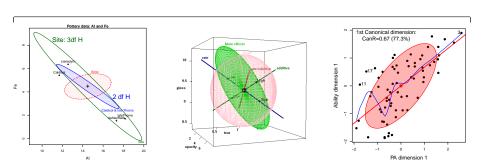
Recent Advances in Visualizing Multivariate Linear Models

Michael Friendly Matthew Sigal with appreciation to Georges Monette & John Fox

Statistics Day @ York, April 5, 2013



Outline

- Background
 - Visual overview
 - Data ellipses
 - The Multivariate Linear Model
 - Motivating example
- 2 Hypothesis-Error (HE) plots
 - Visualizing H and E (co)variation
 - MANOVA designs
 - MREG designs
 - Reduced-rank displays
 - Low-D displays of high-D data
 - Canonical discriminant HE plots
- Recent extensions
 - Canonical correlation
 - Robust MLMs
 - Influence diagnostics for MLMs
 - Conclusions

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Slides: http://datavis.ca/papers/ssc2013/

Precepts of this work

Visualization

Should be fundamental in statistical theory & practice.

"If I can't picture it, I can't understand it." — Albert Einstein

"In certain problems it was necessary to develop the picture as the method before the mathematics could be really done" — Richard Feynman

Theory into Practice

"The practical power of a statistical test is the product of its' statistical power and the probability of use." — J. W. Tukey, 1959

Computation and Implementation

- Modern statistical methods are often mathematically complex and computationally intensive (e.g., bootstrap, MCMC, asymptotics)
- A general implementation allows these to be tested studied as statistical objects and find flaws in theory or implementation.

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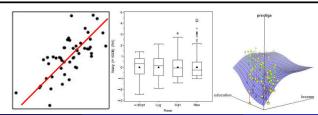
Introduction: The LM family and friends

Models, graphical methods and opportunities

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Classical linear models Generalized linear models LM family: $E(y)=X\beta$, $V(y|X)=\sigma^2I$ GLM: $E(y)=g^{-1}(X\beta)$, $V=V[g^{-1}(X\beta)]$ ANOVA, regression, ... poisson, logistic, loglinear, ... Many graphical methods: effect Some graphical methods: mosaic plots, plots, spread-leverage, influence, ... 4fold plots, diagnostic plots, ... 2+ MLM: $E(Y)=X\beta$, $V(Y|X)=I\otimes\Sigma$ MGLM: ??? MANOVA. MMReg. ... Graphical methods: ??? Graphical methods: ???



Introduction: The LM family and friends

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Classical linear models

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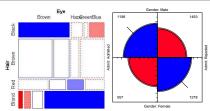
Graphical methods: ???

Generalized linear models

GLM: $E(y)=g^{-1}(X\beta)$, $V=V[g^{-1}(X\beta)]$ poisson, logistic, loglinear, ... Some graphical methods: mosaic plots, 4fold plots, diagnostic plots, ...

MGLM: ???

Graphical methods: ???



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Classical linear models Generalized linear models

- LM family: $E(y)=X\beta$, $V(y|X)=\sigma^2I$ ANOVA, regression, ...
 - Many graphical methods: effect plots, spread-leverage, influence, ...
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4fold plots, diagnostic plots, ...

Not much here

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Fill the gap!

Models, graphical methods and opportunities

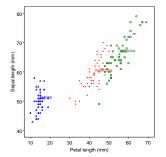
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What we know how to do well (almost)

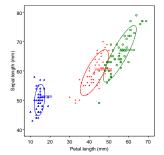
- 2 vars: Scatterplot
- p vars: Scatterplot matrix (all pairs)
- p vars: Reduced-rank display—show max. total variation \mapsto biplot



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

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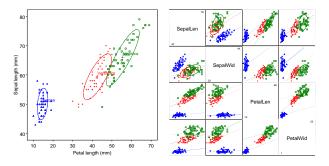
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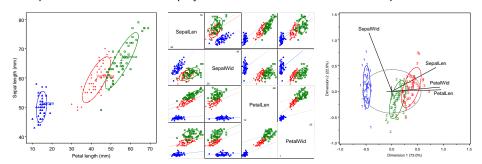
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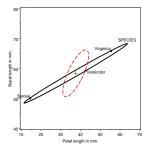
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Visual overview: Multivariate linear model, $\mathbf{Y} = \mathbf{X} \, \mathbf{B} + \mathbf{U}$

What is new here?

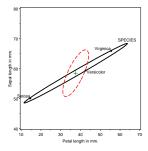
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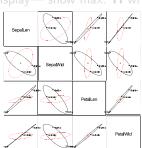


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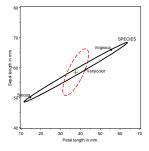


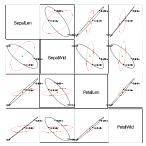


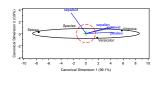
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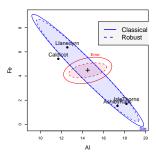




Visual overview: Recent extensions

Extending univariate methods to MLMs:

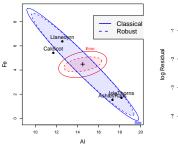
- Robust estimation for MLMs
- Influence measures and diagnostic plots for MLMs
- Visualizing canonical correlation analysis

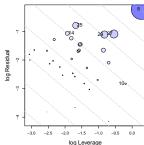


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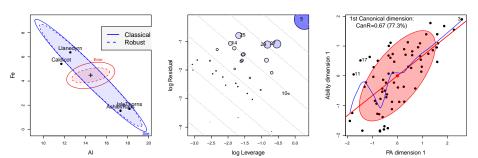




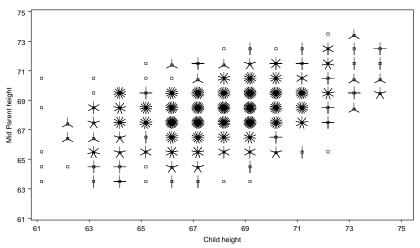
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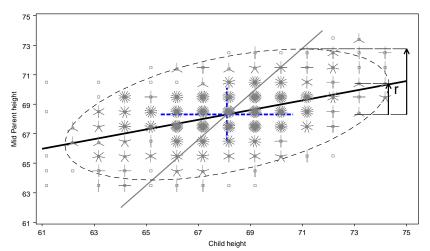
Data Ellipses: Galton's data



Galton's data on Parent & Child height

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Data Ellipses: Galton's data

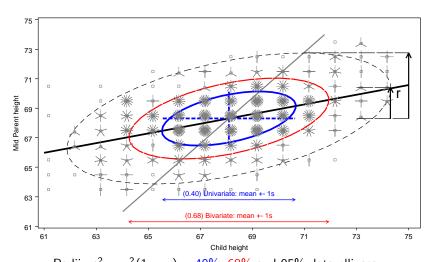


Data ellipse: Shows means, std. devs, regression lines, correlation

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Conclusions

Data Ellipses: Galton's data



Radii: $c^2=\chi_p^2(1-\alpha)$ — 40%, 68% and 95% data ellipses

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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 $< c^2$,

$$D^{2}(\mathbf{y}) \equiv (\mathbf{y} - \overline{\mathbf{y}})^{\mathsf{T}} \mathbf{S}^{-1} (\mathbf{y} - \overline{\mathbf{y}}) \leq c^{2}$$

S =sample variance-covariance matrix

- Radius: when y is \approx bivariate normal, $D^2(y)$ has a large-sample χ^2 distribution with 2 degrees of freedom.
 - $c^2=\chi_2^2(0.40)pprox 1$: 1 std. dev univariate ellipse– 1D shadows: $ar{y}\pm 1s$

 - $c^2 = \chi_2^2(0.68) = 2.28$: 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, $\mathcal{U} = (\sin \theta, \cos \theta)$,

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

 $S^{1/2} = any$ "square root" of S (e.g., Cholesky)

- Robustify: Use robust estimate of S, e.g., MVE (mimimum volume ellipsoid)
- p variables: Extends naturally to p-dimensional ellipsoids

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

$$\mathbf{C}eta = \left[egin{array}{ccc} 0 & 1 & 0 \ 0 & 0 & 1 \end{array}
ight] \left(egin{array}{c} eta_0 \ eta_1 \ eta_2 \end{array}
ight) = \left(egin{array}{c} 0 \ 0 \end{array}
ight)$$

• All \rightarrow F-test: How big is SS_H relative to SS_E ?

$$F = rac{SS_H/\mathrm{df}_h}{SS_F/\mathrm{df}_e} = rac{MS_H}{MS_F} \longrightarrow (MS_H - F \ MS_E) = 0$$

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: $H_0: C_{h\times q} B_{q\times p} = \mathbf{0}_{h\times p}$
- Analogs of sums of squares, SS_H and SS_E are $(p \times p)$ matrices, **H** and **E**,

$$\begin{split} \boldsymbol{H} &= (\boldsymbol{C}\widehat{\boldsymbol{B}})^T [\boldsymbol{C}(\boldsymbol{X}^T\boldsymbol{X})^- \boldsymbol{C}^T]^{-1} (\boldsymbol{C}\widehat{\boldsymbol{B}}) \ , \\ \boldsymbol{E} &= \boldsymbol{U}^T \boldsymbol{U} = \boldsymbol{Y}^T [\boldsymbol{I} - \boldsymbol{H}] \boldsymbol{Y} \ . \end{split}$$

Analog of univariate F is

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

- How big is **H** relative to **E** ?
 - Latent roots $\lambda_1, \lambda_2, \dots \lambda_s$ measure the "size" of **H** relative to **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

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Hypothesis-Error (HE) plots

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 (AI), iron (Fe), magnesium (Mg), calcium (Ca) and sodium (Na)
- One-way MANOVA design, 4 groups, 5 responses

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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:

What have we learned?

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

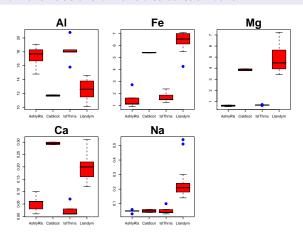
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Hypothesis-Error (HE) plots Reduced-rank displays Recent extensions

Motivating Example: Romano-British Pottery

Univariate plots are limited

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

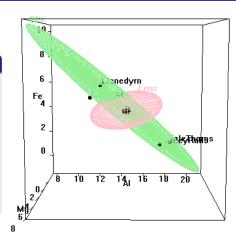


Motivating Example: Romano-British Pottery

Visual answer: HE plot

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

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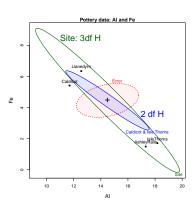


R> heplot3d(pottery.mod)

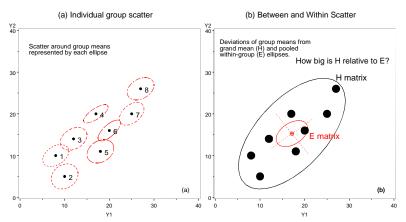
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HE plots: Visualizing **H** and **E** (co) variation

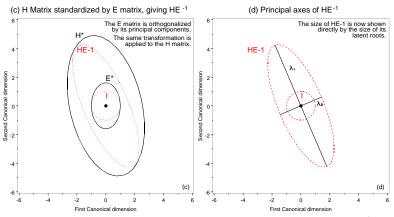


Ideas behind multivariate tests: (a) Data ellipses; (b) H and E matrices

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

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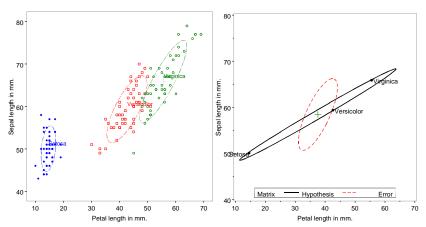
HE plots: Visualizing multivariate hypothesis tests



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

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

HE plot for iris data



- (a) Data ellipses and (b) **H** and **E** matrices (scaled by $1/df_e$: effect size)
- **H** ellipse: data ellipse for fitted values, $\hat{\mathbf{y}}_{ij} = \bar{\mathbf{y}}_{j}$.
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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))

Term: Site

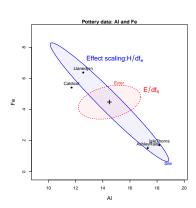
```
Sum of squares and products for hypothesis:
   175.6 -149.3 -130.8 -5.89
Fe -149.3
         134.2
                117.7
Mg - 130.8
         117.7
                 103.4 4.21
          4.8
Ca
    -5.9
                   4.2 0.20
                             0.15
   -5.4
         5.3
Na
          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

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

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

- The E ellipse is divided by $df_e = (n p) \rightarrow$ data ellipse of residuals
 - \bullet Centered at grand means \to show factor means in same plot.
- "Effect size" scaling– $\mathbf{H}/df_e \to \mathrm{data}$ ellipse of fitted values.
- "Significance" scaling

 H ellipse protrudes beyond E ellipse iff H₀ 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 .

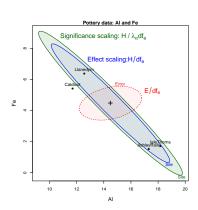


R> heplot(pottery.mod, size="effect")

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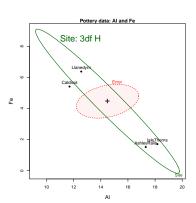
R> heplot(pottery.mod, size="evidence")

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
 H₀: C_{h×q} B_{q×p} = 0_{h×p} → 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 → degenerate 1D ellipses (lines)
- Geometry:
 - Sub-hypotheses are tangent to enclosing hypotheses
 - Orthogonal contrasts form conjugate axes



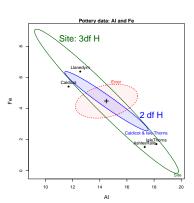
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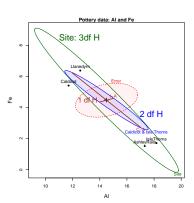
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- Geometry:
 - Sub-hypotheses are tangent to enclosing hypotheses
 - Orthogonal contrasts form conjugate axes

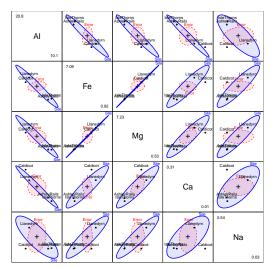


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HE plot matrices: All bivariate views

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

Lump to low-D



R> pairs(pottery.mod)

HE plots for Multivariate Multiple Regression

- Model: Y = XB + U, where cols of X are quantitative.
- **Overall test**: H_0 : $\mathbf{B} = \mathbf{0}$ (all coefficients for all responses are zero)

$$ullet$$
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• Individual predictors: $H_0: \beta_i = 0$

$$ullet$$
 $ullet$ $\mathbf{C} = (0, 0, \dots, 1, 0, \dots, 0)
ightarrow \mathbf{H}_i = \hat{oldsymbol{eta}}_i^\mathsf{T} (\mathbf{X}^\mathsf{T} \mathbf{X})^{-1} \hat{oldsymbol{eta}}_i$

- HE plot
 - Overall H ellipse: how predictors relate collectively to responses
 - Individual H ellipses (rank(H)=1 → vectors):
 - orientation \rightarrow relation of x_i to y_1, y_2
 - length \rightarrow strength of relation
 - ullet collection of individual **H** vectors o how predictors contribute to overall test.

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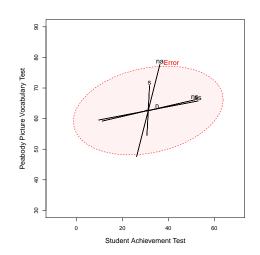
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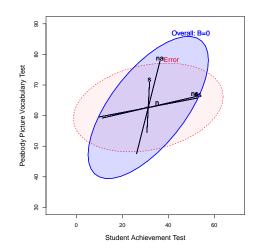
HE plots for MMRA: Example

- 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: Example

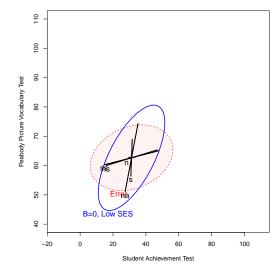
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HE plots for MMRA: MANCOVA

• 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?

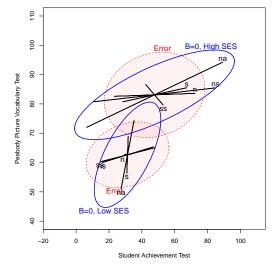


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HE plots for MMRA: MANCOVA

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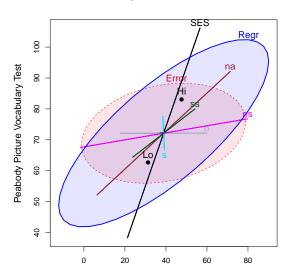
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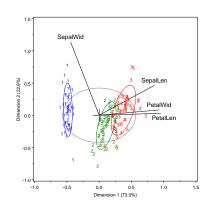
HE plots for MMRA: MANCOVA

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



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 - Motivating example
- 2 Hypothesis-Error (HE) plots
 - Visualizing H and E (co)variation
 - MANOVA designs
 - MREG designs
- Reduced-rank displays
 - Low-D displays of high-D data
 - Canonical discriminant HE plots
- Recent extensions
 - Canonical correlation
 - Robust MI Me
 - Influence diagnostics for MLMs
 - Conclusions



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Low-D displays of high-D data

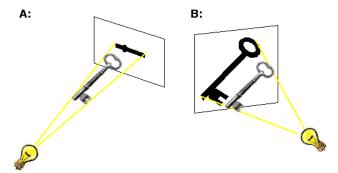
- High-D data often shown in 2D (or 3D) views— orthogonal projections in variable space— scatterplot
- Dimension-reduction techniques: project the data into subspace that has the largest shadow— e.g., accounts for largest variance.
- ullet ightarrow low-D approximation to high-D data

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

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Low-D displays of high-D data

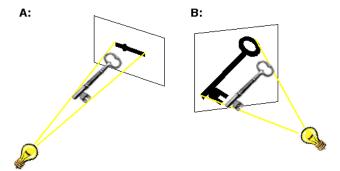
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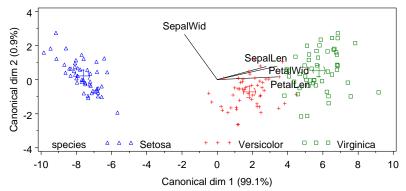
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Hypothesis-Error (HE) plots Reduced-rank displays Recent extensions

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!



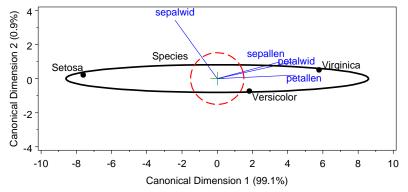
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Hypothesis-Error (HE) plots Reduced-rank displays Recent extensions

Canonical discriminant HE plots

• Canonical HE plot is just the HE plot of canonical scores, (z_1, z_2) in 2D,

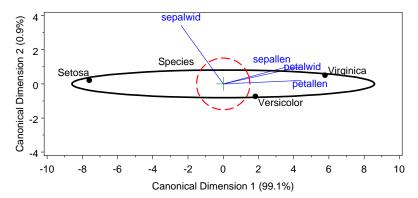
- or, z₁, z₂, z₃, in 3D.
- As in biplot, we add vectors to show relations of the y_i response variables to the canonical variates.
- variable vectors here are structure coefficients = correlations of variables with canonical scores.



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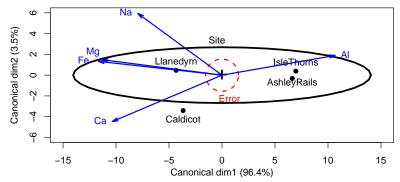
Canonical discriminant HE plots: Properties

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



Canonical discriminant HE plots: Pottery data

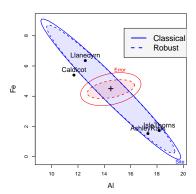
- Canonical HE plots provide 2D (3D) visual summary of **H** vs. **E** variation
- Pottery data: p = 5 variables, 4 groups $\mapsto df_H = 3$
- Variable vectors: Fe, Mg and Al contribute to distingiushing (Caldicot, Llandryn) from (Isle Thorns, Ashley Rails): 96.4% of mean variation
- Na and Ca contribute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



Run heplot-movie.ppt Friendly. Sigal

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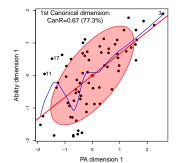
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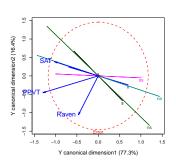
Visualizing Canonical Correlation Analysis

• Basic idea: another instance of low-rank approximation

CCA is to MMReg as CDA is to MANOVA

- ullet For quantitative predictors, provides an alternative view of ${f Y}\sim {f XB}$ 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 (X, Y) relations as heplots for Y in CAN space.

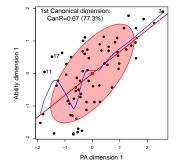


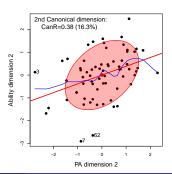


oothesis-Error (HE) plots Reduced-rank displays Recent exte

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





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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, $\psi(D^2)$.

$$D^{2} = (\mathbf{Y} - \widehat{\mathbf{Y}})^{\mathsf{T}} \mathbf{S}_{\mathrm{trob}}^{-1} (\mathbf{Y} - \widehat{\mathbf{Y}}) \sim \chi_{\rho}^{2}$$
 (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.

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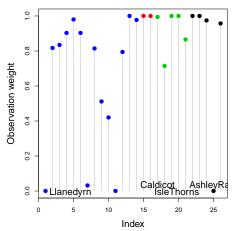
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pothesis-Error (HE) plots Reduced-rank displays

Robust MLMs: Example

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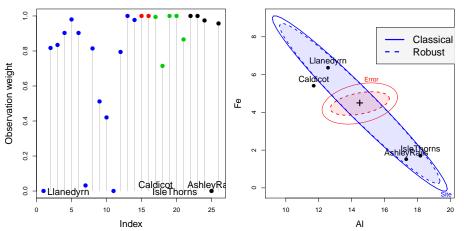


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- The E ellipse is considerably reduced, enhancing apparent significance

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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 have 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:

$$H_{I} = \mathbf{X}_{I} (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}_{I}^{\mathsf{T}}$$
 (2)

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

- Provides deletion diagnostics for subsets (1) of size m > 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.

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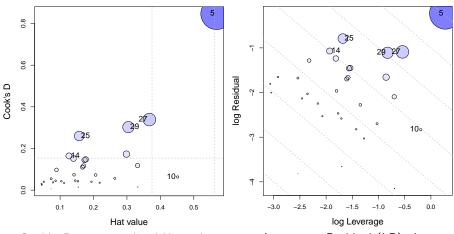
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Influence diagnostics for MLMs: Example

For the Rohwer data:



Cook's D vs. generalized Hat value

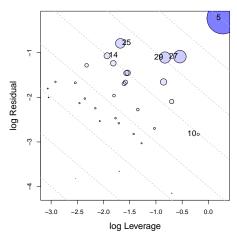
Leverage - Residual (LR) plot

Influence diagnostics for MLMs: LR plots

• Main idea: Influence \sim Leverage (L) \times Residual (R)

- $\bullet \mapsto \log(Infl) = \log(L) + \log(R)$
- contours of constant influence lie

 on lines with slope = -1.
- Bubble size ∼ influence (Cook's D)
- This simplifies interpretation of influence measures



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
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- Beautiful and useful geometries:

 - Opportunities for other extensions

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— FIN —

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