Recent Advances in Visualizing Multivariate Linear Models

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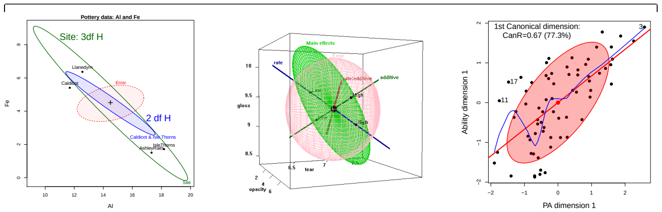
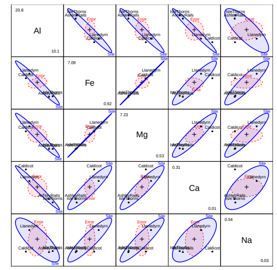


Outline

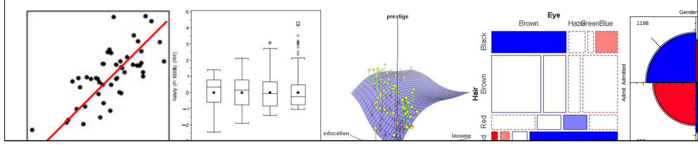


Slides & R scripts: `http://datavis.ca/papers/ssc2013/`

Introduction: The LM family and friends

Models, graphical methods and opportunities

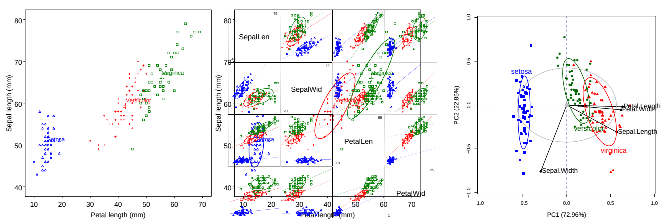
# of response variables	Classical linear models	Generalized linear models
1	LM family: E(y)=Xβ, V(y|X)=σ²I ANOVA, regression, … Many graphical methods: effect plots, spread-leverage, influence, …	GLM: E(y)=g⁻¹(Xβ), V=V[g⁻¹(Xβ)] poisson, logistic, loglinear, … Some graphical methods: mosaic plots, 4fold plots, diagnostic plots, …
2+	MLM: E(Y)=Xβ, V(Y|X)=I⊗Σ MANOVA, MMReg, … Graphical methods: ???	MGLM: ??? Graphical methods: ???



Visual overview: Multivariate data, $\mathbf{Y}_{n\times p}$

What we know how to do well (almost)

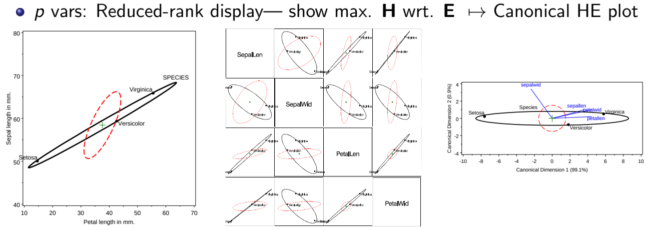
- 2 vars: Scatterplot + annotations (data ellipses, smooths, …)
- p vars: Scatterplot matrix (all pairs)
- p vars: Reduced-rank display– show max. total variation $\mapsto$ biplot



Visual overview: Multivariate linear model, $\mathbf{Y} = \mathbf{X}\,\mathbf{B} + \mathbf{U}$

What is new here?

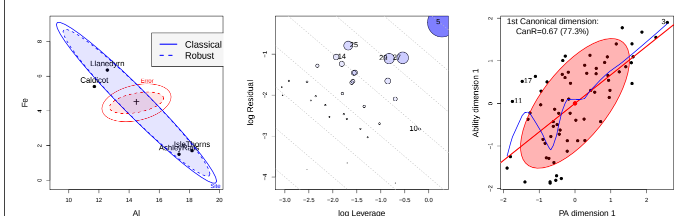
- 2 vars: HE plot— data ellipses of **H** (fitted) and **E** (residual) SSP matrices
- p vars: HE plot matrix (all pairs)
- p vars: Reduced-rank display— show max. **H** wrt. **E** $\mapsto$ Canonical HE plot



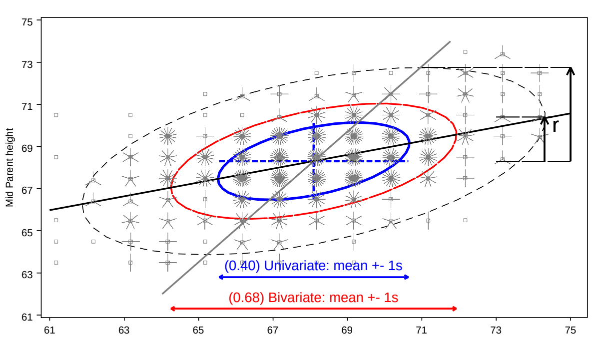
Visual overview: Recent extensions

Extending univariate methods to MLMs:

- Robust estimation for MLMs
- Influence measures and diagnostic plots for MLMs
- Visualizing canonical correlation analysis



Data Ellipses: Galton's data



Galton's data on Parent & Child height: 40%, 68% and 95% data ellipses

The Data Ellipse: Details

- **Visual summary for bivariate relations**
  - **Shows**: means, standard deviations, correlation, regression line(s)
  - **Defined**: set of points whose squared Mahalanobis distance $\le c^2$,

$$D^2(\mathbf{y}) \equiv (\mathbf{y}-\bar{\mathbf{y}})^\mathsf{T}\,\mathbf{S}^{-1}\,(\mathbf{y}-\bar{\mathbf{y}}) \le c^2$$

  $\mathbf{S}$ = sample variance-covariance matrix
  - **Radius**: when $\mathbf{y}$ is ≈ bivariate normal, $D^2(\mathbf{y})$ has a large-sample χ^2_2 distribution with 2 degrees of freedom.
    - $c^2 = \chi^2_2(0.40) \approx 1$: 1 std. dev univariate ellipse– 1D shadows: $\bar{y} \pm 1s$
    - $c^2 = \chi^2_2(0.68) = 2.28$: 1 std. dev bivariate ellipse
    - $c^2 = \chi^2_2(0.95) \approx 6$: 95% data ellipse, 1D shadows: Scheffé intervals
  - **Construction**: Transform the unit circle, $\mathcal{U} = (\sin\boldsymbol{\theta}, \cos\boldsymbol{\theta})$,

$$\mathcal{E}_c = \bar{\mathbf{y}} + c\mathbf{S}^{1/2}\mathcal{U}$$

  $\mathbf{S}^{1/2}$ = any "square root" of $\mathbf{S}$ (e.g., Cholesky)
  - **Robustify**: Use robust estimate of $\mathbf{S}$, e.g., MVE (mimimum volume ellipsoid)
- p **variables**: Extends naturally to p-dimensional ellipsoids

The univariate linear model

- **Model**: $\mathbf{y}_{n\times 1} = \mathbf{X}_{n\times q}\,\boldsymbol{\beta}_{q\times 1} + \boldsymbol{\epsilon}_{n\times 1}$, with $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I}_n)$
- **LS estimates**: $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$
- **General Linear Test**: $H_0 : \mathbf{C}_{h\times q}\,\boldsymbol{\beta}_{q\times 1} = \mathbf{0}$, where $\mathbf{C}$ = matrix of constants; rows specify h linear combinations or contrasts of parameters.
- e.g., Test of $H_0 : \beta_1 = \beta_2 = 0$ in model $y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \epsilon_i$

$$\mathbf{C}\boldsymbol{\beta} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

- All → F-test: How big is SS_H relative to SS_E?

$$F = \frac{SS_H/\mathrm{df}_h}{SS_E/\mathrm{df}_e} = \frac{MS_H}{MS_E} \longrightarrow (MS_H - F\,MS_E) = 0$$

The multivariate linear model

- **Model**: $\mathbf{Y}_{n\times p} = \mathbf{X}_{n\times q}\,\mathbf{B}_{q\times p} + \mathbf{U}$, for p responses, $\mathbf{Y} = (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_p)$
- **General Linear Test**: $H_0 : \mathbf{C}_{h\times q}\,\mathbf{B}_{q\times p} = \mathbf{0}_{h\times p}$
- Analogs of sums of squares, SS_H and SS_E are $(p \times p)$ matrices, $\mathbf{H}$ and $\mathbf{E}$,

$$\mathbf{H} = (\mathbf{C}\widehat{\mathbf{B}})^{\mathsf{T}}\,[\mathbf{C}(\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-}\mathbf{C}^{\mathsf{T}}]^{-1}\,(\mathbf{C}\widehat{\mathbf{B}})\ ,$$

$$\mathbf{E} = \mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{Y}^{\mathsf{T}}[\mathbf{I} - \mathbf{H}]\mathbf{Y}\ .$$

- Analog of univariate F is

$$\det(\mathbf{H} - \lambda\mathbf{E}) = 0\ ,$$

- How big is $\mathbf{H}$ relative to $\mathbf{E}$?
  - Latent roots $\lambda_1, \lambda_2, \dots \lambda_s$ measure the "size" of $\mathbf{H}$ relative to $\mathbf{E}$ in $s = \min(p, df_h)$ orthogonal directions.
  - Test statistics (Wilks' Λ, Pillai trace criterion, Hotelling-Lawley trace criterion, Roy's maximum root) all combine info across these dimensions

Motivating Example: Romano-British Pottery

Tubb, Parker & Nicholson analyzed the chemical composition of 26 samples of Romano-British pottery found at four kiln sites in Britain.

- Sites: Ashley Rails, Caldicot, Isle of Thorns, Llanedryn
- Variables: aluminum (Al), iron (Fe), magnesium (Mg), calcium (Ca) and sodium (Na)
- → One-way MANOVA design, 4 groups, 5 responses

```
R> library(heplots)
R> Pottery

         Site   Al   Fe   Mg   Ca   Na
1   Llanedyrn 14.4 7.00 4.30 0.15 0.51
2   Llanedyrn 13.8 7.08 3.43 0.12 0.17
3   Llanedyrn 14.6 7.09 3.88 0.13 0.20
 . . .
25 AshleyRails 14.8 2.74 0.67 0.03 0.05
26 AshleyRails 19.1 1.64 0.60 0.10 0.03
```


Motivating Example: Romano-British Pottery

Questions:

- **Can** the content of Al, Fe, Mg, Ca and Na differentiate the sites?
- **How to understand** the contributions of chemical elements to discrimination?

Numerical answers:

```
R> pottery.mod <- lm(cbind(Al, Fe, Mg, Ca, Na) ~ Site)
R> Manova(pottery.mod)

Type II MANOVA Tests: Pillai test statistic
     Df test stat approx F num Df den Df  Pr(>F)
Site  3      1.55     4.30     15     60 2.4e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

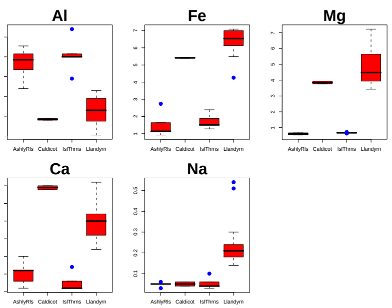
What have we learned?

- **Can**: YES! We can discriminate sites.
- But: **How to understand** the pattern(s) of group differences: ???

Motivating Example: Romano-British Pottery

Univariate plots are limited

- Do not show the *relations* of variables to each other

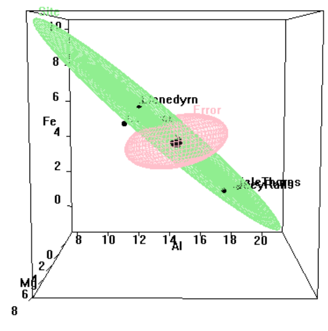


Motivating Example: Romano-British Pottery

Visual answer: HE plot

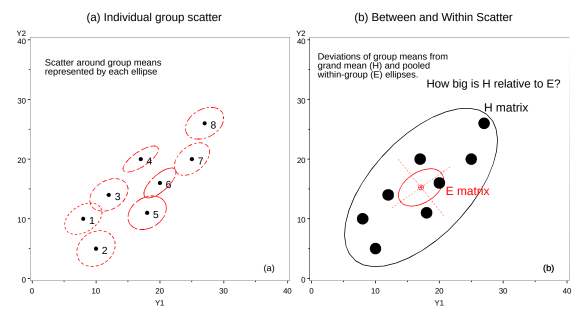
- Shows variation of means ($\mathbf{H}$) relative to residual ($\mathbf{E}$) variation
- Size and orientation of $\mathbf{H}$ wrt $\mathbf{E}$: *how much* and *how* variables contribute to discrimination
- Evidence scaling: $\mathbf{H}$ is scaled so that it projects outside $\mathbf{E}$ *iff* null hypothesis is rejected.

Run heplot-movie.ppt




```
R> heplot3d(pottery.mod)
```

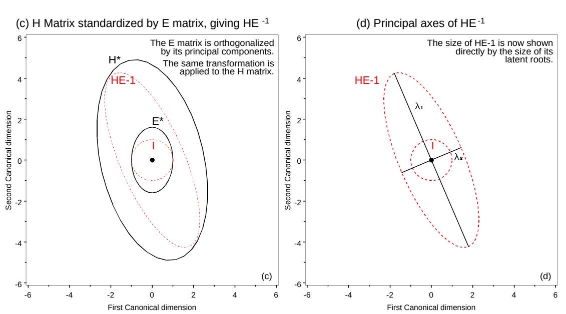

HE plots: Visualizing H and E (co) variation



Ideas behind multivariate tests: (a) Data ellipses; (b) $\mathbf{H}$ and $\mathbf{E}$ matrices

- $\mathbf{H}$ ellipse: data ellipse for fitted values, $\hat{\mathbf{y}}_{ij} = \bar{\mathbf{y}}_j$.
- $\mathbf{E}$ ellipse: data ellipse of residuals, $\hat{\mathbf{y}}_{ij} - \bar{\mathbf{y}}_j$.

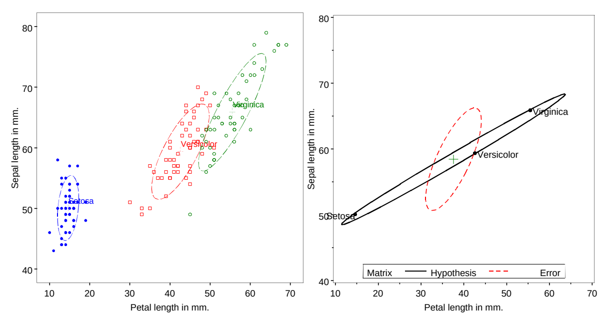
HE plots: Visualizing multivariate hypothesis tests



Ideas behind multivariate tests: latent roots & vectors of $\mathbf{HE}^{-1}$

- $\lambda_i, i = 1, \dots df_h$ show size(s) of $\mathbf{H}$ relative to $\mathbf{E}$.
- latent vectors show canonical directions of maximal difference.

HE plot for iris data



(a) Data ellipses and (b) $\mathbf{H}$ and $\mathbf{E}$ matrices (scaled by $1/df_e$: effect size)

- $\mathbf{H}$ ellipse: data ellipse for fitted values, $\hat{\mathbf{y}}_{ij} = \bar{\mathbf{y}}_j$.
- $\mathbf{E}$ ellipse: data ellipse of residuals, $\hat{\mathbf{y}}_{ij} - \bar{\mathbf{y}}_j$.

HE plot details: H and E matrices

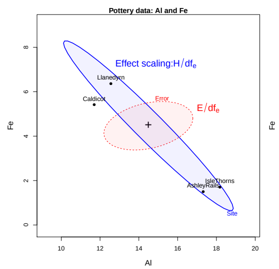
Recall the data on 5 chemical elements in samples of Romano-British pottery from 4 kiln sites:

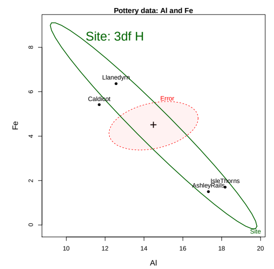
```
R> summary(Manova(pottery.mod))

Sum of squares and products for error:
      Al     Fe     Mg     Ca     Na
Al 48.29  7.080  0.608  0.106  0.589
Fe  7.08 10.951  0.527 -0.155  0.067
Mg  0.61  0.527 15.430  0.435  0.028
Ca  0.11 -0.155  0.435  0.051  0.010
Na  0.59  0.067  0.028  0.010  0.199
------------------------------------

Term: Site

Sum of squares and products for hypothesis:
       Al     Fe     Mg    Ca    Na
Al  175.6 -149.3 -130.8 -5.89 -5.37
Fe -149.3  134.2  117.7  4.82  5.33
Mg -130.8  117.7  103.4  4.21  4.71
Ca   -5.9    4.8    4.2  0.20  0.15
Na   -5.4    5.3    4.7  0.15  0.26
```

- **E matrix**: Within-group (co)variation of residuals
  - diag: SSE for each variable
  - off-diag: ∼ partial correlations
- **H matrix**: Between-group (co)variation of means
  - diag: SSH for each variable
  - off-diag: ∼ correlations of means
- How big is $\mathbf{H}$ relative to $\mathbf{E}$?
- Ellipsoids: $\dim(\mathbf{H}) = \text{rank}(\mathbf{H}) = \min(p, df_h)$

HE plot details: Scaling **H** and **E**

- The E ellipse is divided by $df_e = (n-p) \to$ data ellipse of residuals
  - Centered at grand means $\to$ show factor means in same plot.
- "Effect size" scaling– $\mathbf{H}/df_e \to$ data ellipse of fitted values.
- "Significance" scaling– H ellipse protrudes beyond E ellipse *iff* H_0 can be rejected by Roy maximum root test
  - $H/(\lambda_\alpha df_e)$ where λ_α is critical value of Roy's statistic at level α.
  - direction of **H** wrt **E** $\mapsto$ linear combinations that depart from H_0.






```
R> heplot(pottery.mod, size="effect")   R> heplot(pottery.mod,
size="evidence")
```


HE plot details: Contrasts and linear hypotheses

- An overall effect $\mapsto$ an **H** ellipsoid of $s = \min(p, df_h)$ dimensions
- Linear hypotheses, of the form $H_0 : \mathbf{C}_{h \times q} \mathbf{B}_{q \times p} = \mathbf{0}_{h \times p} \mapsto$ sub-ellipsoid of dimension h, e.g., 2 df test:

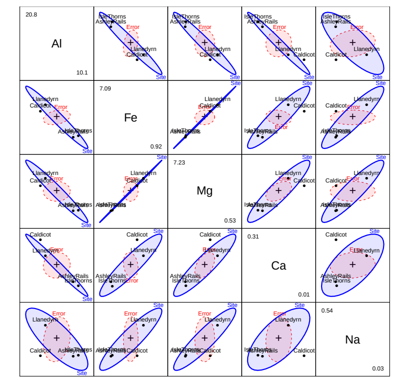
$$\mathbf{C} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

- 1D tests and contrasts $\mapsto$ degenerate 1D ellipses (lines)
- Geometry:
  - Sub-hypotheses are tangent to enclosing hypotheses
  - Orthogonal contrasts form conjugate axes

HE plot matrices: All bivariate views

AL stands out – opposite pattern $r(\overline{Fe}, \overline{Mg}) \approx 1$

Jump to low-D



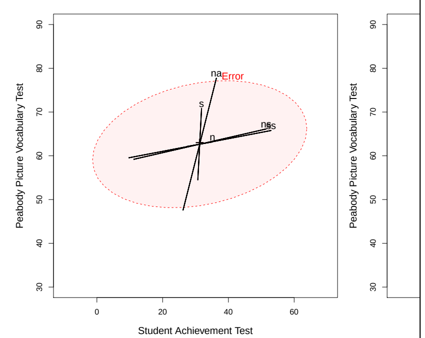

```
R> pairs(pottery.mod)
```


HE plots for Multivariate Multiple Regression

- **Model**: $\mathbf{Y} = \mathbf{X}\mathbf{B} + \mathbf{U}$, where cols of $\mathbf{X}$ are quantitative.
- **Overall test**: $H_0 : \mathbf{B} = \mathbf{0}$ (all coefficients for all responses are zero)
  - $\to \mathbf{C} = \mathbf{I}$ in GLT $\to \mathbf{H} = \widehat{\mathbf{B}}^\mathsf{T} (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1} \widehat{\mathbf{B}} = \widehat{\mathbf{Y}}^\mathsf{T} \widehat{\mathbf{Y}}$
- **Individual predictors**: $H_0 : \beta_i = \mathbf{0}$
  - $\to \mathbf{C} = (0, 0, \ldots, 1, 0, \ldots, 0) \to \mathbf{H}_i = \hat{\beta}_i^\mathsf{T} (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1} \hat{\beta}_i$
- **HE plot**
  - Overall **H** ellipse: how predictors relate collectively to responses
  - Individual **H** ellipses (rank(**H**)=1 $\to$ vectors):
  - orientation $\to$ relation of $\mathbf{x}_i$ to $\mathbf{y}_1, \mathbf{y}_2$
  - length $\to$ strength of relation
  - collection of individual **H** vectors $\to$ how predictors contribute to overall test.

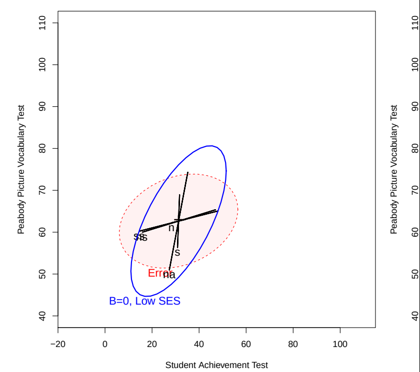
HE plots for MMRA: Example

- Rohwer data on $n = 37$ low SES children, for 5 PA tasks (N, S, NS, NA, SS) predicting intelligence/achievement (PPVT, SAT, Raven)
- Only NA is individually significant (in this view)
- ... but overall test highly significant
- NA & S contribute to predicting PPVT
- NS & SS contribute to predicting SAT



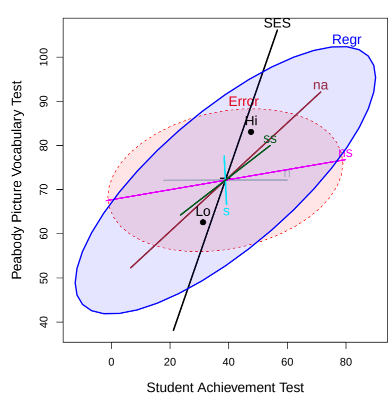
HE plots for MMRA: MANCOVA

- Rohwer data on $n_1 = 37$ low SES, and $n_2 = 32$ high SES children
- Fit separate regressions for each group
- Are regressions parallel?
- Are they coincident?



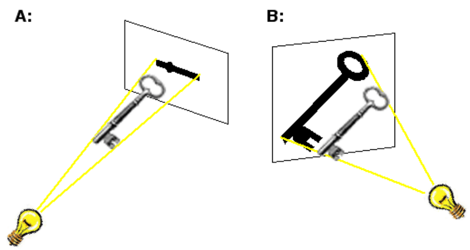
HE plots for MMRA: MANCOVA

- Rohwer data on $n_1 = 37$ low SES, and $n_2 = 32$ high SES children
- Fit MANCOVA model (assuming equal slopes)



Low-D displays of high-D data

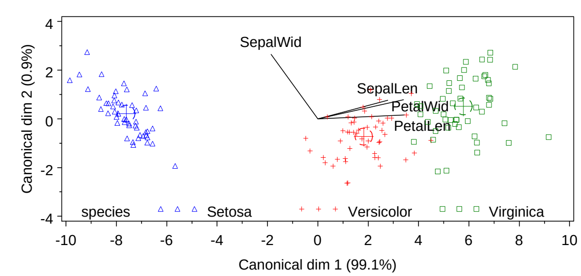
- High-D data often shown in 2D (or 3D) views— orthogonal projections in variable space— scatterplot
- Dimension-reduction techniques: project the data into subspace that has the largest *shadow*— e.g., accounts for largest variance.
- $\to$ low-D approximation to high-D data



A: minimum-variance projection; B: maximum variance projection

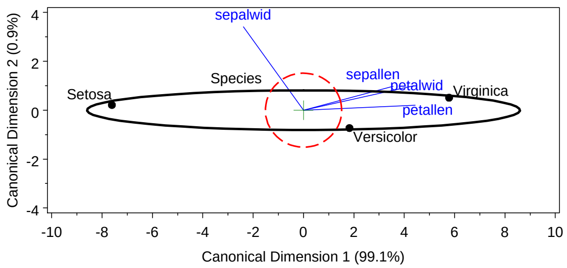
Canonical discriminant HE plots

- As with biplot, we can visualize MLM hypothesis variation for *all* responses by projecting **H** and **E** into low-rank space.
- Canonical projection: $\mathbf{Y}_{n \times p} \mapsto \mathbf{Z}_{n \times s} = \mathbf{Y}\mathbf{E}^{-1/2}\mathbf{V}$, where $\mathbf{V}$ = eigenvectors of $\mathbf{H}\mathbf{E}^{-1}$.
- This is the view that maximally discriminates among groups, ie max. **H** wrt **E** !



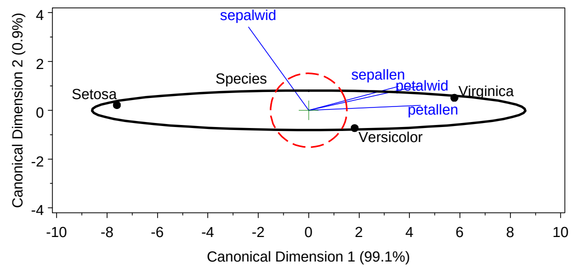
Canonical discriminant HE plots

- Canonical HE plot is just the HE plot of canonical scores, $(\mathbf{z}_1, \mathbf{z}_2)$ in 2D,
- or, $\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3$, in 3D.
- As in biplot, we add vectors to show relations of the $\mathbf{y}_i$ response variables to the canonical variates.
- variable vectors here are structure coefficients = correlations of variables with canonical scores.



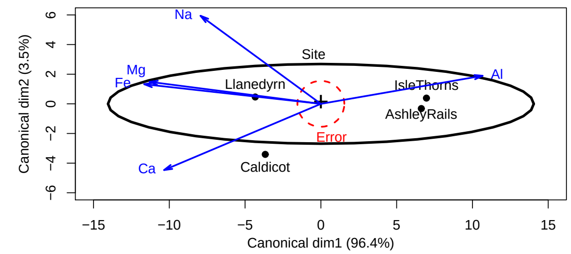
Canonical discriminant HE plots: Properties

- Canonical variates are uncorrelated: **E** ellipse is spherical
- $\mapsto$ axes must be equated to preserve geometry
- Variable vectors show how variables discriminate among groups
- Lengths of variable vectors $\sim$ contribution to discrimination



Canonical discriminant HE plots: Pottery data

- Canonical HE plots provide 2D (3D) visual summary of **H** vs. **E** variation
- Pottery data: $p = 5$ variables, 4 groups $\mapsto df_H = 3$
- Variable vectors: Fe, Mg and Al contribute to distinguishing (Caldicot, Llandryn) from (Isle Thorns, Ashley Rails): 96.4% of mean variation
- Na and Ca contribute an additional 3.5%. End of story!



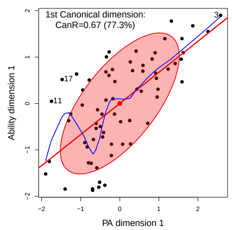
Run heplot-movie.ppt

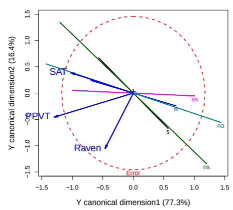
Visualizing Canonical Correlation Analysis

- Basic idea: another instance of low-rank approximation

CCA is to *MMReg* as *CDA* is to *MANOVA*

- $\rightarrow$ For quantitative predictors, provides an alternative view of $\mathbf{Y} \sim \mathbf{XB}$ in space of maximal (canonical) correlations.
- The candisc package implements two new views for CCA:
  - `plot()` method to show canonical (X, Y) variates as data
  - `heplot()` method to show $(\mathbf{X}, \mathbf{Y})$ relations as heplots for $\mathbf{Y}$ in CAN space.

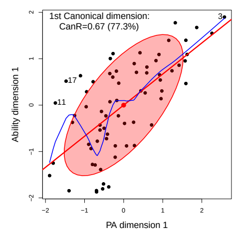


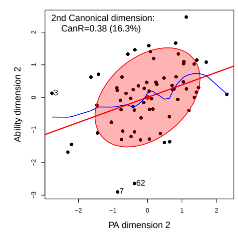


CCA Example: Rohwer data, Ability and PA tests

- `plot()` method shows canonical variates for **X** and **Y** on one dimension
- Smoother shows possible non-linearity
- Point identification highlights unusual observations

```
R> library(candisc)
R> cc <- cancor(cbind(SAT, PPVT, Raven) ~ n + s + ns + na + ss,
+         data=Rohwer, set.names=c("PA", "Ability"))
R> plot(cc, smooth=TRUE, id.n=3)
R> plot(cc, smooth=TRUE, id.n=3, which=2)
```





Robust MLMs

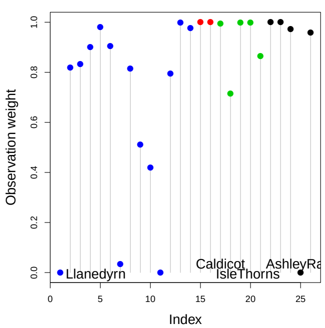
- R has a large collection of packages dealing with robust estimation:
  - `robust::lmrob()`, `MASS::rlm()`, for univariate LMs
  - `robust::glmrob()` for univariate *generalized* LMs
  - High breakdown-bound methods for robust PCA and robust covariance estimation
  - However, none of these handle the fully general MLM
- The heplots package now provides `robmlm()` for robust MLMs:
  - Uses a simple M-estimtor via iteratively re-weighted LS.
  - Weights: calculated from Mahalanobis squared distances, using a simple robust covariance estimator, `MASS::cov.trob()` and a weight function, $\psi(D^2)$.

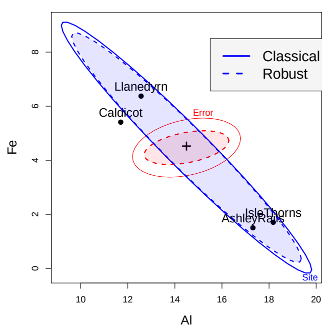
$$D^2 = (\mathbf{Y} - \hat{\mathbf{Y}})^{\mathsf{T}} \mathbf{S}^{-1}_{\mathrm{trob}} (\mathbf{Y} - \hat{\mathbf{Y}}) \sim \chi^2_p \qquad (1)$$

  - This fully extends the `"mlm"` class
  - Compatible with other `mlm` extensions: `car:::Anova` and `heplots::heplot`.
  - Downside: Does not incorporate modern consistency factors or other niceties.

Robust MLMs: Example

For the Pottery data:





- Some observations are given weights ~ 0
- The **E** ellipse is considerably reduced, enhancing apparent significance

Influence diagnostics for MLMs

- Influence measures and diagnostic plots are well-developed for univariate LMs
  - Influence measures: Cook's D, DFFITS, dfbetas, etc.
  - Diagnostic plots: Index plots, `car:::influencePlot()` for LMs
  - However, these are been unavailable for MLMs
- The mvinfluence package now provides:
  - Calculation for multivariate analogs of univariate influence measures (following Barrett & Ling, 1992), e.g., Hat values & Cook's D:

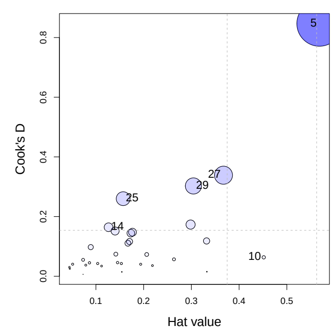
$$H_I = \mathbf{X}_I(\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}_I^{\mathsf{T}} \qquad (2)$$

$$D_I = [vec(\mathbf{B} - \mathbf{B}_{(I)})]^{\mathsf{T}} [\mathbf{S}^{-1} \otimes (\mathbf{X}^{\mathsf{T}}\mathbf{X})][vec(\mathbf{B} - \mathbf{B}_{(I)})] \qquad (3)$$

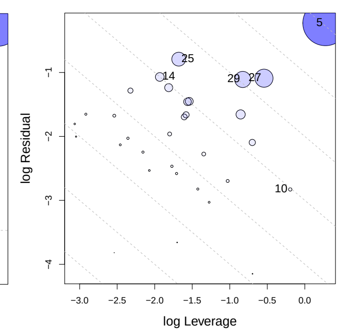
  - Provides deletion diagnostics for subsets (I) of size $m \geq 1$.
  - e.g., $m = 2$ can reveal cases of masking or joint influence.
  - Extension of `influencePlot()` to the multivariate case.
  - A new plot format: leverage-residual (LR) plots (McCulloch & Meeter, 1983)

Influence diagnostics for MLMs: Example

For the Rohwer data:



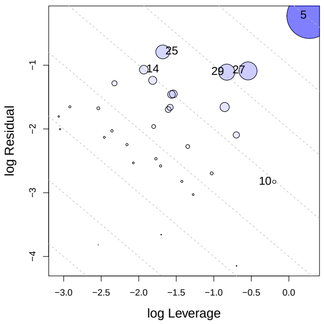
Cook's D vs. generalized Hat value



Leverage - Residual (LR) plot

Influence diagnostics for MLMs: LR plots

- Main idea: Influence $\sim$ Leverage (L) $\times$ Residual (R)
- $\mapsto \log(\mathit{Infl}) = \log(L) + \log(R)$
- $\mapsto$ contours of constant influence lie on lines with slope = -1.
- Bubble size $\sim$ influence (Cook's D)
- This simplifies interpretation of influence measures



Conclusions: Graphical methods for MLMs

Summary & Opportunities

- **Data ellipse**: visual summary of bivariate relations
  - Useful for multiple-group, MANOVA data
  - Embed in scatterplot matrix: pairwise, bivariate relations
  - Easily extend to show partial relations, robust estimators, etc.
- **HE plots**: visual summary of multivariate tests for MANOVA and MMRA
  - Group means (MANOVA) or 1-df H vectors (MMRA) aid interpretation
  - Embed in HE plot matrix: all pairwise, bivariate relations
  - Extend to show partial relations: HE plot of "adjusted responses"
- **Dimension-reduction techniques**: low-rank (2D) visual summaries
  - Biplot: Observations, group means, biplot data ellipses, variable vectors
  - Canonical HE plots: Similar, but for dimensions of maximal discrimination
- **Beautiful and useful geometries**:
  - Ellipses everywhere; eigenvector–ellipse geometries!
  - Visual representation of significance in MLM
  - Opportunities for other extensions

— FIN —