01NAEX - Lecture 03 Factorial design

Jiri Franc

Czech Technical University
Faculty of Nuclear Sciences and Physical Engineering
Department of Mathematics

Introduction to Blocking, Nuisance factors, and Factorial Design D. C. Montgomery, Design and Analysis of Experiment: Section 4.1

- The randomized complete block design (RCBD).
- Extension of the single factor ANOVA to the RCBD.
- General principles of factorial experiments.
- The two factor factorial with fixed effects.
- The ANOVA for factorials.
- Extensions to more than two factors.
- Quantitative and qualitative factors, response curves and surfaces.
- Estimation of Sample Size.
- Other blocking scenarios (Latin square designs, ...) and Incomplete Block design will be covered next lesson.

Introduction to Blocking and Nuisance Factors

Blocking is a technique for dealing with nuisance factors

- A nuisance factor is a factor that probably has some effect on the response, but it s of no interest to the experimenter however, the variability it transmits to the response needs to be minimized.
- Typical nuisance factors include batches of raw material, operators, pieces of test equipment, time (shifts, days, etc.), different experimental units.
- Failure to block is a common flaw in the design of a experiment and data analysis.

If the nuisance variable is known and controllable, we use blocking:

- If the nuisance factor is known and uncontrollable, sometimes we can use the analysis of covariance to remove the effect of the nuisance factor from the analysis.
- If the nuisance factor is unknown and uncontrollable, we hope that randomization balances out its impact across the experiment.
- Sometimes several sources of variability are combined in a block, so the block becomes an aggregate variable.

When to Block vs When to Just Randomize

Nuisance vs noise

- Nuisance factor = known source of systematic variability.
- ▶ **Noise** = unknown, many tiny influences you can't name.

Decision guide

- ► Known & assignable (day/operator/lot) ⇒ block it.
- **Unknown/weak** ⇒ rely on **randomization**, check residuals vs run.
- ▶ **Trade-off:** Blocking uses b-1 **df**; does it noticeably **reduces** MS_E ?.

Practical checklist

- Define blocks so each block is as homogeneous as possible.
- Randomize within each block. (Pre-print run sheets.)
- ▶ If β ^{block} looks tiny and insignificant, consider CRD.

Fun fact: If Monday are a nuisance factors, block it.

Q: In a thermal test, which would you block - oven, operator, or day? Why?

RCBD Model & ANOVA

Model (no treatment-by-block interaction):

$$y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}$$
, $i = 1, ..., a$ (treatments), $j = 1, ..., b$ (blocks), $\sum \tau_i = \sum \beta_j = 0$.

Source	df	SS	MS / Test
Treatments (τ)	a – 1	SS_T	$MS_T = SS_T/df_T$
Blocks (β)	<i>b</i> − 1	SS_B	$MS_B = SS_B/df_B$
Error	abn-a-b+1	SS_E	$MS_E = SS_E/df_E$

Tests: $F_T = MS_T/MS_E$ (treatment), $F_B = MS_B/MS_E$ (block).

N: If treatment-by-block interaction is significant, include it.

What Blocking Buys You

Model: $y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}$, $\varepsilon_{ij} \sim (0, \sigma^2)$, blocks variability $Var(\beta_j) = \sigma_\beta^2$.

Without block (CRD): block shifts leak into error \Rightarrow error variance $\approx \sigma^2 + \sigma_{\beta}^2$. With block (RCBD): the block mean is removed \Rightarrow error variance stays σ^2 .

Gain in signal-to-noise:

$$F = rac{MS_{ au}}{MS_{E}}$$
 increases with: $Gain pprox rac{\sigma^{2} + \sigma_{eta}^{2}}{\sigma^{2}} = 1 + rac{\sigma_{eta}^{2}}{\sigma^{2}}.$

Example: If measurement noise $\sigma = 1$ and day-to-day shifts $\sigma_{\beta} = 2$,

Gain
$$\approx 1 + \frac{4}{1} = 5 \times \text{ (much larger } F \text{ with blocks)}.$$

Always randomize within blocks and check residuals vs run order.

Q: If σ_{β}^2 is nearly zero, what 's the cost/benefit of blocking? *Hint*: You spend df but gain little precision.

- We wish to determine whether different tips produce different (mean) hardness reading on a tester machine.
- 4 different types of tips: conical, ball, cylinder, and cube.
- The test coupons (experimental unit) are a source of nuisance variability.
- Experimental error measures both random error and variability between coupons.
- ➤ To conduct this experiment as a RCBD, assign all 4 tips to each coupon.
- Each coupon is called a **block**; that is, it is a more homogeneous experimental unit on which to test the tips.
- Variability between blocks can be large, variability within a block should be relatively small.

In general, a block is a specific level of the nuisance factor. A complete replicate of the basic experiment is conducted in each block and all runs within a block are randomized.

Randomized Complete Block Design for the Hardness Testing Experiment

Test Coupon (Block)

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

In completely randomized single-factor design, 16 different metal test coupons would be required, one for each run in the design.

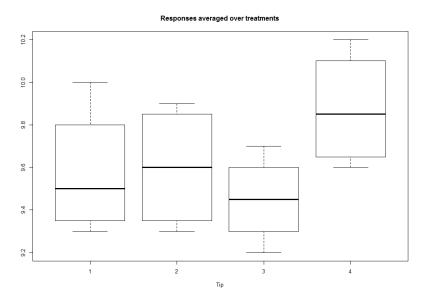
In RCBD, the variability between coupons from the experimental error is removed.

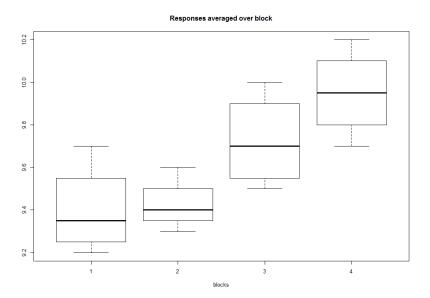
Only randomization of treatments (Tips) is within the blocks, i.e. blocks represent a restriction on randomization.

The two-way structure of the experiment (Tips x Blocks)

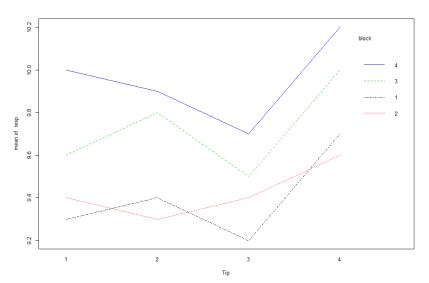
Tip		Test Coup	on (Block)	
Number	1	2	3	4
1	9.3	9.4	9.6	10.0
2	9.4	9.3	9.8	9.9
3	9.2	9.4	9.5	9.7
4	9.7	9.6	10.0	10.2

- We are interested in testing the equality of treatment means (again).
- We have to remove the variability associated with the nuisance factor (the blocks).
- Analysis is identical to the two-factor factorial design without replication.

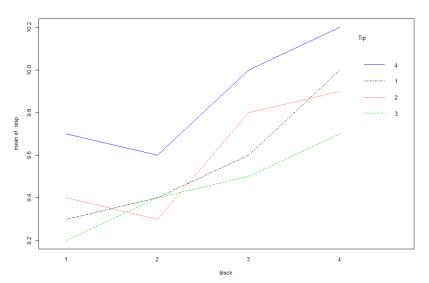




Interaction plot over Tips.



Interaction plot over Blocks.



ANOVAfor the RCBD

Effects model for the RCBD:

$$y_{ij} = \mu_{ij} + \epsilon_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij}$$
 $i = 1, 2, ..., a$ $j = 1, 2, ..., b$,

where μ is an overall mean, τ_i is the effect of the *i*th treatment, β_j is the effect of the *j*th block and $\epsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$ random error term.

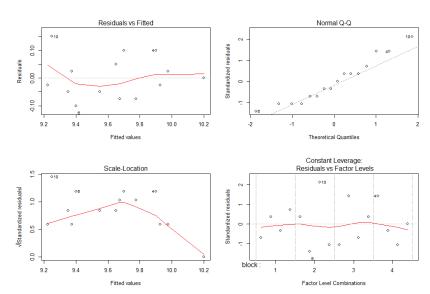
Analysis of Variance for a Randomized Complete Block Design

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Treatments	$SS_{Treatments}$	a – 1	$\frac{SS_{\text{Treatments}}}{a-1}$	$\frac{MS_{\text{Treatment}}}{MS_E}$
Blocks	$SS_{ m Blocks}$	b - 1	$\frac{SS_{\text{Blocks}}}{b-1}$	
Error	SS_E	(a-1)(b-1)	$\frac{SS_E}{(a-1)(b-1)}$	
Total	SS_T	N-1		
	$= SS_T - SS_{Treatm}$ $= \sum_{a}^{a} \sum_{b}^{b} (y_{ij} - \bar{y})$) ²

The results obtained from this experiment and RCBD differ from results obtained from Completely Randomized Design.

Note, that the MS for Residuals has more than tenfold. All of the variability due to blocks is now in the error term.

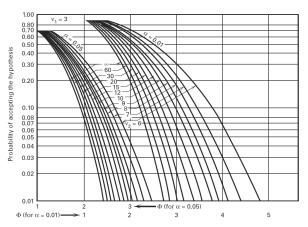
Model adequacy checking:



Suppose that we would like to be able to determine the appropriate number of blocks to run if we are interested in detecting a true max difference in readings of 0.4 with a high probability and the estimate of the standard deviation is 0.1.

$$\Phi^2=rac{bD^2}{2a\sigma^2}$$
 ,where Φ^2 is related to noncentral r.v. $F_0=rac{MS_{\textit{Treatments}}}{MS_{\textit{Error}}}$

OC Curves for the Fixed-Effects Model ANOVA



 $u_1=(a-1)$ Numerator df , $u_2=(a-1)(b-1)$ Denominator df

Power Planning - What Are We Guaranteeing?

Goal: Choose *n* so the test rejects with probability $\geq 1 - \beta$ when *meaningful* differences exist (at level α).

Two common settings

- RCBD (Treatment + Block): Power the treatment main effect A. Factor B is a nuisance that reduces noise.
- **Two-treatment factorial:** Power A, B, and interaction $A \times B$.

Detectable size(s): Specify minimally important differences:

$$D_A$$
, D_B , D_{AB} (difference-of-differences).

Q: Is your study

- confirmatory (stricter Family Wise Error Rate (FWER) control)?
- exploratory (report CIs with less stringent False Discovery Rate (FDR) control)?

RCBD (Treatment + Block) & Operating Characteristic (OC)

Model (balanced, *n* per cell):

$$y_{ijr} = \mu + \tau_i + \beta_j + \varepsilon_{ijr}, \quad i = 1..a, \ j = 1..b, \ r = 1..n, \quad \varepsilon_{ijr} \sim N(0, \sigma^2),$$

$$\sum_i \tau_i = \sum_i \beta_j = 0.$$

Test of interest (treatments): $H_0: \tau_1 = \cdots = \tau_a = 0$ with

$$F_0 = \frac{\textit{MS}_A}{\textit{MS}_E}, \qquad \mathsf{df}_A = a - 1, \quad \mathsf{df}_E = \begin{cases} (a - 1)(b - 1), & n = 1 \\ ab(n - 1), & n > 1 \end{cases}$$

Under H_1 : $F_0 \sim F_{\text{num df, den df}}(\lambda)$ (noncentral F).

Power at level α :

$$1-\beta = \Pr(F_{\text{num df, den df}}(\lambda) > F_{\alpha; \text{ num df, den df}}).$$

Scaled distance (OC parameter): We use

$$\Phi^2 \equiv \frac{\lambda}{\text{num df}},$$

so OC tables/curves are indexed by $(\alpha, df_{num}, df_{den}, \Phi^2)$.

Practical view: Bigger Φ^2 (or λ) \Rightarrow larger separation from $H_0 \Rightarrow$ higher power.

Noncentrality for Treatment (RCBD)

Let μ_i be the block-averaged mean for treatment i and $\bar{\mu}$ the grand mean. For balanced RCBD:

$$\lambda_A = \frac{nb}{\sigma^2} \sum_{i=1}^a (\mu_{i\cdot} - \bar{\mu})^2, \qquad \Phi_A^2 = \frac{\lambda_A}{a-1}.$$

Design target (pairwise): Detect *any* pairwise difference $\geq D_A$. **Least favorable configuration** (hardest to detect):

$$\mu_{1\cdot} = + D_A/2, \quad \mu_{2\cdot} = -D_A/2, \quad \mu_{3\cdot} = \cdots = \mu_{a\cdot} = 0 \Rightarrow \sum (\mu_{i\cdot} - \bar{\mu})^2 = D_A^2/2.$$

Therefore

$$\Phi_A^2 = rac{nb \, D_A^2}{2(a-1)\sigma^2} \, , \qquad \lambda_A = (a-1)\Phi_A^2 = rac{nb \, D_A^2}{2\sigma^2} .$$

Check: If b = 1, this reduces to the one-way formula.

Choosing n in RCBD (From OC Curves)

Given α , target power, a, b, and pilot $\hat{\sigma}^2$:

Recipe

- 1. From OC tables (or software), find $\Phi_{A,\star}^2$ that achieves the power with $df_A = a 1$, df_E as per design.
- 2. Solve for *n* from $\Phi_A^2 = \frac{nb D_A^2}{2(a-1)\hat{\sigma}^2}$:

$$n = \frac{2(a-1)\hat{\sigma}^2}{bD_A^2} \Phi_{A,\star}^2 \quad \text{(round up)}.$$

Heuristics: Halve $\hat{\sigma}^2 \Rightarrow$ halve n; double $D_A \Rightarrow$ quarter n; double $b \Rightarrow$ halve n.

Introduction to Factorial Design

- Factorial Designs are most efficient methods for experiments where we study the effects of two or more factors.
- The effect of the primary factor of interest in the experiment is called main effect.
- If the difference in response between the levels of one factor is not the same at all levels of other factors, the interaction occurs.

The Battery Design Example

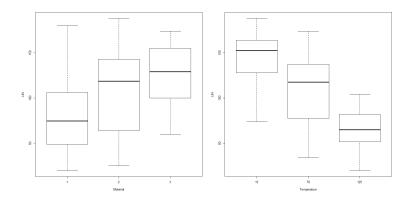
- ► Two factors: A = Material type; B = Temperature (quantitative variable)
- What effects do material type and temperature have on life?
- Is there a choice of material that would give uniformly long life regardless of temperature?

Life (in hours) Data for the Battery Design Example

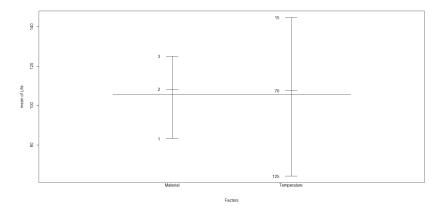
Material Type	Temperature (°F) 15 70				1	125	
	130	155	34	40	20	70	
	74	180	80	75	82	58	
2	150	188	136	122	25	70	
	159	126	106	115	58	45	
3	138	110	174	120	96	104	
	168	160	150	139	82	60	

Since there are two factors at three levels, this design is sometimes called a 3^2 factorial design.

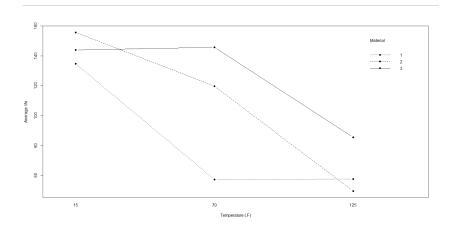
Box plot of data from the Battery Design Example



Effects plot of data from the Battery Design Example



Interactions plot of data from the Battery Design Example



ANOVA for Two-Factor Factorial Fixed-Effects Model

Effects model for the Two Factor - Fixed Factorial Experiment:

$$y_{ijk} = \mu_{ijk} + \epsilon_{ijk} = \mu + \tau_i + \beta_j + (\tau \beta)_{ij} + \epsilon_{ij}$$
 $i = 1, ..., a; j = 1, ..., b; k = 1, ..., n.$
where $(\tau \beta)_{ij}$ is the effect of the interaction between τ_i and β_i .

The Analysis of Variance Table for the Two-Factor Factorial, Fixed Effects Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
A treatments	SS_A	<i>a</i> − 1	$MS_A = \frac{SS_A}{a - 1}$	$F_0 = \frac{MS_A}{MS_E}$
B treatments	SS_B	<i>b</i> – 1	$MS_B = \frac{SS_B}{b-1}$	$F_0 = \frac{MS_B}{MS_E}$
Interaction	SS_{AB}	(a-1)(b-1)	$MS_{AB} = \frac{SS_{AB}}{(a-1)(b-1)}$	$F_0 = \frac{MS_{AB}}{MS_E}$
Error	SS_E	ab(n-1)	$MS_E = \frac{SS_E}{ab(n-1)}$	
Total	SS_T	abn-1		

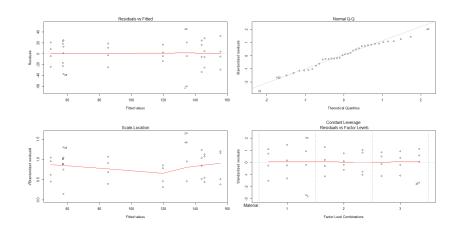
$$SS_E = SS_T - SS_{AB} - SS_A - SS_B = 77646.97 - 10683.72 - 39118.72 - 9613.78 = 18230.75$$

ANOVA for Battery Design Example

ANOVA for Battery Design Example

```
> summary(battery.aov2 <- aov(Life~Material+Temperature,</pre>
         data=battery))
           Df Sum Sg Mean Sg F value Pr(>F)
Material 2 10684 5342 5.947 0.00651 **
Temperature 2 39119 19559 21.776 1.24e-06 ***
Residuals 31 27845 898
> anova(battery.aov2,battery.aov)
Analysis of Variance Table
Model 1: Life ~ Material + Temperature
Model 2: Life ~ Material * Temperature
 Res.Df RSS Df Sum of Sq F Pr(>F)
1 31 27845
2 27 18231 4 9613.8 3.5595 0.01861 *
```

Model checking for Battery Design Example



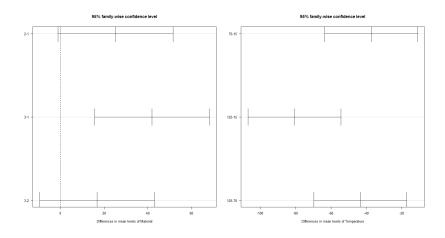
Comparison between groups

```
# Compute means and variance for all levels and factors
>
> with(battery, tapply(Life, list(Material, Temperature), mean))
      15
             70 125
1 134.75 57.25 57.5
2 155.75 119.75 49.5
3 144.00 145.75 85.5
> with(battery, tapply(Life, list(Material, Temperature), var))
                  70 125
1 2056,9167 556,9167 721,0000
2 656.2500 160.2500 371.0000
3 674.6667 508.2500 371.6667
```

Apply Tukey HSD test to test the pairwise comparisons between the treatment group means

```
> TukeyMaterial = TukeyHSD(battery.aov, which="Material")
> Tukey multiple comparisons of means
  95% family-wise confidence level
 Material
       diff lwr upr padj
2x1 25.16667 -1.135677 51.46901 0.0627571
3x1 41.91667 15.614323 68.21901 0.0014162
3x2 16.75000 -9.552344 43.05234 0.2717815
> TukeyTemperature = TukeyHSD(battery.aov, which="Temperature")
> Tukey multiple comparisons of means
  95% family-wise confidence level
 Temperature
           diff lwr upr padj
70 \times 15 -37.25000 -63.55234 -10.94766 0.0043788
125x15 -80.66667 -106.96901 -54.36432 0.0000001
125 \times 70 - 43.41667 - 69.71901 - 17.11432 0.0009787
```

Visualization of Tukey HSD test:



Because interaction is significant, we make the comparison at just one level of temperature, say level 2 ($70\hat{A}$ °F).

```
battery.aov2<-aov(Life~Material,data=battery[battery$Temperature==70,]
TukeyMaterial2=TukeyHSD(battery.aov_70,which="Material")</pre>
```

Tukey multiple comparisons of means 95% family-wise confidence level

diff lwr upr p adj 2-1 62.5 22.59911 102.40089 0.0045670 3-1 88.5 48.59911 128.40089 0.0004209 3-2 26.0 -13.90089 65.90089 0.2177840

$$T_{0.05} = q_{0.05}(3,27)\sqrt{\frac{MS_E}{n}} = 3.5\sqrt{\frac{675.21}{4}} = 45.47$$

Test indicates that at the temperature level 70°F, the mean battery life is the same for material types 2 and 3, and that the mean battery life for material type 1 is significantly lower in comparison to both types 2 and 3

\$Material

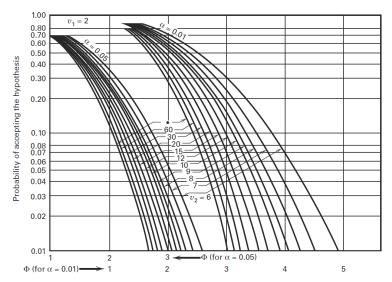
Since the interaction in the model is significant, the effect of Material depends on which level of Temperature is considered. Let us compute the three means at Temperature = 70F, appropriate 95% confidence intervals and compare the observed difference of means with the critical value.

```
mm<- with (subset (battery, Temperature==70),
           aggregate (Life, list (M=Material), mean))
              M x M
  1 57.25 2 119.75 3 145.75
>val.crit <-qtukey(.95,3,27)*sqrt(unlist(summary(battery.aov))</pre>
             [["Mean Sq4"]]/4)
[1] 45.5
T_{0.05} = q_{0.05}(3,27)\sqrt{MS_E/n} = 3.5\sqrt{675.21/4} = 45.5
> diff.mm <- c(d.3.1=mm$x[3]-mm$x[1],d.3.2=mm$x[3]-mm$x[2],
              d.2.1=mm$x[2]-mm$x[1])
d.3.1 d.3.2 d.2.1
 88.5 26.0 62.5
> names(which(diff.mm > val.crit))
[1] "d.3.1" "d.2.1"
```

In conclusion, only Material type 3 vs. type 1 and Material type 2 vs. type 1 appear to be significantly different when Temperature is fixed at $70 \, {\rm \mathring{A}} \, {\rm \mathring{F}}$.

Sample Size Determination - Operating Characteristic Curve

Operating Characteristic Curve Parameters for the Two-Factor Factorial, Fixed Effects Model. (See charts V in the Montgomery DOE book)



Two-Treatment Factorial - What to Power

Model (balanced, *n* per cell):

$$y_{ijr} = \mu + \tau_i + \beta_j + \gamma_{ij} + \varepsilon_{ijr},$$

$$df_A = a - 1$$
, $df_B = b - 1$, $df_{AB} = (a - 1)(b - 1)$, $df_E = ab(n - 1)$.

Noncentrality parameters:

$$\lambda_{A} = \frac{nb}{\sigma^{2}} \sum_{i} (\mu_{i\cdot} - \bar{\mu})^{2}, \quad \lambda_{B} = \frac{na}{\sigma^{2}} \sum_{j} (\mu_{\cdot j} - \bar{\mu})^{2},$$
$$\lambda_{AB} = \frac{n}{\sigma^{2}} \sum_{i,j} (\mu_{ij} - \mu_{i\cdot} - \mu_{\cdot j} + \bar{\mu})^{2}.$$

OC parameters:

$$\begin{split} \Phi_A^2 &= \lambda_A/(a-1) \\ \Phi_B^2 &= \lambda_B/(b-1) \\ \Phi_{AB}^2 &= \lambda_{AB}/((a-1)(b-1)) \end{split}$$

N: Set targets (D_A, D_B, D_{AB}) , choose n to satisfy the strictest β requirement.

Detectable Sizes - Worst-Case Configurations

Main effect A (pairwise $\geq D_A$):

$$\sum_{i}(\mu_{i\cdot}-\bar{\mu})^2\geq D_A^2/2 \ \Rightarrow \boxed{ \Phi_A^2=\frac{nb\,D_A^2}{2(a-1)\sigma^2}}.$$

Main effect B (pairwise $\geq D_B$):

$$\sum_{j} (\mu_{\cdot j} - \bar{\mu})^2 \geq D_B^2/2 \Rightarrow \boxed{\Phi_B^2 = \frac{na D_B^2}{2(b-1)\sigma^2}}.$$

Interaction $A \times B$ (diff-of-diffs $\geq D_{AB}$): Embed a single 2×2 pattern with entries $\pm c$ so that the interaction contrast equals D_{AB} ; this gives $SS = D_{AB}^2/4$ and

$$\Phi_{AB}^2 = \frac{n \, D_{AB}^2}{4 \, (a-1)(b-1)\sigma^2} \ .$$

N: These are least favorable (hardest to detect) alternatives.

Choosing n in Factorial - Per Effect, Take the Max

From OC tables/curves, obtain Φ^2_{\star} for each effect at (α, df) .

Planner formulas

$$n_{A} = \frac{2(a-1)\hat{\sigma}^{2}}{b D_{A}^{2}} \Phi_{A,\star}^{2}, \qquad n_{B} = \frac{2(b-1)\hat{\sigma}^{2}}{a D_{B}^{2}} \Phi_{B,\star}^{2},$$
$$n_{AB} = \frac{4(a-1)(b-1)\hat{\sigma}^{2}}{D_{AB}^{2}} \Phi_{AB,\star}^{2}.$$

Final choice:

$$n = \max\{n_A, n_B, n_{AB}\}$$
 (round up).

N: If interaction is likely, n_{AB} often dominates. If not, size for A and B but still test $A \times B$ and interpret simple effects if needed.

Sample Size Determination for Battery Experiment

```
> n = c(2, 3, 4, 5)
> a = 3
                         # number of treatment levels A
> b = 3
                         # number of treatment levels B
> D = 40
                         # max difference in group means
> sigma = 25
                         # standard deviation
> Fi_sq = (n*b*(D)^2)/(2*a*(sigma^2))
> Fi = sqrt(Fi_sq)
> errorDF = a*b*(n-1)
> powers = power.anova.test(groups=3, n=n,
         between.var = (n*(D^2))/((n-1)), within.var=sigma^2,
          sig.level=.05)$power
> rbind(n , Fi ,errorDF, powers)
           [,1] [,2] [,3] [,4]
    2.0000000 3.0000000 4.000000 5.0000000
n
Fi 1.6000000 1.9595918 2.262742 2.5298221
errorDF 9.0000000 18.0000000 27.000000 36.0000000
powers 0.6391205 0.9116119 0.979752 0.9956568
```

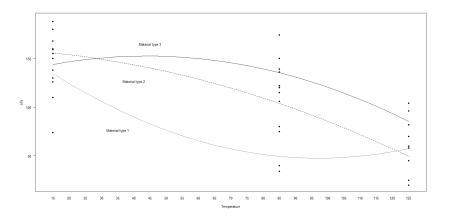
General Factorial Design - Response Curves

Let us assume that temperature is quantitative and use linear regression model to fit data.

```
>Temperature.num=as.numeric(as.character(battery$Temperature))
>battery.aov3=aov(Life~Material+Temperature.num+
             I(Temperature.num^2) +Material:Temperature.num+
             Material:I(Temperature.num^2))
>summary(battery.aov3)
                            Df Sum Sq Mean Sq F value
                                                      Pr(>F)
Material
                               10684 5342 7.911
                                                     0.00198
Temperature.num
                                39043 39043 57.823 3.53e-8
I(Temperature.num^2)
                                   76
                                         76 0.113 0.73975
                             2 2315 1158 1.714 0.19911
Material: Temperature.num
Material:I(Temperature.num^2)
                             2 7299 3649 5.405
                                                     0.01061
Residuals
                                18231 675
                            2.7
```

P-values indicate that A^2 and AB are not significant, whereas the A^2B is significant. By removing A^2 and AB the model is not **hierarchical** any more.

General Factorial Design - Response Curves



P-values indicate that A^2 and AB are not significant, whereas the A^2B is significant. By removing A^2 and AB the model is not **hierarchical** any more.

Homework experiment 01

Perform the homework experiment 01 described in the Rmd/pdf/ipynb files in repo:

01NAEX/projects/01NAEX_HW01_pendulum

The report can be elaborated by group up to 5 students, written in pdf file (R Markdown or Jupyter NB are recommended) and handed till **October 18**.