Linear regression using ordinary least squares

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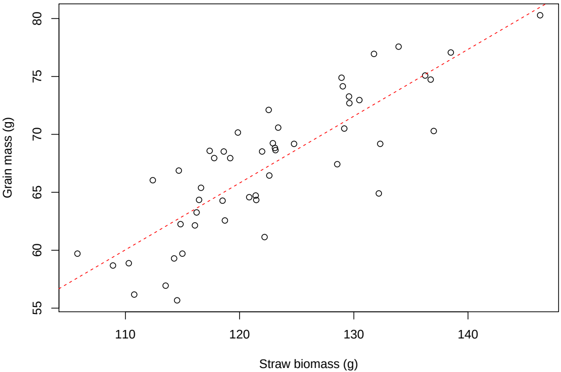
OLS recap

Goal is to find a line that best fits the data

- Best line is one that minimizes the residual sum of squares
- Coefficients for best line are given by $\beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$

$$y_i = \beta_0 + \beta_1 x_i + e_i$$



OLS recap

We are partitioning variability in y into orthogonal components.

$$SS_{Total} = SS_{Regression} + SS_{Error}$$

Total variability in y = Variability explained by the model + Unexplained variability

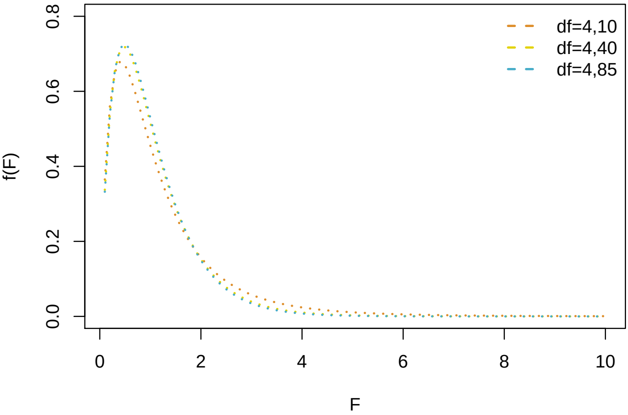
Source	**SS**	**df**	**MS**
Regression	$SSR = \sum_{i=1}^{i}(\hat{y}_i - \bar{y})^2$	$df_{Reg.} = p$	$\frac{SSR}{df_{Reg.}}$
Error	$SSE = \sum_{i=1}^{i}(y_i - \hat{y}_i)^2$	$df_{Err.} = n - p - 1$	$\frac{SS_{Err.}}{df_{Err.}}$
Total	$SS_{Tot.} = \sum_{i=1}^{i}\sum_{j=1}^{j}(y_i - \bar{y})^2$	$df_{Tot.} = n - 1$	

OLS recap

Does the model explain more variability than error?

- $\mathbf{H_0}$: $\beta_1 = 0$
- $\mathbf{H_1}$: $\beta_1 \neq 0$

$$F = \frac{\text{MSR}}{\text{MSE}}$$



F-dist. is parameterized by $\text{df}_{\textbf{Regression mod.}}$ and $\text{df}_{\textbf{Error}}$

Multiple linear regression – OLS with $p > 1$

Motivations:

- Confounding
  - Confounder: An extraneous variable that distorts the association between the dependent variable of interest and the response
- Gain precision
- Scientific reasons

An example

We are interested in looking at the effects of straw biomass (g plant^{-1}) and grain width (mm) on yield (g plant^{-1}) in rice. Fifty varieties were randomly selected and grown in the field. At harvest plant biomass, grain width and yield were collected.

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- Assume grain width and plant biomass are uncorrelated.

	Biomass	**Gr. Width**	**Yld.**
Biomass	1.00	0.00	0.73
Gr. Width	0.00	1.00	0.67
Yld.	0.73	0.67	1.00

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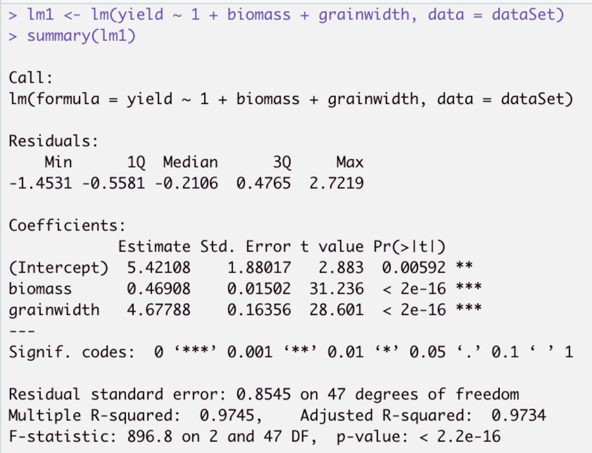
$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + e_i$$

- y_i: grain yield for *i*th experimental unit (plant)
- x_{i1}: biomass for *i*th experimental unit (plant)
- x_{i2}: grain width for *i*th experimental unit (plant)

An example in R



```
> lm1 <- lm(yield ~ 1 + biomass + grainwidth, data = dataSet)
> summary(lm1)

Call:
lm(formula = yield ~ 1 + biomass + grainwidth, data = dataSet)

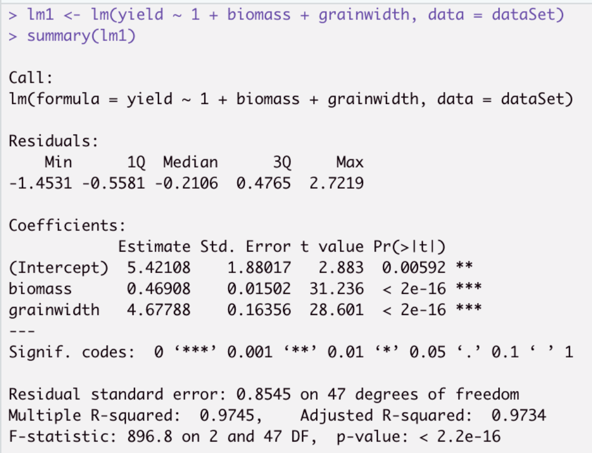
Residuals:
    Min      1Q  Median      3Q     Max 
-1.4531 -0.5581 -0.2106  0.4765  2.7219 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  5.42108    1.88017   2.883  0.00592 ** 
biomass      0.46908    0.01502  31.236  < 2e-16 ***
grainwidth   4.67788    0.16356  28.601  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.8545 on 47 degrees of freedom
Multiple R-squared:  0.9745,	Adjusted R-squared:  0.9734 
F-statistic: 896.8 on 2 and 47 DF,  p-value: < 2.2e-16
```

- Interpreting coefficients: If straw biomass is *held constant*, for every mm increase in grain width grain will result in a 4.7 g increase in yield.

An example in R



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- The F-stat tells us the regression model explains sign. more variability in y than the error.

Model comparisons

Does a subset of predictors have an effect on the response?

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + e_i$$

- H_0: $\beta_3 = \beta_4 = 0$
- H_1: β_3 or $\beta_4 \neq 0$

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- H_1: β_3 or $\beta_4 \neq 0$

An alternative way to view this is as a set of nested models.

- H_0: $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + e_i$ (reduced model)
- H_1: $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + e_i$ (full model)

Model comparisons

- H_0: $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + e_i$ (reduced model)
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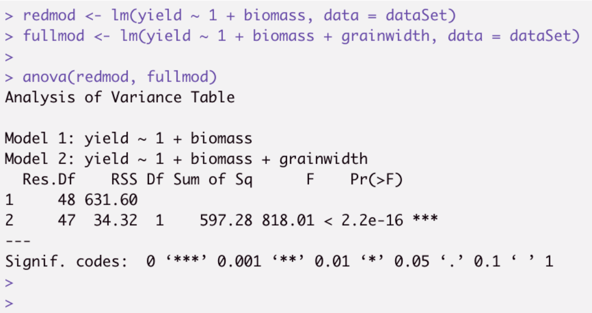
1. Fit “full” and “reduced” models and compute the residual/error SS ($\text{SS}_{\mathrm{Err.}}$).
2. Compare $\text{SS}_{\mathrm{Err.}}$ (SSE) between models using F-test

$$\mathrm{F} = \frac{(\mathrm{SSE}(\mathrm{Reduced}) - \mathrm{SSE}(\mathrm{Full}))/(df_{\mathrm{Reduced}} - df_{\mathrm{Full}})}{\mathrm{SSE}(\mathrm{Full})/df_{\mathrm{Full}}}$$

$$\mathrm{F}(df_{\mathrm{Reduced}} - df_{\mathrm{Full}}, df_{\mathrm{Full}})$$

Model comparisons in R

- The rice example only includes two predictors (biomass and grain width), but the concepts are the same.



```
> redmod <- lm(yield ~ 1 + biomass, data = dataSet)
> fullmod <- lm(yield ~ 1 + biomass + grainwidth, data = dataSet)
>
> anova(redmod, fullmod)
Analysis of Variance Table

Model 1: yield ~ 1 + biomass
Model 2: yield ~ 1 + biomass + grainwidth
  Res.Df    RSS Df Sum of Sq      F    Pr(>F)
1     48 631.60
2     47  34.32  1    597.28 818.01 < 2.2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
>
>
```

Collinearity and multicollinearity

In many real world datasets there will be some dependency among predictors

- Issues:
  - Adding/changing predictor substantially changes coefficient estimates
  - Can no longer interpret meaning of coefficients
  - High standard error for coefficient estimates

- Addressing dependencies
  - Correlation between predictors
  - Variance inflation factors (VIF)

Variance inflation factors

Regress each predictor variable on all other predictors and calculate R^2 **for each predictor**

For example:

- Our regression model: $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + e_i$
- For $\mathbf{x_1}$: $x_{i1} = \alpha + \alpha_2 x_{i2} + \alpha_3 x_{i3} + \alpha_4 x_{i4} + e_i$
- VIF for $\mathbf{x_1}$:

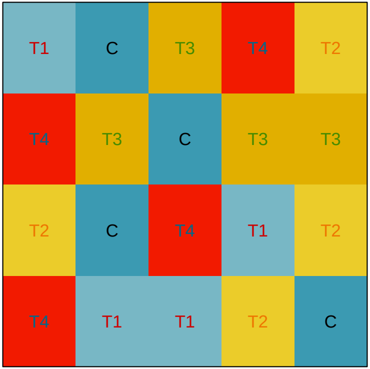
$$VIF_1 = \frac{1}{1 - R_1^2}$$

- Remove predictors with $VIF > 10$

Analyzing one factor designs

Completely randomized designs

Objective: One factor (e.g. treatment) under consideration and levels of the factor are randomly assigned to experimental units



T1	C	T3	T4	T2
T4	T3	C	T3	T3
T2	C	T4	T1	T2
T4	T1	T1	T2	C

Randomization ensures that the systematic difference is treatment (i.e. eliminates confounding)

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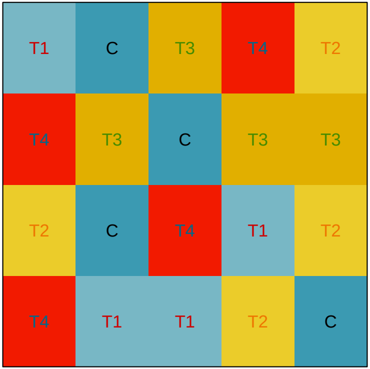

T1	C	T3	T4	T2
T4	T3	C	T3	T3
T2	C	T4	T1	T2
T4	T1	T1	T2	C

The model: $y_{ij} = \mu_i + e_{ij}$

Comparing treatments (means)

Two levels: two-sample t-test

$$t = \frac{\hat{\mu}_1 - \hat{\mu}_2}{\hat{\sigma}\sqrt{2/n}}$$

More than two levels?

Comparing treatments (means)

Two levels: two-sample t-test

$$t = \frac{\hat{\mu}_1 - \hat{\mu}_2}{\hat{\sigma}\sqrt{2/n}}$$

More than two levels: One-way analysis of variance (ANOVA)

- The ANOVA model is often written as $y_{ij} = \mu_i + e_{ij}$
  - y_{ij}: the response for the jth replicate in the ith treatment
  - μ_i: mean of the ith treatment
  - **Cell means model**
- An equivalent model is $y_{ij} = \mu + \alpha_i + e_{ij}$
  - α_i: ith treatment effect (how far the ith treatment deviates from the overall mean)
  - **Additive model**

Example – Single factor CRD

Researchers are interested in studying the effects of three N regimes (180, 200, and 220 lbs. N ac^{-1}) on yield. The field was split into nine plots (experimental units) and treatments were randomly assigned to each plot. Three observations were recorded for each combination of N level ($N = 3 \times 3 = 9$).

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- **Treatment design:** Each Nitro. treatment is assigned to at least one experimental unit
  - One factor: Nitrogen
  - Three levels: 180, 200, and 220
- **Experimental Design:** Treatments are randomly assigned and all are observed an equal number of times → *balanced complete randomized design*

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$$y_{ij} = \mu_i + e_{ij}$$

$\mathbf{H_0}$: Average yield is the same for all Nit.; **$\mathbf{H_1}$**: Average yield is different for at least one comparison of N levels;

$\mathbf{H_0}$: $\mu_{20} = \mu_{25} = \mu_{30}$; **$\mathbf{H_1}$**: $\mu_i \neq \mu_k$

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$$y_{ij} = \mu + \alpha i + e_{ij}$$

$$\mathbf{H_0}\text{: } \alpha_i = 0\text{; } \mathbf{H_1}\text{: } \alpha_i \neq 0$$

ANOVA is just OLS

ANOVA is regression on dummy variables

- Dummy variables: recoding of categorical variables

Cell means: $y_{ij} = \mu_i + e_{ij}$

Nit.	Rep.	Yld.
180	1	173.3
180	2	182.9
180	3	169.6
200	1	205.9
200	2	208.5
200	3	203.9
220	1	229.1
220	2	231.3
220	3	208.7

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

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Additive: $y_{ij} = \mu + \alpha_i + e_{ij}$

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An example in R

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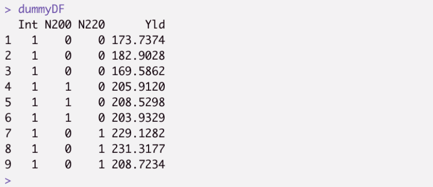
$$\mathbf{H_0}\text{: } \alpha_i = 0\text{; } \mathbf{H_1}\text{: } \alpha_i \neq 0$$

OR

$$\mathbf{H_0}\text{: } \mu_{20} = \mu_{25} = \mu_{30}\text{; } \mathbf{H_1}\text{: } \mu_i \neq \mu_k$$

An example in R

Using dummy variables:



```
> dummyDF
  Int N200 N220      Yld
1   1    0    0 173.7374
2   1    0    0 182.9028
3   1    0    0 169.5862
4   1    1    0 205.9120
5   1    1    0 208.5298
6   1    1    0 203.9329
7   1    0    1 229.1282
8   1    0    1 231.3177
9   1    0    1 208.7234
>
```

Using `aov()`:

An example in R

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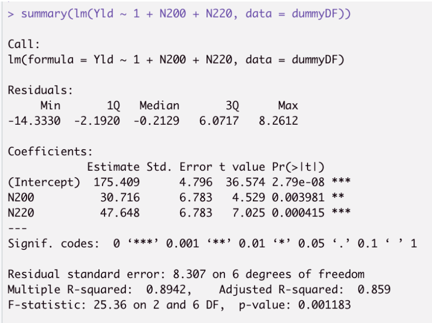

```
> summary(lm(Yld ~ 1 + N200 + N220, data = dummyDF))

Call:
lm(formula = Yld ~ 1 + N200 + N220, data = dummyDF)

Residuals:
     Min       1Q   Median       3Q      Max 
-14.3330  -2.1920  -0.2129   6.0717   8.2612 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  175.409      4.796  36.574 2.79e-08 ***
N200          30.716      6.783   4.529 0.003981 ** 
N220          47.648      6.783   7.025 0.000415 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 8.307 on 6 degrees of freedom
Multiple R-squared:  0.8942,	Adjusted R-squared:  0.859 
F-statistic: 25.36 on 2 and 6 DF,  p-value: 0.001183
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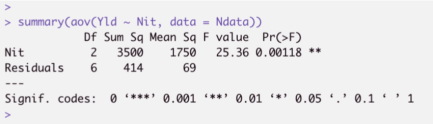
Using `aov()`:



```
> 
> summary(aov(Yld ~ Nit, data = Ndata))
            Df Sum Sq Mean Sq F value  Pr(>F)   
Nit          2   3500    1750   25.36 0.00118 **
Residuals    6    414      69                   
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An example in R

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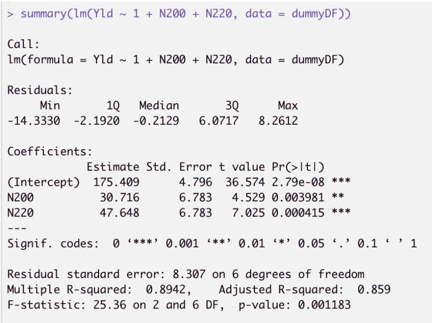

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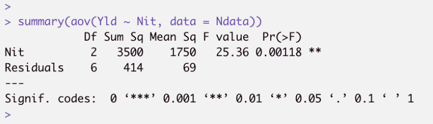

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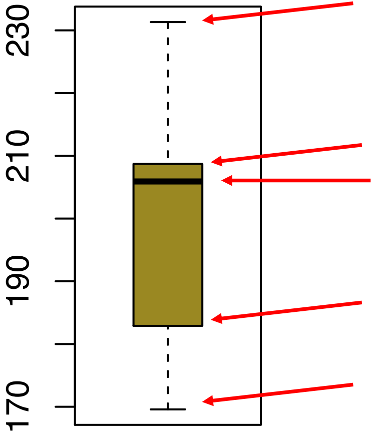
With ANOVA we are interested in drawing conclusions about a factor(s) (set of predictors)

- Equivalent to comparing models

Post-hoc tests



Q3 + 1.5*IQR

3rd quartile (Q3):
median of upper half

Median

1st quartile (Q1):
median of lower half

Q1 – 1.5*IQR

$$IQR = Q3 - Q1$$

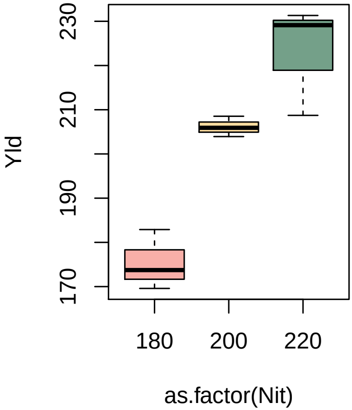
Post-hoc tests

Which treatments are different?

$\mathbf{H_0}$: $\alpha_i = 0$; $\mathbf{H_1}$: $\alpha_i \neq 0$

OR

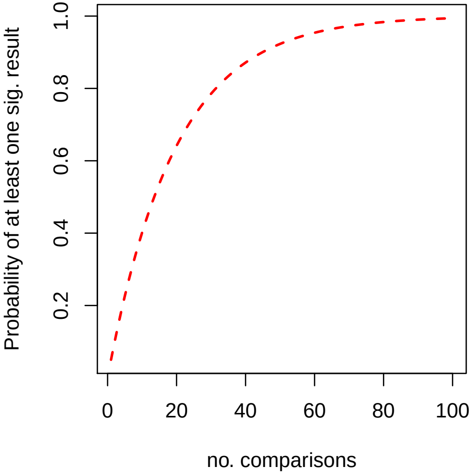
$\mathbf{H_0}$: $\mu_{20} = \mu_{25} = \mu_{30}$; $\mathbf{H_1}$: $\mu_i \neq \mu_k$



Hypothesis testing – multiple testing

We want to compare four levels of nitrogen. For each comparison we assume $\alpha = 0.05$

- $\frac{k(k-1)}{2}$ comparisons
- $1 - \alpha$: probability of failing to reject null when null is true
- Family-wise error rate: Type I error over set of comparisons
    - $FWER = 1 - (1-\alpha)^{\text{no. tests}}$

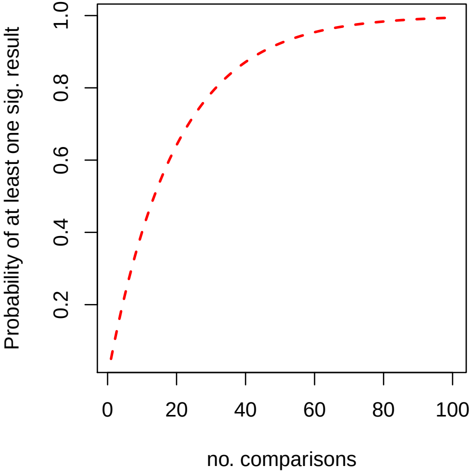


Hypothesis testing – multiple testing

We want to compare four levels of nitrogen. For each comparison we assume $\alpha = 0.05$

Multiple testing correction:

- Bonferroni's correction: $\alpha^* = \alpha/\text{No. tests}$
- Sidak's correction: $\alpha^* = 1-(1-\alpha)^{1/\text{No. tests}}$
- Benjamini-Hochberg: Ranking procedure (see course notes)

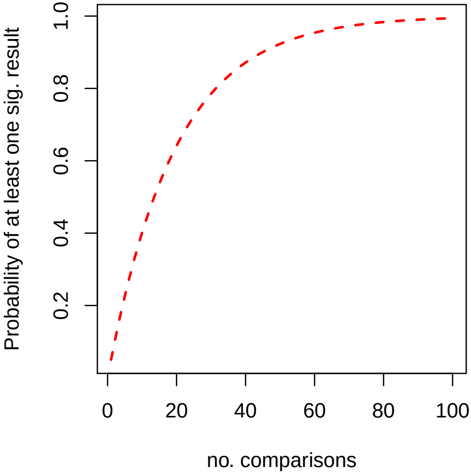


Hypothesis testing – multiple testing

We want to compare four levels of nitrogen. For each comparison we assume $\alpha = 0.05$

Post-hoc tests:

- Tukey's honest significant difference (HSD) test: all pairwise comp.
- Dunnett's test: Control vs treatments



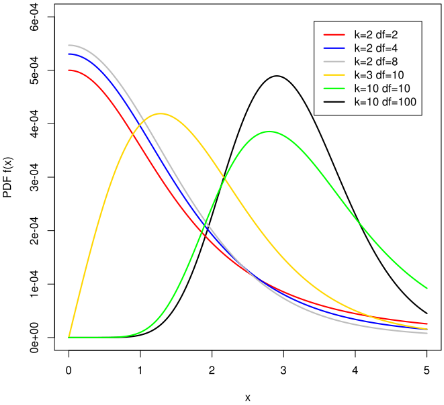
Hypothesis testing – Tukey's HSD

HSD stat. is similar to t-statistic:

$$HSD = \frac{\mu_1 - \mu_2}{\sqrt{MSE_e/n}}$$

$$\mu_1 \geq \mu_2$$

Studentized range distribution:



https://en.wikipedia.org/wiki/Studentized$_{r}$*ange*$_{d}$*istribution*

k = number of levels for factor, $df = n - k$

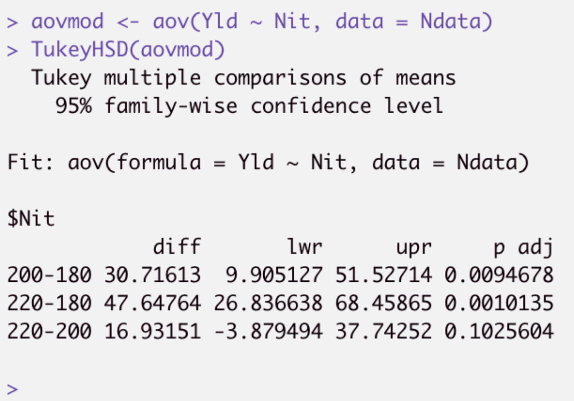
Hypothesis testing – Tukey's HSD

HSD stat. is similar to t-statistic:

$$HSD = \frac{\mu_1 - \mu_2}{\sqrt{MSE_e/n}}$$

$$\mu_1 \geq \mu_2$$

In R:



```
> aovmod <- aov(Yld ~ Nit, data = Ndata)
> TukeyHSD(aovmod)
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = Yld ~ Nit, data = Ndata)

$Nit
            diff       lwr      upr     p adj
200-180 30.71613  9.905127 51.52714 0.0094678
220-180 47.64764 26.836638 68.45865 0.0010135
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