CSCI 3022

intro to data science with probability & statistics

Lecture 26
April 18, 2018

Forward & Backward Selection
+
Analysis of Variance (ANOVA)

Room for final has changed! FLMG 155

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Practicum

- The **Practicum** is posted. It is due at 11:55pm on Wednesday May 2.
- **The Rules**:
  - All work must be your own. Collaboration of any kind is is not permitted.
  - You may use any resources you like, but you may not post to message boards or other online resources asking for help.
  - We will answer general, clarifying questions in office hours.
  - If you have a question for us, post a **PRIVATE** message on Piazza.
  - Use pandas, numpy, scipy as you wish, plus matplotlib. No other packages pls.
  - See clarifying thread on Piazza. I'm adding any clarifications text in blue.

Last time on CSCI 3022:

- Given data $(x_{i1}, x_{i2}, \ldots, x_{ip}, y_i)$ for $i = 1, 2, \ldots, n$ fit a MLR model of the form:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \epsilon_i \quad \text{where} \quad \epsilon_i \sim N(0, \sigma^2)$$

- We can test if any of the features are important:

$$F = \frac{(SST - SSE)/p}{SSE/(n-p-1)} \qquad SST = \sum_{i=1}^{n} (y_i - \bar{y})^2 \qquad SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- The F-statistic follows an F-distribution
- Rejection Region: $F \geq F_{\alpha,p,n-p-1}$ p-value: 1 – stats.f.cdf(F, p, n-p-1)

Deciding on important variables

i = 100

- Suppose that we have 100 data points (n=100), but we have 200 different features (p=200). How can we learn which features are important and which are not?
- **Some options**:
  - Try all the possible combinations of features in models to see which gives the best fit.

Bad!

2^p different models.

p = 30 1,073,741,824 models.

yikes!

Deciding on important variables

- Suppose that we have 100 data points (n=100), but we have 200 different features (p=200). How can we learn which features are important and which are not?
- **Some options**:
  - **Forward selection**:

β_0

do not include any $\beta_1, \beta_2, \beta_3 \ldots$

"baseline"

"baseline + 1 feature"

1. fit null model with an intercept but no predictors.
2. fit p-SLRs, 1 for each feature. Choose the one that gives the lowest SSE.
3. fit p-1 MLRs. Choose that which gives lowest SSE…
4. repeat. step 3, w/ p-2 MLRs, then p-3 MLRs …

Deciding on important variables

- Suppose that we have 100 data points (n=100), but we have 200 different features (p=200). How can we learn which features are important and which are not?
- **Some options**:
  - **Backward selection**:

p features
1. Fit model with *all* predictors

p-1 features
2. Remove the one with the largest *p*-value.
3. Fit model with p-1 predictors.

p-2 features
4. Remove the one with the largest *p-value…*

Quiz. Name That Computation!

1. **Advertising example**. I want to know if the set of {news,radio} together have at least one slope that is significantly different from 0.

F-test! For a subset of features. H_0: $\beta_{news} = \beta_{radio} = 0$

2. **Home prices example**. I have 1000 data points and 30 features. I want to learn the 10 most predictive and significant features.

because $n >> p$ use forward selection to get 10 features, or backward selection.

3. **Home prices example**. I have 100 data points and 200 features. I want to learn the 20 most predictive features.

Forward only. If $n < p$, use forward selection.

4. **Shark attacks example**. I have 50 shark attacks, and I have 20 features. I fit my MLR model. Now I want to compute how well my model fits the data.

R^2_a ← includes penalty for using so many features.

Comparing multiple means

- We're often interested in comparing the means of a response from different groups
- **Example**: Suppose we are doing a study on the effect of diet on weight-loss. We have three different groups in the study:
  - **Control group**: exercise only
  - **Treatment A**: exercise plus Diet A
  - **Treatment B**: exercise plus Diet B
- We record the weight-loss of each participant after one week of the study and find the following results:

Three participants in each group.

	Control	Diet A	Diet B
0	3	5	5
1	2	3	6
2	1	4	7

Comparing multiple means

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- We record the weight-loss of each participant after one week of the study and find the following results:

Question: Are the means of the different groups all the same?

What would we do if there were only two groups?

CI for $\mu_1 - \mu_2$? includes 0

CIs μ_1 and μ_2 ? overlap

t-test

z-test

$H_0: \mu_1 = \mu_2$

$H_1: \mu_1 \neq \mu_2$

Comparing multiple means

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Question: Are the means of the different groups all the same?

Why would a t- or z-test be problematic if we had many different groups?

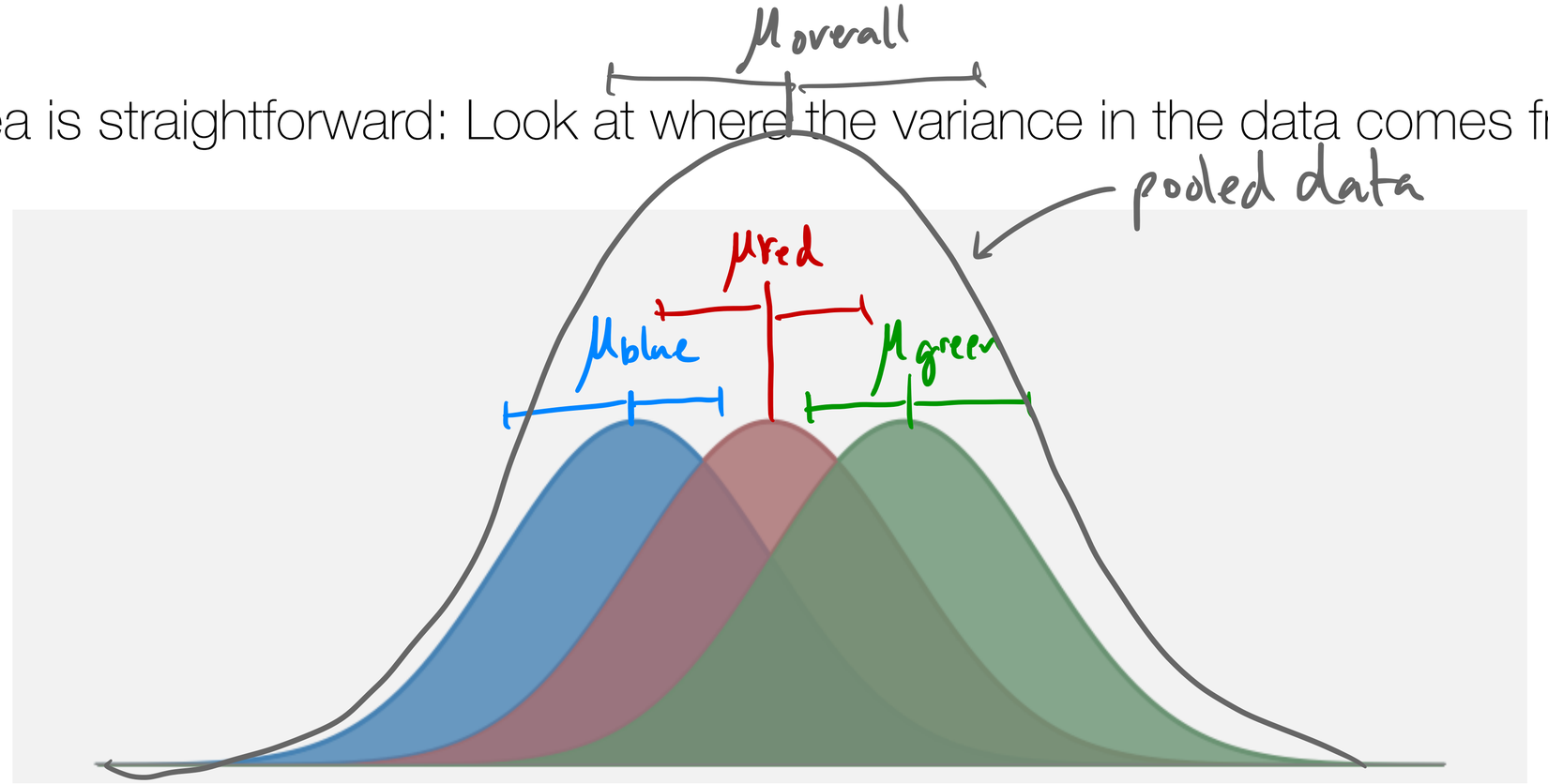
① expensive
k groups
$\binom{k}{2}$ comparison $= \frac{k(k-1)}{2} \sim k^2$

② multiple comparisons problem.

Analysis of variance

- We can answer the question "Are any of the means different?" using a procedure called analysis of variance, or **ANOVA** for short.

- The idea is straightforward: Look at where the variance in the data comes from.



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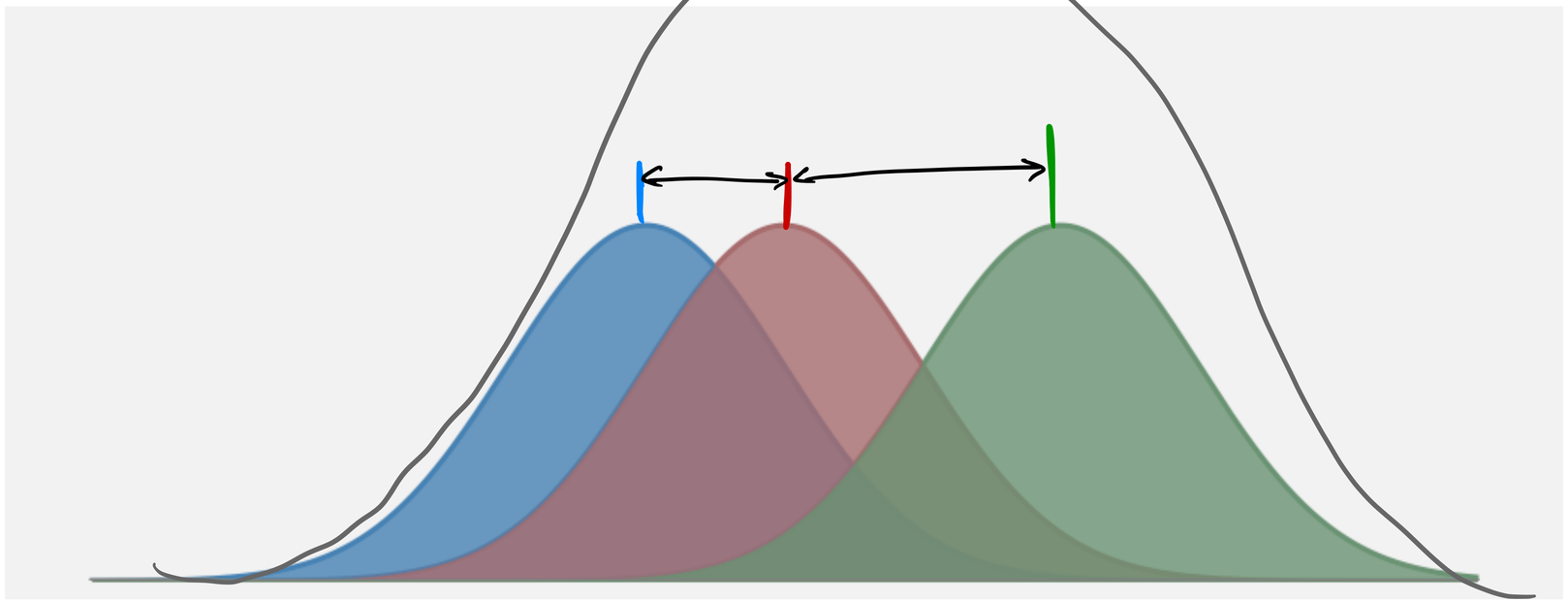

Analysis of variance

overall variance $= \frac{1}{n-1}\sum(y_i - \bar{\bar{y}})^2$ ($\bar{\bar{y}}$ = mean of all data when pooled together. "grand mean")

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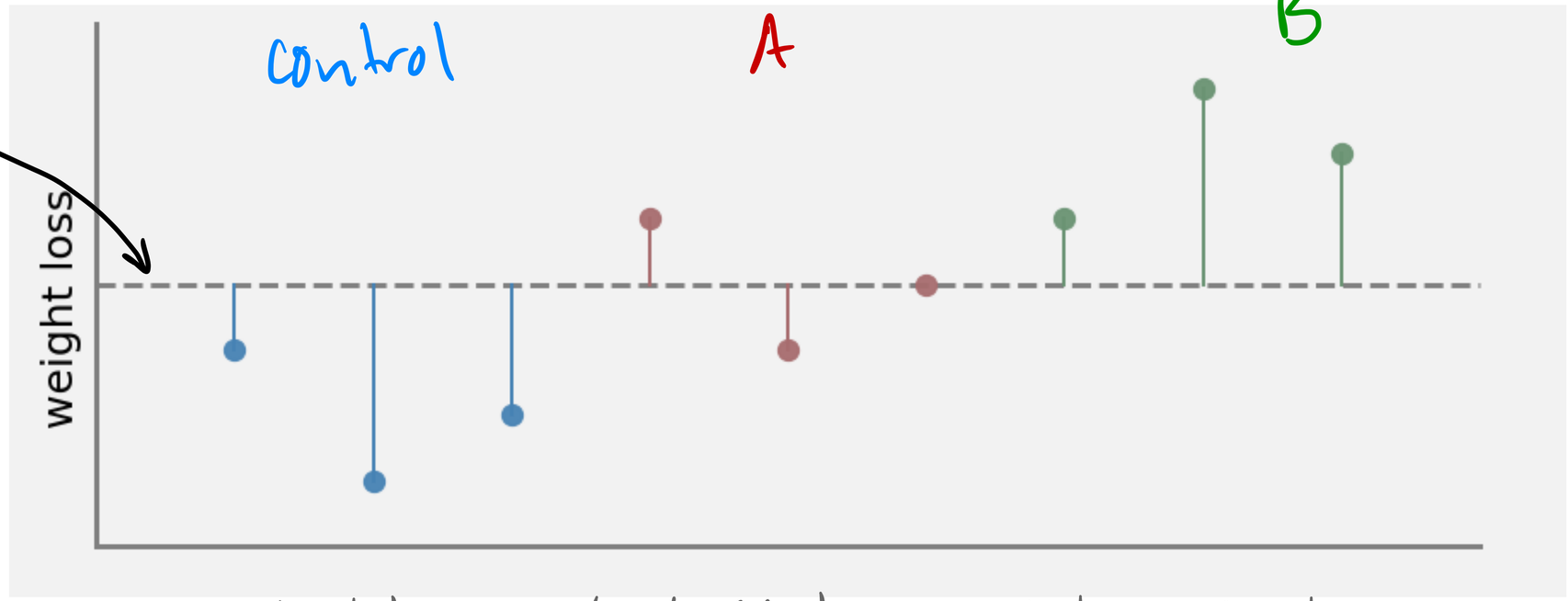

$\bar{\bar{y}} = \frac{1}{n}\sum_{i=1}^{n} y_i$ ← calculation pretends that group labels don't exist.

Analysis of variance

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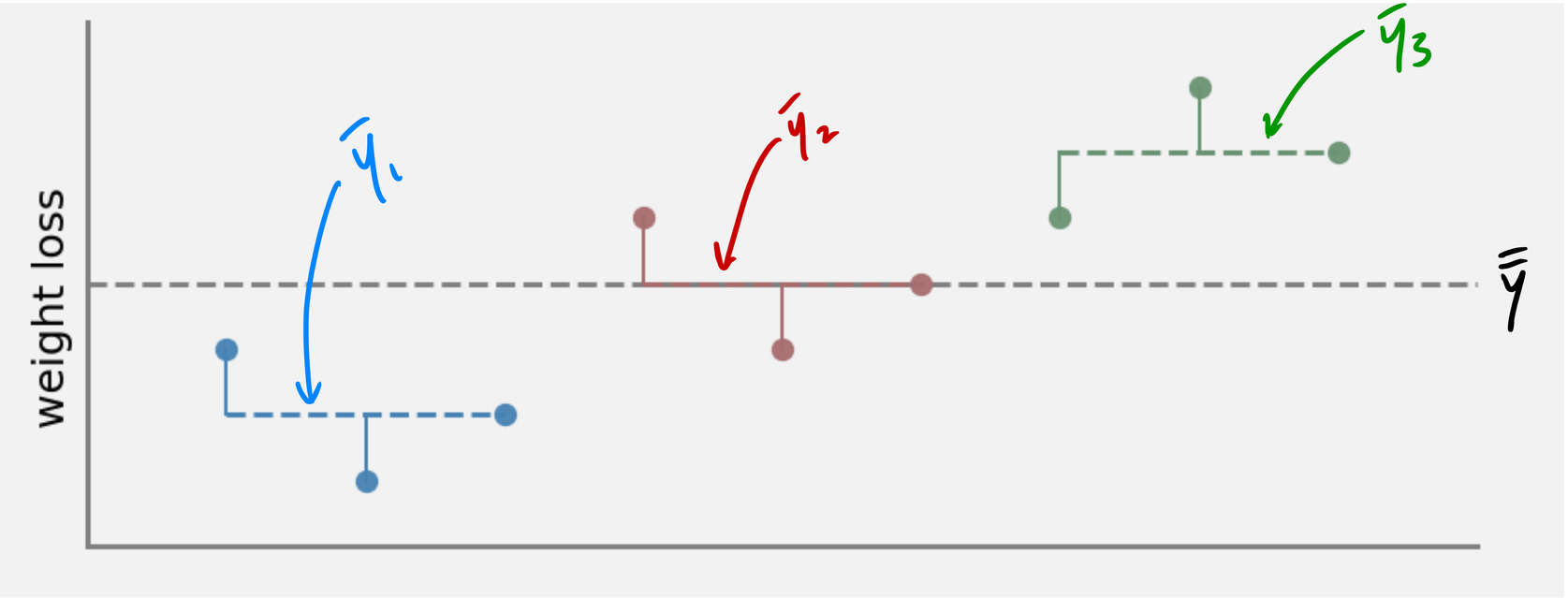
- The idea is straightforward: Look at where the variance in the data comes from.



The one-way ANOVA model

prev example
$n_1 = 3$
$n_2 = 3$
$n_3 = 3$
points

I

- Suppose that we have I groups that we want to compare, each with n_i data
- We model the relationship between responses and group means as follows:

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

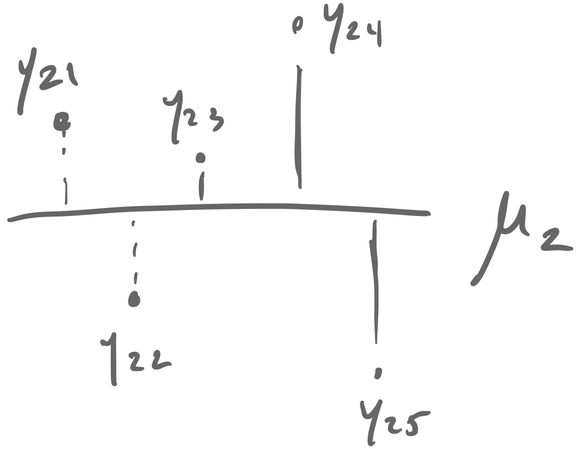
group i

j^{th} data point in that group

mean of group i

noise, error

$\varepsilon_{ij} \sim N(0, \sigma^2)$



Assumptions:

- the responses are i.i.d. samples from normally distributed groups
- the variance of each group is the same

ANOVA is "pretty robust" to violations of these assumptions.
- non-normal data
- slightly non-equal variances.

The one-way ANOVA model

	Control	Diet A	Diet B
0	3	5	5
1	2	3	6
2	1	4	7

Let's compute some means!

- The **grand mean** is the sample mean of all responses.

$$\bar{\bar{y}} = \frac{1}{9}\left[(3+2+1) + (5+3+4) + (5+6+7) \right]$$

$$= \frac{1}{9}\left[6 + 12 + 18 \right] = \frac{1}{9} \cdot 36 = 4$$

$$\boxed{\bar{\bar{y}} = 4}$$

- The **group means** are the sample means within each group.

$$\bar{y}_1 = \frac{1}{3}(3+2+1) = \frac{1}{3}6 = 2$$

$$\bar{y}_2 = \frac{1}{3}(5+3+4) = \frac{1}{3}12 = 4$$

$$\bar{y}_3 = \frac{1}{3}(5+6+7) = \frac{1}{3}18 = 6$$

$$N = n_1 + n_2 + n_3 = 9$$

$$\bar{\bar{y}} = \frac{n_1\bar{y}_1 + n_2\bar{y}_2 + n_3\bar{y}_3}{N}$$

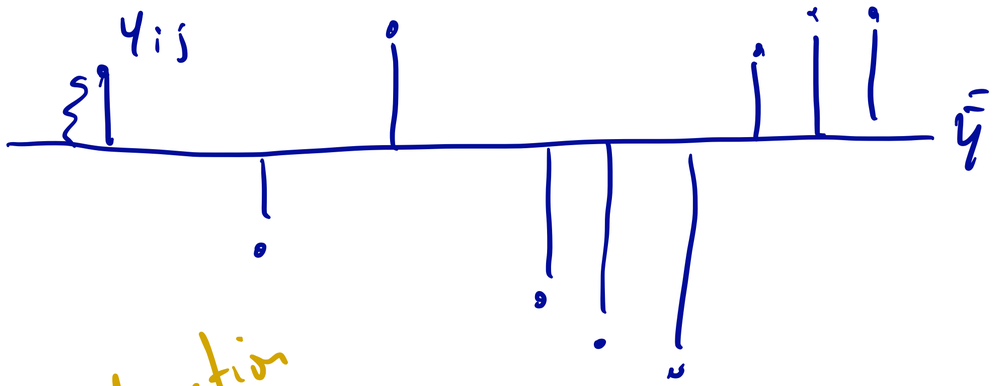
It's the variances, stupid

cf "It's the economy, stupid" 1992 Carville.

- Where does the total variation in the data come from? Remember linear regression:

$$SST = \sum_{i=1}^{I} \sum_{j=1}^{n_i} (y_{ij} - \bar{\bar{y}})^2$$

over all groups; within each group



- A helpful decomposition:

$$y_{ij} - \bar{\bar{y}} + \bar{y}_i - \bar{y}_i = (y_{ij} - \bar{y}_i) + (\bar{y}_i - \bar{\bar{y}})$$

overall deviation; within group deviation; between group deviation

- Then, a minor (mathematical) miracle occurs:

$$SST = \sum_{i=1}^{I} \sum_{j=1}^{n_i} \left[(y_{ij} - \bar{y}_i)^2 + (\bar{y}_i - \bar{\bar{y}})^2 \right]$$

SS_{Within} $SS_{Between}$

The one-way ANOVA model

Let's compute some variances (or at least, sums of squares)!

	Control	Diet A	Diet B
0	3	5	5
1	2	3	6
2	1	4	7

$n_1 = 3 \quad n_2 = 3 \quad n_3 = 3$

$\bar{y}_{i\cdot} = 2 \quad 4 \quad 6$

- The **BETWEEN** group sum of squares is:

$$SSB = \sum_{i=1}^{I} \sum_{j=1}^{n_i} (\bar{y}_{i\cdot} - \bar{\bar{y}})^2 = \sum_{i=1}^{I} n_i (\bar{y}_{i\cdot} - \bar{\bar{y}})^2$$

(# data points in group i)

$$= 3(2-4)^2 + 3(4-4)^2 + 3(6-4)^2 = 24$$

- The **WITHIN** group sum of squares is:

$$SSW = \sum_{i=1}^{I} \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})^2$$

$(3-2)^2\ 1 \quad (6-4)^2\ 1 \quad (5-6)^2\ 1$

$(2-2)^2\ 0 \quad (3-4)^2\ 1 \quad (6-6)^2\ 0$

$(1-2)^2\ 1 \quad (4-4)^2\ 0 \quad (7-6)^2\ 1$

$\rightarrow 6$

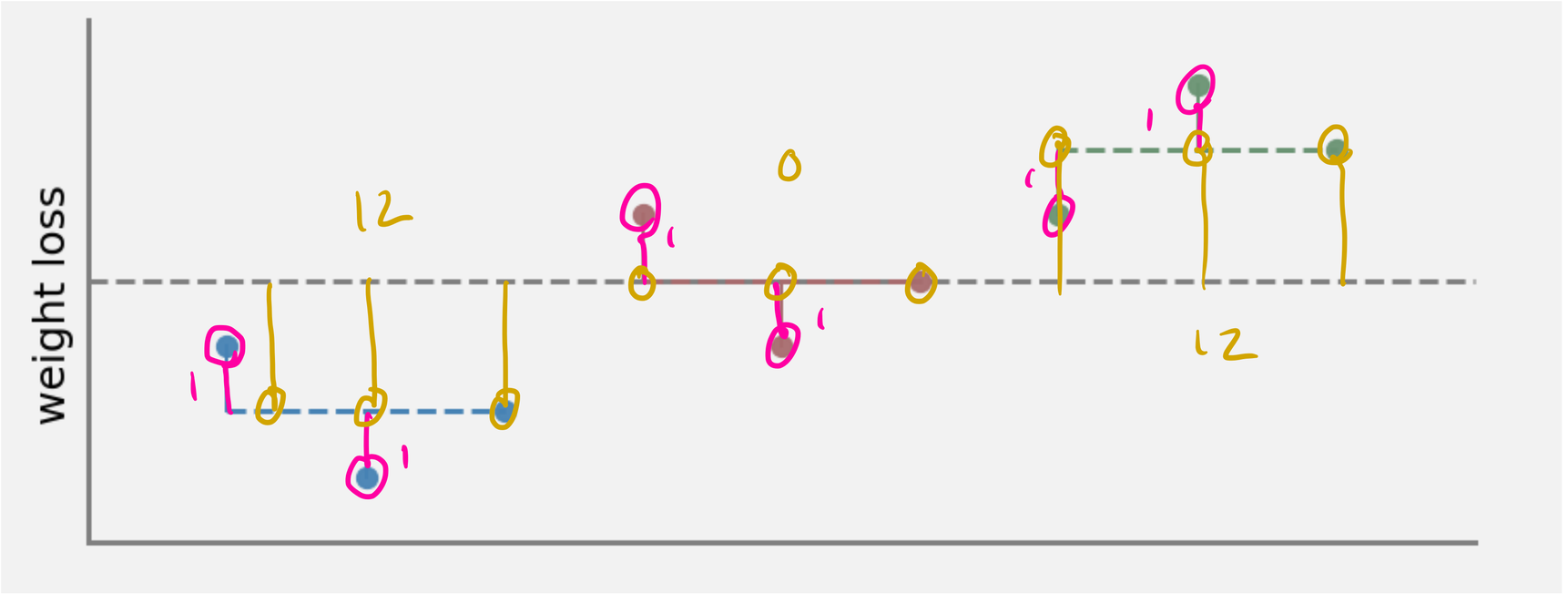
- The **TOTAL** sum of squares is:

$$SST = SSW + SSB = 6 + 24 = 30$$

The one-way ANOVA model

SSB = 24
SSW = 6

- Compare these results to the original picture:



	Control	Diet A	Diet B
0	3	5	5
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The one-way ANOVA model

What about degrees of freedom?

- The **BETWEEN** group degrees of freedom is (are?):

$$SSB = \sum_{i=1}^{I} \sum_{j=1}^{n_i} (\bar{y}_{i\cdot} - \bar{\bar{y}})^2 = \sum_{i=1}^{I} n_i (\bar{y}_{i\cdot} - \bar{\bar{y}})^2$$

treat this like data

computed from the data

$$SSB_{df} = \underbrace{I}_{\#\text{ of groups}} - \underbrace{1}_{\bar{\bar{y}}} = 3 - 1 = 2$$

	Control	Diet A	Diet B
0	3	5	5
1	2	3	6
2	1	4	7

N = total data pts

$$N = \sum_{i=1}^{I} n_i$$

- The **WITHIN** group degrees of freedom is (are?):

$$SSW = \sum_{i=1}^{I} \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})^2$$

data

computed from the data

$$SSW_{df} = N - I = 9 - 3 = 6$$

A hypothesis test

i.e. = id est → that is, specifically

e.g. = exempla gratia → for example.

- We want to perform a hypothesis test to determine if the group means are equal. We have

H_0 : $\mu_1 = \mu_2 = \dots = \mu_I$

H_1 : $\mu_i \neq \mu_j$ for some (i,j) pair i.e. two of the group means are different.

- Our test statistic will be:

$$F = \frac{SSB / SSB_{df}}{SSW / SSW_{df}} = \frac{SSB / I-1}{SSW / N-I} = \frac{SSB(N-I)}{SSW(I-1)}$$

Rej. Region Test: $F \geq F_{\alpha, I-1, N-I}$

p-val : $1 - \text{stats.f.cdf}(F_{21}, I-1, N-I)$

The ANOVA Table

- It is common practice to organize all computations into an ANOVA table

ANOVA	SS	df	SS/df
Between	24	3-1=2	$\frac{24}{2}=12$
Within	6	9-3=6	$\frac{6}{6}=1$
Total	30	8	

	Control	Diet A	Diet B
0	3	5	5
1	2	3	6
2	1	4	7

$F = \frac{12}{1} = 12$

p-val = 0.008

ANOVA as multiple linear regression

- Interestingly, there is a very close relationship between One-Way ANOVA and MLR!
- Suppose you have *I* groups that you want to compare. A random sample of size n_i is taken from the i^{th} group. Then

Tukey's honest significance test

- Suppose that we determine that some of the means are different.
- How can we tell which ones?

Tukey's HST or Tukey's Range Test

Hypothesis Test for pair-wise comp. of means.

Fixes problem of multiple comparisons.

→ Adjusts so that making a Type-I error over all possible pair-wise comparisons = α

rejecting H_0 even though H_0 was true.

same Tukey as 5-number summary EDA

Tukey’s honest significance test

- Suppose that we determine that some of the means are different.
- How can we tell which ones?