SCGLR: An R package for generalized linear regression on supervised components.

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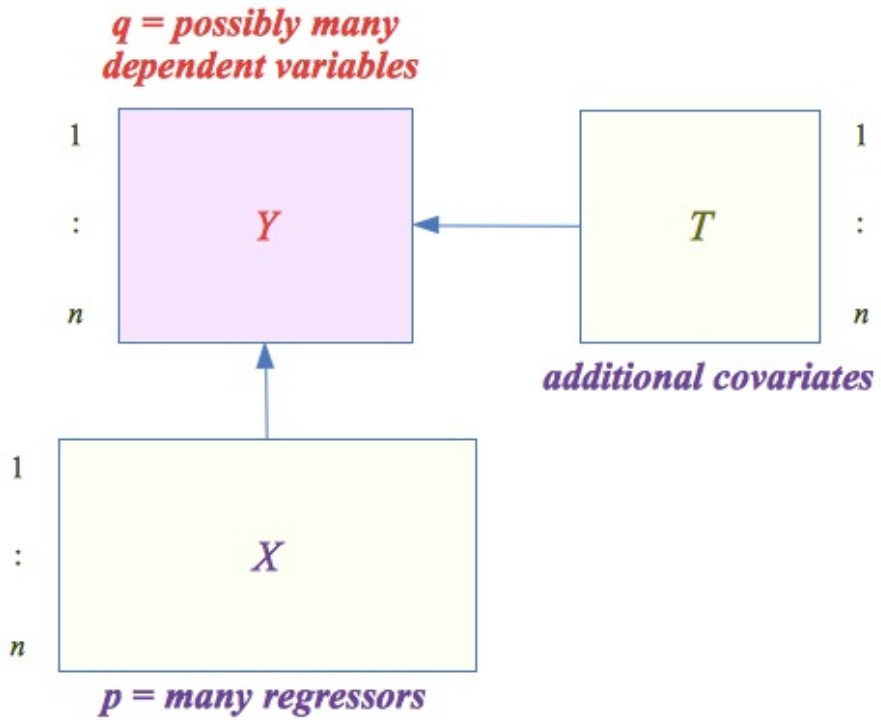
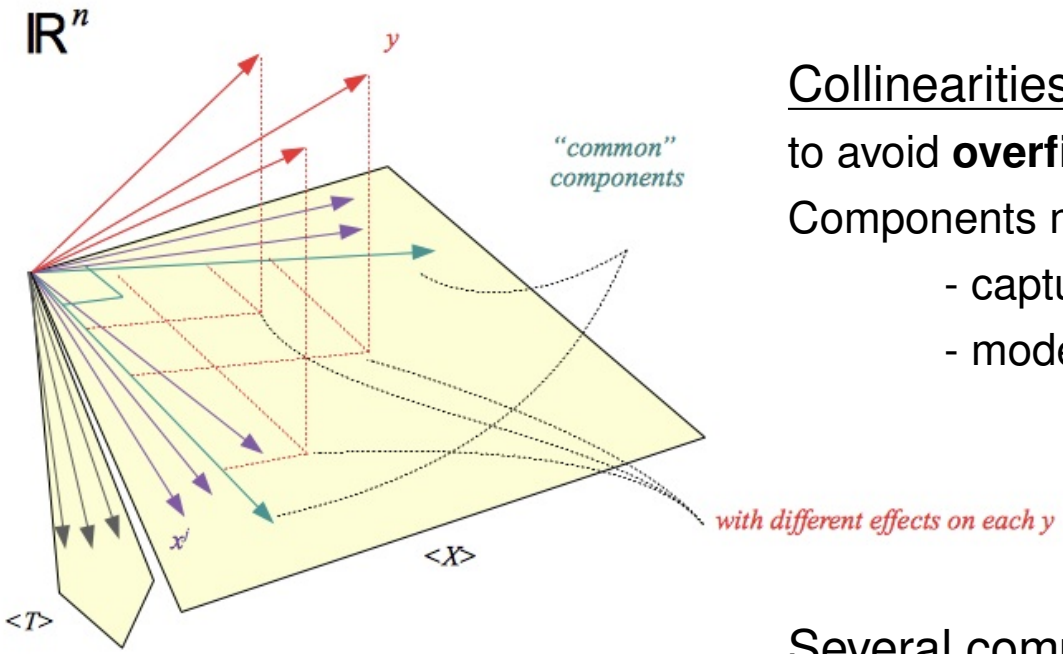
Problematic



$\Rightarrow$ Question: What in X may predict what in Y?

$\hookrightarrow$ *Approach: Dimension reduction by construction of components*



Collinearities:

to avoid **overfitting**, search for **components.**

Components must:

- capture enough variance in X,
- model and predict y.

Several components:

to avoid **redundancy**, search for uncorrelation.

$\rightarrow$ constraint of construction: **orthogonality.**

Multiple y:

same components,

but each y with its **own regression coefficients.**

Exponential family distributed

$\rightarrow$ **generalized linear regression.**

• **First component** is a **compromise** between the direction of X that best predicts y and the first principal component (PC) of X.

↪ *Criterion:* $max_{||u||^2=1} [cov(y, Xu)]$

$$max_{||u||^2=1} \left[\sqrt{var(y)}\ \sqrt{var(Xu)}\ corr(y, Xu)\right]$$

↪ *Program to solve:* $P_1 : max_{||u||^2=1} [< y, Xu >_W]$

• **Further components**: W-orthogonality of components is ensured using the part of X that is not yet used, i.e. the residuals of X regressed on previous components.

PLS2: multiple y

- **First component** can be obtained using several equivalent programs:

$\hookrightarrow \quad P_2 : max_{||u||^2,||v||^2=1} [< Xu, Yv >_W]$

$\hookrightarrow \quad P_3 : max_{||u||^2=1} \left[\sum_{k=1}^{q} < Xu, y^k >_W^2\right]$

P_3 is adapted to the case of multiple weighting :

$\hookrightarrow \quad P_4 : max_{||u||^2=1} \left[\sum_{k=1}^{q} < Xu, y^k >_{W_k}^2\right]$

$\Longrightarrow$ *Solution: eigenvector associated to largest eigenvalue of:*

$$A = X'\Omega X \text{ with } \Omega = \sum_{k=1}^{q} W_k y^k y'^k W_k$$

- **Further components**: idem, subject to constraint of orthogonality to previous components.

Multiple GLM with common predictor

In the GLM, linear predictors are constrained to be collinear to one another:

$$\forall k = 1, q : \quad \eta^k = X\beta_k + T\delta_k = X\gamma_k u + T\delta_k$$

$\longrightarrow$ **modified Fisher Scoring Algorithm**:
u and $\gamma = (\gamma_k)_{k=1,q}$ estimated iterating an alternated least squares two steps sequence:

(1) Given γ, working data $(z^k)_k$ is regressed on matrix $[\gamma \otimes X, 1_q \otimes T]$ with respect to working matrix $W = diag[W_k]_k$

$\longrightarrow$ coefficient vectors $\hat{u}$, $\hat{\delta} = (\hat{\delta}_k)_k$

$\longrightarrow$ $\hat{u}$ made unit norm $\longrightarrow$ updated u

(2) Given Xu, each working vector z^k is regressed on $[Xu, T]$ with respect to working matrix W_k

$\longrightarrow$ updated γ_k, δ_k

Step t of the FSA:

$$min_{\gamma,u:u'u=1}\left[\sum_k ||z^{k[t]} - X\gamma_k u||^2_{W_k^{[t]}}\right]$$

$$\Leftrightarrow min_{u:u'u=1}\left[\sum_k ||z^{k[t]} - \Pi_{Xu} z^{k[t]}||^2_{W_k^{[t]}}\right]$$

$$\Leftrightarrow max_{u:u'u=1}\left[\sum_k ||z^{k[t]}||^2_{W_k^{[t]}} cos^2_{W_k^{[t]}}(z^{k[t]}, Xu)\right]$$

is **replaced** by: $max_{u:u'u=1}\left[\sum_k ||z^{k[t]}||^2_{W_k^{[t]}} cos^2_{W_k^{[t]}}(z^{k[t]}, Xu) \;\; ||Xu||^2_{W_k^{[t]}}\right]$

equivalent to:

$$max_{u:u'u=1}\left[\sum_k < z^{k[t]}, Xu >^2_{W_k^{[t]}}\right]$$

= local extended PLS2

$\Longrightarrow$ *Solution: eigenvector associated to largest eigenvalue of:*

$$A = X'\Omega^{[t]}X \text{ with } \Omega^{[t]} = \sum_{k=1}^{q} W_k^{[t]} z^{k[t]} z'^{k[t]} W_k^{[t]}$$

- **Tuning the attraction of components towards principal components**:

$$A_s = (X'WX)^s A$$

The larger the value of s, the closer the components to PC's
$\Longrightarrow$ if $s = +\infty$, SCGLR components = PC's.

- **Choice of the number of components**:

Cross-validation subsampling $\longrightarrow$ prediction error

$\longrightarrow$ model selection

Functions and methods

1. Main functions
   `scglr()`, `scglrCrossVal()`
2. Utility functions
   `multivariateFormula()`, `multivariateGlm()`, `infoCriterion()`
3. Methods
   `print()`, `summary()`
   `barplot()`, `plot()`, `pairs()`

'genus' sample dataset

1. Samples: 1000 plots (8 by 8 km laid on a grid)
2. Y: abundance of 27 common tree genera in the tropical forest
3. X: 40 environmental variables

First Example, known number of components

Model building

```
> library(SCGLR)
>
> # load sample data
> data(genus)
> # get variable names from dataset
> n <- names(genus)
> ny <- n[grep("^gen", n)]     # Y <- names that begins with "gen"
> nx <- n[-grep("^gen", n)]    # X <- remaining names
> # remove "geology" and "surface" from nx
> # as surface is offset and we want to use geology as additional covariate
> nx <-nx[!nx %in% c("geology", "surface")]
> # define family
> fam <- rep("poisson",length(ny))
>
> # build multivariate formula
> # we also add "lat*lon" as computed covariate
> form <- multivariateFormula(ny,c(nx,"I(lat*lon)"),c("geology"))
```

`form` is a Formula object:

$$y_1 + y_2 + \ldots \sim x_1 + x_2 + \ldots \mid t_1 + \ldots.$$

First Example, known number of components

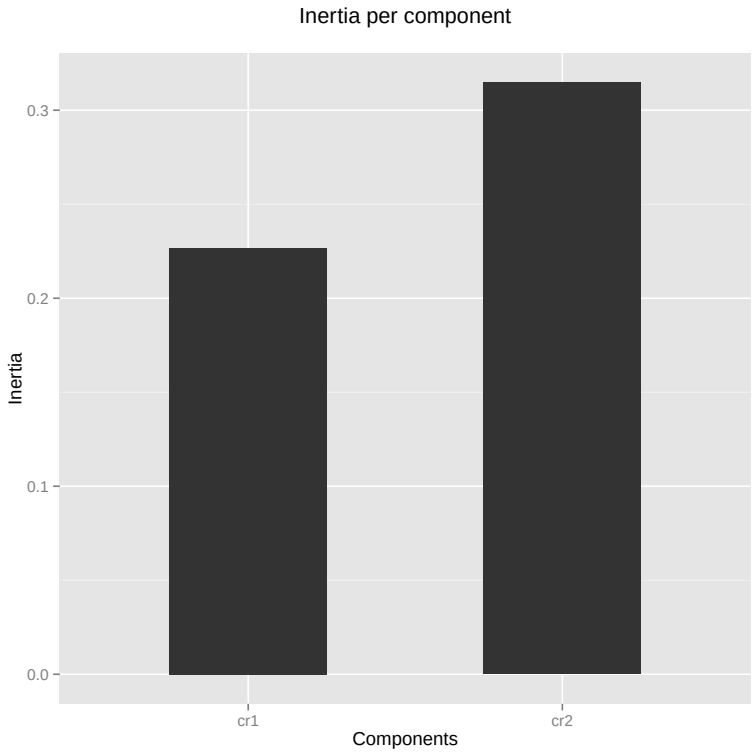
Model fitting

```
> genus.scglr <- scglr(formula=form,data = genus,family=fam, K=2,
+  offset=genus$surface)
> str(genus.scglr, max.level=1)

List of 11
 $ call    : language scglr(formula = form, data = genus, family = fam, K = 2, offset
 $ u       :'data.frame': 46 obs. of  2 variables:
 $ comp    :'data.frame': 1000 obs. of  2 variables:
 $ compr   :'data.frame': 1000 obs. of  2 variables:
 $ gamma   :List of 27
 $ beta    :'data.frame': 51 obs. of  27 variables:
 $ lin.pred:'data.frame': 1000 obs. of  27 variables:
 $ xFactors:'data.frame': 1000 obs. of  1 variable:
 $ xNumeric:'data.frame': 1000 obs. of  40 variables:
 $ inertia : Named num [1:2] 0.227 0.315
  ..- attr(*, "names")= chr [1:2] "cr1" "cr2"
 $ deviance: Named num [1:27] 2307 2790 1632 1479 1468 ...
  ..- attr(*, "names")= chr [1:27] "gen1" "gen2" "gen3" "gen4" ...
 - attr(*, "class")= chr "SCGLR"
```

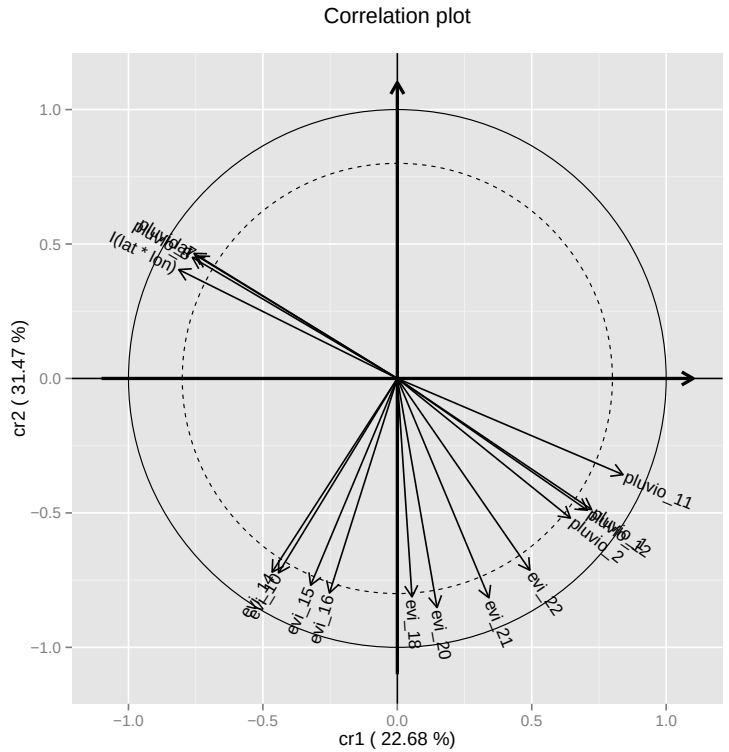
First Example, known number of components

Graphics outputs

```
> barplot(genus.scglr)
```



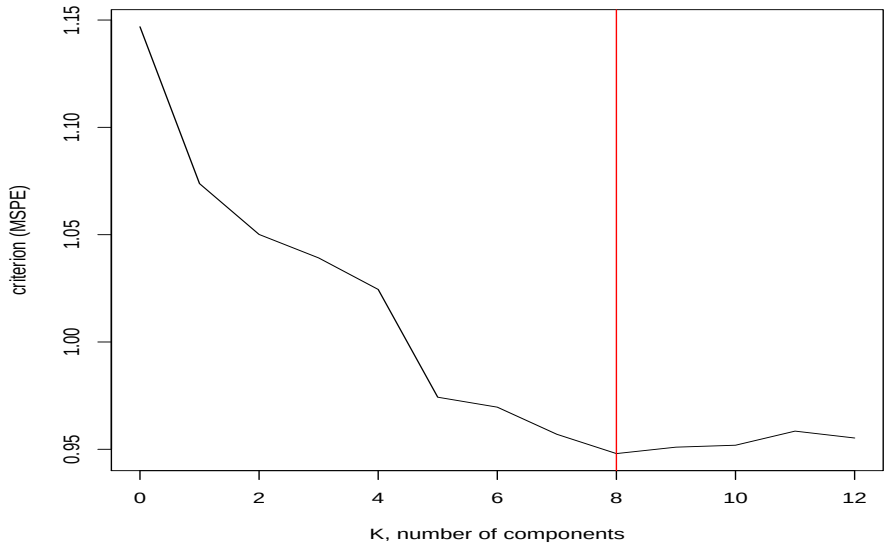

```
> plot(genus.scglr,style="simple,threshold")
```



Second example, unknown number of components

Cross-validation

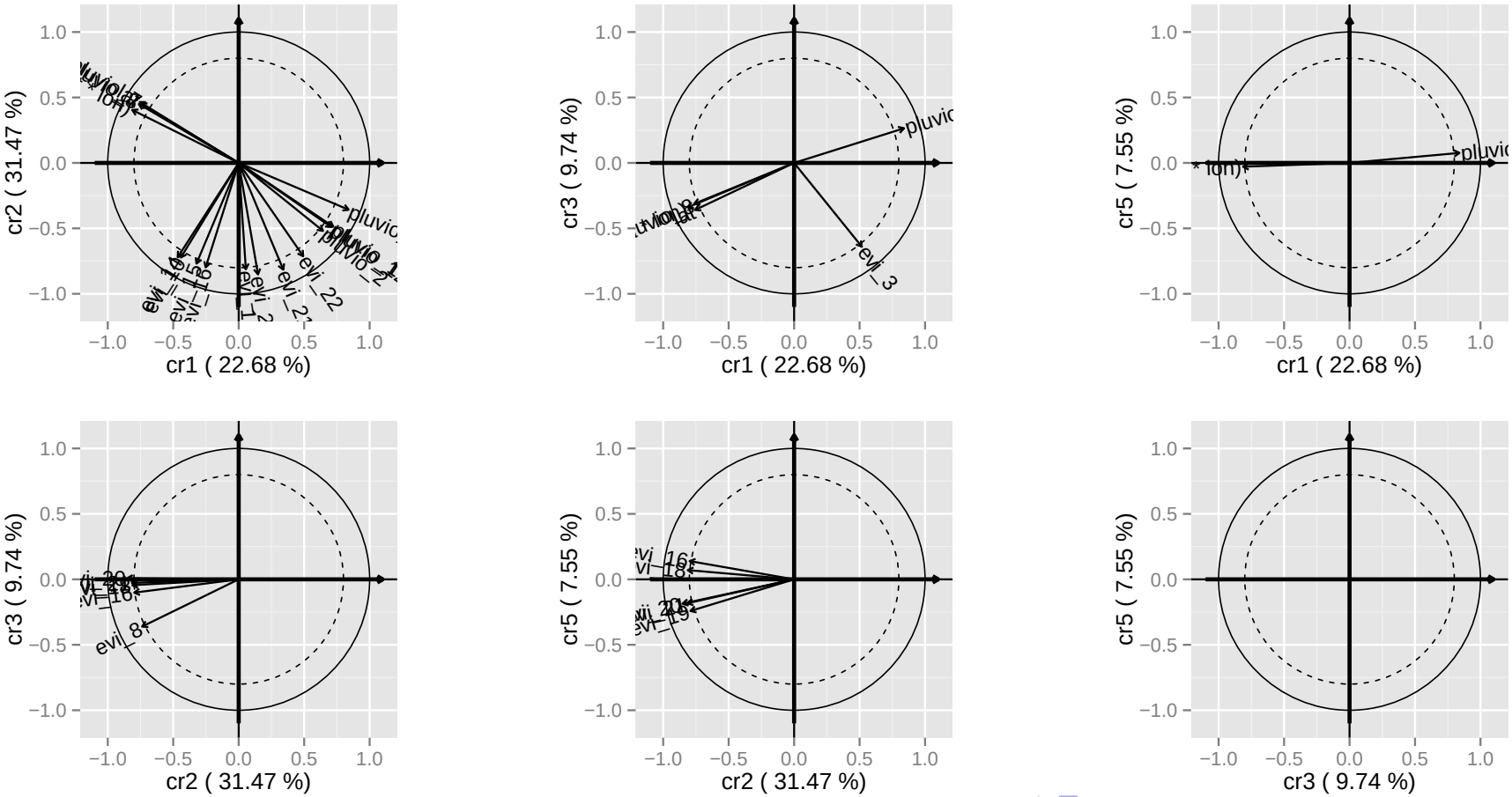
```
> genus.cv <- scglrCrossVal(formula=form, data=genus, family=fam, K=12,
+  offset=genus$surface)
>
> mean.crit <- t(apply(genus.cv,1,function(x) x/mean(x)))
> mean.crit <- apply(mean.crit,2,mean)
> K.cv <- which.min(mean.crit)-1
> cat("Best number of components: ",K.cv)

Best number of components:  8
```



Second example, unknown number of components

Fitting and pairs-Plot

```
> genus.scglr <- scglr(formula=form, data=genus, family=fam, K=K.cv,
+  offset=genus$surface)
> pairs(genus.scglr,components=c(1:3,5),style="simple,threshold")
```



Ongoing works

SCGLR 1.3 version, soon on CRAN

- with new alternate optimization algorithms: Eigen vector and Iterative Normalized Gradient
- Enhancements for plot customization

SCGLR 2 version, in progress

- Multiple explanatory theme support
- New distribution families (Negative-Binomial, Exponential, Inverse Gaussian)

References

1. X. Bry, C. Trottier, T. Verron and F. Mortier (2013). Supervised component generalized linear regression using a PLS-extension of the Fisher scoring algorithm. *Journal of Multivariate Analysis*, 119(0), 47.

2. F. Mortier, C. Trottier, G. Cornu and X. Bry (2014). SCGLR - An R package for Supervised Component Generalized Linear Regression. *Journal of Statitistical Software*. submitted