

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

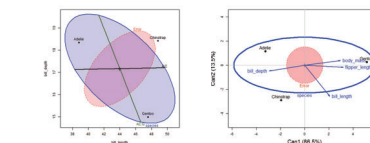
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SCS Short Course
Oct-Nov 2021

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

Today's topics

- Brief review of the GLM & MLM
$$\mathbf{Y} = \mathbf{X} \mathbf{B} + \mathbf{E}$$

 $(n \times p) \quad (n \times q) \quad (q \times p) \quad (n \times p)$
- Data ellipses
 - sufficient visual summaries
- HE plot framework
 - H & E matrices/ellipses
 - Discriminant/canonical views
- Example: Penguins data



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One-way ANOVA vs. MANOVA

ANOVA



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

source: Cooley & Lohnes ((1971))

Do means differ?

(Assume equal within-group variances)

MANOVA

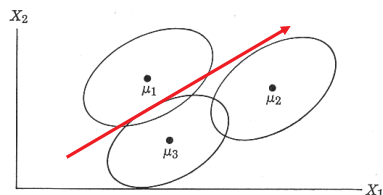


Figure 8.2. The simple manova situation, when the differences among the populations are "real."

How do centroids differ?
How many dimensions?

(Assume equal within-group variance-covariance matrices)

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 , $\log(\text{income})$
 - Polynomial terms: age^2 , 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 $y \sim X$:

```
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
```

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Univariate linear model

- Model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$
 $(n \times 1) \quad (n \times q) \quad (1 \times q) \quad (n \times 1)$
 $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_q)$
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

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

$$= SS_H + SS_E$$

- Hypothesis tests

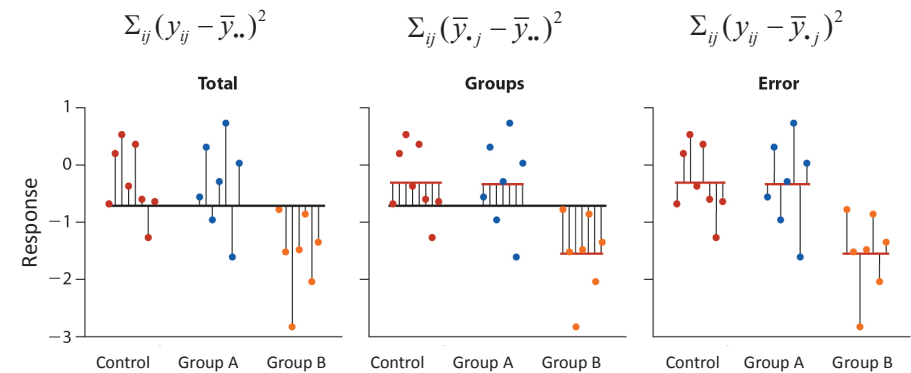
$$F = \frac{SS_H / df_H}{SS_E / df_E} = \frac{MS_H}{MS_E}$$

How big is hypothesis variation relative to error variation?

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Visualizing $SS_T = SS_H + SS_E$

Total variance = Between group variance + Within group variance



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Multivariate linear model

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

- Sums of squares & cross-products

$$SSP_T = (\hat{\mathbf{Y}}'\hat{\mathbf{Y}} - n\bar{\mathbf{y}}\bar{\mathbf{y}}') + \boldsymbol{\epsilon}'\boldsymbol{\epsilon}$$

$$(p \times p)$$

$$= SSP_H + SSP_E = \mathbf{H} + \mathbf{E}$$

- Hypothesis tests

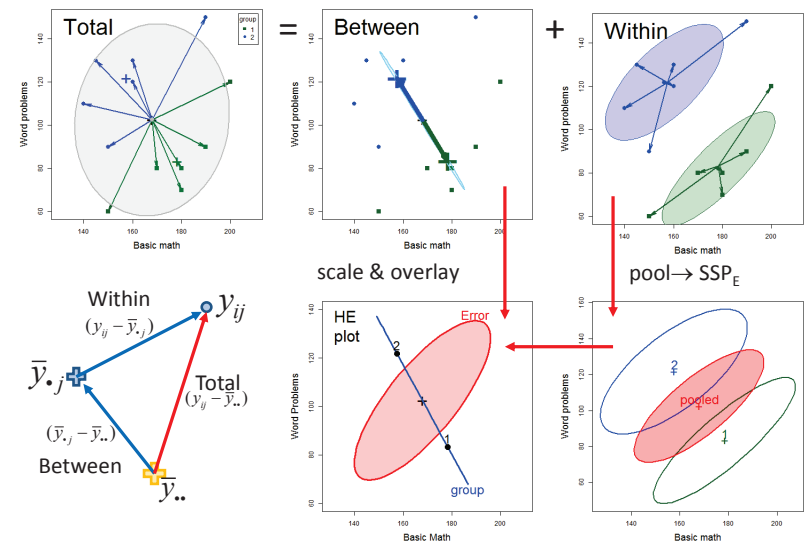
- Eigenvalues $\lambda_i, i=1:p$ of $\mathbf{H}\mathbf{E}^{-1}$
- Wilks' Λ , Pillai & Hotelling trace, Roy's test
- how many dimensions (aspects of responses)?

How big is hypothesis variation relative to error variation?

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

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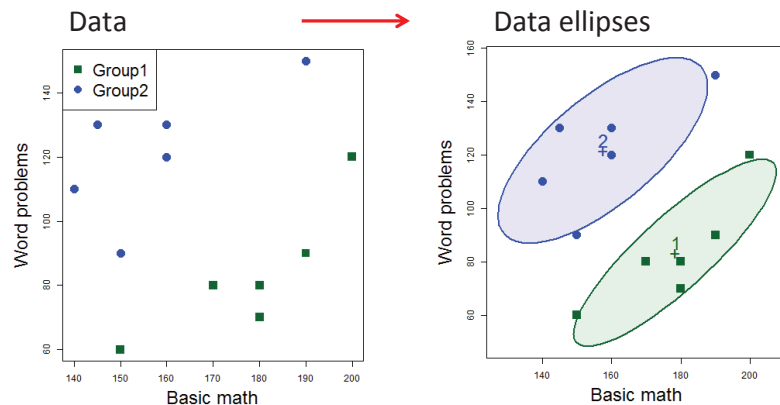
Visualizing $SSP_T = SSP_H + SSP_E$



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Data ellipsoids

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



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Data ellipsoids: definitions

- 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 centered at $\bar{\mathbf{y}}$,

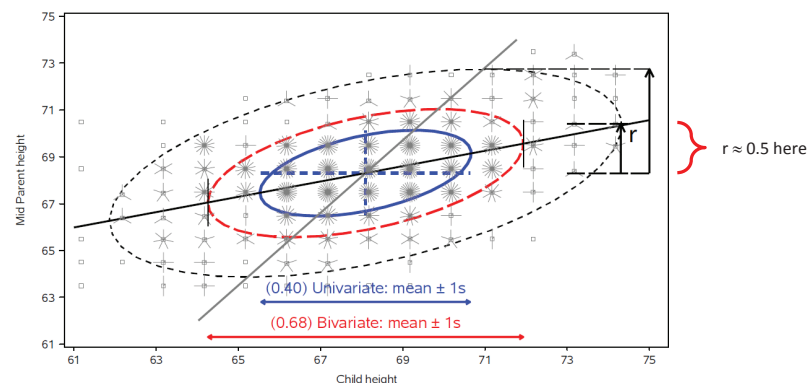
$$\mathcal{E}_c(\bar{\mathbf{y}}, \mathbf{S}) := \{\mathbf{y} : (\mathbf{y} - \bar{\mathbf{y}})^T \mathbf{S}^{-1} (\mathbf{y} - \bar{\mathbf{y}}) \leq c^2\} \quad \text{or,} \quad D_M^2(\mathbf{y}) \leq c^2$$

- 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.

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Data ellipsoids: properties

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



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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!

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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
```

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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.

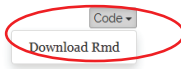
- Examples:
 - Math scores: Simple demo of MLMs [mathscore-simple.R](#)
 - Math scores: HE plot examples [mathscore-ex.R](#) || [mathscore-ex.html](#)
 - Penguins data: [Multivariate EDA vignette](#)
 - Diabetes data: [heplots and candisc examples vignette](#)
- HW: explore other examples

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 to download the R code and comments

Math scores: HE plot examples

Michael Friendly



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

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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](#))?

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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)
```

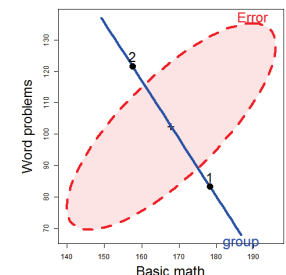
```
Type II MANOVA Tests: Pillai test statistic
      Df test stat approx F num Df den Df    Pr(>F)
group 1  0.86518   28.878      2      9 0.0001213 ***
```

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:

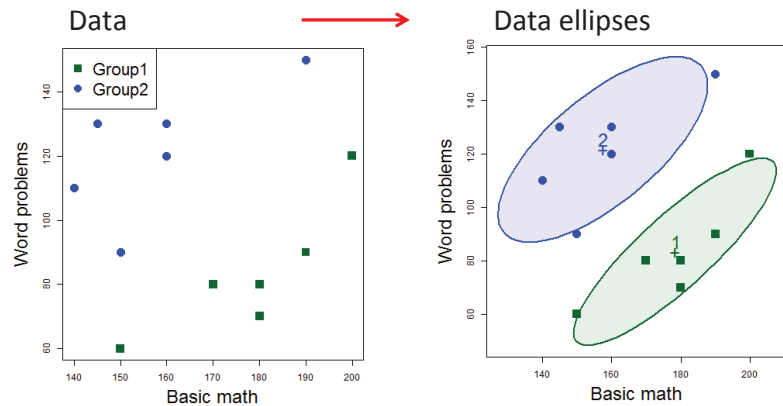
- Group 1 > Group 2 on Basic Math, but worse on Word Problems
- Group 2 > Group 1 on Word Problems, but worse on Basic Math
- BM & WP are + correlated w/in groups



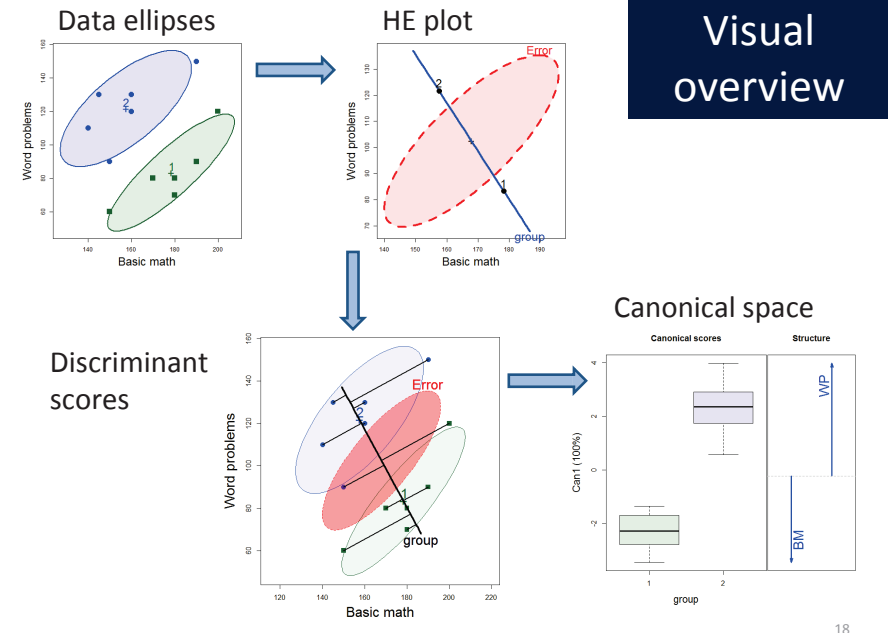
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HE plot framework: Visual overview

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

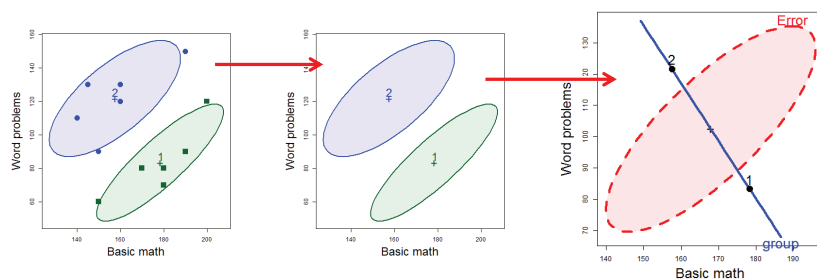


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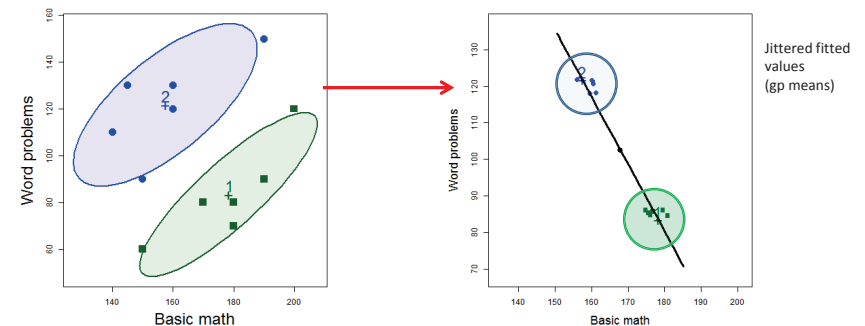
Data → Data ellipses → HE plot



- 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

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The H ellipse

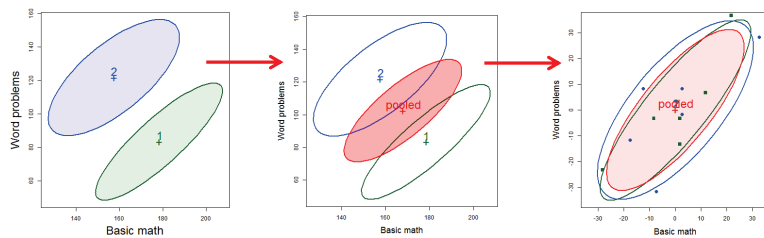


- The **H** ellipse is the data ellipse of the fitted values (group means, here)
 - The **H** matrix is the sum of squares and crossproducts of the fitted values, corrected for the grand mean

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

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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”

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

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

```
> 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
```

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H & E in numbers

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

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

```
> resid <- residuals(math.mod)
> crossprod(resid)
      BM      WP
BM 3070.8 2808.3
WP 2808.3 4216.7
```

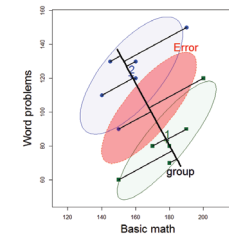
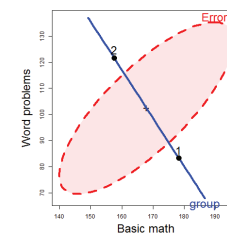
```
> cor(resid)
      BM      WP
BM 1.00 0.78
WP 0.78 1.00
```

```
> 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
```

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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 $\mathbf{H}\mathbf{E}^{-1}$
 - Discriminant weights are eigenvectors of $\mathbf{H}\mathbf{E}^{-1}$



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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))
```

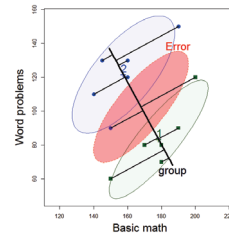
Group means:

	BM	WP
1	178.3	83.33
2	157.5	121.67

Coefficients of linear discriminants:

LD1

	BM	WP
1	-0.08350	0.07527

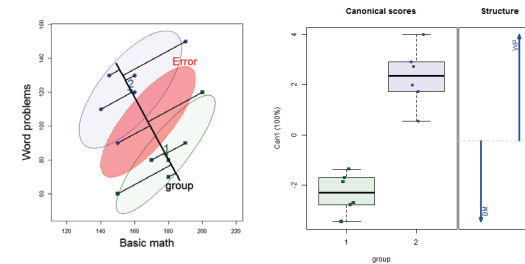


The canonical dimension is Can1 = 0.075 WP - 0.083 BM, a contrast between the two tests

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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)
```

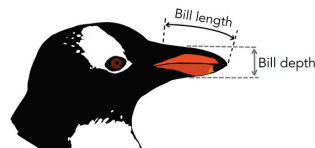
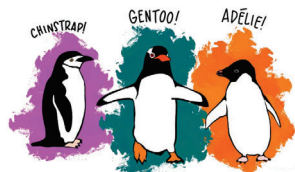
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Penguin data

- 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
```

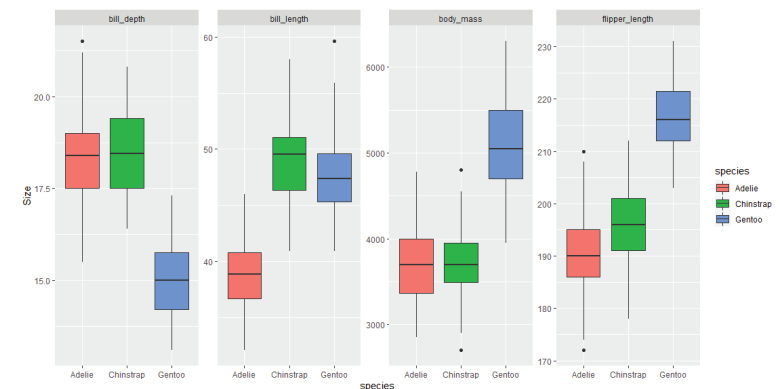


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Penguins: Multivariate EDA

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?



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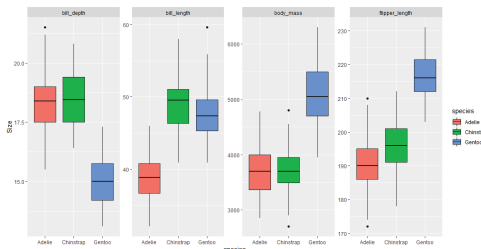
Penguins: Multivariate EDA

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)
```



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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

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PCA

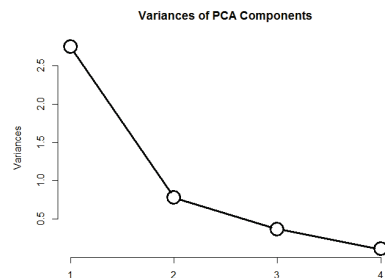
```
peng.pca <- prcomp(~ bill_length + bill_depth + flipper_length + body_mass,
  data=peng,
  na.action=na.omit,
  scale. = TRUE)
screeplot(peng.pca, type = "line", lwd=3, cex=3,
  main="Variances of PCA Components")
```

```
> 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  0.686  0.881  0.9730  1.000
```

2D: 88.1 %

3D: 97.3 %

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



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Biplot

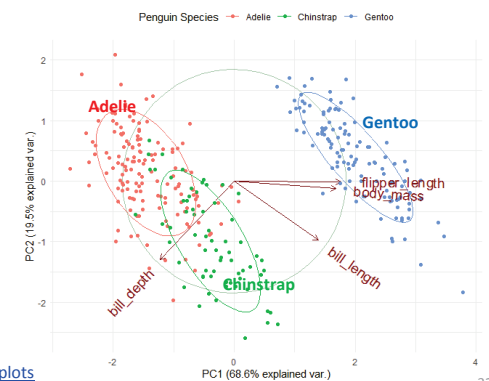
```
library(ggbiplot)
ggbiplot(peng.pca, obs.scale = 1, var.scale = 1,
  groups = peng$species,
  ellipse = TRUE, circle = TRUE) +
  scale_color_discrete(name = 'Penguin Species')
```

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>



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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 species
- Could also use other factors: \sim species + island + 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 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

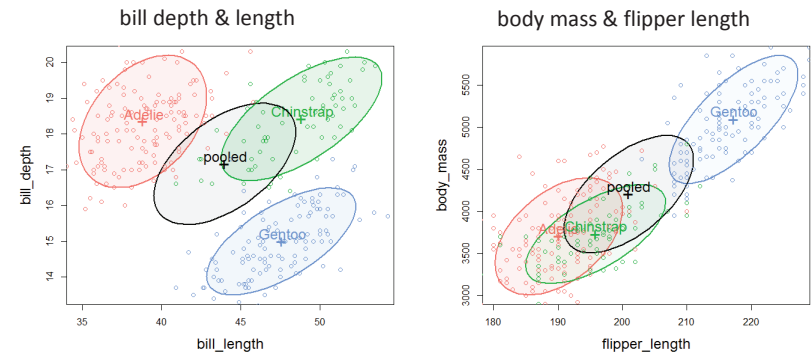
Yet, we are left to understand the nature of this effect wrt. the size variables.

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

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Penguins: view data ellipses

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

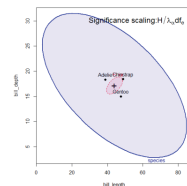
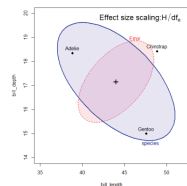


- group means negatively correlated
- within group correlation > 0
- group means positively correlated
- within group correlation > 0

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HE plot details

- **E** ellipse reflects within-group error (co)variation
 - Size: 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 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 $H/\lambda_\alpha df_e$.
 - The **H** ellipse protrudes outside the **E** ellipse somewhere, *iff* an effect is significant (Roy's largest root test) at $p < \alpha$

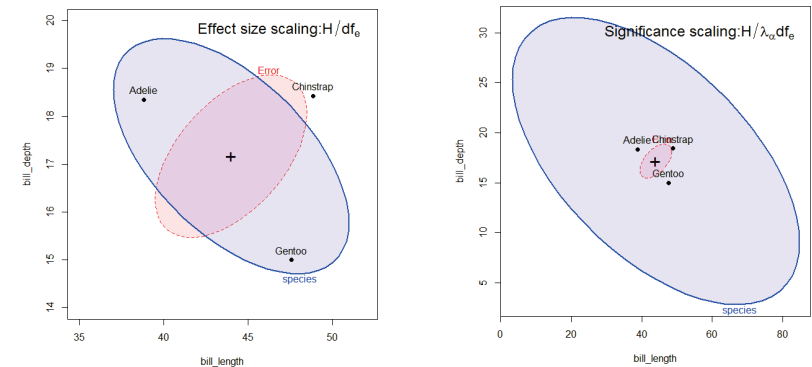


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Penguins: HE plots

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")

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Contrasts

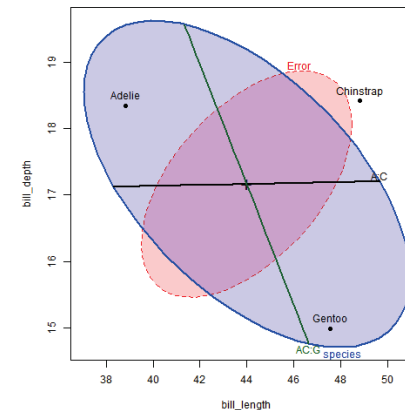
- In linear models, any effect of $df_h > 1$ can be partitioned into df_h separate 1 df tests of contrasts
 - If orthogonal, $H = H_1 + H_2 + \dots H_{df_h}$ -- accounts for total effect
 - Tested as a linear hypothesis, e.g., $x_1 - (x_2 + x_3)/2 = 0$
 - Each H_i has rank=1, so appears as a line in 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
```

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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 (bill shape)

Both of these are large effects!

Together, they are the entire species effect!

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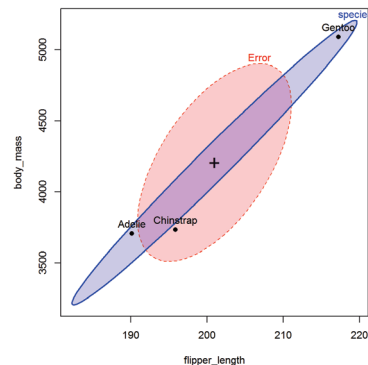
Other HE plots

- 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:

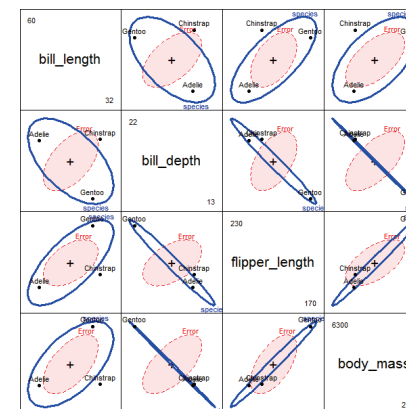
- major axis of the H ellipse measures “penguin size”
- Gentoo are the Big Birds in this story!



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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

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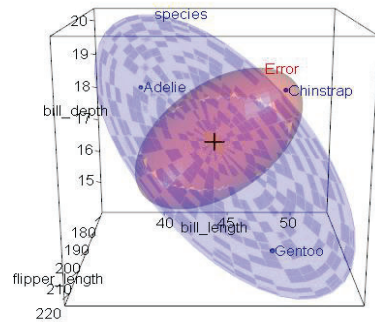
heplot3d()

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



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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

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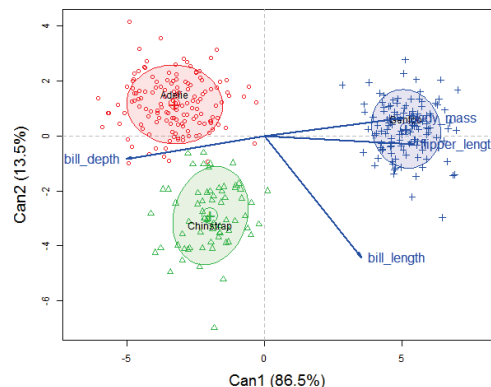
Canonical view

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

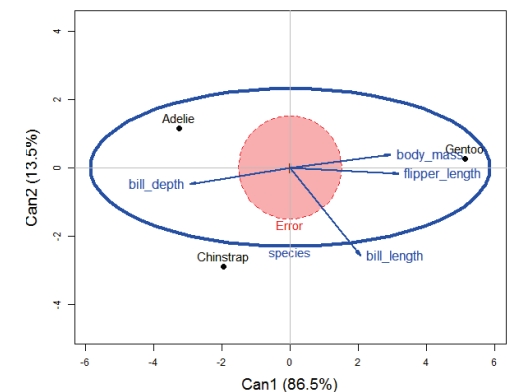
```
heplot(peng.can, size="effect", fill=c(TRUE, FALSE))
```

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

In CAN space, residuals are uncorrelated: $E = \text{circle}$

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

Variable vectors show how the groups are discriminated.



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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.