc)-(1)\right]$$

What is the standard deviation of the main effect estimate A?

1) $\sigma_A = \frac{1}{2}\sqrt{2}\sigma_{\varepsilon}$ 2) $\sigma_A = \frac{1}{4}\sigma_{\varepsilon}$ 3) $\sigma_A = \sqrt{8}\sigma_{\varepsilon}$ 4) $\sigma_A = \sigma_{\varepsilon}$

Response Surface Methodology

- A method to seek improvements in a system by sequential investigation and parameter design
  - Variable screening
  - Steepest ascent
  - Fitting polynomial models
  - Empirical optimization

Box, G. E. P. and Wilson, K. B. (1951), "On the Experimental Attainment of Optimum Conditions," *Journal of the Royal Statistical Society*, B13, 1-38.

Cross (or Product) Arrays

Noise Factors 2_{III}^{3-1}

	a	-1	-1	+1	+1
	b	-1	+1	-1	+1
	c	-1	+1	+1	-1

Control Factors

2_{III}^{7-4}

	A	B	C	D	E	F	G				
1	-1	-1	-1	-1	-1	-1	-1				
2	-1	-1	-1	+1	+1	+1	+1				
3	-1	+1	+1	-1	-1	+1	+1				
4	-1	+1	+1	+1	+1	-1	-1				
5	+1	-1	+1	-1	+1	-1	+1				
6	+1	-1	+1	+1	-1	+1	-1				
7	+1	+1	-1	-1	+1	+1	-1				
8	+1	+1	-1	+1	-1	-1	+1				

$$2_{III}^{7-4} \times 2_{III}^{3-1}$$

Taguchi, G., 1976, *System of Experimental Design*.

Robust Parameter Design

“Robust Parameter Design … is a statistical / engineering methodology that aims at reducing the performance variation of a system (i.e. a product or process) by choosing the setting of its control factors to make it less sensitive to noise variation."

Wu, C. F. J. and M. Hamada, 2000, *Experiments: Planning, Analysis, and Parameter Design Optimization*, John Wiley & Sons, NY.

George Box on Sequential Experimentation

"Because results are usually known quickly, the natural way to experiment is to use information from each group of runs to plan the next …"

"…Statistical training unduly emphasizes mathematics at the expense of science.   This has resulted in undue emphasis on "one-shot" statistical procedures… examples are hypothesis testing and alphabetically optimal designs."

Box, G. E. P. 1999, "Statistics as a Catalyst to Learning by Scientific Method: Part 2", *Journal of Quality Technology*, **31** (1): 16-29.

Majority View on "One at a Time"

One way of thinking of the great advances of the science of experimentation in this century is as **the <u>final demise</u> of the "one factor at a time" method**, although it should be said that there are still organizations which have never heard of factorial experimentation and use up many man hours wandering a crooked path.

Logothetis, N., and Wynn, H.P., 1994, *Quality Through Design: Experimental Design, Off-line Quality Control and Taguchi's Contributions*, Clarendon Press, Oxford.

My Observations of Industry

- Farming equipent company has reliability problems
- Large blocks of robustness experiments had been planned at outset of the design work
- More than 50% were not finished
- Reasons given
  - Unforseen changes
  - Resource pressure
  - Satisficing

"Well, in the third experiment, we found a solution that met all our needs, so we cancelled the rest of the experiments and moved on to other tasks…"

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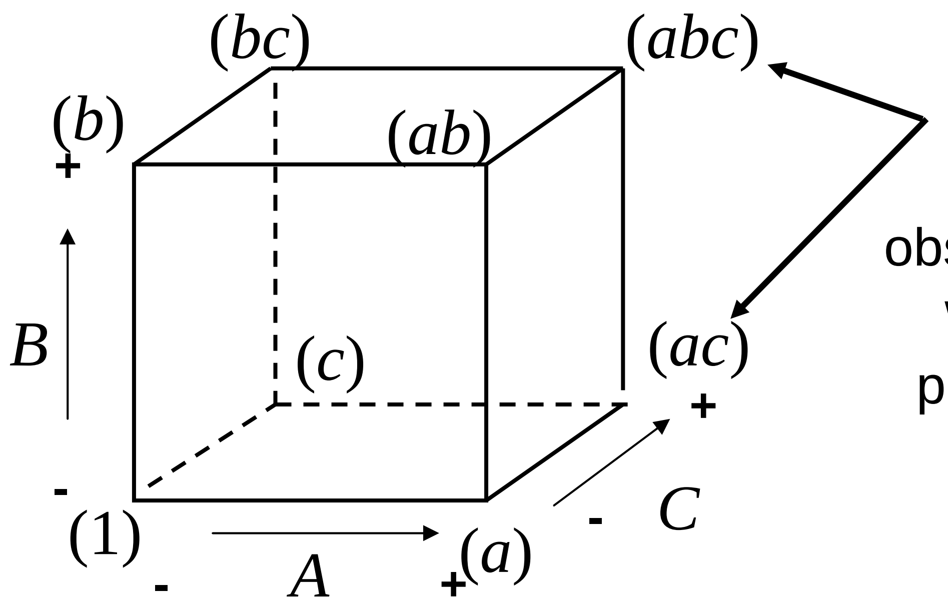
Basic Terms in Factorial DOE

- **Response –** the output of the system you are measuring
- **Factor** – an input variable that may affect the response
- **Level** – a specific value a factor may take
- **Trial** – a single instance of the setting of factors and the measurement of the response
- **Replication** – repeated instances of the setting of factors and the measurement of the response
- **Effect** – what happens to the response when factor levels change
- **Interaction** – joint effects of multiple factors

Cuboidal Representation



This notation indicates observations made with factors at particular levels.

Exhaustive search of the space of 3 discrete 2-level factors is the full factorial 2^3 experimental design

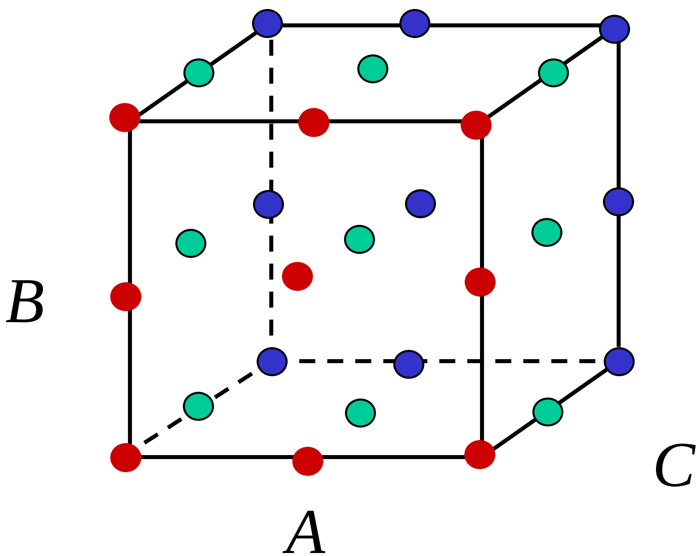
Tabular Representation

Trial	A	B	C
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

A cube has eight vertices

2^3 Design

Three Level Factors



8 vertices +
12 edges +
6 faces +
1 center =
27 points

3^3 Design

Creating and Randomizing Full Factorials in Matlab

```
X = fullfact([4 3]);
r=rand(1,4*3);
[B,INDEX] = sort(r);
Xr(1:4*3,:)=X(INDEX,:);
```

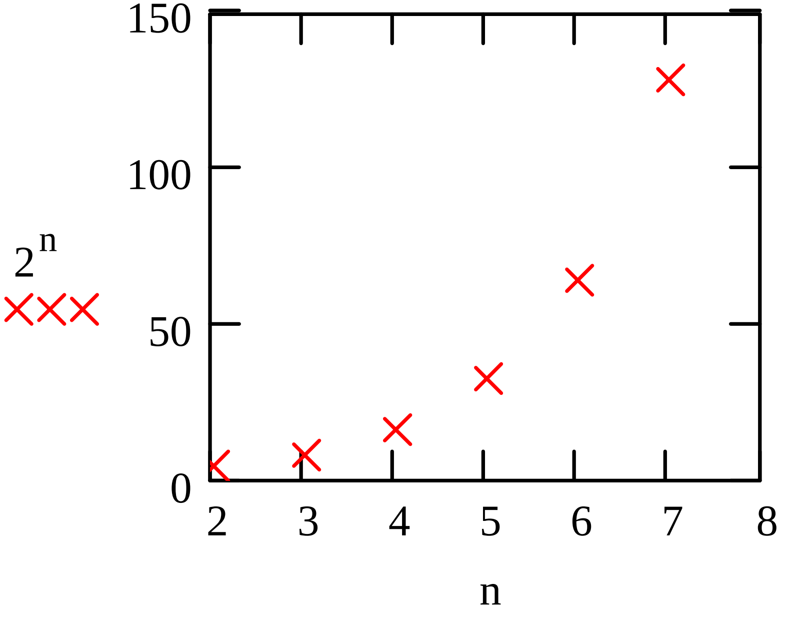
X

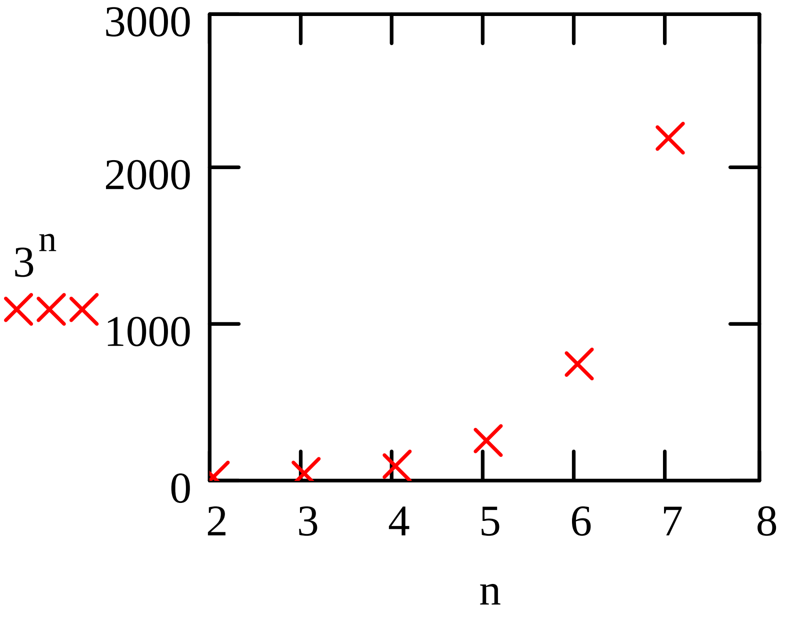
1	1
2	1
3	1
4	1
1	2
2	2
3	2
4	2
1	3
2	3
3	3
4	3

Xr

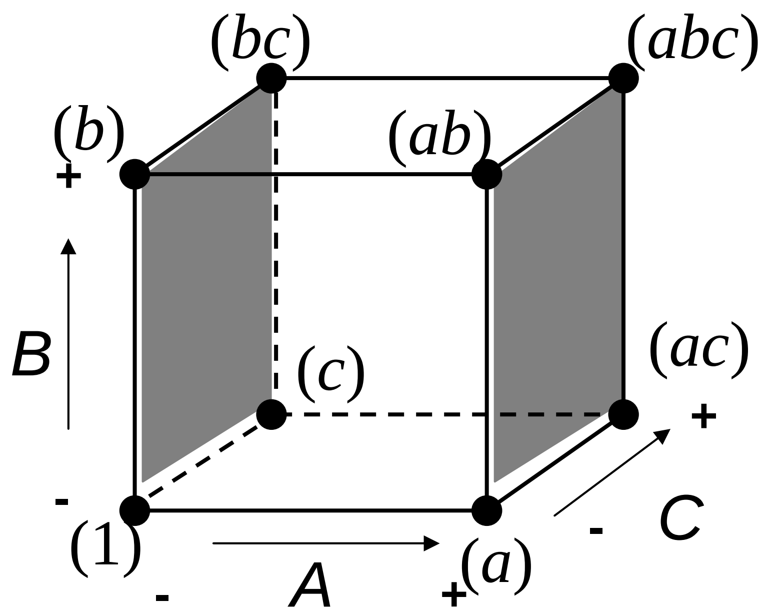
3	2
1	1
3	1
2	2
2	1
1	2
4	3
1	3
3	3
4	1
4	2
2	3

Geometric Growth of Experimental Effort



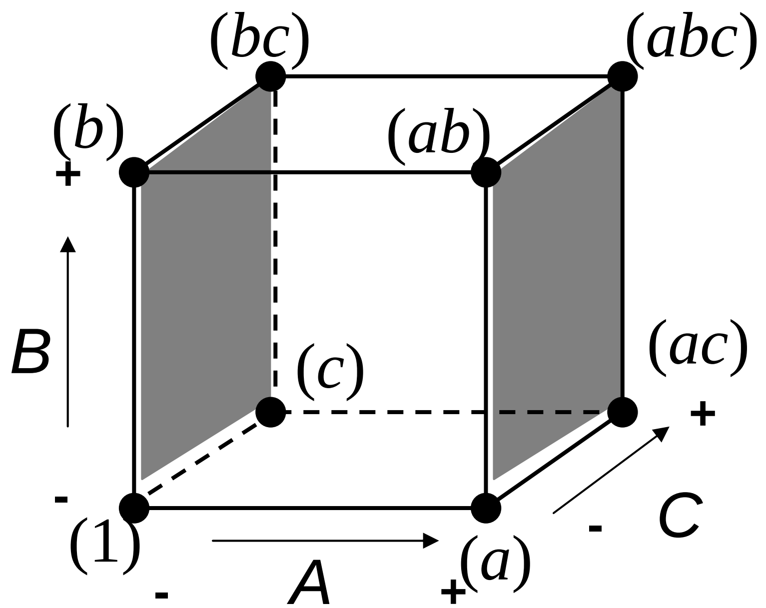


Calculating Main Effects



$$A \equiv \frac{1}{4}\left[(abc)+(ab)+(ac)+(a)-(b)-(c)-(bc)-(1)\right]$$

Concept Test

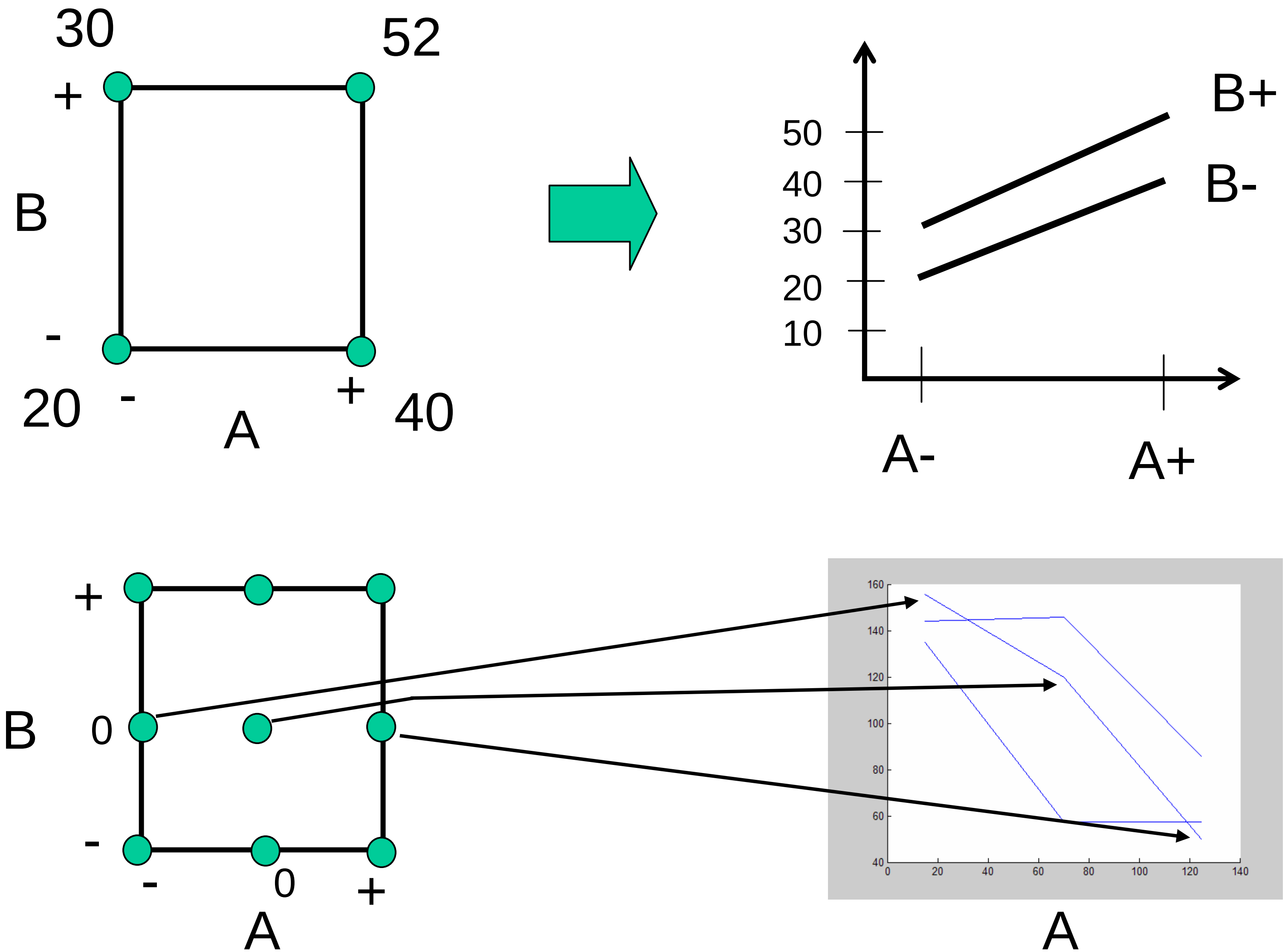


If the standard deviation of (a), (ab), et cetera is σ, what is the standard deviation of the main effect estimate A?

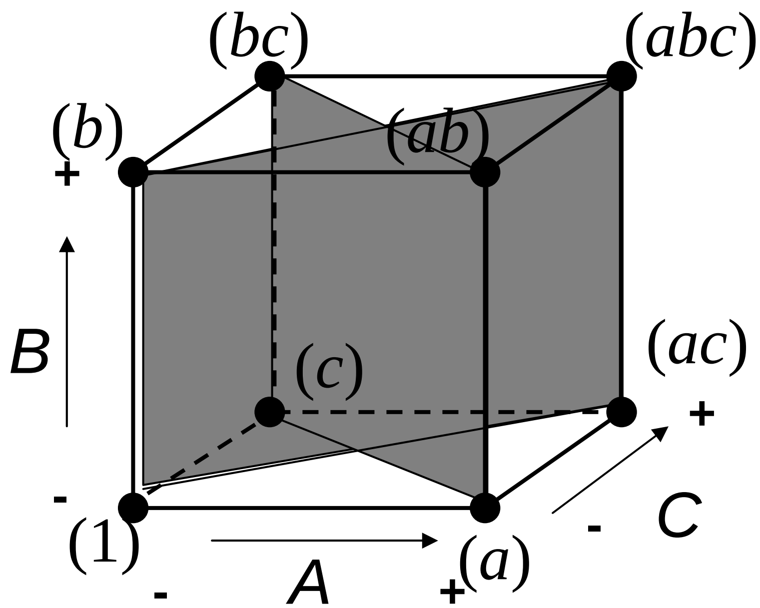
$$A \equiv \frac{1}{4}\left[(abc)+(ab)+(ac)+(a)-(b)-(c)-(bc)-(1)\right]$$

1) σ 2) Less than σ 3) More than σ 4) Not enough info

Factor Effect Plots



Calculating Interactions



$$AC \equiv \frac{1}{4}\left[(abc)+(ac)+(b)+(1)-(ab)-(bc)-(c)-(a)\right]$$

Treatment Effects Model (Two Factors)

$$y_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases}$$

$$\sum \tau_i = 0$$

If factor a has two levels

$$\tau_1 + \tau_2 = 0$$

$$\tau_1 = -\tau_2$$

$$\boxed{\tau_1 = -\frac{A}{2}} \qquad \boxed{\tau_2 = \frac{A}{2}}$$

Treatment Effects Model (Two Factors)

this is not a product

$$y_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases}$$

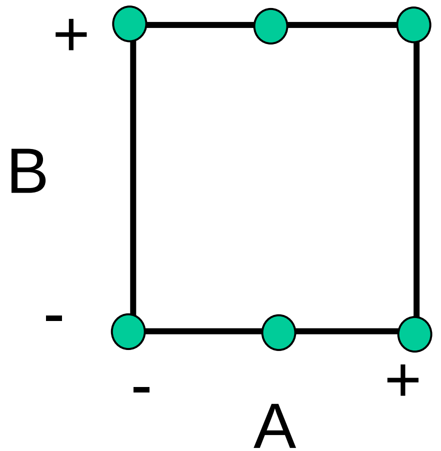
interactions – there are of ab these terms

$$\sum_{i=1}^{a} (\tau\beta)_{ij} = \sum_{j=1}^{b} (\tau\beta)_{ij} = 0$$

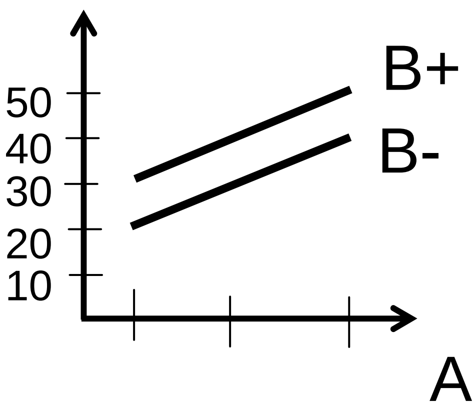
a+b equations
but only a+b-1
are independent

(a-1)(b-1) DOF

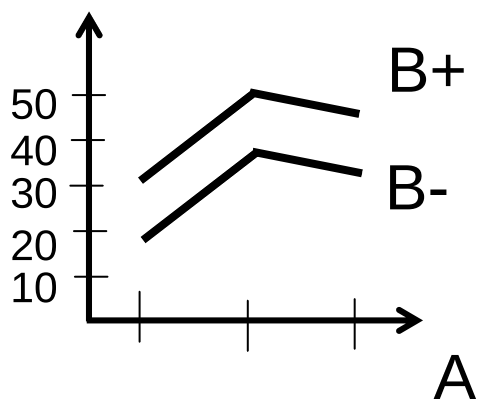
Concept Test



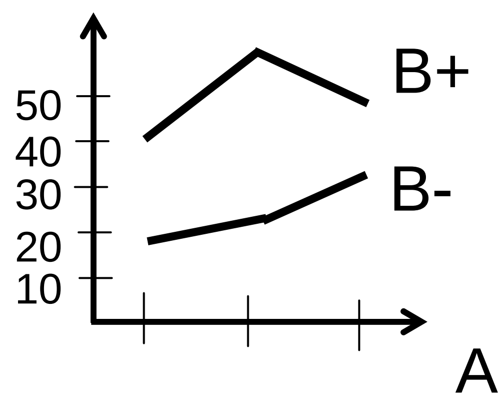
If there are no interactions in this system, then the factor effect plot from this design could look like:



1



2



3

Hold up all cards that apply.

Treatment Effects Model versus the Regression Model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon$$

$$y_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk}$$

- If the factors are <u>two level</u> factors
- And they are coded as (-1,+1)
- Then $\tau_2 = \beta_1 \quad \tau_1 = -\beta_1$
- And $(\tau\beta)_{12} = \beta_{12}$

Recall from the lecture on multiple regression

Estimation of the Parameters β

Assume the model equation

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

We wish to minimize the sum squared error

$$L = \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} = \left(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\right)^T \left(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\right)$$

To minimize, we take the derivative and set it equal to zero

$$\left.\frac{\partial L}{\partial \boldsymbol{\beta}}\right|_{\hat{\boldsymbol{\beta}}} = -2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}}$$

The solution is

$$\boxed{\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}}$$

And we define the fitted model

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$$

Estimation of the Parameters β when $\mathbf{X}$ is a 2^k design

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$$

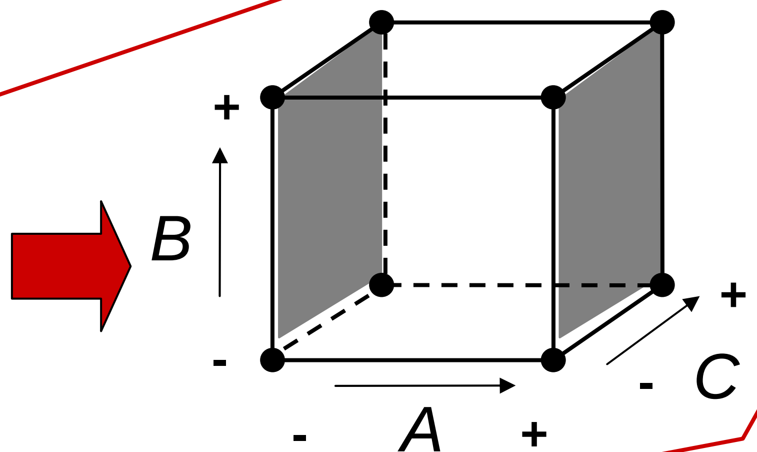
$$\left(\mathbf{X}^T\mathbf{X}\right)_{ij} = 0 \ \text{ if } i \neq j$$

The columns are orthogonal

$$\left(\mathbf{X}^T\mathbf{X}\right)_{ij} = n2^k \ \text{ if } i = j$$

$$\left(\mathbf{X}^T\mathbf{X}\right)^{-1} = \frac{1}{n2^k}\mathbf{I}$$

$$\left[\mathbf{X}^T\mathbf{y}\right]_1$$



Breakdown of Sum Squares

"Grand Total Sum of Squares"

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk}^{\;2}$$

SS due to mean $= N\bar{y}_{...}^{\;2}$

"Total Sum of Squares"

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk} - \bar{y}_{...})^2$$

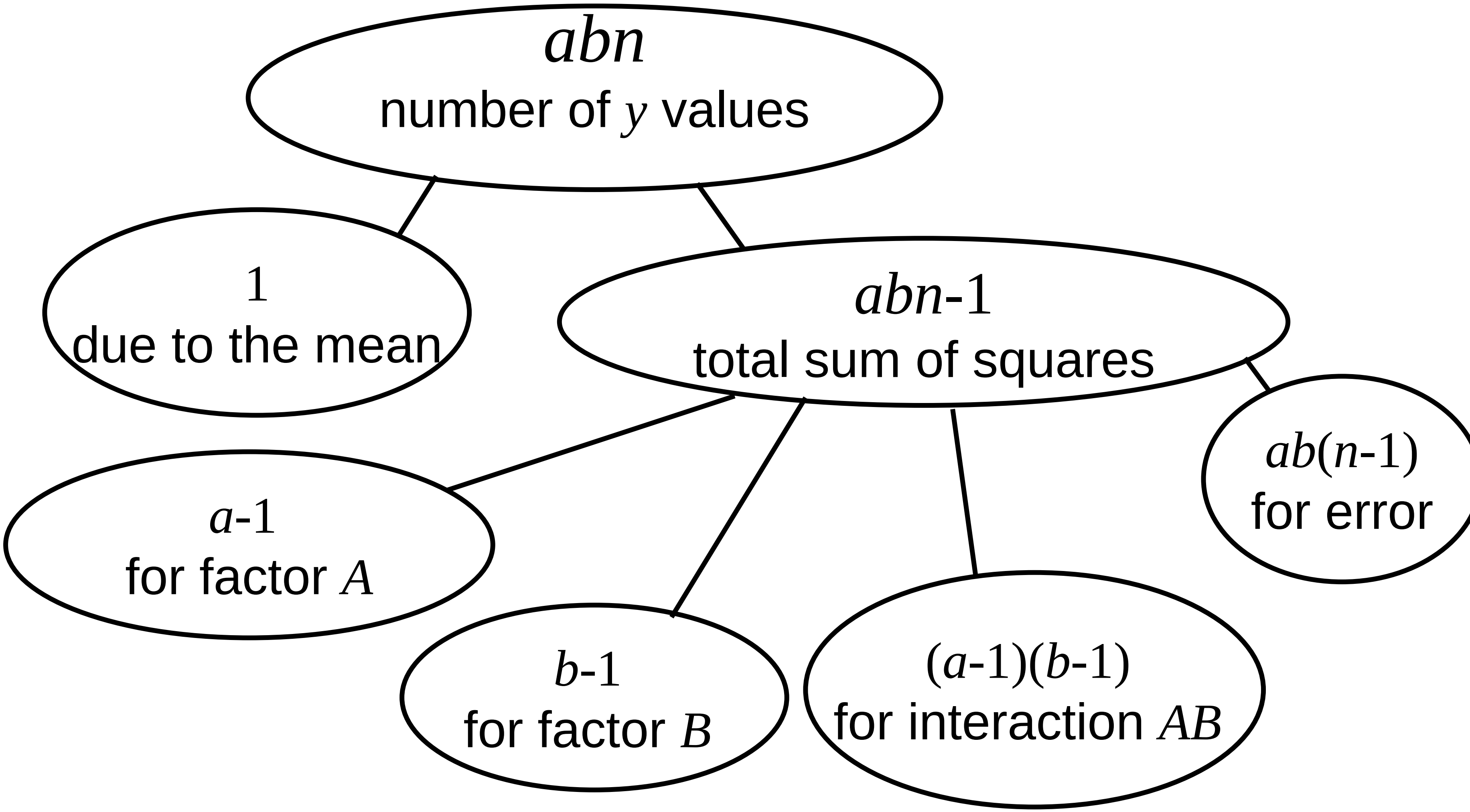
$$SS_E$$

$$SS_A = bn\sum_{i=1}^{a}(\bar{y}_{i..} - \bar{y}_{...})^2$$

$$SS_{AB} = n\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} - \bar{y}_{...})^2$$

$$SS_B = an\sum_{j=1}^{b}(\bar{y}_{.j.} - \bar{y}_{...})^2$$

Breakdown of DOF



Hypothesis Tests in Factorial Exp

- Equality of treatment effects due to factor A or due to factor B

$$H_0: \tau_1 = \tau_2 = \ldots = \tau_a = 0$$

$$H_1: \tau_i \neq 0 \text{ for at least one } i$$

$$H_0: \beta_1 = \beta_2 = \ldots = \beta_a = 0$$

$$H_1: \beta_i \neq 0 \text{ for at least one } i$$

- Test statistic $F_0 = \dfrac{MS_A}{MS_E}$ $\quad F_0 = \dfrac{MS_B}{MS_E}$

- Criterion for rejecting H_0

$$F_0 > F_{\alpha, a-1, ab(n-1)} \qquad F_0 > F_{\alpha, b-1, ab(n-1)}$$

Hypothesis Tests in Factorial Exp

- Significance of *AB* interactions

$$H_0 : \tau\beta_{ij} = 0 \ \text{ for all } i, j$$

$$H_1 : \text{at least one } \ \tau\beta_{ij} \neq 0$$

- Test statistic

$$F_0 = \frac{MS_{AB}}{MS_E}$$

- Criterion for rejecting H_0

$$F_0 > F_{\alpha,(a-1)(b-),ab(n-1)}$$

Example 5-1 – Battery Life

```
FF= fullfact([3 3]);
X=[FF; FF; FF; FF];
Y=[130 150 138 34 136 174  20  25 96 155 188 110 40 122
120 70 70 104 74 159 168 80 106 150 82 58 82 180 126 160
75 115 139 58 45 60]';

[p,table,stats]=anovan(Y,{X(:,1),X(:,2)},'interaction');

hold off; hold on
for i=1:3;  for j=1:3;
intplt(i,j)=(1/4)*sum(Y.*(X(:,1)==j).*(X(:,2)==i)); end
plot([15 70 125],intplt(:,i)); end
```

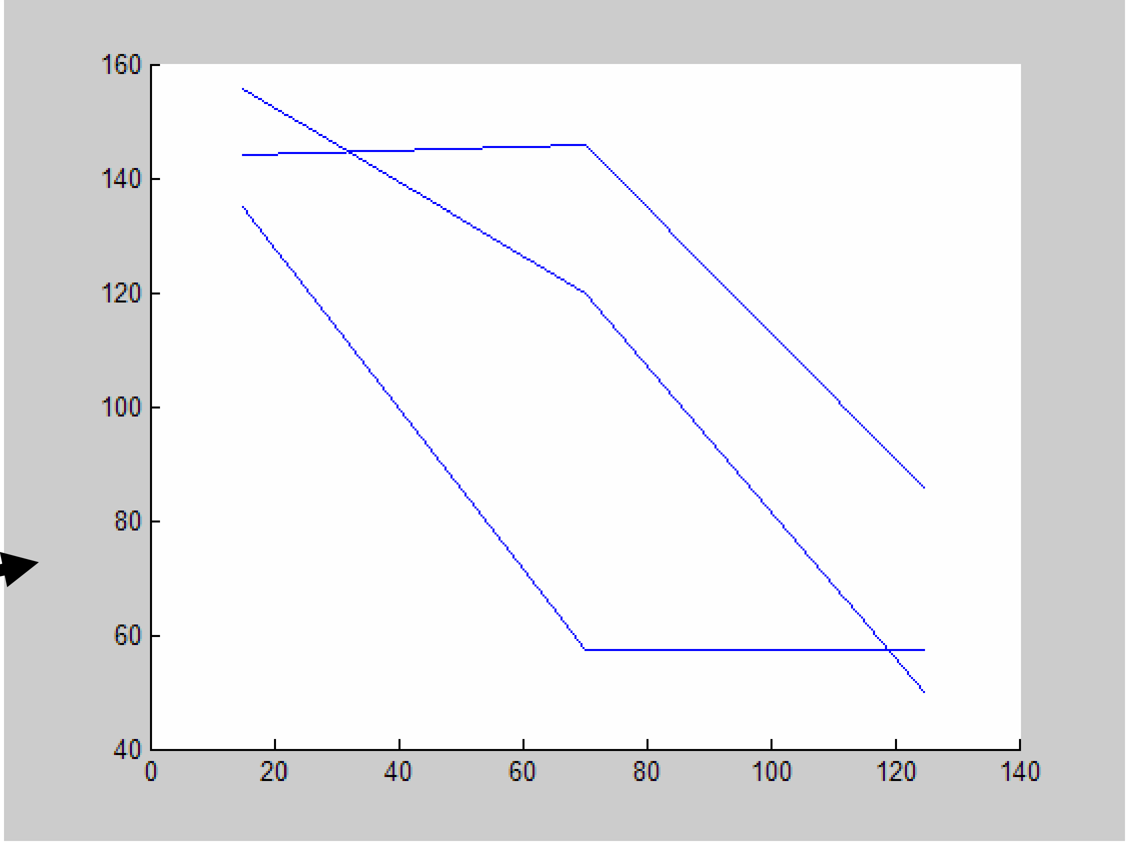
Analysis of Variance

Source	Sum Sq.	d.f.	Mean Sq.	F	Prob>F
X1	10683.7	2	5341.9	7.91	0.002
X2	39118.7	2	19559.4	28.97	0
X1*X2	9613.8	4	2403.4	3.56	0.0186
Error	18230.7	27	675.2		
Total	77647	35			

Constrained (Type III) sums of squares.

ANOVA table

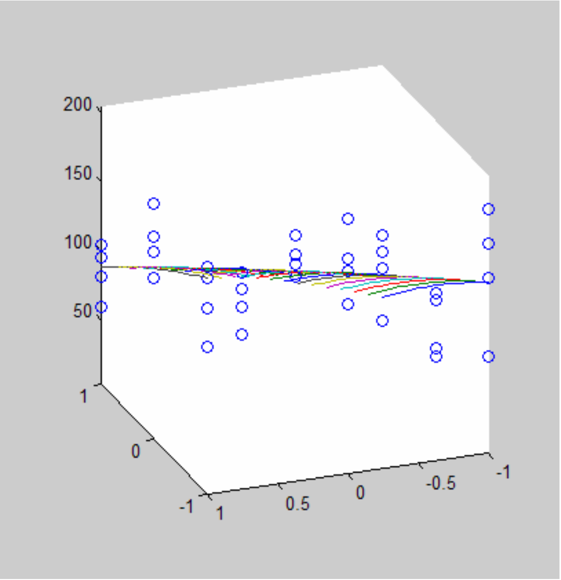
Interaction plot



Regression – Battery Life

```
FF= fullfact([3 3]);
A=FF(:,1)-2;  B=FF(:,2)-2;  ones(1:3*3)=1;
R=[ones' A B A.*A B.*B A.*B ];
X=[R; R; R; R];
Y=[130 150 138 34 136 174  20  25 96 155 188 110 40 122
120 70 70 104 74 159 168 80 106 150 82 58 82 180 126 160
75 115 139 58 45 60]';

[b,bint,r,rint,stats] = regress(Y,X,0.05);
[t,m] = meshgrid(-1:.1:1,-1:.1:1);
Yhat= b(1)+b(2)*t+b(3)*m+b(4)*t.*t+b(5)*r
hold off; h=plot3(t,m,Yhat);
hold on; scatter3(X(:,2),X(:,3),Y);
```



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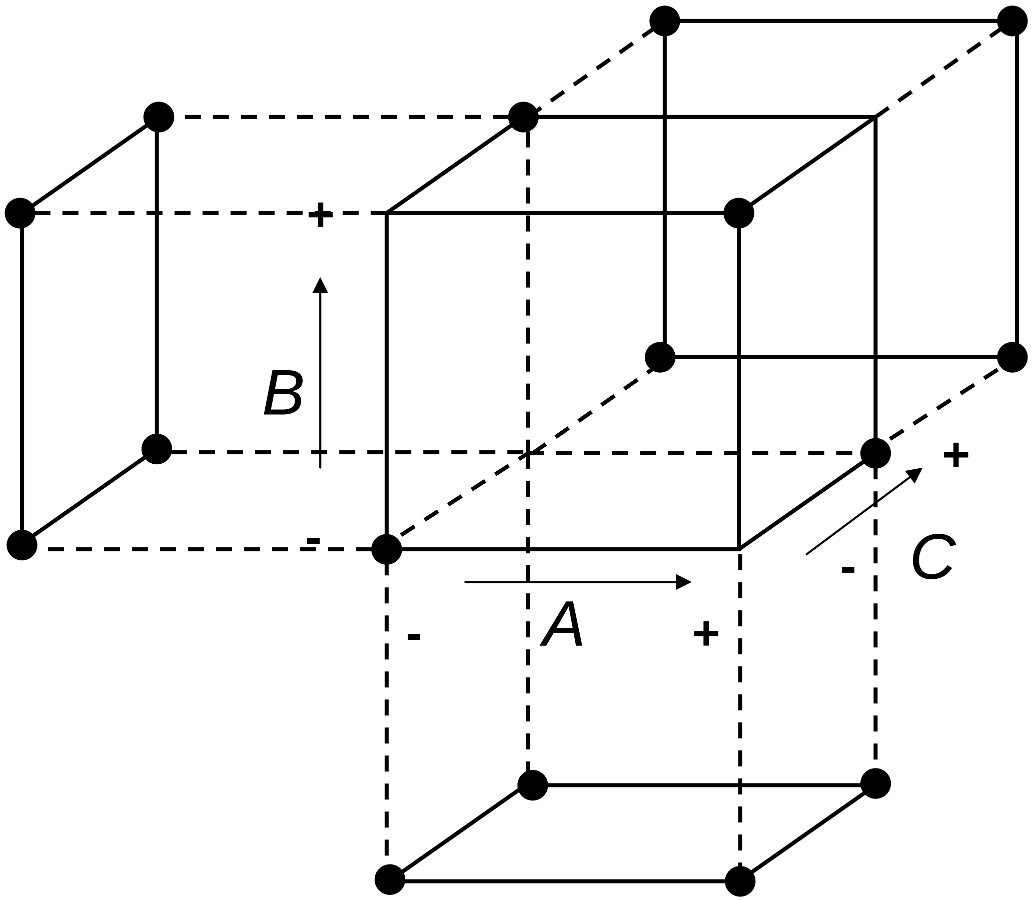
➡ Fractional factorial designs

Fractional Factorial Experiments

Cuboidal Representation



This is the 2^{3-1} fractional factorial.

Fractional Factorial Experiments

Tabular Representation

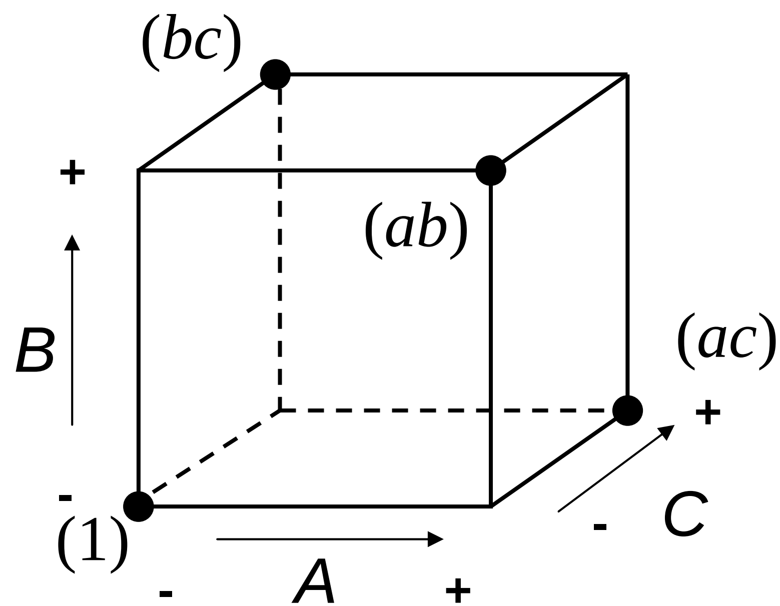
Trial	A	B	C	D	E	F	G	FG=-A
1	-1	-1	-1	-1	-1	-1	-1	+1
2	-1	-1	-1	+1	+1	+1	+1	+1
3	-1	+1	+1	-1	-1	+1	+1	+1
4	-1	+1	+1	+1	+1	-1	-1	+1
5	+1	-1	+1	-1	+1	-1	+1	-1
6	+1	-1	+1	+1	-1	+1	-1	-1
7	+1	+1	-1	-1	+1	+1	-1	-1
8	+1	+1	-1	+1	-1	-1	+1	-1

2^{7-4} Design
Resolution III.

Two-way interactions are aliased with main effects

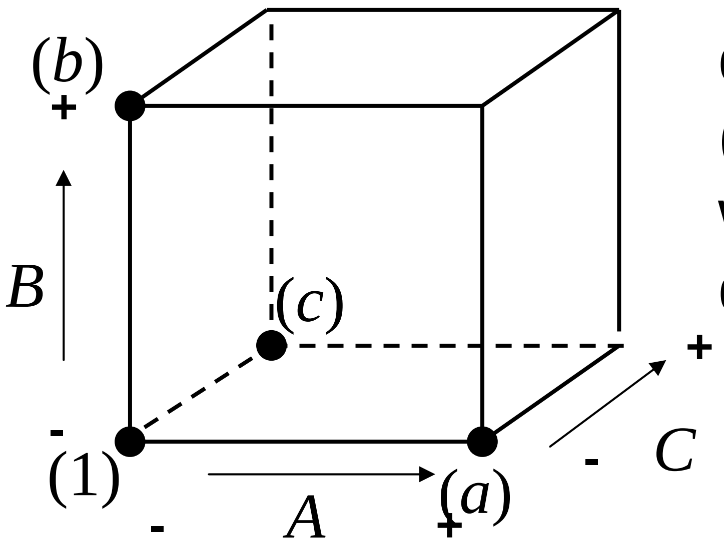
Fractional Factorial Experiments

Cuboidal Representation



$$A = \frac{1}{2}\left[(ab) + (ac) - (1) - (bc)\right]$$

One at a Time Experiments



If the standard deviation of (a) and (1) is σ, what is the standard deviation of A?

Provides resolution of individual factor effects

But the effects may be biased

$$A \approx (a) - (1)$$

Efficiency

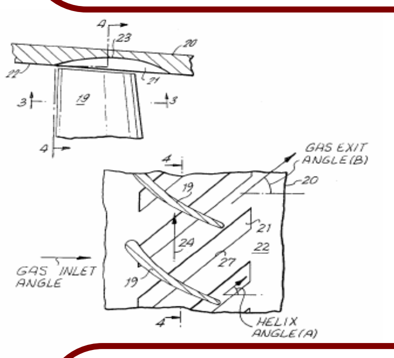
- The variance for OFAT is $\sqrt{2}\sigma$ using 4 experiments
- The standard deviation for 2^{3-1} was σ using 4 experiments
- The inverse ratio of variance per unit is considered a measure of *relative efficiency*

$$\frac{\left[\sqrt{2}\sigma\right]^2}{4} \Bigg/ \frac{\left[\sigma\right]^2}{4} = 2$$

- The 2^{3-1} is considered 2 times more efficient than the OFAT

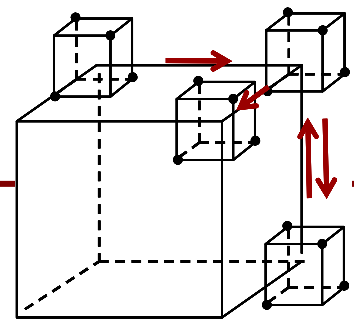
Overview Research

Concept Design



Outreach to K-12

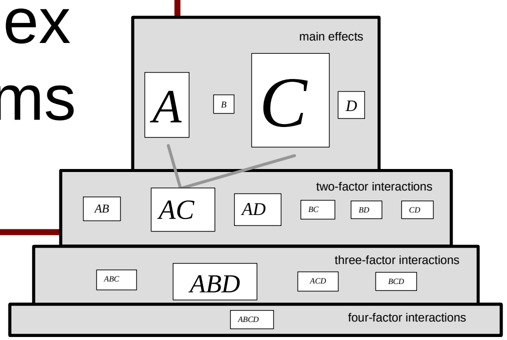
PBS show "Design Squad"

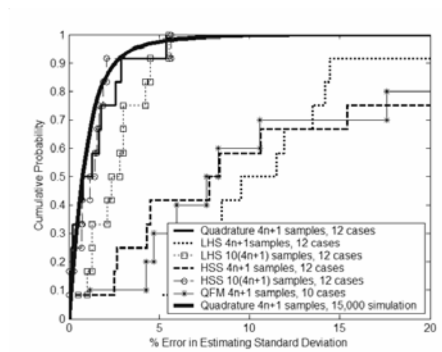


Adaptive Experimentation and Robust Design

$$\Pr\left(\beta_{12}x_1^*x_2^*>0 \middle| \beta_{12}>\beta_{ij}\right)>\frac{1}{\pi}\binom{n}{2}\int_0^\infty\int_{-x_2}^\infty \frac{\left[erf\left(\frac{1}{\sqrt{2}}\frac{x_1}{\sigma_{INT}}\right)\right]^{\binom{n}{2}-1} e^{\frac{-x_1^2}{2\sigma_{INT}^2}+\frac{-x_2^2}{2\left(\sigma_{ME}^2+(n-2)\sigma_{INT}^2+\frac{1}{2}\sigma_\varepsilon^2\right)}}}{\sigma_{INT}\sqrt{\sigma_{ME}^2+(n-2)\sigma_{INT}^2+\frac{1}{2}\sigma_\varepsilon^2}}dx_2dx_1$$

Complex Systems





Methodology Validation

Next Steps

- Friday 27 April
  - Recitation to support the term project
- Monday 30 April
  - Design of Experiments: Part 2
- Wednesday 2 May
  - Design of Computer Experiments
- Friday 4 May
  - Exam review
- Monday 7 May – Frey at NSF
- Wednesday 9 May – Exam #2