

An Introduction to Statistics for Experimental Analysis



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Instructor / Presentor

* **Mark Wineberg** is an Associate Professor at the University of Guelph. He has been actively researching the field of GEC since 1993 while he was still a graduate student. Over the years he has published on various topics including: the intersection of GA and GP, enhancing the GA for improved behavior in dynamic environments through specialized multiple populations, and exploring the concept of distances and diversity in GA populations. Prof. Wineberg also teaches an undergraduate course on computer simulation and modeling of discrete stochastic systems with an emphasis on proper statistical analysis, as well as a graduate course on experimental design and analysis for computer science, which is an outgrowth of the statistical analysis tutorial given at GECCO.



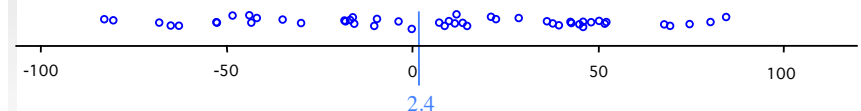
What Are We Interested In?

- For most statistical analysis for EC the question is
 - Is one way better than another way?
 - Statistically this translates into a statement about the difference between means: “Is the difference between ‘my mean’ and ‘the other mean’ greater than zero?”
- We will approach this question in 2 steps:
 1. What can we say about the true mean of a *single* distribution?
 - Called *point estimation*
 2. How can we compare the true means of *two* or more distributions?



Recompute ‘Average’ with different samples

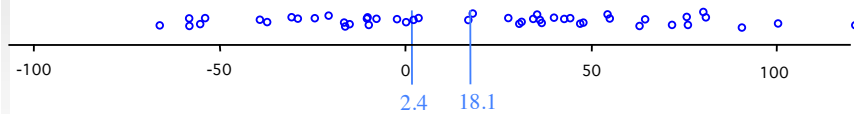
- The system has a true mean ... but where is it?





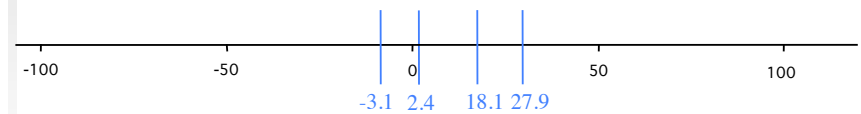
Recompute 'Average' with different samples

- The system has a true mean ... but where is it?



Recompute 'Average' with different samples

- The system has a true mean ... but where is it?
- Averages change from sample to sample ... they are samples from a random variable



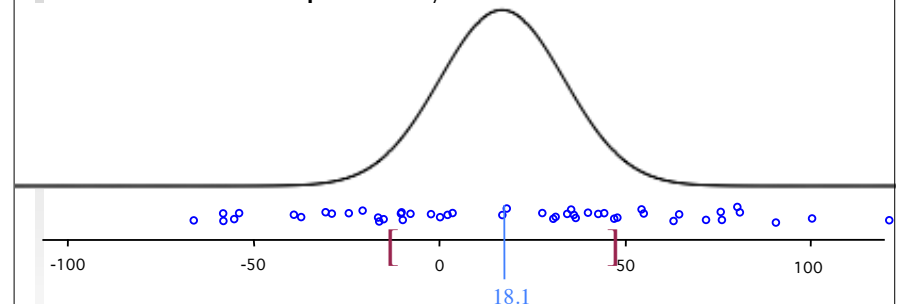
Confidence Intervals

- Can give a range within which it is very likely the true mean lies
 - Called the *confidence interval*
- Also should consider the probability that the true mean lies with the range
 - Called the *confidence level*



Confidence Interval (Formed Around Average)

- True mean probably with confidence interval





Normal (Gaussian) Distribution

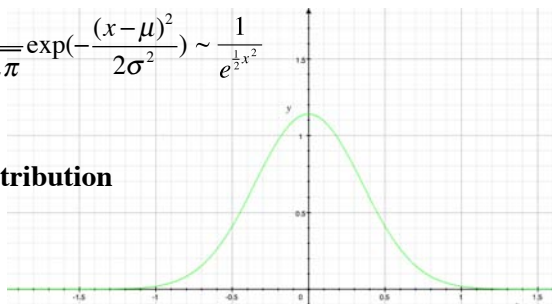
- For now we will assume that we are sampling from (the results are distributed as) a *normal distribution*
 - AKA Bell Curve
 - Most common distribution found in nature thanks to the *Central Limit Theorem*

$$P(X = x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \sim \frac{1}{e^{\frac{1}{2}x^2}}$$

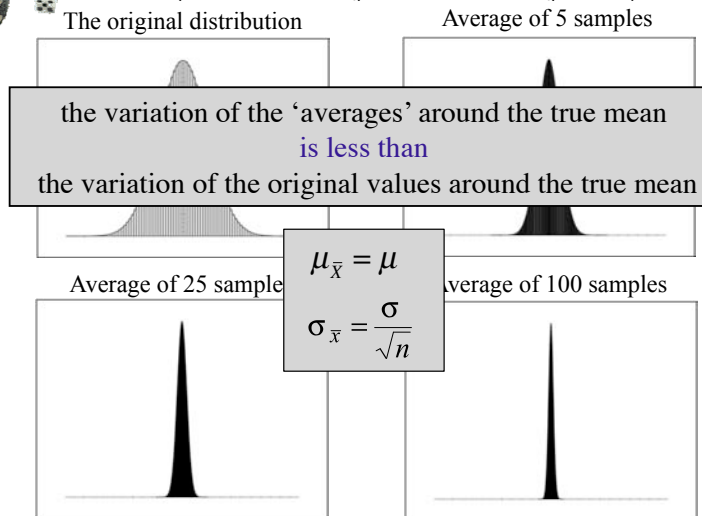
$$X \sim N(\mu, \sigma^2)$$

Standard Normal Distribution

$$X \sim N(0, 1)$$



Distribution of the Average (of a normally distributed system)



Confidence Intervals

- Of course, we don't know the true mean, μ , or true standard deviation, σ
- We *do* know the mean of the samples, \bar{X} , the sample size, n , and the sample standard deviation, s_X
- If the source distribution is *normally distributed*, the shape and size of the “finger” is known exactly!
 - We can determine the odds that the true mean lies within a specified range of \bar{X}



Confidence Intervals

- First since \bar{X} is normally distributed, we can turn it into a standard normal distribution
 - subtract off the mean to zero it
 - divide by the std deviation to give it a std deviation of 1
 - also gives a variance of 1

$$Z = \frac{\bar{X} - \mu_{\bar{X}}}{\sigma_{\bar{X}}} = \frac{\bar{X} - \mu_X}{\sigma_X / \sqrt{n}}$$



t Distribution

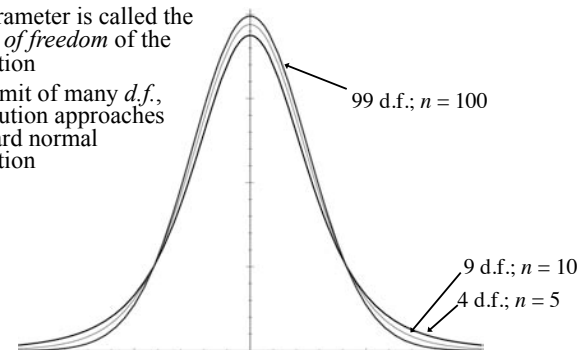
- Want to find μ the true mean in terms of the average
 - But we have not one but two unknowns - σ is also unknown
 - One equation - two unknowns - not good!!!
 - Trick - divide by the known sample standard deviation s instead of σ
- But now we have a normally distributed numerator divided by a non-normally distributed denominator
 - Denominator has a chi distribution
 - A normal distribution over a chi distribution has a Student's t distribution

$$T = \frac{\bar{X} - \mu_{\bar{X}}}{s_{\bar{X}}} = \frac{\bar{X} - \mu_X}{s_X / \sqrt{n}}$$



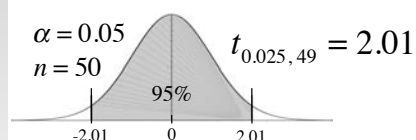
t Distribution

- The t “distribution” is really a family of distributions – the shape of the distribution changes as the number of samples, n , changes
 - This parameter is called the *degrees of freedom* of the distribution
 - In the limit of many *d.f.*, t distribution approaches a standard normal distribution



Estimating the Mean: Confidence Intervals Around the Average

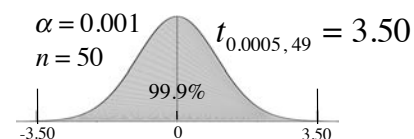
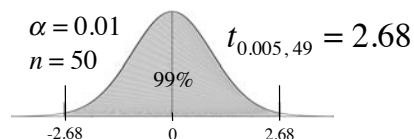
If samples taken from a *standard normal distribution* ($\mu = 0, \sigma = 1$),
Based on $n = 50$ runs the sample average has a t distribution.



- α is the probability of seeing values outside the cutoffs
 - Confidence Level is $1 - \alpha$

Cut off $t_{\frac{\alpha}{2}, n-1}$ values can be computed using Excel: **=TINV($\alpha, n - 1$)**
using R: **> qt($1-\alpha/2, n - 1$)**

- For CI, we can use cutoff t values
- The wider the cutoff values, the more likely the true mean lies between them



Estimating the Mean: Confidence Intervals Around the Average

- We know that
- Using the $\pm t_{\frac{\alpha}{2}, n-1}$ cutoff t -values we can form a Confidence Interval that has a $1 - \alpha$ C.L. with $n - 1$ degrees of freedom
- Substituting the cutoff values from the C.I. into the above equation produces

$$T = \frac{(\bar{X} - \mu_X)}{s_X / \sqrt{n}}$$

$$\pm t_{\frac{\alpha}{2}, n-1} = \frac{\bar{X} - \mu_X}{s_X / \sqrt{n}}$$

which can be rewritten as $\mu_X = \bar{X} \pm t_{\frac{\alpha}{2}, n-1} \frac{s_X}{\sqrt{n}}$



Estimating the Mean: Confidence Intervals Around the Average

- Confidence Intervals can be written in 3 equivalent ways

Error Bounds

$$\mu_X = \bar{X} \pm t_{\frac{\alpha}{2}, n-1} \frac{s_X}{\sqrt{n}}$$

Confidence Intervals

$$\bar{X} - t_{\frac{\alpha}{2}, n-1} \frac{s_X}{\sqrt{n}} \leq \mu_X \leq \bar{X} + t_{\frac{\alpha}{2}, n-1} \frac{s_X}{\sqrt{n}}$$

$$\mu_X \in \left[\bar{X} - t_{\frac{\alpha}{2}, n-1} \frac{s_X}{\sqrt{n}}, \bar{X} + t_{\frac{\alpha}{2}, n-1} \frac{s_X}{\sqrt{n}} \right]$$



Estimating the Mean: Confidence Intervals Around the Average

Example:

- An experimenter runs a New Evolutionary Algorithm on a TSP
- At the end of each run, the smallest length tour that had been found during the run was recorded
- NEA is run 50 times on the same TSP problem
- On average NEA found solutions with a tour length of 272
- The standard deviation of these tours is 87
- We want to compute a Confidence Interval using a 99% Confidence level



Estimating the Mean: Confidence Intervals Around the Average

- From the problem we know that the average NEA run produced tours of

$$\bar{X} = 272 \text{ that had } s_X = 87$$

We know that
$$\mu_X = \bar{X} \pm t_{\frac{\alpha}{2}, n-1} \frac{s_X}{\sqrt{n}}$$

- Also from the problem $n = 50$ and $\alpha = (1 - 0.99) = 0.01$

so the $\pm t$ cutoff value is $t_{\frac{0.01}{2}, 49}$

using Excel/R we see that $\text{TINV}(0.01, 49) = \text{qt}(0.995, 49) = 2.68$

$$\mu_X = 272 \pm 2.68 \frac{87}{\sqrt{50}} = 272 \pm 33$$

and so $239 \leq \mu_X \leq 305$ with a 99% C.L.

i.e. there is only a 1% chance that the true mean lies outside the confidence interval formed around average

Basic Statistical Tests



Part 2 - Comparisons: Non-Overlapping Confidence Intervals and the Student's T Test



Using Confidence Intervals to Determine Whether My Way is Better

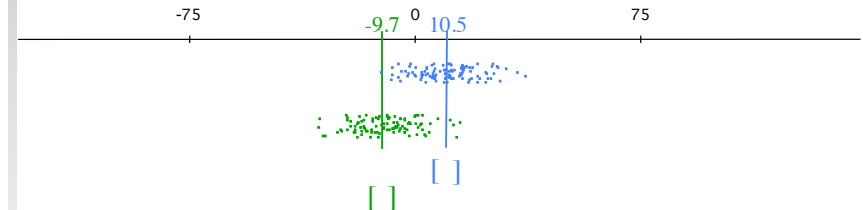
If we have two different EC systems how can we tell if one is better than the other?

Trivial method: Find confidence intervals around both means

- If the CIs don't overlap
 - Then it is a rare occurrence when the two systems do have identical means
 - The system with the better mean can be said to be better on average with a probability better than the Confidence Level
- If the CIs do overlap
 - Can't say that the two systems are different with this technique
 - Either:
 1. The two systems are equivalent
 2. We haven't sampled enough to discriminate between the two



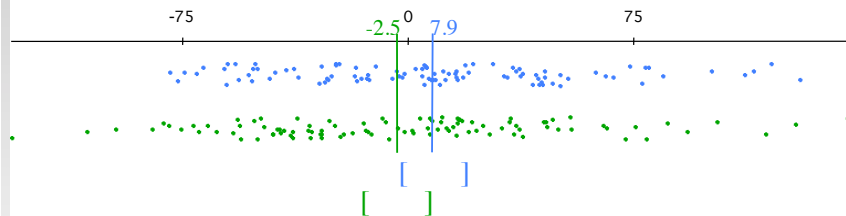
Confidence Interval Example



		95% Confidence Level					
μ	σ	n	\bar{X}	$s_{\bar{X}}$	$1.96 \frac{s_{\bar{X}}}{\sqrt{n}}$	Lower	Upper
+10	10	100	10.5	10.0	3.3	7.2	13.8
-10	10	100	-9.7	10.1	3.3	-13.1	-6.4



Confidence Interval Example



		95% Confidence Level					
μ	σ	n	\bar{X}	$s_{\bar{X}}$	$1.96 \frac{s_{\bar{X}}}{\sqrt{n}}$	Lower	Upper
+10	50	100	7.9	47.1	9.2	-1.3	17.1
-10	50	100	-2.5	52.1	10.2	-12.7	7.7



Improving the Sensitivity: The Student t Test

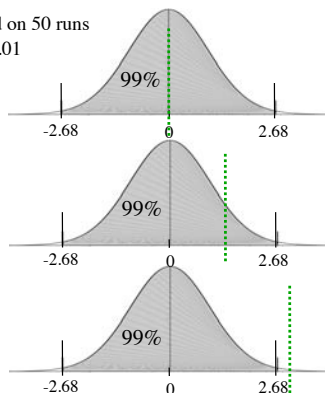
- The Student t Test is the basic test used in statistics
 - Idea: Gain sensitivity by looking at the difference between the means of the two systems



The Student t Test

Where the normalized difference falls on the t distribution determines whether difference expected if both systems were actually performing the same

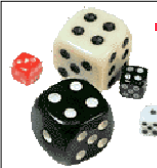
Based on 50 runs
 $\alpha = 0.01$



- Normalized difference called the t value

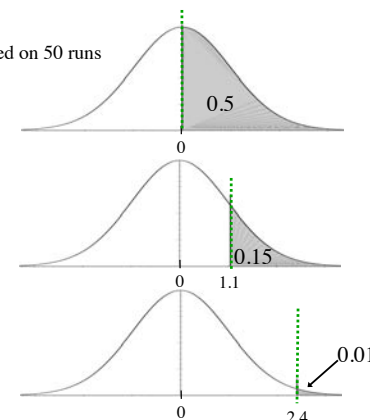
$$t \text{ value} = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_{X_1}^2 + s_{X_2}^2}{n}}}$$

- Distribution again differs for different sample sizes
 - Degrees of Freedom is now $= (n - 1) + (n - 1) = 2n - 2$
- t test either succeeds or fails
 - t value greater than cutoff for a given C.L. or not



The Student t Test: p -values

Based on 50 runs



- The cut-off values produces a binary decision: true or false
 - loses information
- Better to report the probability that two systems are different
- This is the complement of the probability that they are the same
 - $1 - \Pr(T < t \text{ score})$
 - Called the p -value



t Test Step by Step

- Compute the 2 averages \bar{X}_1 and \bar{X}_2
- Compute standard deviations s_1 and s_2
- Compute degrees of freedom: $n_1 + n_2 - 2 = 2n - 2$

- Calculate T statistic:
$$T = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_{X_1}^2 + s_{X_2}^2}{n}}}$$
- Compute the p -value

- p -value = the area under the t distribution outside $[-T, T]$
- In Excel: `=TDIST(T, 2*n - 2, 2)`
 - The final "2" in Excel means "two-sided"
- In R: `> 2*pt(-T, 2*n - 2)`



Variance Assumptions and the T Test

$$\sigma_1 = \sigma_2 = \sigma \text{ and } n_1 = n_2 = n \quad T = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_{X_1}^2 + s_{X_2}^2}{n}}}$$

$$\sigma_1 = \sigma_2 = \sigma \text{ but } n_1 \neq n_2 \quad T = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{(n_1 - 1)s_{X_1}^2 + (n_2 - 1)s_{X_2}^2}{(n_1 + n_2 - 2)} \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}}$$

In Excel: `=ttest(A1:A50, B1:B50, 2, 2)`



Variance Assumptions and the T Test

$$\sigma_1 \neq \sigma_2 \text{ and } n_1 \neq n_2 \quad T = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_{X_1}^2}{n_1} + \frac{s_{X_2}^2}{n_2}}} \leftarrow \begin{array}{l} \text{Approximate variance} \\ \text{not pooled} \end{array}$$

$$D.F. = \frac{(s_1^2 / n_1 + s_2^2 / n_2)^2}{(s_1^2 / n_1)^2 / (n_1 - 1) + (s_2^2 / n_2)^2 / (n_2 - 1)}$$

called the Welch's T test

In Excel: =ttest(A1:A50, B1:B50, 2, 3)



t.test(): Everything in one simple R function

n = 80 for both OEA and NEA

```
> t.test(OEA, NEA)
Welch Two Sample t-test
data:  OEA and NEA
t = -2.2549,      df = 152.68,      p-value = 0.02556
alternative hypothesis:
      true difference in means is not equal to 0
95 percent confidence interval:
 -4.7621535      -0.3143734
average of OEA      average of NEA
5.119665      7.657929
```

slightly modified for legibility



t.test(): Welch's vs Student's

n = 80 for both OEA and NEA

```
> t.test(OEA, NEA, var.equal=TRUE)
Two Sample t-test
data:  OEA and NEA
t = -2.2549,      df = 158,      p-value = 0.02551
alternative hypothesis:
      true difference in means is not equal to 0
95 percent confidence interval:
 -4.7615555      -0.3149714
average of OEA      average of NEA
5.119665      7.657929
```

slightly modified for legibility



Comparing Variances

- For the T test, we are comparing means
 - Difference between averages (after normalization)
 - see if it equals 0
- Now we want to compare variances
 - Won't take the difference between variances
 - Difference between variances not a nice distribution
 - Rather will take the ratio of variances
 - see if it equals 1
 - distribution known: F distribution



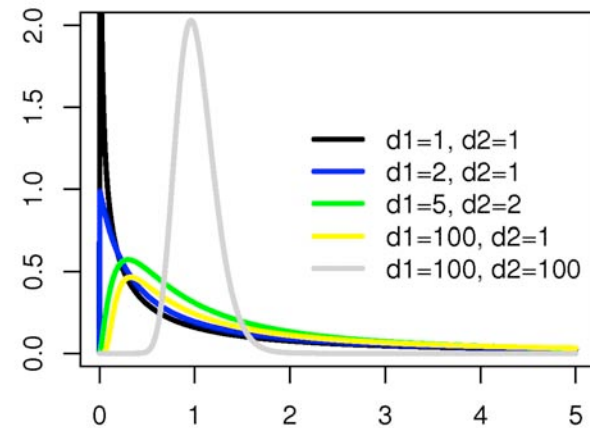
The F Distribution

- The sample variance over the true variance has a χ^2 distribution with a $n - 1$ degrees of freedom
 - seen when creating the T distribution (normal / chi)
- But what about the ratio of two variances?
 - With degrees of freedom of d_1 and d_2
- Answer: It has a $F(d_1, d_2)$ distribution
 - F distribution is the ratio of two χ^2 distribution over their degrees of freedom

$$F(d_1, d_2) = \frac{\chi_1^2 / d_1}{\chi_2^2 / d_2} = \frac{d_2 \chi_1^2}{d_1 \chi_2^2}$$



The F Distribution



From Wikipedia: http://en.wikipedia.org/wiki/F_distribution



The F test

- $H_0: V(X_1) = V(X_2)$
- $H_a: V(X_1) \neq V(X_2)$
- Test Statistic

$$F^* = \frac{V(X_1)}{V(X_2)} \quad \text{has a } F(df_1, df_2) \text{ distribution}$$



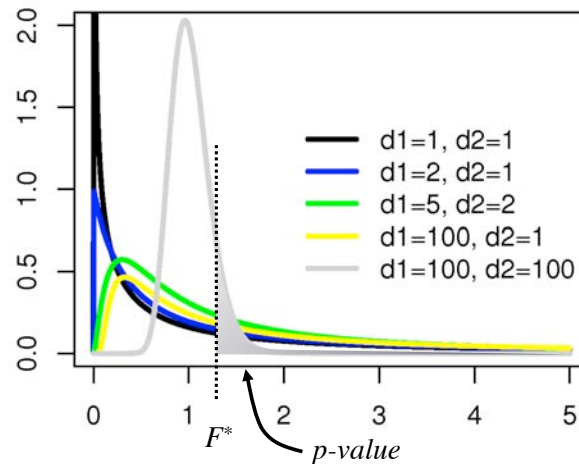
The F test

- $H_0: V(X_1) = V(X_2)$
- $H_a: V(X_1) \neq V(X_2)$
- Test Statistic

$$F^* = \frac{S_{X_1}^2}{S_{X_2}^2} \quad \text{has a } F(n_1 - 1, n_2 - 1) \text{ distribution}$$



The F Test



From Wikipedia: http://en.wikipedia.org/wiki/F_distribution



var.test(): Comparing variances in R

n = 80 for both OEA and NEA

```
> var.test(OEA, NEA)
```

Note:

- F Test is used “backwards”
 - Null Hypothesis should be “variances are different”
 - default should be to use Welch’s T test
 - F test null hypothesis is “variances are the same”
 - default uses Student’s T test

1.280031

slightly modified for legibility



var.test(): Comparing variances in R

n = 80 for both OEA and NEA

```
> var.test(OEA, NEA)      Excel: =fptest(array1,array2)
      F test to compare two variances
data:  OEA and NEA
F = 1.28, num df = 79,  denom df = 79,  p-value = 0.2747
alternative hypothesis:
      true ratio of variances is not equal to 1
95 percent confidence interval:
 0.8209112      1.9959280
ratio of variances
      1.280031
```

slightly modified for legibility



var.test(): Comparing variances in R

n = 80 for both OEA and NEA

```
> var.test(OEA, NEA)
```

Note:

- Consequently
 - look for higher p-values, not lower
 - Using var.test() should be thought of as only a guide, not a true statistical test
- F test used as intended inside other statistical test
 - ANOVA
 - Chi Square test

1.280031

slightly modified for legibility



When The Normality Fails

- Everything so far has depended on the assumption of normality which in turn depends on the Central Limit Theorem holding
 - But this is not always true
 - *In in many areas of CS it rarely holds*
- Problems occur when
 - ...you have a non-zero probability of obtaining infinity
 - Mean and standard deviation are infinite!
 - ...the sample average depends highly on a few scores
 - When the mean of your distribution is not measuring what you want, consider using the median instead (rank-based statistics)
 - ...you don't know how fast your sample series converges to normal
 - if your sample average distribution converges very slowly than the number of samples may be *insufficient to assume normality*



So what should we do?

First test for normality

- Many such tests
- Recommended
 - Normal Probability Plot (QQ plot: sorted data vs Normal quantiles)
 - Lilliefors test (variant of the KS test)



So what should we do?

There are 3 basic remedial measures:

1. Transforming data to make them normally distributed
 - also called *data re-expression*
 - traditional approach (required before the advent of fast computers)
2. Resampling techniques
3. Non-parametric statistics



Non-Parametric Statistics

- Basic Idea
 - Sort the data and then rank them
 - Use Ranks instead of actual values to perform statistics
- Also known as
 - *order statistics*,
 - *ordinal statistics*
 - *rank statistics*
- Measures how interspersed the samples are from the 2 treatments
 - If the result is “alternating” it is assumed that there is no difference
- Can't be affected by outliers (extrememly large or small values)
 - Just the highest or lowest rank



Non-Parametric Tests

- Reason behind the appropriateness of non-parametric tests
 - Both the sum of ranks and average of ranks will be approximately normally distributed
 - because of the Central Limit Theorem,
 - as long as we have 5 or more samples
 - result is independent of the underlying distribution
- Ranked T-test
 - Perform a t test on the ranks of the values
 - instead of the values themselves
- 2 other techniques with similar results are commonly seen
 - Wilcoxon's Rank-Sum test
 - Mann-Whitney U test
 - All are effectively equivalent



Two data sets
combined
into a single
array

Sort

A	0.03
A	0.91
A	0.64
A	0.99
A	0.64
A	0.16
A	0.16
A	0.91
A	0.16
A	0.27
B	0.64
B	0.08
B	0.16
B	0.27
B	0.02
B	0.01
B	0.16
B	0.03
B	0.03
B	0.03
B	0.64

ranks		
A	0.99	1
A	0.91	2
A	0.91	3
A	0.64	4
A	0.64	5
B	0.64	6
B	0.64	7
A	0.27	8
B	0.27	9
A	0.16	10
A	0.16	11
A	0.16	12
B	0.16	13
B	0.16	14
B	0.08	15
A	0.03	16
B	0.03	17
B	0.03	18
B	0.02	19
B	0.01	20

Give each data element
its corresponding rank

Ranked Example



ranks		
A	0.99	1
A	0.91	2.5
A	0.91	2.5
A	0.64	5.5
A	0.64	5.5
B	0.64	5.5
B	0.64	5.5
B	0.64	5.5
A	0.27	8.5
B	0.27	8.5
A	0.16	12
A	0.16	12
A	0.16	12
B	0.16	12
B	0.16	12
B	0.16	12
B	0.08	15
A	0.03	17
B	0.03	17
B	0.03	17
B	0.02	19
B	0.01	20

t1
t1
t2
t2
t2
t2
t3
t3
t4
t4
t4
t4
t4
t4
t5
t5
t5

Average tied ranks
together

t1	2.5
t2	5.5
t3	8.5
t4	12
t5	17

Replace tied ranks
with average tied ranks

Ranked Example



ranks		
A	0.99	1
A	0.91	2.5
A	0.91	2.5
A	0.64	5.5
A	0.64	5.5
A	0.27	8.5
A	0.16	12
A	0.16	12
A	0.16	12
B	0.64	5.5
B	0.64	5.5
B	0.27	8.5
B	0.16	12
B	0.16	12
B	0.08	15
B	0.03	17
B	0.03	17
B	0.02	19
B	0.01	20

Resort by treatment

Perform t test on Ranks

	A _{rank}	B _{rank}
avg	7.85	13.15
stdDev	5.28	5.33

Ranked t Test	
$s_T = \sqrt{\frac{s_A^2}{n_A} + \frac{s_B^2}{n_B}}$	2.37
$(avg_A - avg_B) / s_T$	2.23
p -value	0.038

$n = 10$
 t_R score

Ranked Example



A Non-Parametric ‘Mean’: The Median

- Average of a data set that is not normally distributed produces a value that behaves non-intuitively
 - Especially if the probability distribution is skewed
 - Large values in ‘tail’ can dominate
 - Average tends to reflect the typical value of the “worst” data not the typical value of the data in general
- Instead use the Median
 - 50th percentile
 - Counting from 1, it is the value in the $\frac{n+1}{2}$ position
 - If n is even, $(n+1)/2$ will be between 2 positions, average the values at that position



A Confidence Interval Around the Median: Thompson-Savur

- Find the b the binomial value that has a cumulative upper tail probability of $\alpha/2$
 - b will have a value near $n/2$
- The lower percentile $l = \frac{b}{n-1}$
- The upper percentile $u = 1 - l$
- Confidence Interval is $[value_l, value_u]$
 - i.e. $value_l \leq median \leq value_u$
 - With a confidence level of $1 - \alpha$



A Confidence Interval Around the Median: Thompson-Savur

- Find the b the binomial value that has a cumulative upper tail probability of $\alpha/2$
 - However: Thompson-Savur is not common
- The Usually a Box-Plot is used to show where the “mass” of the data points are (based on interquartile range)
- The Box-Plot has the advantage of finding potential outliers
- Confidence Interval is $[value_l, value_u]$
 - i.e. $value_l \leq median \leq value_u$
 - With a confidence level of $1 - \alpha$



Thompson-Savur: Example

0.03	18	0.99
0.01	17	0.91
0.04	16	0.91
0.09	15	0.64
0.04	14	0.64
0.06	13	0.64
0.06	12	0.64
0.01	11	0.27
0.06	10	0.27
0.07	9	0.16
0.04	8	0.16
0.08	7	0.16
0.06	6	0.16
0.07	5	0.16
0.02	4	0.08
0.06	3	0.03
0.03	2	0.03
0.03	1	0.03
0.04	0	0.02

Sort
Data

$n = 19$ $CL = 99\%$
 $\alpha = 0.01$

$b = \text{qbinom}(\alpha/2, n, 1/2)$
 $= \text{qbinom}(0.005, 19, 0.5)$
 $= 4$

$upper \quad \frac{rank}{(n-1) - b}$
 $median \quad \frac{(n-1)/2}{b}$
 $lower \quad b$

In Excel: $b = \text{CRITBINOM}(n, 1/2, \alpha/2)$

Thompson-Savur: Example



0.03
0.01
0.04
0.09
0.04
0.06
0.06
0.01
0.06
0.07
0.04
0.08
0.06
0.07
0.02
0.06
0.03
0.03
0.04

Sort
Data

18	0.99
17	0.91
16	0.91
15	0.64
14	0.64
13	0.64
12	0.64
11	0.27
10	0.27
9	0.16
8	0.16
7	0.16
6	0.16
5	0.16
4	0.08
3	0.03
2	0.03
1	0.03
0	0.02

$n = 19$

$CL = 99\%$

$\alpha = 0.01$

$b = \text{qbinom}(\alpha/2, n, 1/2)$
 $= \text{qbinom}(0.005, 19, 0.5)$
 $= 4$

	<u>rank</u>	<u>percentile</u>	<u>value</u>
upper	14	78th	0.64
median	9	50th	0.16
lower	4	22nd	0.08

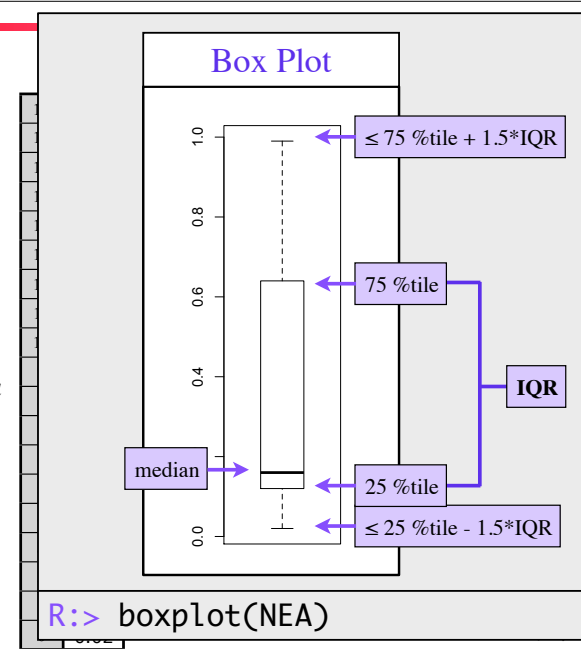
In Excel: $b = \text{CRITBINOM}(n, 1/2, \alpha/2)$

Box Plot



0.04
0.09
0.04
0.06
0.06
0.01
0.06
0.07
0.04
0.08
0.06
0.07
0.02
0.06
0.03
0.03
0.04

Sort
Data



R:> boxplot(NEA)

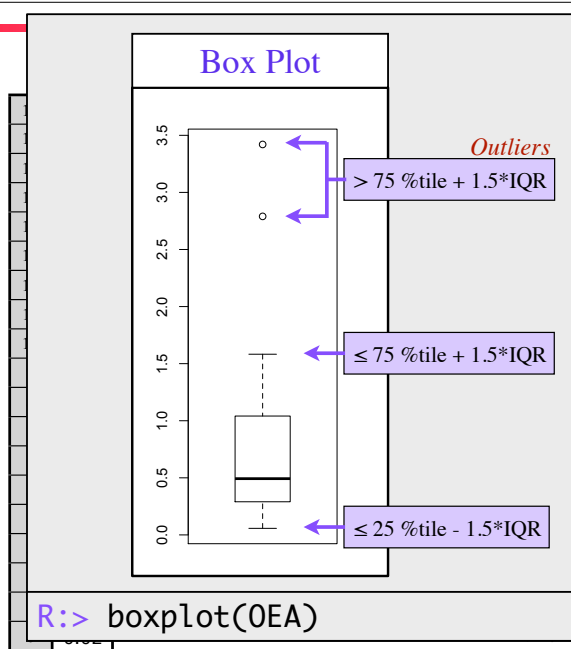
<u>value</u>
0.64
0.16
0.08

Box Plot



0.04
0.09
0.04
0.06
0.06
0.01
0.06
0.07
0.04
0.08
0.06
0.07
0.02
0.06
0.03
0.03
0.04

Sort
Data



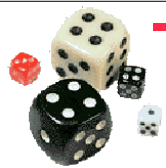
R:> boxplot(OEA)

<u>value</u>
0.64
0.16
0.08

Part 3

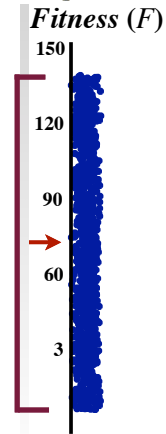


Regression by means of Least Squares



Linear Regression

Simple model of F



$$E(\varepsilon_F) = 0$$

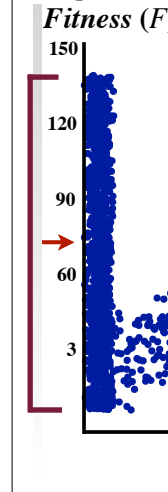
$$V(\varepsilon_F) = \sigma_F^2$$

$$F_i = 72 + \varepsilon_F$$



Linear Regression

Factor in Population Size



$$E(\varepsilon) = 0$$

$$V(\varepsilon) = \sigma^2$$

$$F_i = 0.12 p_i + \varepsilon$$



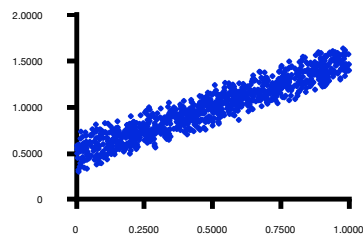
Modeling Response Behavior: Treating X as a factor

- Simplest model - linear relationship

$$Y_i = f(x_i) + \varepsilon \quad \text{with} \quad f(x_i) = \beta_0 + \beta_1 x_i$$



$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon$$



Two parameters β_0 and β_1
define the function

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Linear Regression by Means of Least Squares

- Idea:
 - From sample pairs $\{(Y_1, x_1), (Y_2, x_2), \dots, (Y_n, x_n)\}$ determine b_0, b_1
 - Estimates of the two unknowns β_0, β_1
- $$Y_i = \beta_0 + \beta_1 x_i + \varepsilon \quad \Longrightarrow \quad \hat{Y}_i = b_0 + b_1 x_i$$
- chosen such that the sum of squared errors is minimized
 - i.e. find the model that has the smallest (least) total squared error



Linear Regression

Error

$$e_i = Y_i - b_0 - b_1 x_i$$

Squares

Idea:

- From sample $(Y_1, x_1), \dots, (Y_n, x_n)$ determine

Error

$$e_i = Y_i - \hat{Y}$$

- Estimates of the two unknowns β_0, β_1

$$Y_i = \beta_0 + \beta_1 x_i$$

Sum of Squared Errors

$$e_i^2 = (Y_i - b_0 - b_1 x_i)^2$$

- chosen such that the sum of squared errors is minimized

- i.e. find

Squared Error

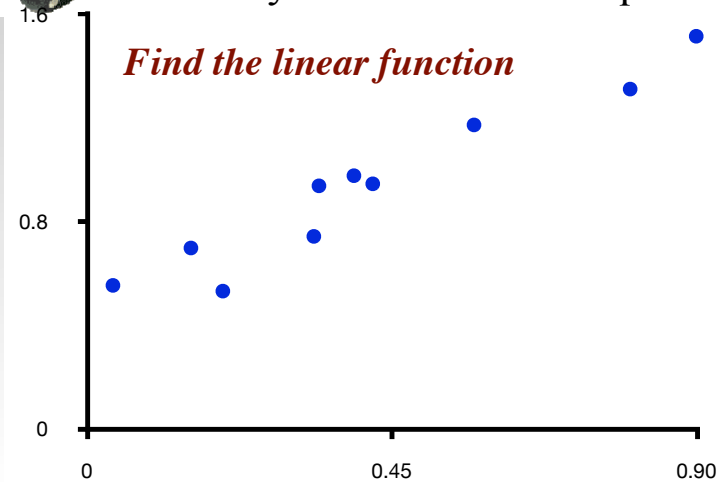
$$SSE = \sum e_i^2$$

ed error

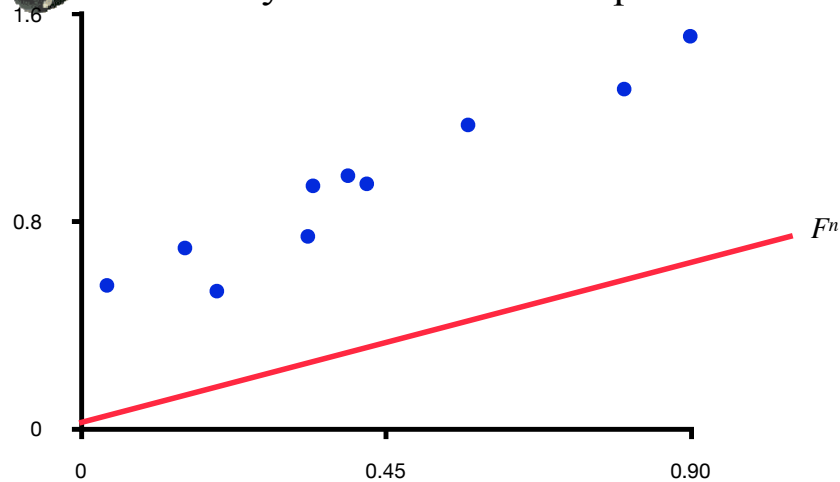


Linear Regression by Means of Least Squares

Find the linear function

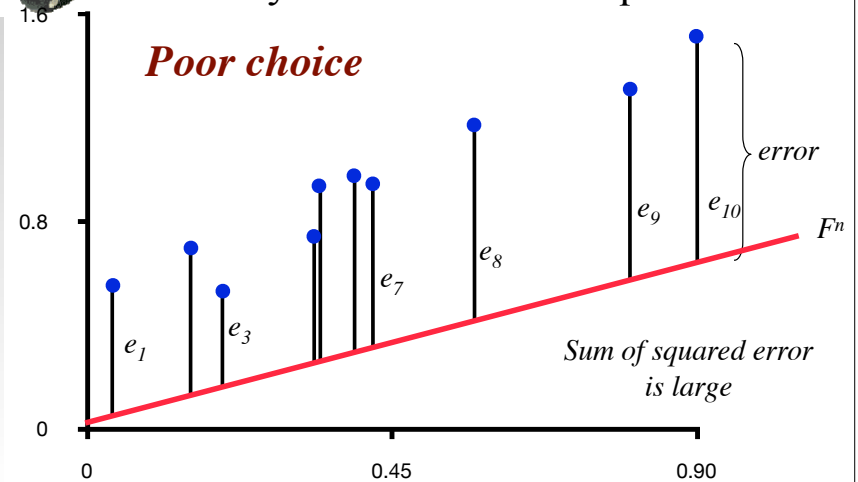


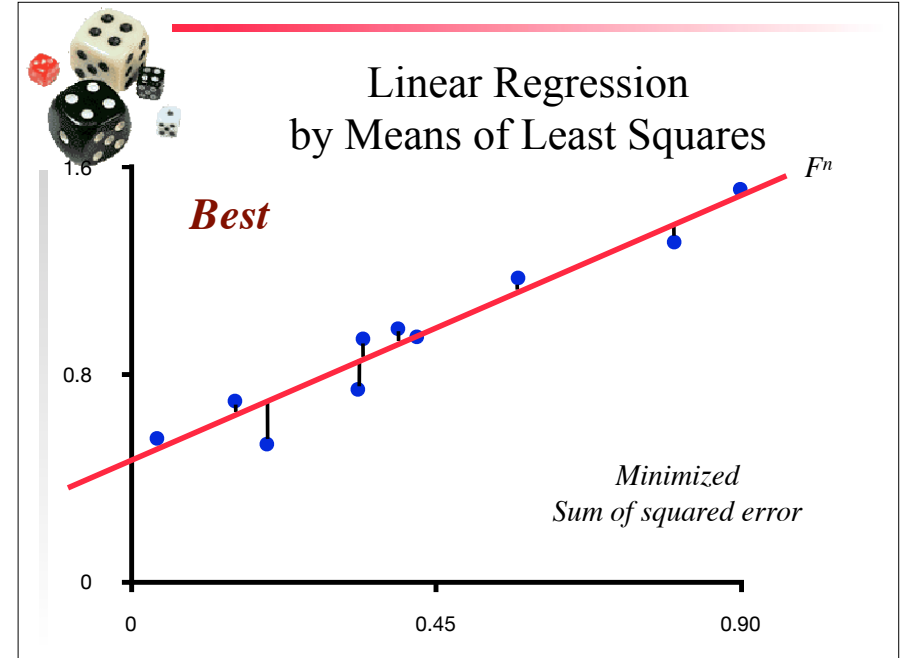
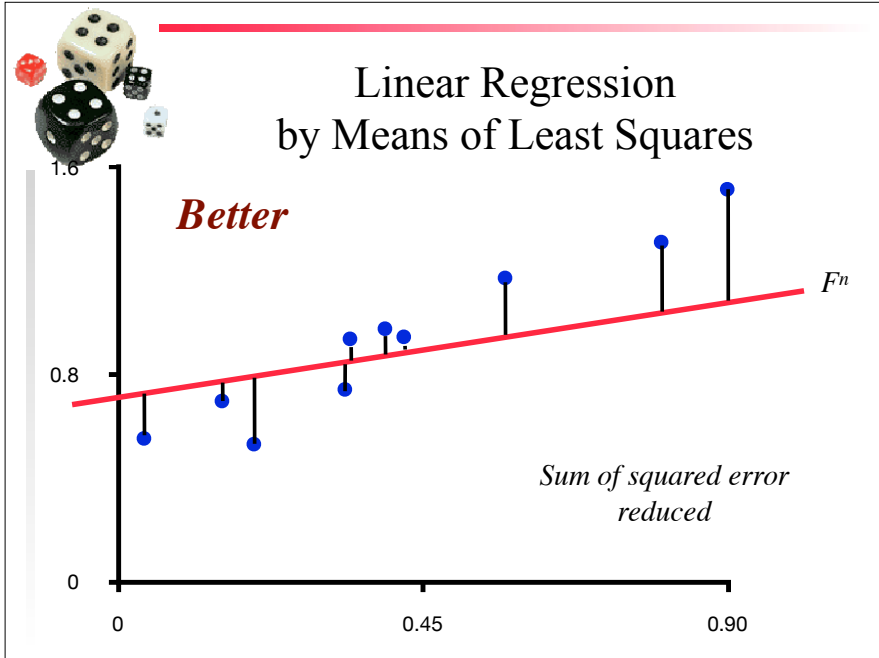
Linear Regression by Means of Least Squares



Linear Regression by Means of Least Squares

Poor choice





Linear Regression by Means of Least Squares

- Determine $\hat{Y}_i = b_0 + b_1 X_i$
- Find b_0, b_1 such that

$$\min \sum_{i=1}^n e_i^2 = \min \sum_{i=1}^n (Y_i - b_0 - b_1 x_i)^2$$
- Use calculus (minimum finding)
 - Take partial derivatives wrt b_0 and b_1
 - set to zero
 - two equations, two unknowns ... solve

Linear Regression by Means of Least Squares

- Determine $\hat{Y}_i = b_0 + b_1 X_i$
- Solution

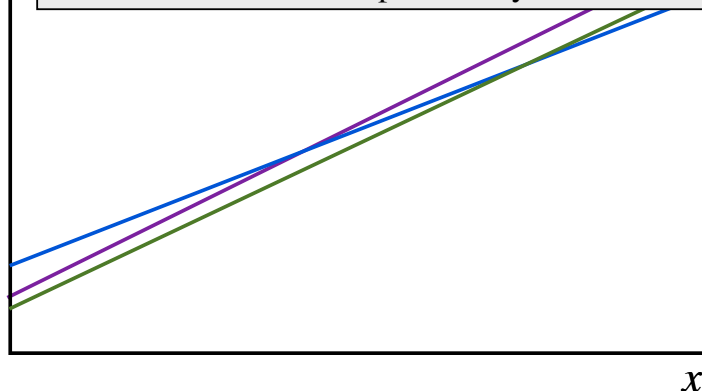
$$b_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(Y - \bar{Y}_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\text{cov}(x, Y)}{\text{var}(x)} = \frac{S_{xy}}{S_x^2}$$

$$b_0 = \bar{Y} - b_1 \bar{x}$$



Different Samples ... Different Regression Line

- Slope (b_1) and Y intercept (b_0) are random variables, each with a probability distribution



Expectation of b_1 and b_0

b_1 and b_0 can be thought of as sample means

$$E(b_0) = \beta_0 \quad E(b_1) = \beta_1$$

and they have associated variances

$$V(b_1) = \frac{\sigma_Y^2}{nS_x^2} \Rightarrow s_{b_1}^2 = \frac{MS_{error}}{nS_x^2}$$

$$V(b_0) = \left(1 + \frac{\bar{x}^2}{S_x^2}\right) \frac{\sigma_Y^2}{n} \Rightarrow s_{b_0}^2 = \left(1 + \frac{\bar{x}^2}{S_x^2}\right) \frac{MS_{error}}{n}$$

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What are the distributions of b_1 and b_0 ?

b_1 can be rewritten as

$$b_1 = \sum_{i=1}^n k_i Y_i \quad \text{where} \quad k_i = \frac{(x_i - \bar{x})}{\sum (x_i - \bar{x})^2}$$

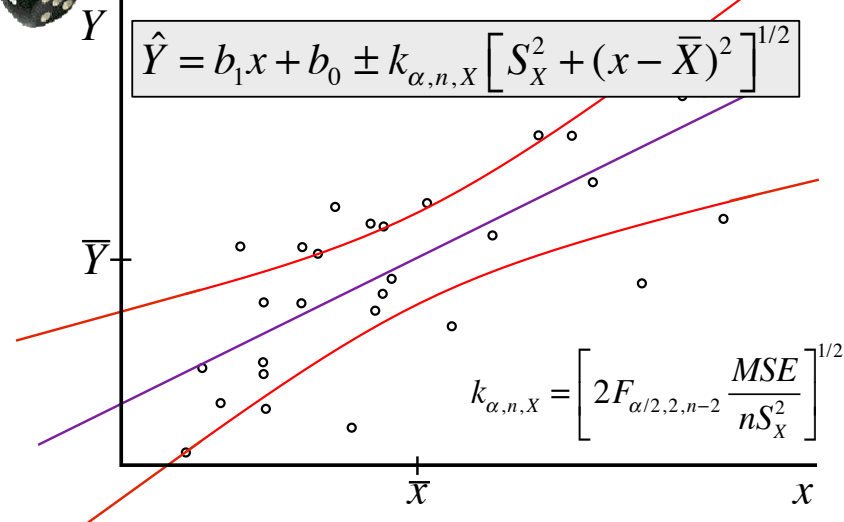
$$\text{and} \quad b_0 = \bar{Y} - b_1 \bar{x}$$

- since the x_i are constant
 b_1 is a linear combination of Y_i 's
- linear combinations of normally distributed random variables are normally distributed
- so ... if Y is normally distributed, b_1 is too (as is b_0)

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Confidence Bands





T test to see if a the slope is statistically significant

- To see if the slope b_1 is statistically different from 0
 - use the T test

$$T = \frac{(b_1 - 0)}{S_{b_1}} = \frac{b_1}{S_{b_1}}$$

- and find the corresponding p-value
- because we we originally estimated 2 parameters use

$$df = n - 2 - 1 = n - 3$$

43



T test to see if a y intercept is statistically significant

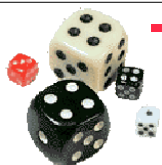
- To see if the regression line goes through the origin check if b_0 is statistically different from 0
 - use the T test

$$T = \frac{(b_0 - 0)}{S_{b_0}} = \frac{b_0}{S_{b_0}}$$

- and find the corresponding p-value
- again because we originally estimated 2 parameters use

$$df = n - 2 - 1 = n - 3$$

43



T test to see if a y intercept is statistically significant

- To see if the regression line goes through the origin check if b_0 is statistically different from 0

These confidence intervals and tests are very important to perform.

Yet they are not commonly done!

and find the corresponding p-value

- again because we originally estimated 2 parameters use

$$df = n - 2 - 1 = n - 3$$

43



Multifactor Regression

- General model for one factor

$$Y_i = f(x_i) + \varepsilon$$

random variable \rightarrow Y_i

\rightarrow non-random variable $f(x_i)$

\rightarrow random variable where $E(\varepsilon) = 0$

represents the true distribution of Y

- General model for multiple factors
 - Note: still not a multivariate analysis – error term still additive to the (now multiple) factors – factors themselves not stochastic

$$Y_i = f(x_{1,i}, x_{2,i}, \dots, x_{k,i}) + \varepsilon$$



Multifactor Regression

- Assume linear combination of factors ... simplest fⁿ

$$Y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \dots + \beta_k x_{k,i} + \varepsilon$$

$$\Rightarrow \hat{Y}_i = b_0 + b_1 x_{1,i} + b_2 x_{2,i} + \dots + b_k x_{k,i}$$

- Just
 - take the partial derivative of the squared error function for each parameter
 - Set each derivative to zero to find the maximum
 - Solve the set of linear equations
 - k unknown parameters, k equations

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T test to see if a factor is statistically significant

- Each factor b_i has known estimated variance
 - Found analogously to b_i and b_0
- To see if the factor is meaningful, see if b_i is statistically different from 0
 - using the T test

$$T = \frac{(b_i - 0)}{S_{b_i}} = \frac{b_i}{S_{b_i}}$$

- find the corresponding p-value
- because we are estimating k parameters use $df = n - k - 1$

This is very important to compute!!! Yet not commonly provided.

43



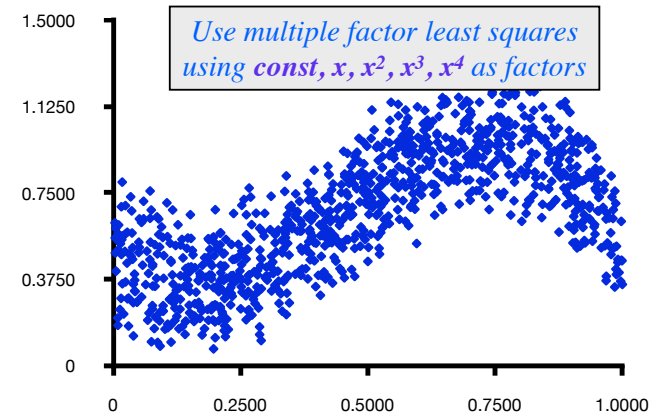
Polynomial Regression

- One trick is to set $x_2 = x^2$, $x_3 = x^3$, etc.
 - This can be done since each factor is not a random variable, just a regular variable
- Since it is known that any function can be formed through a linear combination of polynomial variables (a power series), we can now regress against any function!!
 - We must know the function to regress against
 - Again called the model
 - Must check to see if each term is statistically significant
 - Use T test from previous slide
 - If a term is not significant, eliminate it from the model and apply least squares again on simpler model

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Polynomial Regression E.g.





Polynomial Regression E.g.

$R^2 = 70.2\%$ $R^2 \text{ (adjusted)} = 70.1\%$
 $s = 0.1466$ with $1000 - 5 = 995$ degrees of freedom

Source *X^4 is not statistically significant
... reduce the number of terms by one* F-ratio
 Regression 587
 Residual 21.3783 995 0.0215

Variable	Coefficient	s.e. of Coeff	t-ratio	p-value
Constant	0.515460	0.0236	21.9	≤ 0.0001
X	-2.27114	0.3210	-7.07	≤ 0.0001
X^2	8.87396	1.303	6.81	≤ 0.0001
X^3	-6.94563	1.968	-3.53	0.0004
X^4	0.331472	0.9828	0.337	0.7360

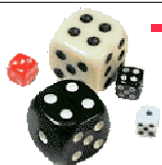


Polynomial Regression E.g.

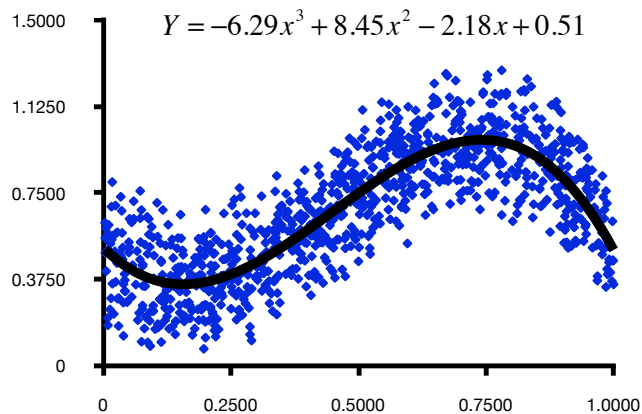
$R^2 = 70.2\%$ $R^2 \text{ (adjusted)} = 70.2\%$
 $s = 0.1465$ with $1000 - 4 = 996$ degrees of freedom

Source *All factors statistically significant
... regression function is a cubic polynomial* F-ratio
 Regression 587
 Residual 21.3783 996 0.0215

Variable	Coefficient	s.e. of Coeff	t-ratio	p-value
Constant	0.510755	0.0190	26.9	≤ 0.0001
X	-2.17801	0.1636	-13.3	≤ 0.0001
X^2	8.45358	0.3813	22.2	≤ 0.0001
X^3	-6.28741	0.2515	-25.0	≤ 0.0001



Polynomial Regression E.g.



Actual model used to generate the data: $Y = -6x^3 + 8x^2 - 2x + 0.5 + \epsilon$

ANOVA: Analysis of Variance



Part 1a: Multi-Level Analysis Basic Concept



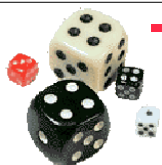
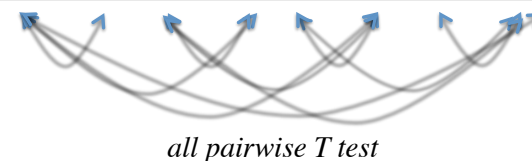
More Than 2 Treatments

- Preceding stats to be used for simple experiment designs
- More sophisticated stats needs to be done if:
 - Comparing multiple systems instead of just 2 treatments
 - E.g. comparing the effect on a Genetic Algorithm of using no mutation, low, medium and high levels of mutation
 - We say there are 4 *levels* of the mutation variable
 - Need $\binom{4}{2} = 6$ possible comparisons to test all pairs of treatments
 - Called a ‘multi-level’ analysis



Analysis of Variance (ANOVA)

	no xover	xover = 1pt	xover = 2pt	xover = 3pt	xover = 4pt
Fitness Values	4.3	8.8	5.0	6.3	5.4
	3.7	7.7	5.3	6.6	5.9
	4.7	8.3	5.1	7.2	5.4
	3.7	8.1	5.2	7.4	5.4
Question: Do crossover settings make a difference at all?					
avg fitness	4.02	8.13	5.09	7.02	5.76
std dev	0.451	0.313	0.424	0.478	0.471

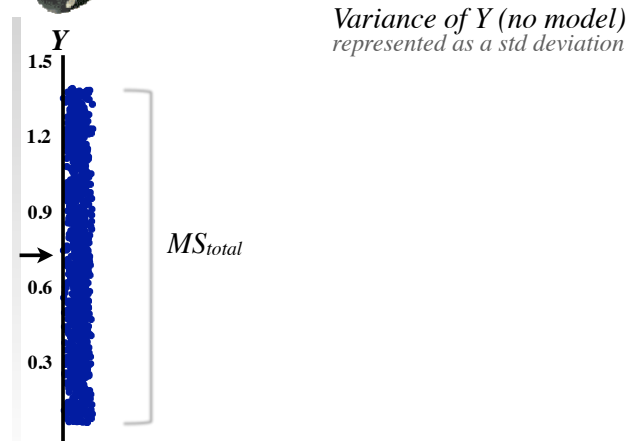


Comparing Variances

- Up to now we have been comparing means
 - Student's T test (difference between means)
- From here on we will be comparing variances
 - This is why it is called “Analysis of *Variance*”
 - Remember - compare the ratio of variances
 - see if it equals 1
 - distribution known: F distribution



ANOVA: Graphical Intuition

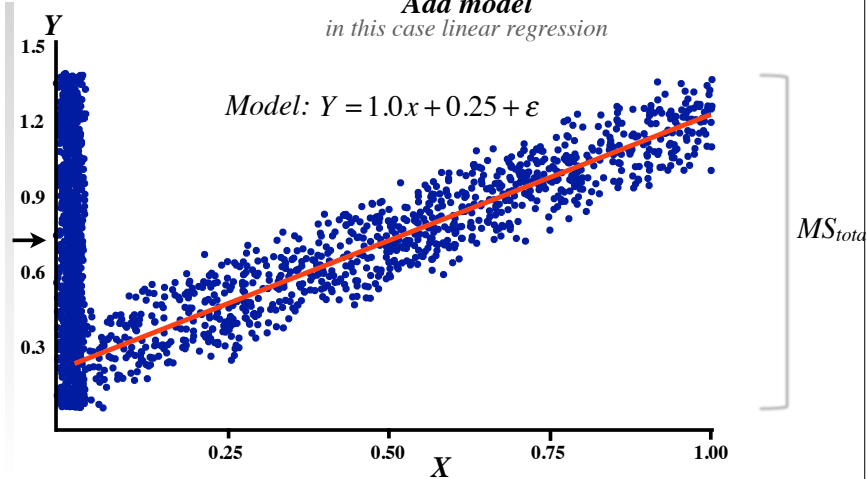




ANOVA: Graphical Intuition

*Add model
in this case linear regression*

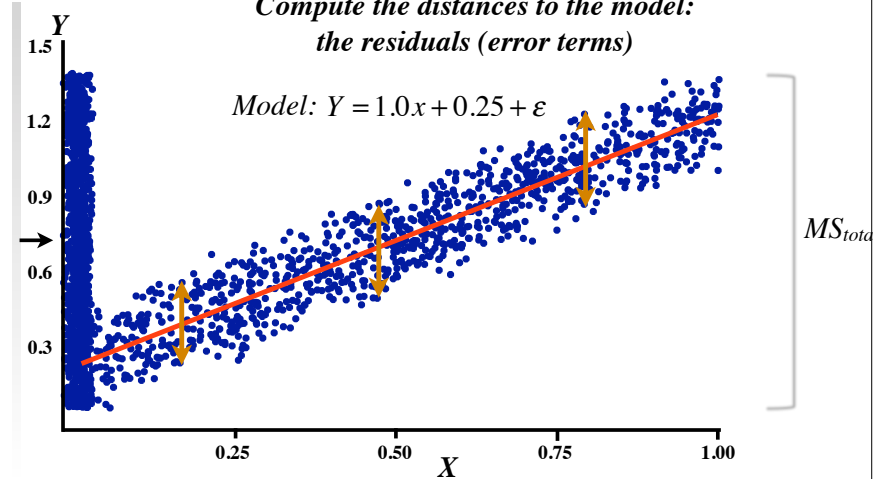
$$\text{Model: } Y = 1.0x + 0.25 + \epsilon$$



ANOVA: Graphical Intuition

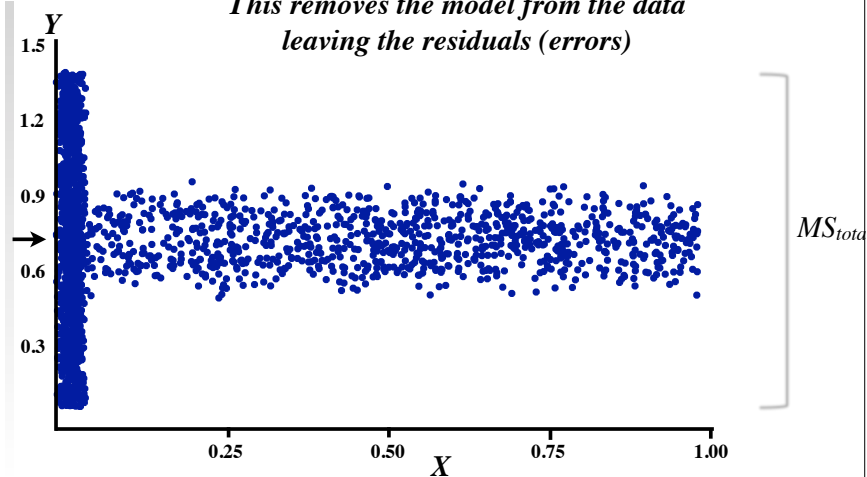
*Compute the distances to the model:
the residuals (error terms)*

$$\text{Model: } Y = 1.0x + 0.25 + \epsilon$$



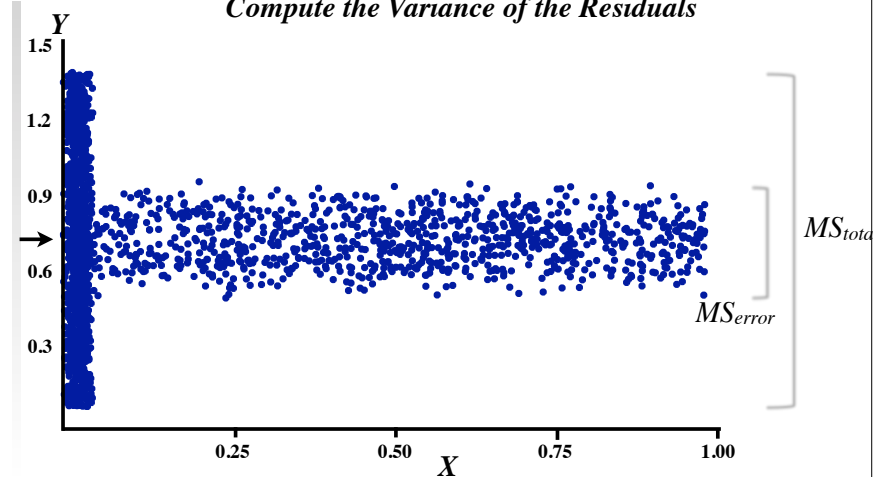
ANOVA: Graphical Intuition

*This removes the model from the data
leaving the residuals (errors)*



ANOVA: Graphical Intuition

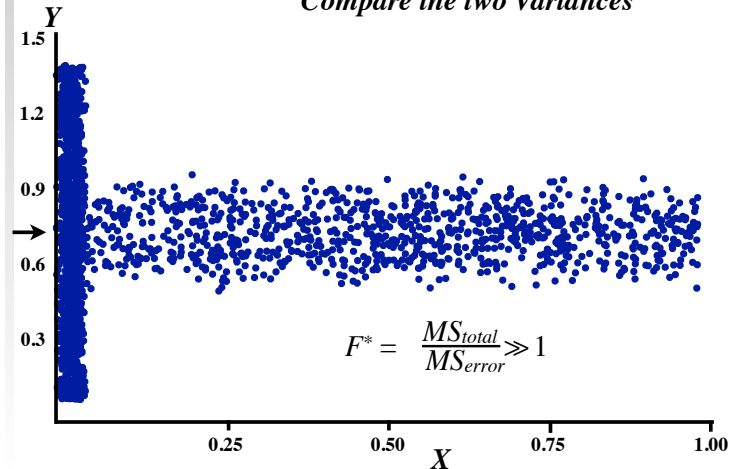
Compute the Variance of the Residuals





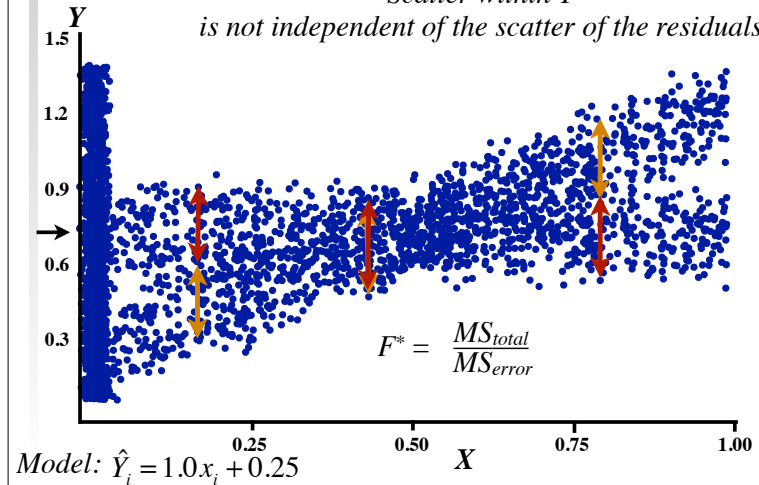
ANOVA: Graphical Intuition

Compare the two Variances



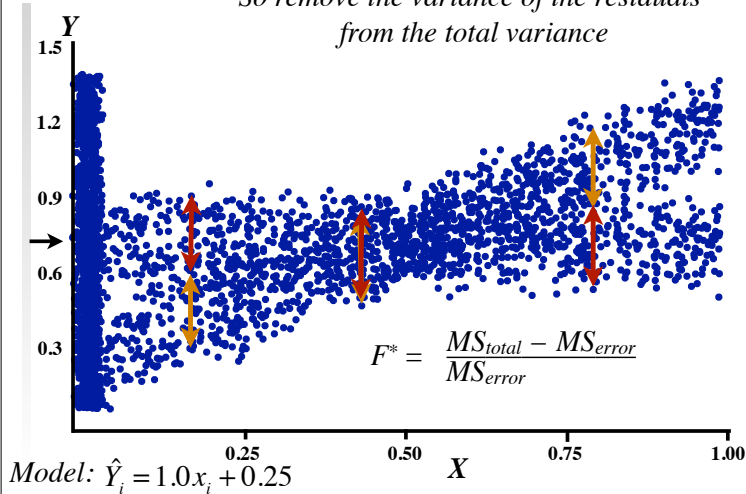
ANOVA: Graphical Intuition

*Scatter within Y
is not independent of the scatter of the residuals*



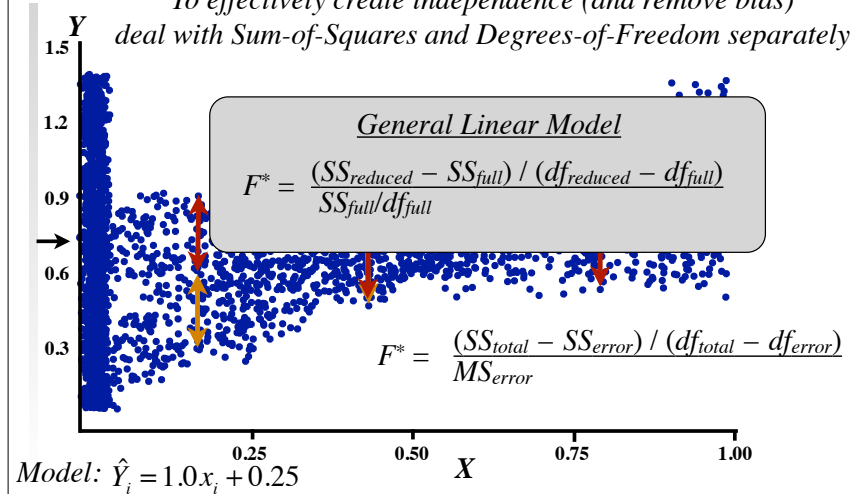
ANOVA: Graphical Intuition

*To remove the variance of the residuals
from the total variance*



ANOVA: Graphical Intuition

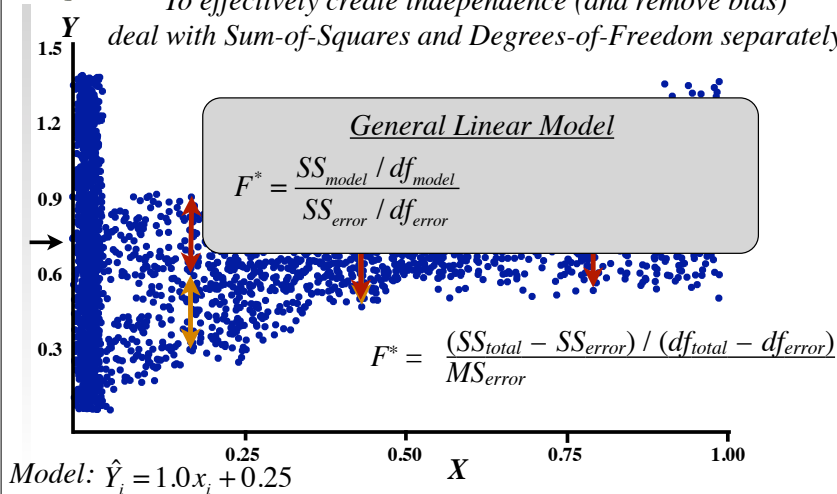
*To effectively create independence (and remove bias)
deal with Sum-of-Squares and Degrees-of-Freedom separately*





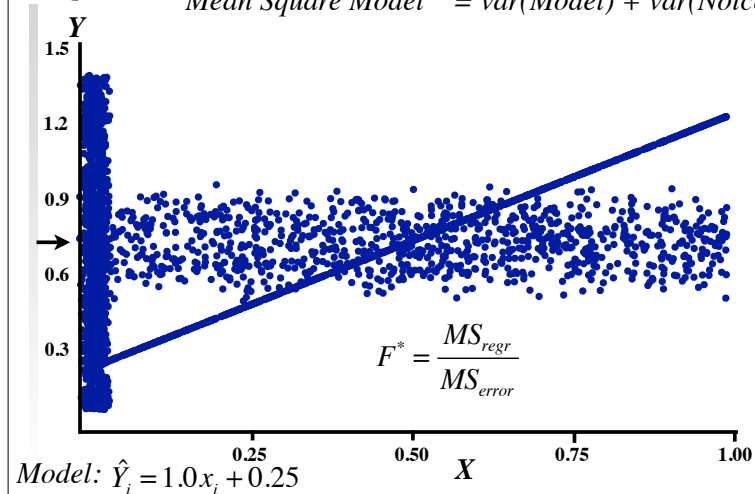
ANOVA: Graphical Intuition

To effectively create independence (and remove bias)
deal with Sum-of-Squares and Degrees-of-Freedom separately

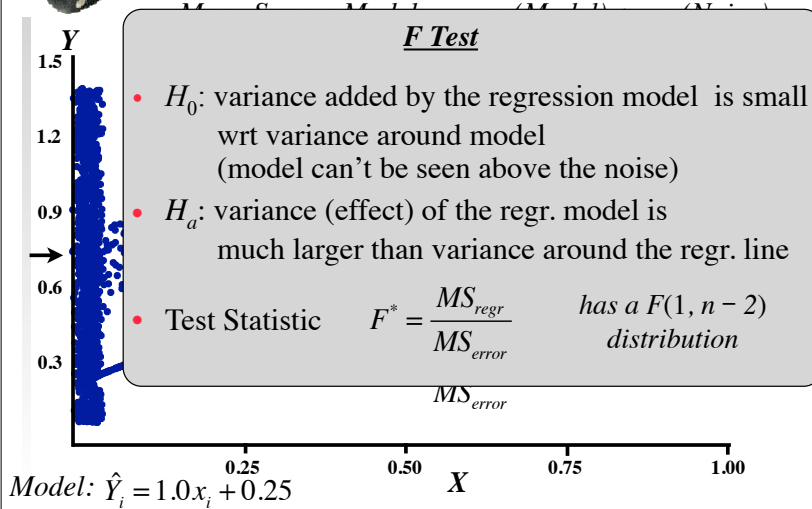


ANOVA: Graphical Intuition

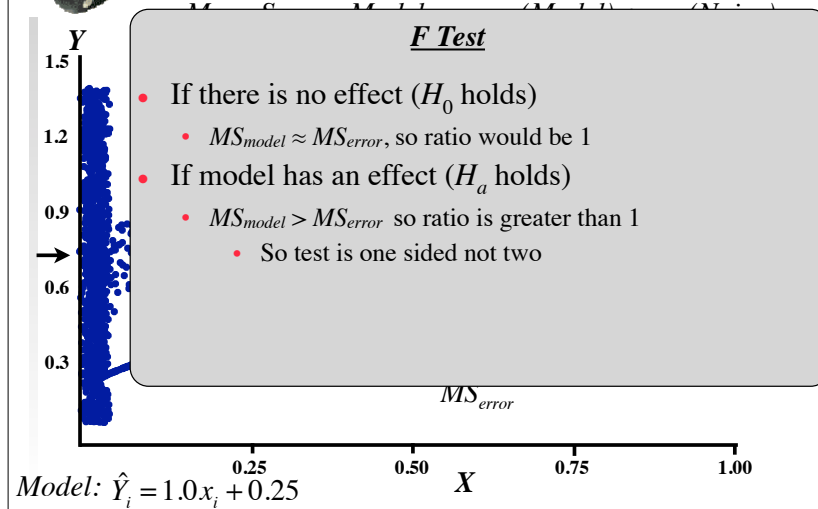
Mean Square Model = var(Model) + var(Noise)



ANOVA: Graphical Intuition



ANOVA: Graphical Intuition





Polynomial Regression E.g.

$R^2 = 70.2\%$ $R^2 \text{ (adjusted)} = 70.2\%$
 $s = 0.1465$ with $1000 - 4 = 996$ degrees of freedom

Source	Sum of Squares	df	Mean Square	F-ratio	p-value
Regression	50.4684	3	16.8228	784	≤ 0.0001
Residual	21.3807	996	0.021467		

Variable	Sum of Squares	df	Mean Square	F-ratio	p-value
Constant	50.4684	1	50.4684	2422.2	≤ 0.0001
X	2.17661	0.1656	13.13	622.2	≤ 0.0001
X^2	8.45358	0.3813	22.2	1062.2	≤ 0.0001
X^3	-6.28741	0.2515	-25.0	-1182.2	≤ 0.0001

Regression model is statistically significant
 $F\text{-ratio} = 784 \gg 1$



ANOVA: Discrete Levels

Fitness
Values

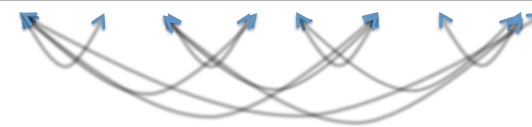
no xover	xover = 1pt	xover = 2pt	xover = 3pt	xover = 4pt
4.3	8.8	5.0	6.3	5.4
3.7	7.7	5.3	6.6	5.9
4.7	8.3	5.1	7.2	5.4
3.7	8.1	5.2	7.4	5.4

Question:

Do crossover settings make a difference at all?

avg fitness
std dev

no xover	xover = 1pt	xover = 2pt	xover = 3pt	xover = 4pt
4.02	8.13	5.09	7.02	5.76
0.451	0.313	0.424	0.478	0.471



all pairwise T test



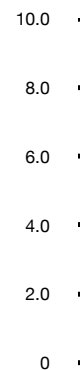
ANOVA: Discrete Levels



Total Reps: $N = 75$



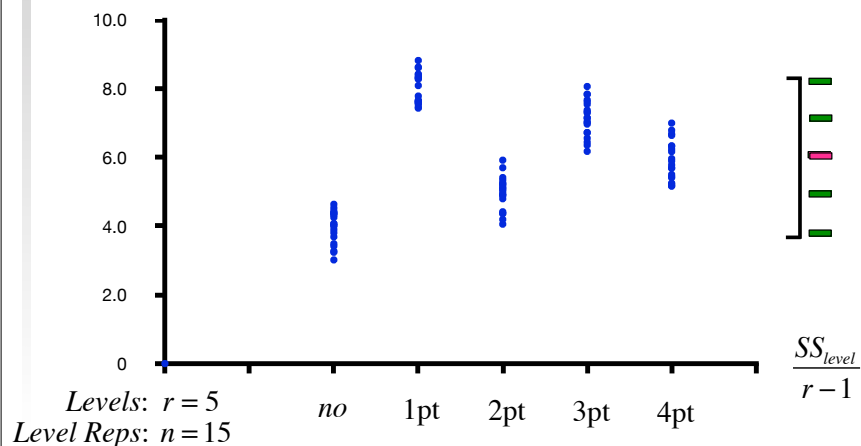
ANOVA: Discrete Levels



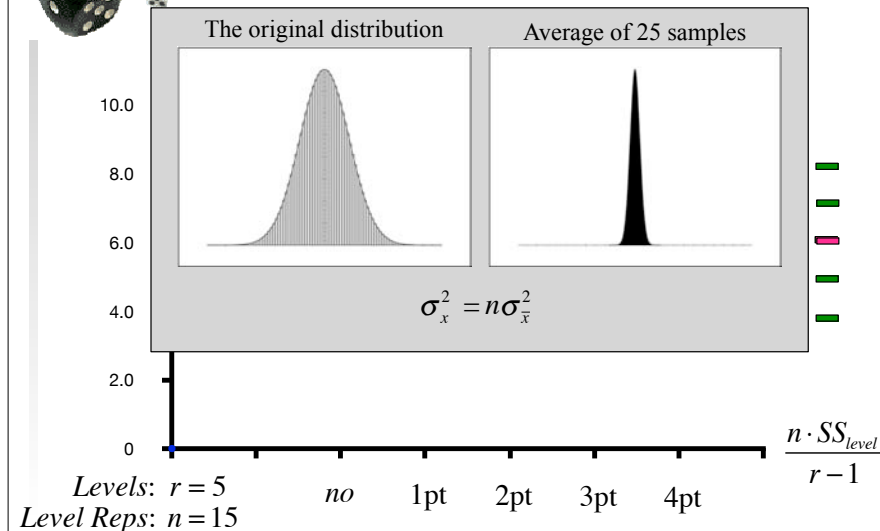
Levels: $r = 5$
Level Reps: $n = 15$



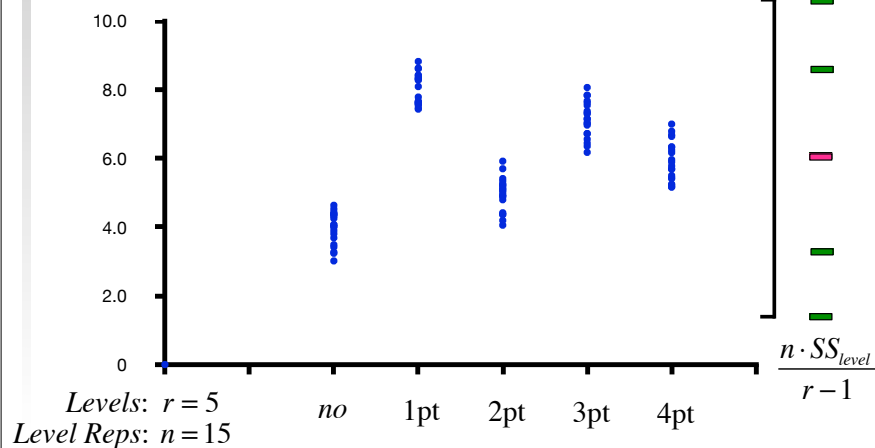
ANOVA: Discrete Levels



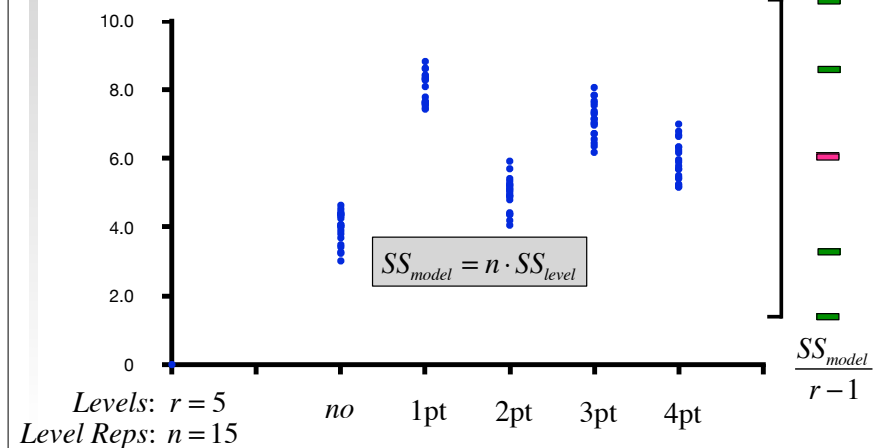
ANOVA: Discrete Levels



ANOVA: Discrete Levels

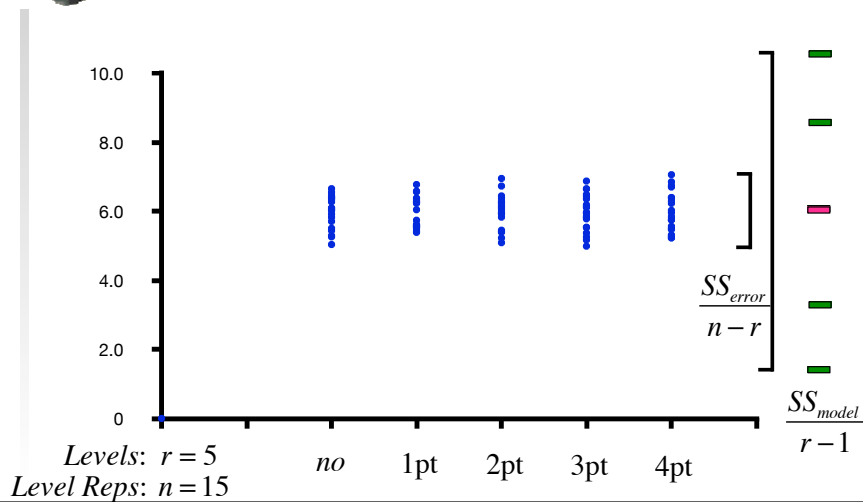


ANOVA: Discrete Levels

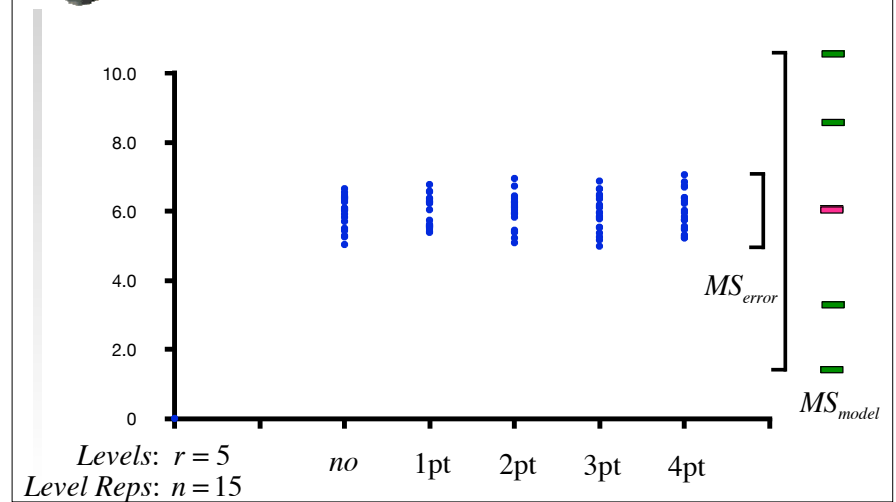




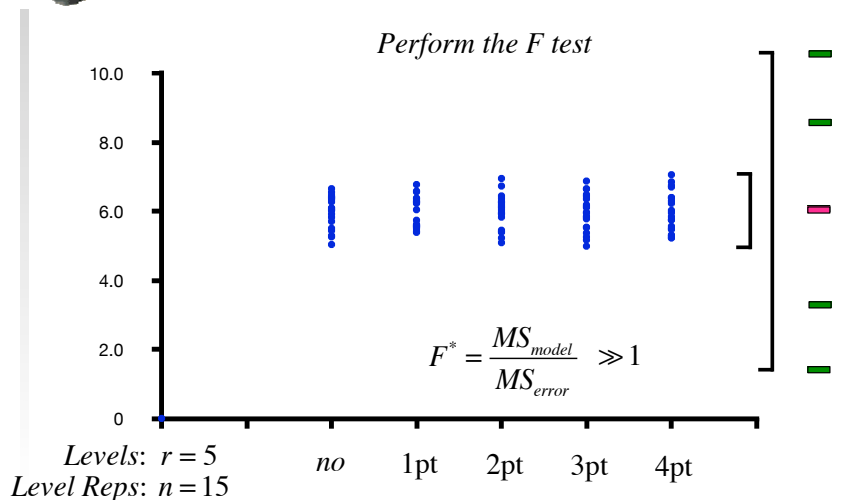
ANOVA: Discrete Levels



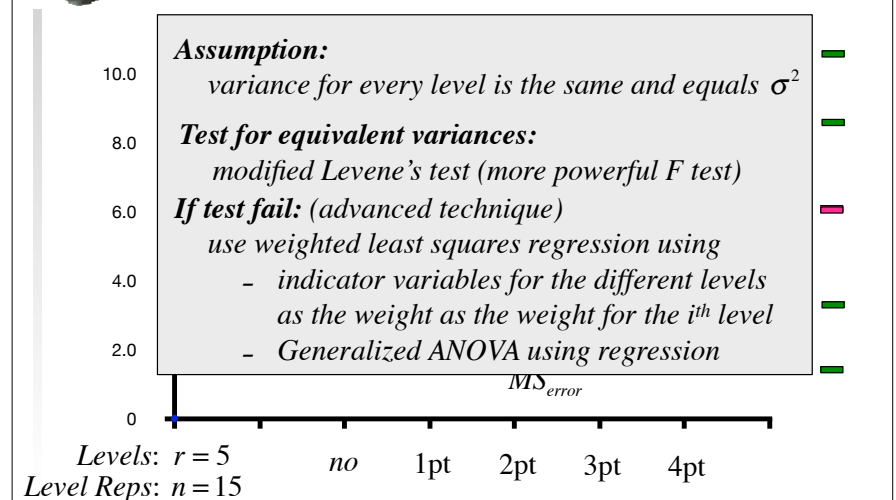
ANOVA: Discrete Levels



ANOVA: Discrete Levels



ANOVA: Discrete Levels





ANOVA table for example

from DataDesk

Source	df	SS	MS	F-ratio	Prob
const	1	3592.9	3592.9	13967	≤ 0.0001
xover	4	210.9	52.7	204.94	≤ 0.0001
Error	95	24.4	0.257		
Total	99	235.3			

$$F^* = \frac{MS_{model}}{MS_{error}} = \frac{52.7}{0.257} = 204.94$$

F test (From Excel)

$f_{dist}(204.94, 4, 95) = 8.19E-46$



Non-parametric ANOVA

- Again, what happens if Y (or actually ϵ) is not normally distributed?
- Various non-parametric techniques
 - Kruskal-Wallis first such test
- However, even simpler technique
 - Like Spearman's correlation coefficient and non-parametric regression, replace the Y_i values with their corresponding ranks
 - Perform ANOVA on ranked values as usual
- A slightly more accurate version is called the Friedman test
 - Same as above, except
 - the F distribution is replaced by the Chi-Squared distribution ($DofF = r - 1$) for large n or r ($n > 15$ or $r > 4$)
 - a special purpose distribution for small n or r

ANOVA: Analysis of Variance



Part 1b: Multi-Level Analysis

Pairwise Comparisons

Post-Hoc Analysis



Pairwise Comparisons between Factor-Level Means

- What if we want to know more detailed information?
 - Which of the means is the significantly different one?
 - Are there more than one significantly different mean?
 - If so, what are the pair-wise differences and are they statistically significant?



Pairwise Comparisons between Factor-Level Means

- This is determined by a series of pair-wise T tests
- However, commonly uses pooled information from the

Assumption: variances for each factor level is the same (σ^2)
which is best estimated by the *MSE*

original T test comparison

comparing level i with level j
across the ANOVA model

$$t \text{ value} = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_{X_1}^2}{n_1} + \frac{s_{X_2}^2}{n_2}}} \rightarrow t \text{ value} = \frac{\bar{X}_i - \bar{X}_j}{\sqrt{\frac{MSE}{n_i} + \frac{MSE}{n_j}}}$$



Pairwise Comparisons between Factor-Level Means

- This is determined by a series of pair-wise T tests
- However, commonly uses pooled information from the model for the variance to provide greater accuracy
 - Called *standard error*

original T test comparison

comparing level i with level j
across the ANOVA model

$$t \text{ value} = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_{X_1}^2}{n_1} + \frac{s_{X_2}^2}{n_2}}} \rightarrow t \text{ value} = \frac{\bar{X}_i - \bar{X}_j}{\sqrt{\frac{2 \cdot MSE}{n}}}$$

when $n_i = n_j = n$



Multiple Levels: Post-hoc Analysis

- For 4 levels of mutation there are 6 comparisons possible
 - Each one of the comparison holds at a 95% C.L. independent of the other comparisons
 - If *all* comparisons are to hold at once the odds are $0.95 \times 0.95 \times 0.95 \times \dots \times 0.95 = (0.95)^6 = 0.735$
 - So in practice we only have 73.5% C.L.
 - Wrong 1/4 of the time
- For 7 levels of mutation there are 21 comparisons possible
 - C.L. = $(0.95)^{21} = 0.341$
 - Chances are better than half that at least one of the decisions may be wrong!



The Bonferroni Correction

- To correct, choose a smaller α

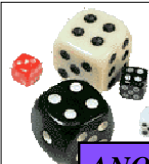
$$\alpha' = \frac{\alpha}{m}$$
 - Where m is the number of comparisons
 - So for 95% CL use $\alpha = 0.025/6 = 0.004167$
 - For a Z test the critical value changes from 1.96 to 2.64
- You should apply the Bonferroni (etc.) correction:
 - To t tests (t tests and ranked t tests)
 - To Confidence Intervals and Error Bounds
 - Whenever you mean "all the significant results we found hold at once"



Pairwise Comparisons between Factor-Level Means

Regular Pair-wise T test (with Bonf. Correction)

	Diff	std. err.	t-value	df	p-value
n - 1	-4.04	0.15	-27.5	18	3.6E-15
n - 3	-3.18	0.16	-20.5	18	6.3E-13
2 - 1	-3.04	0.16	-20.2	18	8.4E-13
3 - 2	2.16	0.17	13.7	18	5.5E-10
4 - 1	-2.09	0.17	-12.7	18	2.0E-09
n - 4	-1.95	0.17	-11.4	18	1.1E-08
4 - 3	-1.22	0.18	-7.1	18	1.3E-05
n - 2	-1.00	0.16	-6.3	18	5.8E-05
4 - 2	0.95	0.16	5.6	18	2.6E-04
3 - 1	-0.86	0.15	-5.6	18	2.6E-04



Pairwise Comparisons between Factor-Level Means

ANOVA Pair-wise T test (with Bonf. Correction)

	Diff	std. err.	t-value	df	p-value
n - 1	-4.04	0.16	-25.2	95	7.7E-43
n - 3	-3.18	0.16	-19.8	95	1.7E-34
2 - 1	-3.04	0.16	-19.0	95	4.8E-33
3 - 2	2.16	0.16	13.6	95	6.0E-23
4 - 1	-2.09	0.16	-13.0	95	7.5E-22
n - 4	-1.95	0.16	-12.2	95	4.4E-20
4 - 3	-1.22	0.16	-7.6	95	1.8E-10
n - 2	-1.00	0.16	-6.2	95	1.2E-07
4 - 2	0.95	0.16	5.9	95	4.8E-07
3 - 1	-0.86	0.16	-5.4	95	5.1E-06



Pairwise Comparisons between Factor-Level Means

ANOVA Pair-wise T test (with Bonf. Correction)

	Diff	std. err.	t-value	df	p-value
n - 1	-4.04	0.16	-25.2	95	7.7E-43

$$Diff = \bar{Y}_{i.} - \bar{Y}_{j.} \quad df = n_T - r = rn - r = 5 * 20 - 5 = 95$$

$$stdError = \sqrt{\frac{MS_{error}}{n_i} + \frac{MS_{error}}{n_j}} = \sqrt{\frac{2 \cdot MS_{error}}{n}} = \sqrt{\frac{2 * 0.257}{20}} = 0.1604$$

Student-T with Bonf. Correction

$$t - value = \frac{Diff}{stdError} \quad p - value = m * tdist(t - value, df, two - sided) = 10 * tdist(t - value, 95, 2)$$


Other Post-Hoc Corrections

- Holm -Sidak (really Bonferroni done “right”)
 - Order the p-values from smallest to largest
 - Compare the smallest p-value to α/k (regular Bonferroni)
 - If that p-value is less than α/k , then accept that alternative hypothesis
 - Now look at the next smallest p-value at $\alpha / (k - 1)$
 - Continue until the p-value is not smaller than the modified value
 - At that point, stop and accept all the rest as null hypotheses



Other Post-Hoc Corrections

- Tukey
 - Used when comparing **all** pair-wise differences
 - produces narrower confidence intervals than Bonferroni in this situation
 - usual situation when trying to order results
 - e.g. comparing 5 different EC systems
 - Found out that $EC_3 > EC_2 \mid EC_5 > EC_1 > EC_4$
 - Note: Although there are 4 comparison symbols above, there are really 6 comparisons
 - actually there are $5C2 = 10$ implicit comparisons
 - because we did not know how many comparisons there would be apriori



Other Post-Hoc Corrections

- Tukey
 - Same as T test except uses the q distribution instead of the t distribution
 - $q(1 - \alpha, r, n_T - r)$ value is the cut off value where the difference observed would be **less than this value** with a probability of $1 - \alpha$ if r values are sampled from a normal distribution $N(0,1)$
 - $DofF = n_T - r$
 - q distribution is called the studentized range distribution
 - q “broader” than t ,
 - q is not as “broad” as t after Bonferroni correction
 - q distribution is not in Excel, but it is in most other stats packages including R



Other Post-Hoc Corrections

- Many others
 - Scheffé
 - used when comparing pairs, and triples and quadruples etc., not just pairs
 - many many others
 - Duncan's multiple range test
 - The Nemenyi test
 - The Bonferroni–Dunn test
 - Newman-Keuls post-hoc analysis



Important Topics Not Covered

- Data Modelling
 - What is a statistical model
 - Correlation, Regression and ANOVA as linear models
 - Generalized Linear Models (GLM)
- Regression
 - Linear Regression by means of least squares
 - Multivariate regression, Polynomial Regression
 - Confidence Intervals around model parameters
 - Statistical Testing for factor relevance
 - Correlation Coefficients: r , r^2 , adjusted r^2
- How to perform ANOVA as a multivariate regression
 - Indicator Variables



Important Topics Not Covered

- Testing for equality (homogeneity) of variance across different factor-levels / treatments
 - Levene's Test
- Correcting for inequality of variance
 - Convert to multivariate regression using indicator variables
 - Perform Weighted Least Squares
- How to perform ANOVA when using different test functions
 - Test functions as *blocking variables*
 - Non-parametric blocking
- What if one EC system has parameters the other EC system doesn't?
 - Nesting factor analysis



References: Books

- Mathematical statistics with applications
 - *Dennis D. Wackerly, William Mendenhall, Richard L. Scheaffer.*
 - *Boston : Duxbury Press, (6th Ed.)*
 - Introductory material - probability distributions, simple sample statistics
 - Easy to understand concrete proofs and examples - good exercises
- Applied linear statistical models
 - *Michael H. Kutner, Christopher J. Nachtsheim, John Neter, William Li*
 - *Boston: McGraw-Hill Irwin, 2005. (5th Ed.)*
 - Advanced Regression techniques, ANOVA, and GLM
- Nonparametric statistical methods
 - *Myles Hollander and Douglas A. Wolfe.*
 - *New York: Wiley, 1973*
 - Classic nonparametric statistics textbook (very practical)