Slide 1
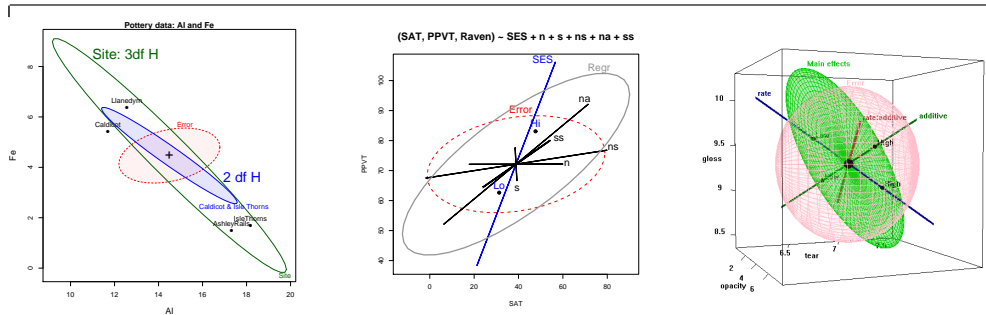
Recent Advances in Visualizing Multivariate Linear Models
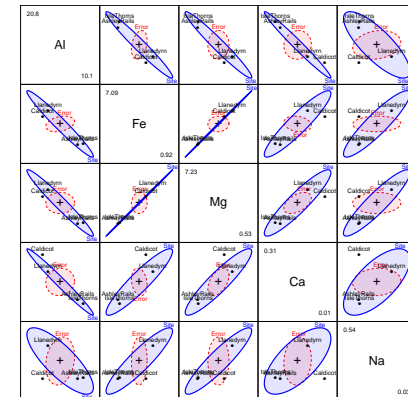
Michael Friendly   Matthew Sigal

May 26–29, 2013, SSC annual Meeting

Slide 2

Outline

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

## Slide 3

Introduction: The LM family and friends

Models, graphical methods and opportunities

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

# of response variables

Slide 4
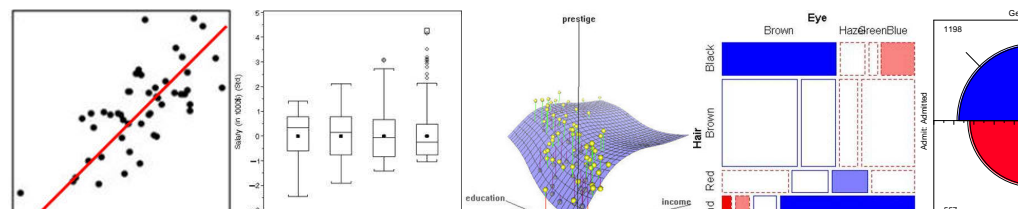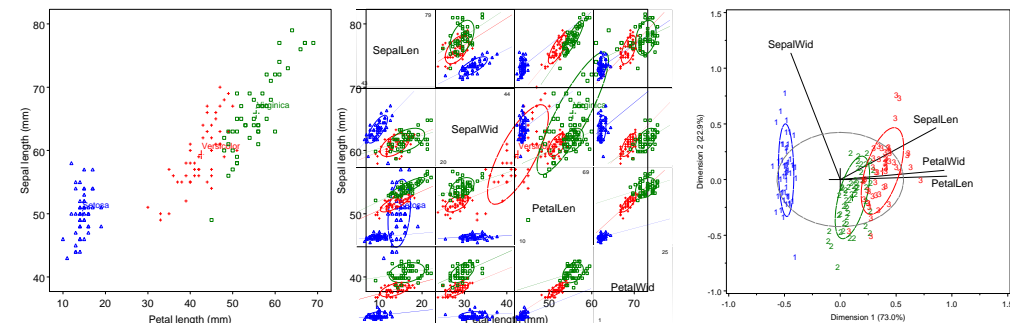
Visual overview: Multivariate data, $\mathbf{Y}_{n\times p}$

What we know how to do well (almost)

- 2 vars: Scatterplot + annotations (data ellipses)
- 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 $\mathbf{H}$ (fitted) and $\mathbf{E}$ (residual) SSP matrices
- p vars: HE plot matrix (all pairs)
- p vars: Reduced-rank display— show max. $\mathbf{H}$ wrt. $\mathbf{E}$ $\mapsto$ Canonical HE plot
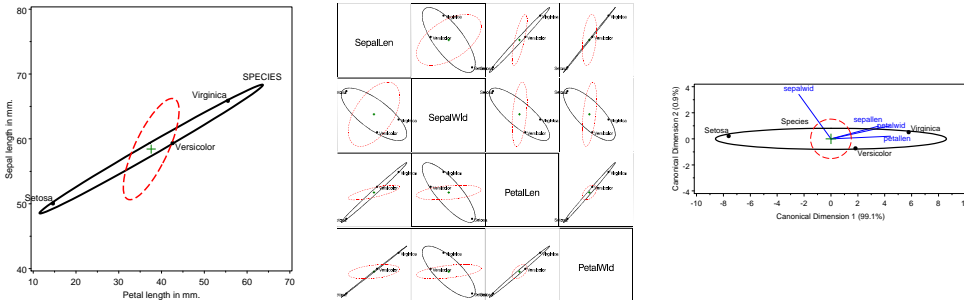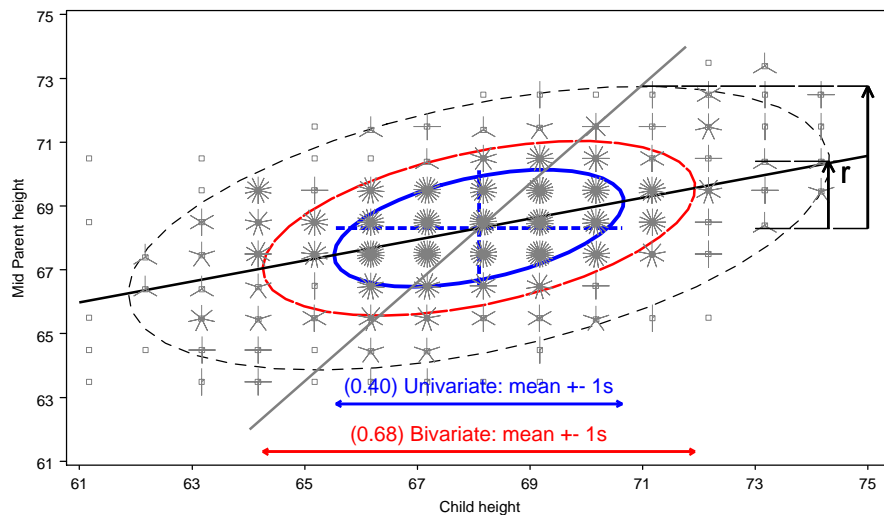
Visual overview: Recent extensions

Extending univariate methods to MLMs:

- Robust estimation for MLMs
- Influence measures and diagnostic plots for MLMs
- Visualizing canonical correlation analysis
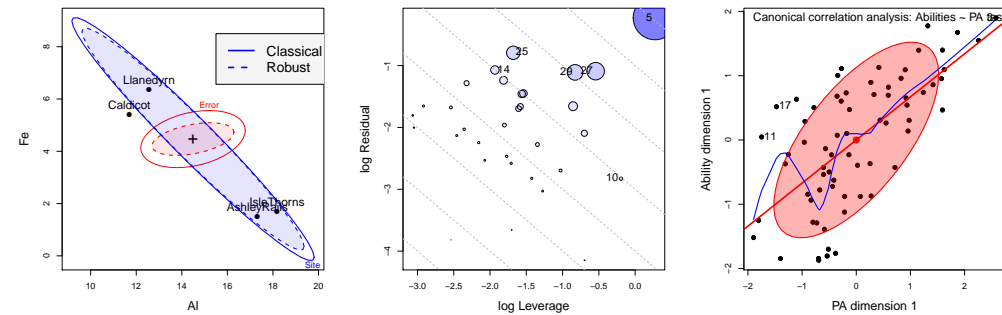
Data Ellipses: Galton's data

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 $\leq c^2$,

  $$D^2(\mathbf{y}) \equiv (\mathbf{y} - \bar{\mathbf{y}})^\top \mathbf{S}^{-1} (\mathbf{y} - \bar{\mathbf{y}}) \leq c^2$$

  $\mathbf{S}$ = sample variance-covariance matrix
  - **Radius**: when $\mathbf{y}$ is $\approx$ 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, $\mathcal{U} = (\sin\theta, \cos\theta)$,

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

  $\mathbf{S}^{1/2}$ = 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**: $\mathbf{y}_{n \times 1} = \mathbf{X}_{n \times q}\,\beta_{q \times 1} + \epsilon_{n \times 1}$, with $\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n)$

- **LS estimates**: $\hat{\beta} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{y}$

- **General Linear Test**: $H_0 : \mathbf{C}_{h \times q}\,\beta_{q \times 1} = \mathbf{0}$, 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 $y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \epsilon_i$

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

- All $\rightarrow$ 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, $\mathbf{Y} = (\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_p)$
- **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 $\lambda_1, \lambda_2, \ldots \lambda_s$ 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)
- $\rightarrow$ 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
```
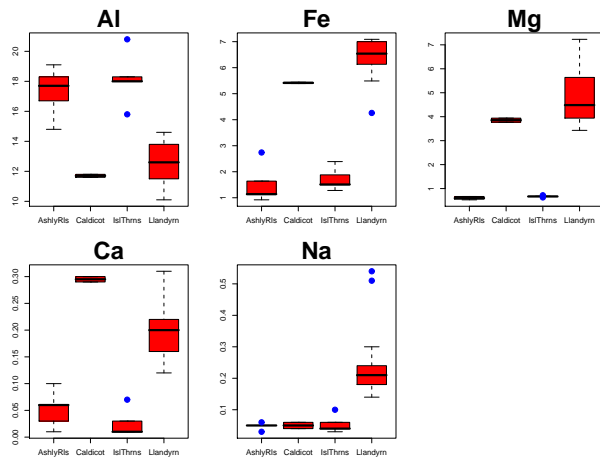
What have we learned?
- **Can**: YES! We can discriminate sites.
- But: **How to understand** the pattern(s) of group differences: ???

Slide 1

Motivating Example: Romano-British Pottery

Univariate plots are limited
- Do not show the *relations* of variables to each other

Slide 2

Motivating Example: Romano-British Pottery
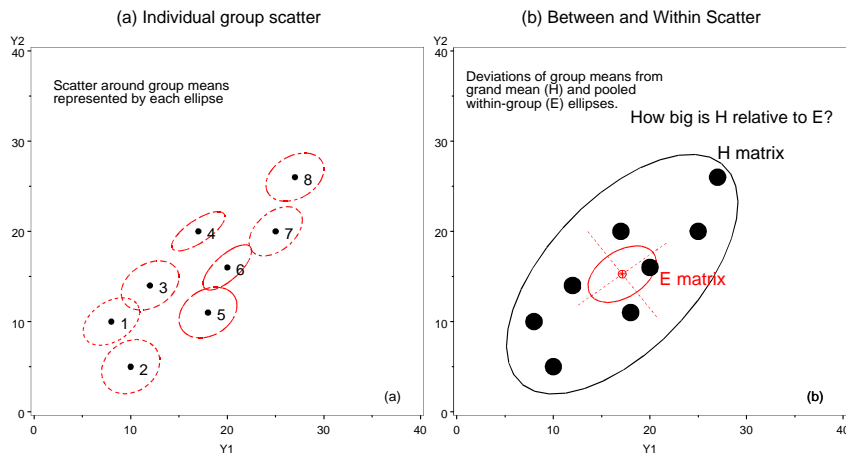
Visual answer: HE plot
- Shows variation of means (**H**) relative to residual (**E**) variation
- Size and orientation of **H** wrt **E**: *how much* and *how* variables contribute to discrimination
- Evidence scaling: **H** is scaled so that it projects outside **E** *iff* null hypothesis is rejected.

Run heplot-movie.ppt
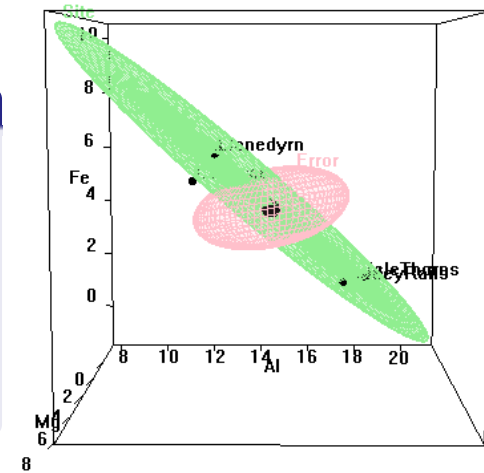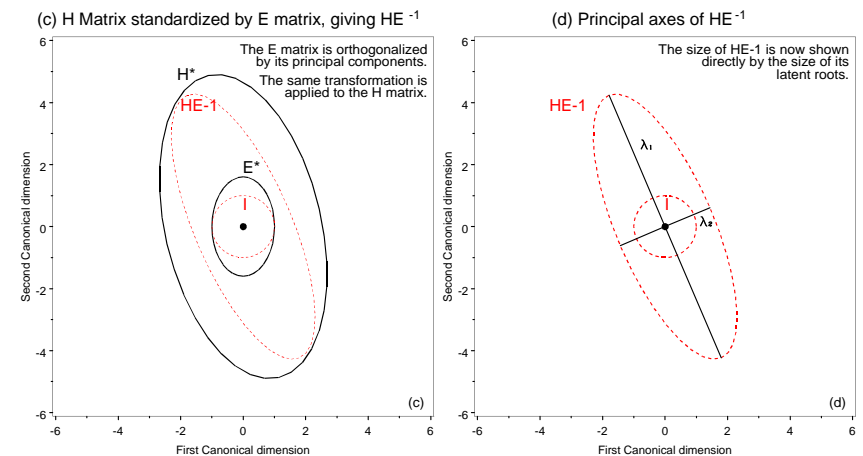

R> heplot3d(pottery.mod)

Slide 3

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, $\hat{\mathbf{y}}_{ij} = \bar{\mathbf{y}}_j$.
- **E** ellipse: data ellipse of residuals, $\hat{\mathbf{y}}_{ij} - \bar{\mathbf{y}}_j$.
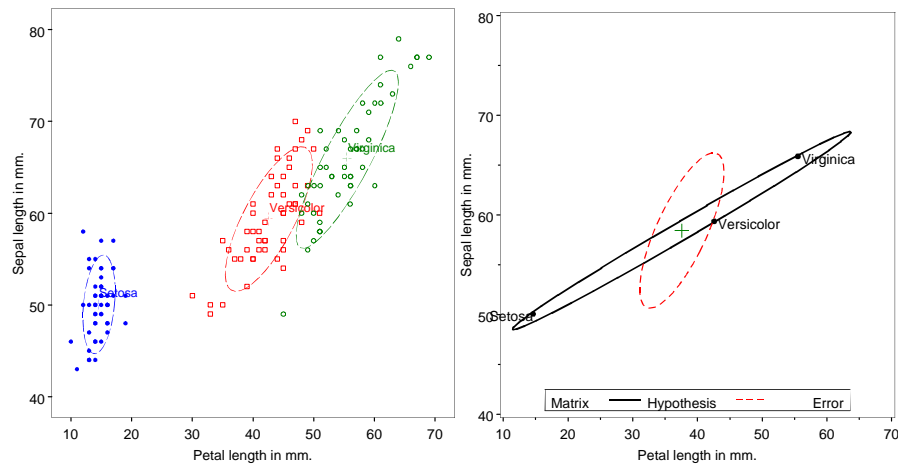
Slide 4

HE plots: Visualizing multivariate hypothesis tests

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

- $\lambda_i, i = 1, \ldots df_h$ 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, $\hat{\mathbf{y}}_{ij} = \bar{\mathbf{y}}_j$.
- **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: $\sim$ partial correlations
- **H** matrix: Between-group (co)variation of means
  - diag: SSH for each variable
  - off-diag: $\sim$ correlations of means
- How big is **H** relative to **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 $df_e = (n - p) \rightarrow$ data ellipse of residuals
  - Centered at grand means $\rightarrow$ show factor means in same plot.
- "Effect size" scaling– $\mathbf{H}/df_e \rightarrow$ 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.
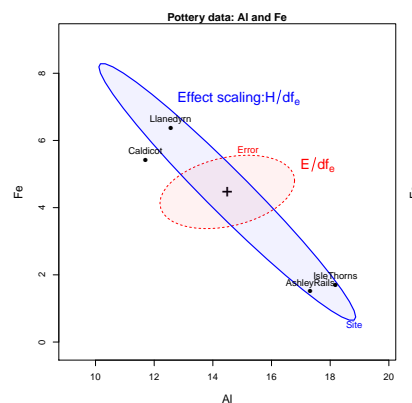
```
R> heplot(pottery.mod, size="effect")   R> heplot(pottery.mod,
size="evidence")
```


Pottery data: Al and Fe

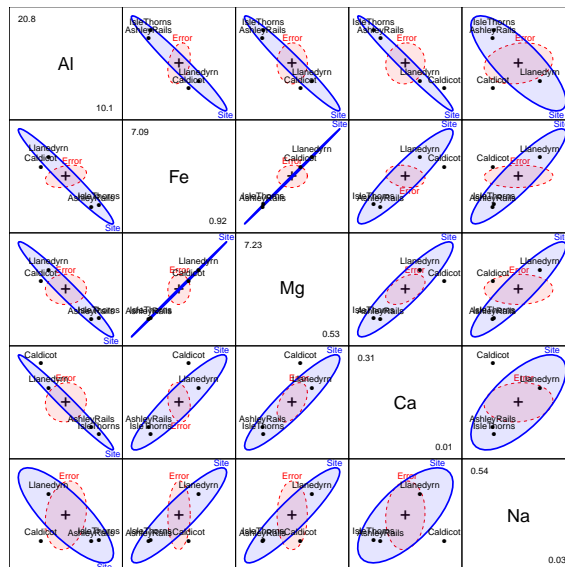
HE plot details: Contrasts and linear hypotheses

- 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
- 1D tests and contrasts $\mapsto$ degenerate 1D ellipses (lines)

Pottery data: Al and Fe
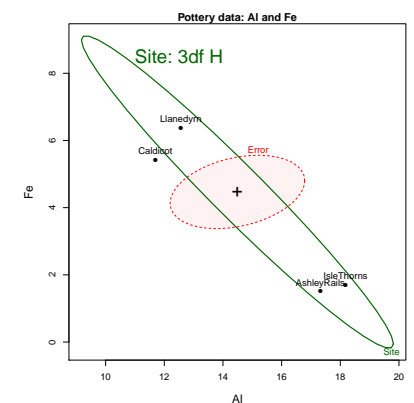
HE plot matrices: All bivariate views

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

R> pairs(pottery.mod)

HE plots for Multivariate Multiple Regression

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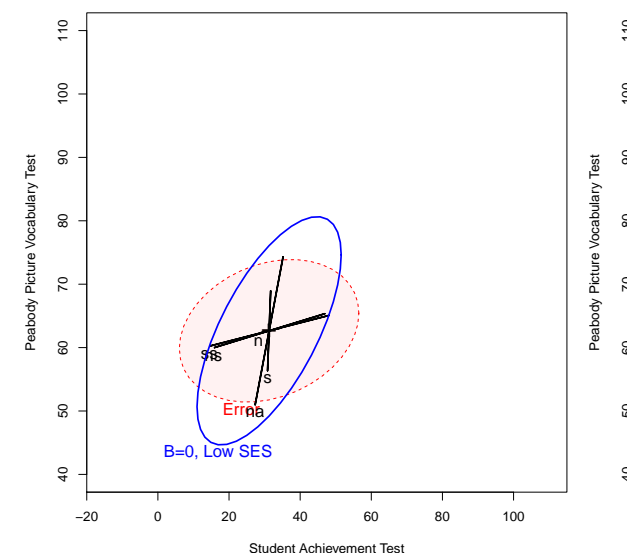
HE plots for MMRA: Example

- 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
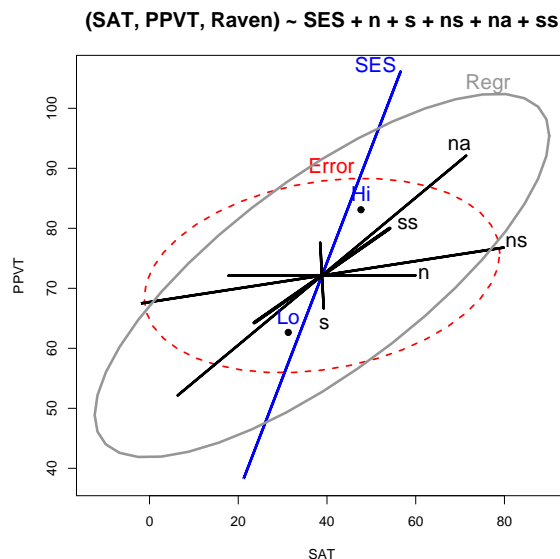- NS & SS contribute to predicting SAT
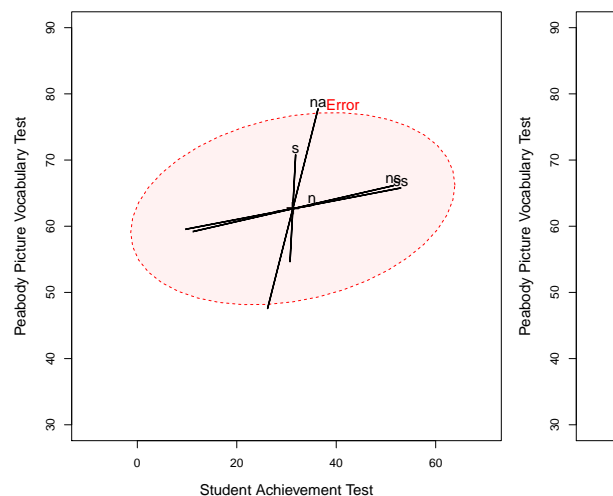
HE plots for MMRA: MANCOVA

- 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)

(SAT, PPVT, Raven) ~ SES + n + s + ns + na + ss

# Low-D displays of high-D data

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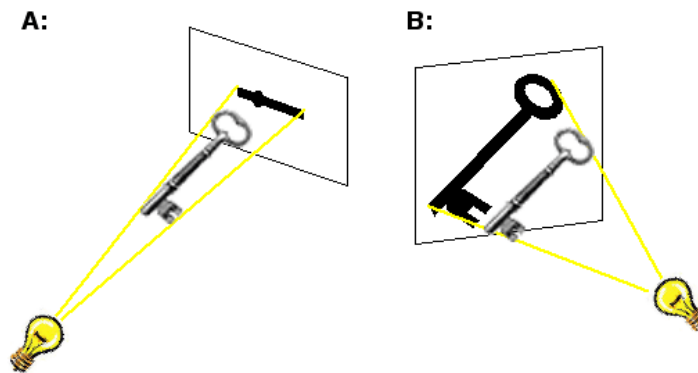

A: minimum-variance projection; B: maximum variance projection

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: $\mathbf{Y}_{n \times p} \mapsto \mathbf{Z}_{n \times s} = \mathbf{YE}^{-1/2}\mathbf{V}$, where $\mathbf{V} =$ eigenvectors of $\mathbf{HE}^{-1}$.
- This is the view that maximally discriminates among groups, ie max. **H** wrt **E** !
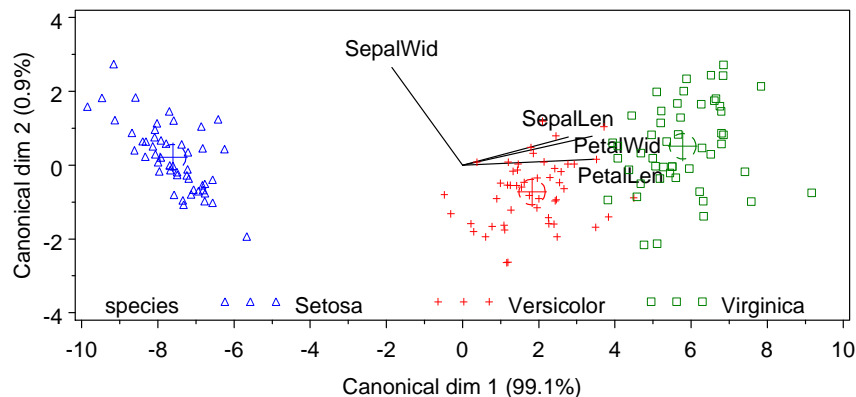
Canonical discriminant HE plots

- 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.
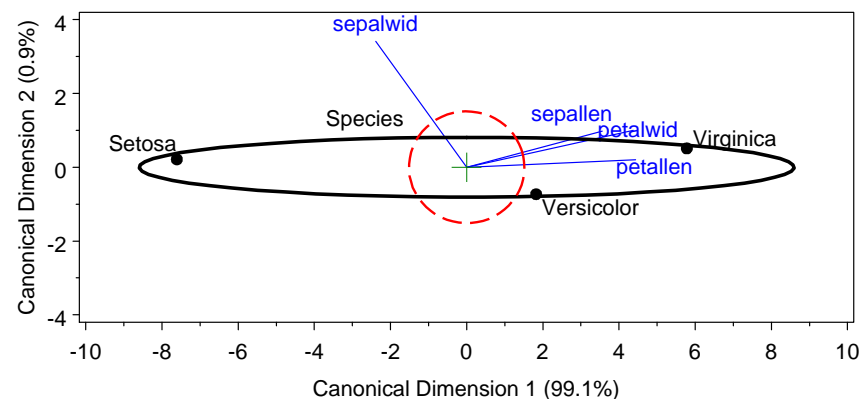
Canonical discriminant HE plots: Properties

- 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
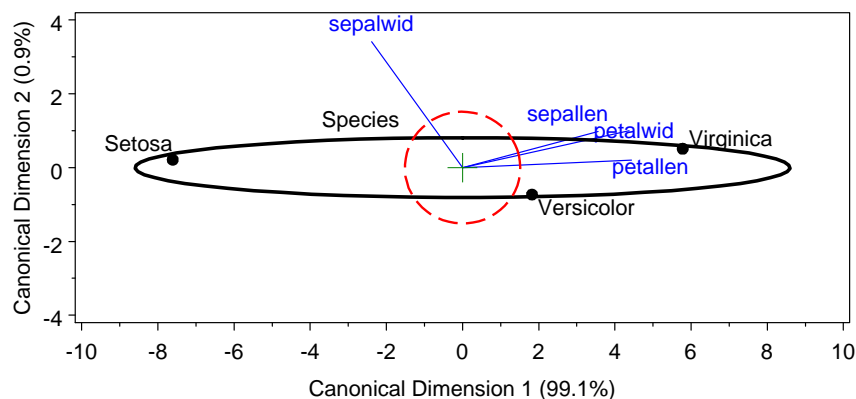
Canonical discriminant HE plots: Pottery data

- 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 distingiushing (Caldicot, Llandryn) from (Isle Thorns, Ashley Rails): 96.4% of mean variation
- Na and Ca contribute an additional 3.5%. End of story!
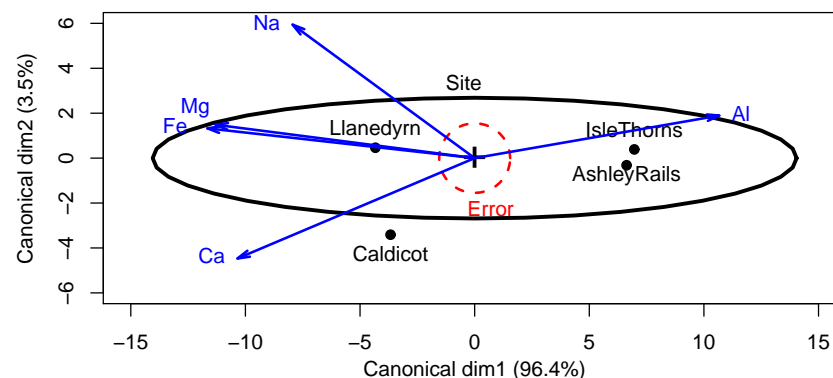

Run heplot-movie.ppt

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, $\psi(D^2)$.

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

  - 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:
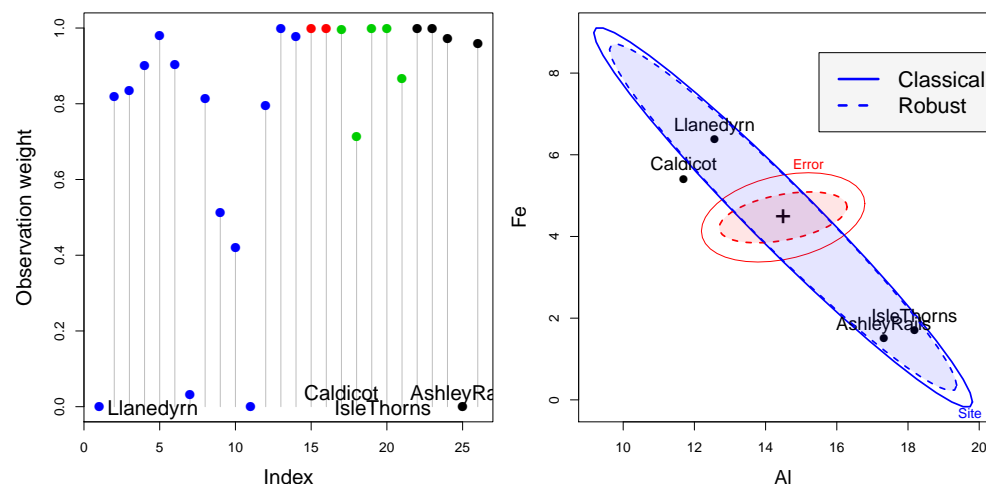
The **E** ellipse is considerably reduced, enhancing apparent significance

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 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:

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

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

  - 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.

Influence diagnostics for MLMs: Example

For the Rohwer data:

Cook's D vs. generalized Hat value   Leverage - Residual (LR) plot
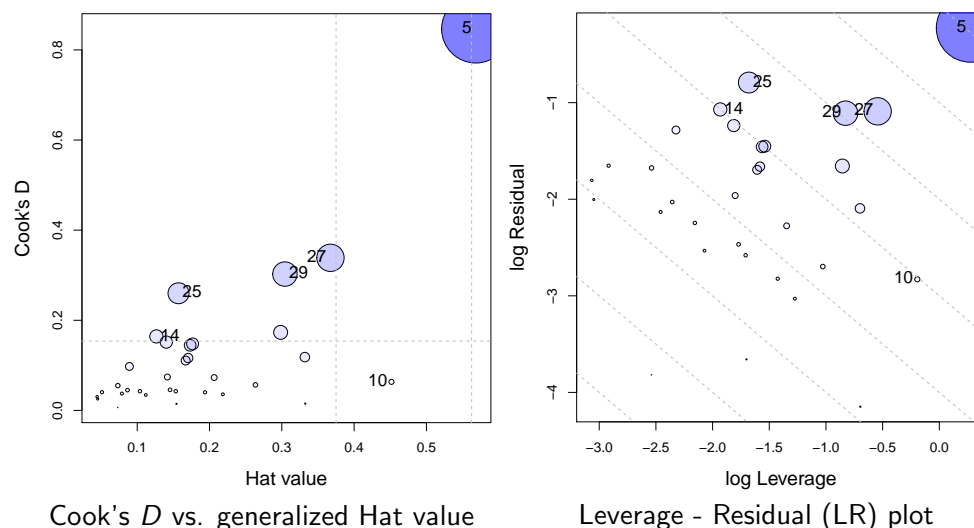
Influence diagnostics for MLMs: LR plots

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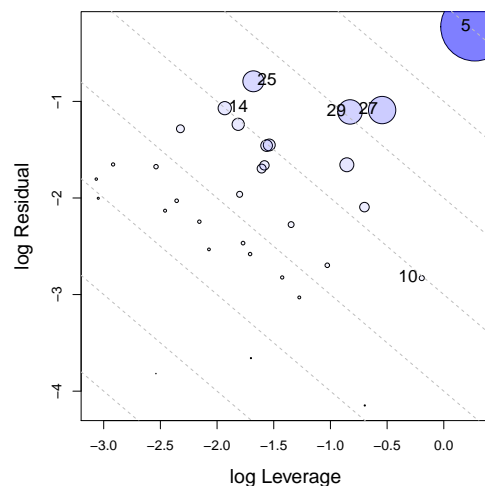
Conclusions: Graphical methods for MLMs

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 —