Università degli Studi di Padova

Department of Industrial Engineering

Design of Experiments
Lesson #6

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Issues on ANOVA modelling

- **ANalysis Of VAriance** (ANOVA) is an appropriate tool to manage experiments if a **single factor** is present
  - deals with factors and levels as **qualitative/categorical variables**
  - indicates if factors influence the response, but nothing about **how the factors influence the response**:
    - does response increase with increasing factor value?

… HOWEVER…

- Usually factors are **quantitative variables** (defined in the domain of real numbers)
- Some of the experimental objectives, such as product or process/system optimization, need a **model for quantitative variables**

Factorial designs

Multiple factors designs basic principles

- **Factorial designs** are appropriate when **two or more factors are present**
  - **all the possible combinations of the levels of all the factors** are investigated in each complete **trial/replicate of the experiment**
  - if there are a levels of factor A and b levels of factor B, each replicate contains all ab treatment combinations
  - when factors are arranged in a factorial design, they are often said to be **crossed**

Factorial designs

- **Factorial designs** are widely used in experiments involving several factors where it is necessary to study the **joint effect of the factors on a response**
- Several special cases of the general factorial design are important because they are widely used in research and also because they form the basis of other designs of **considerable practical value**
- When L levels are considered for K variables, the total number of experiments to be carried out is:

$$N = L^K$$

- The most important of these special cases is that of K **factors** moved on $L = 2$ **levels**, where factors may be:
  - **quantitative**,
    - temperature, pressure, time, etc…
  - **qualitative**
    - machines, operators, the “high” and “low” levels of a factor, presence/absence of a factor
    - the normality assumptions are satisfied

2^K factorial designs

- This is called 2^K **factorial design**:
  - complete replicate of such a design requires:

    $$(2 \cdot 2 \cdot \cdots \cdot 2) = 2^K \text{ observations}$$

  - particularly useful in the early stages of experimental work when **many factors** are likely to be investigated
    - these designs are widely used in **factor screening experiments**
  - it provides the **smallest number of runs with which K factors** can be studied in a complete factorial design
    - since there are only two levels for each factor, the **response is assumed to be approximately** linear over the range of the factor levels chosen
- Assumptions:
  - the **factors are fixed**
  - the designs are completely **randomized**
  - the **normality** assumptions are satisfied

Codification of the experiments

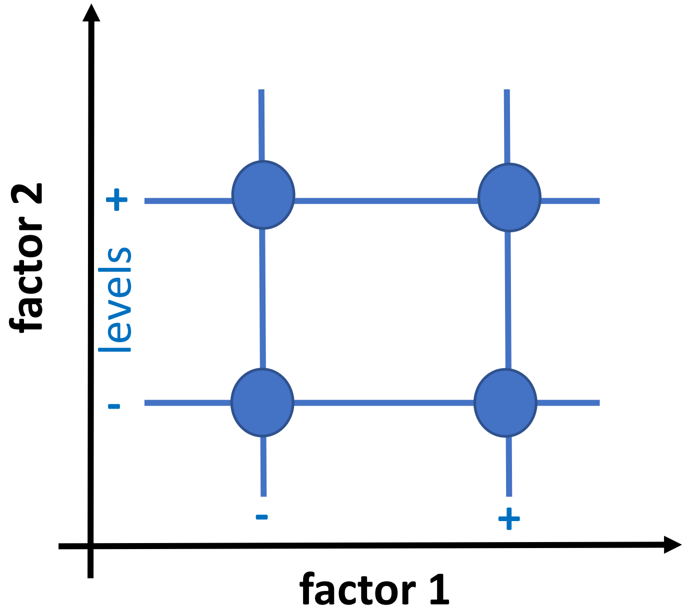
- **Effects**:
  - the effects are usually codified by letters:
    - A is the effect of factor 1
    - B is the effect of factor 2
    - AB is the interaction among the two factors

- **Coded variables** are often used for factors:
  - \- or -1 indicate the lowest factor level
  - \+ or +1 indicate the highest factor level
  - 0 indicates the center point of the factor

Experimental design notations

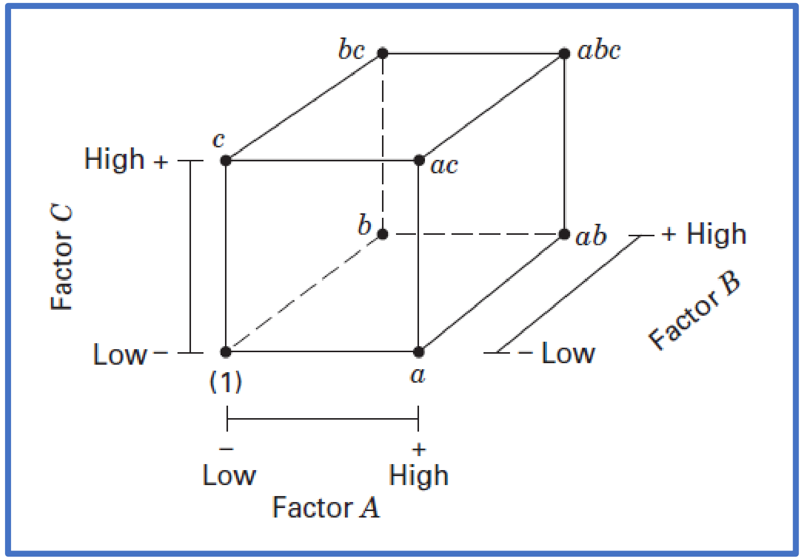
- Alternative experimental design notations can be adopted:
  - **geometric coding**
  - **orthogonal coding**
  - **effects coding**

Run	*A*	*B*	*C*	Labels	*A*	*B*	*C*
1	−	−	−	(1)	0	0	0
2	+	−	−	*a*	1	0	0
3	−	+	−	*b*	0	1	0
4	+	+	−	*ab*	1	1	0
5	−	−	+	*c*	0	0	1
6	+	−	+	*ac*	1	0	1
7	−	+	+	*bc*	0	1	1
8	+	+	+	*abc*	1	1	1



Extension to higher dimension

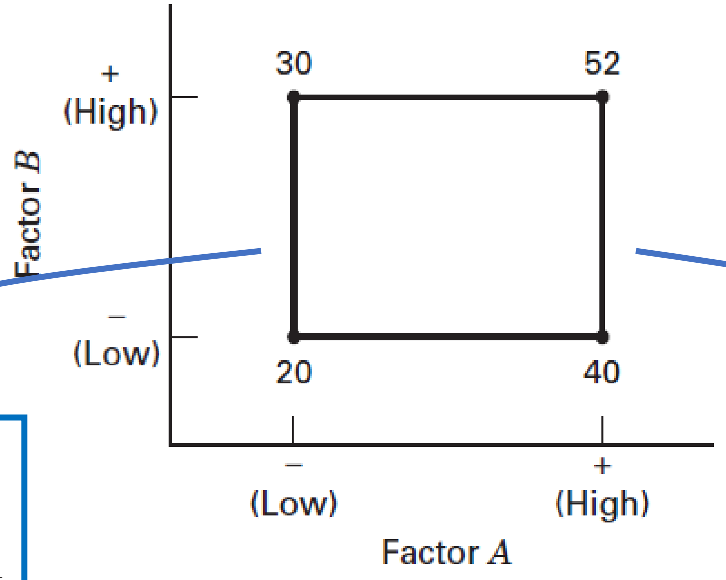
- The methodology of experiment data modelling can be (easily) transferred to the highest dimensional spaces:
  - larger number of factors
- Suppose that 3 factors, *A*, *B*, and *C*, each at two levels, are of interest:
  - the design is called a **2^3 factorial design**
  - the eight treatment combinations can now be displayed geometrically as a cube
- A **design matrix** can be built which represents an orthogonal coding of the low and high levels of the factors using - and + (or 0/1, or -1/1) and listing the experiments



Run	Factor A	Factor B	Factor C
1	−	−	−
2	+	−	−
3	−	+	−
4	+	+	−
5	−	−	+
6	+	−	+
7	−	+	+
8	+	+	+

Main effects

- The **effect of a factor** is defined to be the change in response produced by a change in the level of the factors
  - since it refers to the primary factors, it is called a **main effect**
- **Example #1**: consider a full factorial design with 2 factors varied on two levels



main effect on A

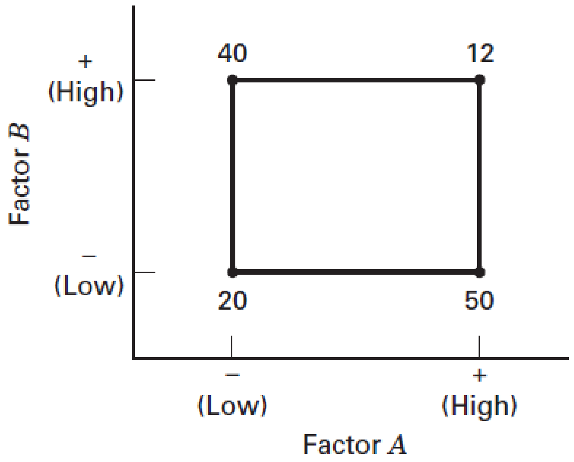
$$A = \frac{40 + 52}{2} - \frac{20 + 30}{2} = 21$$

main effect on B

$$B = \frac{30 + 52}{2} - \frac{20 + 40}{2} = 11$$

Interactions between factors

- When the difference in response between the levels of one factor is not the same at all levels of the other factors an **interaction between the factors** is present
- **Example #2**: consider the two-factor factorial experiment in the following figure

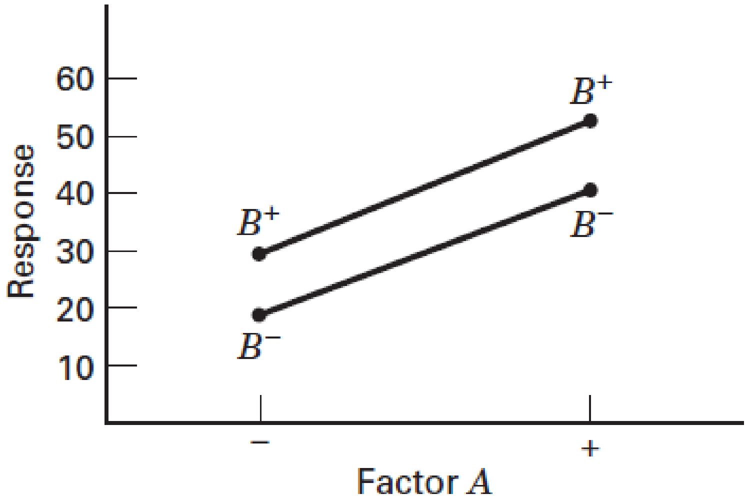


  - at the low level of factor *B*, the *A* effect is: $A = 50 - 20 = 30$
  - at the high level of factor *B*, the *A* effect is: $A = 12 - 40 = -28$
  - since **the effect of *A* depends on the level chosen for factor *B***, we see that there is interaction between *A* and *B*
    - the interaction effect magnitude is the average difference in these two *A* effects, or *AB* = [(12-40)-(50-20)]/2=(-28- 30)/2=-29
    - the interaction is large in this experiment

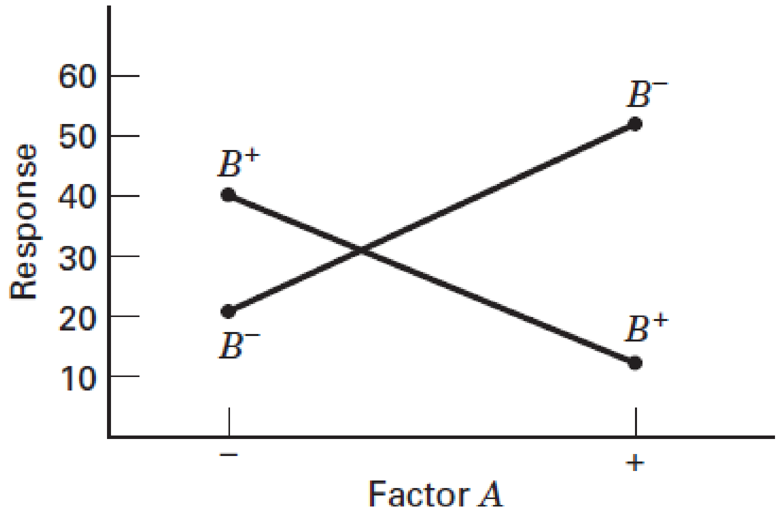
Graphical illustration of interaction

- **Two-factor interaction plots** are very useful in interpreting significant interactions and in reporting results to non-statistically-trained personnel:
  - pay attention that interpretation is subjective and sometimes may be misleading
  - they should not be utilized as a sole technique
- Plot the response data against one factor (i.e., factor *A*) for both levels of the other factor (i.e., *B*)
  - they indicate if the response increases or decreases with the factor
  - if the lines are approximately **parallel**, this indicates a lack of interaction between factors
  - if lines are **not parallel**, this indicates an **interaction between factors**

example #1 - no interaction



example #2 - interaction



Regression model representation

- There is another way to illustrate the concept of interaction
- Suppose that both of our design factors x_1 and x_2 are **quantitative** (such as temperature, pressure, time, etc…)
- A **regression model representation** of the factorial experiment could be written as:

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

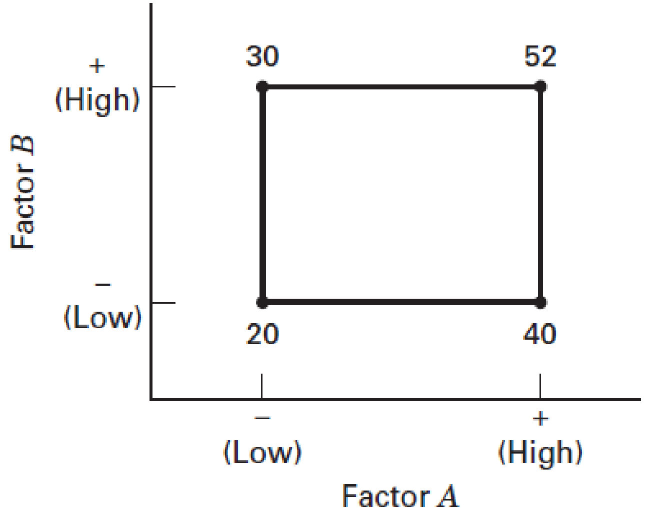
  - variables x_1 and x_2 are defined on a **coded scale** from -1 to 1 (the low and high levels of *A* and *B*, respectively)
  - $x_1 x_2$ represents the **interaction** between x_1 and x_2

Regression model parameter estimation

- **Example #1**: the estimates of the regression coefficients of the regression model:

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

  - β_1 and β_2 can be estimated as one half of the main effects:
    - $\beta_1 = \frac{21}{2} = 10.5$
    - $\beta_2 = \frac{11}{2} = 5.5$
  - β_{12} is the one half of the interaction effect:
    - $\text{AB} = \frac{(52+20)-(40+30)}{2} = 1$:
    - $\beta_{12} = \frac{1}{2} = 0.5$
  - the intercept is the average of the responses:
    - $\beta_0 = \frac{(20+40+30+52)}{4} = 35.5$

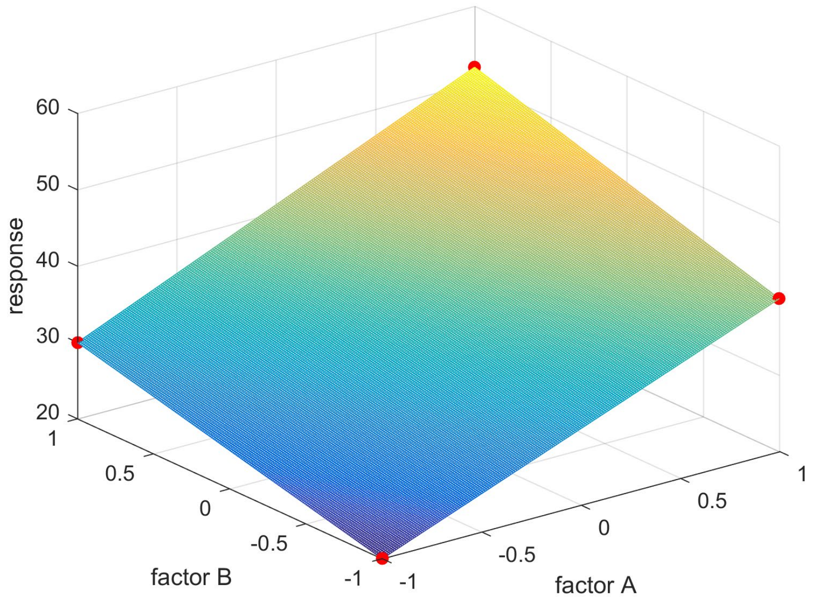


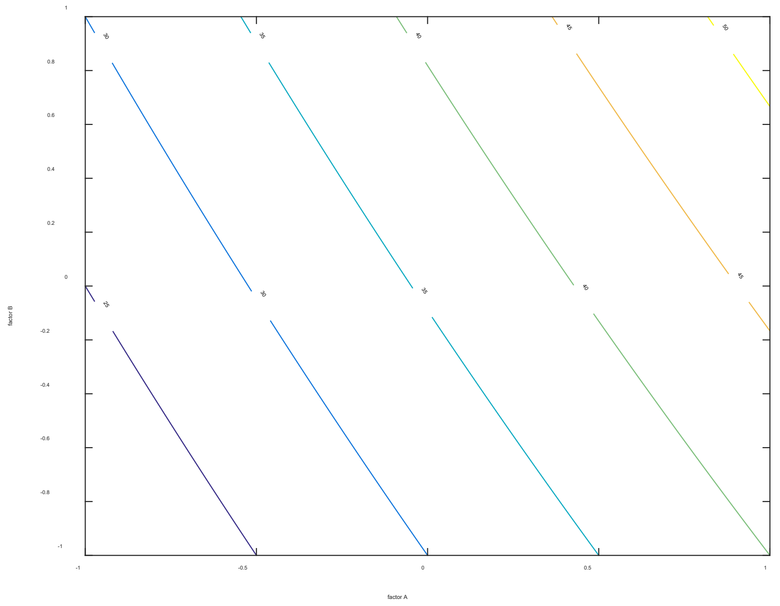
- This means that the interaction term is mall if compared to the main effects ➡ it could be ignored:
  - the regression model can be formulated as:

$$y = 35.5 + 10.5x_1 + 5.5x_2 + 0.5x_1x_2$$

Regression model graphical representations

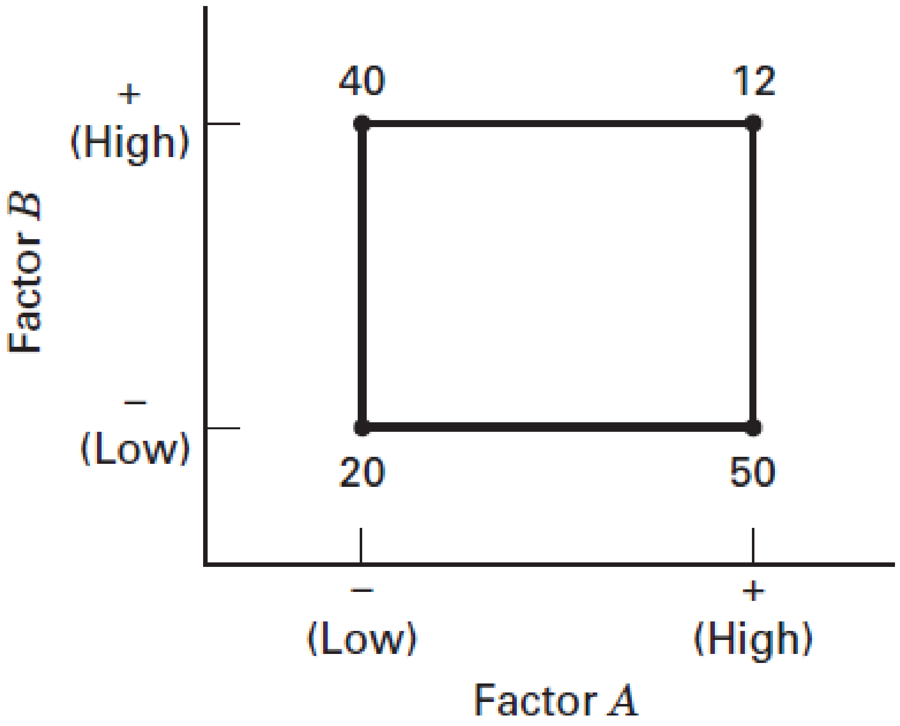
- The main graphical representations of the regression model are:
  - **response surface plot**: a plot of the plane of y-values generated by the various combinations of x_1 and x_2
  - **contour lines**: constant response y in the x_1 - x_2 plane
    - notice that the contour plot contains parallel straight lines when the response surface is a plane, and no interactions are present





… and now:

- Find the solution in the case of **Example #2**:
  1. manual calculations
  2. computational solution

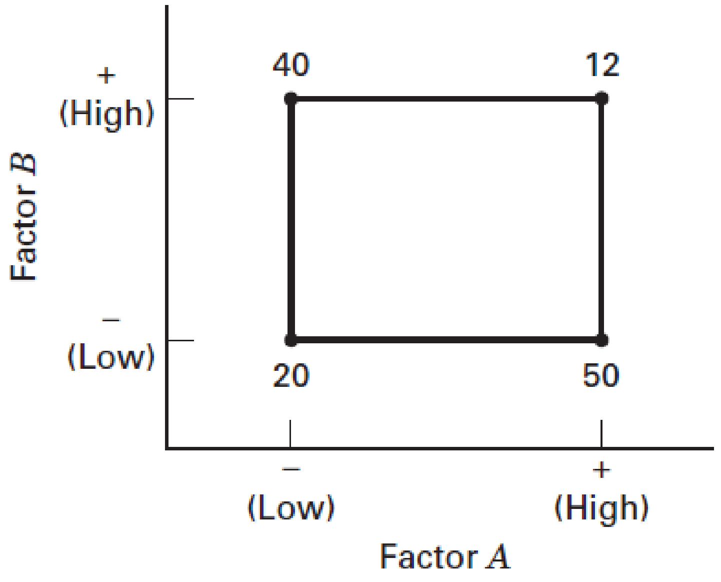


Example #2

- In the example #2 the estimates of the regression coefficients of the regression model:

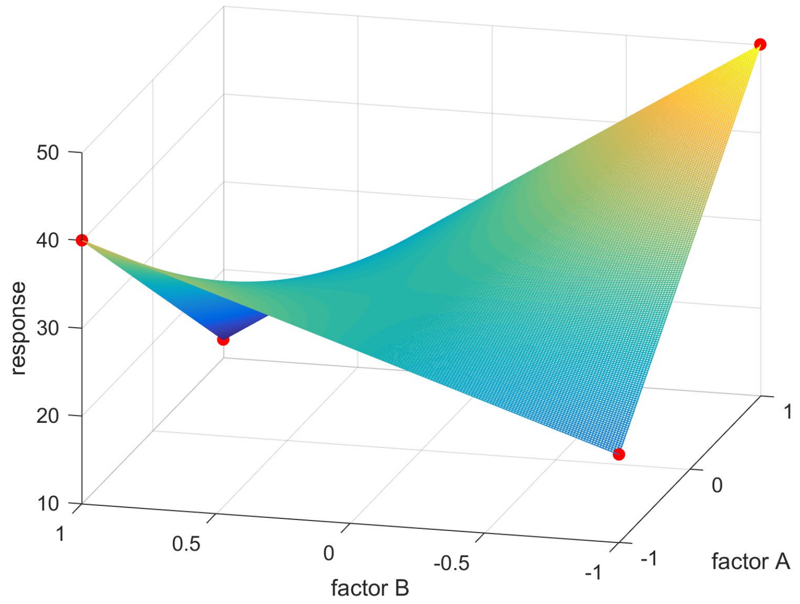
$$y = 30.5 + 0.5x_1 - 4.5x_2 - 14.5x_1x_2$$

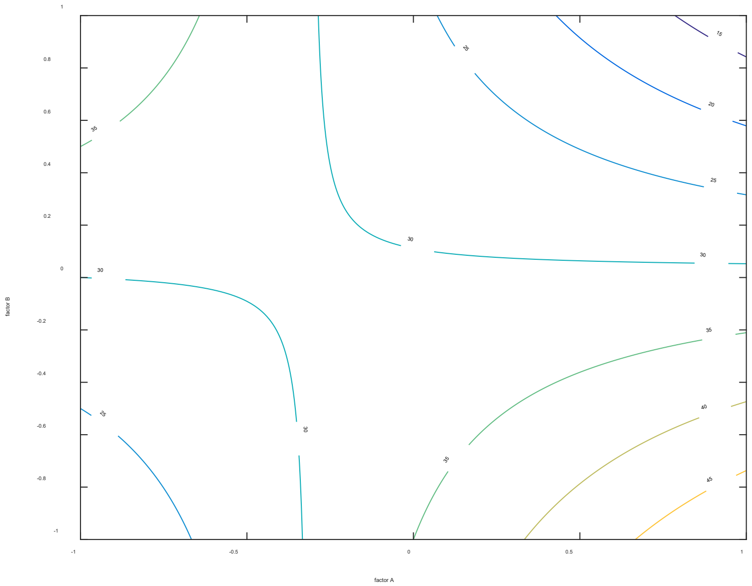
  - the interaction term is the most important one
  - the main effect of A is low
    - however, it *strongly depends on the level of factor B*



Interactions in regression model representation

- Significant **interaction** terms:
  - **twists** the plane
    - the twisting of the response surface results in curved contour lines in the x_1 - x_2 plane
  - **is a form of curvature** in the underlying response surface model for the experiment
  - **masks** the significance of main effects
    - these points are clearly indicated by the interaction plot





Computational solution of the problem

- In Matlab® use command:
  - **`regress`**
  - **`fitlm`**
- Datasets of examples #1 and #2:
  - **`example1.mat`**
- Command line:

```
[b,bint,r,rint,stats]=regress(Y1,[ones(4,1) X1 X1(:,1).*X1(:,2)]);
```

  - **`b`** are the regression coefficients and the respective confidence intervals $\mathbf{b}_{\mathrm{int}}$
  - **`r`** are the residuals and the respective confidence intervals $\mathbf{r}_{\mathrm{int}}$
  - stats are:
    - the determination coefficient
    - the *F* statistic
    - the *p*-value
    - error variance
- The graphical representations of response surface and contour plots can be done with commands:
  - **`mesh`**
  - **`contour`**

Example: extreme temperatures battery design

High temperature battery design

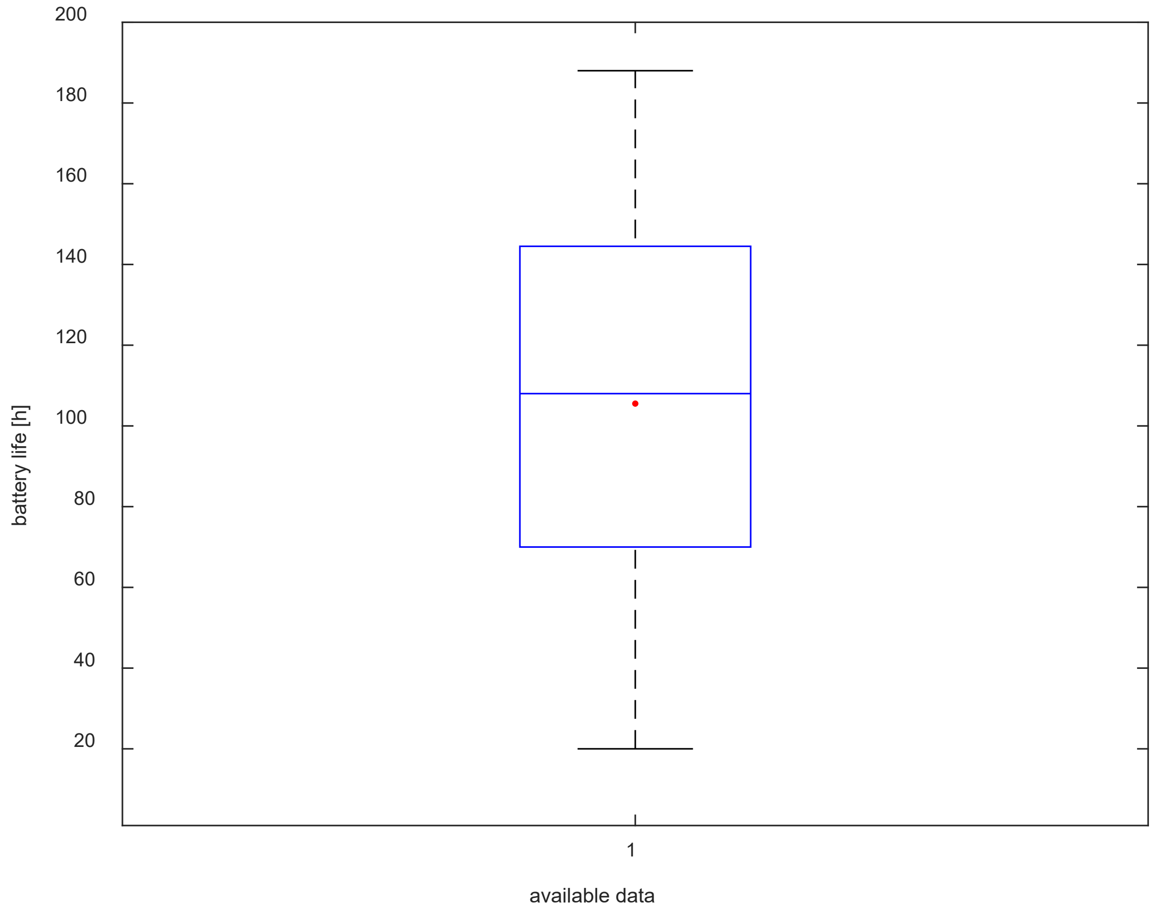
- A battery is designed to be utilized in a device that is subject to extreme temperature variations:
  - design parameter: **plate material** for the battery
    - three possible choices
  - **temperature** can be controlled in the product development laboratory for the purposes of a test
- Available data on **experimental campaign**:
  - **3^2 factorial design** with 4 replicates per experiment
  - response: effective **life of the battery** in hours

Material Type	Temperature (°F) 15		70		125	
1	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

- **Objectives**:
  - what effects do materials and temperature have on the battery life?
  - is there a material that guarantees long life regardless of temperature?

Battery life

- Visualization of the battery life available data



N-way ANOVA

- **Two-factor analysis of variance** is used here:
  - based on the following definitions:

$$y_{i..} = \sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk} \qquad \bar{y}_{i..} = \frac{y_{i..}}{bn}$$

$$y_{.j.} = \sum_{i=1}^{a}\sum_{k=1}^{n} y_{ijk} \qquad \bar{y}_{.j.} = \frac{y_{.j.}}{an}$$

$$y_{ij.} = \sum_{k=1}^{n} y_{ijk} \qquad \bar{y}_{ij.} = \frac{y_{ij.}}{n}$$

$$y_{...} = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk} \qquad \bar{y}_{...} = \frac{y_{...}}{abn}$$

  - the **corrected sum of squares** constituting the **fundamental ANOVA equation** is:
    - the total sum of squares is partitioned into:
      - a sum of squares due to "rows," or factor *A*: SS_A
      - a sum of squares due to "columns," or factor *B*: SS_B
      - a sum of squares due to the interaction between *A* and *B*: SS_{AB}
      - a sum of squares due to error: SS_E
      - there must be at least two replicates ($n = 2$) to obtain an error sum of squares

$$\begin{aligned}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk}-\bar{y}_{...})^2 &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}[(\bar{y}_{i..}-\bar{y}_{...})+(\bar{y}_{.j.}-\bar{y}_{...})\\ &\quad +(\bar{y}_{ij.}-\bar{y}_{i..}-\bar{y}_{.j.}+\bar{y}_{...})+(y_{ijk}-\bar{y}_{ij.})]^2\\ &= bn\sum_{i=1}^{a}(\bar{y}_{i..}-\bar{y}_{...})^2+an\sum_{j=1}^{b}(\bar{y}_{.j.}-\bar{y}_{...})^2\\ &\quad + n\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{y}_{ij.}-\bar{y}_{i..}-\bar{y}_{.j.}+\bar{y}_{...})^2\\ &\quad + \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk}-\bar{y}_{ij.})^2\end{aligned}$$

  - The symbolic form of the equation is:

$$SS_T = SS_A + SS_B + SS_{AB} + SS_E$$

Mean squares

- Each sum of squares divided by respective degrees of freedom is a **mean square**:
  - if the null hypotheses of no row treatment effects, no column treatment effects, and no interaction are true: MS_A, MS_B, MS_{AB}, and MS_E all estimate the variance σ^2
  - if there are differences between row treatment effects:
    $$MS_A > MS_E$$
  - if there are column treatment effects:
    $$MS_B > MS_E$$
  - if there are interaction effects:
    $$MS_{AB} > MS_E$$

$$E(MS_A) = E\left(\frac{SS_A}{a-1}\right) = \sigma^2 + \frac{bn\sum_{i=1}^{a}\tau_i^2}{a-1}$$

$$E(MS_B) = E\left(\frac{SS_B}{b-1}\right) = \sigma^2 + \frac{an\sum_{j=1}^{b}\beta_j^2}{b-1}$$

$$E(MS_{AB}) = E\left(\frac{SS_{AB}}{(a-1)(b-1)}\right) = \sigma^2 + \frac{n\sum_{i=1}^{a}\sum_{j=1}^{b}(\tau\beta)_{ij}^2}{(a-1)(b-1)}$$

$$E(MS_E) = E\left(\frac{SS_E}{ab(n-1)}\right) = \sigma^2$$

Main effects and interactions significance

- To test the **significance of both main effects and interactions**, divide the corresponding mean square by the error mean square:
  - large values of this ratio imply that the data do not support the null hypothesis
- If the model is adequate and the error terms are normally and independently distributed with constant variance
  - the ratios of mean squares MS_A/MS_E, MS_B/MS_E, and MS_{AB}/MS_E is distributed as F with $(a-1)$, $(b-1)$, and $(a-1)(b-1)$ numerator degrees of freedom, respectively, and $ab(n-1)$ denominator degrees of freedom
  - the critical region would be the upper tail of an F distribution
- The test procedure is usually summarized in an **analysis of variance table**

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
A treatments	SS_A	$a-1$	$MS_A = \frac{SS_A}{a-1}$	$F_0 = \frac{MS_A}{MS_E}$
B treatments	SS_B	$b-1$	$MS_B = \frac{SS_B}{b-1}$	$F_0 = \frac{MS_B}{MS_E}$
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	$abn-1$		

ANOVA model building

- Command:

```
[p,tbl,stats]=anovan(Y,X,'model','full')
```

- Outputs: analysis of variance table

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.

the effects of ***both the factors and the interaction*** are higher than the error and **significant**

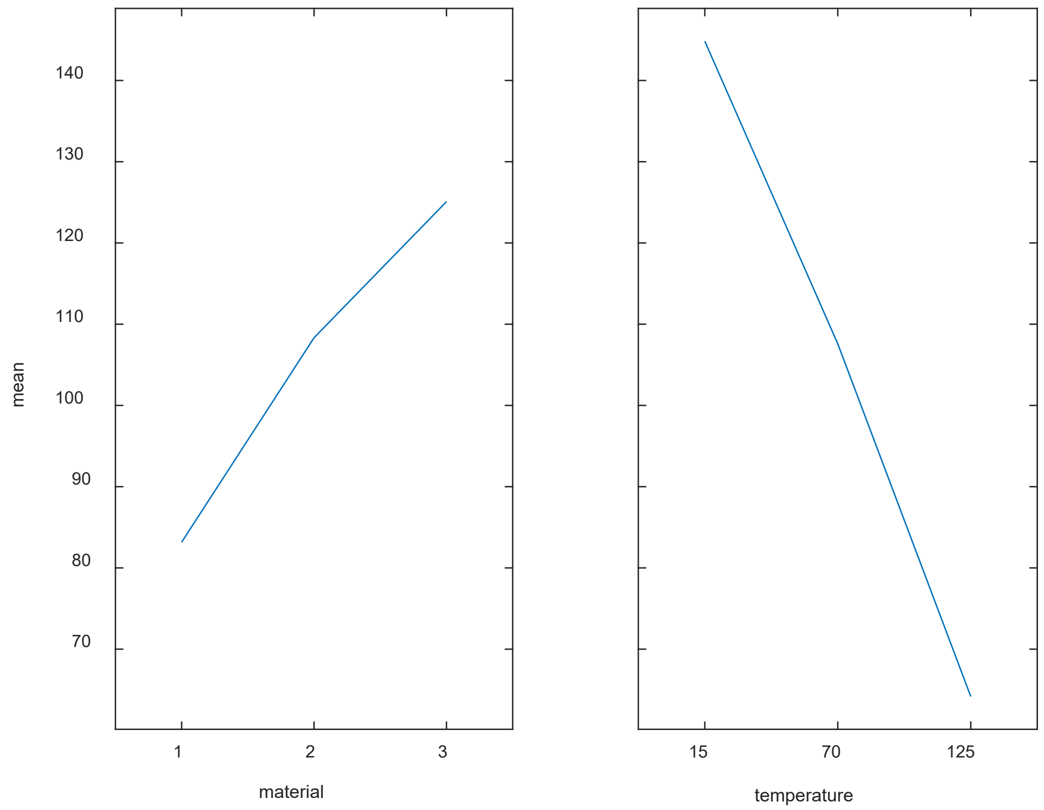
how does this effects affect the battery life???

Main effect plot

- The **main effect plot** is an easy way to visualize how the main effects act on the response variable:
  - the main effect plots are just graphs of the **marginal response averages at the levels of the three factors**

- In this case study:
  - the effect of temperature is much larger than the effect of material
  - material #3 guarantees longer battery life
  - high temperatures decrease battery life
  - command:

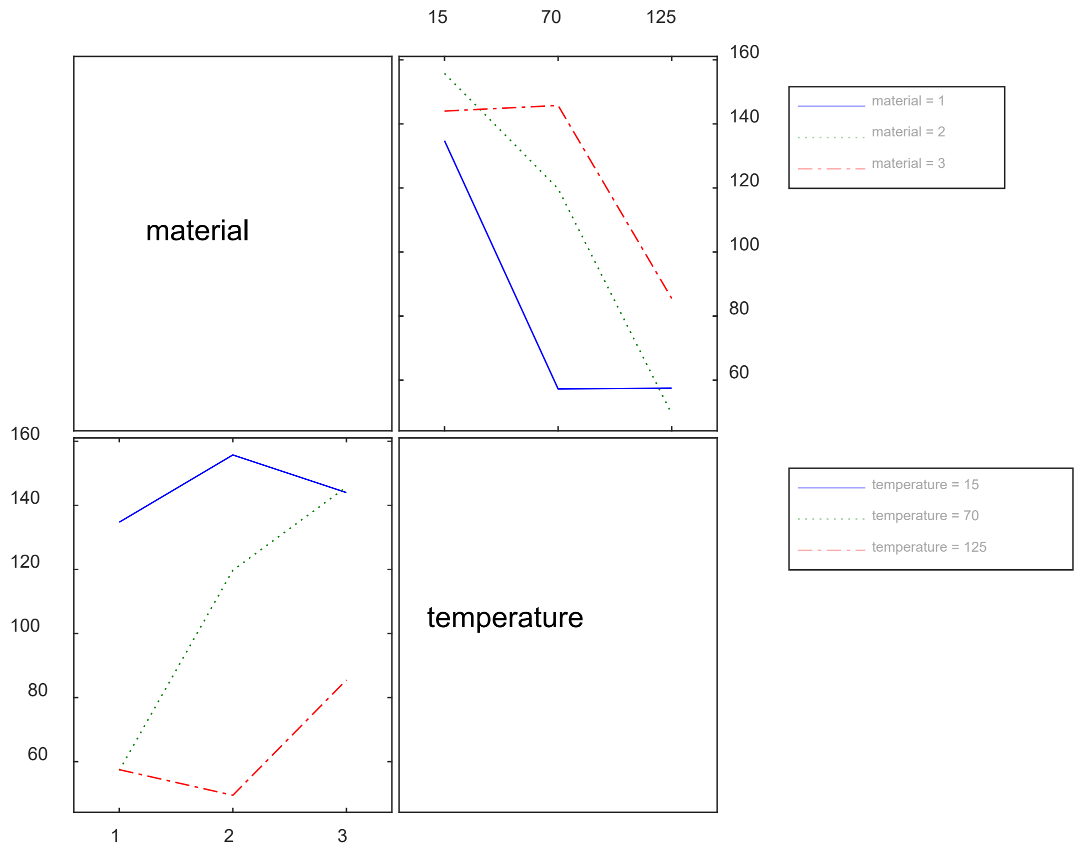
```
maineffectsplot(Y,X1,'varnames',
{'material','temperature'})
```



Interaction plot

- The **interaction plot** is used to visualize how the interaction effects act on the response:
  - lack of parallelism of the lines means significant interaction

- In this case study:
  - a longer life is attained at low temperature, regardless of material type
  - changing from low to intermediate temperature, battery life with material type 3 may actually increase, whereas it decreases for types 1 and 2
  - from intermediate to high temperature, battery life decreases for material types 2 and 3 and is essentially unchanged for type 1
  - material type 3 seems to give the best results if we want less loss of effective life as the temperature changes
  - command:
    `interactionplot(Y,X,'varnames', {'material','temperature'})`



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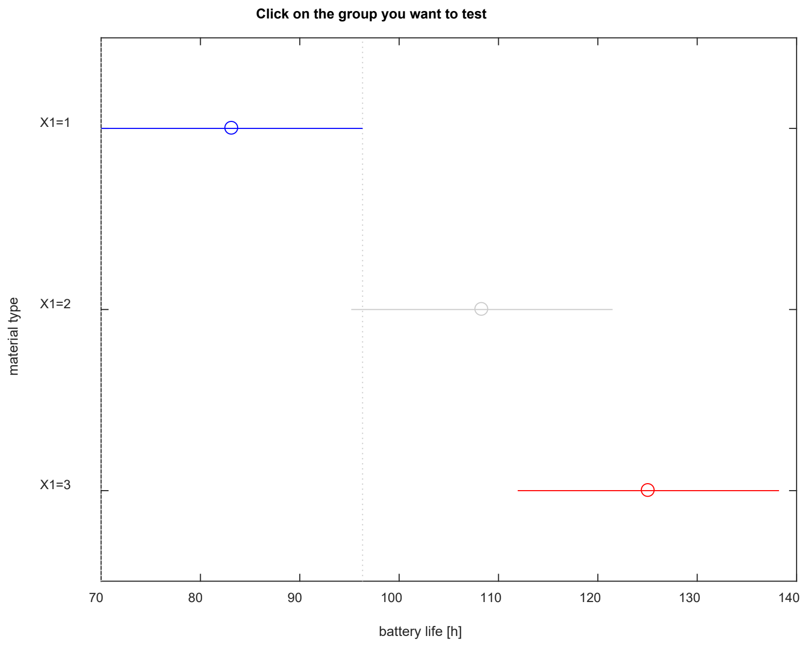
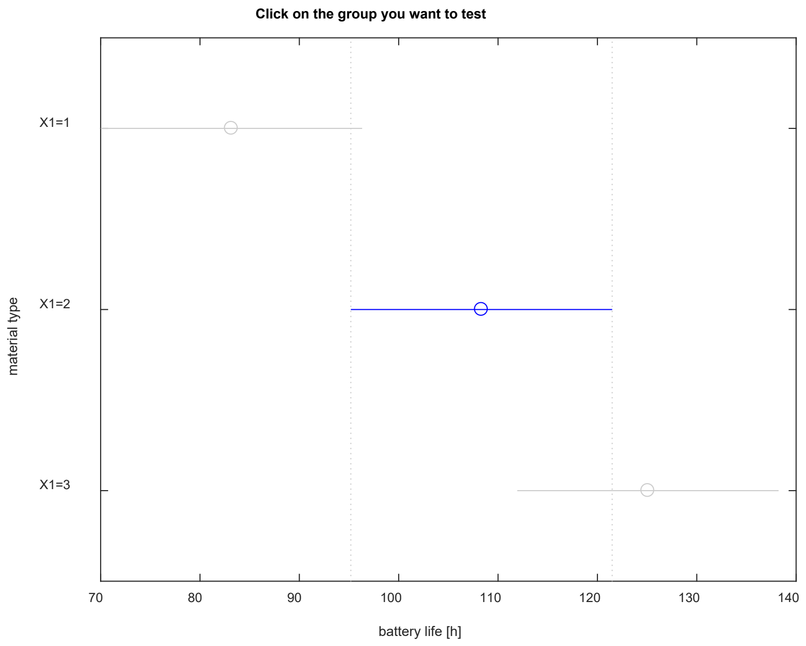
Comparison among treatments

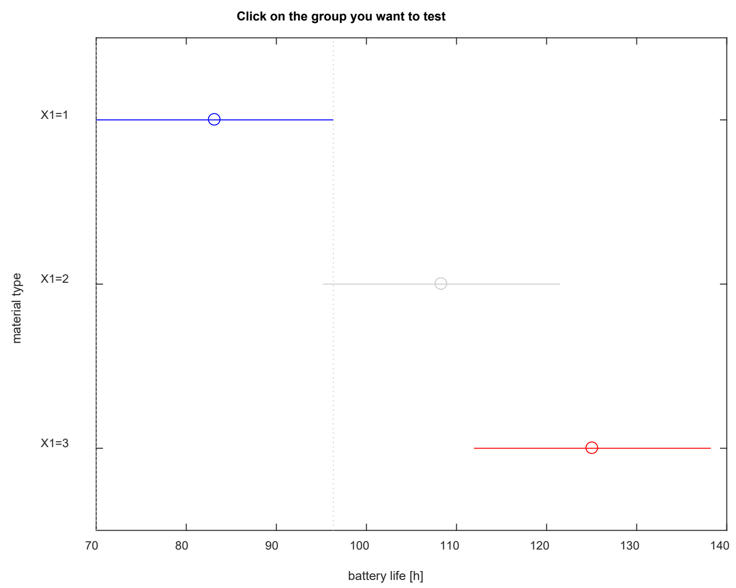
- Confidence intervals in the means of the different treatments can be obtained with command:
  - note that in this experiment, interaction is significant and consequently the comparisons between the means of one factor may be obscured by the interaction
  - one approach to this situation is to fix factor *B* at a specific level and apply Tukey's test to the means of factor *A* at that level

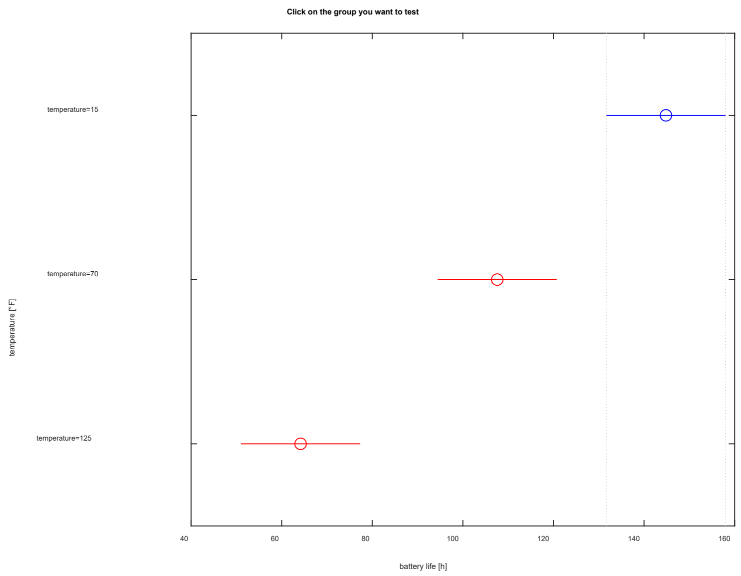




Comparison among materials/temperatures

- Study of the means difference:
  - among materials at a temperature of 70°F
    - material #1 is the one that performs in the worst manner
    - materials #2 and 3 are not clearly distinguishable
  - among temperatures for material #3
    - the highest temperature is the one which deteriorates in a significant manner the battery and decreases the battery life



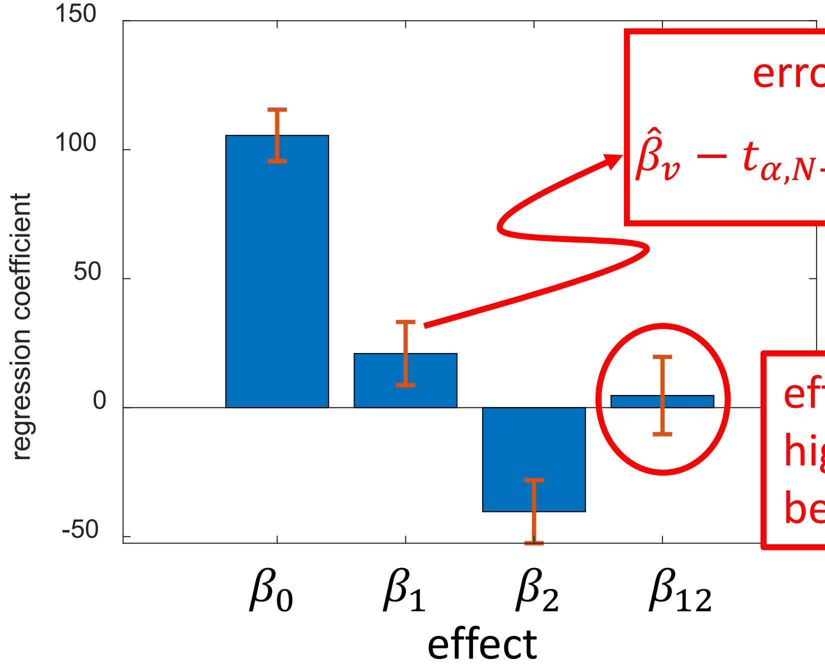


Estimated regression model

- The estimation of the regression coefficients determines a model that is:

$$y = 105.5 + 20.96x_1 - 40.33x_2 + 4.69x_1x_2$$

  - the second factor, the temperature, confirms to be the most influential on the response
  - the battery life:
    - increases passing from material 1, to material 2 and to material 3
    - decreases with increasing temperatures
  - high uncertainty is related to interaction
  - $R^2 = 0.64$



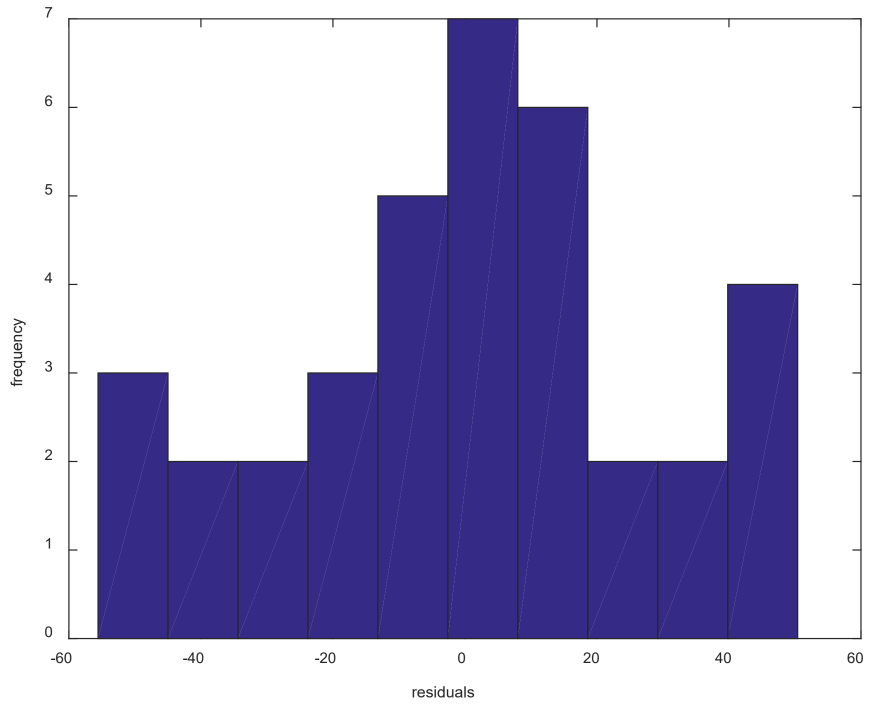
error bars show parameters uncertainty

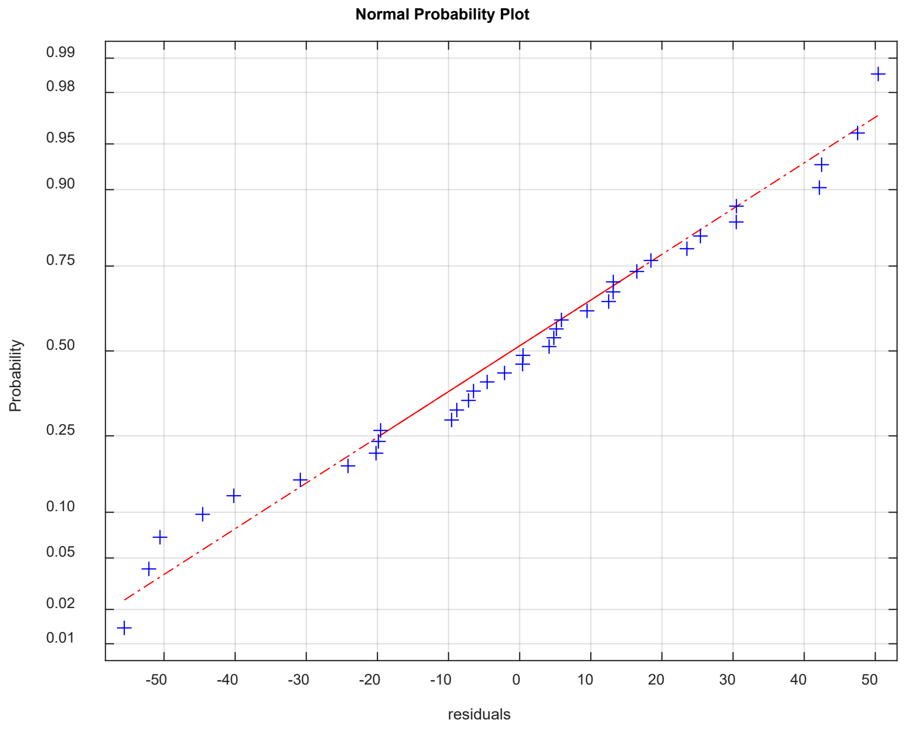
$$\hat{\beta}_v - t_{\alpha,N-V-1}\sqrt{\sigma^2 c_{vv}} \leq \beta_v \leq \hat{\beta}_v + t_{\alpha,N-V-1}\sqrt{\sigma^2 c_{vv}}$$

effects whose parameter uncertainty is too high (i.e., the error bars cross the zero) can be discarded from the model

Checking model adequacy

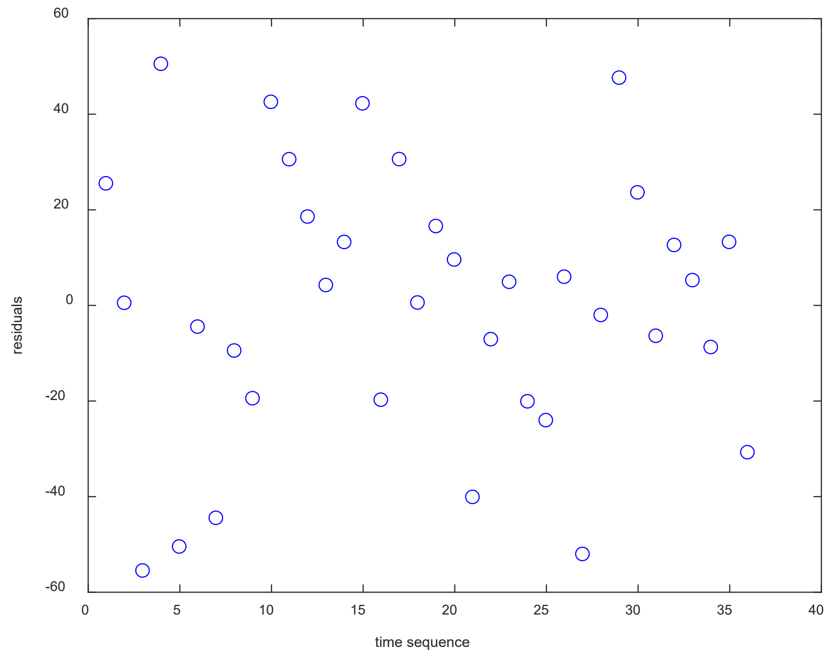
- After fitting a linear regression model ($R^2 = 0.64$), the residuals are studied:
  - residuals histogram can be compatible with a normal distribution
  - the normal probability plot shows a Gaussian behavior of the residuals

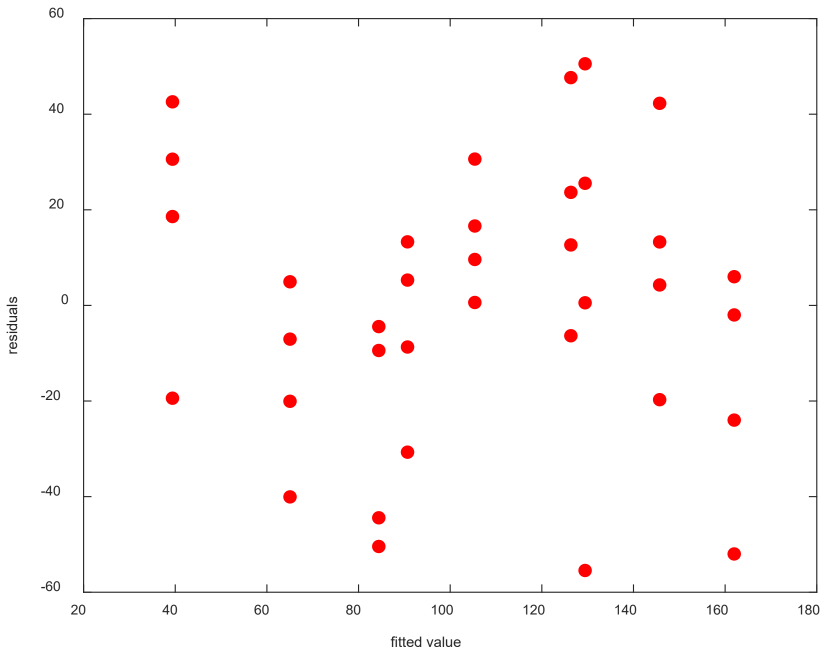




Pattern of the residuals

- The residuals are represented:
  - in time:
    - everything is regular
  - against the fitted value
    - no patterns are found

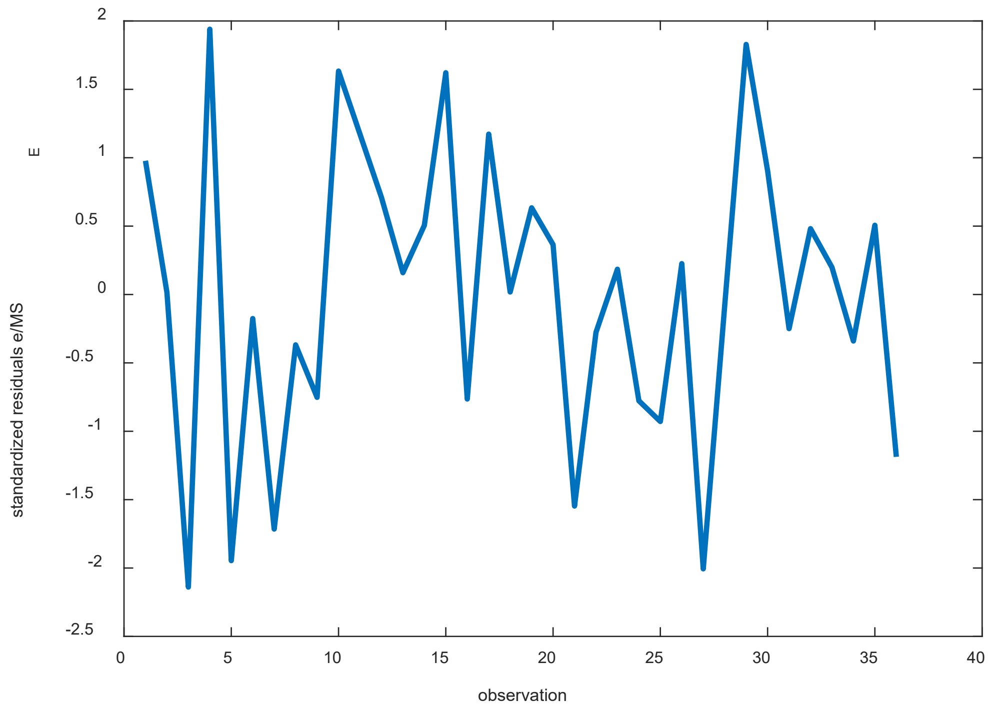




Standardized residuals

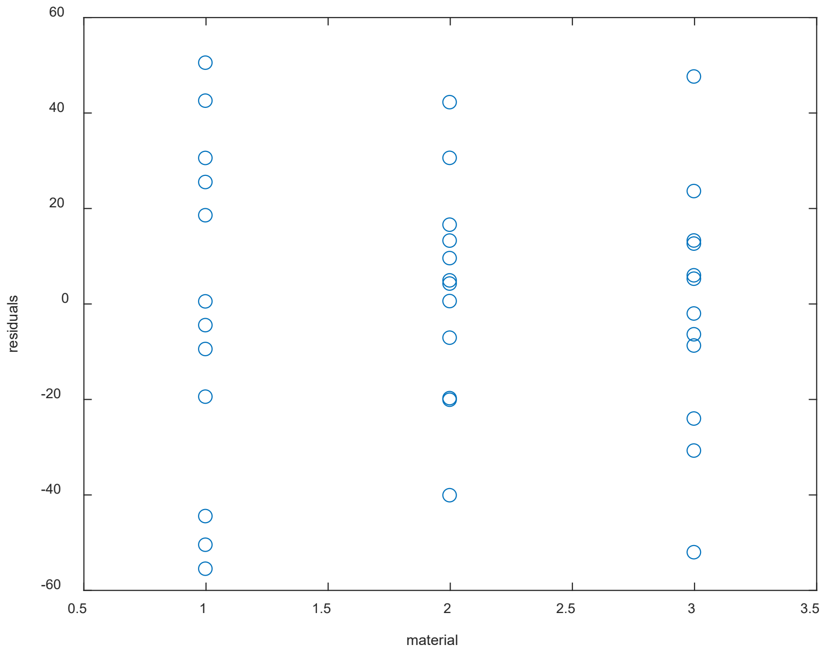
- The standardized residuals show:
  - 12 observations > 1
  - 1 observation > 2

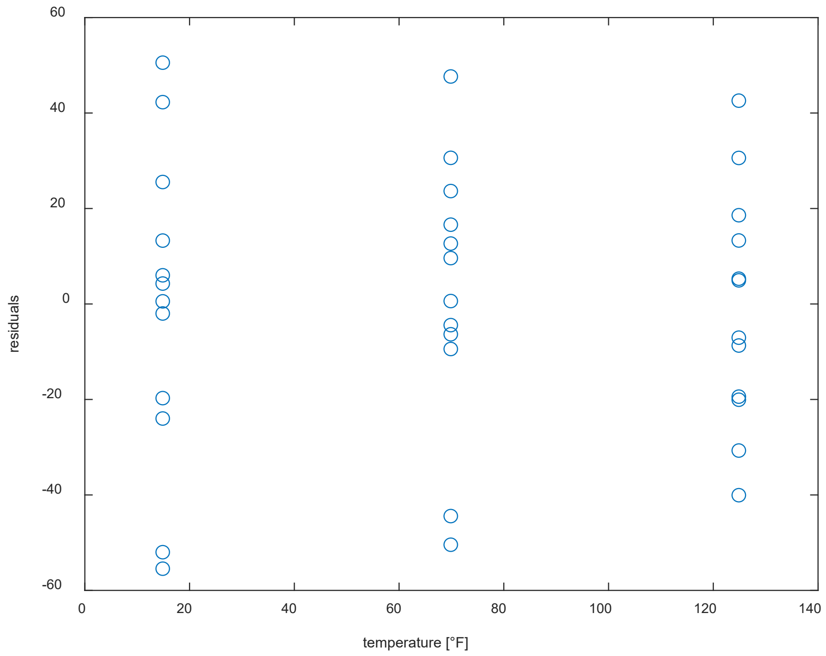
this is compatible with a ***standard normal distribution of the standardized residuals***



Residuals vs. variables

- The plots of the residuals against the factors show that:
  - the variance of the residuals for material #2 is slightly lower than the other materials
  - the residuals slightly decrease with a temperature increase





Take home message

- The **procedure to analyze experiments** goes through the following steps:
  1. preliminary data visualization
  2. building an N-way ANOVA model

  or

  2. build a **response surface model**
     - study the main effects
     - study the treatment means
     - examine the interactions
     - test on the residuals:
       - check residuals normality, independence and standardized values normality
       - visualize trends:
         - in time
         - against fitted values
         - against factors

this is a much powerful modelling methodology!!!

… per sempre a fianco a me!