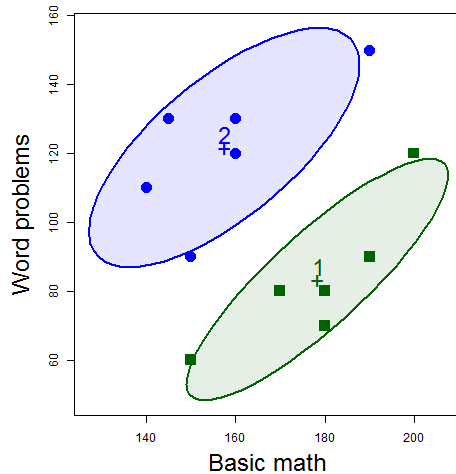
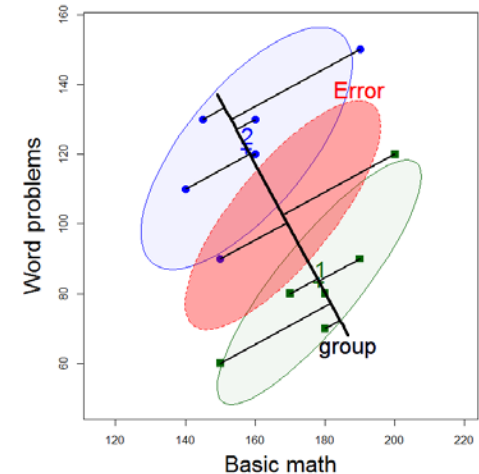
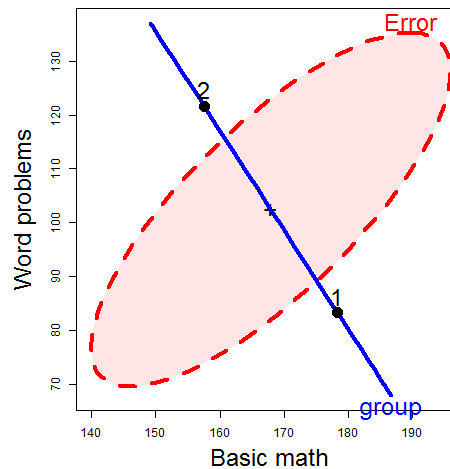


Data ellipses



HE plot



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

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SCS Short Course  
Oct. 2020

# Today's topics

- Brief review of the GLM & MLM

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

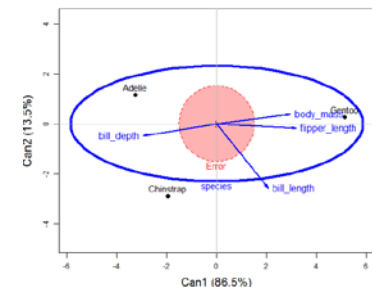
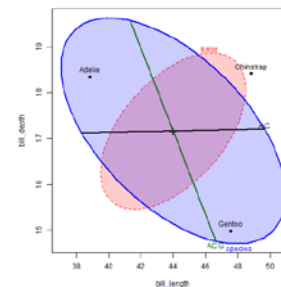
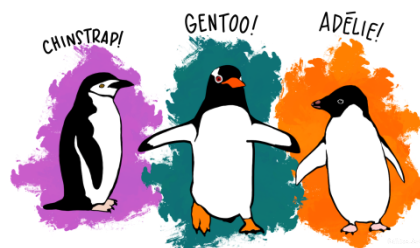
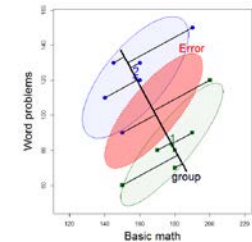
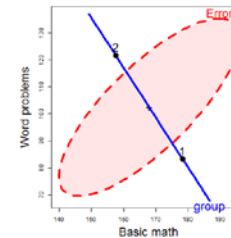
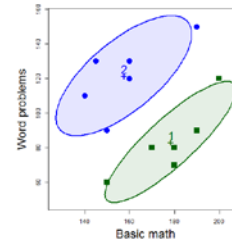
- Data ellipses

- sufficient visual summaries

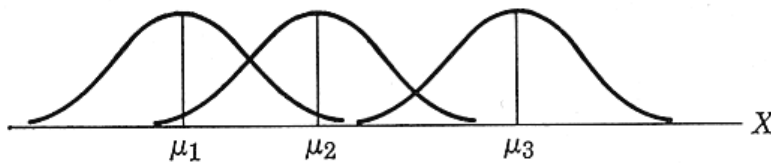
- HE plot framework

- H & E matrices/ellipses
- Discriminant/canonical views

- Example: Penguins data



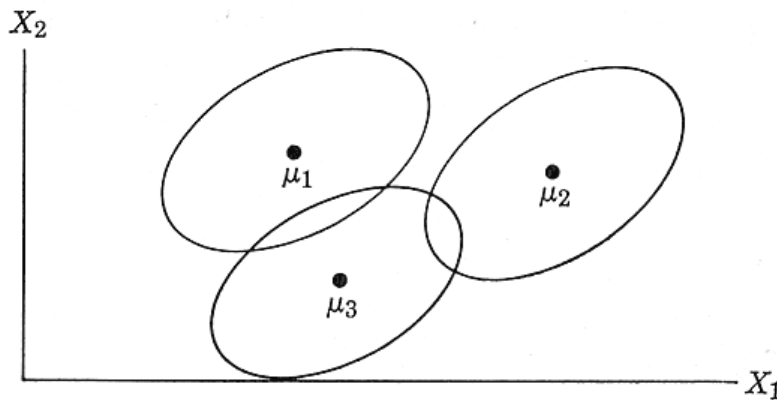
# One-way ANOVA vs. MANOVA



**How do means differ?**  
(Assume equal within-group variances)

**Figure 8.1.** The simple anova situation, when the differences among the populations are “real.”

source: Cooley & Lohnes ((1971)



**How do centroids differ?**  
**How many dimensions?**

(Assume equal within-group variance-covariance matrices)

**Figure 8.2.** The simple manova situation, when the differences among the populations are “real.”

# 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:  $\sqrt{\text{age}}$ ,  $\log(\text{income})$
  - Polynomial terms:  $\text{age}^2$ ,  $\text{age}^3$ , ...
  - Categorical predictors (“factors”, class variables): treatment (control, drug A, drug B), sex
  - Interactions:  $\text{treatment} * \text{sex}$ ,  $\text{age} * \text{sex}$

Model formulae in R define y & X:

```
prestige ~ income + education           # 2 main effects
prestige ~ income * education           # interaction
prestige ~ income + education + women + type # 4 main effects
prestige ~ education + poly(women, 2) + log(income)*type
```

# Univariate linear model

- Model  $\underset{(n \times 1)}{\mathbf{y}} = \underset{(n \times q)}{\mathbf{X}} \underset{(1 \times q)}{\boldsymbol{\beta}} + \underset{(n \times 1)}{\boldsymbol{\epsilon}}$   $\underset{(n \times q)}{\mathbf{X}} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q)$   
matrix of predictors, factors, ...

- Sums of squares

$$\begin{aligned} SS_{\text{Tot}} &= \sum_{i,j} (\hat{y}_{i,j} - \bar{y}_i)^2 + \sum_{i,j} (y_{i,j} - \hat{y}_{i,j})^2 \\ &= SS_H + SS_E \end{aligned}$$

- 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?

# Multivariate linear model

- Model 
$$\underset{(n \times p)}{\mathbf{Y}} = \underset{(n \times q)}{\mathbf{X}} \underset{(q \times p)}{\mathbf{B}} + \underset{(n \times p)}{\mathcal{E}}$$
 
$$\underset{(n \times p)}{\mathbf{Y}} = (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_p)$$
  
matrix of  $p$  responses

- Sums of squares & cross-products

$$\underset{(p \times p)}{\mathbf{SSP}_T} = \left( \hat{\mathbf{Y}}' \hat{\mathbf{Y}} - n \overline{\mathbf{y}} \overline{\mathbf{y}}' \right) + \hat{\mathcal{E}}' \hat{\mathcal{E}}$$

$$= \mathbf{SSP}_H + \mathbf{SSP}_E = \mathbf{H} + \mathbf{E}$$

- Hypothesis tests

- Eigenvalues  $\lambda_i, i=1:p$  of  $\mathbf{H} \mathbf{E}^{-1}$
- Wilks'  $\Lambda$ , 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

# Data ellipsoids

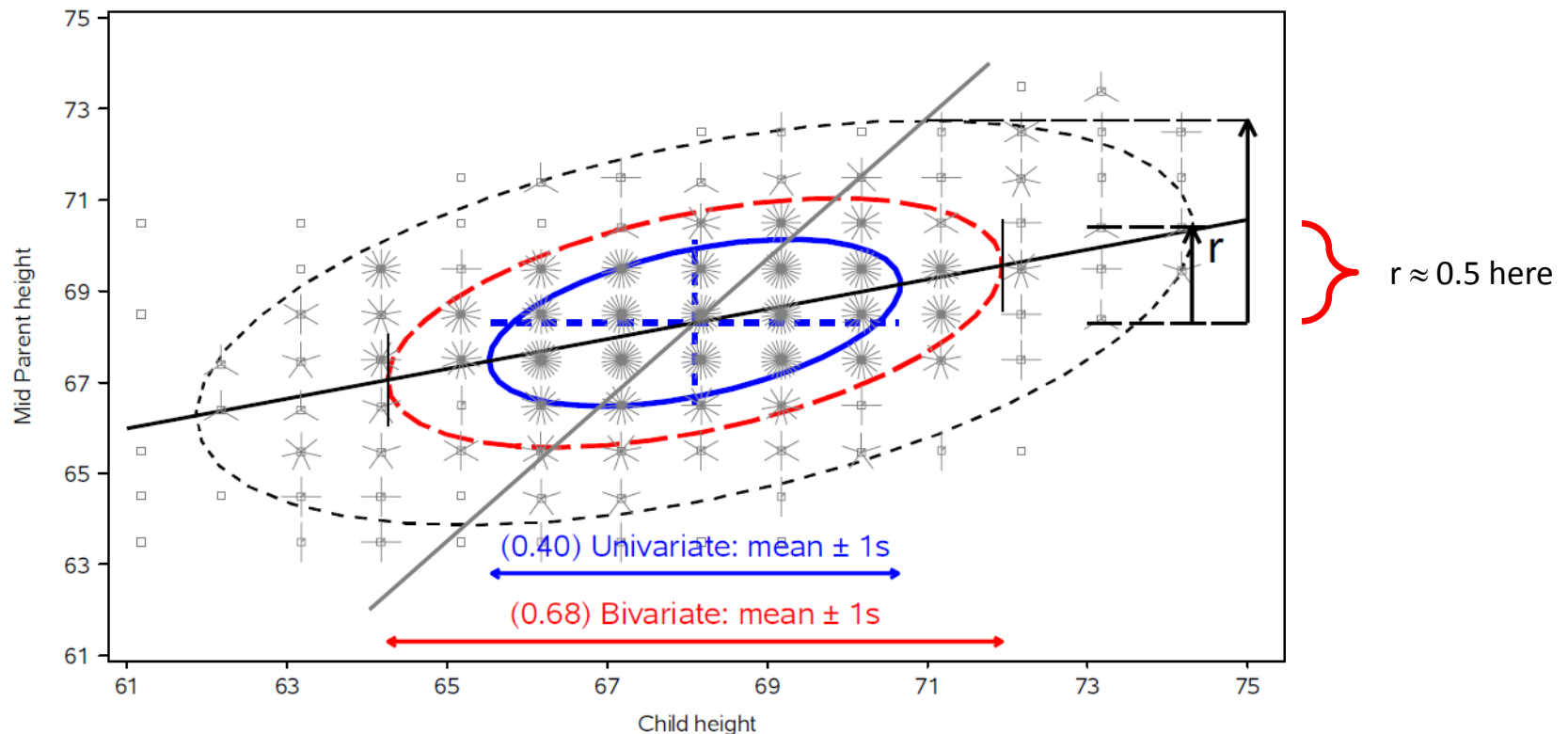
- For a  $p$ -dimensional multivariate sample,  $\mathbf{Y}_{N \times p}$ , the sample mean vector,  $\bar{\mathbf{y}}$ , and sample covariance matrix,  $\mathbf{S}$ , are **minimally sufficient statistics** under classical (gaussian) assumptions.
- These can be represented visually by the  $p$ -dimensional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

$$\mathcal{E}_c(\bar{\mathbf{y}}, \mathbf{S}) := \{\mathbf{y} : (\mathbf{y} - \bar{\mathbf{y}})^T \mathbf{S}^{-1} (\mathbf{y} - \bar{\mathbf{y}}) \leq c^2\}$$

- → 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 ???

```
> data(mathscore, package="heplots")
> mod <- lm(cbind(BM, WP) ~ group, data=mathscore)
> Anova(mod)
```

Type II MANOVA Tests: Pillai test statistic

	Df	test stat	approx F	num Df	den Df	Pr(>F)
group	1	0.86518	28.878	2	9	0.0001213 ***

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

# Why do multivariate tests?

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

```
> Anova(lm(BM ~ group, data=mathscore))  
Anova Table (Type II tests)
```

Response: BM

	Sum Sq	Df	F value	Pr(>F)
group	1302	1	4.24	0.066 .
Residuals	3071	10		

```
> Anova(lm(WP ~ group, data=mathscore))  
Anova Table (Type II tests)
```

Response: WP

	Sum Sq	Df	F value	Pr(>F)
group	4408	1	10.4	0.009 **
Residuals	4217	10		

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

```
> mod <- lm(cbind(BM, WP) ~ group, data=mathscore)
> Anova(mod)
```

Type II MANOVA Tests: Pillai test statistic

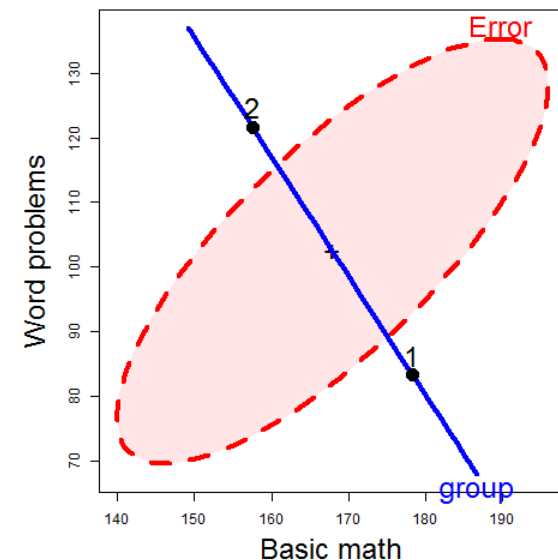
	Df	test stat	approx F	num Df	den Df	Pr(>F)
group	1	0.86518	28.878	2	9	0.0001213 ***

Visual test of significance (Roy's test)

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

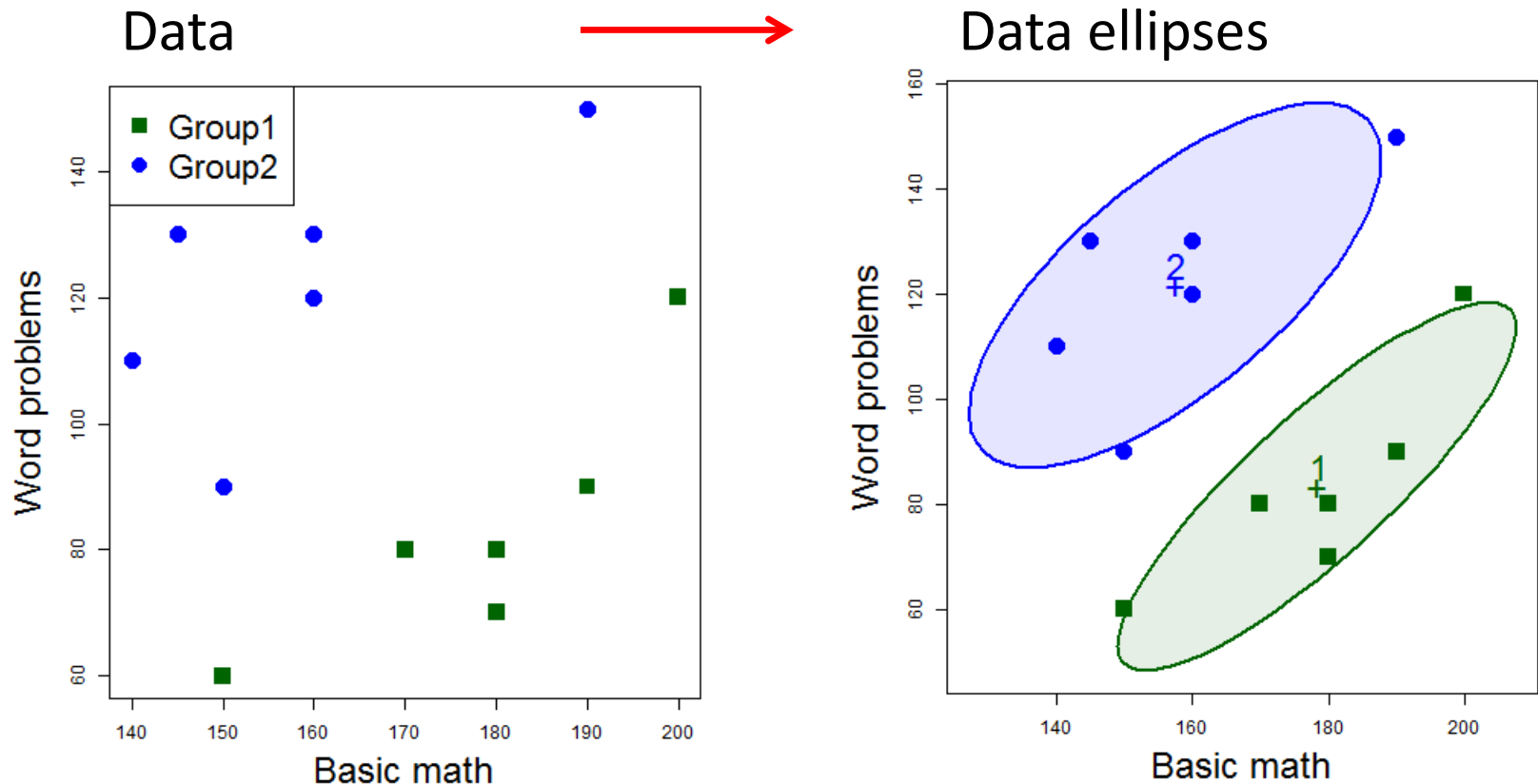
HE plot provides an interpretation:

- 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



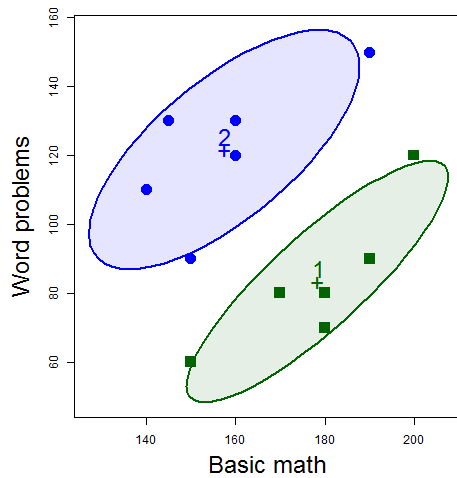
# HE plot framework: Visual overview

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

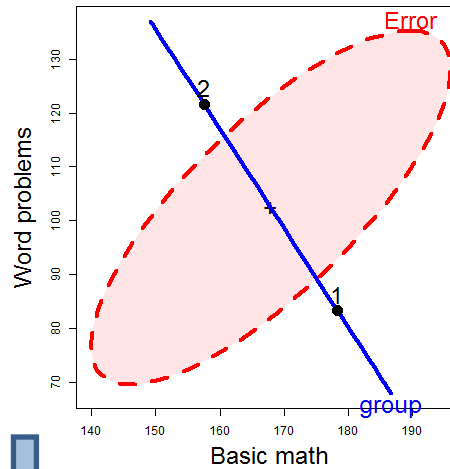


# Visual overview

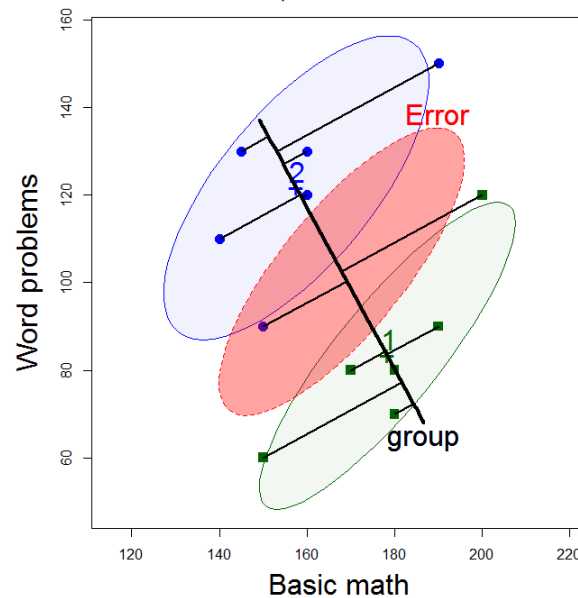
Data ellipses



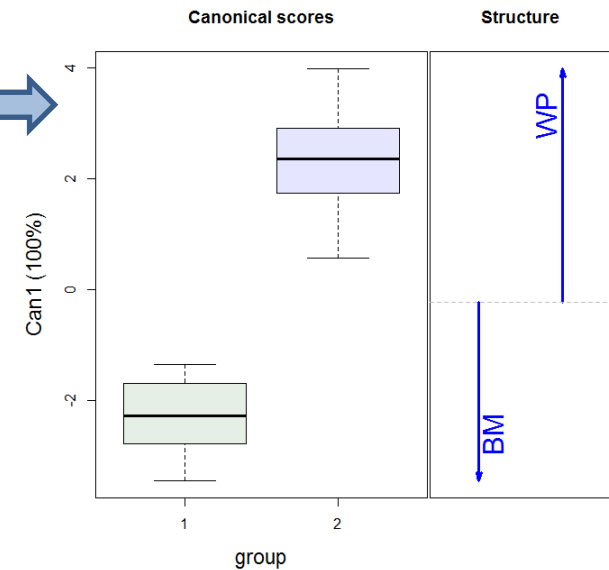
HE plot



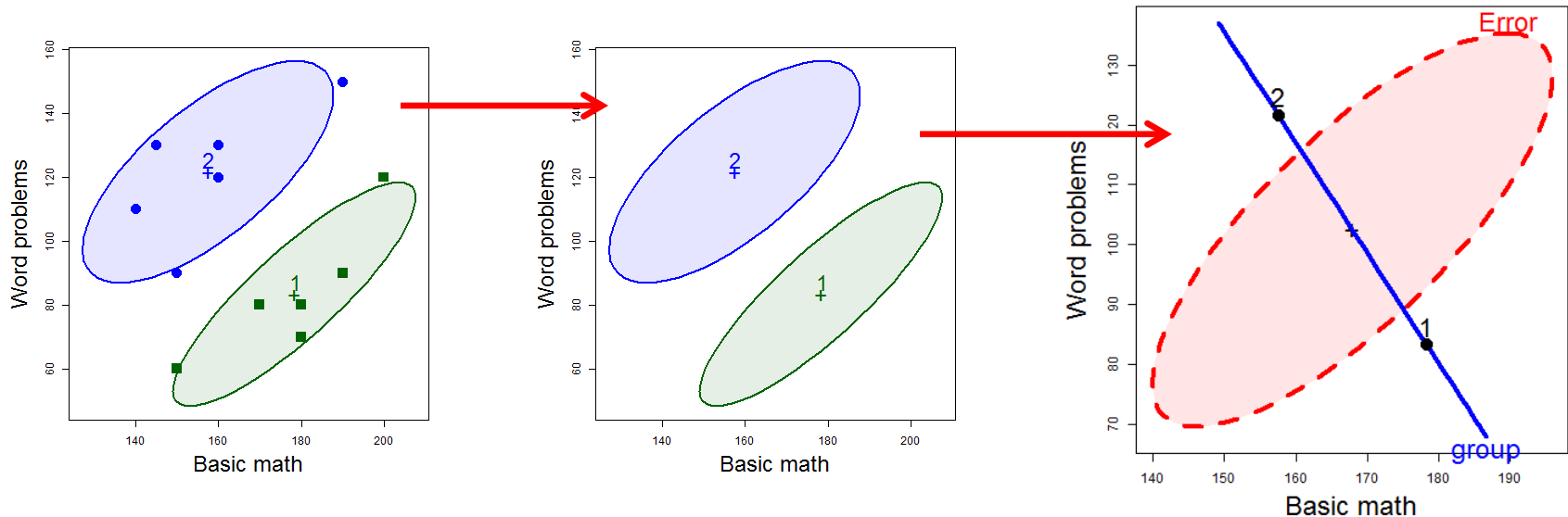
Discriminant scores



Canonical space

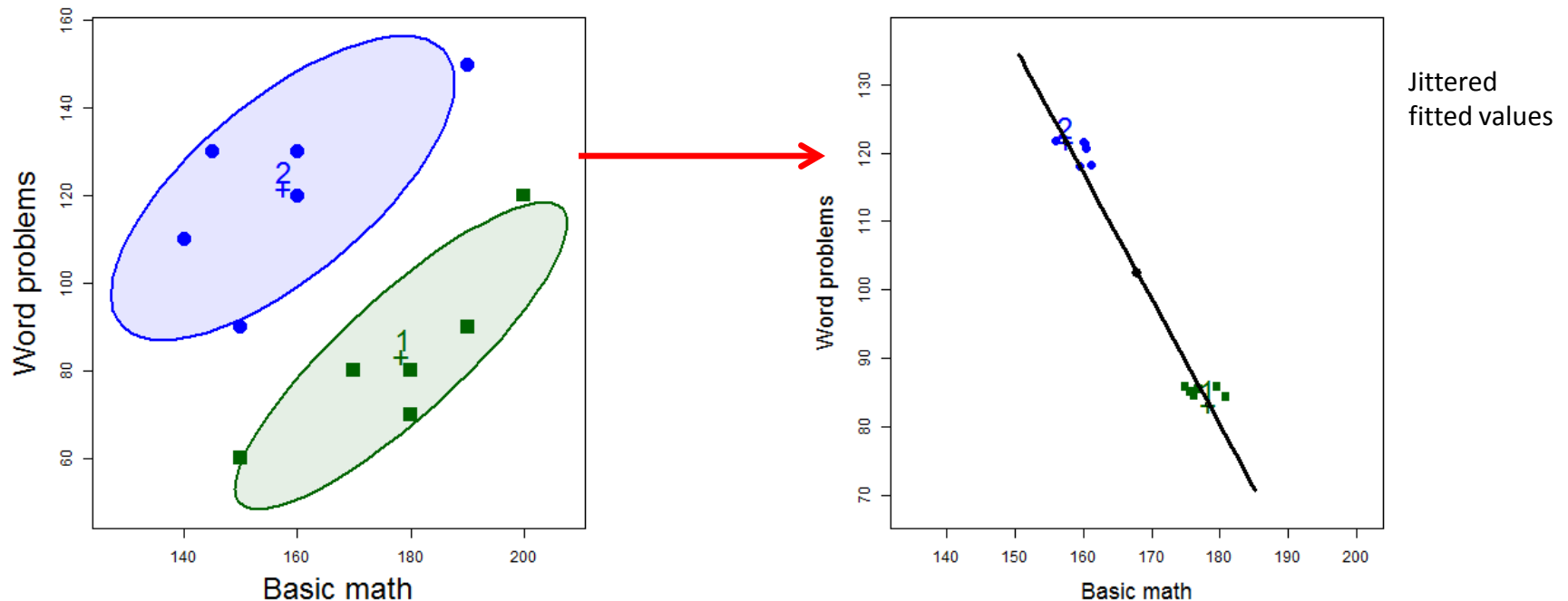


# Data → Data ellipses → HE plot



- 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

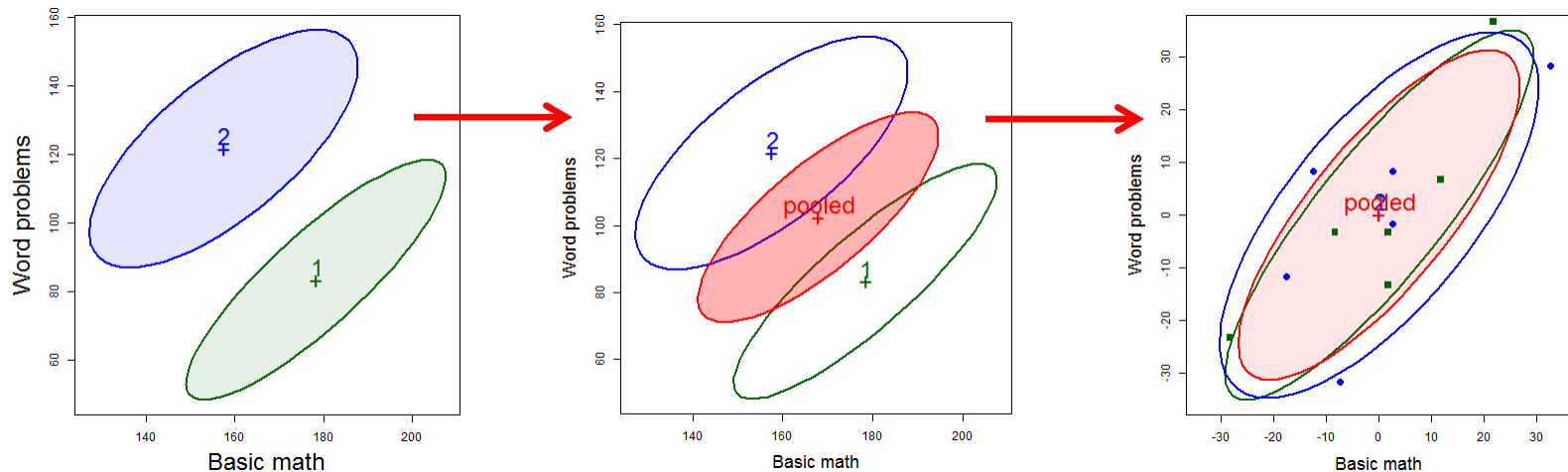


- The **H** ellipse is the data ellipse of the fitted values (group means, here)
  - The **H** matrix is the sum of squares and crossproducts of the fitted values, corrected for the grand mean

$$\mathbf{H} = (\hat{\mathbf{Y}}' \hat{\mathbf{Y}} - n \bar{y} \bar{y}')$$



# 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”

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

# 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.

```
> math.aov <- Anova(math.mod)
> (H <- math.aov$SSP)
$group
```

	BM	WP
BM	1302.1	-2395.8
WP	-2395.8	4408.3

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

```
> fit <- fitted(math.mod)
> ybar <- colMeans(mathscore[,2:3])
> n <- nrow(mathscore)
> crossprod(fit) - n*outer(ybar, ybar)
```

	BM	WP
BM	1302.1	-2395.8
WP	-2395.8	4408.3

```
> 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:  $E = (\hat{\mathbf{Y}} - \bar{\mathbf{Y}})'(\hat{\mathbf{Y}} - \bar{\mathbf{Y}}) = \hat{\mathcal{E}}'\hat{\mathcal{E}}$

```
> resid< residuals(math.mod)
```

```
> crossprod(resids)
```

	BM	WP
BM	3070.8	2808.3
WP	2808.3	4216.7

```
> cor(resids)
```

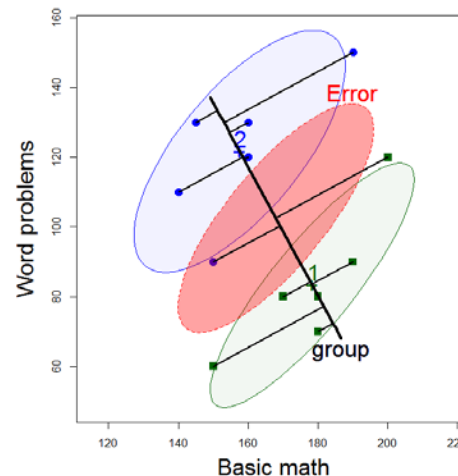
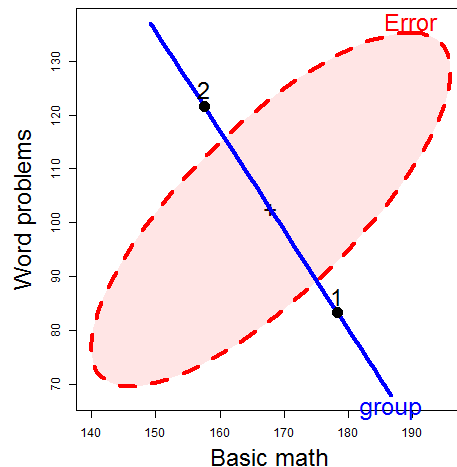
	BM	WP
BM	1.00	0.78
WP	0.78	1.00

```
> resid<
```

	BM	WP
1	11.667	6.667
2	-8.333	-3.333
3	1.667	-3.333
4	21.667	36.667
5	-28.333	-23.333
6	1.667	-13.333
7	2.500	-1.667
8	32.500	28.333
9	-7.500	-31.667
10	2.500	8.333
11	-17.500	-11.667
12	-12.500	8.333

# 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  $HE^{-1}$
  - Discriminant weights are eigenvectors of  $HE^{-1}$



# 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:lda() does this analysis

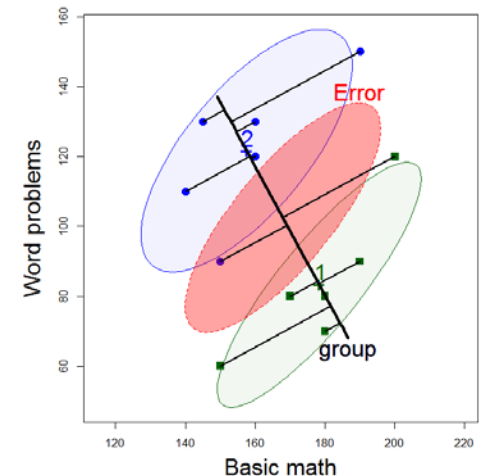
```
> (mod.lda <- MASS::lda(group ~ ., mathscore))
```

Group means:

	BM	WP
1	178.3	83.33
2	157.5	121.67

Coefficients of linear discriminants:

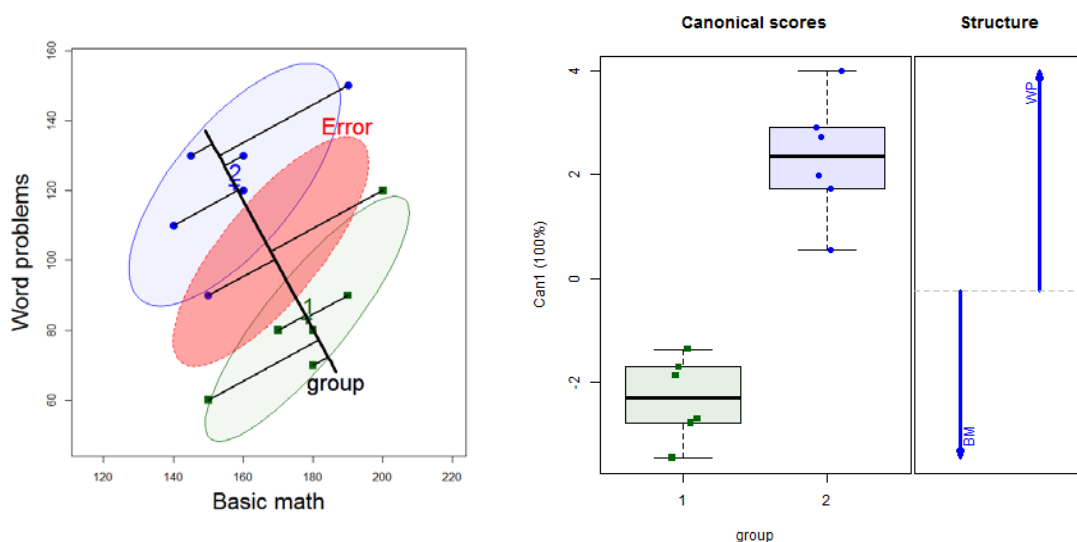
	LD1
BM	-0.08350
WP	0.07527



The canonical dimension is  $\text{Can1} = 0.075 \text{ WP} - 0.083 \text{ BM}$ , 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)
```

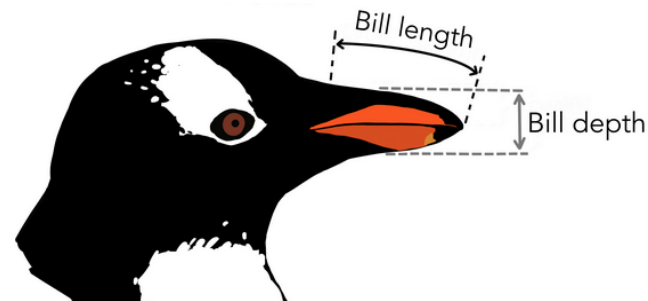
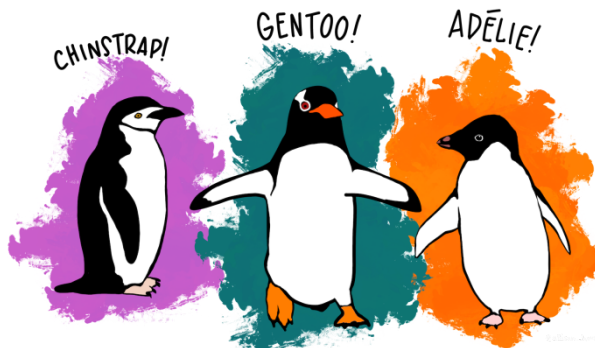
# Penguin data

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

- How does penguin “size” differ by species, island, ... ?



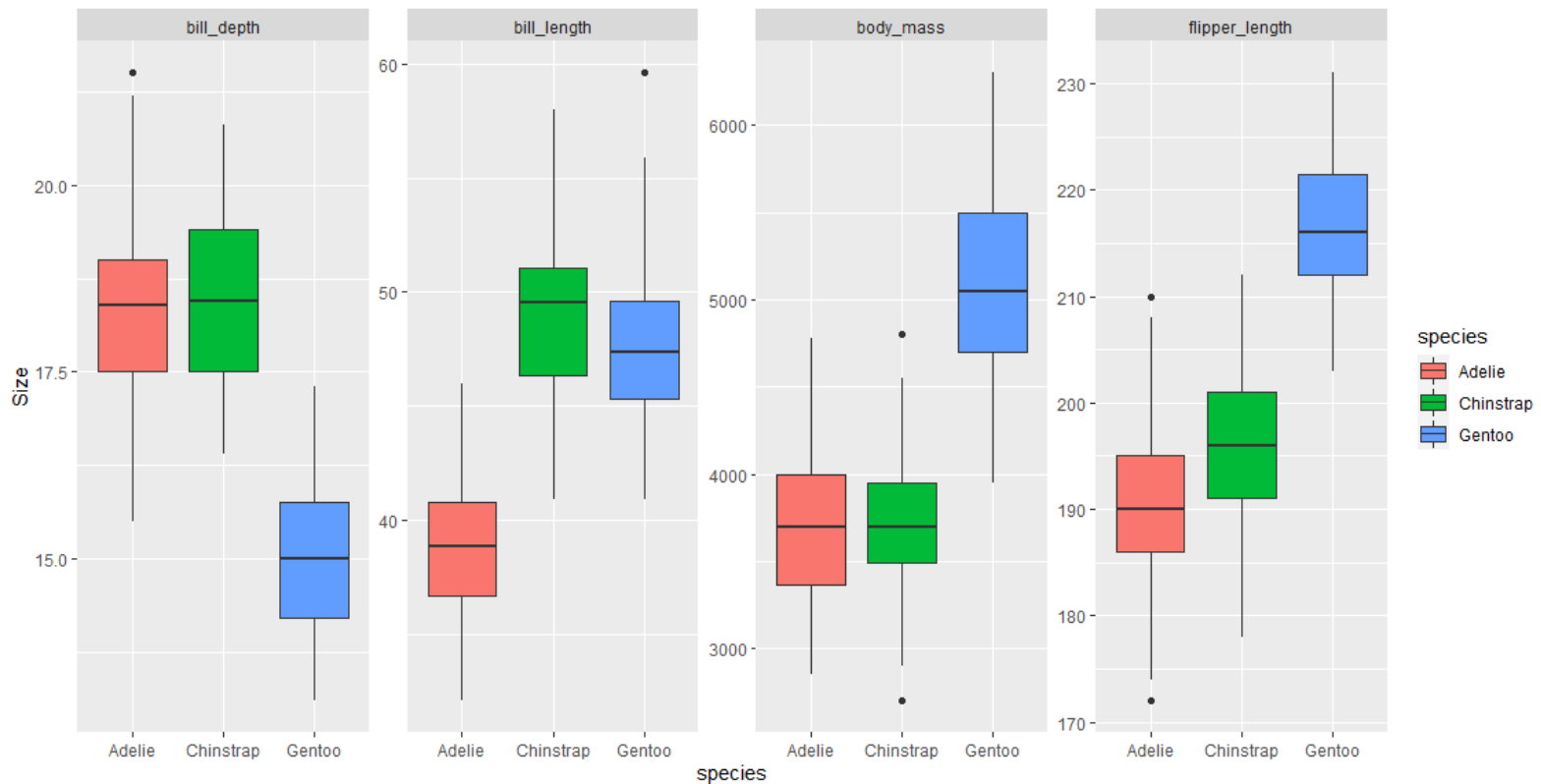
```
> library(palmerpenguins)
> peng <- penguins %>% rename(...) %>% ... # clean up names, etc.
> peng[sample(1:333, 5), ]
# A tibble: 5 x 8
  species island bill_length bill_depth flipper_length body_mass sex year
  <fct>   <fct>   <dbl>      <dbl>      <int>      <int> <fct> <int>
1 Chinstrap Dream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



# 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?



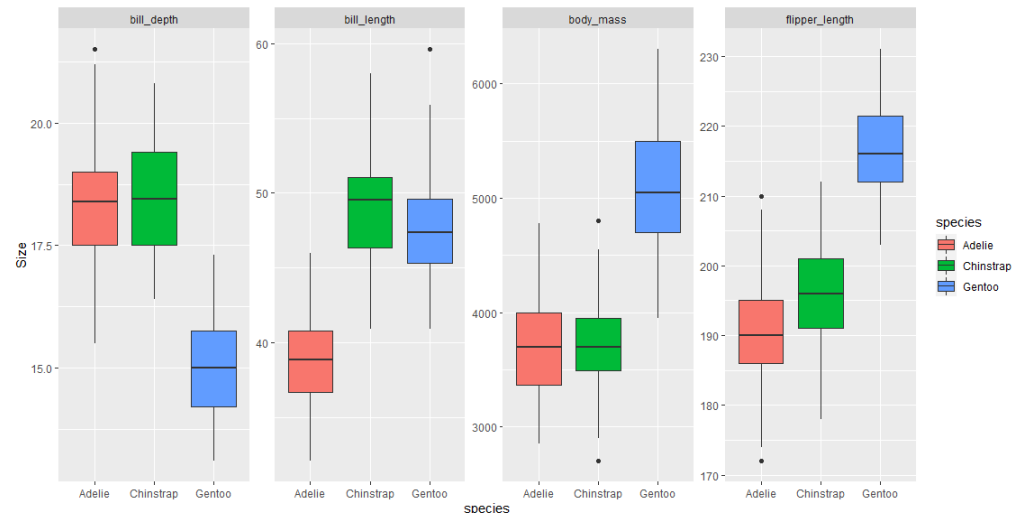


# Penguins: Multivariate EDA

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

```
peng.pca <- prcomp (~ bill_length + bill_depth + flipper_length + body_mass,  
  data=peng,  
  na.action=na.omit,  
  scale. = TRUE)  
screeplot(peng.pca, type = "line", lwd=3, cex=3,  
  main="Variances of PCA Components")
```

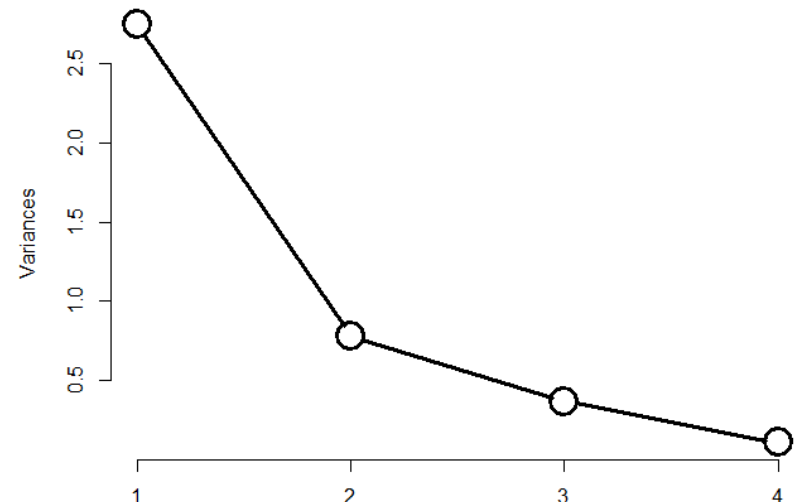
```
> summary(peng.pca)  
Importance of components:
```

	PC1	PC2	PC3	PC4
Standard deviation	1.657	0.882	0.6072	0.328
Proportion of Variance	0.686	0.195	0.0922	0.027
Cumulative Proportion	<b>0.686</b>	<b>0.881</b>	<b>0.9730</b>	<b>1.000</b>

2D: 88.1 %

3D: 97.3 %

Variances of PCA Components



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

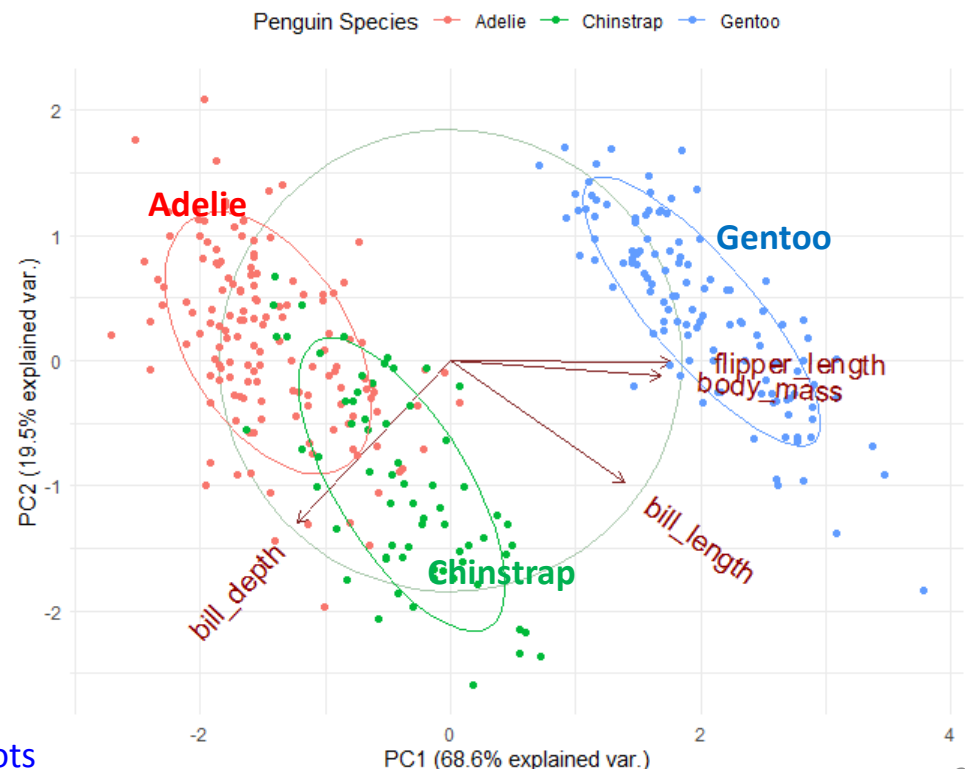
# Biplot

```
library(ggbiplot)
ggbiplot(peng.pca, obs.scale = 1, var.scale = 1,
         groups = peng$species,
         ellipse = TRUE, circle = TRUE) +
  scale_color_discrete(name = 'Penguin Species')
```

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:  $\sim \text{species}$
- Could also use other factors:  $\sim \text{species} + \text{island} + \text{sex}$

```
> peng.mod0 <- lm(cbind(bill_length, bill_depth, flipper_length, body_mass) ~ species,  
                  data=peng)  
> Anova(peng.mod0)
```

Type II MANOVA Tests: Pillai test statistic

	Df	test	stat	approx	F	num	Df	den	Df	Pr(>F)
species	2		1.64		371	8	656			<2e-16 ***

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Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

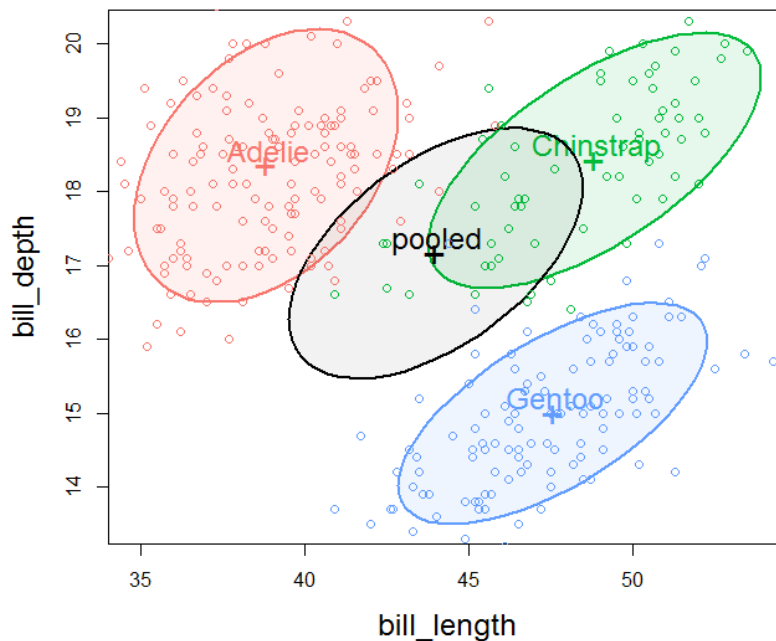
Yet, we are left to understand the nature of this effect wrt. the size variables.

See: <https://rpubs.com/friendly/penguin-manova> for details

# Penguins: view data ellipses

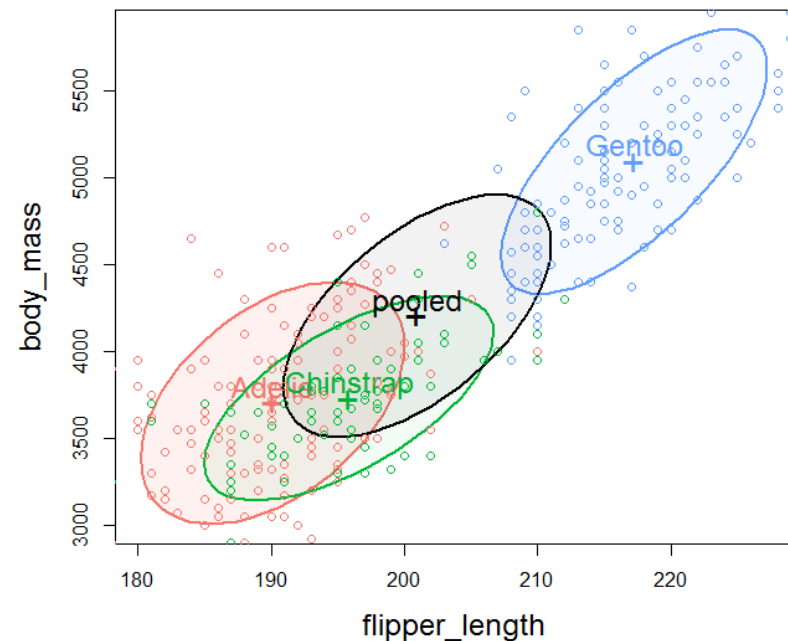
Data ellipses in 2D provide a good start for pairwise relations

bill depth & length



- group means negatively correlated
- within group correlation  $> 0$

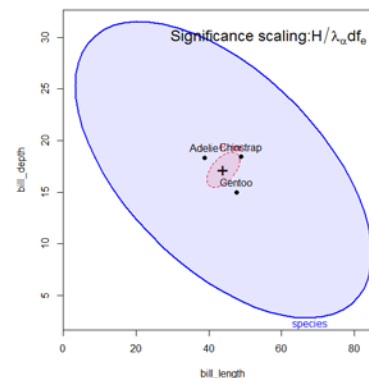
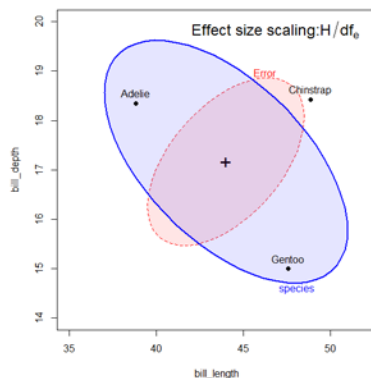
body mass & flipper length



- group means positively correlated
- within group correlation  $> 0$

# HE plot details

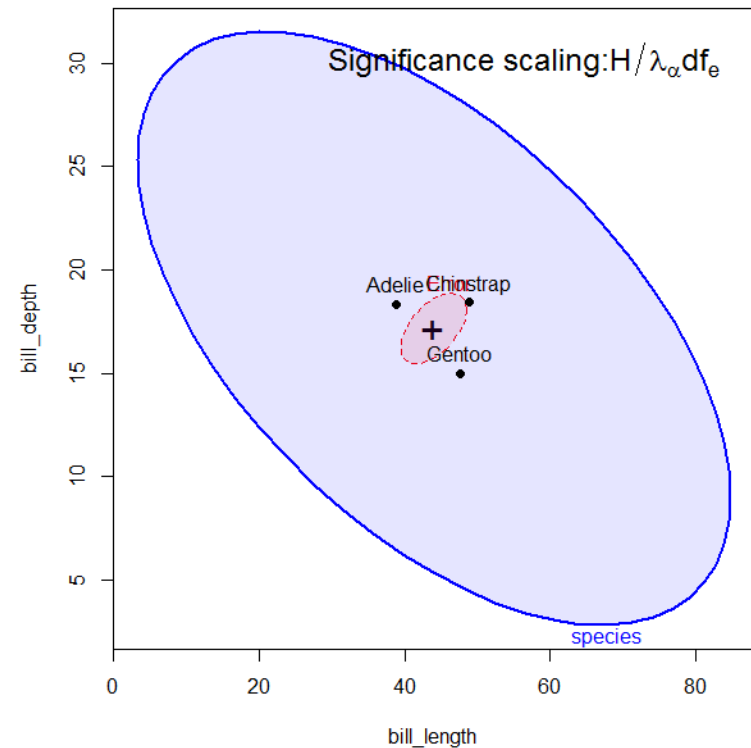
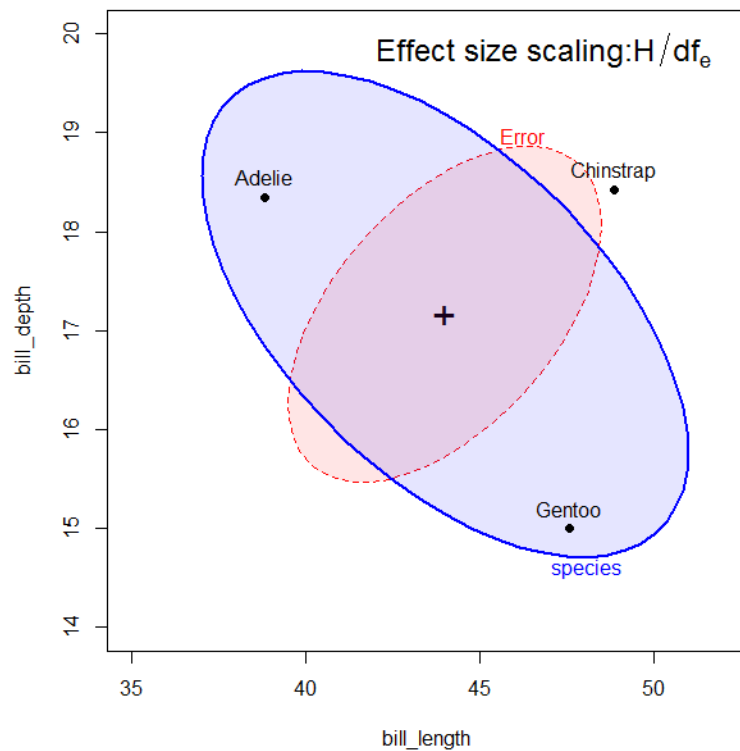
- **E** ellipse reflects within-group error (co)variation
  - Size:  $\mathbf{E} / df_e$  set to cover 68%, an analog of  $\bar{y} \pm 1$  std
  - Shift to grand mean for direct comparison with **H**
- **H** ellipse reflects (co)variation of group means
  - **effect size** scaling, uses  $\mathbf{H}/df_e$  to put this on the same scale as the **E** ellipse. Analog of effect size in univariate designs.
  - **significance** (“evidence”) scaling: uses  $\mathbf{H}/\lambda_\alpha df_e$ .
    - 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.

**E** ellipse: within species, larger bill length → larger bill depth



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

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



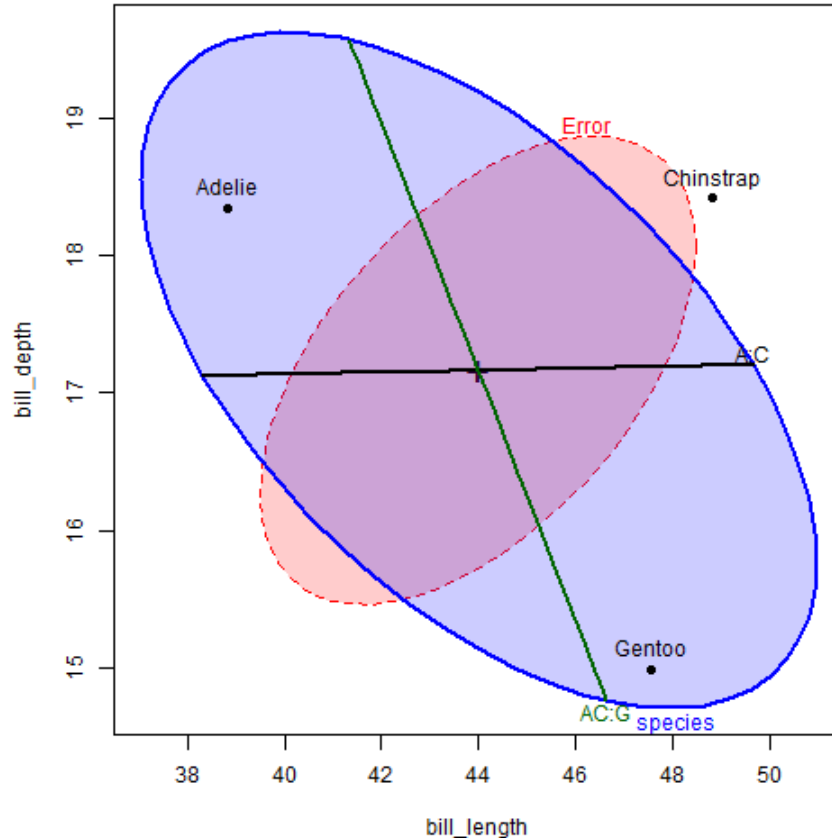
# Contrasts

- In linear models, any effect of  $df_h > 1$  can be partitioned into  $df_h$  separate 1 df tests of contrasts
  - If orthogonal,  $\mathbf{H} = \mathbf{H}_1 + \mathbf{H}_2 + \dots \mathbf{H}_{dfh}$  -- accounts for total effect
  - Tested as a linear hypothesis, e.g.,  $x_1 - (x_2 + x_3)/2 = 0$
  - Each  $\mathbf{H}_i$  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(peng$species)<-matrix(c(1,-1,0, -1, -1, -2), 3,2)
> contrasts(peng$species)
      [,1] [,2]
Adelie    1   -1
Chinstrap -1   -1
Gentoo    0   -2
```

# Contrasts

```
hyp <- list("A:C"="species1","AC:G"="species2") # give names to contrasts  
heplot(peng.mod0, fill=TRUE, fill.alpha=0.2,  
       hypotheses=hyp, size="effect")
```



Result is very clear:

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

Both of these are large effects!

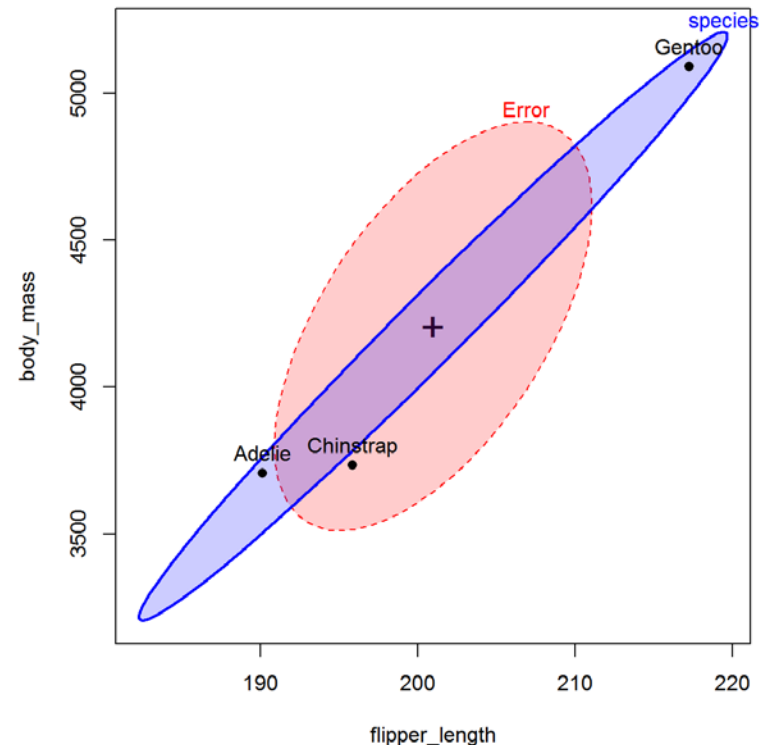
# Other HE plots

- 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")
```

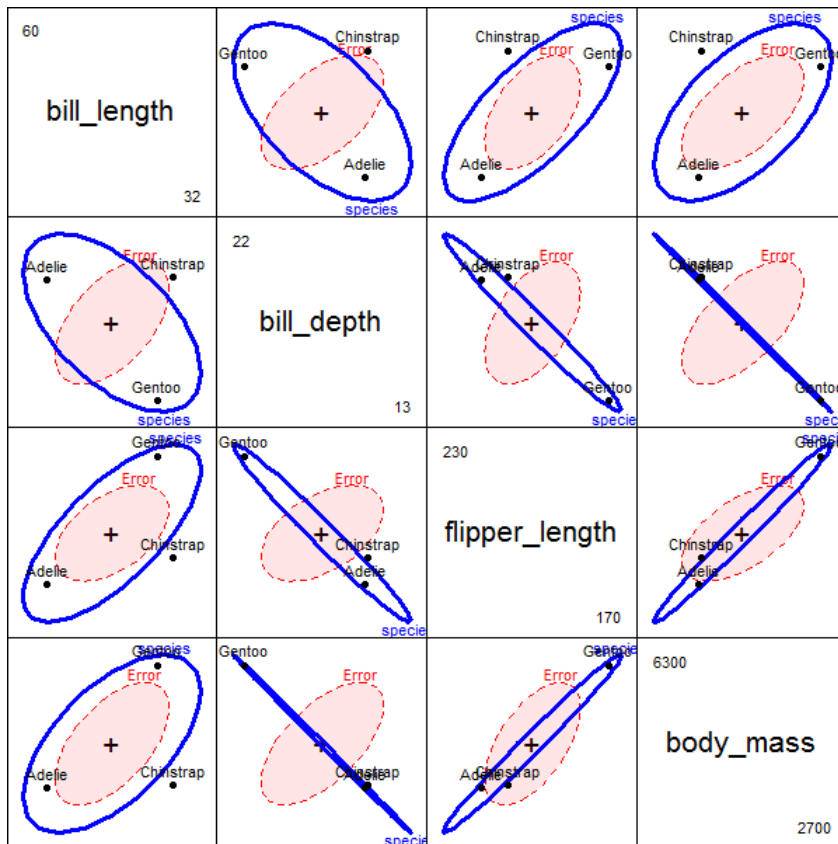
Interpretation:

- 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 a all pairwise HE plots in a scatterplot matrix format.



```
pairs(peng.mod0, size="effect",  
      fill=c(TRUE, FALSE))
```

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

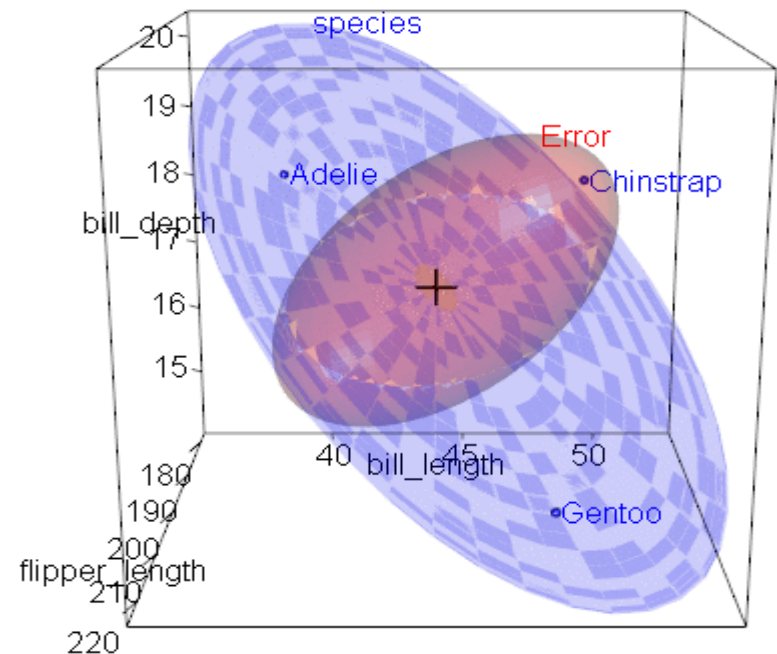
# heplot3d()

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.



# 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))
```

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 H0: The canonical correlations in the current row and all that follow are zero

	LR test stat	approx F	numDF	denDF	Pr(> F)
1	0.0187	516	8	654	<2e-16 ***
2	0.2997	255	3	328	<2e-16 ***

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

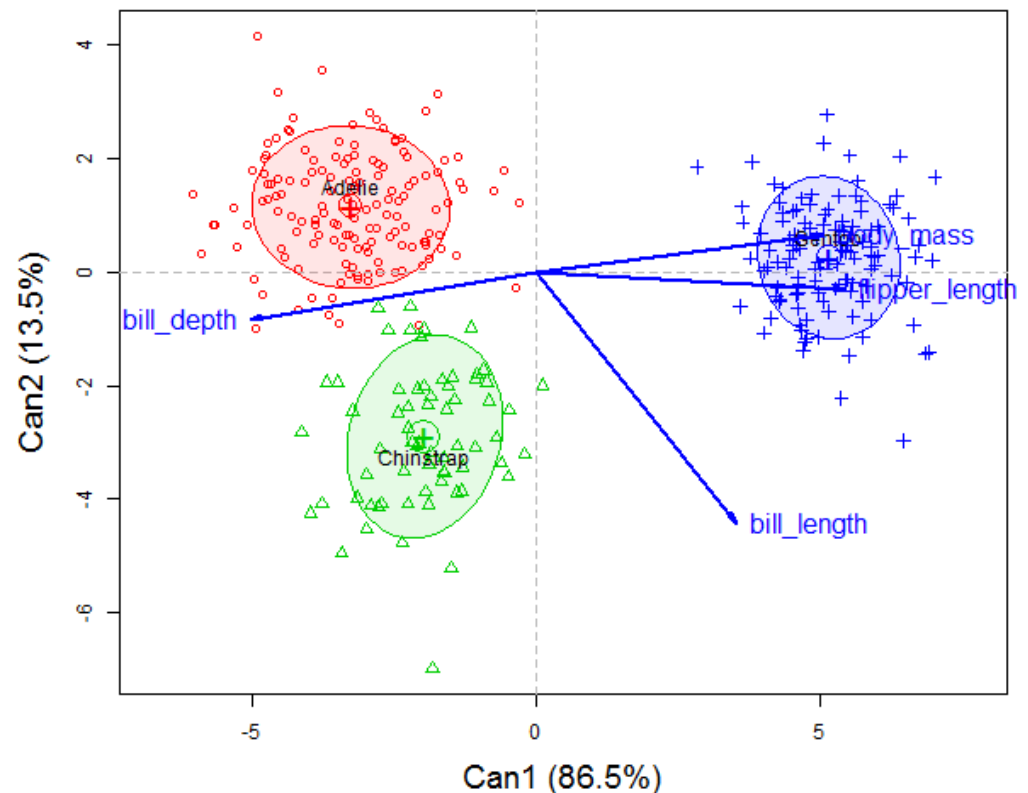
# Canonical view

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

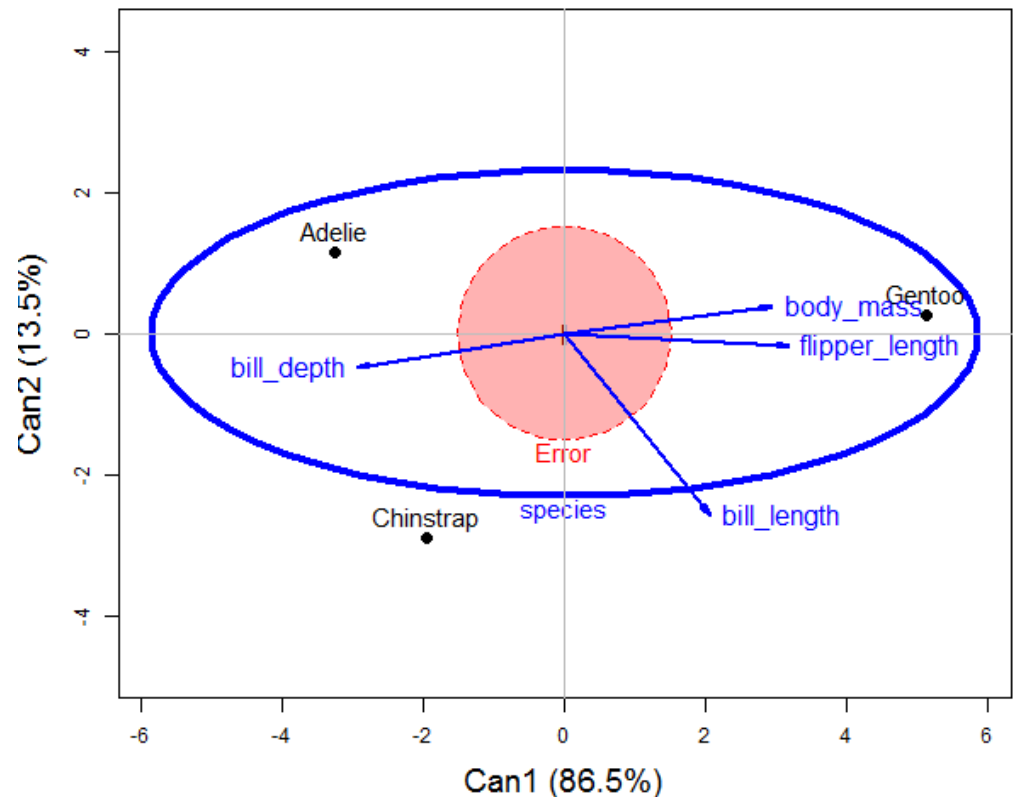
```
heplot(peng.can, size="effect", fill=c(TRUE, FALSE))
```

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
- Data ellipses
  - Summarize bivariate data to show means, variances, correlation
- 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.