Subselect 0.9-99: Selecting variable subsets in multivariate linear models

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<u>THE PROBLEM:</u> Finding a k-variable subset that is a good surrogate for a full p-variable data set

CONTEXT:

- **Exploratory data analysis – Subselect 0.1-- 0.9**

  (Cadima, Cerdeira, Duarte Silva and Minhoto -- useR! 2004)

- **Multivariate Linear Models – Subselect 0.9-99**

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A LINEAR HYPOTHESIS FRAMEWORK

$$X = A\ \Psi + U \qquad H0:\ C\ \Psi = 0$$

- **SELECT COLUMNS OF X IN ORDER TO EXPLAIN H1**

PARTICULAR CASES:

CANONICAL CORRELATION ANALYSIS $A = [1 \mid Y] \quad C = [0 \mid I\,]$

LINEAR DISCRIMINANT ANALYSIS

$$A = [1_g\,] \qquad \Psi = [\mu_g] \qquad C = \begin{bmatrix} 1 & -1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 1 & 0 & \ldots & -1 \end{bmatrix}$$

MULTI-WAY MANOVA/MANCOVA EFFECTS

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$\Omega = \mathcal{R}(A)$ $\omega = \mathcal{R}(A) \cap \mathcal{N}(C)$ **r = dim(Ω) - dim(ω)**

$\mathbf{ccr}_i^2 = \mathbf{Eigval}_i(\mathbf{T}^{-1}\mathbf{H})$ **T = X' (I - P_ω) X** **H = X' (P_Ω - P_ω) X**

Comparison Criteria: **Multivariate Indices**

$$\mathbf{ccr}_1^2$$

(*max* ccr_1^2 ⇔ *max* Roy λ_1)

$$\varsigma^2 = 1 - \frac{\mathbf{r}}{\sum_{i=1}^{r}\left(1 - \mathbf{ccr}_i^2\right)^{-1}}$$

(*max* ς^2 ⇔ *max* Lawley-Hotelling trace)

$$\tau^2 = 1 - \left(\prod_{i=1}^{r}(1 - \mathbf{ccr}_i^2)\right)^{1/r}$$

(*max* τ^2 ⇔ *min* Wilks Λ)

$$\xi^2 = \frac{\sum_{i=1}^{r}\mathbf{ccr}_i^2}{\mathbf{r}}$$

(*max* ξ^2 ⇔ *max* Bartlei-Pillai trace)

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The Subselect Package

Search routines for (combinatorial) criteria optimization

Exact Algorithm:

leaps - **based on Furnival and Wilson´s leaps and bounds algorithm for linear regression**

- **viable with up to 30 - 35 original variables**

Heuristics:

anneal - **simulated annealing**

genetic - **genetic algorithm**

improve - **restricted local improvement**

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Principal arguments of search routines :

mat	- Total SSCP data matrix (T)
H	- Effect SSCP data matrix
r	- Expected rank of the H matrix
criterion	- “ccr12”, “tau2”, “xi2” or “zeta2”
kmin, kmax	- minimum and maximum subset dimensionalities sought

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<u>Other arguments :</u>

- Tuning parameters for heuristics

- Maximum time allowed for exact search

- **Variables forcibly included or excluded in the selected subsets**

- Number of solutions by subset dimensionality

- **Numerical tolerance for detecting singular or non-symmetrical matrices**

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Auxiliary functions:

lmHmat - **creates H and mat matrices for linear regression/canonical correlation analysis**

ldaHmat - **creates H and mat matrices for linear discriminant analysis**

glhHmat - **creates H and mat matrices for an analysis based on a linear hypothesis specified by the user**

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Auxiliary functions :

ccr12.coef, tau2.coef
zeta2.coef, xi2.coef - **computes a comparison criterion for a subset supplied by the user**

trim.matrix - **deletes rows and columns of singular or ill-conditioned matrices**
- **until all linear dependencies (perfect or almost perfect) are removed**

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Example: Hubbard Brook Forest soil data

Source: Morrison (1990)

Description:

58 pits were analyzed before (1983) and after (1986) harvesting (83-84) trees larger than a minimum diameter

Continuous variables: **gr/m^2 of exchangeable cations**

Al - Aluminum

Ca - Calcium

Mg - Magnesium

K - Potassium

Na - Sodium

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Example: Hubbard Brook Forest soil data

Source: Morrison (1990)

Factors:	Factor levels:
F - Forest Type	1 - Spruce- fir
	2 - High elevation hardwood
	3 - Low elevation hardwood
D - Logging Disturbance	0 - Uncut forest
	1 - Cut, undisturbed by machinery
	2 - Cut, disturbed by machinery
Year	1983 or 1986

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Example: Hubbard Brook Forest soil data

Source: Morrison (1990)

Reading and preparing the data:

```
> library(subselect)

> HubForest <- read.table("Hubbard Brook.txt“ ,header=T,
  col.names=c("Pit","F","D","Al","Ca","Mg","K","Na","Year"),
  colClasses=c("factor","factor","factor","numeric",
  "numeric","numeric","numeric","numeric","factor") )
```

Analysis #1: Explaining the levels of calcium

```
> Hmat <- lmHmat(Ca ~ F*D + Al + Mg+ K + Na ,HubForest)
> colnames(Hmat$mat)
> leaps(Hmat$mat,H=Hmat$H,r=1,nsol=3)
```

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Example: Hubbard Brook Forest soil data

Source: Morrison (1990)

<u>Analysis #2:</u> Looking for combinations of Forest type and Disturbance that best explain the nutrient levels

```
> Hmat <- lmHmat(cbind(Al,Ca,Mg,K,Na) ~ F*D,HubForest)
> colnames(Hmat$mat)
> leaps(Hmat$mat,H=Hmat$H,r=5,criterion="tau2",nsol=3)
```

<u>Analysis #3:</u> Finding which subsets of nutrients were most affected by the harvesting in 1983-84

```
> Hmat <- ldaHmat(Year ~  Al + Ca + Mg + K + Na , HubForest)
> leaps(Hmat$mat,H=Hmat$H,r=1,nsol=3)
```

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Example: Hubbard Brook Forest soil data

Source: Morrison (1990)

<u>Analysis #4:</u> Finding which subsets of nutrients are most affected by interactions between harvesting and logging disturbances, after controlling for the effect of forest type

```
> C <- matrix(0.,2,8)
> C[1,7] = C[2,8] = 1.
> Hmat <- glhHmat(cbind(Al,Ca,Mg,K,Na) ~ D*Year + F, C,
  HubForest)
> leaps(Hmat$mat,H=Hmat$H,r=2, criterion="tau2",
  nsol=3,tolsym=1E-10)
```

References

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