Package 'ForeCA'

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Type Package

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Description Implementation of Forecastable Component Analysis ('ForeCA'), including main algorithms and auxiliary function (summary, plotting, etc.) to apply 'ForeCA' to multivariate time series data. 'ForeCA' is a novel dimension reduction (DR) technique for temporally dependent signals. Contrary to other popular DR methods, such as 'PCA' or 'ICA', 'ForeCA' takes time dependency explicitly into account and searches for the most "forecastable" signal. The measure of forecastability is based on the Shannon entropy of the spectral density of the transformed signal.

Depends R (>= 3.5.0)

License GPL-2

Imports astsa (>= 1.10), MASS, graphics, reshape2 (>= 1.4.4), utils

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Fore	CA-package Implementation of Forecastable Component Analysis (ForeCA)	

Description

Forecastable Component Analysis (ForeCA) is a novel dimension reduction technique for multivariate time series \mathbf{X}_t . ForeCA finds a linar combination $y_t = \mathbf{X}_t \mathbf{v}$ that is easy to forecast. The measure of forecastability $\Omega(y_t)$ (Omega) is based on the entropy of the spectral density $f_y(\lambda)$ of y_t : higher entropy means less forecastable, lower entropy is more forecastable.

The main function foreca runs ForeCA on a multivariate time series X_t .

Consult NEWS.md for a history of release notes.

Author(s)

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References

Goerg, G. M. (2013). "Forecastable Component Analysis". Journal of Machine Learning Research (JMLR) W&CP 28 (2): 64-72, 2013. Available at http://jmlr.org/proceedings/papers/v28/goerg13.html.

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Examples

```
XX <- ts(diff(log(EuStockMarkets)))
Omega(XX)

plot(log10(lynx))
Omega(log10(lynx))

## Not run:
ff <- foreca(XX, n.comp = 4)
ff
plot(ff)
summary(ff)

## End(Not run)</pre>
```

common-arguments

List of common arguments

Description

Common arguments used in several functions in this package.

Arguments

series a $T \times K$ array with T observations from the K-dimensional time series X_t . Can be a matrix, data. frame, or a multivariate ts object. U a $T \times K$ array with T observations from the K-dimensional **whitened** (whiten) time series U_t . Can be a matrix, data. frame, or a multivariate ts object. mvspectrum.output an object of class "mvspectrum" representing the multivariate spectrum of \mathbf{X}_t (not necessarily normalized). f.U multivariate spectrum of class 'mvspectrum' with normalize = TRUE. algorithm.control list; control settings for any iterative ForeCA algorithm. See complete_algorithm_control for details. entropy.control list; control settings for entropy estimation. See complete_entropy_control for details. spectrum.control list; control settings for spectrum estimation. See complete_spectrum_control for details. entropy.method string; method to estimate the entropy from discrete probabilities p_i ; here probabilities are the spectral density evaluated at the Fourier frequencies, $\widehat{p}_i = f(\omega_i)$. spectrum.method

string; method for spectrum estimation; see method argument in myspectrum.

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threshold

numeric; values of spectral density below threshold are set to 0; default threshold

= 0.

smoothing

logical; if TRUE the spectrum will be smoothed with a nonparametric estimate using gam and an exponential family (with link = log). Only works for univariate spectrum. The smoothing parameter is chosen automatically using generalized cross-validation (see gam for details). Default: FALSE.

base

logarithm base; entropy is measured in "nats" for base = exp(1); in "bits" if base = 2 (default).

complete-controls

Completes several control settings

Description

Completes algorithm, entropy, and spectrum control lists.

Usage

Arguments

```
algorithm.control
list; control parameters for any iterative ForeCA algorithm.

entropy.control
list; control settings for entropy estimation.

num.outcomes positive integer; number of outcomes for the discrete probability distribution.
Must be specified (no default value).

spectrum.control
list; control settings for spectrum estimation.
```

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Value

A list with fully specified algorithm, entropy, or spectrum controls. Default values are only added if the input {spectrum,entropy,algorithm}.control list does not already set this value.

complete_algorithm_control returns a list containing:

max.iter maximum number of iterations; default: 50.

num. starts number of random starts to avoid local optima; default: 10.

tol tolerance for when convergence is reached in any *iterative* ForeCA algorithm;

default: 1e-03.

type string; type of algorithm. Default: 'EM'.

complete_entropy_control returns a list with:

base logarithm base for the entropy.

method string; method to estimate entropy; default: "MLE".

prior.probs prior distribution; default: uniform rep(1 / num.outcomes, num.outcomes).

prior.weight weight of the prior distribution; default: 1e-3.

threshold non-negative float; set probabilities below threshold to zero; default: 0.

complete_spectrum_control returns a list containing:

kernel R function; function to weigh each Fourier frequency λ ; default: NULL (no re-

weighting).

method string; method to estimate the spectrum; default: 'mvspec' if sapa is installed,

'myspec' if only astsa is installed, and 'pgram' if neither is installed.

smoothing logical; default: FALSE.

Available methods for spectrum estimation are (alphabetical order)

"ar" autoregressive spectrum fit via spec.ar; only for univariate time series.

"mvspec" smoothed estimate using mvspec; many tuning parameters are available – they

can be passed as additional arguments (...) to myspectrum.

"pgram" raw periodogram using spectrum

"pspectrum" advanced non-parametric estimation of a tapered power spectrum using pspectrum.

Setting smoothing = TRUE will smooth the estimated spectrum (again); this option is only available for univariate time series/spectra.

See Also

mvspectrum, discrete_entropy, continuous_entropy

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continuous_entropy

Shannon entropy for a continuous pdf

Description

Computes the Shannon entropy $\mathcal{H}(p)$ for a continuous probability density function (pdf) p(x) using numerical integration.

Usage

```
continuous_entropy(pdf, lower, upper, base = 2)
```

Arguments

pdf R function for the pdf p(x) of a RV $X \sim p(x)$. This function must be non-

negative and integrate to 1 over the interval [lower, upper].

lower, upper lower and upper integration limit. pdf must integrate to 1 on this interval.

base logarithm base; entropy is measured in "nats" for base = exp(1); in "bits" if

base = 2 (default).

Details

The Shannon entropy of a continuous random variable (RV) $X \sim p(x)$ is defined as

$$\mathcal{H}(p) = -\int_{-\infty}^{\infty} p(x) \log p(x) dx.$$

Contrary to discrete RVs, continuous RVs can have negative entropy (see Examples).

Value

scalar; entropy value (real).

Since continuous_entropy uses numerical integration (integrate()) convergence is not garantueed (even if integral in definition of $\mathcal{H}(p)$ exists). Issues a warning if integrate() does not converge.

See Also

```
discrete_entropy
```

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```
continuous_entropy(my_density, -1, 1) # = log(upper - lower)
# a 'triangle' distribution
continuous_entropy(function(x) x, 0, sqrt(2))
```

discrete_entropy

Shannon entropy for discrete pmf

Description

Computes the Shannon entropy $\mathcal{H}(p) = -\sum_{i=1}^n p_i \log p_i$ of a discrete RV X taking values in $\{x_1,\ldots,x_n\}$ with probability mass function (pmf) $P(X=x_i)=p_i$ with $p_i\geq 0$ for all i and $\sum_{i=1}^n p_i=1$.

Usage

```
discrete_entropy(
  probs,
  base = 2,
  method = c("MLE"),
  threshold = 0,
  prior.probs = NULL,
  prior.weight = 0
)
```

Arguments

probs	numeric:	probabilities	(empirical	frequencies)	Must be	non-negative and add
אט זע	mumenc,	probabilities	(empirical	mequencies).	wiust be	non-negative and add

up to 1.

base logarithm base; entropy is measured in "nats" for base = exp(1); in "bits" if

base = 2 (default).

method string; method to estimate entropy; see Details below.

threshold numeric; frequencies below threshold are set to 0; default threshold = 0, i.e.,

no thresholding. If prior.weight > 0 then thresholding will be done before

smoothing.

prior.probs optional; only used if prior.weight > 0. Add a prior probability distribution

to probs. By default it uses a uniform distribution putting equal probability on

each outcome.

prior.weight numeric; how much weight does the prior distribution get in a mixture model

between data and prior distribution? Must be between 0 and 1. Default: 0 (no

prior).

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Details

discrete_entropy uses a plug-in estimator (method = "MLE"):

$$\widehat{\mathcal{H}}(p) = -\sum_{i=1}^{n} \widehat{p}_i \log \widehat{p}_i.$$

If prior.weight > 0, then it mixes the observed proportions \hat{p}_i with a prior distribution

$$\widehat{p}_i \leftarrow (1 - \lambda) \cdot \widehat{p}_i + \lambda \cdot prior_i, \quad i = 1, \dots, n,$$

where $\lambda \in [0, 1]$ is the prior weight parameter. By default the prior is a uniform distribution, i.e., $prior_i = \frac{1}{n}$ for all i.

Note that this plugin estimator is biased. See References for an overview of alternative methods.

Value

numeric; non-negative real value.

References

Archer E., Park I. M., Pillow J.W. (2014). "Bayesian Entropy Estimation for Countable Discrete Distributions". Journal of Machine Learning Research (JMLR) 15, 2833-2868. Available at http://jmlr.org/papers/v15/archer14a.html.

See Also

continuous_entropy

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foreca

Forecastable Component Analysis

Description

foreca performs Forecastable Component Analysis (ForeCA) on \mathbf{X}_t – a K-dimensional time series with T observations. Users should only call foreca, rather than foreca.one_weightvector or foreca.multiple_weightvectors.

foreca.one_weightvector is a wrapper around several algorithms that solve the ForeCA optimization problem for a single weightvector \mathbf{w}_i and whitened time series \mathbf{U}_t .

foreca.multiple_weightvectors applies foreca.one_weightvector iteratively to \mathbf{U}_t in order to obtain multiple weightvectors that yield most forecastable, uncorrelated signals.

Usage

```
foreca(series, n.comp = 2, algorithm.control = list(type = "EM"), ...)
foreca.one_weightvector(
 U,
  f.U = NULL,
  spectrum.control = list(),
  entropy.control = list(),
  algorithm.control = list(),
  keep.all.optima = FALSE,
  dewhitening = NULL,
)
foreca.multiple_weightvectors(
  spectrum.control = list(),
  entropy.control = list(),
  algorithm.control = list(),
  n.comp = 2,
  plot = FALSE,
  dewhitening = NULL,
)
```

Arguments

series a $T \times K$ array with T observations from the K-dimensional time series \mathbf{X}_t . Can be a matrix, data. frame, or a multivariate ts object.

n.comp positive integer; number of components to be extracted. Default: 2.

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algorithm.control

list; control settings for any *iterative* ForeCA algorithm. See complete_algorithm_control

for details.

... additional arguments passed to available ForeCA algorithms.

U a $T \times K$ array with T observations from the K-dimensional **whitened** (whiten)

time series \mathbf{U}_t . Can be a matrix, data.frame, or a multivariate ts object.

f.U multivariate spectrum of class 'mvspectrum' with normalize = TRUE.

spectrum.control

list; control settings for spectrum estimation. See complete_spectrum_control for details.

entropy.control

list; control settings for entropy estimation. See complete_entropy_control for details.

keep.all.optima

logical; if TRUE, it keeps the optimal solutions of each random start. Default:

FALSE (only returns the best solution).

dewhitening optional; if provided (returned by whiten) then it uses the dewhitening transfor-

mation to obtain the original series X_t and it uses that vector (normalized) as the initial weightvector which corresponds to the series $X_{t,i}$ with larges Omega.

plot logical; if TRUE a plot of the current optimal solution \mathbf{w}_i^* will be shown and

updated for each iteration i=1,...,n. comp of any iterative algorithm. Default:

FALSE.

Value

An object of class foreca, which is similar to the output from princomp, with the following components (amongst others):

- center: sample mean $\widehat{\mu}_X$ of each series,
- whitening: whitening matrix of size $K \times K$ from whiten: $\mathbf{U}_t = (\mathbf{X}_t \widehat{\mu}_X) \cdot whitening$; note that \mathbf{X}_t is centered prior to the whitening transformation,
- weightvectors: orthonormal matrix of size $K \times n.comp$, which converts whitened data to n.comp forecastable components (ForeCs) $\mathbf{F}_t = \mathbf{U}_t \cdot weightvectors$,
- loadings: combination of whitening \times weightvectors to obtain the final loadings for the original data: $\mathbf{F}_t = (\mathbf{X}_t \widehat{\mu}_X) \cdot whitening \cdot weightvectors$; again, it centers \mathbf{X}_t first,
- loadings.normalized: normalized loadings (unit norm). Note though that if you use these normalized loadings the resulting signals do not have variance 1 anymore.
- scores: n. comp forecastable components F_t. They have mean 0, variance 1, and are uncorrelated.
- Omega: forecastability score of each ForeC of \mathbf{F}_t .

ForeCs are ordered from most to least forecastable (according to Omega).

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Warning

Estimating Omega directly from the ForeCs \mathbf{F}_t can be different to the reported \$0mega estimates from foreca. Here is why:

In theory $f_y(\lambda)$ of a linear combination $y_t = \mathbf{X}_t \mathbf{w}$ can be analytically computed from the multivariate spectrum $f_{\mathbf{X}}(\lambda)$ by the quadratic form $f_y(\lambda) = \mathbf{w}' f_{\mathbf{X}}(\lambda) \mathbf{w}$ for all λ (see spectrum_of_linear_combination).

In practice, however, this identity does not hold always exactly since (often data-driven) control setting for spectrum estimation are not identical for the high-dimensional, noisy \mathbf{X}_t and the combined univariate time series y_t (which is usually more smooth, less variable). Thus estimating \hat{f}_y directly from y_t can give slightly different estimates to computing it as $\mathbf{w}'\hat{f}_{\mathbf{X}}\mathbf{w}$. Consequently also Omega estimates can be different.

In general, these differences are small and have no relevant implications for estimating ForeCs. However, in rare occasions the obtained ForeCs can have smaller Omega than the maximum Omega across all original series. In such a case users should not re-estimate Ω from the resulting ForeCs \mathbf{F}_t , but access them via \$Omega provided by 'foreca' output (the univariate estimates are stored in \$Omega.univ).

References

Goerg, G. M. (2013). "Forecastable Component Analysis". Journal of Machine Learning Research (JMLR) W&CP 28 (2): 64-72, 2013. Available at http://jmlr.org/proceedings/papers/v28/goerg13.html.

```
XX <- diff(log(EuStockMarkets)) * 100
plot(ts(XX))
## Not run:
ff <- foreca(XX[,1:4], n.comp = 4, plot = TRUE, spectrum.control=list(method="pspectrum"))</pre>
summary(ff)
plot(ff)
## End(Not run)
## Not run:
PW <- whiten(XX)
one.weight.em <- foreca.one_weightvector(U = PW$U,</pre>
                                          dewhitening = PW$dewhitening,
                                          algorithm.control =
                                            list(num.starts = 2,
                                                 type = "EM"),
                                          spectrum.control =
                                            list(method = "mvspec"))
plot(one.weight.em)
## End(Not run)
## Not run:
```

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foreca-utils

Plot, summary, and print methods for class 'foreca'

Description

```
A collection of S3 methods for estimated ForeCA results (class "foreca"). summary.foreca computes summary statistics. print.foreca prints a human-readable summary in the console. biplot.foreca shows a biplot of the ForeCA loadings (wrapper around biplot.princomp). plot.foreca shows biplots, screeplots, and white noise tests.
```

Usage

```
## S3 method for class 'foreca'
summary(object, lag = 10, alpha = 0.05, ...)
## S3 method for class 'foreca'
print(x, ...)
## S3 method for class 'foreca'
biplot(x, ...)
## S3 method for class 'foreca'
plot(x, lag = 10, alpha = 0.05, ...)
```

Arguments

```
lag integer; how many lags to test in Box. test; default: 10.

alpha significance level for testing white noise in Box. test; default: 0.05.

... additional arguments passed to biplot.princomp, biplot, plot, or summary.

x, object an object of class "foreca".
```

```
# see examples in 'foreca'
```

foreca.EM-aux

foreca.EM-aux

ForeCA EM auxiliary functions

Description

foreca.EM.one_weightvector relies on several auxiliary functions:

foreca.EM.E_step computes the spectral density of $y_t = \mathbf{U}_t \mathbf{w}$ given the weightvector \mathbf{w} and the normalized spectrum estimate $f_{\mathbf{U}}$. A wrapper around spectrum_of_linear_combination.

foreca.EM.M_step computes the minimizing eigenvector $(\rightarrow \widehat{\mathbf{w}}_{i+1})$ of the weighted covariance matrix, where the weights equal the negative logarithm of the spectral density at the current $\widehat{\mathbf{w}}_i$.

 $foreca. {\tt EM.E_} and {\tt _M_} step \ is \ a \ wrapper \ around \ foreca. {\tt EM.E_} step \ followed \ by \ foreca. {\tt EM.M_} step.$

foreca. EM. h evaluates (an upper bound of) the entropy of the spectral density as a function of \mathbf{w}_i (or \mathbf{w}_{i+1}). This is the objective funcion that should be minimized.

Usage

```
foreca.EM.E_step(f.U, weightvector)
foreca.EM.M_step(f.U, f.current, minimize = TRUE, entropy.control = list())
foreca.EM.E_and_M_step(
 weightvector,
  f.U,
 minimize = TRUE,
  entropy.control = list()
)
foreca.EM.h(
 weightvector.new,
  f.U,
 weightvector.current = weightvector.new,
  f.current = NULL,
  entropy.control = list(),
  return.negative = FALSE
)
```

Arguments

f.U	multivariate spectrum of class 'mvspectrum' with normalize = TRUE.
weightvector	numeric; weights \mathbf{w} for $y_t = \mathbf{U}_t \mathbf{w}$. Must have unit norm in ℓ^2 .
f.current	numeric; spectral density estimate of $y_t = \mathbf{U}_t \mathbf{w}$ for the current estimate $\widehat{\mathbf{w}}_i$ (required for foreca.EM.M_step; optional for foreca.EM.h).
minimize	logical; if TRUE (default) it returns the eigenvector corresponding to the smallest eigenvalue; otherwise to the largest eigenvalue.

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```
entropy.control list; control settings for entropy estimation. See complete_entropy_control for details. Weightvector.new weightvector \widehat{\mathbf{w}}_{i+1} of the new iteration (i+1). Weightvector.current weightvector \widehat{\mathbf{w}}_i of the current iteration (i). return.negative logical; if TRUE it returns the negative spectral entropy. This is useful when maximizing forecastibility which is equivalent (up to an additive constant) to
```

Value

foreca.EM.E_step returns the normalized univariate spectral density (normalized such that its sum equals 0.5).

maximizing negative entropy. Default: FALSE.

foreca.EM.M_step returns a list with three elements:

- matrix: weighted covariance matrix, where the weights are the negative log of the spectral density. If density is estimated by discrete probabilities, then this matrix is positive semi-definite, since − log(p) ≥ 0 for p ∈ [0, 1]. See weightvector2entropy_wcov.
- vector: minimizing (or maximizing if minimize = FALSE) eigenvector of matrix,
- value: corresponding eigenvalue.

Contrary to foreca.EM.M_step, foreca.EM.E_and_M_step only returns the optimal weightvector as a numeric.

foreca.EM.h returns non-negative real value (see References for details):

- entropy, if weightvector.new = weightvector.current,
- an upper bound of that entropy for weightvector.new, otherwise.

See Also

weightvector2entropy_wcov

```
## Not run:
XX <- diff(log(EuStockMarkets)) * 100
UU <- whiten(XX)$U
ff <- mvspectrum(UU, 'mvspec', normalize = TRUE)
ww0 <- initialize_weightvector(num.series = ncol(XX), method = 'rnorm')
f.ww0 <- foreca.EM.E_step(ff, ww0)
plot(f.ww0, type = "1")
## End(Not run)
## Not run:</pre>
```

```
one.step <- foreca.EM.M_step(ff, f.ww0,
                             entropy.control = list(prior.weight = 0.1))
image(one.step$matrix)
requireNamespace(LICORS)
# if you have the 'LICORS' package use
LICORS::image2(one.step$matrix)
ww1 <- one.step$vector
f.ww1 <- foreca.EM.E_step(ff, ww1)</pre>
layout(matrix(1:2, ncol = 2))
matplot(seq(0, pi, length = length(f.ww0)), cbind(f.ww0, f.ww1),
        type = "1", lwd =2, xlab = "omega_j", ylab = "f(omega_j)")
plot(f.ww0, f.ww1, pch = ".", cex = 3, xlab = "iteration 0",
     ylab = "iteration 1", main = "Spectral density")
abline(0, 1, col = 'blue', lty = 2, lwd = 2)
Omega(mvspectrum.output = f.ww0) # start
Omega(mvspectrum.output = f.ww1) # improved after one iteration
## End(Not run)
## Not run:
ww0 <- initialize_weightvector(NULL, ff, method = "rnorm")</pre>
ww1 <- foreca.EM.E_and_M_step(ww0, ff)</pre>
ww0
ww1
barplot(rbind(ww0, ww1), beside = TRUE)
abline(h = 0, col = "blue", lty = 2)
## End(Not run)
## Not run:
foreca.EM.h(ww0, ff)
                           # iteration 0
foreca.EM.h(ww1, ff, ww0) # min eigenvalue inequality
                           # KL divergence inequality
foreca.EM.h(ww1, ff)
one.step$value
# by definition of Omega, they should equal 1 (modulo rounding errors)
Omega(mvspectrum.output = f.ww0) / 100 + foreca.EM.h(ww0, ff)
Omega(mvspectrum.output = f.ww1) / 100 + foreca.EM.h(ww1, ff)
## End(Not run)
```

foreca.EM.one_weightvector

EM-like algorithm to estimate optimal ForeCA transformation

Description

foreca. EM. one_weightvector finds the optimal weightvector \mathbf{w}^* that gives the most forecastable signal $y_t^* = \mathbf{U}_t \mathbf{w}^*$ using an EM-like algorithm (see References).

Usage

```
foreca.EM.one_weightvector(
    U,
    f.U = NULL,
    spectrum.control = list(),
    entropy.control = list(),
    algorithm.control = list(),
    init.weightvector = initialize_weightvector(num.series = ncol(U), method = "rnorm"),
    ...
)
```

Arguments

```
U
                  a T \times K array with T observations from the K-dimensional whitened (whiten)
                  time series U_t. Can be a matrix, data. frame, or a multivariate ts object.
f.U
                  multivariate spectrum of class 'mvspectrum' with normalize = TRUE.
spectrum.control
                  list; control settings for spectrum estimation. See complete_spectrum_control
                  for details.
entropy.control
                  list; control settings for entropy estimation. See complete_entropy_control
                  for details.
algorithm.control
                  list; control settings for any iterative ForeCA algorithm. See complete_algorithm_control
                  for details.
init.weightvector
                  numeric; starting point \mathbf{w}_0 for several iterative algorithms. By default it uses a
                  (normalized) random vector from a standard Normal distribution (see initialize_weightvector).
                  other arguments passed to myspectrum
```

Value

A list with useful quantities like the optimal weighvector, the corresponding signal, and its fore-castability.

See Also

```
foreca.one_weightvector, foreca.EM-aux
```

```
foreca.one_weightvector-utils
```

Plot, summary, and print methods for class 'foreca.one_weightvector'

Description

S3 methods for the one weightvector optimization in ForeCA (class "foreca.one_weightvector"). summary.foreca.one_weightvector computes summary statistics.

plot.foreca.one_weightvector shows the results of an (iterative) algorithm that obtained the i-th optimal a weightvector \mathbf{w}_i^* . It shows trace plots of the objective function and the weightvector, and a time series plot of the transformed signal y_t^* along with its spectral density estimate $\widehat{f}_y(\omega_i)$.

Usage

```
## S3 method for class 'foreca.one_weightvector'
summary(object, lag = 10, alpha = 0.05, ...)
## S3 method for class 'foreca.one_weightvector'
plot(x, main = "", cex.lab = 1.1, ...)
```

Arguments

```
lag integer; how many lags to test in Box.test; default: 10.

alpha significance level for testing white noise in Box.test; default: 0.05.

additional arguments passed to plot, or summary.

x, object an object of class "foreca.one_weightvector".

main an overall title for the plot: see title.

cex.lab size of the axes labels.
```

Examples

```
# see examples in 'foreca.one_weightvector'
```

```
initialize_weightvector
```

Initialize weightvector for iterative ForeCA algorithms

Description

initialize_weightvector returns a unit norm (in ℓ^2) vector $\mathbf{w}_0 \in R^K$ that can be used as the starting point for any iterative ForeCA algorithm, e.g., foreca.EM.one_weightvector. Several quickly computable heuristics are available via the method argument.

Usage

```
initialize_weightvector(
   U = NULL,
   f.U = NULL,
   num.series = ncol(U),
   method = c("rnorm", "max", "SFA", "PCA", "rcauchy", "runif", "SFA.slow", "SFA.fast",
        "PCA.large", "PCA.small"),
   seed = sample(1e+06, 1),
   ...
)
```

Arguments

U	a $T \times K$ array with T observations from the K -dimensional whitened (whiten) time series \mathbf{U}_t . Can be a matrix, data.frame, or a multivariate ts object.
f.U	multivariate spectrum of class 'mvspectrum' with normalize = TRUE.
num.series	positive integer; number of time series K (determines the length of the weightvector). If num. series = 1 it simply returns a 1×1 array equal to 1.
method	string; which heuristics should be used to generate a good starting \mathbf{w}_0 ? Default: "rnorm"; see Details.
seed	non-negative integer; seed for random initialization which will be returned for reproducibility. By default it sets a random seed.
	additional arguments

Details

The method argument specifies the heuristics that is used to get a good starting vector \mathbf{w}_0 :

- "max" vector with all 0s, but a 1 at the position of the maximum forecastable series in U.
- "reauchy" random start using reauchy(k).
- "rnorm" random start using rnorm(k, 0, 1).
- "runif" random start using runif(k, -1, 1).
- "PCA.large" first eigenvector of PCA (largest variance signal).
- "PCA. small" last eigenvector of PCA (smallest variance signal).
- "PCA" checks both small and large, and chooses the one with higher forecastability as computed by Omega..
- "SFA. fast" last eigenvector of SFA (fastest signal).
- "SFA. slow" first eigenvector of SFA (slowest signal).
- "SFA" checks both slow and fast, and chooses the one with higher forecastability as computed by Omega.

Each vector has length K and is automatically normalized to have unit norm in ℓ^2 .

For the 'SFA*' methods see sfa. Note that maximizing (or minimizing) the lag 1 auto-correlation does not necessarily yield the most forecastable signal, but it's a good start.

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Value

numeric; a vector of length K with unit norm in ℓ^2 .

Examples

```
XX <- diff(log(EuStockMarkets))
## Not run:
initialize_weightvector(U = XX, method = "SFA")
## End(Not run)
initialize_weightvector(num.series = ncol(XX), method = "rnorm")</pre>
```

mvspectrum

Estimates spectrum of multivariate time series

Description

The spectrum of a multivariate time series is a matrix-valued function of the frequency $\lambda \in [-\pi, \pi]$, which is symmetric/Hermitian around $\lambda = 0$.

mvspectrum estimates it and returns a 3D array of dimension $num.freqs \times K \times K$. Since the spectrum is symmetric/Hermitian around $\lambda=0$ it is sufficient to store only positive frequencies. In the implementation in this package we thus usually consider only positive frequencies (omitting 0); num. freqs refers to the number of positive frequencies only.

normalize_mvspectrum normalizes the spectrum such that it adds up to 0.5 over all positive frequencies (by symmetry it will add up to 1 over the whole range – thus the name *normalize*).

For a K-dimensional time series it adds up to a Hermitian $K \times K$ matrix with 0.5 in the diagonal and imaginary elements (real parts equal to 0) in the off-diagonal. Since it is Hermitian the myspectrum will add up to the identity matrix over the whole range of frequencies, since the off-diagonal elements are purely imaginary (real part equals 0) and thus add up to 0.

check_mvspectrum_normalized checks if the spectrum is normalized (see normalize_mvspectrum for the requirements).

mvpgram computes the multivariate periodogram estimate using bare-bone multivariate fft (mvfft). Use mvspectrum(..., method = 'pgram') instead of mvpgram directly.

This function is merely included to have one method that does not require the **astsa** nor the **sapa** R packages. However, it is strongly encouraged to install either one of them to get (much) better estimates. See Details.

get_spectrum_from_mvspectrum extracts the spectrum of one time series from an "mvspectrum" object by taking the i-th diagonal entry for each frequency.

spectrum_of_linear_combination computes the spectrum of the linear combination $\mathbf{y}_t = \mathbf{X}_t \boldsymbol{\beta}$ of K time series \mathbf{X}_t . This can be efficiently computed by the quadratic form

$$f_{y}(\lambda) = \boldsymbol{\beta}' f_{\mathbf{X}}(\lambda) \boldsymbol{\beta} \ge 0,$$

for each λ . This holds for any β (even $\beta = 0$ – not only for $||\beta||_2 = 1$. For $\beta = e_i$ (the i-th basis vector) this is equivalent to get_spectrum_from_mvspectrum(..., which = i).

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Usage

```
mvspectrum(
    series,
    method = c("mvspec", "pgram", "pspectrum", "ar"),
    normalize = FALSE,
    smoothing = FALSE,
    ...
)

normalize_mvspectrum(mvspectrum.output)

check_mvspectrum_normalized(f.U, check.attribute.only = TRUE)

mvpgram(series)

get_spectrum_from_mvspectrum(
    mvspectrum.output,
    which = seq_len(dim(mvspectrum.output)[2])
)

spectrum_of_linear_combination(mvspectrum.output, beta)
```

Arguments

series a $T \times K$ array with T observations from the K-dimensional time series \mathbf{X}_t . Can

be a matrix, data. frame, or a multivariate ts object.

method string; method for spectrum estimation: use "pspectrum" for pspectrum; use

"mvspec" to use mvspec (astsa package); or use "pgram" to use spec.pgram.

normalize logical; if TRUE the spectrum will be normalized (see Value below for details).

smoothing logical; if TRUE the spectrum will be smoothed with a nonparametric estimate us-

ing gam and an exponential family (with link = log). Only works for univariate spectrum. The smoothing parameter is chosen automatically using generalized

cross-validation (see gam for details). Default: FALSE.

... additional arguments passed to pspectrum or mvspec (e.g., taper)

mvspectrum.output

an object of class "myspectrum" representing the multivariate spectrum of \mathbf{X}_t

(not necessarily normalized).

f.U multivariate spectrum of class 'mvspectrum' with normalize = TRUE.

check.attribute.only

logical; if TRUE it checks the attribute only. This is much faster (it just needs to look up one attribute value), but it might not surface silent bugs. For sake of performance the package uses the attribute version by default. However, for

testing/debugging the full computational version can be used.

which integer(s); the spectrum of which series whould be extracted. By default, it

returns all univariate spectra as a matrix (frequencies in rows).

beta numeric; vector β that defines the linear combination.

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Details

For an orthonormal time series \mathbf{U}_t the raw periodogram adds up to I_K over all (negative and positive) frequencies. Since we only consider positive frequencies, the normalized multivariate spectrum should add up to $0.5 \cdot I_K$ plus a Hermitian imaginary matrix (which will add up to zero when combined with its symmetric counterpart.) As we often use non-parametric smoothing for less variance, the spectrum estimates do not satisfy this identity exactly. normalize_mvspectrum thus adjust the estimates so they satisfy it again exactly.

mvpgram has no options for improving spectrum estimation whatsoever. It thus yields very noisy (in fact, inconsistent) estimates of the multivariate spectrum $f_{\mathbf{X}}(\lambda)$. If you want to obtain better estimates then please use other methods in mvspectrum (this is highly recommended to obtain more reasonable/stable estimates).

Value

myspectrum returns a 3D array of dimension $num.freqs \times K \times K$, where

- num.freqs is the number of frequencies
- K is the number of series (columns in series).

It also has an "normalized" attribute, which is FALSE if normalize = FALSE; otherwise TRUE. See normalize_mvspectrum for details.

normalize_mvspectrum returns a normalized spectrum over positive frequencies, which:

univariate: adds up to 0.5,

multivariate: adds up to Hermitian $K \times K$ matrix with 0.5 in the diagonal and purely imaginary elements in the off-diagonal.

check_mvspectrum_normalized throws an error if spectrum is not normalized correctly.

get_spectrum_from_mvspectrum returns either a matrix of all univariate spectra, or one single column (if which is specified.)

spectrum_of_linear_combination returns a vector with length equal to the number of rows of mvspectrum.output.

References

See References in spectrum, pspectrum, mvspec.

```
set.seed(1)
XX <- cbind(rnorm(100), arima.sim(n = 100, list(ar = 0.9)))
ss3d <- mvspectrum(XX)
dim(ss3d)

ss3d[2,,] # at omega_1; in general complex-valued, but Hermitian identical(ss3d[2,,], Conj(t(ss3d[2,,]))) # is Hermitian
## Not run:
    ss <- mvspectrum(XX[, 1], method="pspectrum", smoothing = TRUE)
    mvspectrum(XX, normalize = TRUE)</pre>
```

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```
## End(Not run)
ss <- mvspectrum(whiten(XX)$U, normalize = TRUE)</pre>
xx <- scale(rnorm(100), center = TRUE, scale = FALSE)</pre>
sum(mvspectrum(xx, normalize = FALSE, method = "pgram")) * 2
sum(mvspectrum(xx, normalize = FALSE, method = "mvspec")) * 2
## Not run:
  sum(mvspectrum(xx, normalize = FALSE, method = "pspectrum")) * 2
## End(Not run)
## Not run:
xx <- scale(rnorm(100), center = TRUE, scale = FALSE)</pre>
ss <- mvspectrum(xx)</pre>
ss.n <- normalize_mvspectrum(ss)</pre>
sum(ss.n)
# multivariate
UU <- whiten(matrix(rnorm(40), ncol = 2))$U</pre>
S.U <- mvspectrum(UU, method = "mvspec")</pre>
mvspectrum2wcov(normalize_mvspectrum(S.U))
## End(Not run)
XX <- matrix(rnorm(1000), ncol = 2)</pre>
SS <- mvspectrum(XX, "mvspec")</pre>
ss1 <- mvspectrum(XX[, 1], "mvspec")</pre>
SS.1 <- get_spectrum_from_mvspectrum(SS, 1)</pre>
plot.default(ss1, SS.1)
abline(0, 1, lty = 2, col = "blue")
XX \leftarrow matrix(arima.sim(n = 1000, list(ar = 0.9)), ncol = 4)
beta.tmp <- rbind(1, -1, 2, 0)
yy <- XX %*% beta.tmp
SS <- mvspectrum(XX, "mvspec")</pre>
ss.yy.comb <- spectrum_of_linear_combination(SS, beta.tmp)</pre>
ss.yy <- mvspectrum(yy, "mvspec")</pre>
plot(ss.yy, log = TRUE) # using plot.mvspectrum()
lines(ss.yy.comb, col = "red", lty = 1, lwd = 2)
```

mvspectrum-utils

S3 methods for class 'mvspectrum'

Description

S3 methods for multivariate spectrum estimation.

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plot.mvspectrum plots all univariate spectra. Analogouos to spectrum when plot = TRUE.

Usage

```
## S3 method for class 'mvspectrum'
plot(x, log = TRUE, ...)
```

Arguments

```
x an object of class "foreca.one_weightvector".logical; if TRUE (default), it plots the spectra on log-scale.additional arguments passed to matplot.
```

See Also

```
get_spectrum_from_mvspectrum
```

Examples

mvspectrum2wcov

Compute (weighted) covariance matrix from frequency spectrum

Description

mvspectrum2wcov computes a (weighted) covariance matrix estimate from the frequency spectrum (see Details).

weightvector2entropy_wcov computes the weighted covariance matrix using the negative entropy of the univariate spectrum (given the weightvector) as kernel weights. This matrix is the objective matrix for many foreca.* algorithms.

Usage

```
mvspectrum2wcov(mvspectrum.output, kernel.weights = 1)
weightvector2entropy_wcov(
  weightvector = NULL,
  f.U,
  f.current = NULL,
  entropy.control = list()
)
```

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Arguments

mvspectrum.output

an object of class "mvspectrum" representing the multivariate spectrum of \mathbf{X}_t (not necessarily normalized).

kernel.weights numeric; weights for each frequency. By default uses weights that average out

weightvector numeric; weights w for $y_t = \mathbf{U}_t \mathbf{w}$. Must have unit norm in ℓ^2 .

f.U multivariate spectrum of class 'mvspectrum' with normalize = TRUE.

f.current numeric; spectral density estimate of $y_t = \mathbf{U}_t \mathbf{w}$ for the current estimate $\hat{\mathbf{w}}_i$ (required for foreca.EM.M_step; optional for foreca.EM.h).

entropy.control

list; control settings for entropy estimation. See complete_entropy_control for details.

Details

The covariance matrix of a multivariate time series satisfies the identity

$$\Sigma_X \equiv \int_{-\pi}^{\pi} S_X(\lambda) d\lambda.$$

A generalized covariance matrix estimate can thus be obtained using a weighted average

$$\tilde{\Sigma}_X = \int_{-\pi}^{\pi} K(\lambda) S_X(\lambda) d\lambda,$$

where $K(\lambda)$ is a kernel symmetric around 0 which averages out to 1 over the interval $[-\pi,\pi]$, i.e., $\frac{1}{2\pi}\int_{-\pi}^{\pi}K(\lambda)d\lambda=1$. This allows one to remove or amplify specific frequencies in the covariance matrix estimation.

For ForeCA myspectrum2wcov is especially important as we use

$$K(\lambda) = -\log f_u(\lambda),$$

as the *weights* (their average is not 1!). This particular kernel weight is implemented as a wrapper in weightvector2entropy_wcov.

Value

A symmetric $n \times n$ matrix.

If kernel.weights ≥ 0 , then it is positive semi-definite; otherwise, it is symmetric but not necessarily positive semi-definite.

See Also

mvspectrum

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Examples

```
nn <- 50
YY <- cbind(rnorm(nn), arima.sim(n = nn, list(ar = 0.9)), rnorm(nn))
XX <- YY %*% matrix(rnorm(9), ncol = 3) # random mix
XX <- scale(XX, scale = FALSE, center = TRUE)
# sample estimate of covariance matrix
Sigma.hat <- cov(XX)</pre>
dimnames(Sigma.hat) <- NULL</pre>
# using the frequency spectrum
SS <- mvspectrum(XX, "mvspec")
Sigma.hat.freq <- mvspectrum2wcov(SS)</pre>
layout(matrix(1:4, ncol = 2))
par(mar = c(2, 2, 1, 1))
plot(c(Sigma.hat/Sigma.hat.freq))
abline(h = 1)
image(Sigma.hat)
image(Sigma.hat.freq)
image(Sigma.hat / Sigma.hat.freq)
# examples for entropy wcov
XX <- diff(log(EuStockMarkets)) * 100
UU <- whiten(XX)$U
ff <- mvspectrum(UU, "mvspec", normalize = TRUE)</pre>
ww0 <- initialize_weightvector(num.series = ncol(XX), method = 'rnorm')</pre>
weightvector2entropy_wcov(ww0, ff,
                           entropy.control =
                             list(prior.weight = 0.1))
```

Omega

Estimate forecastability of a time series

Description

An estimator for the forecastability $\Omega(x_t)$ of a univariate time series x_t . Currently it uses a discrete plug-in estimator given the empirical spectrum (periodogram).

Usage

```
Omega(
   series = NULL,
   spectrum.control = list(),
   entropy.control = list(),
   mvspectrum.output = NULL
)
```

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Arguments

series

a univariate time series; if it is multivariate, then Omega works component-wise (i.e., same as apply(series, 2, Omega)).

spectrum.control

list; control settings for spectrum estimation. See complete_spectrum_control for details.

entropy.control

list; control settings for entropy estimation. See complete_entropy_control for details.

mvspectrum.output

an object of class "mvspectrum" representing the multivariate spectrum of \mathbf{X}_t (not necessarily normalized).

Details

The forecastability of a stationary process x_t is defined as (see References)

$$\Omega(x_t) = 1 - \frac{-\int_{-\pi}^{\pi} f_x(\lambda) \log f_x(\lambda) d\lambda}{\log 2\pi} \in [0, 1]$$

where $f_x(\lambda)$ is the normalized spectral density of x_t . In particular $\int_{-\pi}^{\pi} f_x(\lambda) d\lambda = 1$.

For white noise ε_t forecastability $\Omega(\varepsilon_t)=0$; for a sum of sinusoids it equals 100 %. However, empirically it reaches 100% only if the estimated spectrum has exactly one peak at some ω_j and $\widehat{f}(\omega_k)=0$ for all $k\neq j$.

In practice, a time series of length T has T Fourier frequencies which represent a discrete probability distribution. Hence entropy of $f_x(\lambda)$ must be normalized by $\log T$, not by $\log 2\pi$.

Also we can use several smoothing techniques to obtain a less variance estimate of $f_x(\lambda)$.

Value

A real-value between 0 and 100 (%). 0 means not forecastable (white noise); 100 means perfectly forecastable (a sinusoid).

References

Goerg, G. M. (2013). "Forecastable Component Analysis". Journal of Machine Learning Research (JMLR) W&CP 28 (2): 64-72, 2013. Available at http://jmlr.org/proceedings/papers/v28/goerg13.html.

See Also

spectral_entropy, discrete_entropy, continuous_entropy

quadratic_form 27

Examples

```
nn <- 100
eps <- rnorm(nn) # white noise has Omega() = 0 in theory
Omega(eps, spectrum.control = list(method = "pgram"))
# smoothing makes it closer to 0
Omega(eps, spectrum.control = list(method = "mvspec"))
xx <- \sin(\text{seq\_len(nn}) * \text{pi } / 10)
Omega(xx, spectrum.control = list(method = "pgram"))
Omega(xx, entropy.control = list(threshold = 1/40))
Omega(xx, spectrum.control = list(method = "mvspec"),
      entropy.control = list(threshold = 1/20))
# an AR(1) with phi = 0.5
yy \leftarrow arima.sim(n = nn, model = list(ar = 0.5))
Omega(yy, spectrum.control = list(method = "mvspec"))
# an AR(1) with phi = 0.9 is more forecastable
yy \leftarrow arima.sim(n = nn, model = list(ar = 0.9))
Omega(yy, spectrum.control = list(method = "mvspec"))
```

quadratic_form

Computes quadratic form x' A x

Description

quadratic_form computes the quadratic form $\mathbf{x}'\mathbf{A}\mathbf{x}$ for an $n \times n$ matrix \mathbf{A} and an n-dimensional vector \mathbf{x} , i.e., a wrapper for $\mathbf{t}(\mathbf{x})$ %*% A %*% \mathbf{x} .

fill_symmetric and quadratic_form work with real and complex valued matrices/vectors.

fill_hermitian fills up the lower triangular part (NA) of an upper triangular matrix to its Hermitian (symmetric if real matrix) version, such that it satisfies $\mathbf{A} = \bar{\mathbf{A}}'$, where \bar{z} is the complex conjugate of z. If the matrix is real-valued this makes it simply symmetric.

Note that the input matrix must have a **real-valued** diagonal and NAs in the lower triangular part.

Usage

```
quadratic_form(mat, vec)
fill_hermitian(mat)
```

Arguments

```
mat numeric; n \times n matrix (real or complex).
vec numeric; n \times 1 vector (real or complex).
```

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Value

A real/complex value x'Ax.

Examples

```
## Not run:
    set.seed(1)
    AA <- matrix(1:4, ncol = 2)
    bb <- matrix(rnorm(2))
    t(bb) %*% AA %*% bb
    quadratic_form(AA, bb)

## End(Not run)

AA <- matrix(1:16, ncol = 4)
    AA[lower.tri(AA)] <- NA
    AA

fill_hermitian(AA)</pre>
```

sfa

Slow Feature Analysis

Description

sfa performs Slow Feature Analysis (SFA) on a K-dimensional time series with T observations.

Important: This implementation of SFA is just the most basic version; it is merely included here for convenience in initialize_weightvector. If you want to actually use full functionality of SFA in R use the **rSFA** package, which has a much more advanced and efficient implementations. sfa() here corresponds to sfa1.

Usage

```
sfa(series, ...)
```

Arguments

```
series a T \times K array with T observations from the K-dimensional time series \mathbf{X}_t. Can be a matrix, data. frame, or a multivariate ts object.
```

.. additional arguments

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Details

Slow Feature Analysis (SFA) finds *slow* signals (see References below). The problem has an analytic solution and thus can be computed quickly using generalized eigen-value solvers. For ForeCA it is important to know that SFA is equivalent to finding a linear combination signal with largest lag 1 autocorrelation.

The disadvantage of SFA for forecasting is that, e.g., white noise (WN) is ranked higher than an AR(1) with negative autocorrelation coefficient $\rho_1 < 0$. While it is true that WN is slower, it is not more forecastable. Thus we are also interested in the fastest signal, i.e., the last eigenvector. The so obtained fastest signal corresponds to minimizing the lag 1 auto-correlation (possibly $\rho_1 < 0$).

Note though that maximizing (or minimizing) the lag 1 auto-correlation does not necessarily yield the most forecastable signal (as measured by Omega), but it is a good start.

Value

An object of class sfa which inherits methods from princomp. Signals are ordered from slowest to fastest.

References

Laurenz Wiskott and Terrence J. Sejnowski (2002). "Slow Feature Analysis: Unsupervised Learning of Invariances", Neural Computation 14:4, 715-770.

See Also

```
initialize_weightvector
```

Examples

```
XX <- diff(log(EuStockMarkets[-c(1:100),])) * 100
plot(ts(XX))
ss <- sfa(XX[,1:4])

summary(ss)
plot(ss)
plot(ts(ss$scores))
apply(ss$scores, 2, function(x) acf(x, plot = FALSE)$acf[2])
biplot(ss)</pre>
```

spectral_entropy

Estimates spectral entropy of a time series

Description

Estimates spectral entropy from a univariate (or multivariate) normalized spectral density.

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Usage

```
spectral_entropy(
  series = NULL,
  spectrum.control = list(),
  entropy.control = list(),
  mvspectrum.output = NULL,
  ...
)
```

Arguments

series

univariate time series of length T. In the rare case that users want to call this for a multivariate time series, note that the estimated spectrum is in general not normalized for the computation. Only if the original data is whitened, then it is normalized.

spectrum.control

list; control settings for spectrum estimation. See complete_spectrum_control for details.

entropy.control

list; control settings for entropy estimation. See complete_entropy_control for details.

mvspectrum.output

optional; one can directly provide an estimate of the spectrum of series. Usually the output of myspectrum.

... additional arguments passed to myspectrum.

Details

The *spectral entropy* equals the Shannon entropy of the spectral density $f_x(\lambda)$ of a stationary process x_t :

 $H_s(x_t) = -\int_{-\pi}^{\pi} f_x(\lambda) \log f_x(\lambda) d\lambda,$

where the density is normalized such that $\int_{-\pi}^{\pi} f_x(\lambda) d\lambda = 1$. An estimate of $f(\lambda)$ can be obtained by the (smoothed) periodogram (see myspectrum); thus using discrete, and not continuous entropy.

Value

A non-negative real value for the spectral entropy $H_s(x_t)$.

References

Jerry D. Gibson and Jaewoo Jung (2006). "The Interpretation of Spectral Entropy Based Upon Rate Distortion Functions". IEEE International Symposium on Information Theory, pp. 277-281.

L. L. Campbell, "Minimum coefficient rate for stationary random processes", Information and Control, vol. 3, no. 4, pp. 360 - 371, 1960.

See Also

Omega, discrete_entropy

whiten 31

Examples

```
set.seed(1)
eps <- rnorm(100)</pre>
spectral_entropy(eps)
phi.v \leftarrow seq(-0.95, 0.95, by = 0.1)
kMethods <- c("mvspec", "pgram")</pre>
SE <- matrix(NA, ncol = length(kMethods), nrow = length(phi.v))
for (ii in seq_along(phi.v)) {
  xx.tmp <- arima.sim(n = 200, list(ar = phi.v[ii]))</pre>
  for (mm in seq_along(kMethods)) {
    SE[ii, mm] <- spectral_entropy(xx.tmp, spectrum.control =</pre>
                                       list(method = kMethods[mm]))
  }
}
matplot(phi.v, SE, type = "1", col = seq_along(kMethods))
legend("bottom", kMethods, lty = seq_along(kMethods),
       col = seq_along(kMethods))
# AR vs MA
SE.arma <- matrix(NA, ncol = 2, nrow = length(phi.v))
SE.arma[, 1] <- SE[, 2]</pre>
for (ii in seq_along(phi.v)){
  yy.temp <- arima.sim(n = 1000, list(ma = phi.v[ii]))</pre>
  SE.arma[ii, 2] <-</pre>
    spectral_entropy(yy.temp, spectrum.control = list(method = "mvspec"))
}
matplot(phi.v, SE.arma, type = "l", col = 1:2, xlab = "parameter (phi or theta)",
        ylab = "Spectral entropy")
abline(v = 0, col = "blue", lty = 3)
legend("bottom", c("AR(1)", "MA(1)"), lty = 1:2, col = 1:2)
```

whiten

whitens multivariate data

Description

whiten transforms a multivariate K-dimensional signal X with mean μ_X and covariance matrix Σ_X to a *whitened* signal U with mean 0 and $\Sigma_U = I_K$. Thus it centers the signal and makes it contemporaneously uncorrelated. See Details.

check_whitened checks if data has been whitened; i.e., if it has zero mean, unit variance, and is uncorrelated.

 $\operatorname{sqrt_matrix}$ computes the square root B of a square matrix A. The matrix B satisfies $\operatorname{BB} = \operatorname{A}$.

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Usage

```
whiten(data)
check_whitened(data, check.attribute.only = TRUE)
sqrt_matrix(mat, return.sqrt.only = TRUE, symmetric = FALSE)
```

Arguments

data $n \times K$ array representing n observations of K variables.

check.attribute.only

logical; if TRUE it checks the attribute only. This is much faster (it just needs to look up one attribute value), but it might not surface silent bugs. For sake of performance the package uses the attribute version by default. However, for testing/debugging the full computational version can be used.

mat a square $K \times K$ matrix.

return.sqrt.only

logical; if TRUE (default) it returns only the square root matrix; if FALSE it returns other auxiliary results (eigenvectors and eigenvalues, and inverse of the square root matrix).

symmetric

logical; if TRUE the eigen-solver assumes that the matrix is symmetric (which makes it much faster). This is in particular useful for a covariance matrix (which is used in whiten). Default: FALSE.

Details

whiten uses zero component analysis (ZCA) (aka zero-phase whitening filters) to whiten the data; i.e., it uses the inverse square root of the covariance matrix of **X** (see sqrt_matrix) as the whitening transformation. This means that on top of PCA, the uncorrelated principal components are backtransformed to the original space using the transpose of the eigenvectors. The advantage is that this makes them comparable to the original **X**. See References for details.

The square root of a quadratic $n \times n$ matrix \mathbf{A} can be computed by using the eigen-decomposition of \mathbf{A}

$$\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}'$$

where Λ is an $n \times n$ matrix with the eigenvalues $\lambda_1, \ldots, \lambda_n$ in the diagonal. The square root is simply $\mathbf{B} = \mathbf{V}\Lambda^{1/2}\mathbf{V}'$ where $\Lambda^{1/2} = diag(\lambda_1^{1/2}, \ldots, \lambda_n^{1/2})$.

Similarly, the *inverse square root* is defined as $\mathbf{A}^{-1/2} = \mathbf{V}\Lambda^{-1/2}\mathbf{V}'$, where $\Lambda^{-1/2} = diag(\lambda_1^{-1/2}, \dots, \lambda_n^{-1/2})$ (provided that $\lambda_i \neq 0$).

Value

whiten returns a list with the whitened data, the transformation, and other useful quantities.

check_whitened throws an error if the input is not whitened, and returns (invisibly) the data with an attribute 'whitened' equal to TRUE. This allows to simply update data to have the attribute and thus only check it once on the actual data (slow) but then use the attribute lookup (fast).

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sqrt_matrix returns an $n \times n$ matrix. If \mathbf{A} is not semi-positive definite it returns a complex-valued \mathbf{B} (since square root of negative eigenvalues are complex).

If return.sqrt.only = FALSE then it returns a list with:

values eigenvalues of A, vectors eigenvectors of A, square root matrix B,

sqrt.inverse inverse of B.

References

```
See appendix in http://www.cs.toronto.edu/~kriz/learning-features-2009-TR.pdf. See http://ufldl.stanford.edu/wiki/index.php/Implementing_PCA/Whitening.
```

```
## Not run:
XX <- matrix(rnorm(100), ncol = 2) %*% matrix(runif(4), ncol = 2)
cov(XX)
UU <- whiten(XX)$U
cov(UU)
## End(Not run)</pre>
```

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