

# Visualizing Linear Models: An R Bag of Tricks Session 2: Multivariate Models

Michael Friendly SCS Short Course Oct-Nov 2021

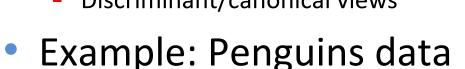
https://friendly.github.io/VisMLM-course/

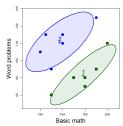
# Today's topics

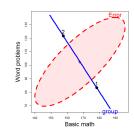
Brief review of the GLM & MLM

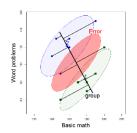
$$\mathbf{Y}_{(n \times p)} = \mathbf{X}_{(n \times q)} \mathbf{B}_{(q \times p)} + \mathcal{E}_{(n \times p)}$$

- Data ellipses
  - sufficient visual summaries
- HE plot framework
  - H & E matrices/ellipses
  - Discriminant/canonical views

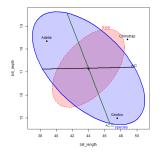


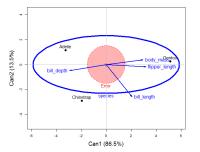






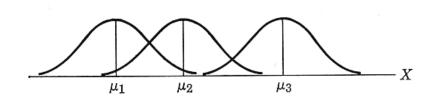






### One-way ANOVA vs. MANOVA

#### **ANOVA**



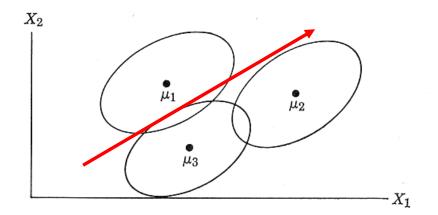
#### Do means differ?

(Assume equal withingroup variances)

Figure 8.1. The simple anova situation, when the differences among the populations are "real."

source: Cooley & Lohnes ((1971)

#### **MANOVA**



### How do centroids differ? How many dimensions?

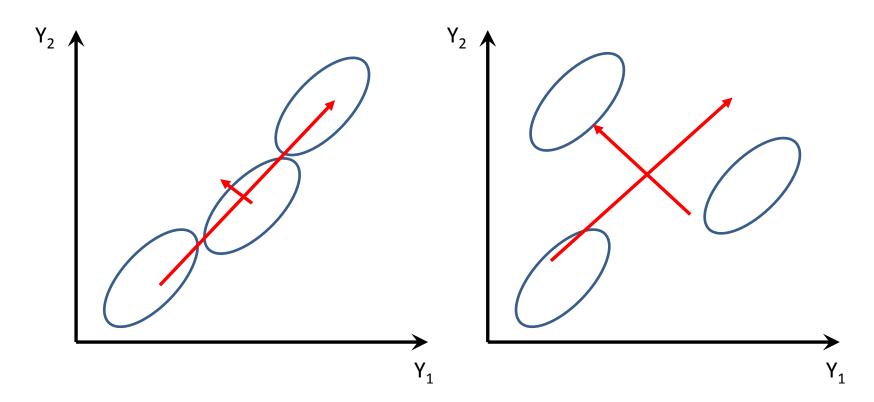
(Assume equal withingroup variance-covariance matrices)

Figure 8.2. The simple manova situation, when the differences among the populations are "real."

### Response dimensions

Means on Y<sub>1</sub> and Y<sub>2</sub> are nearly perfectly correlated

Means on Y<sub>1</sub> and Y<sub>2</sub> have a low correlation



Only 1 dimension required to understand the group effect

Two different aspects are reflected in group means

## GLM: the design matrix (X)

- In the full GLM, the design matrix (X) may consist of:
  - A constant, 1, for the intercept (usually implicit)
  - Quantitative regressors: age, income, education
  - Transformed regressors: Vage, log(income)
  - Polynomial terms: age<sup>2</sup>, age<sup>3</sup>, ...
  - Categorical predictors ("factors", class variables): treatment (control, drug A, drug B), sex
  - Interactions: treatment \* sex, age \* sex

Model formulae in R define y ~ X:

### Univariate linear model

Model

$$\mathbf{y} = \mathbf{X} \mathbf{\beta} + \boldsymbol{\epsilon}_{(n \times 1)}$$

$$\mathbf{X}_{(n\times q)} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q)$$

matrix of predictors, factors, ...

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_q x_{iq} + \epsilon_i$$

Sums of squares

data fit residuals  $SS_{\text{Tot}} = \sum_{i,j} (y_{i,j} - \overline{y}_i)^2 + \sum_{i,j} (y_{i,j} - \hat{y}_i)^2$   $= SS_H + SS_E$ 

Hypothesis tests

$$F = \frac{SS_H / df_H}{SS_E / df_E} = \frac{MS_H}{MS_E}$$

How big is hypothesis variation relative to error variation?

mean square is a variance estimate

# Regression: Visualizing $SS_T = SS_H + \overline{SS_E}$

Total variance

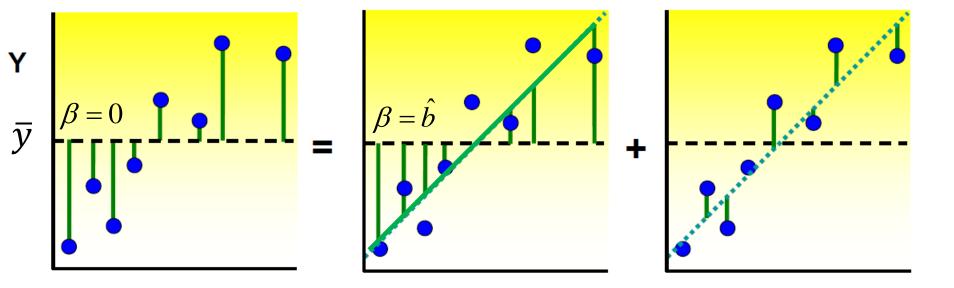
$$\sum_{i}(y_{i}-\overline{y})^{2}$$

Regression variance

$$\sum_{i} (\hat{y}_{i} - \overline{y})^{2}$$

+ Residual variance

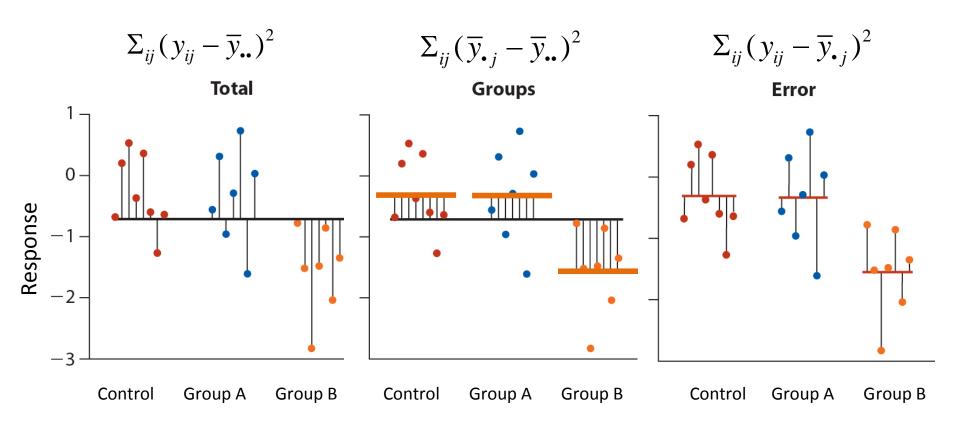
$$\sum_{i}(y_{i}-\hat{y}_{i})^{2}$$



F test: How much better is the fitted regression line ( $\beta = \beta$ ) than the flat line ( $\beta = 0$ )?

# ANOVA: Visualizing $SS_T = SS_H + \overline{SS_F}$

Total variance = Between group variance + Within group variance



F test: How much better is the groups model than the model ignoring groups?

### Multivariate linear model

Model

$$\mathbf{Y} = \mathbf{X} \mathbf{B} + \mathcal{E}_{(n \times p)}$$

$$\mathbf{Y}_{(n \times p)} = (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_p)$$

matrix of *p* responses

Sums of squares & cross-products

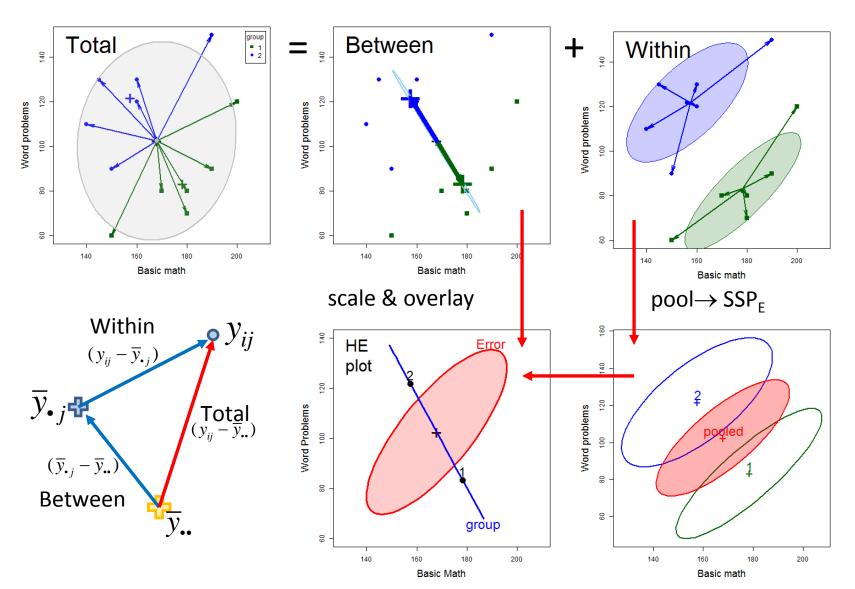
$$\begin{aligned} \mathbf{SSP}_{T} &= \left(\hat{\mathbf{Y}}'\hat{\mathbf{Y}} - n\overline{\mathbf{y}}\overline{\mathbf{y}}'\right) + \mathcal{E}'\mathcal{E} \\ &= \mathbf{SSP}_{H} + \mathbf{SSP}_{E} = \mathbf{H} + \mathbf{E} \end{aligned}$$

- Hypothesis tests
  - Eigenvalues  $\lambda_i$ , i=1:p of H E<sup>-1</sup>
  - Wilks' Λ, Pillai & Hotelling trace, Roy's test
  - how many dimensions (aspects of responses)?

How big is hypothesis variation relative to error variation?

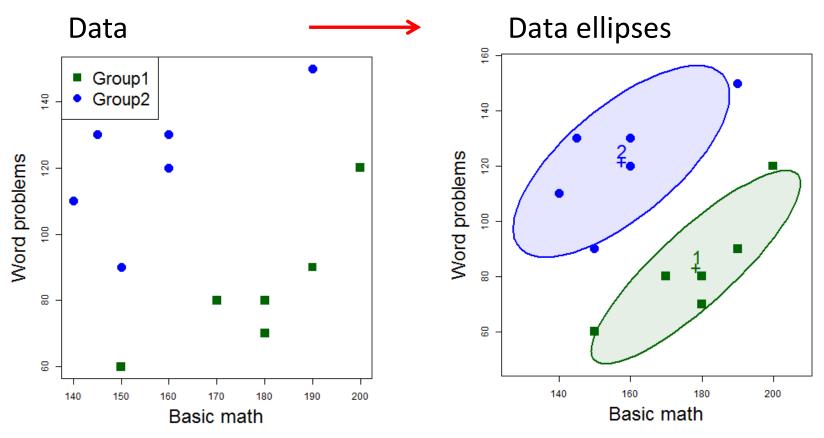
Ah, but there are up to  $s = min(p, df_h)$  dimensions of size

# Visualizing $SSP_T = SSP_H + SSP_E$



### Data ellipsoids

The data ellipsoid is a sufficient visual summary for multivariate location & scatter, just as  $(\bar{y}, S)$  are sufficient for  $(\mu, \Sigma)$ 



### Data ellipsoids: definitions

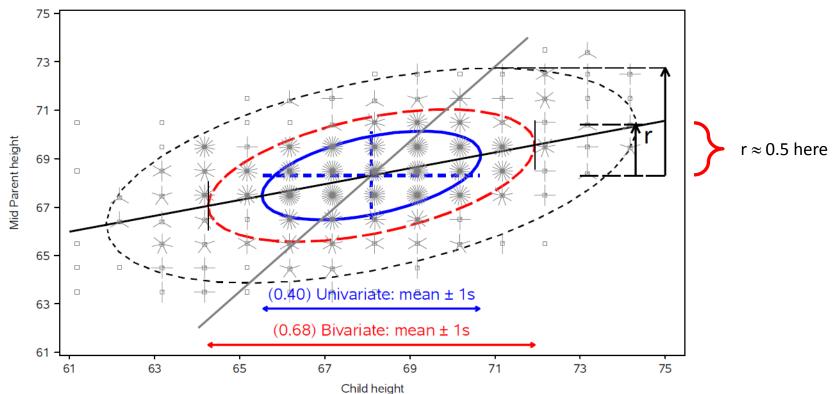
- For a p-dimensional multivariate sample,  $\mathbf{Y}_{N\times p}$ , the sample mean vector,  $\overline{\mathbf{y}}$ , and sample covariance matrix,  $\mathbf{S}$ , are minimally sufficient statistics under classical (gaussian) assumptions.
- These can be represented visually by the p-dimensional data ellipsoid,  $\mathcal{E}_c$  of size ("radius") c centered at  $\overline{y}$ ,

$$\mathcal{E}_c(\overline{\mathbf{y}},\mathbf{S}) := \{\mathbf{y} : (\mathbf{y} - \overline{\mathbf{y}})^T \mathbf{S}^{-1} (\mathbf{y} - \overline{\mathbf{y}}) \le c^2 \}$$
 or,  $D_M^2(\mathbf{y}) \le c^2$ 

- → an ellipsoid centered at the means whose size & shape reflects variances & covariances
- We consider this a minimally sufficient visual summary of multivariate location and scatter.

## Data ellipsoids: properties

- Ellipsoid boundary: Mahalanobis  $D_M^2(y_i) \sim \chi_p^2$ 
  - p=2: shadows generalize univariate confidence intervals
  - eccentricity: precision; visual estimate of correlation



# The HE plot framework

- Hypothesis-Error (HE) plots
  - Visualize multivariate tests in the MLM
  - Linear hypotheses--- lower-dimensional ellipsoids
  - Extension: HE plot matrices
- Canonical displays
  - low-dimensional multivariate juicers
  - shows data in the space of maximal effects
- Covariance ellipsoids
  - visualize tests of homogeneity of covariance matrices
- For all: robust methods are available or good research projects!

## HE plot framework: Trivial example

Two groups of middle-school students are taught algebra by instructors using different methods, and then tested on:

- **BM**: basic math problems (7 \* 23 2 \* 9 = ?)
- WP: word problems ("a train travels at 23 mph for 7 hours, but for 2 hours ...")

Do the groups differ on (BM, WP) by a multivariate test? If so, how ???

### Follow along

The R script (mathscore-ex.R) for this example is linked on the course page. Download and open in R Studio to follow along.

Examples: 
 Math scores: Simple demo of MLMs mathscore-simple.R
 Math scores: HE plot examples mathscore-ex.R || mathscore-ex.html
 Penguins data: Multivariate EDA vignette
 Diabetes data: heplots and candisc examples vignette

HW: explore other examples

The script was run with `knitr` (ctrl+shift+K) in R Studio to create the HTML output (mathscore-ex.html)

The Code button there allows you do download the R code and comments



(R notebooks are a simple way to turn R scripts into finished documents)

### Why do multivariate tests?

Could do univariate ANOVAs (or t-tests) on each response variable (BM, WP)

#### From this, might conclude that:

- Groups don't differ on Basic Math score \*
- Groups are significantly different on Word problems ✓

#### Multivariate tests:

- Do not require correcting for multiple tests (e.g., Bonferroni)
- Combine evidence from multiple response variables ("pooling strength")
- Show how the multivariate responses are jointly related to the predictors
  - How many aspects (dimensions?)

### Why do multivariate tests?

#### Overall test is highly significant:

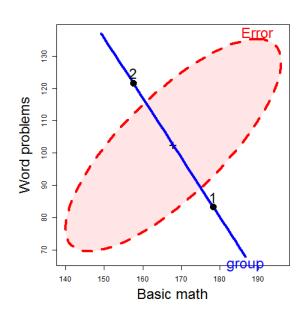
- Combines the evidence for all predictors
- Takes response correlations into account

#### Visual test of significance (Roy's test)

 The H ellipse projects outside the E ellipse iff the effect is significant.

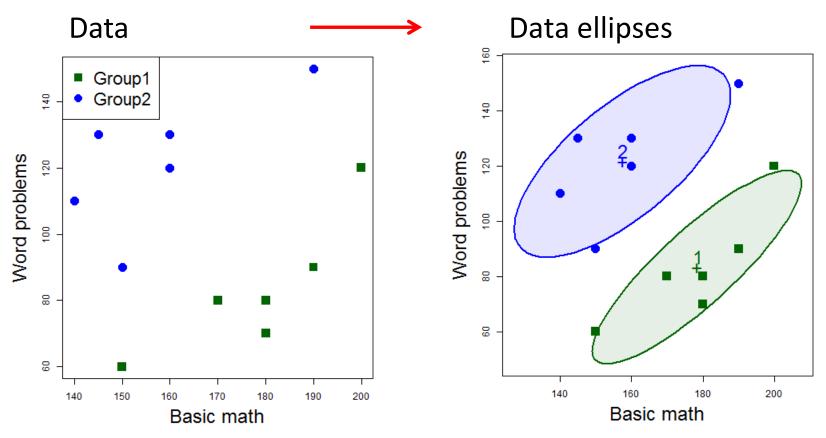
#### HE plot provides an interpretation:

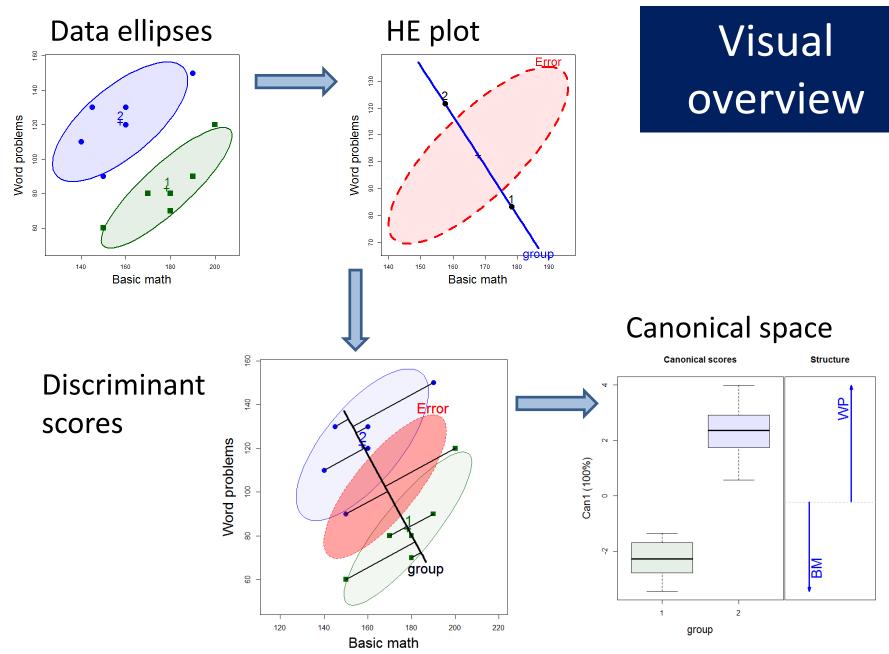
- Group 1 > Group 2 on Basic Math, but worse on Word Problems
- Group 2 > Group 1 on Word Problems, but worse on Basic Math
- BM & WP are + correlated w/in groups



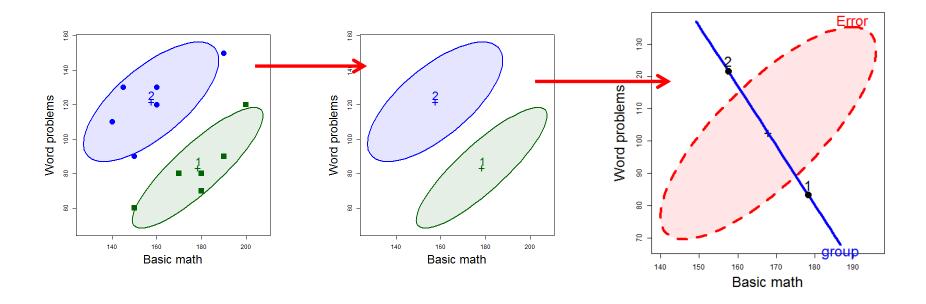
### HE plot framework: Visual overview

The data ellipsoid is a sufficient visual summary for multivariate location & scatter, just as  $(\bar{y}, S)$  are sufficient for  $(\mu, \Sigma)$ 



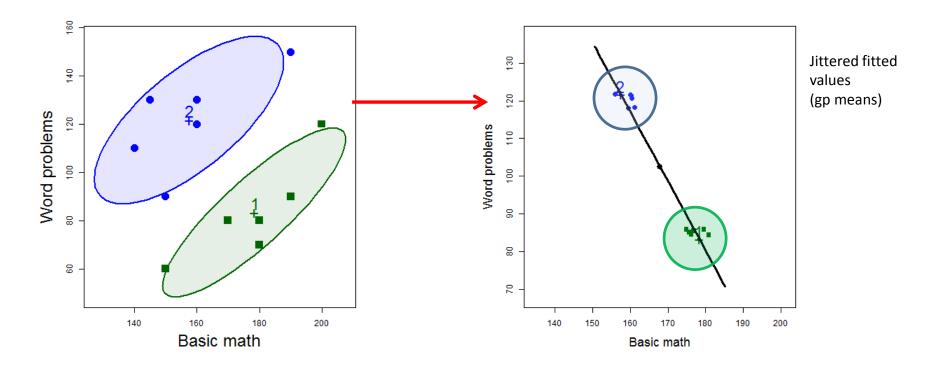


### Data $\rightarrow$ Data ellipses $\rightarrow$ HE plot



- Differences between group means are shown by the H ellipsoid—data ellipsoid
  of the fitted values (w/ 1 df, degenerates to a line)
  - Direction shows relation of groups to response variables
  - Size shows "how big is H relative to E"
- Variation within groups is reflected in the E ellipsoid-- data ellipsoid of the residuals
  - Direction: residual (partial) correlation between BM & WP
  - Size/shape: residual variance

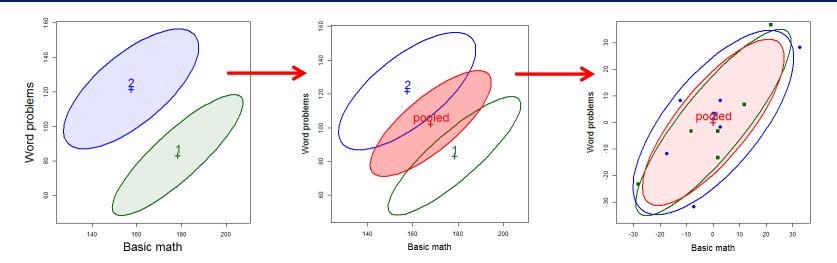
### The H ellipse



- The H ellipse is the data ellipse of the fitted values (group means, here)
  - The H matrix is the sum of squares and crossproducts of the fitted values, corrected for the grand mean

$$\mathbf{H} = \left(\hat{\mathbf{Y}}'\hat{\mathbf{Y}} - n\overline{\mathbf{y}}\overline{\mathbf{y}}'\right)$$

### The E ellipse



- The **E** ellipse is the data ellipse of the residuals
  - What you get when you subtract the group means from all observations, shifting them to the grand means.
  - E matrix called the "within-group pooled covariance matrix"

$$\mathbf{E} = (\hat{\mathbf{Y}} - \overline{\mathbf{Y}})'(\hat{\mathbf{Y}} - \overline{\mathbf{Y}}) = \mathcal{E}'\mathcal{E}$$

### H & E in numbers

The **H** and **E** matrices are calculated in the car::Anova() function and saved as the SSP and SSPE components, used in the statistical tests.

```
Direct calculation: \mathbf{H} = (\hat{\mathbf{Y}}'\hat{\mathbf{Y}} - n\overline{\mathbf{y}}\overline{\mathbf{y}}')
```

```
> fit
BM WP
1 178.33 83.333
2 178.33 83.333
3 178.33 83.333
4 178.33 83.333
5 178.33 83.333
6 178.33 83.333
7 157.50 121.667
8 157.50 121.667
9 157.50 121.667
10 157.50 121.667
11 157.50 121.667
12 157.50 121.667
```

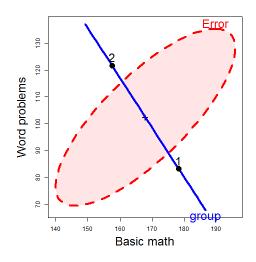
### H & E in numbers

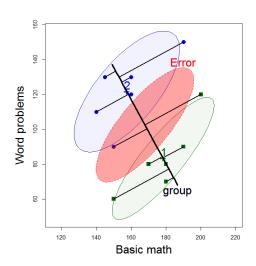
```
> (E <- math.aov$SSPE)
BM WP
BM 3070.8 2808.3
WP 2808.3 4216.7
```

Direct calculation:  $\mathbf{E} = (\hat{\mathbf{Y}} - \overline{\mathbf{Y}})'(\hat{\mathbf{Y}} - \overline{\mathbf{Y}}) = \mathcal{E}'\mathcal{E}$ 

### Discriminant analysis

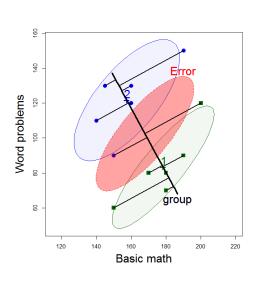
- MANOVA and linear discriminant analysis (LDA) are intimately related and differ mainly in perspective:
  - MANOVA: Do means of groups on 2+ responses differ?
  - LDA: Find weighted sums of responses that best discriminate groups
- In both cases,
  - Group differences are represented by the H matrix; residuals: E matrix
  - Test statistics based on eigenvalues of HE<sup>-1</sup>
  - Discriminant weights are eigenvectors of HE<sup>-1</sup>





### Discriminant analysis

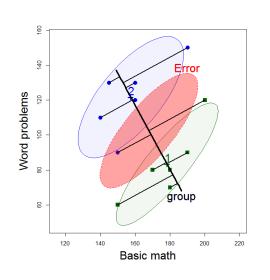
- For 2 groups,
  - the discriminant axis is the line joining the two group centroids,
  - discriminant scores are the projections of observations on this line.
- MASS:Ida() does this analysis

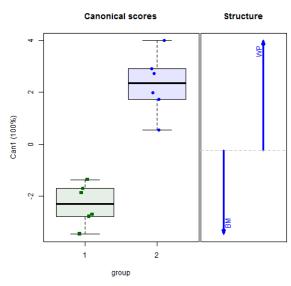


The canonical dimension is Can1 = 0.075 WP - 0.083 BM, a contrast between the two tests

### Canonical space

- The HE plot view shows the data in data space
- Easier to see effects by projecting scores to canonical space –
   the best-discriminating axes.
- For a 1 df effect, there is only one canonical dimension
  - Arrows show the relative size & direction of discriminant weights





library(candisc)
mod.can <- candisc(math.mod)
plot(mod.can)</pre>

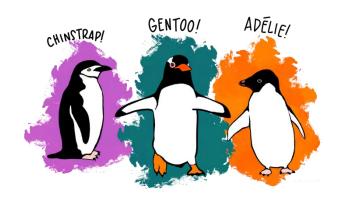
### Penguin data

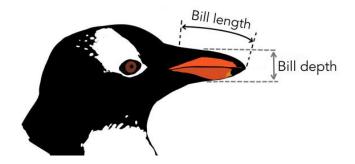
Data on 3 species of penguins, measured on 3 Antarctic islands



How does penguin "size" differ by species, island, ...?

```
> library(palmerpengiuns)
> peng <- penguins %>% rename(...) %>% ... # clean up names, etc.
> peng[sample(1:333, 5), ]
# A tibble: 5 x 8
  species island
                     bill_length bill_depth flipper_length body_mass sex
                                                                             year
 <fct>
           <fct>
                            <dbl>
                                       <dbl>
                                                      <int>
                                                                <int> <fct> <int>
                                        17.8
                                                                 3700 f
1 Chinstrap Dream
                             58
                                                        181
                                                                             2007
2 Adelie Torgersen
                             39.6
                                        17.2
                                                        196
                                                                 3550 f
                                                                             2008
                                        14.1
                                                                 4375 f
3 Gentoo
           Biscoe
                             46.2
                                                        217
                                                                             2009
4 Chinstrap Dream
                             49
                                        19.5
                                                        210
                                                                 3950 m
                                                                             2008
                             50.4
                                        15.7
                                                        222
                                                                             2009
5 Gentoo
            Biscoe
                                                                 5750 m
```

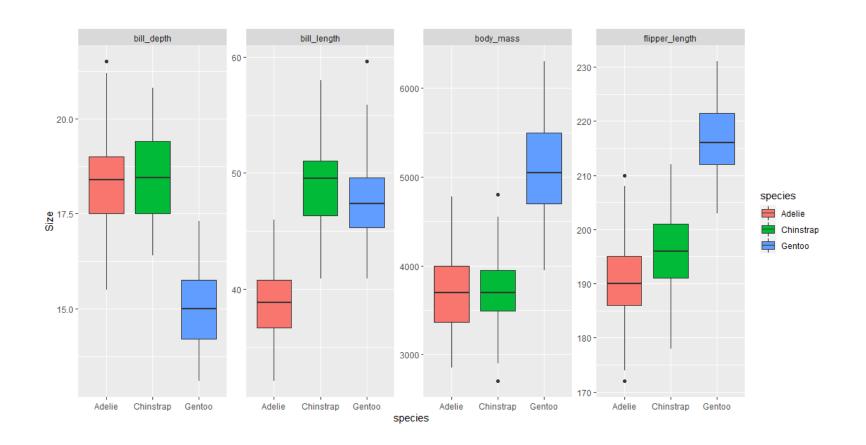




# Penguins: Multivariate EDA

Boxplots by grouping variables (factors) are often useful for an initial overview

- Can show multiple variables, but hard for >1 factor.
- What is the pattern here?



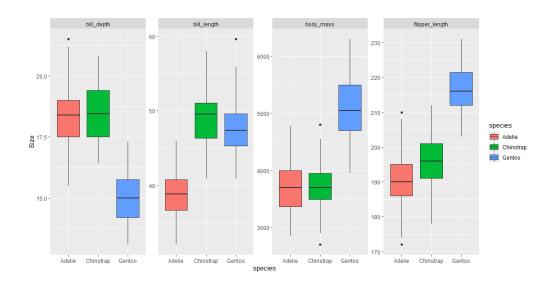
### Penguins: Multivariate EDA

Boxplots by grouping variables (factors) are often useful for an initial overview

Need to reshape data from wide to long format

```
peng_long <- peng %>%
  tidyr::gather(Measure, Size, bill_length:body_mass)

ggplot(peng_long, aes(x=species, y=Size, fill=species)) +
  geom_boxplot() +
  facet_wrap(. ~ Measure, scales="free_y", nrow=1)
```



### PCA & Biplots

- For multivariate data, often want to view the data in a low-D space that shows the most total variance
- PCA: finds weighted sums of variables which are:
  - Uncorrelated
  - Account for maximum variance
  - How many dimensions are necessary?
- A biplot is a 2D (or 3D) plot of the largest PCA dimensions
  - Vectors in this plot show the original data variables
  - Points in this plot show the observations
    - Data ellipses here show within group relations

### **PCA** animation

#### PCA:

- PC1 is the direction along which points have max. variance
- Equivalently, the perp. deviations from the line have min. residual SS

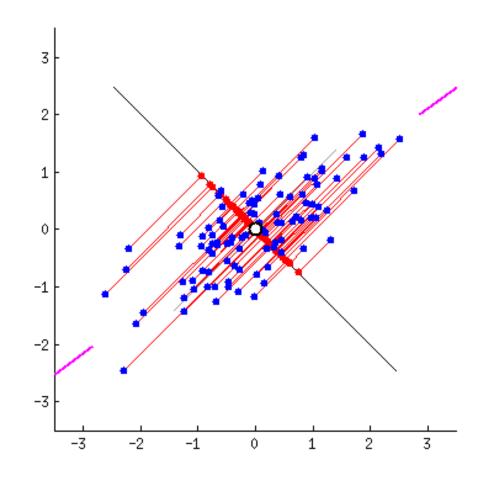
### PCA by springs

- Imagine each pt connected to a possible PC1 line by springs
- Force ~ deviation<sup>2</sup>

Forces balance, naturally seek the min. residual SS position.

#### Voila, QED!

A visual proof

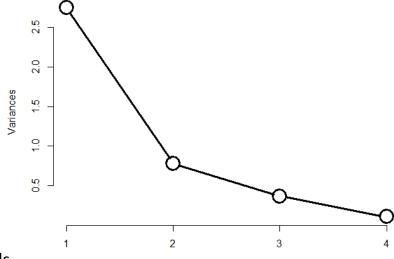


### **PCA**

#### 

2D: 88.1 % 3D: 97.3 %

#### Variances of PCA Components



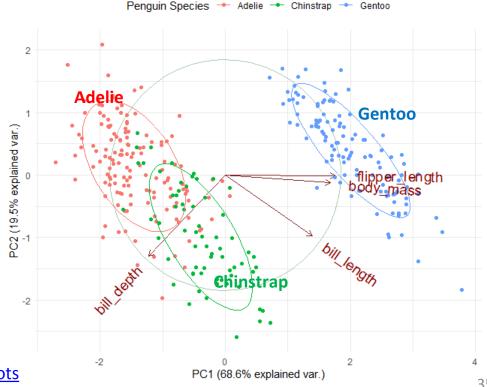
See: https://rpubs.com/friendly/penguin-biplots for details

## Biplot

PC1, PC2 ~ 88.1% of variance

- PC1: largely flipper length & body mass: "penguin size"
- PC2 (& PC1): relates to "bill shape"

Easy to characterize the species in terms of these variables



See: https://rpubs.com/friendly/penguin-biplots

### Penguins: MANOVA

Assume the goal is to determine whether/how the penguins differ in size by species

- A MLM tests all 4 size variables together: ~ species
- Could also use other factors: ~ species + island + sex

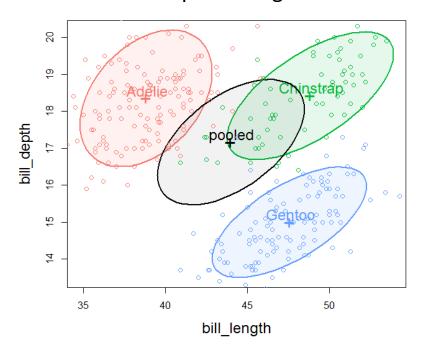
Yet, we are left to understand the nature of this effect wrt. the size variables.

See: <a href="https://rpubs.com/friendly/penguin-manova">https://rpubs.com/friendly/penguin-manova</a> for details

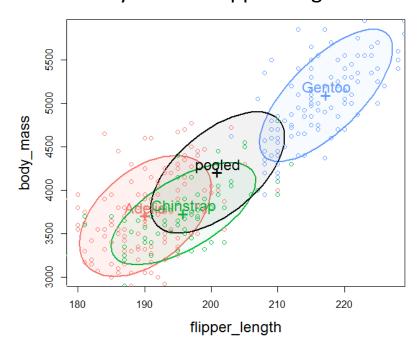
## Penguins: view data ellipses

Data ellipses in 2D provide a good start for pairwise relations

#### bill depth & length



#### body mass & flipper length

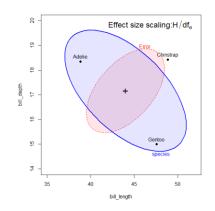


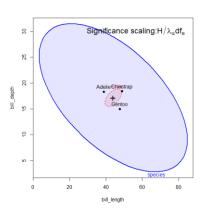
- group means negatively correlated
- within group correlation > 0

- group means positively correlated
- within group correlation > 0

# HE plot details

- E ellipse reflects within-group error (co)variation
  - Size: **E** / df<sub>e</sub> set to cover 68%, an analog of  $\overline{y} \pm 1$  std
  - Shift to grand mean for direct comparison with H
- H ellipse reflects (co)variation of group means
  - effect size scaling, uses H/df<sub>e</sub> to put this on the same scale as the E ellipse.
     Analog of effect size in univariate designs.
  - **significance** ("evidence") scaling: uses  $H/\lambda_{\alpha}$  df<sub>e</sub>.
    - The **H** ellipse protrudes outside the **E** ellipse somewhere, *iff* an effect is significant (Roy's largest root test) at  $p < \alpha$

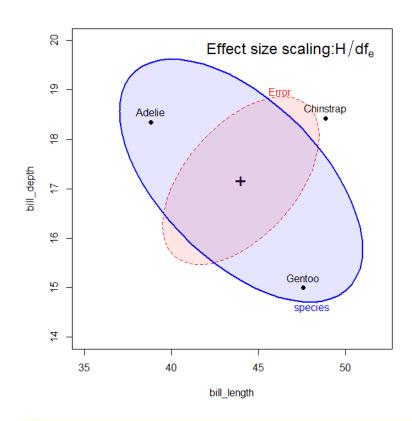


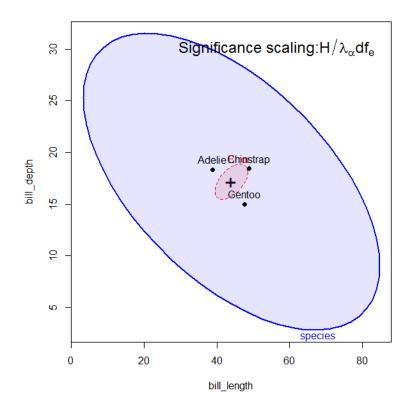


# Penguins: HE plots

Orientation of the **H** ellipse reflects negative correlation of the species means: species with larger bill depth have smaller bill length (bill "shape"?)

**E** ellipse: within species, larger bill length  $\rightarrow$  larger bill depth





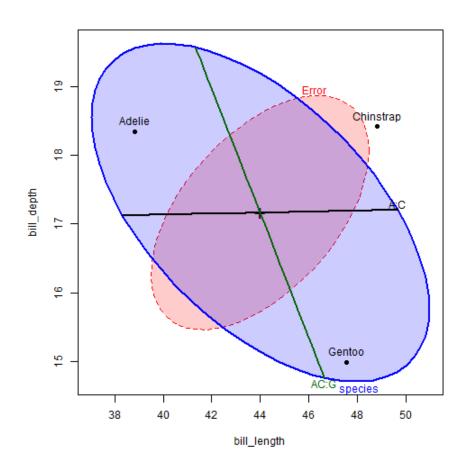
heplot(peng.mod0, size="effect")

heplot(peng.mod0, size="evidence")

### Contrasts

- In linear models, any effect of df<sub>h</sub> > 1 can be partitioned into df<sub>h</sub> separate 1 df tests of contrasts
  - If orthogonal, **H** = **H**<sub>1</sub> + **H**<sub>2</sub> + ... **H**<sub>dfh</sub> -- accounts for total effect
  - Tested as a linear hypothesis, e.g.,  $x_1 (x_2 + x_3)/2 = 0$
  - Each H<sub>i</sub> has rank=1, so appears as a line in HE plots
- Assume we want to compare the species as two contrasts:
  - Do Adelie differ from Chinstrap?
  - Do Gentoo penguins differ from the other two?

### Contrasts



#### Result is very clear:

- Adelie & Chinstrap differ only in bill length
- Gentoo differ from other two –
   longer, but less deep bills (bill shape)

Both of these are large effects!

Together, they are the entire species effect!

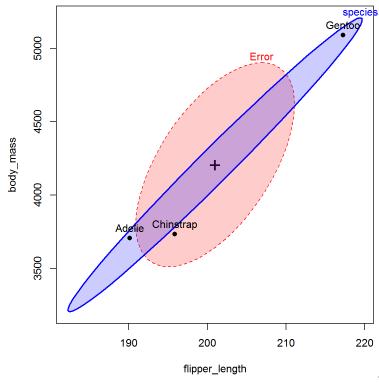
# Other HE plots

- 2D: can plot any pair of responses in data space
- pairs.mlm(): all pairwise 2D views
- heplot3d(): plots in 3D, can rotate, spin, zoom, ...

heplot(peng.mod0, variables=3:4, fill=TRUE, fill.alpha=0.2, size="effect")

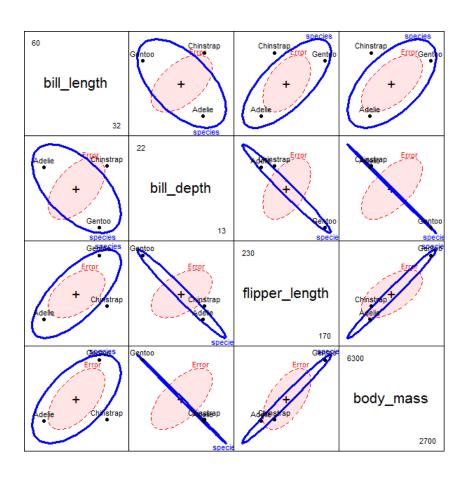
#### Interpretation:

- major axis of the H ellipse measures "penguin size"
- Gentoo are the Big Birds in this story!



# **HE Pairs plots**

The pairs() method for mlm objects gives all pairwise HE plots in a scatterplot matrix format.



#### Something new here:

- avg. bill depth is negatively correlated with "size" variables – larger penguin species have smaller bill depths (curvature?)
- correlation of avg. bill depth with body mass nearly -1

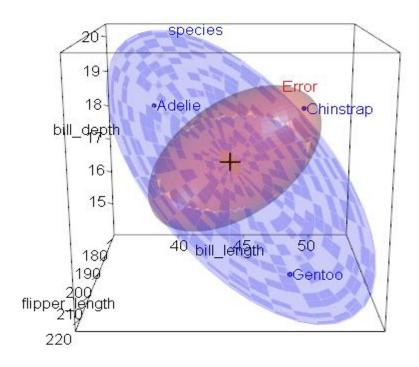
# heplot3d()

3D HE plots can show other features

heplot3d(peng.mod0, size="effect")

The H ellipsoid here is flat (2D), because the species effect has 2 df

In this 3D view, the 3 species form a triangle, suggesting some further interpretation, not seen in 2D views



### Canonical view

- 4 response variables, but only s=min(q, dfh)=2 dimensions.
  - Here, both dimensions are significant
  - Can1 accounts for 86.5% of between-species variance
  - Can 2 accounts for the rest: 13.5%

```
> library(candisc)
> (peng.can <- candisc(peng.mod0))</pre>
Canonical Discriminant Analysis for species:
 CanRsq Eigenvalue Difference Percent Cumulative
1 0.938
             15.03
                          12.7
                                  86.5
                                            86.5
2 0.700
              2.34
                         12.7
                                 13.5
                                           100.0
Test of HO: The canonical correlations in the
current row and all that follow are zero
 LR test stat approx F numDF denDF Pr(> F)
       0.0187
                    516
                               654 <2e-16 ***
       0.2997
                   255 3
                               328 <2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

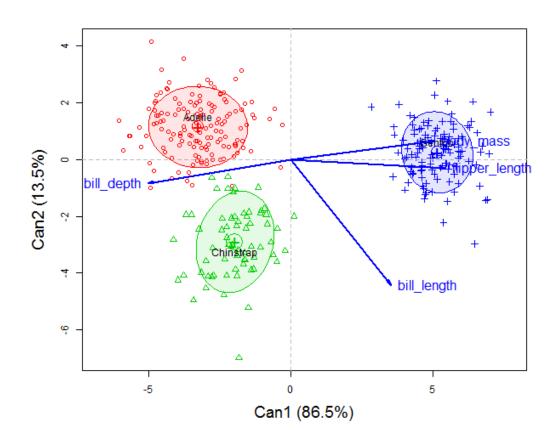
### Canonical view

The plot() method for candisc objects shows points for observations and vector for variables

```
plot(peng.can, ellipse = TRUE ... ) #plot CAN scores with ellipses
```

Can1: largely body mass & flipper length, that separate Gentoo from (Adelie, Chinstrap)

Can2: bill length distinguishes Chinstrap from others.



### Canonical HE plot

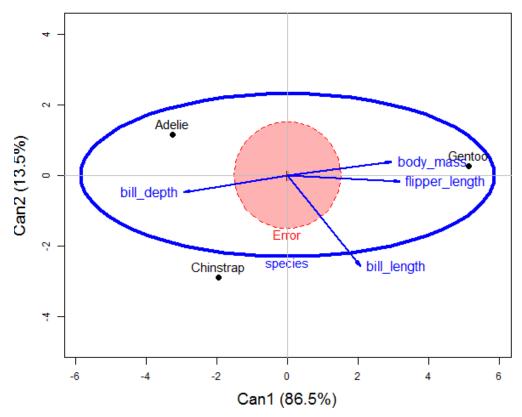
heplot(peng.can, size="effect", fill=c(TRUE, FALSE))

Here is the entire effect of species shown in one HE plot

In CAN space, residuals are uncorrelated: **E** = circle

Size of **H** shows the total effect of species

Variable vectors show how the groups are discriminated.



### Summary

- MLM just like univariate LM, but for multiple responses
  - Simultaneous tests no need for p-value adjustment
  - Take correlations among responses into account
  - Indicates # of dimensions of responses
- Data ellipses
  - Summarize bivariate data to show means, variances, correlation
  - MANOVA: shows how groups differ in these
- HE framework
  - Visualize multivariate tests in the MLM
  - Canonical displays show these results in the 2D (or 3D) space that accounts for largest between-group variance.