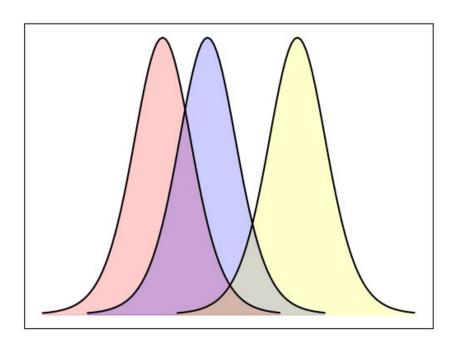
Analysis of Variance (ANOVA)

Jolla Kullgren Department of Chemistry - Ångström

one-way ANOVA F-test



- The F-test can be used to assess whether the expected values of a quantitative variable within several pre-defined groups differ from each other.
- It can be seen as a generalization of the t-test for more than two data-sets.



F-test main formula

$$F = rac{ ext{"beetween-group variablity"}}{ ext{"within-group variablity"}} = rac{\sum_{i=1}^K n_i (ar{x}_i - ar{x})^2 / (K-1)}{\sum_{i=1}^K \sum_{j=1}^{n_i} (x_{ij} - ar{x}_i)^2 / (N-K)}$$

K: Number of groups

 n_i : Samples in group i

 \bar{x}_i : Mean of group i

 $\bar{x}: \text{Overall mean}$

 $x_{ij}:j^{ ext{th}}$ observation in the $i^{ ext{th}}$ group.

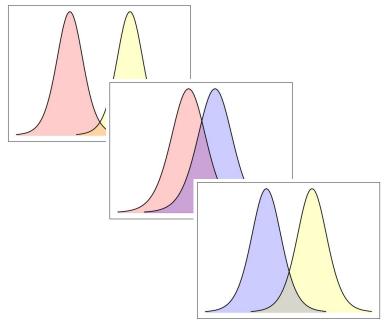
N: Overall sample size

Example: ANOVA in python:

```
import numpy as np
N1=5; off1 = 0.1; w1=0.4
N2=4; off2 = 0.6; w2=0.3
N3=6; off3 = 0.3; w3=0.2
data 2 = w2*np.random.rand(N2)+off2
t-test: 15.011495298649004 -> P-value: 0.0005422077738381697
```

P-value suggest we can reject null hypothesis. The mean value are not significantly the same. However, we do not know if they are all different or if one is different from the other two...

Pair-wise independent two-sample t-test



Using multiple *independent two-sample t-test* we can try to locate the "outlier".

- Using multiple independent two-sample t-test we can identify "outlier"
- With 95 % confidence "mislabel" 5 % of the times. With many comparisons, this become a substantial problem.
- The *Bonferroni correction*: Scale the significance level with the number of comparisons. With a 5 % significance level, p-values should be $0.05/N_{\rm pairs}$ or less.



Example: pair-wise t-tests in python:

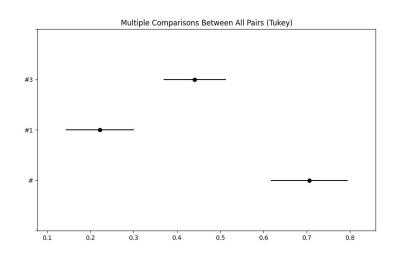
```
print("Pair 1-2")
print("Pair 1-3")
print("Pair 2-3")
print(t test,p value)
```

Example: pair-wise t-tests in python (continued):

```
Pair 1-2
-7.294292120993236 0.00016356196701124712
Pair 1-3
-3.6621612014725207 0.00521797192193281
Pair 2-3
5.023586272797825 0.0010222980431426679
```

P-values suggest we can reject all null hypothesis. This is true also when applying the Bonferroni correction, in which case our threshold should be 0.05/3.

Tukey's-test

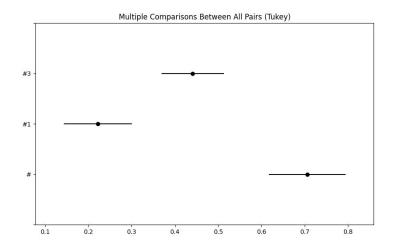


Using multiple *independent two-sample t-test* we can try to locate the "outlier".

- Another way of performing a post hoc-test is the so-called Tukey's test.
- The result from the test can be summarized in a plot a shown to the left.
- Note: There can be "logical contradictions" between ANOVA and Tukey test (doi:10.3390/sym13081387).



Tukey's-test



Using multiple *independent two-sample t-test* we can try to locate the "outlier".

We use the following test statistics for a pair A-B:

$$q^{test} = rac{ar{x}_A - ar{x}_B}{s_{A+B}/\sqrt{n_{A+B}}}$$

 s_{A+B} and n_{A+B} refer to the variance and number of samples in the combined "A+B" group.

• The comparison is made to the studentized range distribution from the entire set of groups.

$$q=rac{ar{x}_{max}-ar{x}_{min}}{\sqrt{2}s_{Tot}/\sqrt{n_{Tot}}}$$

Where max, min and Tot, refer to minimum, maximum, and the total numbers of samples,

Example: Tukey's test in python:

Import pandas as pd data 1=pd.DataFrame({"data-set": len(data 1)*["#1"], "data":data 1 }) #2 #1 -0.4845 0.0 -0.652 -0.317 #2 #3 -0.2649 0.0024 -0.4261 -0.1037 True #1 #3 0.2196 0.0058 0.0684 0.3708 True

The test is consistent with the pair-wise t-tests.

Summary

- ANOVA can be used to assess whether the expected values of a quantitative variable within several pre-defined groups differ from each other.
- ANOVA cannot identify which(s) group(s) that differ from the others.
- Outliers can be identified by performing pair-wise t-tests, or with Tukey's test.
- One should note that the results from ANOVA and Tukey's test need not be consistent.

