Package 'SuperGauss'

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Title Superfast Likelihood Inference for Stationary Gaussian Time Series

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Description

Likelihood evaluations for stationary Gaussian time series are typically obtained via the Durbin-Levinson algorithm, which scales as $O(n^2)$ in the number of time series observations. This package provides a "superfast" $O(n \log^2 n)$ algorithm written in C++, crossing over with Durbin-Levinson around n = 300. Efficient implementations of the score and Hessian functions are also provided, leading to superfast versions of inference algorithms such as Newton-Raphson and Hamiltonian Monte Carlo. The C++ code provides a Toeplitz matrix class packaged as a header-only library, to simplify low-level usage in other packages and outside of R.

License GPL-3

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Author Yun Ling [aut], Martin Lysy [aut, cre]

Maintainer Martin Lysy <mlysy@uwaterloo.ca>

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Description

Likelihood evaluations for stationary Gaussian time series are typically obtained via the Durbin-Levinson algorithm, which scales as O(n^2) in the number of time series observations. This package provides a "superfast" O(n log^2 n) algorithm written in C++, crossing over with Durbin-Levinson around n = 300. Efficient implementations of the score and Hessian functions are also provided, leading to superfast versions of inference algorithms such as Newton-Raphson and Hamiltonian Monte Carlo. The C++ code provides a Toeplitz matrix class packaged as a header-only library, to simplify low-level usage in other packages and outside of R.

Details

While likelihood calculations with stationary Gaussian time series generally scale as O(N^2) in the number of observations, this package implements an algorithm which scales as O(N log^2 N). "Superfast" algorithms for loglikelihood gradients and Hessians are also provided. The underlying C++ code is distributed through a header-only library found in the installed package's include directory.

Author(s)

Maintainer: Martin Lysy <mlysy@uwaterloo.ca>

Authors:

• Yun Ling

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Examples

```
# Superfast inference for the timescale parameter
# of the exponential autocorrelation function
exp_acf \leftarrow function(lambda) exp(-(1:N-1)/lambda)
# simulate data
lambda0 <- 1
N <- 1000
X <- rnormtz(n = 1, acf = exp_acf(lambda0))</pre>
# loglikelihood function
# allocate memory for a NormalToeplitz distribution object
NTz <- NormalToeplitz$new(N)</pre>
loglik <- function(lambda) {</pre>
  NTz$logdens(z = X, acf = exp_acf(lambda))
  ## dSnorm(X = X, acf = Toep, log = TRUE)
}
# maximum likelihood estimation
optimize(f = loglik, interval = c(.2, 5), maximum = TRUE)
```

acf2incr

Convert position autocorrelations to increment autocorrelations.

Description

```
Convert the autocorrelation of a stationary sequence x = (x_1, ..., x_N) to that of its increments, dx = (x_2 - x_1, ..., x_N - x_N).
```

Usage

```
acf2incr(acf)
```

Arguments

acf

Length-N vector of position autocorrelations.

Value

Length N-1 vector of increment autocorrelations.

```
acf2incr(acf = exp(-(0:10)))
```

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acf2msd	Convert autocorrelation of stationary increments to mean squared dis-
	placement of posititions.

Description

Converts the autocorrelation of a stationary increment sequence $dx = (x_1 - x_0, ..., x_N - x_{N-1})$ to the mean squared displacement (MSD) of the corresponding positions, i.e., MSD_i = E[(x_i - x_0)^2].

Usage

```
acf2msd(acf)
```

Arguments

acf

Length-N autocorrelation vector of a stationary increment sequence.

Value

Length-N MSD vector of the corresponding positions.

Examples

```
acf2msd(acf = exp(-(0:10)))
```

Cholesky

Cholesky multiplication with Toeplitz variance matrices.

Description

Multiplies the Cholesky decomposition of the Toeplitz matrix with another matrix, or solves a system of equations with the Cholesky factor.

Usage

```
cholZX(Z, acf)
cholXZ(X, acf)
```

Arguments

acf Length-N autocorrelation vector of the Toeplitz variance matrix.

X Length-N or N x p matrix of observations.

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Details

If C == t(chol(toeplitz(acf))), then cholZX() computes C % % Z and cholZX() computes Solve(C, X). Both functions use the Durbin-Levinson algorithm.

Value

Size N x p residual or observation matrix.

Examples

```
N <- 10
p <- 2
acf <- exp(-(1:N - 1))

Z <- matrix(rnorm(N * p), N, p)
cholZX(Z = Z, acf = acf) - (t(chol(toeplitz(acf))) %*% Z)

X <- matrix(rnorm(N * p), N, p)
cholXZ(X = X, acf = acf) - solve(t(chol(toeplitz(acf))), X)</pre>
```

Circulant

Constructor and methods for Circulant matrix objects.

Description

Constructor and methods for Circulant matrix objects.

Methods

Public methods:

- Circulant\$new()
- Circulant\$size()
- Circulant\$set_acf()
- Circulant\$get_acf()
- Circulant\$set_psd()
- Circulant\$get_psd()
- Circulant\$has_acf()
- Circulant\$prod()
- Circulant\$solve()
- Circulant\$log_det()
- Circulant\$clone()

Method new(): Class constructor.

Usage:

Circulant\$new(N, uacf, upsd)

```
Arguments:
 N Size of Circulant matrix.
 uacf Optional vector of Nu = floor(N/2) + 1 unique elements of the autocorrelation.
 upsd Optional vector of Nu = floor(N/2)+1 unique elements of the PSD.
 Returns: A Circulant object.
Method size(): Get the size of the Circulant matrix.
 Usage:
 Circulant$size()
 Returns: Size of the Circulant matrix.
Method set_acf(): Set the autocorrelation of the Circulant matrix.
 Usage:
 Circulant$set_acf(uacf)
 Arguments:
 uacf Vector of Nu = floor(N/2) + 1 unique elements of the autocorrelation.
Method get_acf(): Get the autocorrelation of the Circulant matrix.
 Usage:
 Circulant$get_acf()
 Returns: The complete autocorrelation vector of length N.
Method set_psd(): Set the PSD of the Circulant matrix.
The power spectral density (PSD) of a Circulant matrix Ct = Circulant(acf) is defined as psd
= iFFT(acf).
 Usage:
 Circulant$set_psd(upsd)
 Arguments:
 upsd Vector of Nu = floor(N/2)+1 unique elements of the psd.
Method get_psd(): Get the PSD of the Circulant matrix.
 Usage:
 Circulant$get_psd()
 Returns: The complete PSD vector of length N.
Method has_acf(): Check whether the autocorrelation of the Circulant matrix has been set.
 Usage:
 Circulant$has_acf()
 Returns: Logical; TRUE if Circulant$set_acf() has been called.
Method prod(): Circulant matrix-matrix product.
 Usage:
 Circulant$prod(x)
```

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Arguments:

x Vector or matrix with N rows.

Returns: The matrix product Ct %*% x.

Method solve(): Solve a Circulant system of equations.

Usage:

Circulant\$solve(x)

Arguments:

x Optional vector or matrix with N rows.

Returns: The solution in z to the system of equations Ct %% z = x. If x is missing, returns the inverse of Ct.

Method log_det(): Calculate the log-determinant of the Circulant matrix.

Usage:

Circulant\$log_det()

Returns: The log-determinant log(det(Ct)).

Method clone(): The objects of this class are cloneable with this method.

Usage:

Circulant\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

dnormtz

Density of a multivariate normal with Toeplitz variance matrix.

Description

Density of a multivariate normal with Toeplitz variance matrix.

Usage

```
dnormtz(X, mu, acf, log = FALSE, method = c("gschur", "ltz"))
```

Arguments

method

Χ	Vector of length N or N x n matrix, of which each column is a multivariate
	observation.
mu	Vector or matrix of mean values of compatible dimensions with X. Defaults to

all zeros.

vector of length N containing the first column of the Toeplitz variance matrix.

Logical; whether to return the multivariate normal density on the log scale.

Which calculation method to use. Choices are: gschur for a modified version of the Generalized Schur algorithm of Ammar & Gragg (1988), or 1tz for the Levinson-Trench-Zohar method. The former scales as 0(N log^2 N) whereas

the latter scales as $O(N^2)$ and should only be used for N < 300.

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Value

Vector of n (log-)densities, one for each column of X.

Examples

```
# simulate data
N <- 10 # length of each time series
n <- 3 # number of time series
theta <- 0.1
lambda <- 2
mu <- theta^2 * rep(1, N)
acf <- exp(-lambda * (1:N - 1))

X <- rnormtz(n, acf = acf) + mu
# evaluate log-density
dnormtz(X, mu, acf, log = TRUE)</pre>
```

fbm_msd

Mean square displacement of fractional Brownian motion.

Description

Mean square displacement of fractional Brownian motion.

Usage

```
fbm_msd(tseq, H)
```

Arguments

```
tseq Length-N vector of timepoints.

H Hurst parameter (between 0 and 1).
```

Details

The mean squared displacement (MSD) of a stochastic process X_t is defined as

```
MSD(t) = E[(X_t - X_0)^2].
```

Fractional Brownian motion (fBM) is a continuous Gaussian process with stationary increments, such that its covariance function is entirely defined the MSD, which in this case is $MSD(t) = |t|^{(2H)}$.

Value

Length-N vector of mean square displacements.

```
fbm_msd(tseq = 1:10, H = 0.4)
```

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matern_acf

Matern autocorrelation function.

Description

Matern autocorrelation function.

Usage

```
matern_acf(tseq, lambda, nu)
```

Arguments

tseq Vector of N time points at which the autocorrelation is to be calculated.

lambda Timescale parameter.nu Smoothness parameter.

Details

The Matern autocorrelation is given by

$$\mathrm{ACF}(t) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{t}{\lambda} \right)^{\nu} K_{\nu} \left(\sqrt{2\nu} \frac{t}{\lambda} \right),$$

where $K_{\nu}(x)$ is the modified Bessel function of second kind.

Value

An autocorrelation vector of length N.

Examples

```
matern\_acf(tseq = 1:10, lambda = 1, nu = 3/2)
```

msd2acf

Convert mean square displacement of positions to autocorrelation of increments.

Description

Converts the mean squared displacement (MSD) of a stationary increments sequence $x = (x_0, x_1, ..., x_N)$ positions to the autocorrelation of the corresponding increments $dx = (x_1 - x_0, ..., x_N - x_N)$.

Usage

msd2acf(msd)

NormalCirculant NormalCirculant

Arguments

msd

Length-N MSD vector, i.e., excluding x_0 which is assumed to be zero.

Value

Length-N autocorrelation vector.

Examples

```
# autocorrelation of fBM increments
msd2acf(msd = fbm_msd(tseq = 0:10, H = .3))
```

NormalCirculant

Multivariate normal with Circulant variance matrix.

Description

Provides methods for the Normal-Circulant (NCt) distribution, which for a random vector \boldsymbol{z} of length N is defined as

Methods

Public methods:

- NormalCirculant\$new()
- NormalCirculant\$size()
- NormalCirculant\$logdens()
- NormalCirculant\$grad_full()
- NormalCirculant\$clone()

Method new(): Class constructor.

Usage:

NormalCirculant\$new(N)

Arguments:

N Size of the NCt random vector.

Returns: A NormalCirculant object.

Method size(): Get the size of the NCt random vector.

Usage:

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NormalCirculant\$size()

Returns: Size of the NCt random vector.

Method logdens(): Log-density function.

Usage:

NormalCirculant\$logdens(z, uacf)

Arguments:

z Density argument. A vector of length N or an N x n_obs matrix where each column is an N-dimensional observation.

uacf A vector of length Nu = floor(N/2) containing the first half of the autocorrelation (i.e., first row/column) of the Circulant variance matrix.

Returns: A scalar or vector of length n_obs containing the log-density of the NCt evaluated at its arguments.

Method grad_full(): Full gradient of log-density function.

Usage:

NormalCirculant\$grad_full(z, uacf, calc_dldz = TRUE, calc_dldu = TRUE)

Arguments:

z Density argument. A vector of length N.

uacf A vector of length Nu = floor(N/2) containing the first half of the autocorrelation (i.e., first row/column) of the Circulant variance matrix.

calc_dldz Whether or not to calculate the gradient with respect to z.

calc_dldu Whether or not to calculate the gradient with respect to uacf.

Returns: A list with elements:

ldens The log-density evaluated at z and uacf.

dldz The length-N gradient vector with respect to z, if calc_dldz = TRUE.

dldu The length-Nu = floor(N/2)+1 gradient vector with respect to uacf, if calc_dldu = TRUE.

Method clone(): The objects of this class are cloneable with this method.

Usage:

NormalCirculant\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

NormalToeplitz NormalToeplitz

NormalToeplitz

Multivariate normal with Toeplitz variance matrix.

Description

Provides methods for the Normal-Toeplitz (NTz) distribution defined as

```
z ~ NTz(acf) <=> z ~ Normal(0, toeplitz(acf)),
```

i.e., for a multivariate normal with mean zero and variance Tz = toeplitz(acf).

Methods

Public methods:

- NormalToeplitz\$new()
- NormalToeplitz\$size()
- NormalToeplitz\$logdens()
- NormalToeplitz\$grad()
- NormalToeplitz\$hess()
- NormalToeplitz\$grad_full()
- NormalToeplitz\$clone()

Method new(): Class constructor.

Usage:

NormalToeplitz\$new(N)

Arguments:

N Size of the NTz random vector.

Returns: A NormalToeplitz object.

Method size(): Get the size of the NTz random vector.

Usage:

NormalToeplitz\$size()

Returns: Size of the NTz random vector.

Method logdens(): Log-density function.

Usage:

NormalToeplitz\$logdens(z, acf)

Arguments:

- z Density argument. A vector of length N or an N x n_obs matrix where each column is an N-dimensional observation.
- acf A vector of length N containing the autocorrelation (i.e., first row/column) of the Toeplitz variance matrix.

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Returns: A scalar or vector of length n_obs containing the log-density of the NTz evaluated at its arguments.

Method grad(): Gradient of the log-density with respect to parameters.

Usage:

NormalToeplitz\$grad(z, dz, acf, dacf, full_out = FALSE)

Arguments:

z Density argument. A vector of length N.

dz An N x n_theta matrix containing the gradient dz/dtheta.

acf A vector of length N containing the autocorrelation of the Toeplitz variance matrix.

dacf An N x n_theta matrix containing the gradient dacf/dtheta.

full_out If TRUE, returns the log-density as well (see 'Value').

Returns: A vector of length n_theta containing the gradient of the NTz log-density with respect to theta, or a list with elements 1dens and grad consisting of the log-density and the gradient vector.

Method hess(): Hessian of log-density with respect to parameters.

Usage:

NormalToeplitz\$hess(z, dz, d2z, acf, dacf, d2acf, full_out = FALSE)

Arguments:

z Density argument. A vector of length N.

dz An N x n_theta matrix containing the gradient dz/dtheta.

d2z An N x n_theta x n_theta array containing the Hessian d^2z/dtheta^2.

acf A vector of length N containing the autocorrelation of the Toeplitz variance matrix.

dacf An N x n_theta matrix containing the gradient dacf/dtheta.

d2acf An N x n_theta x n_theta array containing the Hessian dacf^2/dtheta^2.

full_out If TRUE, returns the log-density and its gradient as well (see 'Value').

Returns: An n_theta x n_theta matrix containing the Hessian of the NTz log-density with respect to theta, or a list with elements 1dens, grad, and hess consisting of the log-density, its gradient (a vector of size n_theta), and the Hessian matrix, respectively.

Method grad_full(): Full gradient of log-density function.

Usage:

NormalToeplitz\$grad_full(z, acf, calc_dldz = TRUE, calc_dlda = TRUE)

Arguments:

z Density argument. A vector of length N.

acf A vector of length N containing the autocorrelation of the Toeplitz variance matrix.

calc_dldz Whether or not to calculate the gradient with respect to z.

calc_dlda Whether or not to calculate the gradient with respect to acf.

Returns: A list with elements:

ldens The log-density evaluated at z and acf.

dldz The length-N gradient vector with respect to z, if calc_dldz = TRUE.

pex_acf

dlda The length-N gradient vector with respect to acf, if calc_dlda = TRUE.

Method clone(): The objects of this class are cloneable with this method.

Usage:

NormalToeplitz\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

pex_acf

Power-exponential autocorrelation function.

Description

Power-exponential autocorrelation function.

Usage

```
pex_acf(tseq, lambda, rho)
```

Arguments

tseq Vector of N time points at which the autocorrelation is to be calculated.

lambda Timescale parameter.
rho Power parameter.

Details

The power-exponential autocorrelation function is given by:

$$ACF(t) = \exp \left\{ -(t/\lambda)^{\rho} \right\}.$$

Value

An autocorrelation vector of length N.

```
pex_acf(tseq = 1:10, lambda = 1, rho = 2)
```

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Description

Simulate a stationary Gaussian time series.

Usage

```
rnormtz(n = 1, acf, Z, fft = TRUE, nkeep, tol = 1e-06)
```

Arguments

n	Number of time series to generate.
acf	Length-N vector giving the autocorrelation of the series.
Z	Optional size (2N-2) \times n or N \times n matrix of iid standard normals, to use in the FFT and Durbin-Levinson methods, respectively.
fft	Logical; whether or not to use the O(N log N) FFT-based algorithm of Wood and Chan (1994) or the more stable O(N^2) Durbin-Levinson algorithm. See Details.
nkeep	Length of time series. Defaults to N = length(acf). See Details.
tol	Relative tolerance on negative eigenvalues. See Details.

Details

The FFT method fails when the embedding circulant matrix is not positive definite. This is typically due to one of two things:

- 1. Roundoff error can make tiny eigenvalues appear negative. For this purpose, argument tol can be used to replace all negative eigenvalues by tol * ev_max, where ev_max is the largest eigenvalue.
- 2. The autocorrelation is decaying too slowly on the given timescale. To mitigate this, argument nkeep can be used to supply a longer acf than is required, and keep only the first nkeep time series observations. For consistency, nkeep also applies to Durbin-Levinson method.

Value

Length-nkeep vector or size nkeep x n matrix with time series as columns.

```
N < -10
acf < -\exp(-(1:N - 1)/N)
rnormtz(n = 3, acf = acf)
```

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SuperGauss-defunct

Defunct functions in SuperGauss.

Description

Defunct functions in SuperGauss.

The following functions have been removed from the SuperGauss package

```
rSnorm() Please use rnormtz() instead.
dSnorm() Please use dnormtz() instead.
Snorm.grad() Please use the grad() method in the NormalToeplitz class.
Snorm.hess() Please use the hess() method in the NormalToeplitz class.
```

toep.mult

Toeplitz matrix multiplication.

Description

Efficient matrix multiplication with Toeplitz matrix and arbitrary matrix or vector.

Usage

```
toep.mult(acf, X)
```

Arguments

acf Length-N vector giving the first column (or row) of the Toeplitz matrix.

X Vector or matrix of compatible dimensions with acf.

Value

An N-row matrix corresponding to toeplitz(acf) %*% X.

```
N <- 20
d <- 3
acf <- exp(-(1:N))
X <- matrix(rnorm(N*d), N, d)
toep.mult(acf, X)</pre>
```

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Toeplitz

Constructor and methods for Toeplitz matrix objects.

Description

The Toeplitz class contains efficient methods for linear algebra with symmetric positive definite (i.e., variance) Toeplitz matrices.

Usage

```
is.Toeplitz(x)
as.Toeplitz(x)
## S3 method for class 'Toeplitz'
dim(x)
```

Arguments

Χ

An R object.

Details

An N x N Toeplitz matrix Tz is defined by its length-N "autocorrelation" vector acf, i.e., first row/column Tz. Thus, for the function stats::toeplitz(), we have Tz = toeplitz(acf).

It is assumed that acf defines a valid (i.e., positive definite) variance matrix. The matrix multiplication methods still work when this is not the case but the other methods do not (return values typically contain NaNs).

as. Toeplitz(x) attempts to convert its argument to a Toeplitz object by calling Toeplitz\$new(acf = x). is.Toeplitz(x) checks whether its argument is a Toeplitz object.

Methods

Public methods:

- Toeplitz\$new()
- Toeplitz\$print()
- Toeplitz\$size()
- Toeplitz\$set_acf()
- Toeplitz\$get_acf()
- Toeplitz\$has_acf()
- Toeplitz\$prod()
- Toeplitz\$solve()
- Toeplitz\$log_det()
- Toeplitz\$trace_grad()
- Toeplitz\$trace_hess()

Toeplitz

• Toeplitz\$clone() Method new(): Class constructor. Usage: Toeplitz\$new(N, acf) Arguments: N Size of Toeplitz matrix. acf Autocorrelation vector of length N. Returns: A Toeplitz object. Method print(): Print method. Usage: Toeplitz\$print() **Method** size(): Get the size of the Toeplitz matrix. Usage: Toeplitz\$size() Returns: Size of the Toeplitz matrix. ncol(), nrow(), and dim() methods for Toeplitz objects also work as expected. **Method** set_acf(): Set the autocorrelation of the Toeplitz matrix. Usage: Toeplitz\$set_acf(acf) Arguments: acf Autocorrelation vector of length N. **Method** get_acf(): Get the autocorrelation of the Toeplitz matrix. Usage: Toeplitz\$get_acf() Returns: The autocorrelation vector of length N. Method has_acf(): Check whether the autocorrelation of the Toeplitz matrix has been set. Usage: Toeplitz\$has_acf() Returns: Logical; TRUE if Toeplitz\$set_acf() has been called. Method prod(): Toeplitz matrix-matrix product. Usage: Toeplitz\$prod(x) Arguments: x Vector or matrix with N rows.

Returns: The matrix product Tz %*% x. Tz %*% x and x %*% Tz also work as expected.

Method solve(): Solve a Toeplitz system of equations.

Usage.

Toeplitz\$solve(x, method = c("gschur", "pcg"), tol = 1e-10)

Arguments:

x Optional vector or matrix with N rows.

method Solve method to use. Choices are: gschur for a modified version of the Generalized Schur algorithm of Ammar & Gragg (1988), or pcg for the preconditioned conjugate gradient method of Chen et al (2006). The former is faster and obtains the log-determinant as a direct biproduct. The latter is more numerically stable for long-memory autocorrelations.

tol Tolerance level for the pcg method.

Returns: The solution in z to the system of equations Tz % % z = x. If x is missing, returns the inverse of Tz. solve(Tz, x) and solve(Tz, x, method, tol) also work as expected.

Method log_det(): Calculate the log-determinant of the Toeplitz matrix.

Usage:

Toeplitz\$log_det()

Returns: The log-determinant log(det(Tz)). determinant(Tz) also works as expected.

Method trace_grad(): Computes the trace-gradient with respect to Toeplitz matrices.

Usage:

Toeplitz\$trace_grad(acf2)

Arguments:

acf2 Length-N autocorrelation vector of the second Toeplitz matrix. This matrix must be symmetric but not necessarily positive definite.

Returns: Computes the trace of

solve(Tz, toeplitz(acf2)).

This is used in the computation of the gradient of log(det(Tz(theta))) with respect to theta.

Method trace_hess(): Computes the trace-Hessian with respect to Toeplitz matrices.

Usage:

Toeplitz\$trace_hess(acf2, acf3)

Arguments:

acf2 Length-N autocorrelation vector of the second Toeplitz matrix. This matrix must be symmetric but not necessarily positive definite.

acf3 Length-N autocorrelation vector of the third Toeplitz matrix. This matrix must be symmetric but not necessarily positive definite.

Returns: Computes the trace of

solve(Tz, toeplitz(acf2)) %*% solve(Tz, toeplitz(acf3)).

This is used in the computation of the Hessian of log(det(Tz(theta))) with respect to theta.

Method clone(): The objects of this class are cloneable with this method.

Usage:

Toeplitz\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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```
# construct a Toeplitz matrix
acf <- exp(-(1:5))
Tz <- Toeplitz$new(acf = acf)</pre>
# alternatively, can allocate space first
Tz <- Toeplitz$new(N = length(acf))</pre>
Tz$set_acf(acf = acf)
# basic methods
Tz$get_acf() # extract the acf
dim(Tz) # == c(nrow(Tz), ncol(Tz))
Tz # print method
# linear algebra methods
X <- matrix(rnorm(10), 5, 2)</pre>
Tz %*% X
t(X) %*% Tz
solve(Tz, X)
determinant(Tz) # log-determinant
```

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