Package 'SFSI'

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Title Sparse Family and Selection Index

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Description Here we provide tools for the estimation of coefficients in penalized regressions when the (co)variance matrix of predictors and the covariance vector between predictors and response, are provided. These methods are extended to the context of a Selection Index (commonly used for breeding value prediction). The approaches offer opportunities such as the integration of high-throughput traits in genetic evaluations ('Lopez-Cruz et al., 2020') <doi:10.1038/s41598-020-65011-2> and solutions for training set optimization in Genomic Prediction ('Lopez-Cruz & de los Campos, 2021') <doi:10.1093/genetics/iyab030>.

LazyLoad true

Depends R (>= 3.5)

Imports stats, grDevices

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R topics documented:

`BinaryFiles` *Binary files*

Description

Save/read a numeric data as a fortran-formatted binary file at a defined precision (single or double).

Usage

```
saveBinary(X, file = paste0(tempdir(), "/file.bin"),
 type = c("float","double"), verbose = TRUE)

readBinary(file = paste0(tempdir(), "/file.bin"),
  indexRow = NULL, indexCol = NULL, verbose = TRUE)
```

Arguments

`X`	(numeric matrix) Data to save
`file`	(character) Name of the binary file to save/read
`type`	(character) Either 'float' or 'double' for single (4 bytes) or double precision (8 bytes), respectively, that matrix to save will occupy
`indexRow`	(integer vector) Which rows are to be read from the file. Default `indexRow=NULL` will read all the rows
`indexCol`	(integer vector) Which columns are to be read from the file. Default `indexCol=NULL` will read all the columns
`verbose`	`TRUE` or `FALSE` to whether printing file information

Value

Function 'saveBinary' does not return any value but print a description of the file saved.

Function 'readBinary' returns the data that was read.

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)

# Simulate matrix
X = matrix(rnorm(5000),ncol=5)
head(X)

# Save matrix
saveBinary(X,paste0(tempdir(),"/Matrix1.bin"),type="double") # as double-precision
saveBinary(X,paste0(tempdir(),"/Matrix2.bin"),type="float")  # as single-precision

# Read the double-precision matrix
X2 = readBinary(paste0(tempdir(),"/Matrix1.bin"))
head(X2)
max(abs(X-X2))     # No loss of precision
object.size(X2)    # Size of the object

# Read the single-precision matrix
X3 = readBinary(paste0(tempdir(),"/Matrix2.bin"))
head(X3)
max(abs(X-X3))     # Loss of precision
object.size(X3)    # But smaller-size object

# Read specific rows and columns
indexRow = c(2,4,5,8,10)
indexCol = c(1,2,5)
X2 = readBinary(paste0(tempdir(),"/Matrix1.bin"),indexRow=indexRow,indexCol=indexCol)
X2
# Equal to:
X[indexRow,indexCol]
```

---

collect *collect function*

Description

Collects all outputs saved at the provided `saveAt` parameter from the SSI analysis when testing data was splited according to argument `subset`.

Usage

```
collect(prefix = "")
```

Arguments

prefix	(character) Prefix that was added to the output files name, this may include a path

Value

An object of the class 'SSI' for which methods `fitted`, `plot` and `summary` exist

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV == 1)             # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))   # Subset and scale markers
G = tcrossprod(M)                    # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))  # Subset response variable

prefix <- paste0(tempdir(),"/testSSI")

# Run the analysis into 4 subsets and save them at a given prefix
fm <- SSI(y,K=G,tst=1:80,trn=81:length(y),subset=c(1,4),saveAt=prefix)
fm <- SSI(y,K=G,tst=1:80,trn=81:length(y),subset=c(2,4),saveAt=prefix)
fm <- SSI(y,K=G,tst=1:80,trn=81:length(y),subset=c(3,4),saveAt=prefix)
fm <- SSI(y,K=G,tst=1:80,trn=81:length(y),subset=c(4,4),saveAt=prefix)

# Collect all results after completion
fm <- collect(prefix)
```

---

covariance_matrix *Conversion of a covariance matrix to a distance or correlation matrix*

Description

Computes a correlation matrix or a Euclidean distance matrix from a covariance matrix

Usage

```
cov2dist(V, void = FALSE)

cov2cor2(V, a = 1, void = FALSE)
```

Arguments

V	(numeric matrix) Symmetric variance-covariance matrix among p variables. It can be of the "float32" type as per the 'float' R-package
void	TRUE or FALSE to whether return or not return the output. When FALSE no result is displayed but the input V is modified. Default void=FALSE
a	(numeric) A number to multiply the whole resulting matrix by. Default a=1

Details

For any variables X_i and X_j with mean zero and with sample vectors $\mathbf{x}_i = (x_{i1}, ..., x_{in})'$ and $\mathbf{x}_j = (x_{j1}, ..., x_{jn})'$, their (sample) variances are equal (up-to a constant) to their cross-products, this is, $var(X_i) = \mathbf{x}_i'\mathbf{x}_i$ and $var(X_j) = \mathbf{x}_j'\mathbf{x}_j$. Likewise, the covariance is $cov(X_i, X_j) = \mathbf{x}_i'\mathbf{x}_j$.

Distance. The square of the distance $d(X_i, X_j)$ between the variables expressed in terms of cross-products is

$$d^2(X_i, X_j) = \mathbf{x}_i'\mathbf{x}_i + \mathbf{x}_j'\mathbf{x}_j - 2\mathbf{x}_i'\mathbf{x}_j$$

Therefore, the output (square) distance matrix will contain as off-diagonal entries

$$d^2(X_i, X_j) = var(X_i) + var(X_j) - 2cov(X_i, X_j)$$

while in the diagonal, the distance between one variable with itself is $d^2(X_i, X_i) = 0$

Correlation. The correlation between the variables is obtained from variances y covariances as

$$cor(X_i, X_j) = cov(X_i, X_j)/(var(X_i)var(X_j))$$

while in the diagonal, the correlation between one variable with itself is $cor(X_i, X_i) = 1$

Variances are obtained from the diagonal values while covariances are obtained from the out-diagonal.

Value

Function 'cov2dist' returns a matrix containing the (square) Euclidean distances. Function 'cov2cor2' returns a correlation matrix

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

X = scale(Y[,4:7])
(V = crossprod(X))             # Covariance matrix

# Covariance matrix to distance matrix
```

```
(D1 = cov2dist(V))
# it must equal (but faster) to:
D0 = as.matrix(dist(t(X)))^2
max(abs(D0-D1))

# Covariance to a correlation matrix
(R1 = cov2cor2(V))
# it must equal (but faster) to:
R0 = cov2cor(V)
max(abs(R0-R1))

if(requireNamespace("float")){
 # Using a 'float' type variable
 V2 = float::fl(V)
 D2 = cov2dist(V2)
 max(abs(D1-D2))   # discrepancy with previous matrix
 R2 = cov2cor2(V2)
 max(abs(R1-R2))   # discrepancy with previous matrix
}

# Using void=TRUE
cov2dist(V,void=TRUE)
V       # notice that V was modified
cov2dist(V2,void=TRUE)
V2       # notice that V2 was modified
```

`fitBLUP` *Function fitBLUP*

Description

Solves the Linear Mixed Model and calculates the Best Linear Unbiased Predictor (BLUP)

Usage

```
fitBLUP(y, X = NULL, Z = NULL, K = NULL, U = NULL,
        d = NULL, h2 = NULL, BLUP = TRUE,
        method = c("REML","ML"), return.Hinv = FALSE,
        tol = 1E-5, maxIter = 1000, interval = c(1E-9,1E9),
        warn = TRUE)
```

Arguments

`y`	(numeric vector) Response variable
`X`	(numeric matrix) Design matrix for fixed effects. When `X=NULL` a vector of ones is constructed only for the intercept (default)
`Z`	(numeric matrix) Design matrix for random effects. When `Z=NULL` an identity matrix is considered (default) thus **G = K**; otherwise **G** $=$ **Z K Z'** is used

`K`	(numeric matrix) Kinship relationships. This can be of the "float32" type as per the 'float' R-package, or a (character) name of a binary file where the matrix is stored
`U`	(numeric matrix) Eigenvectors from spectral value decomposition of **G = U D U'**
`d`	(numeric vector) Eigenvalues from spectral value decomposition of **G = U D U'**
`h2`	(numeric) Heritability of the response variable. When it is not `NULL`, the variance components are not estimated and only fixed and random effects are computed
`BLUP`	`TRUE` or `FALSE` to whether return the random effects estimates
`method`	(character) Either 'REML' (Restricted Maximum Likelihood) or 'ML' (Maximum Likelihood)
`return.Hinv`	`TRUE` or `FALSE` to whether return the inverse of the matrix H
`tol`	(numeric) Maximum error between two consecutive solutions (convergence tolerance) when finding the root of the log-likelihood's first derivative
`maxIter`	(integer) Maximum number of iterations to run before convergence is reached
`interval`	(numeric vector) Range of values in which the root is searched
`warn`	`TRUE` or `FALSE` to whether show warnings

Details

The basic linear mixed model that relates phenotypes with genetic values is of the form

$$\mathbf{y} = \mathbf{Xb} + \mathbf{Zu} + \mathbf{e}$$

where **y** is a vector with the response, **b** is the vector of fixed effects, **u** is the vector of the (random) genetic values of the genotypes, **e** is the vector of environmental residuals (random error), and **X** and **Z** are design matrices conecting the fixed and genetic effects with replicates. Genetic values are assumed to follow a Normal distribution as $\mathbf{u} \sim N(\mathbf{0}, \sigma_u^2\mathbf{K})$, and the error terms are assumed $\mathbf{e} \sim N(\mathbf{0}, \sigma_e^2\mathbf{D})$, with $\mathbf{D} = \mathbf{I}$ being an identity matrix.

The resulting vector of genetic values $\mathbf{g} = \mathbf{Zu}$ will therefore follow $\mathbf{g} \sim N(\mathbf{0}, \sigma_u^2\mathbf{G})$ where $\mathbf{G} = \mathbf{ZKZ}'$. In the un-replicated case, $\mathbf{Z} = \mathbf{I}$ is an identity matrix, and hence $\mathbf{g} = \mathbf{u}$ and $\mathbf{G} = \mathbf{K}$.

Only information from observed data (training set) is used to derive predictions of the values $\mathbf{u}_{trn} = (u_i)$, $i = 1, 2, ..., n_{trn}$, as

$$\mathbf{u}_{tst} = \mathbf{H}(\mathbf{y}_{trn} - \mathbf{X}_{trn}\mathbf{b})$$

where **H** is a matrix of weights given by

$$\mathbf{H} = \mathbf{G}_{trn}(\mathbf{G}_{trn} + \theta\mathbf{D})^{-1}$$

where $\mathbf{G}_{trn}$ is the sub-matrix corresponding to the training set, and $\theta = \sigma_e^2/\sigma_u^2$ is the variance components ratio representing a shrinkage parameter. This parameter is expressed in terms of the heritability, $h^2 = \sigma_u^2/(\sigma_u^2 + \sigma_e^2)$, as $\theta = (1 - h^2)/h^2$.

The prediction of values $\mathbf{u}_{tst}$ corresponding to un-observed data (testing set) can be done by using

$$\mathbf{H} = \mathbf{G}_{tst,trn}(\mathbf{G}_{trn} + \lambda_0\mathbf{D})^{-1}$$

where $\mathbf{G}_{tst,trn}$ is the sub-matrix of $\mathbf{G}$ corresponding to the testing set (in rows) and training set (in columns).

Solutions are found using the GEMMA (Genome-wide Efficient Mixed Model Analysis) approach (Zhou & Stephens, 2012). GEMMA implements the Brent's method to efficiently optimize the first derivative of the log-likelihood to solve for the variance components ratio.

Value

Returns a list object that contains the elements:

- b: (vector) fixed effects solutions (including the intercept).
- u: (vector) random effects solutions.
- varU: random effect variance.
- varE: error variance.
- h2: heritability.
- convergence: (logical) whether Brent's method converged.
- method: either 'REML' or 'ML' method used.

Author(s)

Paulino Perez-Rodriguez, Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

References

VanRaden PM (2008). Efficient methods to compute genomic predictions. *Journal of Dairy Science*, **91**(11), 4414–4423.

Zhou X, Stephens M (2012). Genome-wide efficient mixed-model analysis for association studies. *Nature Genetics*, **44**(7), 821-824

Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV %in% 1:2)       # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))   # Subset and scale markers
G = tcrossprod(M)                    # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))  # Subset response variable

# Training and testing sets
tst = seq(1,length(y),by=3)
trn = seq_along(y)[-tst]

yNA <- y
yNA[tst] <- NA
fm1 = fitBLUP(yNA, K=G)
plot(y[tst],fm1$u[tst])      # Predicted vs observed values in testing set
cor(y[tst],fm1$u[tst])       # Prediction accuracy in testing set
cor(y[trn],fm1$u[trn])       # Prediction accuracy in training set
```

```
fm1$h2                      # Heritability


if(requireNamespace("float")){
 # Using a 'float' type variable
 G2 = float::fl(G)
 fm2 = fitBLUP(yNA, K=G2)
 max(abs(fm1$u-fm2$u))  # Check for discrepances
}
```

---

getGenCov *Genetic covariances*

Description

Pairwise genetic covariances for variables with the same experimental design and equal variance

Usage

```
getGenCov(y1, y2, X = NULL, Z = NULL, K = NULL,
          U = NULL, d = NULL, scale = TRUE,
          mc.cores = 1, warn = FALSE, ...)
```

Arguments

y1	(numeric vector) Response variable 1
y2	(numeric matrix) Response variable 2. The number of rows must be equal to length of vector y1
X	(numeric matrix) Design matrix for fixed effects. When X=NULL a vector of ones is constructed only for the intercept (default)
Z	(numeric matrix) Design matrix for random effects. When Z=NULL an identity matrix is considered (default) thus **G = K**; otherwise **G = Z K Z'** is used
K	(numeric matrix) Kinship relationships
U	(numeric matrix) Eigenvectors from spectral value decomposition of **G = U D U'**
d	(numeric vector) Eigenvalues from spectral value decomposition of **G = U D U'**
scale	TRUE or FALSE to scale y1 and y2 by their corresponding standard deviations so the resulting variables will have unit variance
mc.cores	(integer) Number of cores used. The analysis is run in parallel when mc.cores is greater than 1. Default is mc.cores=1
warn	TRUE or FALSE to whether show warnings
...	Other arguments passed to the function 'fitBLUP'

Details

Assumes that both $\mathbf{y}_1$ and $\mathbf{y}_2$ follow the basic linear mixed model that relates phenotypes with genetic values of the form

$$\mathbf{y}_1 = \mathbf{X}\mathbf{b}_1 + \mathbf{Z}\mathbf{u}_1 + \mathbf{e}_1$$

$$\mathbf{y}_2 = \mathbf{X}\mathbf{b}_2 + \mathbf{Z}\mathbf{u}_2 + \mathbf{e}_2$$

where $\mathbf{b}_1$ and $\mathbf{b}_2$ are the specific fixed effects, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the specific genetic values of the genotypes, $\mathbf{e}_1$ and $\mathbf{e}_2$ are the vectors of specific environmental residuals, and $\mathbf{X}$ and $\mathbf{Z}$ are common design matrices conecting the fixed and genetic effects with replicates. Genetic values are assumed to follow a Normal distribution as $\mathbf{u}_1 \sim N(\mathbf{0}, \sigma^2_{u_1}\mathbf{K})$ and $\mathbf{u}_2 \sim N(\mathbf{0}, \sigma^2_{u_2}\mathbf{K})$, and environmental terms are assumed $\mathbf{e}_1 \sim N(\mathbf{0}, \sigma^2_{e_1}\mathbf{I})$ and $\mathbf{e}_2 \sim N(\mathbf{0}, \sigma^2_{e_2}\mathbf{I})$.

The genetic covariance $\sigma^2_{u_1u_2}$ is estimated from the formula for the variance for the sum of two variables as

$$\sigma^2_{u_1u_2} = \frac{1}{2}(\sigma^2_{u_3} - \sigma^2_{u_1} - \sigma^2_{u_2})$$

where $\sigma^2_{u_3}$ is the genetic variance of the variable $\mathbf{y}_3 = \mathbf{y}_1 + \mathbf{y}_2$ that also follows the same model as for $\mathbf{y}_1$ and $\mathbf{y}_2$.

Likewise, the environmental covariance $\sigma^2_{e_1e_2}$ is estimated as

$$\sigma^2_{e_1e_2} = \frac{1}{2}(\sigma^2_{e_3} - \sigma^2_{e_1} - \sigma^2_{e_2})$$

where $\sigma^2_{e_3}$ is the error variance of the variable $\mathbf{y}_3$.

Solutions are found using the function 'fitBLUP' (see `help(fitBLUP)`) to sequentialy fit mixed models for all the variables $\mathbf{y}_1$, $\mathbf{y}_2$ and $\mathbf{y}_3$.

Value

Returns a list object that contains the elements:

- `varU1`: genetic variance for response variable 1.
- `varU2`: (vector) genetic variances for response variable 2.
- `varE1`: error variance for response variable 1.
- `varE2`: (vector) error variances for response variable 2.
- `covU`: (vector) genetic covariances between response variables 1 and 2.
- `covE`: (vector) environmental covariances between response variables 1 and 2.

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV %in% 1:2)        # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))    # Subset and scale markers
G = tcrossprod(M)                     # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))   # Subset response variable
X = scale(X_E1[index,20:50])          # Subset reflectance data

fm = getGenCov(y,X,K=G)

covU = fm$covU                      # Genetic covariance
covP_corrected = fm$covU+fm$covE    # Phenotypic covariance
covP_uncorrected = cov(y,X)         # Sample phenotypic covariance

plot(covP_corrected,covP_uncorrected)
plot(covU,covP_uncorrected)
plot(covU,covP_corrected)
```

`lars2` *Least Angle Regression to solve LASSO-type problems*

Description

Computes the entire LASSO solution for the regression coefficients, starting from zero, to the least-squares estimates, via the Least Angle Regression (LARS) algorithm (Efron, 2004). It uses as inputs a variance matrix among predictors and a covariance vector between response and predictors.

Usage

```
lars2(Sigma, Gamma, method = c("LAR", "LAR-LASSO"), maxDF = NULL,
  eps = .Machine$double.eps, scale = TRUE, verbose = FALSE)
```

Arguments

`Sigma`	(numeric matrix) Variance-covariance matrix of predictors. It can be of the "float32" type as per the 'float' R-package
`Gamma`	(numeric vector) Covariance between response variable and predictors
`method`	(character) Either: • `'LAR'`: Computes the entire sequence of all coefficients. Values of lambdas are calculated at each step. • `'LAR-LASSO'`: Similar to `'LAR'` but solutions when a predictor leaves the solution are also returned. Default is `method='LAR'`
`maxDF`	(integer) Maximum number of non-zero coefficients in the last LARS solution. Default `maxDF=NULL` will calculate solutions for the entire lambda sequence

eps	(numeric) An effective zero. Default is the machine precision
scale	TRUE or FALSE to scale matrix Sigma for variables with unit variance and scale Gamma by the standard deviation of the corresponding predictor taken from the diagonal of Sigma
verbose	TRUE or FALSE to whether printing each LARS step

Details

Finds solutions for the regression coefficients in a linear model

$$y_i = \mathbf{x}_i'\boldsymbol{\beta} + e_i$$

where y_i is the response for the i^{th} observation, $\mathbf{x}_i = (x_{i1}, ..., x_{ip})'$ is a vector of p predictors assumed to have unit variance, $\boldsymbol{\beta} = (\beta_1, ..., \beta_p)'$ is a vector of regression coefficients, and e_i is a residual.

The regression coefficients $\boldsymbol{\beta}$ are estimated as function of the variance matrix among predictors ($\boldsymbol{\Sigma}$) and the covariance vector between response and predictors ($\boldsymbol{\Gamma}$) by minimizing the penalized mean squared error function

$$-\boldsymbol{\Gamma}'\boldsymbol{\beta} + 1/2\boldsymbol{\beta}'\boldsymbol{\Sigma}\boldsymbol{\beta} + 1/2\lambda||\boldsymbol{\beta}||_1$$

where λ is the penalization parameter and $||\boldsymbol{\beta}||_1 = \sum_{j=1}^{p} |\beta_j|$ is the L1-norm.

The algorithm to find solutions for each β_j is fully described in Efron (2004) in which the "current correlation" between the predictor x_{ij} and the residual $e_i = y_i - \mathbf{x}_i'\boldsymbol{\beta}$ is expressed (up-to a constant) as

$$r_j = \Gamma_j - \boldsymbol{\Sigma}_j'\boldsymbol{\beta}$$

where Γ_j is the j^{th} element of $\boldsymbol{\Gamma}$ and $\boldsymbol{\Sigma}_j$ is the j^{th} column of the matrix $\boldsymbol{\Sigma}$

Value

Returns a list object with the following elements:

- lambda: (vector) all the sequence of values of the LASSO penalty.
- beta: (matrix) regression coefficients for each predictor (in rows) associated to each value of the penalization parameter lambda (in columns).
- df: (vector) degrees of freedom, number of non-zero predictors associated to each value of lambda.

The returned object is of the class 'LASSO' for which methods fitted exist. Function plotPath can be also used

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos. Adapted from the 'lars' function in package 'lars' (Hastie & Efron, 2013)

References

Efron B, Hastie T, Johnstone I, Tibshirani R (2004). Least angle regression. *The Annals of Statistics*, **32**(2), 407–499.

Friedman J, Hastie T, Tibshirani R(2010). Regularization paths for generalized linear models via coordinate descent. *Journal of Statistical Software*, **33**(1), 1–22.

Hastie T, Efron B (2013). lars: least angle regression, Lasso and forward stagewise. https://cran.r-project.org/package=lars.

Tibshirani R (1996). Regression shrinkage and selection via the LASSO. *Journal of the Royal Statistical Society B*, **58**(1), 267–288.

Examples

```
require(SFSI)
data(wheatHTP)

y = as.vector(Y[,"E1"])  # Response variable
X = scale(X_E1)           # Predictors

# Training and testing sets
tst = 1:ceiling(0.3*length(y))
trn = seq_along(y)[-tst]

# Calculate covariances in training set
XtX = var(X[trn,])
Xty = cov(y[trn],X[trn,])

# Run the penalized regression
fm1 = lars2(XtX,Xty,method="LAR-LASSO")

# Predicted values
yHat1 = fitted(fm1, X=X[trn,])  # training data
yHat2 = fitted(fm1, X=X[tst,])  # testing data

# Penalization vs correlation
plot(-log(fm1$lambda[-1]),cor(y[trn],yHat1[,-1]), main="training")
plot(-log(fm1$lambda[-1]),cor(y[tst],yHat2[,-1]), main="testing")


if(requireNamespace("float")){
 # Using a 'float' type variable
 XtX2 = float::fl(XtX)
 fm2 = lars2(XtX2,Xty,method="LAR-LASSO")
 max(abs(fm1$beta-fm2$beta))      # Check for discrepances in beta
 max(abs(fm1$lambda-fm2$lambda))  # Check for discrepances in lambda
}
```

Methods_LASSO *LASSO methods*

Description

Predicted values for a provided matrix of predictors X

Usage

```
## S3 method for class 'LASSO'
fitted(object, ...)
```

Arguments

object	An object of the class 'LASSO' returned either by the function 'lars2' or 'solveEN'
...	Other arguments: X (numeric matrix) scores for as many predictors there are in ncol(object$beta) (in columns) for a desired number n of observations (in rows)

Value

Returns a matrix that contains, for each value of lambda (in columns), the predicted values corresponding to each row of the matrix X

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

y = as.vector(Y[,"E1"])  # Response variable
X = scale(X_E1)          # Predictors

# Training and testing sets
tst = seq(1,length(y),by=3)
trn = seq_along(y)[-tst]

# Calculate covariances in training set
XtX = var(X[trn,])
Xty = cov(y[trn],X[trn,])

# Run the penalized regression
fm = solveEN(XtX,Xty,alpha=0.5)

# Predicted values
yHat1 = fitted(fm, X=X[trn,])  # training data
```

```
yHat2 = fitted(fm, X=X[tst,])  # testing data

# Penalization vs correlation
plot(-log(fm$lambda[-1]),cor(y[trn],yHat1[,-1]), main="training")
plot(-log(fm$lambda[-1]),cor(y[tst],yHat2[,-1]), main="testing")
```

Methods_SSI *SSI methods*

Description

Useful methods for retrieving, summarizing and visualizing important results from an object of the class 'SSI'

Usage

```
## S3 method for class 'SSI'
coef(object, ..., df=NULL, tst=NULL)

## S3 method for class 'SSI'
fitted(object, ...)

## S3 method for class 'SSI'
summary(object, ...)

## S3 method for class 'SSI'
plot(..., title=NULL, py=c("accuracy","MSE"))
```

Arguments

`object`	An object of the class 'SSI'. One or more objects must be passed as `...` in the method `plot`
`df`	(numeric) Average (across testing individuals) number of non-zero regression coefficients
`tst`	(integer vector) Which elements from vector `y` (stored in `object$y`) are in testing set. Default `tst=NULL` will consider all individuals in `object$tst`
`py`	(character) Either 'accuracy' or 'MSE' to plot the correlation between observed and predicted values or the mean squared error, respectively, in the y-axis
`title`	(character or expression) Title of the plot
`...`	Arguments to be passed: • `object`: One or more objects of the class 'SSI' (for method `plot`) • Not needed for methods `summary` and `fitted`

Value

Method `fitted` returns a matrix with the predicted values for each individual in the testing set (in rows) for each value of lambda (in columns).

Method `coef` (list of matrices) returns the regression coefficients for each testing set individual (elements of the list). Each matrix contains the coefficients for each value of lambda (in rows) associated to each training set individual (in columns). If `tst` is specified, the elements of the list will correspond only to the testing individuals given in `tst`. If `df` is specified, only the coefficients for the lambda associated to `df` are returned as a 'matrix' with testing individuals in rows.

Method `summary` returns a list object containing:

- `lambda`: (vector) sequence of (across testing individuals) values of lambda used in the coefficients' estimation.
- `df`: (vector) degrees of freedom (across testing individuals) at each solution associated to each value of lambda.
- `accuracy`: (vector) correlation between observed and predicted values associated to each value of lambda.
- `MSE`: (vector) mean squared error associated to each value of lambda.
- `optCOR`: (vector) summary of the SSI with maximum accuracy.
- `optMSE`: (vector) summary of the SSI with minimum MSE.

Method `plot` creates a plot of either accuracy or MSE versus the (average across testing individuals) number of predictors (with non-zero regression coefficient) and versus lambda.

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV %in% 1:2)        # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))    # Subset and scale markers
G = tcrossprod(M)                     # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))   # Subset ans scale response variable

# Training and testing sets
tst = seq(1,length(y),by=5)
trn = seq_along(y)[-tst][1:200]

fm1 = SSI(y,K=G,tst=tst,trn=trn)

yHat = fitted(fm1)              # Predicted values for each SSI
out = summary(fm1)              # Useful function to get results
corTST = out$accuracy           # Testing set accuracy (correlation cor(y,yHat))
out$optCOR                      # SSI with maximum accuracy
out$optMSE                      # SSI with minimum MSE
B = coef(fm1)                   # Regression coefficients
```

```
B = coef(fm1,df=out$optCOR$df)  # Regression coefficients associated with one 'df'
plot(fm1,title=expression('corr('*y[obs]*','*y[pred]*') vs sparsity'))
plot(fm1,py="MSE",title='Mean Square Error vs sparsity')
```

`Methods_SSI_CV` *SSI_CV methods*

Description

Useful methods for retrieving, summarizing and visualizing important results from an object of the class 'SSI_CV'

Usage

```
## S3 method for class 'SSI_CV'
summary(object, ...)

## S3 method for class 'SSI_CV'
plot(..., py=c("accuracy","MSE"), title=NULL, showFolds=FALSE)
```

Arguments

`object`	An object of the class 'SSI_CV'
`...`	Arguments to be passed: • Not needed for method `summary` • `object`: One or more objects of the class 'SSI_CV' (for method `plot`)
`py`	(character) Either 'accuracy' or 'MSE' to plot the correlation between observed and predicted values or the mean squared error, respectively, in the y-axis
`title`	(character/expression) Title of the plot
`showFolds`	`TRUE` or `FALSE` to whether add results for individuals folds

Value

Method `summary` returns a list object containing:

- `lambda`: (matrix) sequence of (average across folds) values of lambda (in columns) used in each CV partition (in rows).
- `df`: (matrix) degrees of freedom (average across folds) at each solution associated to each value of lambda for each CV partition (in rows).
- `accuracy`: (matrix) correlation between observed and predicted values (average across folds) given by each value of lambda (in columns) in each CV partition (in rows).
- `MSE`: (matrix) mean squared error (average across folds) given by each value of lambda (in columns) in each CV partition (in rows).

- optCOR: (matrix) summary of the SSI with maximum accuracy within and across CV partitions (in rows).
- optMSE: (matrix) summary of the SSI with minimum MSE within and across CV partitions (in rows).

Method plot creates a plot of either accuracy or MSE versus the (average across folds and partitions) number of predictors (with non-zero regression coefficient) and versus lambda.

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV %in% 1:2)        # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))    # Subset and scale markers
G = tcrossprod(M)                     # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))   # Subset ans scale response variable

trn = seq(1,length(y),by=2)
fm1 = SSI_CV(y,K=G,trn=trn,nFolds=5,nCV=1)

out = summary(fm1)    # Useful results
out$accuracy          # Testing set accuracy (cor(y,yHat))
out$optCOR            # SSI with maximum accuracy
out$optMSE            # SSI with minimum MSE

plot(fm1,title=expression('corr('*y[obs]*','*y[pred]*') vs sparsity'))
plot(fm1,showFolds=TRUE)
```

---

plotNet *Network plot*

Description

Network plot of testing and training individuals from an object of the class 'SSI'

Usage

```
plotNet(fm, B, Z = NULL, K, subsetG = NULL, tst = NULL,
        U = NULL, d = NULL, group = NULL, group.shape = NULL,
        set.color = NULL, set.size = NULL, df = NULL, title,
        axis.labels = TRUE, curve = FALSE, bg.color = "gray20",
        unified = TRUE, ntst = 36, line.color = "gray90",
        line.tick = 0.3, legend.pos="right", point.color = "gray20",
        sets = c("Testing","Supporting","Non-active"))
```

Arguments

fm	An object of the 'SSI' class
B	(numeric matrix) (Optional) Regression coefficients for individuals corresponding to fm$tst (in rows) and to fm$trn (in columns)
Z	(numeric matrix) Design matrix for random effects. When Z=NULL an identity matrix is considered (default) thus **G = K**; otherwise **G** $=$ **Z K Z'** is used
K	(numeric matrix) Kinship relationships. This can be a (character) name of a binary file where the matrix is stored
subsetG	(integer vector) Which columns (and rows) from G the vectors fm$trn and fm$tst refer to. Default subsetG=NULL considers that elements fm$trn and fm$tst refer to columns (and rows) from G; otherwise elements in training and testing in G have indices subsetG[fm$trn] and subsetG[fm$tst]
tst	(integer vector) Which elements from vector y (stored in fm$y) are in testing set and to plot. They must be contained in fm$tst. Default tst=NULL will consider the whole vector fm$tst to plot
U	(numeric matrix) Eigenvectors from spectral value decomposition of **G** $=$ **U D U'**
d	(numeric vector) Eigenvalues from spectral value decomposition of **G** $=$ **U D U'**
group	(data.frame) Column grouping for the individuals. The rows must match with the rows in G matrix
df	(numeric) Average number of training individuals contributing to the prediction (active) of testing individuals. Default df=NULL will use the df that yielded the optimal accuracy
title	(character/expression) Title of the plot
bg.color	(character) Plot background color
line.color	(character) Color of lines connecting 'active' training individuals with each individual in testing set
line.tick	(numeric) Tick of lines connecting 'active' training individuals with each individual in testing set
set.color	(character vector) Color point of each level of 'testing', 'active', and 'non-active' elements, respectively
set.size	(numeric vector) Size of 'testing', 'active', and 'non-active' elements, respectively
group.shape	(integer vector) Shape of each level of the grouping column provided as group
curve	TRUE or FALSE to whether draw curve of rect lines connecting 'active' training individuals with each individual in testing set
axis.labels	TRUE or FALSE to whether show labels in both axes
unified	TRUE or FALSE to whether show an unified plot or separated for each individual in 'testing'
point.color	(character) Color of the points in the plot
ntst	(integer) Maximum number of individuals in 'testing' that are plotted separated as indicated by unified=FALSE

legend.pos	(character) Either "right", topright","bottomleft","bottomright","topleft", or "none" indicating where the legend is positioned in the plot
sets	(character vector) Names of the sets: testing group, predictors with non-zero coefficient, and predictors with zero coefficient in the SSI, respectively

Value

Returns the top-2 PC's plot connecting testing (predicted) individuals with training (predictors) individuals

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV == 1)              # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))    # Subset and scale markers
G = tcrossprod(M)                     # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))   # Subset ans scale response variable

# Training and testing sets
tst = seq(1,length(y),by=6)
trn = seq_along(y)[-tst]

fm = SSI(y,K=G,tst=tst,trn=trn)

# Basic setting
plotNet(fm,K=G,bg.color="white",line.color="gray25")
plotNet(fm,K=G,unified=FALSE)


# Passing a matrix of coefficients
B = as.matrix(coef(fm,df=15))
plotNet(fm,B=B,K=G,curve=TRUE,set.size=c(3.5,1.5,1))

# Using Spectral Value Decomposition and grouping
EVD = eigen(G)
gp = data.frame(group=kmeans(EVD$vectors[,1:3],centers=5)$cluster)
plotNet(fm,curve=TRUE,group=gp,U=EVD$vectors,d=EVD$values)
```

---

plotPath *Coefficients path plot*

Description

Coefficients evolution path plot from an object of the class 'LASSO' or 'SSI'

Usage

```
plotPath(fm, Z = NULL, K = NULL, tst = NULL,
         title = NULL, maxCor = 0.85)
```

Arguments

fm	An object of the 'LASSO' or 'SSI' class
Z	(numeric matrix) Design matrix for random effects. When Z=NULL an identity matrix is considered (default) thus **G = K**; otherwise $\mathbf{G} = \mathbf{Z}\,\mathbf{K}\,\mathbf{Z}'$ is used. Only needed for a fm object of the class 'SSI'
K	(numeric matrix) Kinship relationships. This can be a name of a binary file where the matrix is stored. Only needed for a fm object of the class 'SSI'
tst	(integer vector) Which elements from vector y (stored in fm$y) are in testing set and to plot. They must be contained in fm$tst. Default tst=NULL will consider the whole vector fm$tst to plot
title	(character/expression) Title of the plot
maxCor	(numeric) Maximum correlation allowed for two different coefficients. A group of coeffcients with a correlation greater than maxCor are likely to overlap in the plot thus only one is kept

Value

Returns the plot of the coefficients' evolution path along the regularization parameter

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV == 1)              # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))    # Subset and scale markers
G = tcrossprod(M)                     # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))   # Subset response variable
X = scale(X_E1[index,])               # Reflectance data

# Sparse phenotypic regression
fm1 = lars2(var(X),cov(y,X))

# Sparse family index
fm2 = SSI(y,K=G,tst=1:10,trn=11:50)
```

```
plotPath(fm1)
plotPath(fm2,maxCor=0.6)
plotPath(fm2,K=G,maxCor=0.6)


# Path plot for the first individual in testing set for the SSI
plotPath(fm2,K=G,tst=fm2$tst[1])
```

`solveEN` *Coordinate Descent algorithm to solve Elastic-Net-type problems*

Description

Computes the entire Elastic-Net solution for the regression coefficients for all values of the penalization parameter, via the Coordinate Descent (CD) algorithm (Friedman, 2007). It uses as inputs a variance matrix among predictors and a covariance vector between response and predictors

Usage

```
solveEN(Sigma, Gamma, alpha = 1, lambda = NULL,
        nLambda = 100, minLambda = .Machine$double.eps^0.5,
        maxDF = NULL, scale = TRUE, tol = 1e-05,
        maxIter = 1000, verbose = FALSE)
```

Arguments

`Sigma`	(numeric matrix) Variance-covariance matrix of predictors. It can be of the "float32" type as per the 'float' R-package
`Gamma`	(numeric vector) Covariance between response variable and predictors
`lambda`	(numeric vector) Penalization parameter sequence. Default is `lambda=NULL`, in this case a decreasing grid of `'nLambda'` lambdas will be generated starting from a maximum equal to `max(abs(Gamma)/alpha)` to a minimum equal to zero. If `alpha=0` the grid is generated starting from a maximum equal to 5
`nLambda`	(integer) Number of lambdas generated when `lambda=NULL`
`minLambda`	(numeric) Minimum value of lambda that are generated when `lambda=NULL`
`alpha`	(numeric) Value between 0 and 1 for the weights given to the L1 and L2-penalties
`scale`	`TRUE` or `FALSE` to scale matrix `Sigma` for variables with unit variance and scale `Gamma` by the standard deviation of the corresponding predictor taken from the diagonal of `Sigma`

`tol`	(numeric) Maximum error between two consecutive solutions of the CD algorithm to declare convergence
`maxIter`	(integer) Maximum number of iterations to run the CD algorithm at each lambda step before convergence is reached
`maxDF`	(integer) Maximum number of non-zero coefficients in the last solution. Default `maxDF=NULL` will calculate solutions for the entire lambda sequence
`verbose`	`TRUE` or `FALSE` to whether printing each CD step

Details

Finds solutions for the regression coefficients in a linear model

$$y_i = \mathbf{x}_i'\boldsymbol{\beta} + e_i$$

where y_i is the response for the i^{th} observation, $\mathbf{x}_i = (x_{i1}, ..., x_{ip})'$ is a vector of p predictors assumed to have unit variance, $\boldsymbol{\beta} = (\beta_1, ..., \beta_p)'$ is a vector of regression coefficients, and e_i is a residual.

The regression coefficients $\boldsymbol{\beta}$ are estimated as function of the variance matrix among predictors ($\boldsymbol{\Sigma}$) and the covariance vector between response and predictors ($\boldsymbol{\Gamma}$) by minimizing the penalized mean squared error function

$$-\boldsymbol{\Gamma}'\boldsymbol{\beta} + 1/2\boldsymbol{\beta}'\boldsymbol{\Sigma}\boldsymbol{\beta} + \lambda J(\boldsymbol{\beta})$$

where λ is the penalization parameter and $J(\boldsymbol{\beta})$ is a penalty function given by

$$1/2(1-\alpha)||\boldsymbol{\beta}||_2^2 + \alpha||\boldsymbol{\beta}||_1$$

where $0 \leq \alpha \leq 1$, and $||\boldsymbol{\beta}||_1 = \sum_{j=1}^{p} |\beta_j|$ and $||\boldsymbol{\beta}||_2^2 = \sum_{j=1}^{p} \beta_j^2$ are the L1 and (squared) L2-norms, respectively.

The "partial residual" excluding the contribution of the predictor x_{ij} is

$$e_i^{(j)} = y_i - \mathbf{x}_i'\boldsymbol{\beta} + x_{ij}\beta_j$$

then the ordinary least-squares (OLS) coefficient of x_{ij} on this residual is (up-to a constant)

$$\beta_j^{(ols)} = \Gamma_j - \boldsymbol{\Sigma}_j'\boldsymbol{\beta} + \beta_j$$

where Γ_j is the j^{th} element of $\boldsymbol{\Gamma}$ and $\boldsymbol{\Sigma}_j$ is the j^{th} column of the matrix $\boldsymbol{\Sigma}$.

Coefficients are updated for each $j = 1, ..., p$ from their current value β_j to a new value $\beta_j(\alpha, \lambda)$, given α and λ, by "soft-thresholding" their OLS estimate until convergence as fully described in Friedman (2007).

Value

Returns a list object containing the elements:

- `lambda`: (vector) all the sequence of values of the penalty.
- `beta`: (matrix) regression coefficients for each predictor (in rows) associated to each value of the penalization parameter lambda (in columns).
- `df`: (vector) degrees of freedom, number of non-zero predictors associated to each value of lambda.

The returned object is of the class 'LASSO' for which methods `fitted` exist. Function 'plotPath' can be also used

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

References

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Zou H, Hastie T (2005). Regularization and variable selection via the elastic net. *Journal of the Royal Statistical Society B*, **67**(2), 301–320.

Examples

```
require(SFSI)
data(wheatHTP)

y = as.vector(Y[,"E1"])  # Response variable
X = scale(X_E1)          # Predictors

# Training and testing sets
tst = seq(1,length(y),by=3)
trn = seq_along(y)[-tst]

# Calculate covariances in training set
XtX = var(X[trn,])
Xty = cov(y[trn],X[trn,])

# Run the penalized regression
fm1 = solveEN(XtX,Xty,alpha=0.5)

# Predicted values
yHat1 = fitted(fm1, X=X[trn,])  # training data
yHat2 = fitted(fm1, X=X[tst,])  # testing data
```

```
# Penalization vs correlation
plot(-log(fm1$lambda[-1]),cor(y[trn],yHat1[,-1]), main="training")
plot(-log(fm1$lambda[-1]),cor(y[tst],yHat2[,-1]), main="testing")


if(requireNamespace("float")){
 # Using a 'float' type variable
 XtX2 = float::fl(XtX)
 fm2 = solveEN(XtX2,Xty,alpha=0.5)
 max(abs(fm1$beta-fm2$beta))  # Check for discrepances
}
```

SSI *Sparse Selection Index*

Description

Computes the entire Elastic-Net solution for the regression coefficients of a Selection Index for a grid of values of the penalization parameter.

An optimal penalization can be chosen using cross-validation (CV) within a specific training set.

Usage

```
SSI(y, X = NULL, b = NULL, Z = NULL, K, D = NULL,
    h2 = NULL, trn = seq_along(y), tst = seq_along(y),
    subset = NULL, alpha = 1, lambda = NULL, nLambda = 100,
    minLambda = .Machine$double.eps^0.5, commonLambda = TRUE,
    tol = 1E-4, maxIter = 500, method = c("REML","ML"),
    saveAt = NULL, name = NULL, mc.cores = 1, verbose = TRUE)

SSI_CV(y, X = NULL, b = NULL, Z = NULL, K, D = NULL,
      h2 = NULL, trn = seq_along(y), alpha = 1, lambda = NULL,
      nLambda = 100, minLambda = .Machine$double.eps^0.5,
      nCV = 1, nFolds = 5, seed = NULL, commonLambda = TRUE,
      tol = 1E-4, maxIter = 500, method = c("REML","ML"),
      name = NULL, mc.cores = 1, verbose = TRUE)
```

Arguments

y	(numeric vector) Response variable
X	(numeric matrix) Design matrix for fixed effects. When X=NULL, a vector of ones is constructed only for the intercept (default)
b	(numeric vector) Fixed effects. When b=NULL, only the intercept is estimated from training data using generalized least squares (default)

Z	(numeric matrix) Design matrix for random effects. When Z=NULL an identity matrix is considered (default) thus **G = K**; otherwise **G** $=$ **Z K Z'** is used
K	(numeric matrix) Kinship relationships. This can be of the "float32" type as per the 'float' R-package, or a (character) name of a binary file where the matrix is stored
D	(numeric matrix) Relationships among residuals (usually an identity matrix). When D=NULL an identity matrix is considered (default)
h2	(numeric) Heritability of the response variable. When h2=NULL (default), it is calculated from training data estimated using the function 'fitBLUP' (see help(fitBLUP)). It is used to set the residual to genetic variance ratio given by (1-h2)/h2
trn	(integer vector) Which elements from vector y are in training set. Default trn=seq_along(y) will consider all individuals as training
tst	(integer vector) Which elements from vector y are in testing set (prediction set). Default tst=seq_along(y) will consider all individuals as testing
subset	(integer vector) $c(m, M)$ to fit the model only for the m^{th} subset out of M subsets that the testing set will be divided into. Results can be automatically saved when saveAt argument is provided and can be retrieved later using function 'collect' (see help(collect)). Default is subset=NULL for no subsetting, then the model is fitted for all testing data
alpha	(numeric) Value between 0 and 1 for the weights given to the L1 and L2-penalties
lambda	(numeric vector) Penalization parameter sequence. Default is lambda=NULL, in this case a decreasing grid of nLambda lambdas will be generated starting from a maximum equal to `max(abs(G[trn,tst])/alpha)` to a minimum equal to zero. If alpha=0 the grid is generated starting from a maximum equal to 5
nLambda	(integer) Number of lambdas generated when lambda=NULL
minLambda	(numeric) Minimum value of lambda that are generated when lambda=NULL
nFolds	(integer/character) Either 2,3,5,10 or 'n' indicating the number of non-overlaping folds in which the data is split into to do cross-validation. When nFolds='n' leave-one-out CV is performed
seed	(numeric vector) Seed to fix randomization when creating folds for cross-validation. If it is a vector, a number equal to its length of CV repetitions are performed
nCV	(integer) Number of CV repetitions to be performed. Default is nCV=1
commonLambda	TRUE or FALSE to whether computing the coefficients for a grid of lambdas common to all individuals in testing set or for a grid of lambdas specific to each individual in testing set. Default is commonLambda=TRUE
mc.cores	(integer) Number of cores used. The analysis is run in parallel when mc.cores is greater than 1. Default is mc.cores=1
tol	(numeric) Maximum error between two consecutive solutions of the CD algorithm to declare convergence

maxIter	(integer) Maximum number of iterations to run the CD algorithm at each lambda step before convergence is reached
saveAt	(character) Prefix name that will be added to the output files name to be saved, this may include a path. Regression coefficients are saved as a binary file (single-precision: 32 bits, 7 significant digits). Default saveAt=NULL will no save any output
method	(character) Either 'REML' (Restricted Maximum Likelihood) or 'ML' (Maximum Likelihood) to calculate variance components as per the function 'fitBLUP'
name	(character) Name given to the output for tagging purposes. Default name=NULL will give the name of the method used
verbose	TRUE or FALSE to whether printing each step

Details

The basic linear mixed model that relates phenotypes with genetic values is of the form

$$\mathbf{y} = \mathbf{Xb} + \mathbf{Zg} + \mathbf{e}$$

where **y** is a vector with the response, **b** is the vector of fixed effects, **g** is the vector of the genetic values of the genotypes, **e** is the vector of environmental residuals, and **X** and **Z** are design matrices conecting the fixed and genetic effects with replicates. Genetic values are assumed to follow a Normal distribution as $\mathbf{g} \sim N(\mathbf{0}, \sigma_u^2\mathbf{K})$, and environmental terms are assumed $\mathbf{e} \sim N(\mathbf{0}, \sigma_e^2\mathbf{D})$, usually $\mathbf{D} = \mathbf{I}$.

The resulting vector of genetic values $\mathbf{u} = \mathbf{Zg}$ will therefore follow $\mathbf{u} \sim N(\mathbf{0}, \sigma_u^2\mathbf{G})$ where $\mathbf{G} = \mathbf{ZKZ}'$. In the un-replicated case, $\mathbf{Z} = \mathbf{I}$ is an identity matrix, and hence $\mathbf{u} = \mathbf{g}$ and $\mathbf{G} = \mathbf{K}$.

The values $\mathbf{u}_{tst} = (u_i)$, $i = 1, 2, ..., n_{tst}$, for a testing set are estimated individual-wise using (as predictors) all available observations in a training set as

$$u_i = \boldsymbol{\beta}_i'(\mathbf{y}_{trn} - \mathbf{X}_{trn}\mathbf{b})$$

where $\boldsymbol{\beta}_i$ is a vector of weights that are found separately for each individual in the testing set, by minimizing the penalized mean squared error function

$$-\mathbf{G}'_{trn,tst(i)}\boldsymbol{\beta}_i + 1/2\boldsymbol{\beta}_i'(\mathbf{G}_{trn} + \theta\mathbf{D})\boldsymbol{\beta}_i + \lambda J(\boldsymbol{\beta}_i)$$

where $\mathbf{G}_{trn,tst(i)}$ is the i^{th} column of the sub-matrix of **G** whose rows correspond to the training set and columns to the testing set; $\mathbf{G}_{trn}$ is the sub-matrix corresponding to the training set; $\theta = \sigma_e^2/\sigma_u^2$ is the residual to genetic variance ratio that can be expressed in terms of the heritability, $h^2 = \sigma_u^2/(\sigma_u^2 + \sigma_e^2)$, as $\theta = (1 - h^2)/h^2$; λ is the penalization parameter; and $J(\boldsymbol{\beta}_i)$ is a penalty function given by

$$1/2(1 - \alpha)||\boldsymbol{\beta}_i||_2^2 + \alpha||\boldsymbol{\beta}_i||_1$$

where $0 \leq \alpha \leq 1$, and $||\boldsymbol{\beta}_i||_1 = \sum_{j=1}^{n_{trn}} |\beta_{ij}|$ and $||\boldsymbol{\beta}_i||_2^2 = \sum_{j=1}^{n_{trn}} \beta_{ij}^2$ are the L1 and (squared) L2-norms, respectively.

Function 'SSI' calculates each individual solution using the function 'solveEN' (via the Coordinate Descent algorithm, see `help(solveEN)`) by setting the argument `Sigma` equal to $\mathbf{G}_{trn} + \theta\mathbf{D}$ and `Gamma` equal to $\mathbf{G}_{trn,tst(i)}$.

Function 'SSI_CV' performs cross-validation within the training data specified in argument `trn`. Training data is divided into k folds and the SSI is sequentially calculated for (all individuals in) one fold (testing set) using information from the remaining folds (training set).

Value

Function 'SSI' returns a list object of the class 'SSI' for which methods `coef`, `fitted`, `plot`, and `summary` exist. Functions 'plotNet' and 'plotPath' can be also used. It contains the elements:

- `b`: (vector) fixed effects solutions (including the intercept).
- `Xb`: (vector) product of the design matrix 'X' times the fixed effects solutions.
- `varU`, `varE`, `h2`: variance components solutions.
- `alpha`: value for the elastic-net weights used.
- `lambda`: (matrix) sequence of values of lambda used (in columns) for each testing individual (in rows).
- `df`: (matrix) degrees of freedom (number of non-zero predictors) at each solution given by lambda for each testing individual (in rows).
- `file_beta`: path where regression coefficients are saved.

Function 'SSI_CV' returns a list object of length `nCV` of the class 'SSI_CV' for which methods `plot` and `summary` exist. Each element is also a list containing the elements:

- `b`: (vector) solutions for the fixed effects (including the intercept) for each fold.
- `varU`, `varE`, `h2`: variance components estimated within each fold.
- `folds`: (matrix) assignation of training individuals to folds used for the cross-validation.
- `accuracy`: (matrix) correlation between observed and predicted values (in testing set) within each fold (in rows).
- `MSE`: (matrix) mean squared error of prediction (in testing set) within each fold (in rows).
- `lambda`: (matrix) with the sequence of values of lambda used (averaged across individuals) within each fold (in rows).
- `df`: (matrix) with the degrees of freedom (averaged across individuals) within each fold (in rows).

Author(s)

Marco Lopez-Cruz (<maraloc@gmail.com>) and Gustavo de los Campos

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Examples

```
require(SFSI)
data(wheatHTP)

index = which(Y$CV == 1)              # Use only a subset of data
M = scale(M[index,])/sqrt(ncol(M))    # Subset and scale markers
G = tcrossprod(M)                     # Genomic relationship matrix
y = as.vector(scale(Y[index,"E1"]))   # Subset ans scale response variable

# Training and testing sets
tst = seq(1,length(y),by=3)
trn = (seq_along(y))[-tst]

# Calculate heritability using training data
yNA <- y
yNA[tst] <- NA
fm0 = fitBLUP(yNA,K=G)
h2 = fm0$varU/(fm0$varU + fm0$varE)

# Sparse selection index
fm1 = SSI(y,K=G,h2=h2,trn=trn,tst=tst)
summary(fm1)$optCOR


if(requireNamespace("float")){
# Using a 'float' type variable for K
G2 = float::fl(G)
fm2 = SSI(y,K=G2,h2=h2,trn=trn,tst=tst)
summary(fm2)$optCOR  # compare with above results
}


#-----------------------------------------------------
# Predicting a testing set using a value of lambda
# obtained from cross-validation in a traning set
#-----------------------------------------------------
# Run a cross validation in training set
fm2 = SSI_CV(y,K=G,h2=h2,trn=trn,nFolds=5,name="1 5CV")
lambda = summary(fm2)$optCOR["mean","lambda"]
```

```
# Fit the index with the obtained lambda
fm3 = SSI(y,K=G,h2=h2,trn=trn,tst=tst,lambda=lambda)
summary(fm3)$accuracy        # Testing set accuracy

# Compare the accuracy with that of the non-sparse index (G-BLUP)
cor(fm0$u[tst],y[tst])


# Obtain an 'optimal' lambda by repeating the CV several times
fm22 = SSI_CV(y,K=G,h2=h2,trn=trn,nCV=5,name="5 5CV")
plot(fm22,fm2)
```

`wheat` *Wheat dataset*

Description

The dataset consists of 1,092 inbred wheat lines grouped into 39 trials and grown during the 2013-2014 season at the Norman Borlaug experimental research station in Ciudad Obregon, Sonora, Mexico. Each trial consisted of 28 breeding lines that were arranged in an alpha-lattice design with three replicates and six sub-blocks. The trials were grown in four different environments:

- E1: Flat-Drought (sowing in flat with irrigation of 180 mm through drip system)
- E2: Bed-2IR (sowing in bed with 2 irrigations approximately 250 mm)
- E3: Bed-5IR (bed sowing with 5 normal irrigations)
- E4: Bed-EHeat (bed sowing 30 days before optimal planting date with 5 normal irrigations approximately 500 mm)

1. Phenotypic data. Measurements of grain yield (YLD) were reported as the total plot yield after maturity. Records for YLD are reported as adjusted means from which trial, replicate and sub-block effects were removed. Measurements for days to heading (DTH), days to maturity (DTM), and plant height (PH) were recorded only in the first replicate at each trial and thus no phenotype adjustment was made.

2. Reflectance data. Reflectance data was collected from the fields using both infrared and hyper-spectral cameras mounted on an aircraft on 9 different dates (time-points) between January 10 and March 27th, 2014. During each flight, data from 250 wavelengths ranging from 392 to 850 nm were collected for each pixel in the pictures. The average reflectance of all the pixels for each wavelength was calculated from each of the geo-referenced trial plots and reported as each line reflectance. Data for reflectance and Green NDVI and Red NDVI are reported as adjusted phenotypes from which trial, replicate and sub-block effects were removed. Each data-point matches to each data-point in phenotypic data.

3. Marker data. Lines were sequenced for GBS at 192-plexing on Illumina HiSeq2000 or HiSeq2500 with 1 x 100 bp reads. SNPs were called across all lines anchored to the genome assembly of Chinese Spring (International Wheat Genome Sequencing Consortium 2014). Next, SNP were extracted and filtered so that lines >50% missing data were removed. Markers were recoded as –1, 0,

and 1, corresponding to homozygous for the minor allele, heterozygous, and homozygous for the major allele, respectively. Next, markers with a minor allele frequency <0.05 and >15% of missing data were removed. Remaining SNPs with missing values were imputed using the mean of the observed marker genotypes at a given locus.

Replicated and Un-replicated data. The CRAN version includes the `wheatHTP` dataset containing (un-replicated) YLD from all environments E1,...,E4, and reflectance (latest time-point only) data from the environment E1 only. Marker data is also included in the dataset. The phenotypic and reflectance data are averages (line effects from mixed models) for 776 lines evaluated in 28 trials (with at least 26 lines each) for which marker information on 3,438 SNPs is available.

The GitHub (development) version of the SFSI R-package (https://github.com/MarcooLopez/SFSI) includes also the `wheatHTP` dataset plus `wheatHTP.E1`,...,`wheatHTP.E4` datasets containing replicated (adjusted) phenotypic and reflectance data for all four environments, respectively.

Cross-validation partitions. One random partition of 4-folds is provided for the un-replicated data (`wheatHTP` dataset) containing 776 individuals and 28 trials. Data from 7 entire trials (25% of 28 the trials) were arbitrarily assigned to each of the 4 folds. The partition consist of an array of length 776 with indices 1, 2, 3, and 4 denoting the fold.

Genetic covariances. Multi-variate Gaussian mixed models were fitted to phenotypes from the un-replicated data (`wheatHTP` dataset) containing 776 individuals. Bi-variate models were fitted to YLD with each of the 250 wavelengths from environment E1. Tetra-variate models were fitted for YLD from all environments. All models were fitted within each fold (provided partition) using scaled (null mean and unit variance) phenotypes from the remaining 3 folds as training data. Bayesian models were implemented using the 'Multitrait' function from the `BGLR` R-package with 30,000 iterations discarding 5,000 runs for burning. A marker-derived relationships matrix as in VanRaden (2008) was used to model between-individuals genetic effects; both between-traits genetic and residual covariances were assumed unstructured.

Genetic and residual covariances between YLD and each wavelength (environment E1) are storaged in a matrix of 250 rows and 4 columns (folds). Genetic and residual covariances matrices among YLD within each environment are storaged in a list with 4 elements (folds).

Usage

```
data(wheatHTP)
# data(wheatHTP.E1) # GitHub version
# data(wheatHTP.E2) # GitHub version
# data(wheatHTP.E3) # GitHub version
# data(wheatHTP.E4) # GitHub version
```

Format

Replicated data (`wheatHTP.E1`,...,`wheatHTP.E4` datasets):

- `Y`: (matrix) phenotypic data for YLD, DTH, DTM, and PH; and the trial in which each genotype was tested.
- `X`: (9-dimensional list) reflectance data for time-points 1,2,...,9.
- `VI`: (9-dimensional list) green and red NDVI for time-points 1,2,...,9.

Un-replicted data (`wheatHTP` dataset):

- `Y`: (matrix) phenotypic data for YLD in environments E1, E2, E3, and E4; and columns 'trial' and 'CV' (indicating the 4-folds partition).
- `M`: (matrix) marker data with SNPs in columns.
- `X_E1`: (matrix) reflectance data for time-point 9 in environment E1.
- `genCOV_xy`: (matrix) genetic covariances between YLD and each reflectance trait, for each fold (in columns).
- `resCOV_xy`: (matrix) residual covariances between YLD and each reflectance trait, for each fold (in columns).
- `genCOV_yy`: (4-dimensional list) genetic covariances matrices for YLD among environments, for each fold.
- `resCOV_yy`: (4-dimensional list) residual covariances matrices for YLD among environments, for each fold.

Source

International Maize and Wheat Improvement Center (CIMMYT), Mexico.

References

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Index