

Package ‘decorrelate’

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Type Package

Title Decorrelation Projection Scalable to High Dimensional Data

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Description Data whitening is a widely used preprocessing step to remove correlation structure since statistical models often assume independence. Here we use a probabilistic model of the observed data to apply a whitening transformation. This Gaussian Inverse Wishart Empirical Bayes model substantially reduces computational complexity, and regularizes the eigen-values of the sample covariance matrix to improve out-of-sample performance.

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Encoding UTF-8

URL <https://gabrielhoffman.github.io/decorrelate/>

BugReports <https://github.com/GabrielHoffman/decorrelate/issues>

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| | |
|--------------|--------------------------------|
| autocorr.mat | Create auto-correlation matrix |
|--------------|--------------------------------|

Description

Create auto-correlation matrix

Usage

autocorr.mat(p, rho)

Arguments

- | | |
|-----|-----------------------|
| p | dimension of matrix |
| rho | autocorrelation value |

Value

auto-matrix of size p with parameter ρ

Examples

```
# Create 4x4 matrix with correlation between adjacent enties is 0.9
autocorr.mat(4, .9)
```

| | |
|-------------|-------------------------------------|
| averageCorr | <i>Summarize correlation matrix</i> |
|-------------|-------------------------------------|

Description

Summarize correlation matrix as a scalar scalar value, given its SVD and shrinkage parameter. `averageCorr()` computes the average correlation, and `averageCorrSq()` computes the average squared correlation, where both exclude the diagonal terms. `sumInverseCorr()` computes the sum of entries in the inverse correlation matrix to give the 'effective number of independent features'. `effVariance()` evaluates effective variance of the correlation (or covariance) matrix. These values can be computed using the correlation matrix using standard MLE, or EB shrinkage.

Usage

```
averageCorr(ecl, method = c("EB", "MLE"))

averageCorrSq(ecl, method = c("EB", "MLE"))

sumInverseCorr(ecl, method = c("EB", "MLE"), absolute = TRUE)

effVariance(ecl, method = c("EB", "MLE"))

tr(ecl, method = c("EB", "MLE"))
```

Arguments

| | |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------|
| <code>ecl</code> | estimate of correlation matrix from <code>eclairs()</code> storing U , d_1^2 , λ and ν |
| <code>method</code> | compute average correlation for either the empirical Bayes (EB) shinken correlation matrix or the MLE correlation matrix |
| <code>absolute</code> | if TRUE (default) evaluate on absolute correlation matrix |

Details

`tr()`: trace of the matrix. Sum of diagonals is the same as the sum of the eigen-values.

`averageCorr()`: The average correlation is computed by summing the off-diagonal values in the correlation matrix. The sum of all elements in a matrix is $g = \sum_{i,j} C_{i,j} = 1^T C 1$, where 1 is a vector of p elements with all entries 1. This last term is a quadratic form of the correlation matrix

that can be computed efficiently using the SVD and shrinkage parameter from `eclairs()`. Given the value of g , the average is computed by subtracting the diagonal values and dividing by the number of off-diagonal values: $(g - p)/(p(p - 1))$.

`averageCorrSq()`: The average squared correlation is computed using only the eigen-values. Surprisingly, this is a function of the variance of the eigen-values. This is reviewed by Watanabe (2022) and Durand and Le Roux (2017). Letting λ_i be the i^{th} sample or shrunk eigen-value, and $\tilde{\lambda}$ be the mean eigen-value, then $\sum_i (\lambda_i - \tilde{\lambda})^2 / p(p - 1) \tilde{\lambda}^2$.

`sumInverseCorr()`: The 'effective number of independent features' is computed by summing the entires of the inverse covariance matrix. This has the form $\sum_{i,j} C_{i,j}^{-1} = 1^T C^{-1} 1$. This last term is a quadratic form of the correlation matrix that can be computed efficiently using the SVD and shrinkage parameter from `eclairs()` as described above.

`effVariance()`: Compute a metric of the amount of variation represented by a correlation (or covariance) matrix that is comparable across matrices of difference sizes. Proposed by Peña and Rodriguez (2003), the 'effective variance' is $|C|^{\frac{1}{p}}$ where C is a correlation (or covariance matrix) between p variables. The effective variance is the mean of the log eigen-values.

Value

value of summary statistic

References

- Durand, J. L., & Le Roux, B. (2017). Linkage index of variables and its relationship with variance of eigenvalues in PCA and MCA. *Statistica Applicata-Italian Journal of Applied Statistics*, (2-3), 123-135.
- Peña, D., & Rodriguez, J. (2003). Descriptive measures of multivariate scatter and linear dependence. *Journal of Multivariate Analysis*, 85(2), 361-374.
- Watanabe, J. (2022). Statistics of eigenvalue dispersion indices: Quantifying the magnitude of phenotypic integration. *Evolution*, 76(1), 4-28.

Examples

```
library(Rfast)
n <- 200 # number of samples
p <- 800 # number of features

# create correlation matrix
Sigma <- matrix(.2, p, p)
diag(Sigma) <- 1

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# eclairs decomposition
ecl <- eclairs(Y, compute = "cor")

# Average correlation value
```

```

averageCorr(ecl)

# Average squared correlation value
averageCorrSq(ecl)

# Sum elements in inverse correlation matrix
# Gives the effective number of independent features
sumInverseCorr(ecl)

# Effective variance
effVariance(ecl)

```

cov_transform

Estimate covariance matrix after applying transformation

Description

Given covariance between features in the original data, estimate the covariance matrix after applying a transformation to each feature. Here we use the eclairs decomposition of the original covariance matrix, perform a parametric bootstrap and return the eclairs decomposition of the covariance matrix of the transformed data.

Usage

```

cov_transform(
  ecl,
  f,
  n.boot,
  lambda = NULL,
  compute = c("covariance", "correlation"),
  seed = NULL
)

```

Arguments

| | |
|---------|--------------------------------------------------------------------------------------------|
| ecl | covariance/correlation matrix as an eclairs object |
| f | function specifying the transformation. |
| n.boot | number of parametric bootstrap samples. Increasing n gives more precise estimates. |
| lambda | shrinkage parameter. If not specified, it is estimated from the data. |
| compute | evaluate either the "covariance" or "correlation" of X |
| seed | If you want the same to be generated again use a seed for the generator, an integer number |

Details

When the transformation is linear, these covariance matrices are the same.

Value

eclairs decomposition representing correlation/covariance on the transformed data

Examples

```
library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# sample matrix from MVN with covariance Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma, seed = 1)

# perform eclairs decomposition
ecl <- eclairs(Y)

# Parametric bootstrap to estimate covariance
# after transformation

# transformation function
f <- function(x) log(x^2 + 1e-3)

# number of bootstrap samples
n_boot <- 5000

# Evaluate eclairs decomposition on bootstrap samples
ecl2 <- cov_transform(ecl, f = f, n_boot, lambda = 1e-4)

# Get full covariance matrix from eclairs decomposition
C1 <- getCov(ecl2)

# Parametric bootstrap samples directly from full covariance matrix
X <- rmvnorm(n_boot, rep(0, p), getCov(ecl))

# get covariance of transformed data
C2 <- cov(f(X))

# Evaluate differences
# small differences are due to Monte Carlo error from bootstrap sampling
range(C1 - C2)

# Plot entries from two covariance estimates
par(pty = "s")
plot(C1, C2, main = "Concordance between covariances")
abline(0, 1, col = "red")

# Same above but compute eclairs for correlation matrix
#-----
```

```

# Evaluate eclairs decomposition on bootstrap samples
ecl2 <- cov_transform(ecl, f = f, n_boot, compute = "correlation", lambda = 1e-4)

# Get full covariance matrix from eclairs decomposition
C1 <- getCor(ecl2)

# Parametric bootstrap samples directly from full covariance matrix
X <- rmvnorm(n_boot, rep(0, p), getCov(ecl))

# get correlation of transformed data
C2 <- cor(f(X))

# Evaluate differences
# small differences are due to Monte Carlo error from bootstrap sampling
range(C1 - C2)

# Plot entries from two correlation estimates
oldpar <- par(pty = "s")
plot(C1, C2, main = "Correlation between covariances")
abline(0, 1, col = "red")

par(oldpar)

```

decorrelate

*Decorrelation projection***Description**

Efficient decorrelation projection using [eclairs](#) decomposition

Usage

```
decorrelate(X, ecl, lambda, transpose = FALSE, alpha = -1/2)
```

Arguments

| | |
|-----------|--------------------------------------------------------------------------------------------------------------------|
| X | matrix to be transformed so <i>*columns*</i> are independent |
| ecl | estimate of covariance/correlation matrix from eclairs storing U , d_1^2 , λ and ν |
| lambda | specify lambda and override value from ecl |
| transpose | logical, (default FALSE) indicating if X should be transposed first |
| alpha | default = -1/2. Exponent of eigen-values |

Details

Apply a decorrelation transform using the implicit covariance approach to avoid directly evaluating the covariance matrix

Value

a matrix following the decorrelation transformation

Examples

```
library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)

# eclairs decomposition
ecl <- eclairs(Y)

# whitened Y
Y.transform <- decorrelate(Y, ecl)
#
```

dmult

Multiply by diagonal matrix

Description

Multiply by diagonal matrix using efficient algorithm

Usage

```
dmult(M, v, side = c("left", "right"))
```

Arguments

| | |
|------|-----------------------------------------------------------------------------------------------------------|
| M | matrix |
| v | vector with entries forming a diagonal matrix matching the dimensions of M depending on the value of side |
| side | is the matrix M "left" or "right" multiplied by the diagonal matrix |

Details

Naively multiplying by a diagonal matrix with p entries takes $\mathcal{O}(p^2)$, even though most values in the diagonal matrix are zero. R has built in syntax to scale *columns*, so `diag(v) %*% M` can be evaluated with `v * M`. This is often difficult to remember, hard to look up, and scaling *rows* requires `t(t(M) * v)`. This is hard to read and write, and requires two transpose operations.

Here, `dmult()` uses Rcpp to evaluate the right multiplication efficiently, and uses $v * M$ for left multiplication. This gives good performance and readability.

In principle, the Rcpp code can be modified to use BLAS for better performance by treating a `NumericMatrix` as a C array. But this is not currently a bottleneck

Value

matrix product

Examples

```
# right multiply
# mat %%% diag(v)
n <- 30
p <- 20
mat <- matrix(n * p, n, p)
v <- rnorm(p)

A <- dmult(mat, v, side = "right")
B <- mat %%% diag(v)
range(A - B)

# left multiply
# diag(v) %%% mat
n <- 30
p <- 20
mat <- matrix(n * p, p, n)
v <- rnorm(p)

A <- dmult(mat, v, side = "left")
B <- diag(v) %%% mat
range(A - B)
```

eclairs

Estimate covariance/correlation with low rank and shrinkage

Description

Estimate the covariance/correlation between columns as the weighted sum of a low rank matrix and a scaled identity matrix. The weight acts to shrink the sample correlation matrix towards the identity matrix or the sample covariance matrix towards a scaled identity matrix with constant variance. An estimate of this form is useful because it is fast, and enables fast operations downstream. The method is based on the Gaussian Inverse Wishart Empirical Bayes (GIW-EB) model.

Usage

```
eclairs(
  X,
  k,
```

```

lambda = NULL,
compute = c("covariance", "correlation"),
n.samples = nrow(X)
)

```

Arguments

| | |
|------------------|--------------------------------------------------------------------------------------------|
| X | data matrix with n samples as rows and p features as columns |
| k | the rank of the low rank component |
| lambda | shrinkage parameter. If not specified, it is estimated from the data. |
| compute | evaluate either the "covariance" or "correlation" of X |
| n.samples | number of samples data is from. Usually nrow(X), but can be other values in special cases. |

Details

Compute U, d^2 to approximate the correlation matrix between columns of data matrix X by $U \text{diag}(d^2(1-\lambda))U^T + I\nu\lambda$. When computing the covariance matrix, scale by the standard deviation of each feature.

Value

eclairs object storing:

U: orthonormal matrix with k columns representing the low rank component

dSq: eigen-values so that $U \text{diag}(d^2)U^T$ is the low rank component

lambda: shrinkage parameter λ for the scaled diagonal component

sigma: standard deviations of input columns

nu: diagonal value, ν , of target matrix in shrinkage

n: number of samples (i.e. rows) in the original data

p: number of features (i.e. columns) in the original data

k: rank of low rank component

rownames: sample names from the original matrix

colnames: features names from the original matrix

method: method used for decomposition

call: the function call

Examples

```

library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

```

```
# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# eclairs decomposition: covariance
ecl <- eclairs(Y, compute = "covariance")

ecl

# eclairs decomposition: correlation
ecl <- eclairs(Y, compute = "correlation")

ecl
```

eclairs-class

*Class eclairs***Description**

Class eclairs

Details

Object storing:

U: orthonormal matrix with k columns representing the low rank component**dSq:** eigen-values so that $U \text{diag}(d^2) U^T$ is the low rank component**lambda:** shrinkage parameter λ for the scaled diagonal component**sigma:** standard deviations of input columns**nu:** diagonal value, ν , of target matrix in shrinkage**n:** number of samples (i.e. rows) in the original data**p:** number of features (i.e. columns) in the original data**k:** rank of low rank component**rownames:** sample names from the original matrix**colnames:** features names from the original matrix**method:** method used for decomposition**call:** the function call

| | |
|----------------|--------------------------------------------------------------------|
| eclairs_corMat | <i>Estimate covariance/correlation with low rank and shrinkage</i> |
|----------------|--------------------------------------------------------------------|

Description

Estimate covariance/correlation with low rank and shrinkage from the correlation matrix

Usage

```
eclairs_corMat(C, n, k = min(n, nrow(C)), lambda = NULL)
```

Arguments

| | |
|--------|-------------------------------------------------------------------------------------------------------|
| C | sample correlation matrix between features |
| n | number of samples used to estimate the sample correlation matrix |
| k | the rank of the low rank component. Defaults to min of sample size and feature number, $\min(n, p)$. |
| lambda | shrinkage parameter. If not specified, it is estimated from the data. |

Value

[eclairs](#) object storing:

U: orthonormal matrix with k columns representing the low rank component

dSq: eigen-values so that $U \text{diag}(d^2) U^T$ is the low rank component

lambda: shrinkage parameter λ for the scaled diagonal component

sigma: standard deviations of input columns

nu: diagonal value, ν , of target matrix in shrinkage

n: number of samples (i.e. rows) in the original data

p: number of features (i.e. columns) in the original data

k: rank of low rank component

rownames: sample names from the original matrix

colnames: features names from the original matrix

method: method used for decomposition

call: the function call

Examples

```
library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)
rownames(Y) <- paste0("sample_", 1:n)
colnames(Y) <- paste0("gene_", 1:p)

# eclairs decomposition
eclairs(Y, compute = "correlation")

# eclairs decomposition from correlation matrix
eclairs_corMat(cor(Y), n = n)
```

eclairs_sq*Compute eclairs decomp of squared correlation matrix*

Description

Given the eclairs decomp of C, compute the eclairs decomp of C^2

Usage

```
eclairs_sq(ecl, rank1 = ecl$k, rank2 = Inf, varianceFraction = 1)
```

Arguments

| | |
|------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ecl | estimate of correlation matrix from eclairs() storing U , d_1^2 , λ and ν |
| rank1 | use the first 'rank' singular vectors from the SVD. Using increasing rank1 will increase the accuracy of the estimation. But note that the computational complexity is $O(P \text{ choose}(\text{rank}, 2))$, where P is the number of features in the dataset |
| rank2 | rank of eclairs() decomposition returned |
| varianceFraction | fraction of variance to retain after truncating trailing eigen values |

Details

Consider a data matrix $X_{N \times P}$ of P features and N samples where $N \ll P$. Let the columns of X be scaled so that $C_{P \times P} = XX^T$. C is often too big to compute directly since it is $O(P^2)$ and $O(P^3)$ to invert. But we can compute the SVD of X in $O(PN^2)$. The goal is to compute the SVD of the matrix C^2 , given only the SVD of C in less than $O(P^2)$ time. Here we compute this SVD

of C^2 in $O(PN^4)$ time, which is tractible for small N . Moreover, if we use an SVD $X = UDV^T$ with of rank R , we can approximate the SVD of C^2 in $O(PR^4)$ using only D and V

Value

compute the eclairs of C^2

Examples

```
# Compute correlations directly and using eclairs decomp

n <- 600 # number of samples
p <- 100 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- Rfast::rmvnorm(n, rep(0, p), sigma = Sigma, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# correlation computed directly
C <- cor(Y)

# correlation from eclairs decomposition
ecl <- eclairs(Y, compute = "cor")
C.eclairs <- getCor(ecl, lambda = 0)

all.equal(C, C.eclairs)

# Correlation of Y^2
#-----

# exact quadratic way
C <- 2 * cor(Y)^2

# faster low rank
ecl2 <- eclairs_sq(ecl)
C.eclairs <- 2 * getCor(ecl2, lambda = 0)

all.equal(C.eclairs, C)
```

fastcca-class

Class fastcca

Description

Class fastcca

Details

Object storing:

n.comp: number of canonical components

cors: canonical correlations

x.coefs: canonical coefficients for X

x.vars: canonical variates for X

y.coefs: canonical coefficients for Y

y.vars: canonical variates for Y

lambdas: shrinkage parameters from eclairs

getCov

Get full covariance/correlation matrix from [eclairs](#)

Description

Get full covariance/correlation matrix from [eclairs](#) decomposition

Usage

```
getCov(ecl, lambda, ...)
```

```
getCor(ecl, lambda, ...)
```

```
## S4 method for signature 'eclairs'
getCov(ecl, lambda, ...)
```

```
## S4 method for signature 'eclairs'
getCor(ecl, lambda, ...)
```

Arguments

ecl eclairs decomposition

lambda shrinkage parameter for the convex combination.

... other arguments

Details

The full matrix is computationally expensive to compute and uses a lot of memory for large p. So it is better to use [decorrelate](#) or [mult_eclairs](#) to perform projections in $O(np)$ time.

Value

p x p covariance/correlation matrix

Examples

```

library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# eclairs decomposition
ecl <- eclairs(Y)

# extract covariance implied by eclairs decomposition
getCov(ecl)[1:3, 1:3]

```

| | |
|--------------------|--------------------------------------------------------|
| getShrinkageParams | <i>Estimate shrinkage parameter by empirical Bayes</i> |
|--------------------|--------------------------------------------------------|

Description

Estimate shrinkage parameter by empirical Bayes

Usage

```
getShrinkageParams(ecl, k = ecl$k, minimum = 1e-04, lambda = NULL)
```

Arguments

| | |
|---------|-------------------------------------------------------------------------------------------------------|
| ecl | eclairs() decomposition |
| k | number of singular vectors to use |
| minimum | minimum value of lambda |
| lambda | (default: NULL) If NULL, estimate lambda from data. Else evaluate logML using specified lambda value. |

Details

Estimate shrinkage parameter for covariance matrix estimation using empirical Bayes method (Han-nart and Naveau, 2014; Leday and Richardson 2019). The shrinkage estimate of the covariance matrix is $(1 - \lambda)\hat{\Sigma} + \lambda\nu I$, where $\hat{\Sigma}$ is the sample covariance matrix, given a value of λ . A large value of λ indicates more weight on the prior.

Value

value λ and ν indicating the shrinkage between sample and prior covariance matrices.

References

Hannart, A., & Naveau, P. (2014). Estimating high dimensional covariance matrices: A new look at the Gaussian conjugate framework. *Journal of Multivariate Analysis*, 131, 149-162.

Leday, G. G., & Richardson, S. (2019). Fast Bayesian inference in large Gaussian graphical models. *Biometrics*, 75(4), 1288-1298.

Examples

```
library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# eclairs decomposition: covariance
ecl <- eclairs(Y, compute = "correlation")

# For full SVD
getShrinkageParams(ecl)

# For truncated SVD at k = 20
getShrinkageParams(ecl, k = 20)
```

| | |
|--------------------|-----------------------------|
| getWhiteningMatrix | <i>Get whitening matrix</i> |
|--------------------|-----------------------------|

Description

Get whitening matrix implied by [eclairs](#) decomposition

Usage

```
getWhiteningMatrix(ecl, lambda)
```

Arguments

ec1 estimate of covariance/correlation matrix from [eclairs](#) storing U , d_1^2 , λ and ν
 lambda specify lambda and override value from ec1

Value

whitening matrix

Examples

```
library(Rfast)

n <- 2000
p <- 3

Y <- matnorm(n, p, seed = 1) * 10

# decorrelate with implicit whitening matrix
# give same result as explicit whitening matrix
ec1 <- eclairs(Y, compute = "covariance")

# get explicit whitening matrix
W <- getWhiteningMatrix(ec1)

# apply explicit whitening matrix
Z1 <- tcrossprod(Y, W)

# use implicit whitening matrix
Z2 <- decorrelate(Y, ec1)

range(Z1 - Z2)
```

kappa,eclairs-method *Compute condition number*

Description

Compute condition number of matrix from eclairs decomposition

Usage

```
## S4 method for signature 'eclairs'
kappa(z, lambda = NULL)
```

Arguments

z eclairs() decomposition
 lambda specify lambda to override value from z

Value

condition number of the correlation matrix. If z is a covariance matrix, kappa is only computed for the correlation component

Examples

```
library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# eclairs decomposition
ecl <- eclairs(Y, compute = "correlation")

# compute condition number
kappa(ecl)
```

lm_each_eclairs

Fit linear model on each feature after decorrelating

Description

Fit linear model on each feature after applying decorrelation projection to response and predictors.

Usage

```
lm_each_eclairs(
  formula,
  data,
  X,
  ecl,
  subset,
  weights,
  na.action,
  method = "qr",
  model = TRUE,
  x = FALSE,
  y = FALSE,
  qr = TRUE,
```

```

    singular.ok = TRUE,
    contrasts = NULL,
    offset,
    ...
  )

```

Arguments

| | |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| formula | an object of class 'formula' (or one that can be coerced to that class): a symbolic description of the model to be fitted. |
| data | a matrix or data.frame containing the variables in the model |
| X | matrix or data.frame where each column stores a predictor to be evaluated by the regression model one at a time. The i^{th} model includes $X[, i]$ as a predictor. |
| ecl | estimate of covariance/correlation matrix from eclairs storing U , d_1^2 , λ and ν |
| subset | same as for lm |
| weights | same as for lm |
| na.action | same as for lm |
| method | same as for lm |
| model | same as for lm |
| x | same as for lm |
| y | same as for lm |
| qr | same as for lm |
| singular.ok | same as for lm |
| contrasts | same as for lm |
| offset | same as for lm |
| ... | other arguments passed to <code>lm()</code> |

Value

data.frame with columns beta, se, tsat, pvalue storing results for regression model fit for each feature

Examples

```

library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)

```

```

# eclairs decomposition
ecl <- eclairs(Y)

# simulate covariates
data <- data.frame(matrnorm(p, 2, seed = 1))
colnames(data) <- paste0("v", 1:2)

# simulate response
y <- rnorm(p)

# Simulate 1000 features to test
X <- matrnorm(p, 1000, seed = 1)
colnames(X) <- paste0("set_", seq(ncol(X)))

# Use linear model to test each feature stored as columns in X
res <- lm_each_eclairs(y ~ v1 + v2, data, X, ecl)

head(res)

# Analysis after non-linear transform
#-----

# Apply function to transforme data
f <- function(x) log(x^2 + 0.001)

# evaluate covariance of transformed data
ecl_transform <- cov_transform(ecl, f, 100)

# Use linear model to test each feature stored as columns in X
# in data transformed by f()
res2 <- lm_each_eclairs(f(y) ~ v1 + v2, data, X, ecl_transform)

head(res)

```

lm_eclairs

Fit linear model after decorrelating

Description

Fit linear model after applying decorrelation projection to response and predictors.

Usage

```

lm_eclairs(
  formula,
  data,
  ecl,
  subset,
  weights,

```

```

na.action,
method = "qr",
model = TRUE,
x = FALSE,
y = FALSE,
qr = TRUE,
singular.ok = TRUE,
contrasts = NULL,
offset,
...
)

```

Arguments

| | |
|-------------|----------------------------------------------------------------------------------------------------------------------------|
| formula | an object of class 'formula' (or one that can be coerced to that class): a symbolic description of the model to be fitted. |
| data | a matrix or data.frame containing the variables in the model |
| ecl | estimate of covariance/correlation matrix from eclairs storing U , d_1^2 , λ and ν |
| subset | same as for lm |
| weights | same as for lm |
| na.action | same as for lm |
| method | same as for lm |
| model | same as for lm |
| x | same as for lm |
| y | same as for lm |
| qr | same as for lm |
| singular.ok | same as for lm |
| contrasts | same as for lm |
| offset | same as for lm |
| ... | same as for lm |

Details

This function fit a linear regression to the transformed response, and transformed design matrix. Note that the design matrix, not just the data.frame of variables is transformed so that 1) factors are transformed and 2) the intercept term is transformed.

Value

Object of class `lm` returned by function [lm](#)

Examples

```

library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)

# eclairs decomposition
ecl <- eclairs(Y)

# simulate covariates
data <- data.frame(matrnorm(p, 2, seed = 1))
colnames(data) <- paste0("v", 1:2)

# simulate response
y <- rnorm(p)

# fit linear model on transformed data
lm_eclairs(y ~ v1 + v2, data, ecl)

```

logDet

Evaluate the log determinant

Description

Evaluate the log determinant of the matrix

Usage

```
logDet(ecl, alpha = 1)
```

Arguments

| | |
|-------|------------------------------------------------------------------------------------------------------|
| ecl | estimate of covariance/correlation matrix from eclairs() storing U , d_1^2 , λ and ν |
| alpha | exponent to be applied to eigen-values |

Value

log determinant

Examples

```

library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# eclairs decomposition
ecl <- eclairs(Y)

logDet(ecl)

```

mahalanobisDistance *Mahalanobis Distance*

Description

Mahalanobis Distance using eclairs() decomposition

Usage

```
mahalanobisDistance(ecl, X, lambda, center = FALSE)
```

Arguments

| | |
|--------|----------------------------------------------------------------------------------------------------|
| ecl | estimate of covariance/correlation matrix from eclairs storing U , d_1^2 , λ and ν |
| X | data matrix |
| lambda | specify lambda and override value from 'ecl' |
| center | logical: should columns be centered internally |

Details

Evaluate quadratic form $(X - \mu)^T \Sigma^{-1} (X - \mu)$ where covariance is estimated from finite sample

Value

array of distances

Examples

```

library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)

# eclairs decomposition
ecl <- eclairs(Y)

# Mahalanobis distance after mean centering
Y_center <- scale(Y, scale = FALSE)
mu <- colMeans(Y)

# Standard R method
a <- mahalanobis(Y, mu, cov = cov(Y))

# distance using eclairs decomposition, no shrinkage
b <- mahalanobisDistance(ecl, Y_center, lambda = 0)
range(a - b)

# with shrinkage
d <- mahalanobisDistance(ecl, Y_center)

# centering internally
e <- mahalanobisDistance(ecl, Y, center = TRUE)
range(d - e)
#

```

| | |
|--------------|-----------------------------------|
| mult_eclairs | <i>Multiply by eclairs matrix</i> |
|--------------|-----------------------------------|

Description

Multiply by [eclairs](#) matrix using special structure to achieve linear instead of cubic time complexity.

Usage

```
mult_eclairs(X, U1, dSq1, lambda, nu, alpha, sigma, transpose = FALSE)
```

Arguments

| | |
|----|-----------------------------------------------------------------------|
| X | matrix to be transformed so <i>*columns*</i> are independent |
| U1 | orthonormal matrix with k columns representing the low rank component |

| | |
|-----------|-------------------------------------------------------------------------------|
| dSq1 | eigen values so that $U_1 \text{diag}(d_1^2) U_1^T$ is the low rank component |
| lambda | shrinkage parameter for the convex combination. |
| nu | diagonal value of target matrix in shrinkage |
| alpha | exponent to be evaluated |
| sigma | standard deviation of each feature |
| transpose | logical, (default FALSE) indicating if X should be transposed first |

Details

Let $\Sigma = U_1 \text{diag}(d_1^2) U_1^T * (1 - \lambda) + \text{diag}(\nu \lambda, p)$, where λ shrinkage parameter for the convex combination between a low rank matrix and the diagonal matrix with values ν .

Evaluate $X \Sigma^\alpha$ using special structure of the [eclairs](#) decomposition in $O(k^2 p)$ when there are k components in the decomposition.

Value

a matrix product

| | |
|-------------------|---------------------------------------------------|
| optimal_SVHT_coef | <i>Optimal Hard Threshold for Singular Values</i> |
|-------------------|---------------------------------------------------|

Description

A function for the calculation of the coefficient determining optimal location of hard threshold for matrix denoising by singular values hard thresholding when noise level is known or unknown. Recreation of MATLAB code by Matan Gavish and David Donoho.

Usage

```
optimal_SVHT_coef(beta, sigma_known = FALSE)
```

Arguments

| | |
|-------------|----------------------------------------------------------------------------------------------------------------------|
| beta | A single value or a vector that represents aspect ratio m/n of the matrix to be denoised. $0 < \text{beta} \leq 1$. |
| sigma_known | A logical value. TRUE if noise level known, FALSE if unknown. |

Value

Optimal location of hard threshold, up the median data singular value (sigma unknown) or up to $\text{sigma} * \sqrt{n}$ (sigma known); a vector of the same dimension as beta, where $\text{coef}[i]$ is the coefficient corresponding to $\text{beta}[i]$.

References

Gavish, M., & Donoho, D. L. (2014). The optimal hard threshold for singular values is $4/\sqrt{3}$. IEEE Transactions on Information Theory, 60(8), 5040-5053.

| | |
|---------------------|----------------------------|
| plot,eclairs-method | <i>Plot eclairs object</i> |
|---------------------|----------------------------|

Description

Plot eclairs object

Usage

```
## S4 method for signature 'eclairs'
plot(x, y, ...)
```

Arguments

| | |
|-----|--------------------------|
| x | eclairs object |
| y | extra argument, not used |
| ... | additional arguments |

Value

plot

| | |
|----------|--------------------------------|
| quadForm | <i>Evaluate quadratic form</i> |
|----------|--------------------------------|

Description

Evaluate quadratic form

Usage

```
quadForm(ecl, A, alpha = -1/2)
```

Arguments

| | |
|-------|----------------------------------------------------------------------------------------------------|
| ecl | estimate of covariance/correlation matrix from eclairs storing U , d_1^2 , λ and ν |
| A | matrix |
| alpha | default = -1/2. Exponent of eigen-values |

Details

Evaluate quadratic form $A^T \Sigma^{2\alpha} A$

Value

scalar value

Examples

```

library(Rfast)
n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)

# eclairs decomposition
ecl <- eclairs(Y)

# return scalar
quadForm(ecl, Y[1, ])

# return matrix
quadForm(ecl, Y[1:2, ])

```

reform_decomp

*Recompute eclairs after dropping features***Description**

Recompute eclairs after dropping features

Usage

```
reform_decomp(ecl, k = ecl$k, drop = NULL)
```

Arguments

| | |
|------|--------------------------------------------------------------------|
| ecl | covariance/correlation matrix as an eclairs object |
| k | the rank of the low rank component |
| drop | array of variable names to drop. |

Details

Reform the dataset from the eclairs decomposition, drop features, then recompute the eclairs decomposition. If the original SVD/eigen was truncated, then the reconstruction of the original data will be approximate. Note that the target shrinkage matrix is the same as in ecl, so ν is not recomputed from the retained features.

Value

[eclairs](#) decomposition for a subset of features

Examples

```

library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)
rownames(Y) <- paste0("sample_", seq(n))
colnames(Y) <- paste0("gene_", seq(p))

# Correlation
#-----

# eclairs decomposition
Sigma.eclairs <- eclairs(Y, compute = "correlation")

# features to drop
drop <- paste0("gene_", 1:100)

# Compute SVD on subset of eclairs decomposition
ec11 <- reform_decomp(Sigma.eclairs, drop = drop)

ec11

```

rmvnorm_eclairs

Draw from multivariate normal and t distributions

Description

Draw from multivariate normal and t distributions using eclairs decomposition

Usage

```
rmvnorm_eclairs(n, mu, ec1, v = Inf, seed = NULL)
```

Arguments

| | |
|------|--------------------------------------------------------------------------------------------|
| n | sample size |
| mu | mean vector |
| ec1 | covariance matrix as an eclairs object |
| v | degrees of freedom, defaults to Inf. If finite, uses a multivariate t distribution |
| seed | If you want the same to be generated again use a seed for the generator, an integer number |

Details

Draw from multivariate normal and t distributions using eclairs decomposition. If the (implied) covariance matrix is $p \times p$, the standard approach is $O(p^3)$. Taking advantage of the previously computed eclairs decomposition of rank k , this can be done in $O(pk^2)$.

Value

matrix where rows are samples from multivariate normal or t distribution where columns have covariance specified by ecl

Examples

```
library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma, seed = 1)

# perform eclairs decomposition
ecl <- eclairs(Y)

# draw from multivariate normal
n <- 10000
mu <- rep(0, ncol(Y))

# using eclairs decomposition
X.draw1 <- rmvnorm_eclairs(n, mu, ecl)

# using full covariance matrix implied by eclairs model
X.draw2 <- rmvnorm(n, mu, getCov(ecl))

# assess difference between covariances from two methods
range(cov(X.draw1) - cov(X.draw2))

# compare covariance to the covariance matrix used to simulated the data
range(cov(X.draw1) - getCov(ecl))
```

sv_threshold

Singular value thresholding

Description

Singular value thresholding evaluates the optimal number of singular values to retain

Usage

```
sv_threshold(n, p, d)
```

Arguments

| | |
|---|--------------------|
| n | number of samples |
| p | number of features |
| d | singular values |

Value

Number of singular values to retain

References

Gavish, M., & Donoho, D. L. (2014). The optimal hard threshold for singular values is $4/\sqrt{3}$. *IEEE Transactions on Information Theory*, 60(8), 5040-5053.

Examples

```
# simulate data

n <- 500
p <- 5000
Y <- Rfast::matrnorm(n, p, seed = 1)

# SVD
dcmp <- svd(Y)

# how many components to retain
sv_threshold(n, p, dcmp$d)

# in this case the data has no structure, so no components are retained
```

whiten

Decorrelation projection + eclairs

Description

Efficient decorrelation projection using eclairs decomposition

Usage

```
whiten(X, k = ncol(X), lambda = NULL)
```

Arguments

| | |
|--------|----------------------------------------------------------|
| X | matrix to be transformed so *columns* are independent |
| k | the rank of the low rank component |
| lambda | specify lambda and override value estimated by eclairs() |

Value

data rotated and scaled according to the regularized sample covariance of the input data

Examples

```
library(Rfast)

n <- 800 # number of samples
p <- 200 # number of features

# create correlation matrix
Sigma <- autocorr.mat(p, .9)

# draw data from correlation matrix Sigma
Y <- rmvnorm(n, rep(0, p), sigma = Sigma * 5.1, seed = 1)

# eclairs decomposition
ecl <- eclairs(Y)

# whitened Y
Y.transform <- decorrelate(Y, ecl)

# Combine eclairs and decorrelate into one step
Y.transform2 <- whiten(Y)
```


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