Design of Experiments
Lesson #5

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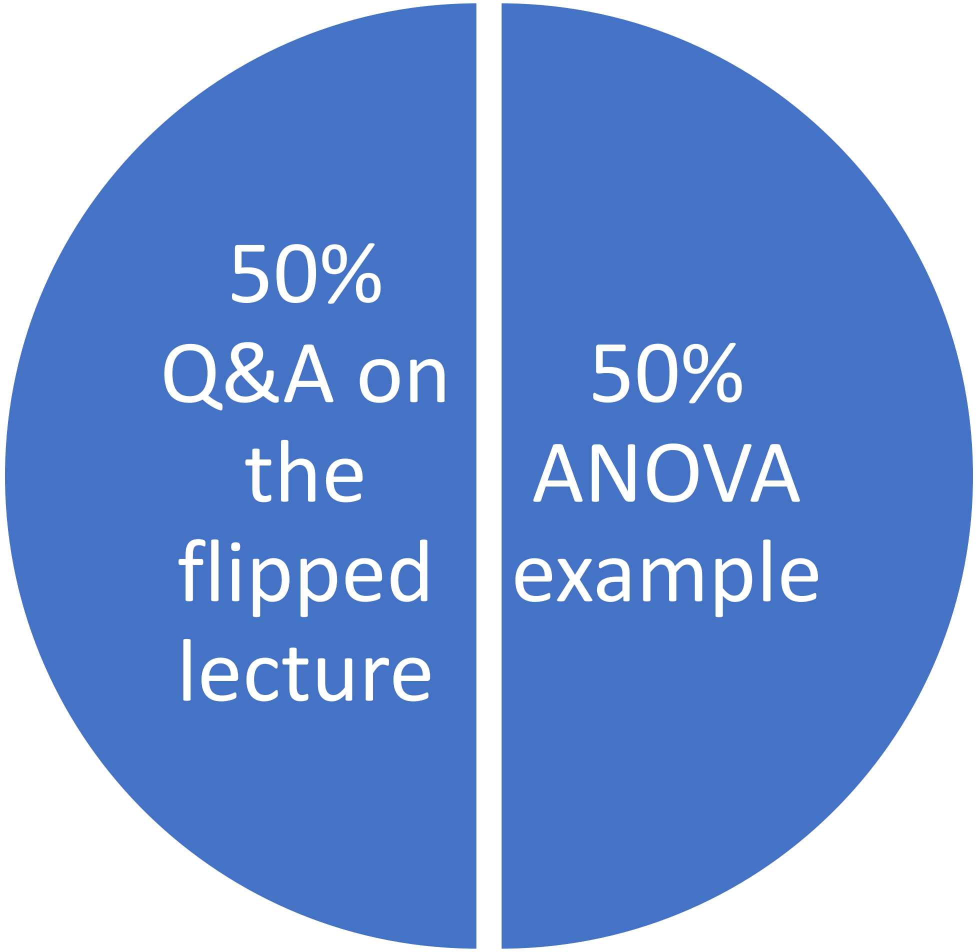
Today's lecture



Q&A on the flipped lecture

White slide because now YOU have to build the lecture with your questions!

Recap on the ANOVA model

- **Objective**: to understand if different treatments on a single factor determine differences on a response (selected because it is representative of the system under study)
- A **model on the effect of different levels of a single factor** on the response is desired:

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij}$$

- Two equivalent formulations of the **hypothesis testing**

$$H_0: \mu_1 = \mu_2 = \cdots = \mu_a$$
$$H_1: \mu_i \neq \mu_j \quad \text{for at least one pair } (i, j)$$

$$H_0: \tau_1 = \tau_2 = \cdots \tau_a = 0$$
$$H_1: \tau_i \neq 0 \quad \text{for at least one } i$$

- The problem can be solved analyzing the aliquot of variance that different treatments determine on the response:

$$SS_T = SS_{\text{Treatments}} + SS_E$$

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

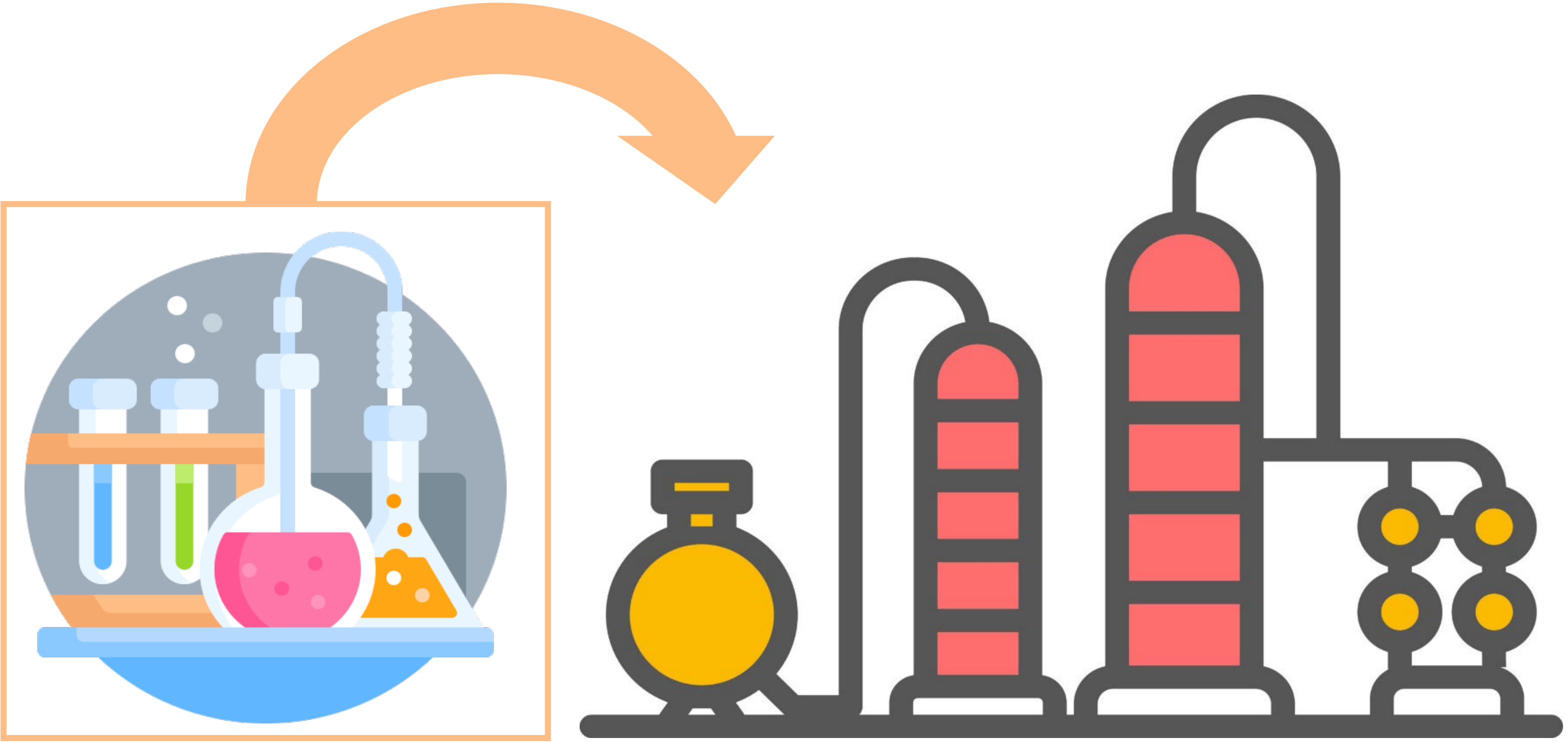
- The hypothesis testing formulation is a comparison between variances, hence it requires an F test:

$$F_0 = \frac{SS_{\text{Treatments}}/(a-1)}{SS_E/(N-a)} = \frac{MS_{\text{Treatments}}}{MS_E}$$

$$F_0 > F_{\alpha, a-1, N-a}$$

Taday’s lesson

- Procedure for ANOVA application



ANOVA procedure

- The **procedure for a comprehensive analysis of variance** goes through the following steps:
  1. computation of the effects
  2. comparison of the significance of effects with respect to error
     - F-test
       - see Matlab® commands: `anova; fitlm; anova1; anovan`
  3. determination of what determines the difference in treatment means
     - Schaffè method
     - Tuckey method
       - see Matlab® command: `multcompare`
  4. model adequacy checking
     - normality tests on the residuals
     - standardized residual normality test
     - residuals autocorrelation
     - residuals vs. fitted values pattern
     - residuals vs. original variables patterns
     - Anderson-Darling test for outlier detection
  5. homoscedasticity test
     - Bartlett test
       - see Matlab® command: `barttest`
     - Levene test
       - see Matlab® command: `vartestn`
  6. empirical modelling if quantitative factors are present

Empirical modelling and model interpretation

Linear regression models

Practical results interpretation: empirical modelling

- The analysis of variance treats **the design factor as if it was qualitative or categorical**:
  - when a factor is qualitative, it is meaningless to consider the response for a subsequent run at an intermediate level of the factor
- With a **quantitative factor**, the experimenter is usually interested in the entire range of values used
  - particularly the response from a subsequent run at an intermediate factor level

- Experimenters are frequently interested in developing **empirical regression models** to describe the relation among factors and responses

Linear regression models

- If examining a scatter diagram among factors and responses a strong relationship between factors and responses is found regression models can be built to describe the relation among factors and responses:
  - **linear model**:

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

  - sometimes an improvement can be obtained by adding a quadratic term in a **quadratic model**:

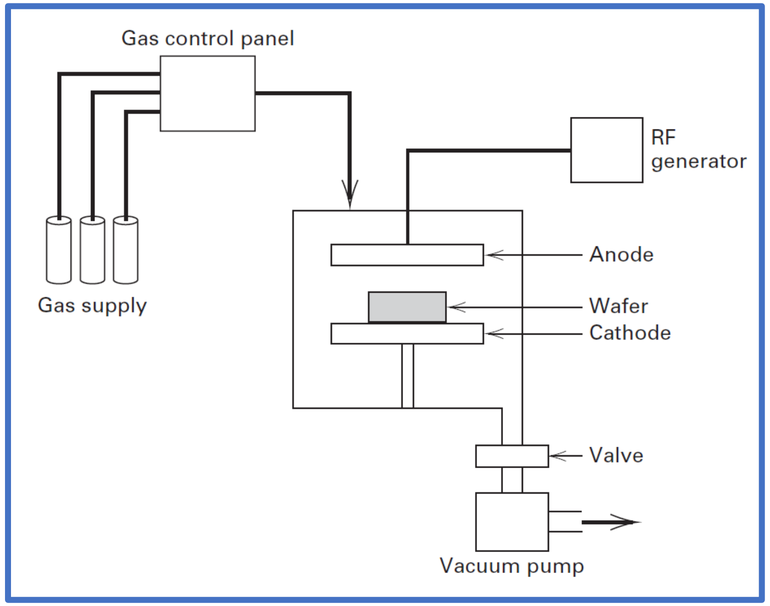
$$y = \beta_0 + \beta_1 x_1 + \beta_1 x_1^2 + \varepsilon$$

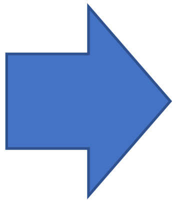
- The model parameters can be estimated from available data through the **method of least squares**
  - selecting estimates of the parameters β_i such that the sum of the squares of the errors is minimized
- It is desirable to fit the lowest order polynomial that adequately describes the system or process
  - models of higher complexity are appropriate if the extra complexity allows obtaining a much better model representativeness without overfitting the available data
- The empirical model could then be used to predict the response within the factors’ domain of experimentation and for **process optimization**
  - finding the levels of the design variables that result in the best values of the response

Example: integrated circuits manufacturing

Example: integrated circuits manufacturing

- Context: **integrated circuit manufacturing**
  - wafers are completely coated with a layer of material such as silicon dioxide or a metal
  - the unwanted material is then selectively removed by photolotography through a mask, thereby creating circuit patterns
  - a plasma etching process is widely used for creating zones at different conductivity in small geometries
  - energy is supplied by a radio-frequency (RF) generator causing plasma to be generated in the gap between two electrodes





- <u>Objective</u>: investigating the relationship between the **RF power** setting and the **etch rate**
  - to model the relationship between:
    - etch rate
    - RF power

04/05/2026

Experimental campaign

- Experimental campaign:
  - 4 levels of RF power were tested: 160, 180, 200, and 220 W
  - 5 wafers are tested at each level
- Available data: `wafer_anova.mat`

Power (W)	Observations 1	2	3	4	5
160	575	542	530	539	570
180	565	593	590	579	610
200	600	651	610	637	629
220	725	700	715	685	710

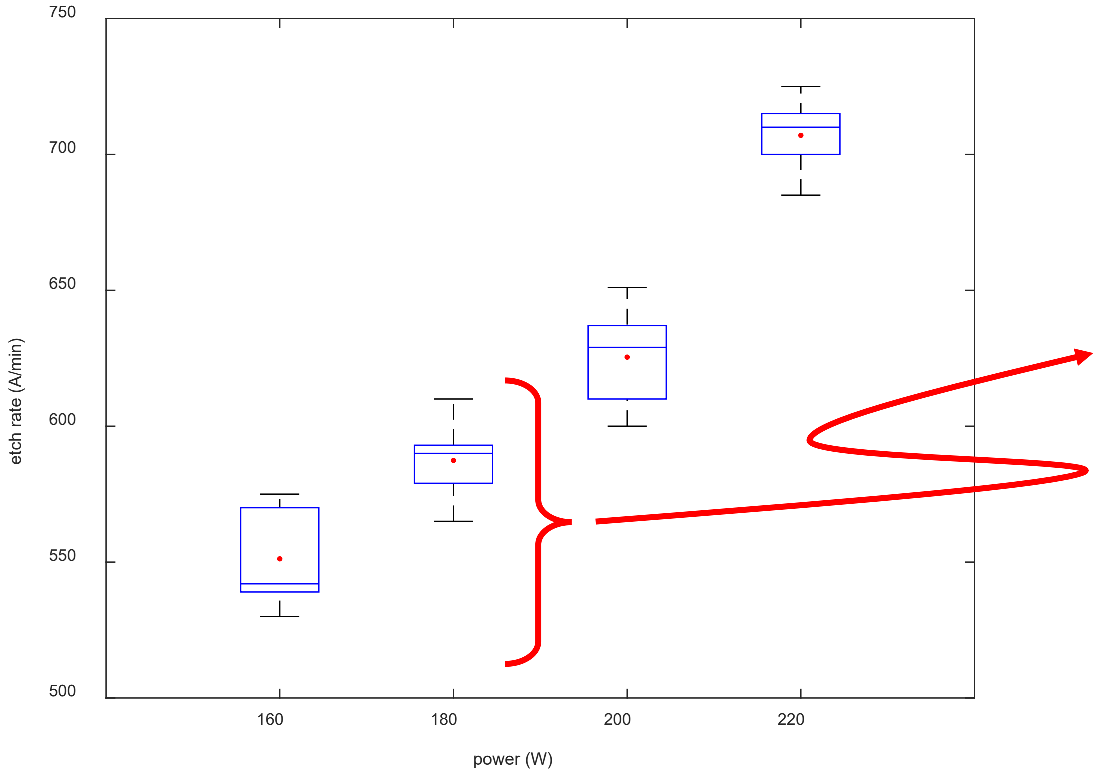
- This is an example of single-factor experiment with:
  - $a = 4$ levels of the factor
  - $n = 5$ replicates

→ $N = 20$ measurements (one for each of the 20 performed experiments)

- The 20 runs are made in random order
  - an efficient way to generate the run order is to use software:
    - Excel: enter the 20 runs in a spreadsheet; generate a column of random numbers using the rand(…) function; sort by that column
    - Matlab®: `randsample`

Initial analysis

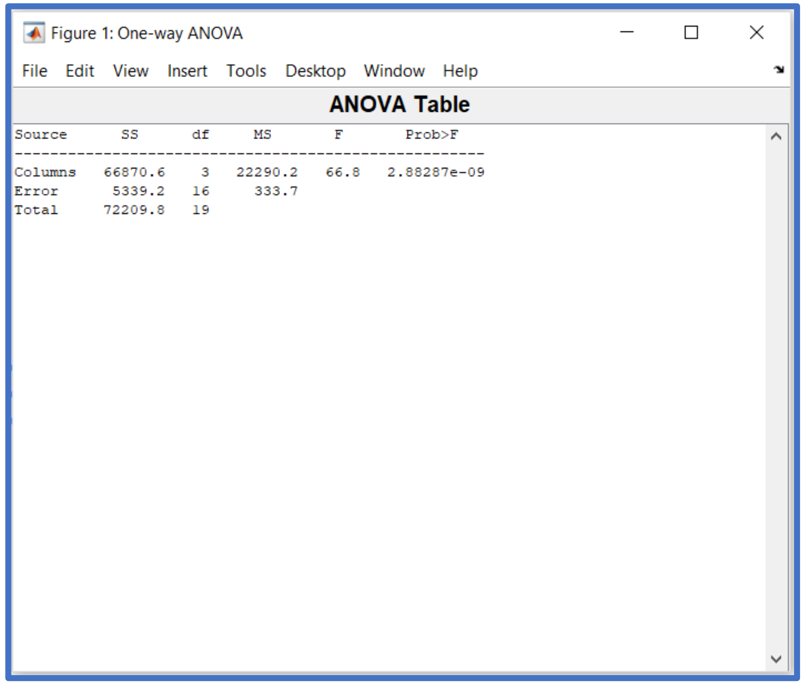
- Data visualization:
  - boxplot
  - `boxplot(Y1,X1);xlabel('power (W)');ylabel('etch rate (A/min)')`



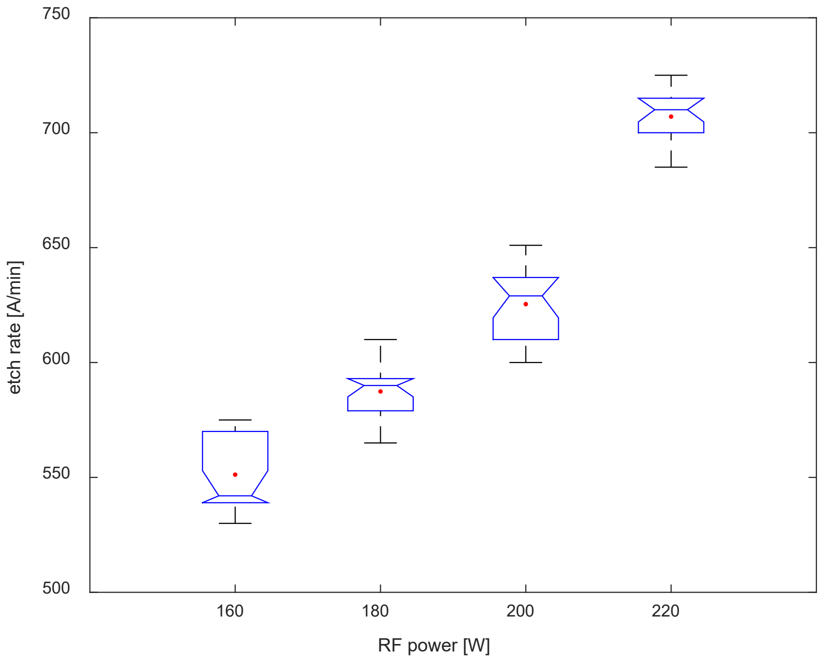
Some differences are evident.
Are they meaningful?

ANOVA model building

- Command: `[p,tbl,stats]=anova1(Y')`
- Outputs:
  - the treatment is significant: $MS_{Treatments} \gg MS_E$
    - the effect of the treatment is much higher than the noise
  - the null hypothesis is rejected ($F_0 \gg F_{\alpha,a-1,N-a}$ and $p < 0.05$)
    - the treatments determine substantial difference in treatments means



Source	SS	df	MS	F	Prob>F
Columns	66870.6	3	22290.2	66.8	2.88287e-09
Error	5339.2	16	333.7		
Total	72209.8	19			



ANOVA model outputs

- In Matlab® (and also other software) the ANOVA model outputs are calculated automatically:
  - $SS_{Treatments}$ and SS_E
  - $MS_{Treatments}$ and MS_E
  - F_0
  - the *p*-value associated to F_0
- Command:
  - `[p,tbl,stats]=anova1(Y')`
  - alternative command (which produces the same results):
    - construct the vectorized form of matrices $\mathbf{X}$ and $\mathbf{Y}$
    - `[p,tbl,stats]=anova1(Y1,X1)`

ANOVA via Matlab® commands

- Commands:
  - SS_T=sum(sum(Y'.^2))-sum(sum(Y'))^2/numel(Y)
  - $SS_{Treatments}$=sum(sum(Y').^2)/size(Y,2)-sum(sum(Y'))^2/numel(Y)
  - $SS_E=SS_T-SS_{Treatments}$
  - degrees of freedom:
    - treatment: size(Y,1)-1
    - error: numel(Y)-size(Y,1)
    - total: numel(Y)-1
  - mean errors:
    - treatment: $MS_{Treatments}=SS_{Treatments}$/(size(Y,1)-1)
    - error: $MS_E=SS_E$/(numel(Y)-size(Y,1))
  - F_0: $F_0=MS_{Treatments}/MS_E$
    - F distribution 95% confidence limit: finv(0.95,3,16)
  - *p*-value: 1-fcdf(F_0,3,16)

Comparison among treatments

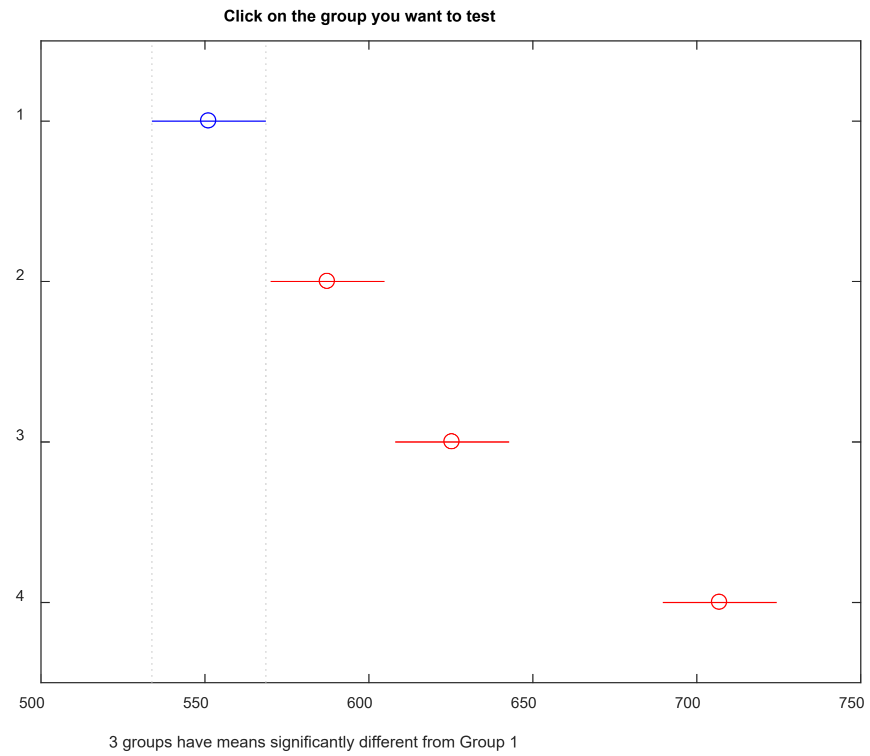
- Confidence intervals in the means of the different treatments can be obtained with command:

```
[c,m,h] = multcompare(stats)
```

- The Bonferroni method can be utilized with command:

```
[c,m,h] =
multcompare(stats,'CType','bonferroni')
```

- The **multcompare** command is utilized for implementing:
  - Scheffè's method
  - Tuckey's test on pair of means, etc.



Checking model adequacy

- The residuals are the difference among the models predictions and the ground truth (the real measured values)

- The **residuals** ε_{ij} of the means effect model are calculated from the difference the measured response y_{ij} and the means μ_i of the treatments:

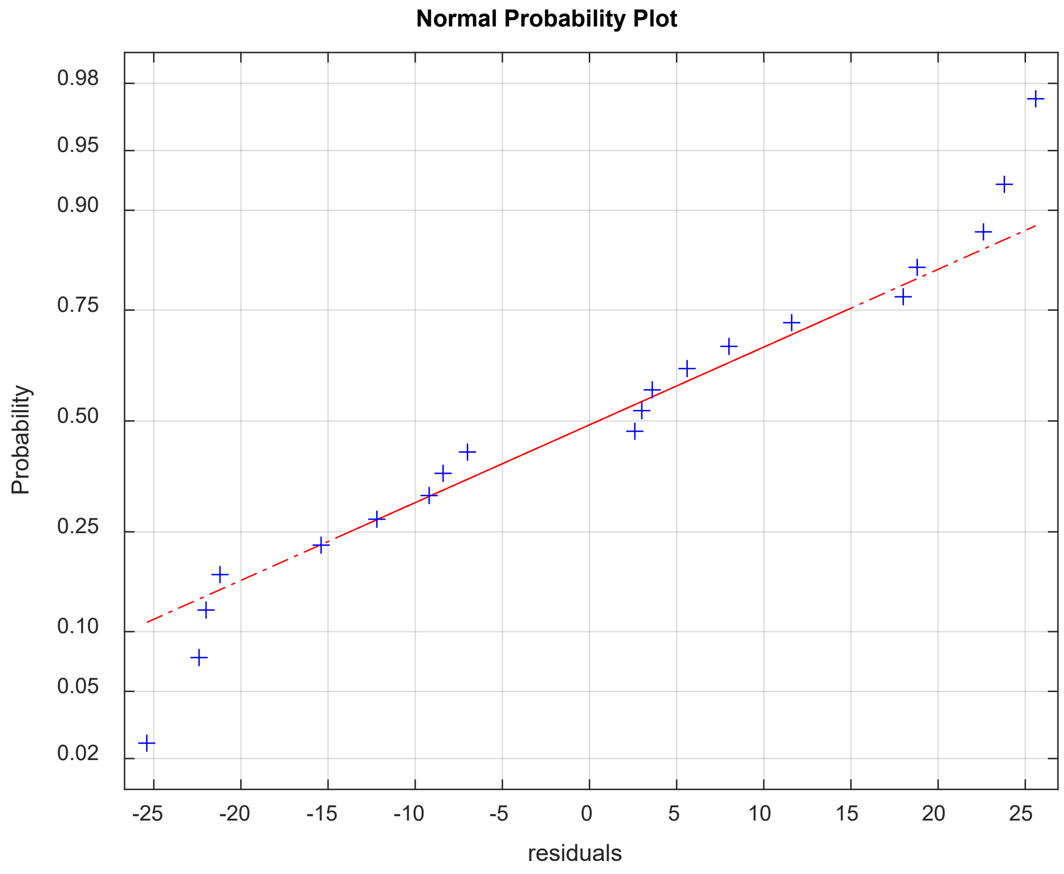
$$\varepsilon_{ij} = y_{ij} - \mu_i$$

  - `r = reshape(Y-repmat(stats.means',1,5),20,1)`

- Normal probability plot can be used to test if residuals are normally distributed:
  - `normplot(r);xlabel('residuals');box on`
  - `normplot(model.Residuals.Raw);xlabel('residuals');box on`

Normal probability lot of the residuals

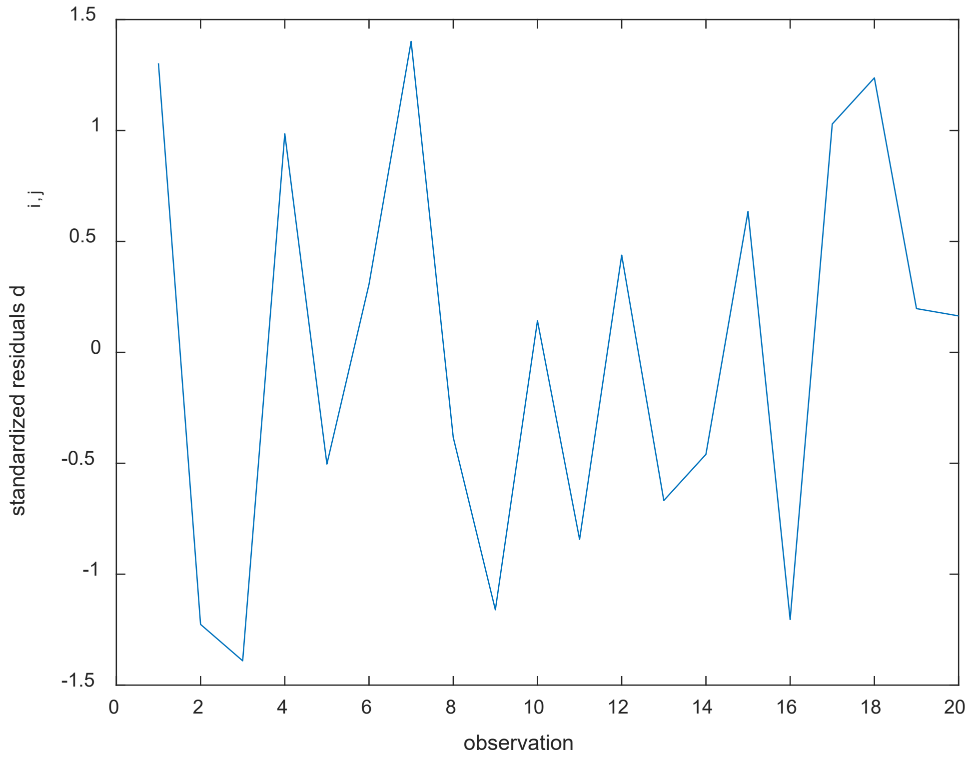
- The normal probability plot does not show significant departures from a normal distribution



Residuals analysis

- Anderson-Darling verifies if data come from a normal distribution:
  - `[h,p] = adtest(r)`
  - fails to reject the null hypothesis at the default 5% significance level (with $p = 0.3863$)

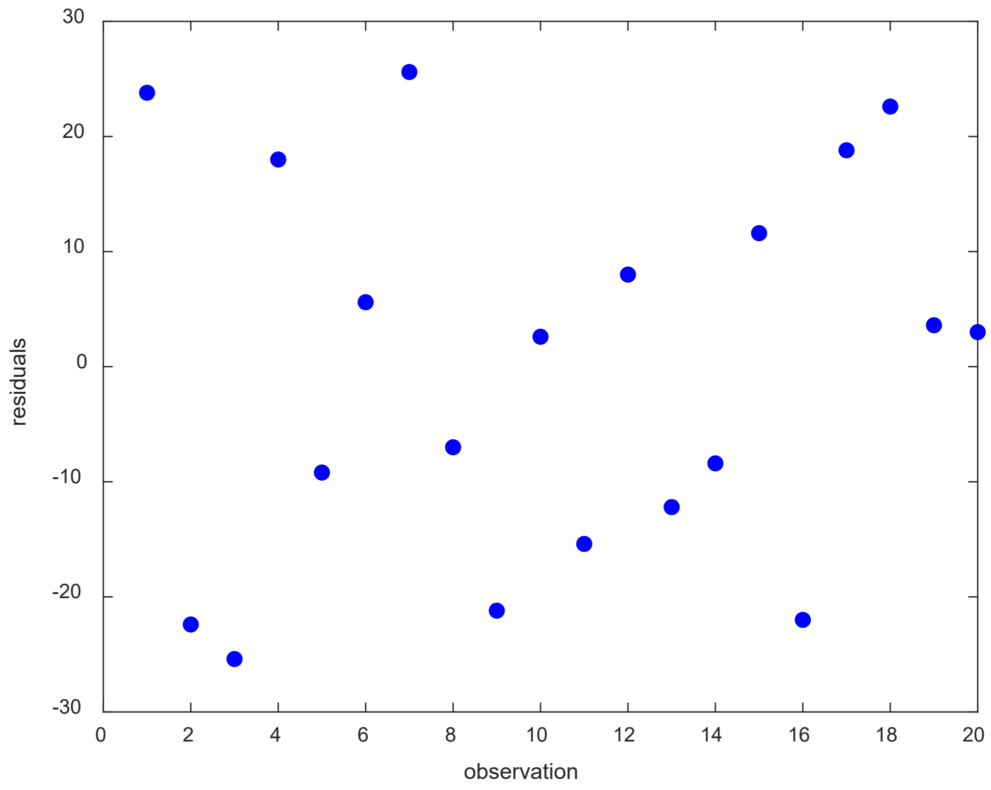
- Outliers can be detected through standardized residuals d_{ij} :
  - the standardized residuals should stay in the interval $d_{ij} \in [-3,3]$



Pattern of the residuals in time

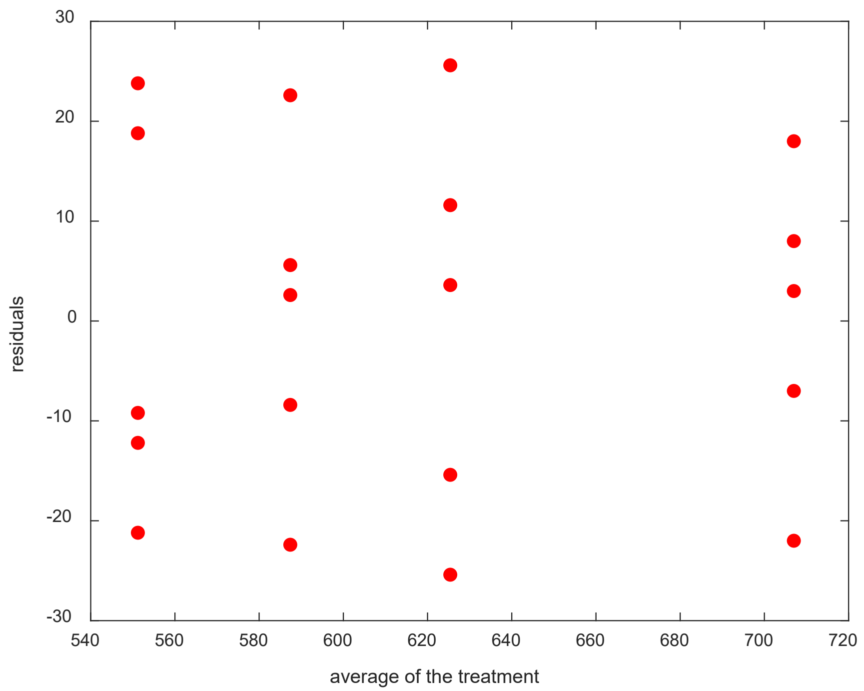
- The residuals are represented in time to observe if they are independent (autocorrelation is not present)
  - no significant autocorrelation is present in the residuals

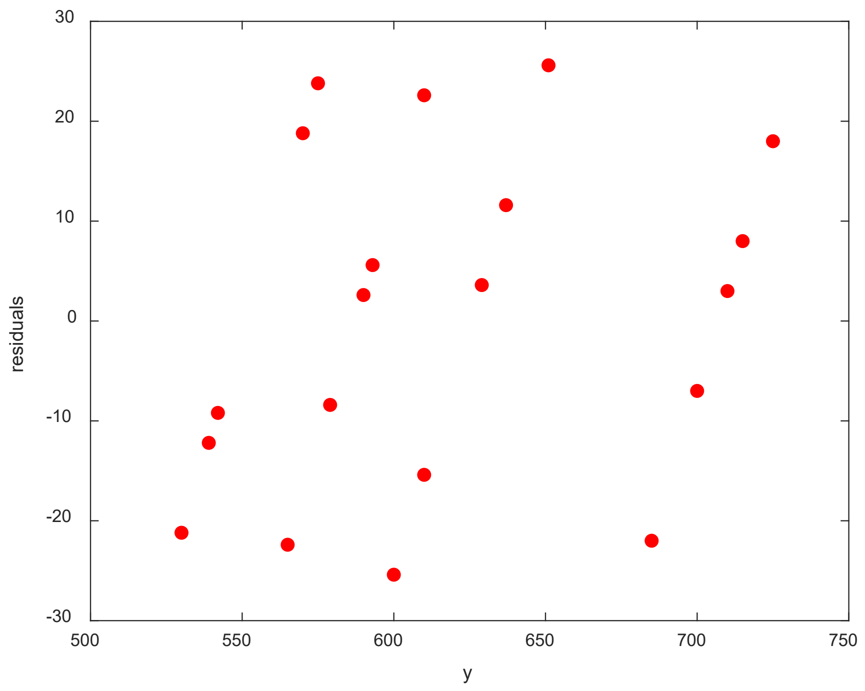
- Command:
  - `scatter(1:20,r,'ob','filled');xlabel('observation');ylabel('residuals');box on`



Residuals versus fitted values

- Residuals do not show particular patterns vs:
  - average treatment:
    - `scatter(repmat(mean(Y')',5,1),r,'or','filled'); xlabel('average of the treatment');ylabel('residuals');box on`
  - the response y





Residuals variance equality testing

- **Bartlett's test**:
  - failed to reject the null hypothesis of the equality between variances
    - $p = 0.93324$
  - command:
    - `[p,stats] = vartestn(Y')`
- **Modified Levene test**:
  - failed to reject the null hypothesis of the equality between variances
    - $p = 0.66116$
  - command:
    - `[p,stats] = vartestn(Y','TestType','LeveneAbsolute')`
- Variances are verified to be equal:
  - data from different treatments are homoscedastic

Summary of the ANOVA code (1/3)

```
close all
clear all
clc


load('…where the dataset file is…')


%ANOVA
[p,tbl,stats]=anova1(Y');
% or [p,tbl,stats]=anova1(Y1,X1);
```

Summary of the ANOVA code (2/3)

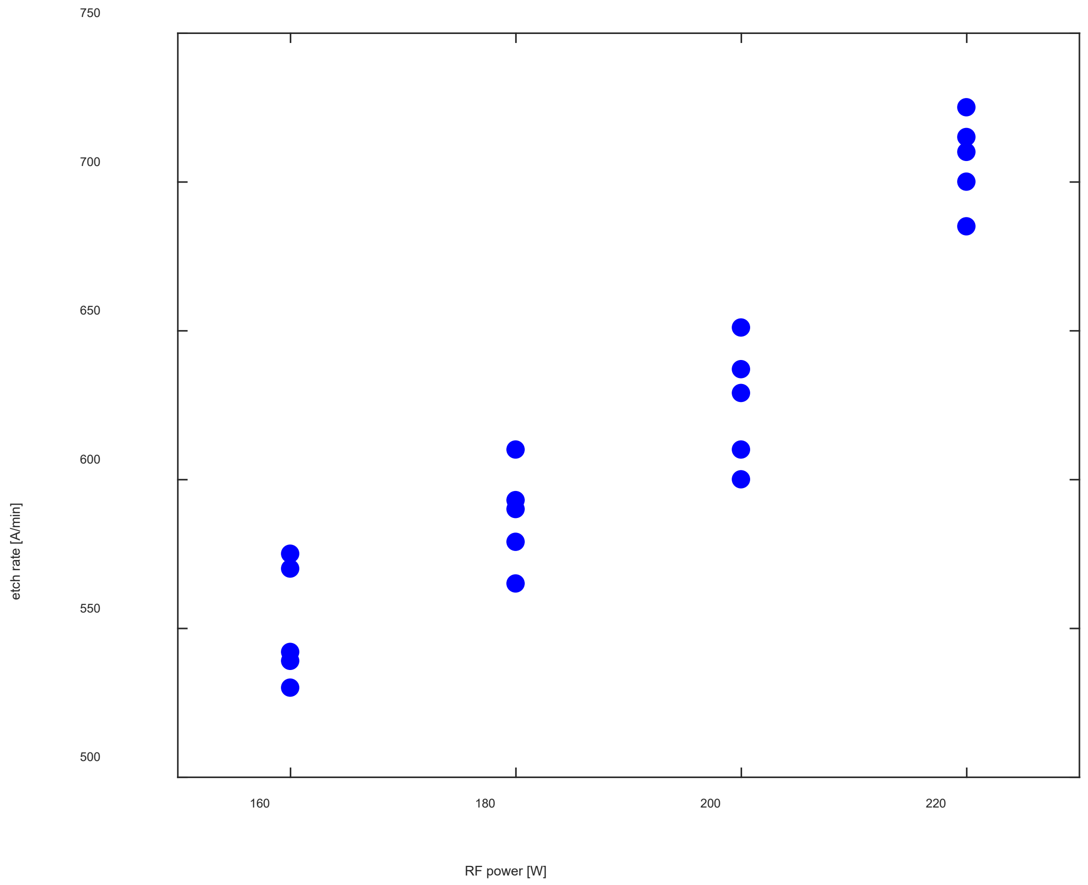
```
SST=sum(sum(Y'.^2))-sum(sum(Y'))^2/numel(Y)
SSTreatments=sum(sum(Y').^2)/size(Y,2)-sum(sum(Y'))^2/numel(Y)
SSE=SST-SSTreatments
% degrees of freedom:
% treatment
size(Y,1)-1
%error
numel(Y)-size(Y,1)
% total
numel(Y)-1
% mean errors
% treatment
MSTreatments=SSTreatments/(size(Y,1)-1)
% error
MSE=SSE/(numel(Y)-size(Y,1))
% F0
Fo=MSTreatments/MSE
% F distribution 95% confidence limit
F95ci=finv(0.95,3,16)
% p-value
pvalue=1-fcdf(Fo,3,16)
```

Summary of the ANOVA code (3/3)

```
% Bonferroni test on what treatments are significantly different
[c,m]=multcompare(stats,'CType','bonferroni')
% residuals
r=reshape(Y-repmat(stats.means',1,5),20,1)
d=r/sqrt(MSE);
figure;plot(d);xlabel('observation');ylabel('standardized residuals d_i_,_j');box on
% Normal probability plot can be easily displayed:
figure;normplot(r);xlabel('residuals');box on
% normplot(model.Residuals.Raw);xlabel('residuals');box on
[h,pad]=adtest(r)
figure;scatter(1:20,r,'ob','filled');xlabel('observation');ylabel('residuals');box on
figure;scatter(repmat(mean(Y')',5,1),r,'or','filled');xlabel('average of the treatment’);
ylabel('residuals');box on
figure;scatter(Y1,r,'or','filled');xlabel('y');ylabel('residuals');box on
% Bartlett’s test
[pb,statsb] = vartestn(Y')
% Modified Levene test
[pl,statsl] = vartestn(Y','TestType','LeveneAbsolute’)
```

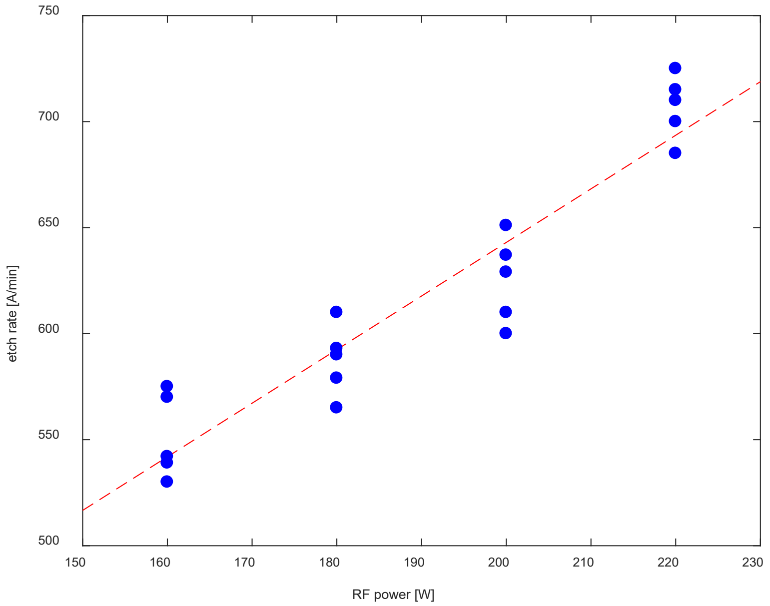
Example of plasma etching

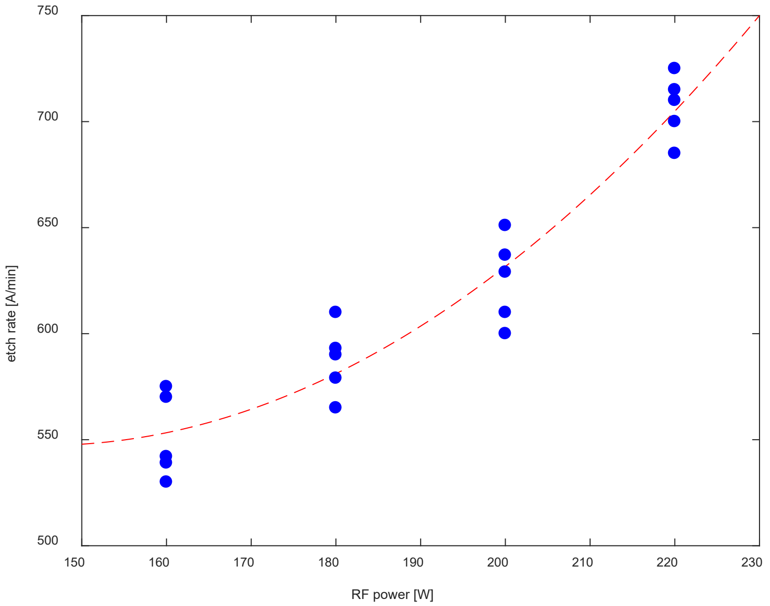
- A strong correlation is evident among the etch rate and the RF power



Fitted regression model in plasma etching

- The fitted empirical models are:
  - linear model: $y = 137.62 + 2.527x_1$
  - quadratic model: $y = 1147.8 - 8.2555x_1 + 0.0284x_1^2$
- A visual inspections seems to highlight that the quadratic models fits better the data:
  - total sum of squared residuals:
    - 8352.5 for the linear model
    - 5776 for the quadratic model
  - however, higher parameters uncertainty was found in the quadratic model…





… per sempre a fianco a me!