CSCI 3022

intro to data science with probability & statistics

November 28, 2018

Forward & Backward Selection

+

Analysis of Variance (ANOVA)

Arkaive! :)

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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)

Is a Subset of Features Important?

- **Full Model**: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4$ (p=4 features in full model)
- **Reduced Model**: $y = \beta_0 + \beta_2 x_2 + \beta_4 x_4$ (k=2 features in reduced model)
- **Question**: Are the missing features important, or are we OK going with the reduced model?
- **Partial F-Test**: $H_0 : \beta_1 = \beta_3 = 0$
- Since the features in the reduced model are also in the full model, we expect the full model to perform at least as well as the reduced model.
- **Strategy**: Fit the Full and Reduced models. Determine if the difference in performance is real or due to just chance.

Is a Subset of Features Important?

p features

- SSE_{full} =variation unexplained by the full model

k features

$(k < p)$

- SSE_{red} =variation unexplained by the reduced model

Intuitively, if <u>SSEfull</u> is much smaller than <u>SSEred</u> , the full model fits the data much better than the reduced model. The appropriate test statistic should depend on the difference <u>SSEred - SSEfull</u> in unexplained variation.

- Test Statistic: $$F = \frac{(SSE_{\text{red}} - SSE_{\text{full}})/(p-k)}{SSE_{\text{full}}/(n-p-1)} \sim F_{p-k,n-p-1}$$

- Rejection Region: $F \geq F_{\alpha,p-k,n-p-1}$

http://homepage.divms.uiowa.edu/~mbognar/applets/f.html

F… why even?

- Why compute the p-value for F-statistic when instead, we already have p-values for each of the covariates?
- Doing so would not be testing one hypothesis, but rather *p* hypotheses!
- At α=0.05, how many *p* values do we expect to be significant if the null hypothesis is, in fact, true?

```
In [27]:  1 model.summary()
Out[27]:
```

OLS Regression Results

Dep. Variable:	sales	**R-squared:**	0.897
Model:	OLS	**Adj. R-squared:**	0.896
Method:	Least Squares	**F-statistic:**	570.3
Date:	Tue, 28 Nov 2017	**Prob (F-statistic):**	1.58e-96
Time:	20:28:02	**Log-Likelihood:**	-386.18
No. Observations:	200	**AIC:**	780.4
Df Residuals:	196	**BIC:**	793.6
Df Model:	3		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
const	2.9389	0.312	9.422	0.000	2.324	3.554
tv	0.0458	0.001	32.809	0.000	0.043	0.049
radio	0.1885	0.009	21.893	0.000	0.172	0.206
news	-0.0010	0.006	-0.177	0.860	-0.013	0.011

?

?

Suppose 100 features. $(0.05 \cdot 100) = 5$ false pos. features simply by chance!

The road to R^2 for MLR

- Just as with simple regression, the error sum of squares is:

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$\boxed{\hat{\sigma}^2 = \frac{SSE}{n-(p+1)} = \frac{SSE}{n-p-1}}$$

Note: you may see SSE written as RSS: "residual sum of squares"

- It is again interpreted as a measure of how much variation in the observed y values is not explained by (not attributed to) the model relationship.

- The number of df associated with SSE is n–(p+1) because p+1 df are lost in estimating the p+1 β coefficients.

The road to R^2

- Just as before, the **total sum of squares** is:

$$SST = \sum_{i=1}^{n} (y_i - \bar{y})^2 \qquad df: n-1$$

see prev slide!

- And the **sum of squared errors** is:

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \qquad df: n-p-1$$

- Then the coefficient of multiple determination R^2 is:

$$R^2 = 1 - \frac{SSE}{SST} \quad (SLR)$$

- It is interpreted in the same way as before. (Do you remember?)

Hacking R^2

Unfortunately, there is a problem with R^2: Its value can be inflated by adding lots of predictors into the model even if most of these predictors are frivolous!

Hacking R^2

- For example, suppose y is the sale price of a house. Then:
- Sensible predictors include
  x_1 = the interior size of the house,
  x_2 = the size of the lot on which the house sits,
  x_3 = the number of bedrooms,
  x_4 = the number of bathrooms, and
  x_5 = the house's age.
- But now suppose we add in
  x_6 = the diameter of the doorknob on the coat closet,
  x_7 = the thickness of the cutting board in the kitchen,
  x_8 = the thickness of the patio slab.

Adjusted R^2

- The objective in multiple regression is not simply to explain most of the observed y variation, but to do so using a model with relatively few predictors that are easily interpreted.
- It is thus desirable to adjust R^2 to take account of the size of the model:

$$R^2 = 1 - \frac{SSE}{SST}$$

$$R_a^2 = 1 - \frac{SSE/df_{SSE}}{SST/df_{SST}} = 1 - \frac{SSE/(n-p-1)}{SST/(n-1)}$$

adjusted

$$= 1 - \frac{SSE\,(n-1)}{SST\,(n-p-1)}$$

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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**:
  - Try all the possible combinations of features in models to see which gives the best fit.

Bad idea! Reason. 2^p diff. models.

$p=3 \rightarrow 8$ models

$p=30 \rightarrow 1,073,741,824$ 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**:

baseline. 1. fit null model with an intercept but no predictors.

baseline + 1 feature. 2. fit p-SLRs, 1 for each feature. Choose the one that gives the lowest SSE. Keep that one! e.g. ft^2

3. fit p-1 MLRs. Choose that which gives lowest SSE…

ft^2 + bathrooms, ft^2 + patio, ft^2 + dogs, ...

4. repeat.

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**:
    1. Fit model with *all* predictors
    2. Remove the one with the largest *p*-value.
    3. Fit model with p-1 predictors.
    4. Remove the one with the largest *p-value…*

Quiz

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

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

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

Forward 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 *but they are unlabeled*. I want to compute how well my model fits the data.

Use R_a^2 ← penalty for # 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:

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

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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?

CI for μ_1, CI for μ_2? non-overlapping?

t-test $H_0: \mu_1 = \mu_2$

$H_1: \mu_1 \neq \mu_2$

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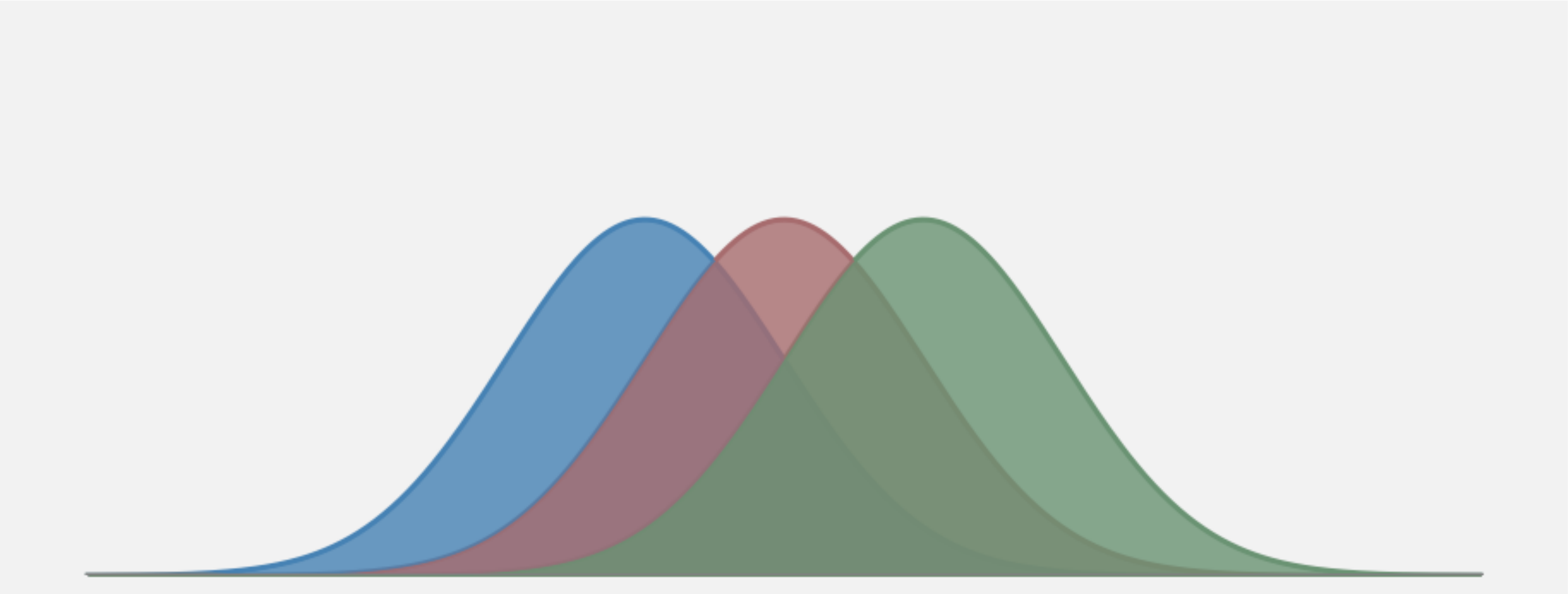
Question: Are the means of the different groups all the same?

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

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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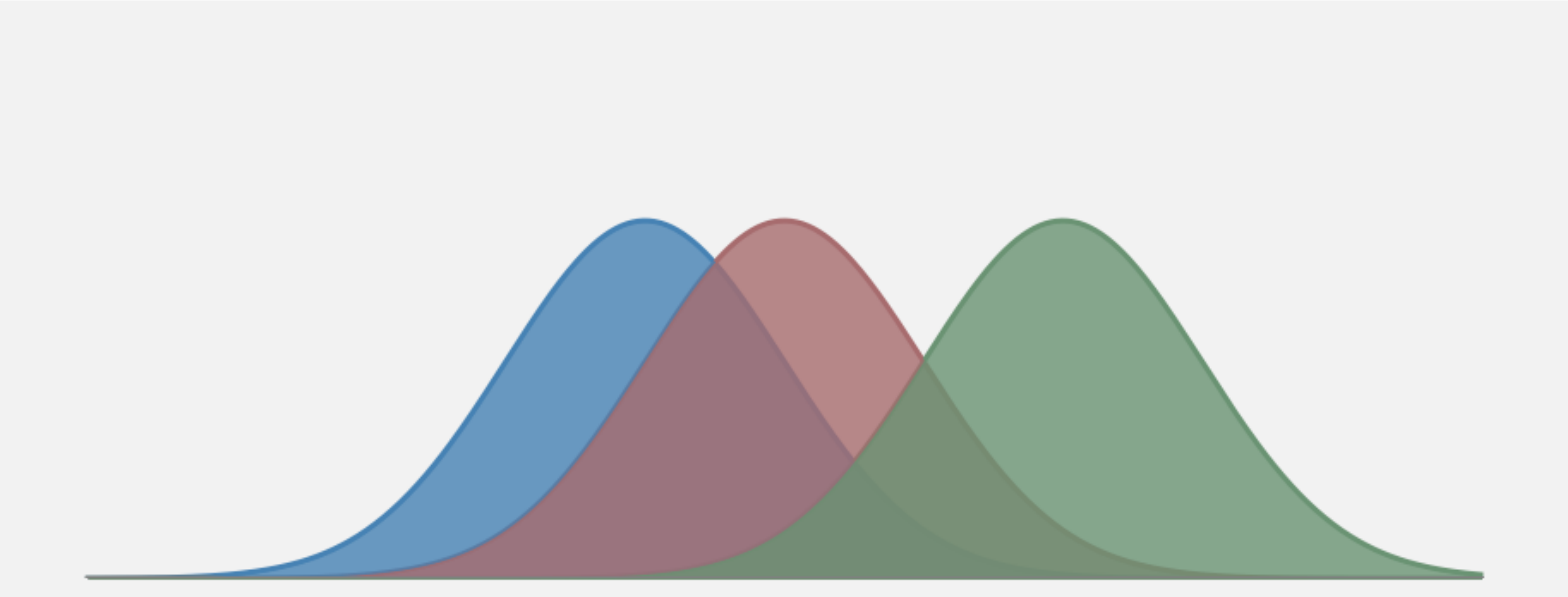

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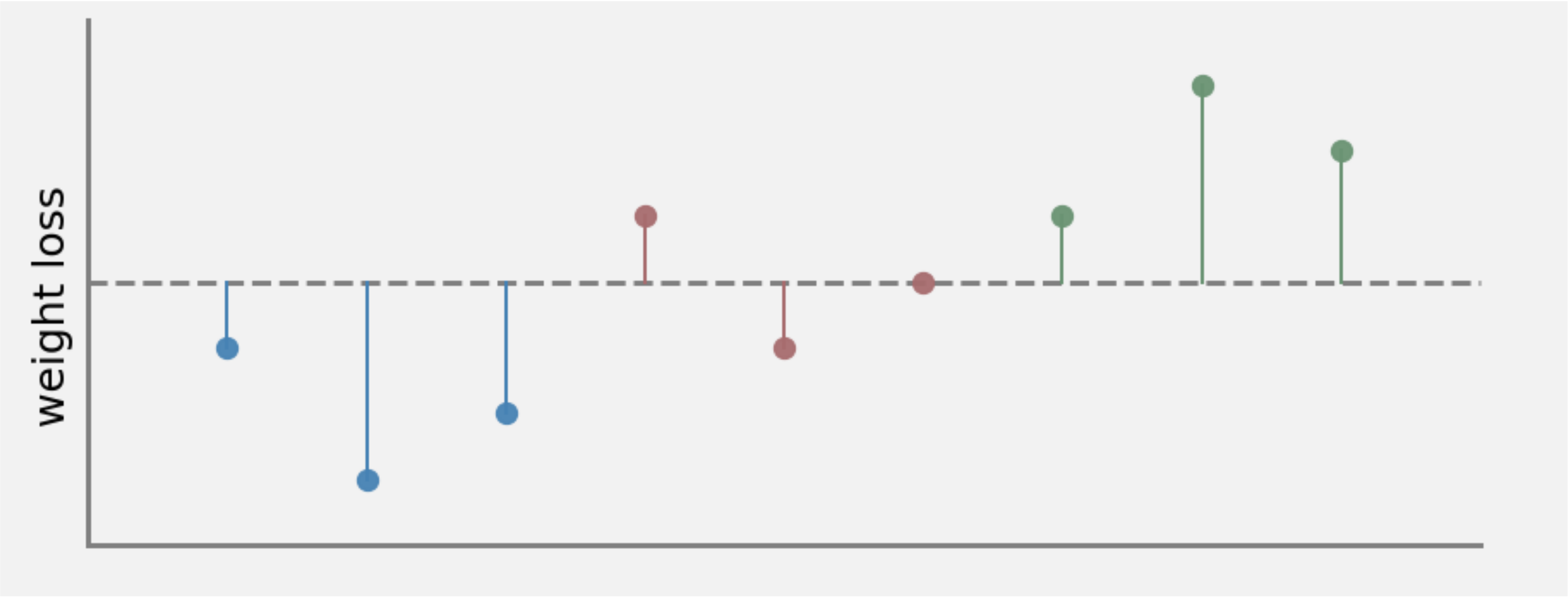

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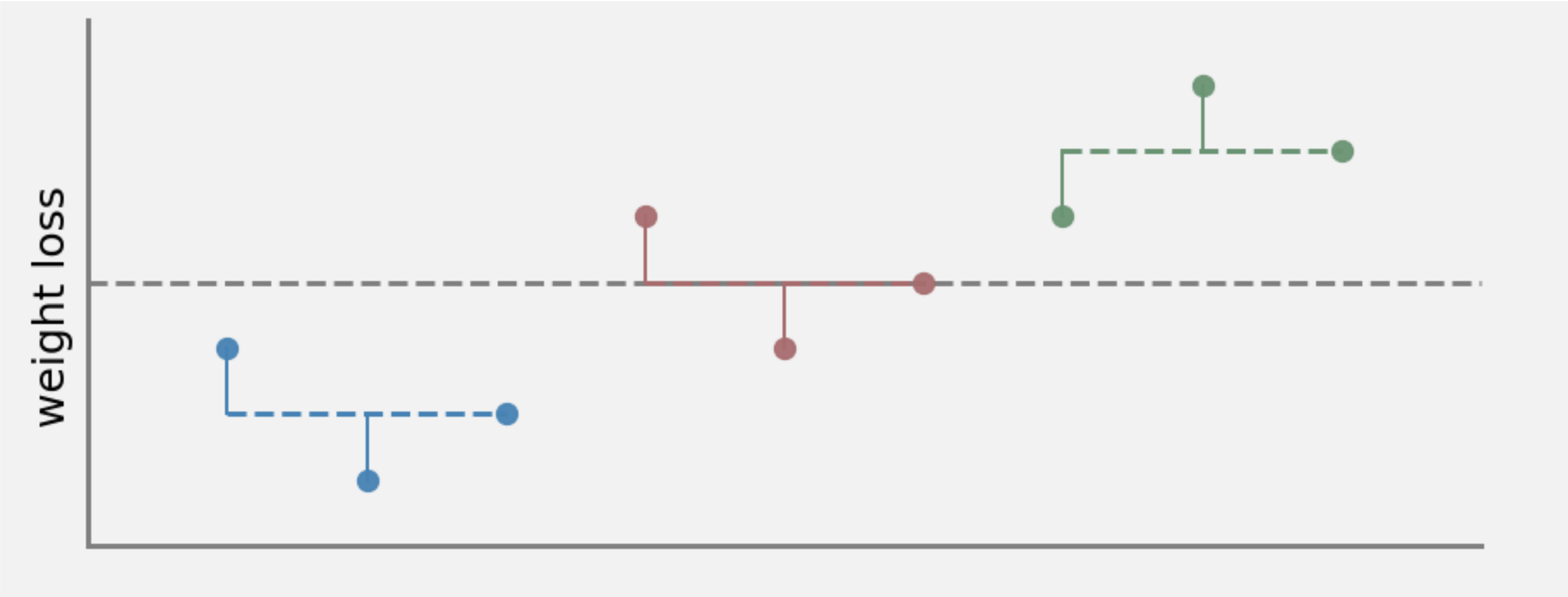

The one-way ANOVA model

- 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:

Assumptions:

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

The one-way ANOVA model

Let's compute some means!

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

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

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

It’s the variances, stupid

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

- A helpful decomposition:

- Then, a minor (mathematical) miracle occurs:

The one-way ANOVA model

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

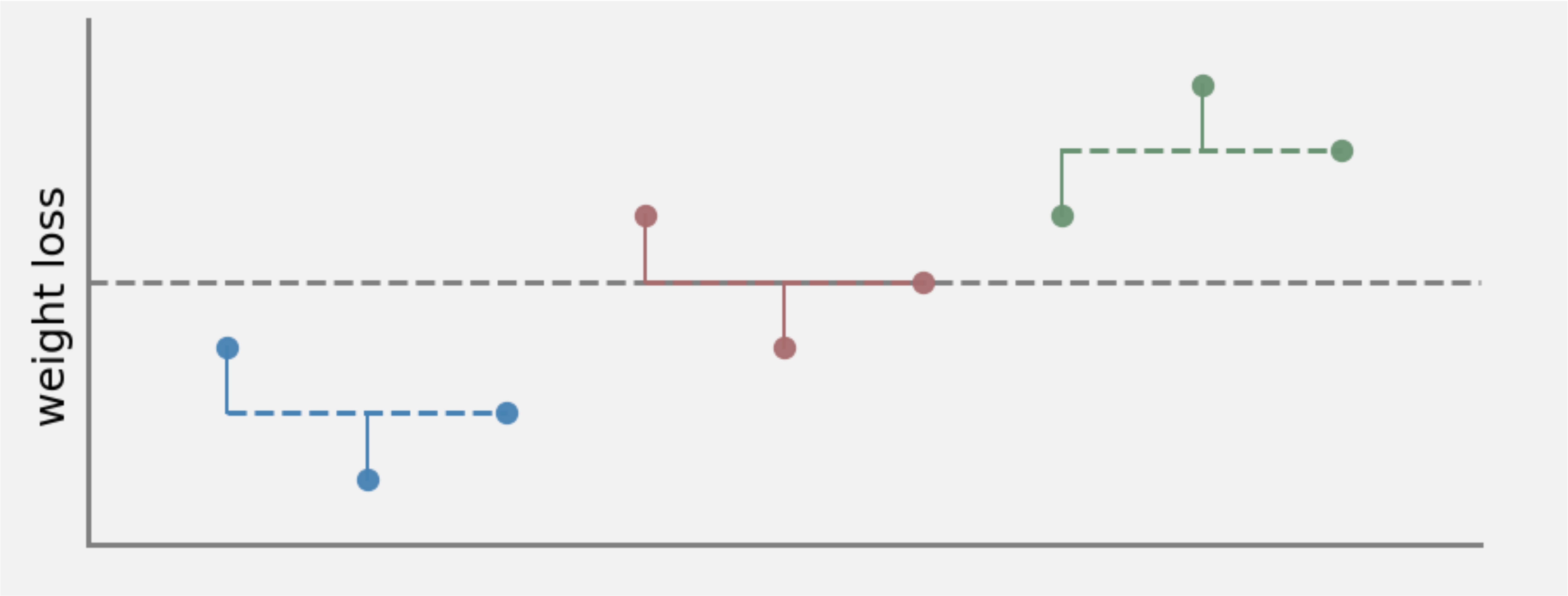
- The **BETWEEN** group sum of squares is:

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

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

The one-way ANOVA model

- Compare these results to the original picture:



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The one-way ANOVA model

What about degrees of freedom?

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

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1	2	3	6
2	1	4	7

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

A hypothesis test

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

$$H_0 \;:$$

$$H_1 \;:$$

- Our test statistic will be:

The ANOVA Table

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

	Control	Diet A	Diet B
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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

ANOVA as multiple linear regression

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- 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?