Package 'sdetorus'

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Type Package

Title Statistical Tools for Toroidal Diffusions

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Description Implementation of statistical methods for the estimation of toroidal diffusions. Several diffusive models are provided, most of them belonging to the Langevin family of diffusions on the torus. Specifically, the wrapped normal and von Mises processes are included, which can be seen as toroidal analogues of the Ornstein-Uhlenbeck diffusion. A collection of methods for approximate maximum likelihood estimation, organized in four blocks, is given: (i) based on the exact transition probability density, obtained as the numerical solution to the Fokker-Plank equation; (ii) based on wrapped pseudo-likelihoods; (iii) based on maximum likelihood of the stationary densities. The package allows the replicability of the results in García-Portugués et al. (2019) <doi:10.1007/s11222-017-9790-2>.

License GPL-3

Depends R (>= 3.6.0), Rcpp, mvtnorm

Suggests rgl, Bessel, manipulate

LinkingTo Rcpp, RcppArmadillo

URL https://github.com/egarpor/sdetorus

BugReports https://github.com/egarpor/sdetorus

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```
alphaToA
```

Valid drift matrices for the Ornstein–Uhlenbeck diffusion in 2D

Description

Constructs drift matrices A such that solve(A) %*% Sigma is symmetric.

Usage

```
alphaToA(alpha, sigma = NULL, rho = 0, Sigma = NULL)
```

aToAlpha(A, sigma = NULL, rho = 0, Sigma = NULL)

Arguments

alpha	vector of length 3 containing the A matrix. The first two elements are the diagonal.
sigma	vector of length 2 containing the square root of the diagonal of Sigma.
rho	correlation of Sigma.
Sigma	the diffusion matrix of size c(2, 2).
A	matrix of size c(2, 2).

Details

The parametrization enforces that solve(A) %*% Sigma is symmetric. Positive definiteness is guaranteed if alpha[3]^2 < rho^2 * (alpha[1] - alpha[2])^2 / 4 + alpha[1] * alpha[2].

Value

The drift matrix A or the alpha vector.

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Examples

```
# Parameters
alpha <- 3:1
Sigma <- rbind(c(1, 0.5), c(0.5, 4))
# Covariance matrix
A <- alphaToA(alpha = alpha, Sigma = Sigma)
S <- 0.5 * solve(A) %*% Sigma
det(S)
# Check
aToAlpha(A = alphaToA(alpha = alpha, Sigma = Sigma), Sigma = Sigma)
alphaToA(alpha = aToAlpha(A = A, Sigma = Sigma), Sigma = Sigma)
```

approxMleWn1D Approximate MLE of the WN diffusion in 1D

Description

Approximate Maximum Likelihood Estimation (MLE) for the Wrapped Normal (WN) in 1D using the wrapped Ornstein–Uhlenbeck diffusion.

Usage

```
approxMleWn1D(data, delta, start, alpha = NA, mu = NA, sigma = NA,
lower = c(0.01, -pi, 0.01), upper = c(25, pi, 25), vmApprox = FALSE,
maxK = 2, ...)
```

Arguments

data	a matrix of dimension c(n, p).
delta	discretization step.
start	starting values, a matrix with p columns, with each entry representing a different starting value.
alpha, mu, sigma	
	if their values are provided, the likelihood function is optimized with respect to the rest of unspecified parameters. The number of elements in start, lower and upper has to be modified accordingly (see examples).
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
vmApprox	flag to indicate von Mises approximation to wrapped normal. See momentMatchWnVm and scoreMatchWnBvm.
maxK	maximum absolute winding number used if circular = TRUE.
	further parameters passed to mleOptimWrapper.

Details

See Section 3.3 in García-Portugués et al. (2019) for details.

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approxMleWn2D

Value

Output from mleOptimWrapper.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Examples

approxMleWn2D	Approximate MLE of the WN diffusion in 2D
---------------	---

Description

Approximate Maximum Likelihood Estimation (MLE) for the Wrapped Normal (WN) in 2D using the wrapped Ornstein–Uhlenbeck diffusion.

Usage

```
approxMleWn2D(data, delta, start, alpha = rep(NA, 3), mu = rep(NA, 2),
sigma = rep(NA, 2), rho = NA, lower = c(0.01, 0.01, -25, -pi, -pi,
0.01, 0.01, -0.99), upper = c(rep(25, 3), pi, pi, 25, 25, 0.99),
maxK = 2, ...)
```

Arguments

data	a matrix of dimension c(n, p).	
delta	discretization step.	
start	starting values, a matrix with p columns, with each entry representing a different starting value.	
alpha, mu, sigma, rho		
	if their values are provided, the likelihood function is optimized with respect to	

if their values are provided, the likelihood function is optimized with respect to the rest of unspecified parameters. The number of elements in start, lower and upper has to be modified accordingly (see examples).

lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
maxK	maximum absolute winding number used if circular = TRUE.
	further parameters passed to mleOptimWrapper.

Details

See Section 3.3 in García-Portugués et al. (2019) for details.

Value

Output from mleOptimWrapper.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Examples

approxMleWnPairs Approximate MLE of the WN diffusion in 2D from a sample of initial and final pairs of angles.

Description

Approximate Maximum Likelihood Estimation (MLE) for the Wrapped Normal (WN) diffusion, using the wrapped Ornstein–Uhlenbeck diffusion and assuming initial stationarity.

Usage

```
approxMleWnPairs(data, delta, start = c(0, 0, 1, 1, 0, 1, 1),
alpha = rep(NA, 3), mu = rep(NA, 2), sigma = rep(NA, 2), rho = NA,
lower = c(-pi, -pi, 0.01, 0.01, -25, 0.01, 0.01, -0.99), upper = c(pi,
pi, 25, 25, 25, 25, 25, 0.99), maxK = 2, expTrc = 30, ...)
```

crankNicolson1D

Arguments

data	a matrix of dimension c(n, p).
delta	discretization step.
start	starting values, a matrix with p columns, with each entry representing a different starting value.
alpha	vector of length 3 parametrizing the A matrix as in alphaToA.
mu	a vector of length 2 giving the mean.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.
	further parameters passed to mleOptimWrapper.

Value

Output from mleOptimWrapper.

Examples

crankNicolson1D

Crank–Nicolson finite difference scheme for the 1D Fokker–Planck equation with periodic boundaries

Description

Implementation of the Crank-Nicolson scheme for solving the Fokker-Planck equation

$$p(x,t)_t = -(p(x,t)b(x))_x + \frac{1}{2}(\sigma^2(x)p(x,t))_{xx},$$

where p(x, t) is the transition probability density of the circular diffusion

$$dX_t = b(X_t)dt + \sigma(X_t)dW_t$$

Usage

•

```
crankNicolson1D(u0, b, sigma2, N, deltat, Mx, deltax, imposePositive = 0L)
```

Arguments

uØ	matrix of size $c(Mx, 1)$ giving the initial condition. Typically, the evaluation of a density highly concentrated at a given point. If $nt == 1$, then u0 can be a matrix $c(Mx, nu0)$ containing different starting values in the columns.
b	vector of length Mx containing the evaluation of the drift.
sigma2	vector of length Mx containing the evaluation of the squared diffusion coefficient.
Ν	increasing integer vector of length nt giving the indexes of the times at which the solution is desired. The times of the solution are delta $* c(0:max(N))[N + 1]$.
deltat	time step.
Mx	size of the equispaced spatial grid in $[-\pi, \pi)$.
deltax	space grid discretization.
imposePositive	flag to indicate whether the solution should be transformed in order to be always larger than a given tolerance. This prevents spurious negative values. The tolerance will be taken as imposePositiveTol if this is different from FALSE or 0.

Details

The function makes use of solvePeriodicTridiag for obtaining implicitly the next step in time of the solution.

If imposePositive = TRUE, the code implicitly assumes that the solution integrates to one at any step. This might b unrealistic if the initial condition is not properly represented in the grid (for example, highly concentrated density in a sparse grid).

Value

- If nt > 1, a matrix of size c(Mx, nt) containing the discretized solution at the required times.
- If nt == 1, a matrix of size c(Mx, nu0) containing the discretized solution at a fixed time for different starting values.

crankNicolson2D

References

Thomas, J. W. (1995). *Numerical Partial Differential Equations: Finite Difference Methods*. Springer, New York. doi:10.1007/9781489972781

Examples

```
# Parameters
Mx <- 200
N <- 200
x \le seq(-pi, pi, 1 = Mx + 1)[-c(Mx + 1)]
times <- seq(0, 1, 1 = N + 1)
u0 <- dWn1D(x, pi/2, 0.05)
b <- driftWn1D(x, alpha = 1, mu = pi, sigma = 1)</pre>
sigma2 <- rep(1, Mx)</pre>
# Full trajectory of the solution (including initial condition)
u <- crankNicolson1D(u0 = cbind(u0), b = b, sigma2 = sigma2, N = 0:N,
                     deltat = 1 / N, Mx = Mx, deltax = 2 * pi / Mx)
# Mass conservation
colMeans(u) * 2 * pi
# Visualization of tpd
plotSurface2D(times, x, z = t(u), levels = seq(0, 3, 1 = 50))
# Only final time
v <- crankNicolson1D(u0 = cbind(u0), b = b, sigma2 = sigma2, N = N,</pre>
                     deltat = 1 / N, Mx = Mx, deltax = 2 * pi / Mx)
sum(abs(u[, N + 1] - v))
```

crankNicolson2D	Crank–Nicolson finite difference scheme for the 2D Fokker–Planck
	equation with periodic boundaries

Description

Implementation of the Crank-Nicolson scheme for solving the Fokker-Planck equation

$$p(x, y, t)_t = -(p(x, y, t)b_1(x, y))_x - (p(x, y, t)b_2(x, y))_y + \frac{1}{2}(\sigma_1^2(x, y)p(x, y, t))_{xx} + \frac{1}{2}(\sigma_2^2(x, y)p(x, y, t))_{yy} + (\sigma_{12}(x, y)p(x, y, t))_{xy}$$

where p(x, y, t) is the transition probability density of the toroidal diffusion

$$dX_t = b_1(X_t, Y_t)dt + \sigma_1(X_t, Y_t)dW_t^1 + \sigma_{12}(X_t, Y_t)dW_t^2,$$

$$dY_t = b_2(X_t, Y_t)dt + \sigma_{12}(X_t, Y_t)dW_t^1 + \sigma_2(X_t, Y_t)dW_t^2.$$

Usage

```
crankNicolson2D(u0, bx, by, sigma2x, sigma2y, sigmaxy, N, deltat, Mx, deltax,
My, deltay, imposePositive = 0L)
```

Arguments

u0	matrix of size $c(Mx * My, 1)$ giving the initial condition matrix column-wise stored. Typically, the evaluation of a density highly concentrated at a given point. If $nt == 1$, then u0 can be a matrix $c(Mx * My, nu0)$ containing different starting values in the columns.
bx, by	matrices of size $c(Mx, My)$ containing the evaluation of the drift in the first and second space coordinates, respectively.
sigma2x, sigma2	y, sigmaxy
	matrices of size c(Mx, My) containing the evaluation of the entries of the diffu- sion matrix (it has to be positive definite) rbind(c(sigma2x, sigmaxy), c(sigmaxy, sigma2y)).
N	
N	increasing integer vector of length nt giving the indexes of the times at which the solution is desired. The times of the solution are delta $* c(0:max(N))[N + 1]$.
deltat	time step.
Mx, My	sizes of the equispaced spatial grids in $[-\pi,\pi)$ for each component.
deltax, deltay	space grid discretizations for each component.
imposePositive	flag to indicate whether the solution should be transformed in order to be always larger than a given tolerance. This prevents spurious negative values. The tolerance will be taken as imposePositiveTol if this is different from FALSE or 0 .

Details

The function makes use of solvePeriodicTridiag for obtaining implicitly the next step in time of the solution.

If imposePositive = TRUE, the code implicitly assumes that the solution integrates to one at any step. This might b unrealistic if the initial condition is not properly represented in the grid (for example, highly concentrated density in a sparse grid).

Value

- If nt > 1, a matrix of size c(Mx * My, nt) containing the discretized solution at the required times with the c(Mx, My) matrix stored column-wise.
- If nt == 1, a matrix of size c(Mx * My, nu0) containing the discretized solution at a fixed time for different starting values.

References

Thomas, J. W. (1995). *Numerical Partial Differential Equations: Finite Difference Methods*. Springer, New York. doi:10.1007/9781489972781

dBvm

Examples

```
# Parameters
Mx <- 100
My <- 100
N <- 200
x \le seq(-pi, pi, 1 = Mx + 1)[-c(Mx + 1)]
y <- seq(-pi, pi, 1 = My + 1)[-c(My + 1)]
m <- c(pi / 2, pi)
p <- c(0, 1)
u0 <- c(outer(dWn1D(x, p[1], 0.5), dWn1D(y, p[2], 0.5)))
bx <- outer(x, y, function(x, y) 5 * sin(m[1] - x))
by <- outer(x, y, function(x, y) 5 * sin(m[2] - y))
sigma2 <- matrix(1, nrow = Mx, ncol = My)</pre>
sigmaxy <- matrix(0.5, nrow = Mx, ncol = My)</pre>
# Full trajectory of the solution (including initial condition)
u <- crankNicolson2D(u0 = cbind(u0), bx = bx, by = by, sigma2x = sigma2,
                     sigma2y = sigma2, sigmaxy = sigmaxy,
                     N = 0:N, deltat = 1 / N, Mx = Mx, deltax = 2 * pi / Mx,
                     My = My, deltay = 2 * pi / My)
# Mass conservation
colMeans(u) * 4 * pi^2
# Only final time
v <- crankNicolson2D(u0 = cbind(u0), bx = bx, by = by, sigma2x = sigma2,</pre>
                     sigma2y = sigma2, sigmaxy = sigmaxy,
                     N = N, deltat = 1 / N, Mx = Mx, deltax = 2 * pi / Mx,
                     My = My, deltay = 2 * pi / My)
sum(abs(u[, N + 1] - v))
## Not run:
# Visualization of tpd
library(manipulate)
manipulate({
  plotSurface2D(x, y, z = matrix(u[, j + 1], Mx, My),
                main = round(mean(u[, j + 1]) * 4 * pi^2, 4),
                levels = seq(0, 2, 1 = 21))
  points(p[1], p[2], pch = 16)
  points(m[1], m[2], pch = 16)
}, j = slider(0, N))
## End(Not run)
```

dB∨m

Bivariate Sine von Mises density

Description

Evaluation of the bivariate Sine von Mises density and its normalizing constant.

Usage

```
dBvm(x, mu, kappa, logConst = NULL)
```

constBvm(M = 25, kappa)

Arguments

х	a matrix of size c(nx, 2) for evaluating the density.
mu	two-dimensional vector of circular means.
kappa	three-dimensional vector with concentrations $(\kappa_1, \kappa_2, \lambda)$.
logConst	logarithm of the normalizing constant. Computed if NULL.
М	number of terms considered in the series expansion used for evaluating the nor- malizing constant.

Details

If $\kappa_1 = 0$ or $\kappa_2 = 0$ and $\lambda \neq 0$, then constBvm will perform a Monte Carlo integration of the constant.

Value

A vector of length nx with the evaluated density (dBvm) or a scalar with the normaalizing constant (constBvm).

References

Singh, H., Hnizdo, V. and Demchuk, E. (2002) Probabilistic model for two dependent circular variables, *Biometrika*, 89(3):719–723, doi:10.1093/biomet/89.3.719

Examples

diffCirc

Lagged differences for circular time series

Description

Returns suitably lagged and iterated circular differences.

Usage

diffCirc(x, circular = TRUE, ...)

Arguments

x	wrapped or unwrapped angles to be differenced. Must be a vector or a matrix, see details.
circular	convenience flag to indicate whether wrapping should be done. If FALSE, the function is exactly diff.
	parameters to be passed to diff.

Details

If x is a matrix then the difference operations are carried out row-wise, on each column separately.

Value

The value of diff(x, ...), circularly wrapped. Default parameters give an object of the kind of x with one less entry or row.

Examples

dJp

Jones and Pewsey (2005)'s circular distribution

Description

Computes the circular density of Jones and Pewsey (2005).

Usage

dJp(x, mu, kappa, psi, const = NULL)
constJp(mu, kappa, psi, M = 200)

Arguments

x	evaluation angles, not necessary in $[\pi, \pi)$.
mu	circular mean.
kappa	non-negative concentration parameter.
psi	shape parameter, see details.
const	normalizing constant, computed with constJp if not provided.
М	grid size for computing the normalizing constant by numerical integration.

Details

Particular interesting choices for the shape parameter are:

- psi = -1: gives the Wrapped Cauchy as stationary density.
- psi = 0: is the sinusoidal drift of the vM diffusion.
- psi = 1: gives the Cardioid as stationary density.

Value

A vector of the same length as x containing the density.

References

Jones, M. C. and Pewsey, A. (2005). A family of symmetric distributions on the circle. *Journal of the American Statistical Association*, 100(472):1422–1428. doi:10.1198/01621450500000286

Examples

dPsTpd	Wrapped Euler and Shoji–Ozaki pseudo-transition probability densi-
	ties

Description

Wrapped pseudo-transition probability densities.

Usage

```
dPsTpd(x, x0, t, method = c("E", "SO", "SO2"), b, jac.b, sigma2, b1, b2,
circular = TRUE, maxK = 2, vmApprox = FALSE, twokpi = NULL, ...)
```

dPsTpd

Arguments

x	a matrix of dimension $c(n, p)$. If a vector is provided, is assumed that $p = 1$.
x0	a matrix of dimension $c(n, p)$. If all x0 are the same, a matrix of dimension $c(1, p)$ can be passed for better performance. If a vector is provided, is assumed that $p = 1$.
t	time step between x and x0.
method	a string for choosing "E" (Euler), "S0" (Shoji–Ozaki) or "S02" (Shoji–Ozaki with Ito's expansion in the drift) method.
b	drift function. Must return a matrix of the same size as x.
jac.b	jacobian of the drift function.
sigma2	diagonal of the diffusion matrix (if univariate, this is the square of the diffusion coefficient). Must return an object of the same size as x.
b1	first derivative of the drift function (univariate). Must return a vector of the same length as x.
b2	second derivative of the drift function (univariate). Must return a vector of the same length as x.
circular	flag to indicate circular data.
maxK	maximum absolute winding number used if circular = TRUE.
vmApprox	flag to indicate von Mises approximation to wrapped normal. See momentMatchWnVm and scoreMatchWnBvm.
twokpi	optional matrix of winding numbers to avoid its recomputation. See details.
	additional parameters passed to b, b1, b2, jac.b and sigma2.

Details

See Section 3.2 in García-Portugués et al. (2019) for details. "S02" implements Shoji and Ozai (1998)'s expansion with for p = 1. "S0" is the same expansion, for arbitrary p, but considering null second derivatives.

twokpi is repRow(2 * pi * c(-maxK:maxK), n = n) if p = 1 and as.matrix(do.call(what = expand.grid,args = rep(list(2 * pi * c(-maxK:maxK)), p))) otherwise.

Value

Output from mleOptimWrapper.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Shoji, I. and Ozaki, T. (1998) A statistical method of estimation and simulation for systems of stochastic differential equations. *Biometrika*, 85(1):240–243. doi:10.1093/biomet/85.1.240

Examples

```
# 1D
grid <- seq(-pi, pi, l = 501)[-501]
alpha <- 1
sigma <- 1
t <- 0.5
x0 <- pi/2
# manipulate::manipulate({
  # Drifts
  b <- function(x) driftWn1D(x = x, alpha = alpha, mu = 0, sigma = sigma)</pre>
  b1 <- function(x, h = 1e-4) {
    1 \le length(x)
    res <- driftWn1D(x = c(x + h, x - h), alpha = alpha, mu = 0,
                     sigma = sigma)
   drop(res[1:1] - res[(1 + 1):(2 * 1)])/(2 * h)
  }
  b2 <- function(x, h = 1e-4) \{
   1 <- length(x)
    res <- driftWn1D(x = c(x + h, x, x - h), alpha = alpha, mu = 0,
                     sigma = sigma)
    drop(res[1:1] - 2 * res[(1 + 1):(2 * 1)] +
          res[(2 * 1 + 1):(3 * 1)]) / (h^2)
  }
  # Squared diffusion
  sigma2 <- function(x) rep(sigma^2, length(x))</pre>
  # Plot
  plot(grid, dTpdPde1D(Mx = length(grid), x0 = x0, t = t, alpha = alpha,
                       mu = 0, sigma = sigma), type = "1",
       ylab = "Density", xlab = "", ylim = c(0, 0.75), lwd = 2)
  lines(grid, dTpdWou1D(x = grid, x0 = rep(x0, length(grid)), t = t,
                       alpha = alpha, mu = 0, sigma = sigma), col = 2)
  lines(grid, dPsTpd(x = grid, x0 = x0, t = t, method = "E", b = b,
                     b1 = b1, b2 = b2, sigma2 = sigma2), col = 3)
  lines(grid, dPsTpd(x = grid, x0 = x0, t = t, method = "S0", b = b,
                     b1 = b1, b2 = b2, sigma2 = sigma2), col = 4)
  lines(grid, dPsTpd(x = grid, x0 = x0, t = t, method = "S02", b = b,
                     b1 = b1, b2 = b2, sigma2 = sigma2),
        col = 5)
  lines(grid, dPsTpd(x = grid, x0 = x0, t = t, method = "E", b = b,
                     b1 = b1, b2 = b2, sigma2 = sigma2, vmApprox = TRUE),
        col = 6)
  lines(grid, dPsTpd(x = grid, x0 = x0, t = t, method = "S0", b = b,
                     b1 = b1, b2 = b2, sigma2 = sigma2, vmApprox = TRUE),
        col = 7)
  lines(grid, dPsTpd(x = grid, x0 = x0, t = t, method = "SO2", b = b,
                     b1 = b1, b2 = b2, sigma2 = sigma2, vmApprox = TRUE),
        col = 8)
  legend("topright", legend = c("PDE", "WOU", "E", "SO1", "SO2", "EvM",
                                "SO1vM", "SO2vM"), lwd = 2, col = 1:8)
```

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```
# }, x0 = manipulate::slider(-pi, pi, step = 0.1, initial = -pi),
# alpha = manipulate::slider(0.1, 5, step = 0.1, initial = 1),
# sigma = manipulate::slider(0.1, 5, step = 0.1, initial = 1),
# t = manipulate::slider(0.1, 5, step = 0.1, initial = 1))
# 2D
grid <- seq(-pi, pi, 1 = 76)[-76]
alpha1 <- 2
alpha2 <- 1
alpha3 <- 0.5
sig1 <- 1
sig2 <- 2
t <- 0.5
x01 <- pi/2
x02 <- -pi/2
# manipulate::manipulate({
 alpha <- c(alpha1, alpha2, alpha3)</pre>
 sigma <- c(sig1, sig2)</pre>
 x0 <- c(x01, x02)
 # Drifts
 b <- function(x) driftWn2D(x = x, A = alphaToA(alpha = alpha,</pre>
                                                  sigma = sigma),
                             mu = rep(0, 2), sigma = sigma)
 jac.b <- function(x, h = 1e-4) {
   1 <- nrow(x)
   res <- driftWn2D(x = rbind(cbind(x[, 1] + h, x[, 2]),</pre>
                                cbind(x[, 1] - h, x[, 2]),
                                cbind(x[, 1], x[, 2] + h),
                                cbind(x[, 1], x[, 2] - h)),
                     A = alphaToA(alpha = alpha, sigma = sigma),
                     mu = rep(0, 2), sigma = sigma)
    cbind(res[1:1, ] - res[(1 + 1):(2 * 1), ],
          res[2 * 1 + 1:1, ] - res[2 * 1 + (1 + 1):(2 * 1), ]) / (2 * h)
 }
 # Squared diffusion
 sigma2 <- function(x) matrix(sigma^2, nrow = length(x) / 2L, ncol = 2)</pre>
 # Plot
 old_par <- par(mfrow = c(3, 2))
 plotSurface2D(grid, grid, z = dTpdPde2D(Mx = length(grid),
                                           My = length(grid), x0 = x0,
                                           t = t, alpha = alpha,
                                           mu = rep(0, 2), sigma = sigma),
                levels = seq(0, 1, 1 = 20), main = "Exact")
 plotSurface2D(grid, grid,
                f = function(x) drop(dTpdWou2D(x = x,
                                                x0 = repRow(x0, nrow(x)),
                                                t = t, alpha = alpha,
                                                mu = rep(0, 2),
```

```
sigma = sigma)),
                levels = seq(0, 1, 1 = 20), fVect = TRUE, main = "WOU")
 plotSurface2D(grid, grid,
                f = function(x) dPsTpd(x = x, x0 = rbind(x0), t = t,
                                       method = "E", b = b, jac.b = jac.b,
                                       sigma2 = sigma2),
                levels = seq(0, 1, 1 = 20), fVect = TRUE, main = "E")
 plotSurface2D(grid, grid,
                f = function(x) dPsTpd(x = x, x0 = rbind(x0), t = t,
                                       method = "SO", b = b, jac.b = jac.b,
                                       sigma2 = sigma2),
                levels = seq(0, 1, 1 = 20), fVect = TRUE, main = "SO")
 plotSurface2D(grid, grid,
                f = function(x) dPsTpd(x = x, x0 = rbind(x0), t = t,
                                       method = "E", b = b, jac.b = jac.b,
                                       sigma2 = sigma2, vmApprox = TRUE),
                levels = seq(0, 1, 1 = 20), fVect = TRUE, main = "EvM")
 plotSurface2D(grid, grid,
                f = function(x) dPsTpd(x = x, x0 = rbind(x0), t = t,
                                       method = "SO", b = b, jac.b = jac.b,
                                       sigma2 = sigma2, vmApprox = TRUE),
                levels = seq(0, 1, 1 = 20), fVect = TRUE, main = "SOvM")
 par(old_par)
# }, x01 = manipulate::slider(-pi, pi, step = 0.1, initial = -pi),
# x02 = manipulate::slider(-pi, pi, step = 0.1, initial = -pi),
# alpha1 = manipulate::slider(0.1, 5, step = 0.1, initial = 1),
# alpha2 = manipulate::slider(0.1, 5, step = 0.1, initial = 1),
# alpha3 = manipulate::slider(-5, 5, step = 0.1, initial = 0),
# sig1 = manipulate::slider(0.1, 5, step = 0.1, initial = 1),
# sig2 = manipulate::slider(0.1, 5, step = 0.1, initial = 1),
# t = manipulate::slider(0.01, 5, step = 0.01, initial = 1))
```

driftJp

Drift for the JP diffusion

Description

Drift for the Langevin diffusion associated to the Jones and Pewsey (JP) family of circular distributions.

Usage

driftJp(x, alpha, mu, psi)

Arguments

х	vector with the evaluation points for the drift.
alpha	strength of the drift.
mu	unconditional mean of the diffusion.
psi	shape parameter, see details.

Details

Particular interesting choices for the shape parameter are:

- psi = -1: gives the Wrapped Cauchy as stationary density.
- psi = 0: is the sinusoidal drift of the vM diffusion.
- psi = 1: gives the Cardioid as stationary density.

See Section 2.2.3 in García-Portugués et al. (2019) for details.

Value

A vector of the same length as x containing the drift.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Jones, M. C. and Pewsey, A. (2005). A family of symmetric distributions on the circle. *Journal of the American Statistical Association*, 100(472):1422–1428. doi:10.1198/01621450500000286

Examples

driftMixIndVm Drift for the mivM diffusion

Description

Drift for the Langevin diffusion associated to a mixture of m independent (multivariate) von Mises (mivM) of dimension p.

Usage

```
driftMixIndVm(x, A, M, sigma, p, expTrc = 30)
```

Arguments

x	matrix of size c(n, p) with the evaluation points for the drift.
A	matrix of size c(m, p) giving the strengths of the drifts.
Μ	matrix of size c(m, p) giving the means.
sigma	diffusion coefficient.
р	vector of length m giving the proportions. Must add to one.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Details

driftMixVm is more efficient for the circular case. The diffusion matrix is σI . See Section 2.2.4 in García-Portugués et al. (2019) for details.

Value

A matrix of the same size as x containing the drift.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

driftMixVm

Description

Drift for the Langevin diffusion associated to a mixture of m independent von Mises (mivM) of dimension one.

Usage

driftMixVm(x, alpha, mu, sigma, p, expTrc = 30)

Arguments

х	vector with the evaluation points for the drift.
alpha	vector of length m giving the strengths of the drifts.
mu	vector of length m giving the means.
sigma	diffusion coefficient.
р	vector of length m giving the proportions. Must add to one.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Details

driftMixIndVm is more general, but less efficient for the circular case. See Section 2.2.4 in García-Portugués et al. (2019) for details.

Value

A vector of the same length as x containing the drift.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

driftMvm

Description

Drift for the Langevin diffusion associated to the Multivariate von Mises (MvM) in dimension p.

Usage

driftMvm(x, alpha, mu, A = 0)

Arguments

х	matrix of size c(n, p) with the evaluation points for the drift.
alpha	vector of length p with the strength of the drift in the diagonal (sin terms).
mu	vector of length p with the unconditional mean of the diffusion.
А	matrix of size c(p, p) with the strength of the drift in cross terms (cos-sin
	terms). The diagonal has to be zero.

Details

See Section 2.2.1 in García-Portugués et al. (2019) for details.

Value

A matrix of the same size as x containing the drift.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

driftWn

Description

Drift for the Langevin diffusion associated to the (multivariate) Wrapped Normal (WN) in dimension p.

Usage

```
driftWn(x, A, mu, Sigma, invSigmaA = NULL, maxK = 2, expTrc = 30)
```

Arguments

х	matrix of size c(n, p) with the evaluation points for the drift.
Α	matrix of size c(p, p) giving the drift strength.
mu	vector of length p with the unconditional mean of the diffusion.
Sigma	diffusion matrix, of size c(p, p).
invSigmaA	the matrix solve(Sigma) %*% A (optional).
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Details

See Section 2.2.2 in García-Portugués et al. (2019) for details.

driftWn1D and driftWn2D are more efficient for the 1D and 2D cases.

Value

A matrix of the same size as x containing the drift.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Examples

```
driftWn1D
```

Drift of the WN diffusion in 1D

Description

Computes the drift of the WN diffusion in 1D in a vectorized way.

Usage

```
driftWn1D(x, alpha, mu, sigma, maxK = 2L, expTrc = 30)
```

Arguments

x	a vector of length n containing angles. They all must be in $[\pi, \pi)$ so that the truncated wrapping by maxK windings is able to capture periodicity.
alpha	drift parameter.
mu	mean parameter. Must be in $[\pi, \pi)$.
sigma	diffusion coefficient.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

A vector of length n containing the drift evaluated at x.

Examples

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driftWn2D

Description

Computes the drift of the WN diffusion in 2D in a vectorized way.

Usage

driftWn2D(x, A, mu, sigma, rho = 0, maxK = 2L, expTrc = 30)

Arguments

x	a matrix of dimension c(n, 2) containing angles. They all must be in $[\pi, \pi)$ so that the truncated wrapping by maxK windings is able to capture periodicity.
А	drift matrix of size c(2, 2).
mu	a vector of length 2 giving the mean.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

A matrix of size c(n, 2) containing the drift evaluated at x.

```
alpha <- 3:1
mu <- c(0, 0)
sigma <- 1:2
rho <- 0.5
Sigma <- diag(sigma^2)
Sigma[1, 2] <- Sigma[2, 1] <- rho * prod(sigma)
A <- alphaToA(alpha = alpha, sigma = sigma, rho = rho)
x <- rbind(c(0, 1), c(1, 0.1), c(pi, pi), c(-pi, -pi), c(pi / 2, 0))
driftWn2D(x = x, A = A, mu = mu, sigma = sigma, rho = rho)
driftWn(x = x, A = A, mu = c(0, 0), Sigma = Sigma)</pre>
```

dStatWn2D

Description

Stationary density of the WN diffusion.

Usage

```
dStatWn2D(x, alpha, mu, sigma, rho = 0, maxK = 2L, expTrc = 30)
```

Arguments

x	a matrix of dimension c(n, 2) containing angles. They all must be in $[\pi, \pi)$ so that the truncated wrapping by maxK windings is able to capture periodicity.
alpha	vector of length 3 parametrizing the A matrix as in alphaToA.
mu	a vector of length 2 giving the mean.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

A vector of size n containing the stationary density evaluated at x.

dTpdMou

Description

Transition probability density of the multivariate Ornstein-Uhlenbeck (OU) diffusion

$$dX_t = A(\mu - X_t)dt + \Sigma^{\frac{1}{2}}dW_t, X_0 = x_0.$$

Usage

dTpdMou(x, x0, t, A, mu, Sigma, eigA = NULL, log = FALSE)
meantMou(t, x0, A, mu, eigA = NULL)
covtMou(t, A, Sigma, eigA = NULL)

Arguments

x	matrix of with p columns containing the evaluation points.
xØ	initial point.
t	time between observations.
A	the drift matrix, of size c(p, p).
mu	unconditional mean of the diffusion.
Sigma	square of the diffusion matrix, a matrix of size c(p, p).
eigA	optional argument containing eigen(A) for reuse.
log	flag to indicate whether to compute the logarithm of the density.

Details

The transition probability density is a multivariate normal with mean meantMou and covariance covtMou. See dTpdOu for the univariate case (more efficient).

solve(A) %*% Sigma has to be a covariance matrix (symmetric and positive definite) in order to have a proper transition density. For the bivariate case, this can be ensured with the alphaToA function. In the multivariate case, it is ensured if Sigma is isotropic and A is a covariance matrix.

Value

A matrix of the same size as x containing the evaluation of the density.

Examples

dTpd0u

Transition probability density of the univariate OU diffusion

Description

Transition probability density of the univariate Ornstein-Uhlenbeck (OU) diffusion

 $dX_t = \alpha(\mu - X_t)dt + \sigma dW_t, X_0 = x_0.$

Usage

```
dTpdOu(x, x0, t, alpha, mu, sigma, log = FALSE)
meantOu(x0, t, alpha, mu)
vartOu(t, alpha, sigma)
covstOu(s, t, alpha, sigma)
```

Arguments

х	vector with the evaluation points.
x0	initial point.
t,s	time between observations.
alpha	strength of the drift.
mu	unconditional mean of the diffusion.
sigma	diffusion coefficient.
log	flag to indicate whether to compute the logarithm of the density.

Details

The transition probability density is a normal density with mean meantOu and variance vartOu. See dTpdMou for the multivariate case (less efficient for dimension one).

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dTpdPde1D

Value

A vector of the same length as x containing the evaluation of the density.

Examples

```
x <- seq(-4, 4, by = 0.01)
plot(x, dTpdOu(x = x, x0 = 3, t = 0.1, alpha = 1, mu = -1, sigma = 1),
    type = "1", ylim = c(0, 1.5), xlab = "x", ylab = "Density",
    col = rainbow(20)[1])
for (i in 2:20) {
    lines(x, dTpdOu(x = x, x0 = 3, t = i / 10, alpha = 1, mu = -1, sigma = 1),
        col = rainbow(20)[i])
}</pre>
```

dTpdPde1D

Transition probability density in 1D by PDE solving

Description

Computation of the transition probability density (tpd) of the Wrapped Normal (WN) or von Mises (vM) diffusion, by solving its associated Fokker–Planck Partial Differential Equation (PDE) in 1D.

Usage

```
dTpdPde1D(Mx = 500, x0, t, alpha, mu, sigma, type = "WN",
    Mt = ceiling(100 * t), sdInitial = 0.1, ...)
```

Arguments

Mx	size of the equispaced spatial grid in $[-\pi, \pi)$.
x0	point giving the mean of the initial circular density, a WN with standard deviation equal to sdInitial.
t	time separating x0 and the evaluation of the tpd.
alpha	drift parameter.
mu	mean parameter. Must be in $[\pi, \pi)$.
sigma	diffusion coefficient.
type	either "WN" or "vM".
Mt	size of the time grid in $[0, t]$.
sdInitial	the standard deviation of the concentrated WN giving the initial condition.
	Further parameters passed to crankNicolson1D.

Details

A combination of small sdInitial and coarse space-time discretization (small Mx and Mt) is prone to create numerical instabilities. See Sections 3.4.1, 2.2.1 and 2.2.2 in García-Portugués et al. (2019) for details.

Value

A vector of length Mx with the tpd evaluated at seq(-pi, pi, 1 = Mx + 1)[-(Mx + 1)].

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Examples

```
Mx <- 100
x \le seq(-pi, pi, 1 = Mx + 1)[-c(Mx + 1)]
x0 <- pi
t <- 0.5
alpha <- 1
mu <- 0
sigma <- 1
isRStudio <- identical(.Platform$GUI, "RStudio")</pre>
if (isRStudio) {
  manipulate::manipulate({
  plot(x, dTpdPde1D(Mx = Mx, x0 = x0, t = t, alpha = alpha, mu = 0,
                    sigma = sigma), type = "l", ylab = "Density",
       xlab = "", ylim = c(0, 0.75))
  lines(x, dTpdWou1D(x = x, x0 = rep(x0, Mx), t = t, alpha = alpha, mu = 0,
                      sigma = sigma), col = 2)
  }, x0 = manipulate::slider(-pi, pi, step = 0.01, initial = 0),
  alpha = manipulate::slider(0.01, 5, step = 0.01, initial = 1),
  sigma = manipulate::slider(0.01, 5, step = 0.01, initial = 1),
  t = manipulate::slider(0.01, 5, step = 0.01, initial = 1))
}
```

dTpdPde2D

```
Transition probability density in 2D by PDE solving
```

Description

Computation of the transition probability density (tpd) of the Wrapped Normal (WN) or Multivariate von Mises (MvM) diffusion, by solving its associated Fokker–Planck Partial Differential Equation (PDE) in 2D.

Usage

```
dTpdPde2D(Mx = 50, My = 50, x0, t, alpha, mu, sigma, rho = 0,
    type = "WN", Mt = ceiling(100 * t), sdInitial = 0.1, ...)
```

dTpdPde2D

Arguments

Mx, My	sizes of the equispaced spatial grids in $[-\pi, \pi)$ for each component.
x0	point giving the mean of the initial circular density, an isotropic WN with stan- dard deviations equal to sdInitial.
t	time separating $x0$ and the evaluation of the tpd.
alpha	for "WN", a vector of length 3 parametrizing the A matrix as in alphaToA. For "vM", a vector of length 3 containing c(alpha[1:2], A[1, 2]), from the arguments alpha and A in driftMvm.
mu	vector of length 2 giving the mean.
sigma	for "WN", a vector of length 2 containing the square root of the diagonal of the diffusion matrix. For "vM", the standard deviation giving the isotropic diffusion matrix.
rho	for "WN", the correlation of the diffusion matrix.
type	either "WN" or "vM".
Mt	size of the time grid in $[0, t]$.
sdInitial	standard deviations of the concentrated WN giving the initial condition.
	Further parameters passed to crankNicolson2D.

Details

A combination of small sdInitial and coarse space-time discretization (small Mx and Mt) is prone to create numerical instabilities. See Sections 3.4.2, 2.2.1 and 2.2.2 in García-Portugués et al. (2019) for details.

Value

A matrix of size c(Mx, My) with the tpd evaluated at the combinations of seq(-pi, pi, 1 = Mx + 1)[-(Mx + 1)] and seq(-pi, pi, 1 = My + 1)[-(My + 1)].

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

dTpdWou

Description

Conditional probability density of the Wrapped Ornstein-Uhlenbeck (WOU) process.

Usage

```
dTpdWou(x, t, A, mu, Sigma, x0, maxK = 2, eigA = NULL, invASigma = NULL)
```

Arguments

matrix of size c(n, p) with the evaluation points in $[-\pi, \pi)^p$.
a scalar containing the times separating x and $x0$.
matrix of size c(p, p) giving the drift strength.
mean parameter. Must be in $[\pi, \pi)$.
diffusion matrix, of size c(p, p).
vector of length p with the initial point in $[-\pi, \pi)^p$.
maximum absolute value of the windings considered in the computation of the WN.
optional argument containing eigen(A) for reuse.
the matrix solve(Sigma) %*% A (optional).

Details

See Section 3.3 in García-Portugués et al. (2019) for details. dTpdWou1D and dTpdWou2D are more efficient implementations for the 1D and 2D cases, respectively.

Value

A vector of length n with the density evaluated at x.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

dTpdWou1D

Examples

```
# 1D
t <- 0.5
alpha <- 1
mu <- 0
sigma <- 1
x0 <- pi
x <- seq(-pi, pi, l = 10)
dTpdWou(x = cbind(x), x0 = x0, t = t, A = alpha, mu = 0, Sigma = sigma^2) -
dTpdWou1D(x = cbind(x), x0 = rep(x0, 10), t = t, alpha = alpha, mu = 0,
          sigma = sigma)
# 2D
t <- 0.5
alpha <- c(2, 1, -1)
sigma <- c(1.5, 2)
rho <- 0.9
Sigma <- diag(sigma^2)</pre>
Sigma[1, 2] <- Sigma[2, 1] <- rho * prod(sigma)</pre>
A <- alphaToA(alpha = alpha, sigma = sigma, rho = rho)
mu <- c(pi, 0)
x0 <- c(0, 0)
x <- seq(-pi, pi, 1 = 5)
x <- as.matrix(expand.grid(x, x))</pre>
dTpdWou(x = x, x0 = x0, t = t, A = A, mu = mu, Sigma = Sigma) -
dTpdWou2D(x = x, x0 = rbind(x0), t = t, alpha = alpha, mu = mu,
          sigma = sigma, rho = rho)
```

dTpdWou1D	Approximation of the transition probability density of the WN diffusion
	in 1D

Description

Computation of the transition probability density (tpd) for a WN diffusion.

Usage

dTpdWou1D(x, x0, t, alpha, mu, sigma, maxK = 2L, expTrc = 30, vmApprox = 0L, kt = 0, logConstKt = 0)

Arguments

x	a vector of length n containing angles. They all must be in $[\pi, \pi)$ so that the truncated wrapping by maxK windings is able to capture periodicity.
x0	a vector of length n containing the starting angles. They all must be in $[\pi, \pi)$.
t	a scalar containing the times separating x and $x0$.
alpha	drift parameter.

mu	mean parameter. Must be in $[\pi, \pi)$.
sigma	diffusion coefficient.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.
vmApprox	whether to use the von Mises approximation to a wrapped normal (1) or not (0 , default).
kt	concentration for the von Mises, a suitable output from momentMatchWnVm (see examples).
logConstKt	the logarithm of the von Mises normalizing constant associated to the concen- tration kt (see examples)

Details

See Section 3.3 in García-Portugués et al. (2019) for details. See dTpdWou for the general case (less efficient for 2D).

Value

A vector of size n containing the tpd evaluated at x.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

dTpdWou2D

Description

Computation of the transition probability density (tpd) for a WN diffusion (with diagonal diffusion matrix)

Usage

```
dTpdWou2D(x, x0, t, alpha, mu, sigma, rho = 0, maxK = 2L, expTrc = 30)
```

Arguments

x	a matrix of dimension c(n, 2) containing angles. They all must be in $[\pi, \pi)$ so that the truncated wrapping by maxK windings is able to capture periodicity.
ר	a matrix of dimension $c(n, 2)$ containing the starting angles. They all must be in $[\pi, \pi)$. If all x0 are the same, a matrix of dimension $c(1, 2)$ can be passed for better performance.
t	a scalar containing the times separating x and x0.
alpha	vector of length 3 parametrizing the A matrix as in alphaToA.
mu	a vector of length 2 giving the mean.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Details

The function checks for positive definiteness. If violated, it resets A such that solve(A) %*% Sigma is positive definite.

See Section 3.3 in García-Portugués et al. (2019) for details. See dTpdWou for the general case (less efficient for 1D).

Value

A vector of size n containing the tpd evaluated at x.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

```
set.seed(3455267)
alpha <- c(2, 1, -1)
sigma <- c(1.5, 2)
rho <- 0.9
Sigma <- diag(sigma^2)</pre>
Sigma[1, 2] <- Sigma[2, 1] <- rho * prod(sigma)</pre>
A <- alphaToA(alpha = alpha, sigma = sigma, rho = rho)
solve(A) %*% Sigma
mu <- c(pi, 0)
x <- t(euler2D(x0 = matrix(c(0, 0), nrow = 1), A = A, mu = mu,</pre>
               sigma = sigma, N = 500, delta = 0.1)[1, , ])
sum(sapply(1:49, function(i) log(dTpdWou(x = matrix(x[i + 1, ], ncol = 2)))
                                          x0 = x[i, ], t = 1.5, A = A,
                                          Sigma = Sigma, mu = mu))))
sum(log(dTpdWou2D(x = matrix(x[2:50, ], ncol = 2),
                  x0 = matrix(x[1:49, ], ncol = 2), t = 1.5, alpha = alpha,
                  mu = mu, sigma = sigma, rho = rho)))
lgrid <- 56
grid <- seq(-pi, pi, l = lgrid + 1)[-(lgrid + 1)]
image(grid, grid, matrix(dTpdWou(x = as.matrix(expand.grid(grid, grid)),
                                  x0 = c(0, 0), t = 0.5, A = A,
                                  Sigma = Sigma, mu = mu),
                         nrow = 56, ncol = 56), zlim = c(0, 0.25),
      main = "dTpdWou")
image(grid, grid, matrix(dTpdWou2D(x = as.matrix(expand.grid(grid, grid)),
                                    x0 = matrix(0, nrow = 56^{2}, ncol = 2),
                                    t = 0.5, alpha = alpha, sigma = sigma,
                                   mu = mu),
                          nrow = 56, ncol = 56), zlim = c(0, 0.25),
      main = "dTpdWou2D")
x <- seq(-pi, pi, l = 100)
t <- 1
image(x, x, matrix(dTpdWou2D(x = as.matrix(expand.grid(x, x)),
                             x0 = matrix(rep(0, 100 * 2), nrow = 100 * 100,
                                          ncol = 2),
                              t = t, alpha = alpha, mu = mu, sigma = sigma,
                              maxK = 2, expTrc = 30),
                             nrow = 100, ncol = 100),
      zlim = c(0, 0.25))
points(stepAheadWn2D(x0 = rbind(c(0, 0)), delta = t / 500,
                     A = alphaToA(alpha = alpha, sigma = sigma), mu = mu,
```
```
sigma = sigma, N = 500, M = 1000, maxK = 2,
expTrc = 30))
```

dVm

Density of the von Mises

Description

Computes the density of a von Mises in a numerically stable way.

Usage

dVm(x, mu, kappa)

Arguments

х	evaluation angles, not necessary in $[\pi, \pi)$.
mu	circular mean.
kappa	non-negative concentration parameter.

Value

A vector of the same length as x containing the density.

References

Jammalamadaka, S. R. and SenGupta, A. (2001) *Topics in Circular Statistics*. World Scientific, Singapore. doi:10.1142/4031

```
x <- seq(-pi, pi, l = 200)
plot(x, x, type = "n", ylab = "Density", ylim = c(0, 1))
for (i in 0:20) {
    lines(x, dVm(x = x, mu = 0, kappa = 5 * i / 20),
        col = rainbow(21)[i + 1])
}</pre>
```

dWn1D

Description

Computation of the WN density in 1D.

Usage

```
dWn1D(x, mu, sigma, maxK = 2L, expTrc = 30, vmApprox = 0L, kt = 0,
logConstKt = 0)
```

Arguments

x	a vector of length n containing angles. They all must be in $[\pi, \pi)$ so that the truncated wrapping by maxK windings is able to capture periodicity.
mu	mean parameter. Must be in $[\pi, \pi)$.
sigma	diffusion coefficient.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.
vmApprox	whether to use the von Mises approximation to a wrapped normal (1) or not $(0, default)$.
kt	concentration for the von Mises, a suitable output from momentMatchWnVm (see examples).
logConstKt	the logarithm of the von Mises normalizing constant associated to the concen- tration kt (see examples)

Value

A vector of size n containing the density evaluated at x.

euler1D

Description

Simulation of the Wrapped Normal (WN) diffusion or von Mises (vM) diffusion by the Euler method in 1D, for several starting values.

Usage

```
euler1D(x0, alpha, mu, sigma, N = 100L, delta = 0.01, type = 1L,
maxK = 2L, expTrc = 30)
```

Arguments

x0	vector of length nx0 giving the initial points.
alpha	drift parameter.
mu	mean parameter. Must be in $[\pi, \pi)$.
sigma	diffusion coefficient.
Ν	number of discretization steps.
delta	discretization step.
type	integer giving the type of diffusion. Currently, only 1 for WN and 2 for vM are supported.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

A matrix of size c(nx0, N+1) containing the nx0 discretized trajectories. The first column corresponds to the vector x0.

```
euler2D
```

Description

Simulation of the Wrapped Normal (WN) diffusion or Multivariate von Mises (MvM) diffusion by the Euler method in 2D, for several starting values.

Usage

```
euler2D(x0, A, mu, sigma, rho = 0, N = 100L, delta = 0.01, type = 1L,
maxK = 2L, expTrc = 30)
```

Arguments

x0	matrix of size $c(nx0, 2)$ giving the initial points.
A	drift matrix of size c(2, 2).
mu	a vector of length 2 giving the mean.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
Ν	number of discretization steps.
delta	discretization step.
type	integer giving the type of diffusion. Currently, only 1 for WN and 2 for vM are supported.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

An array of size c(nx0, 2, N + 1) containing the nx0 discretized trajectories. The first slice corresponds to the matrix x0.

linesCirc

linesCirc

Lines and arrows with vertical wrapping

Description

Joins the corresponding points with line segments or arrows that exhibit wrapping in $[-\pi, \pi)$ in the vertical axis.

Usage

linesCirc(x = seq_along(y), y, col = 1, lty = 1, ltyCross = lty, arrows = FALSE, ...)

Arguments

х	vector with horizontal coordinates.
У	vector with vertical coordinates, wrapped in $[-\pi, \pi)$.
col	color vector of length 1 or the same length of x and y .
lty	line type as in par.
ltyCross	specific line type for crossing segments.
arrows	flag for drawing arrows instead of line segments.
	further graphical parameters passed to segments or arrows.

Details

y is wrapped to $[-\pi, \pi)$ before plotting.

Value

Nothing. The functions are called for drawing wrapped lines.

```
x <- 1:100
y <- toPiInt(pi * cos(2 * pi * x / 100) + 0.5 * runif(50, -pi, pi))
plot(x, y, ylim = c(-pi, pi))
linesCirc(x = x, y = y, col = rainbow(length(x)), ltyCross = 2)
plot(x, y, ylim = c(-pi, pi))
linesCirc(x = x, y = y, col = rainbow(length(x)), arrows = TRUE)
```

```
linesTorus
```

Description

Joins the corresponding points with line segments or arrows that exhibit wrapping in $[-\pi, \pi)$ in the horizontal and vertical axes.

Usage

```
linesTorus(x, y, col = 1, lty = 1, ltyCross = lty, arrows = FALSE, ...)
```

Arguments

х	vector with horizontal coordinates, wrapped in $[-\pi, \pi)$.
У	vector with vertical coordinates, wrapped in $[-\pi, \pi)$.
col	color vector of length 1 or the same length of x and y .
lty	line type as in par.
ltyCross	specific line type for crossing segments.
arrows	flag for drawing arrows instead of line segments.
	further graphical parameters passed to segments or arrows.

Details

x and y are wrapped to $[-\pi, \pi)$ before plotting.

Value

Nothing. The functions are called for drawing wrapped lines.

```
x <- toPiInt(rnorm(50, mean = seq(-pi, pi, l = 50), sd = 0.5))
y <- toPiInt(x + rnorm(50, mean = seq(-pi, pi, l = 50), sd = 0.5))
plot(x, y, xlim = c(-pi, pi), ylim = c(-pi, pi), col = rainbow(length(x)),
    pch = 19)
linesTorus(x = x, y = y, col = rainbow(length(x)), ltyCross = 2)
plot(x, y, xlim = c(-pi, pi), ylim = c(-pi, pi), col = rainbow(length(x)),
    pch = 19)
linesTorus(x = x, y = y, col = rainbow(length(x)), arrows = TRUE)
```

linesTorus3d

Description

Joins the corresponding points with line segments or arrows that exhibit wrapping in $[-\pi, \pi)$ in the horizontal and vertical axes.

Usage

linesTorus3d(x, y, z, col = 1, arrows = FALSE, ...)

Arguments

х, у	vectors with horizontal coordinates, wrapped in $[-\pi, \pi)$.
z	vector with vertical coordinates, wrapped in $[-\pi, \pi)$.
col	color vector of length 1 or the same length of x , y , and z .
arrows	flag for drawing arrows instead of line segments.
	further graphical parameters passed to segments or arrows.

Details

x, y, and z are wrapped to $[-\pi,\pi)$ before plotting. arrows = TRUE makes sequential calls to arrow3d, and is substantially slower than arrows = FALSE.

Value

Nothing. The functions are called for drawing wrapped lines.

```
if (requireNamespace("rgl")) {
 n <- 20
 x \leftarrow toPiInt(rnorm(n, mean = seq(-pi, pi, 1 = n), sd = 0.5))
 y \le toPiInt(rnorm(n, mean = seq(-pi, pi, 1 = n), sd = 0.5))
 z \leftarrow toPiInt(x + y + rnorm(n, mean = seq(-pi, pi, 1 = n), sd = 0.5))
 rgl::plot3d(x, y, z, xlim = c(-pi, pi), ylim = c(-pi, pi),
              zlim = c(-pi, pi), col = rainbow(n), size = 2,
              box = FALSE, axes = FALSE)
 linesTorus3d(x = x, y = y, z = z, col = rainbow(n), lwd = 2)
 torusAxis3d()
 rgl::plot3d(x, y, z, xlim = c(-pi, pi), ylim = c(-pi, pi),
              zlim = c(-pi, pi), col = rainbow(n), size = 2,
              box = FALSE, axes = FALSE)
 linesTorus3d(x = x, y = y, z = z, col = rainbow(n), ltyCross = 2,
               arrows = TRUE, theta = 0.1 \times pi / 180, barblen = 0.1)
 torusAxis3d()
```

}

logBesselI0Scaled Efficient computation of Bessel related functions

Description

```
Computation of \log(I_0(x)) - x and the inverse of A_1(k) = \frac{I_0(k)}{I_1(k)}.
```

Usage

```
logBesselI0Scaled(x, splineApprox = TRUE)
```

```
a1Inv(x, splineApprox = TRUE)
```

Arguments

х	evaluation vector. For logBesselI0Scaled, x must contain non-negative val-
	ues. For allnv, x must be in $[0, 1]$.
splineApprox	whether to use a pre-computed spline approximation (faster) or not.

Details

Both functions may rely on pre-computed spline interpolations (logBesselI0ScaledSpline and alInvSpline). Otherwise, a call to besselI is done for $\log(I_0(x)) - x$ and $A_1(k) = x$ is solved numerically. The data in which the interpolation is based is given in the examples.

For x larger than 5e4, the asymptotic expansion of bessellasym is employed.

Value

A vector of the same length as x.

logLikWouPairs

```
alInvEvalGrid <- sapply(x2, function(k) {
  uniroot(f = function(x) k - bessell(x, nu = 1, expon.scaled = TRUE) /
        besselI(x, nu = 0, expon.scaled = TRUE),
        lower = 1e-06, upper = 1e+05, tol = 1e-15)$root
})
# save(list = "alInvEvalGrid", file = "alInvEvalGrid.rda", compress = TRUE)
# Accuracy logBesselI0Scaled
x <- seq(0, 1e3, l = 1e3)
summary(logBesselI0Scaled(x = x, splineApprox = TRUE) -
        logBesselI0Scaled(x = x, splineApprox = FALSE))
# Accuracy alInv
y <- seq(0, 1 - 1e-4, l = 1e3)
summary(alInv(x = y, splineApprox = TRUE) -
        alInv(x = y, splineApprox = FALSE))</pre>
```

```
logLikWouPairs Loglikelihood of WN in 2D when only the initial and final points are observed
```

Description

Computation of the loglikelihood for a WN diffusion (with diagonal diffusion matrix) from a sample of initial and final pairs of angles.

Usage

```
logLikWouPairs(x, t, alpha, mu, sigma, rho = 0, maxK = 2L, expTrc = 30)
```

Arguments

x	a matrix of dimension c(n, 4) of initial and final pairs of angles. Each row is an observation containing $(\phi_0, \psi_0, \phi_t, \psi_t)$. They all must be in $[\pi, \pi)$ so that the truncated wrapping by maxK windings is able to capture periodicity.
t	either a scalar or a vector of length n containing the times the initial and final dihedrals. If t is a scalar, a common time is assumed.
alpha	vector of length 3 parametrizing the A matrix as in alphaToA.
mu	a vector of length 2 giving the mean.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Details

A negative penalty is added if positive definiteness is violated. If the output value is Inf, -100 * N is returned instead.

Value

A scalar giving the final loglikelihood, defined as the sum of the loglikelihood of the initial angles according to the stationary density and the loglikelihood of the transitions from initial to final angles.

Examples

mleMou

Maximum likelihood estimation of the multivariate OU diffusion

Description

Computation of the maximum likelihood estimator of the parameters of the *multivariate* Ornstein–Uhlenbeck (OU) diffusion from a discretized trajectory $\{X_{\Delta i}\}_{i=1}^{N}$. The objective function to minimize is

$$\sum_{i=2}^{n} \log p_{\Delta}(X_{\Delta i} | X_{\Delta(i-1)}).$$

Usage

```
mleMou(data, delta, alpha = rep(NA, 3), mu = rep(NA, 2), sigma = rep(NA,
2), start, lower = c(0.01, 0.01, -25, -pi, -pi, 0.01, 0.01),
upper = c(25, 25, 25, pi, pi, 25, 25), ...)
```

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mleOptimWrapper

Arguments

data	a matrix of size c(N, p) with the discretized trajectory of the diffusion.
delta	time discretization step.
alpha, mu, sigma	
	arguments to fix a parameter to a given value and perform the estimation on the rest. Defaults to NA, meaning that the parameter is estimated. Note that start, lower and upper must be changed accordingly if parameters are fixed, see examples.
start	starting values, a matrix with p columns, with each entry representing a different starting value.
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
	further arguments to be passed to mleOptimWrapper.

Details

The first row in data is not taken into account for estimation. See mleOu for the univariate case (more efficient).

mleMou only handles p = 2 currently. It imposes that Sigma is diagonal and handles the parametrization of A by alphaToA.

Value

Output from mleOptimWrapper.

Examples

mleOptimWrapper Optimization wrapper for likelihood-based procedures

Description

A convenient wrapper to perform local optimization of the likelihood function via nlm and optim including several practical utilities.

```
mleOptimWrapper(minusLogLik, region = function(pars) list(pars = pars,
    penalty = 0), penalty = 1e+10, optMethod = "Nelder-Mead", start,
    lower = rep(-Inf, ncol(start)), upper = rep(Inf, ncol(start)),
    selectSolution = "lowestLocMin", checkCircular = TRUE, maxit = 500,
    tol = 1e-05, verbose = 0, eigTol = 1e-04, condTol = 10000, ...)
```

Arguments

minusLogLik	function computing the minus log-likelihood function. Must have a single argument containing a vector of length p.
region	function to impose a feasibility region via a penalty. See details.
penalty	imposed penalty if value is not finite.
optMethod	one of the following strings: "nlm", "Nelder-Mead", "BFGS", "CG", "L-BFGS-B", "SANN", or "Brent".
start	starting values, a matrix with p columns, with each entry representing a different starting value.
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
selectSolution	which criterion is used for selecting a solution among possible ones, either "lowest", "lowestConv" or "lowestLocMin". "lowest" returns the solution with lowest value in the minusLogLik function. "lowestConv" restricts the search of the best solution among the ones for which the optimizer has converged. "lowestLocMin" in addition imposes that the solution is guaranteed to be a local minimum by examining the Hessian matrix.
checkCircular	logical indicating whether to automatically treat the variables with lower and upper entries equal to -pi and pi as circular. See details.
maxit	maximum number of iterations.
tol	tolerance for convergence (passed to reltol, pgtol or gradtol).
verbose	an integer from 0 to 2 if optMethod = "Nelder-Mead" or from 0 to 4 otherwise giving the amount of information displayed.
eigTol, condTol	
	eigenvalue and condition number tolerance for the Hessian in order to guarantee a local minimum. Used only if selectSolution = "lowestLocMin".
	further arguments passed to the optMethod selected. See options in nlm or optim.

Details

If checkCircular = TRUE, then the corresponding lower and upper entries of the circular parameters are set to -Inf and Inf, respectively, and minusLogLik is called with the *principal value* of the circular argument.

If no solution is found satisfying the criterion in selectSolution, NAs are returned in the elements of the main solution.

The Hessian is only computed if selectSolution = "lowestLocMin".

mleOptimWrapper

Region feasibility can be imposed by a function with the same arguments as minusLogLik that resets pars in to the boundary of the feasibility region and adds a penalty proportional to the violation of the feasibility region. Note that this is *not the best procedure at all* to solve the constrained optimization problem, but just a relatively flexible and quick approach (for a more advanced treatment of restrictions, see optimization-focused packages). The value must be a list with objects pars and penalty. By default no region is imposed, i.e., region = function(pars) list("pars" = pars, "penalty" = 0). Note that the Hessian is computed from the unconstrained problem, hence localMinimumGuaranteed might be FALSE even if a local minimum to the constrained problem was found.

Value

A list containing the following elements:

- par: estimated minimizing parameters
- value: value of minusLogLik at the minimum.
- convergence: if the optimizer has converged or not.
- message: a character string giving any additional information returned by the optimizer.
- eigHessian: eigenvalues of the Hessian at the minimum. Recall that for the same solution slightly different outputs may be obtained according to the different computations of the Hessian of nlm and optim.
- localMinimumGuaranteed: tests if the Hessian is positive definite (all eigenvalues larger than the tolerance eigTol and condition number smaller than condTol).
- solutionsOutput: a list containing the complete output of the selected method for the different starting values. It includes the extra objects convergence and localMinimumGuaranteed.

```
# No local minimum
head(mleOptimWrapper(minusLogLik = function(x) - sum((x - 1:4)^2),
                     start = rbind(10:13, 1:2), selectSolution = "lowest"))
head(mleOptimWrapper(minusLogLik = function(x) - sum((x - 1:4)^2),
                     start = rbind(10:13, 1:2),
                     selectSolution = "lowestConv"))
head(mleOptimWrapper(minusLogLik = function(x) - sum((x - 1:4)^2),
                     start = rbind(10:13, 1:2),
                     selectSolution = "lowestLocMin"))
# Local minimum
head(mleOptimWrapper(minusLogLik = function(x) sum((x - 1:4)^2),
                     start = rbind(10:13), optMethod = "BFGS"))
head(mleOptimWrapper(minusLogLik = function(x) sum((x - 1:4)<sup>2</sup>),
                     start = rbind(10:13), optMethod = "Nelder-Mead"))
# Function with several local minimum and a 'spurious' one
f <- function(x) 0.75 * (x[1] - 1)^2 -
                  10 / (0.1 + 0.1 * ((x[1] - 15)^2 + (x[2] - 2)^2)) -
                  9.5 / (0.1 + 0.1 * ((x[1] - 15)^2 + (x[2] + 2)^2))
plotSurface2D(x = seq(0, 20, 1 = 100), y = seq(-3, 3, 1 = 100), f = f)
```

```
head(mleOptimWrapper(minusLogLik = f,
                     start = rbind(c(15, 2), c(15, -2), c(5, 0)),
                     selectSolution = "lowest"))
head(mleOptimWrapper(minusLogLik = f,
                     start = rbind(c(15, 2), c(15, -2), c(5, 0)),
                     selectSolution = "lowestConv"))
head(mleOptimWrapper(minusLogLik = f,
                     start = rbind(c(15, 2), c(15, -2), c(5, 0)),
                     selectSolution = "lowestLocMin", eigTol = 0.01))
# With constraint region
head(mleOptimWrapper(minusLogLik = function(x) sum((x - 1:2)^2),
                     start = rbind(10:11),
                     region = function(pars) {
                       x <- pars[1]
                       y <- pars[2]
                       if (y <= x^2) {
                         return(list("pars" = pars, "penalty" = 0))
                       } else {
                        return(list("pars" = c(sqrt(y), y),
                                    "penalty" = y - x^2)
                       }
                     }, lower = c(0.5, 1), upper = c(Inf, Inf),
                optMethod = "Nelder-Mead", selectSolution = "lowest"))
head(mleOptimWrapper(minusLogLik = function(x) sum((x - 1:2)^2),
                     start = rbind(10:11), lower = c(0.5, 1),
                     upper = c(Inf, Inf),optMethod = "Nelder-Mead"))
```

mleOu

Maximum likelihood estimation of the OU diffusion

Description

Computation of the maximum likelihood estimator of the parameters of the *univariate* Ornstein–Uhlenbeck (OU) diffusion from a discretized trajectory $\{X_{\Delta i}\}_{i=1}^{N}$. The objective function to minimize is

$$\sum_{i=2}^{n} \log p_{\Delta}(X_{\Delta i}|X_{\Delta(i-1)}).$$

Usage

mleOu(data, delta, alpha = NA, mu = NA, sigma = NA, start, lower = c(0.01, -5, 0.01), upper = c(25, 5, 25), ...)

Arguments

data	a vector of size N with the discretized trajectory of the diffusion.
delta	time discretization step.

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alpha, mu, sigma	9
	arguments to fix a parameter to a given value and perform the estimation on the rest. Defaults to NA, meaning that the parameter is estimated. Note that start, lower and upper must be changed accordingly if parameters are fixed, see examples.
start	starting values, a matrix with p columns, with each entry representing a different starting value.
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
	further arguments to be passed to mleOptimWrapper.

Details

The first element in data is not taken into account for estimation. See mleMou for the multivariate case (less efficient for dimension one).

Value

Output from mleOptimWrapper.

Examples

mlePde1D

MLE for toroidal process via PDE solving in 1D

Description

Maximum Likelihood Estimation (MLE) for arbitrary diffusions, based on the transition probability density (tpd) obtained as the numerical solution of the Fokker–Planck Partial Differential Equation (PDE) in 1D.

```
mlePde1D(data, delta, b, sigma2, Mx = 500, Mt = ceiling(100 * delta),
    sdInitial = 0.1, linearBinning = FALSE, start, lower, upper, ...)
```

Arguments

data	a vector of size N with the discretized trajectory of the diffusion.
delta	time discretization step.
b	drift function. Must return a vector of the same size as its argument.
sigma2	function giving the squared diffusion coefficient. Must return a vector of the same size as its argument.
Mx	size of the equispaced spatial grid in $[-\pi, \pi)$.
Mt	size of the time grid in $[0, t]$.
sdInitial	the standard deviation of the concentrated WN giving the initial condition.
linearBinning	flag to indicate whether linear binning should be applied for the initial values of the tpd, instead of usual simple binning (cheaper). Linear binning is always done in the evaluation of the tpd.
start	starting values, a matrix with p columns, with each entry representing a different starting value.
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
•••	Further parameters passed to crankNicolson1D.

Details

See Sections 3.4.1 and 3.4.4 in García-Portugués et al. (2019) for details.

Value

Output from mleOptimWrapper.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

```
sigma2 = sigma2, start = c(1, 1, 2),
                  lower = c(0.1, -pi, -10), upper = c(10, pi, 10),
                  verbose = 2)
pdeOuLin <- mlePde1D(data = traj, delta = 0.5, Mx = 100, Mt = 100, b = b,
                     sigma2 = sigma2, start = c(1, 1, 2),
                     lower = c(0.1, -pi, -10), upper = c(10, pi, 10),
                     linearBinning = TRUE, verbose = 2)
head(exactOu)
head(pdeOu)
head(pdeOuLin)
# Test in WN diffusion
alpha <- 2
mu <- 0
sigma <- 1
set.seed(234567)
traj <- rTrajWn1D(x0 = 0, alpha = alpha, mu = mu, sigma = sigma, N = 500,</pre>
                 delta = 0.5)
exactOu <- mleOu(traj, delta = 0.5, start = c(1, 1, 2),
                 lower = c(0.1, -pi, 0.1), upper = c(10, pi, 10))
pdeWn <- mlePde1D(data = traj, delta = 0.5, Mx = 100, Mt = 100,
                  b = function(x, pars)
                    driftWn1D(x = x, alpha = pars[1], mu = pars[2],
                              sigma = pars[3]),
                  sigma2 = function(x, pars) rep(pars[3]^2, length(x)),
                  start = c(1, 1, 2), lower = c(0.1, -pi, -10),
                  upper = c(10, pi, 10), verbose = 2)
pdeWnLin <- mlePde1D(data = traj, delta = 0.5, Mx = 100, Mt = 100,
                     b = function(x, pars)
                       driftWn1D(x = x, alpha = pars[1], mu = pars[2],
                                 sigma = pars[3]),
                     sigma2 = function(x, pars) rep(pars[3]^2, length(x)),
                     start = c(1, 1, 2), lower = c(0.1, -pi, -10),
                     upper = c(10, pi, 10), linearBinning = TRUE,
                     verbose = 2)
head(exactOu)
head(pdeWn)
head(pdeWnLin)
```

mlePde2D

MLE for toroidal process via PDE solving in 2D

Description

Maximum Likelihood Estimation (MLE) for arbitrary diffusions, based on the transition probability density (tpd) obtained as the numerical solution of the Fokker–Planck Partial Differential Equation (PDE) in 2D.

Usage

Arguments

data	a matrix of dimension c(n, p).
delta	discretization step.
b	drift function. Must return a vector of the same size as its argument.
sigma2	function giving the diagonal of the diffusion matrix. Must return a vector of the same size as its argument.
Mx, My	sizes of the equispaced spatial grids in $[-\pi,\pi)$ for each component.
Mt	size of the time grid in $[0, t]$.
sdInitial	standard deviations of the concentrated WN giving the initial condition.
linearBinning	flag to indicate whether linear binning should be applied for the initial values of the tpd, instead of usual simple binning (cheaper). Linear binning is always done in the evaluation of the tpd.
start	starting values, a matrix with p columns, with each entry representing a different starting value.
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
	further parameters passed to mleOptimWrapper.

Details

See Sections 3.4.2 and 3.4.4 in García-Portugués et al. (2019) for details. The function currently includes the region function for imposing a feasibility region on the parameters of the bivariate WN diffusion.

Value

Output from mleOptimWrapper.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

```
# Test in OU process
alpha <- c(1, 2, -0.5)
mu <- c(0, 0)
sigma <- c(0.5, 1)
set.seed(2334567)
```

```
data <- rTrajMou(x0 = c(0, 0), A = alphaToA(alpha = alpha, sigma = sigma),
                 mu = mu, Sigma = diag(sigma^2), N = 500, delta = 0.5)
b <- function(x, pars) sweep(-x, 2, pars[4:5], "+") %*%</pre>
                       t(alphaToA(alpha = pars[1:3], sigma = sigma))
sigma2 <- function(x, pars) repRow(sigma^2, nrow(x))</pre>
exactOu <- mleMou(data = data, delta = 0.5, sigma = sigma,
                  start = c(1, 1, 0, 2, 2),
                  lower = c(0.1, 0.1, -25, -10, -10),
                  upper = c(25, 25, 25, 10, 10)
head(exactOu, 2)
pdeOu <- mlePde2D(data = data, delta = 0.5, b = b, sigma2 = sigma2,
                  Mx = 10, My = 10, Mt = 10,
                  start = rbind(c(1, 1, 0, 2, 2)),
                  lower = c(0.1, 0.1, -25, -10, -10),
                  upper = c(25, 25, 25, 10, 10), verbose = 2)
head(pdeOu, 2)
pdeOuLin <- mlePde2D(data = data, delta = 0.5, b = b, sigma2 = sigma2,</pre>
                     Mx = 10, My = 10, Mt = 10,
                     start = rbind(c(1, 1, 0, 2, 2)),
                     lower = c(0.1, 0.1, -25, -10, -10),
                     upper = c(25, 25, 25, 10, 10), verbose = 2,
                     linearBinning = TRUE)
head(pdeOuLin, 2)
# Test in WN diffusion
alpha <- c(1, 0.5, 0.25)
mu < - c(0, 0)
sigma <- c(2, 1)
set.seed(234567)
data <- rTrajWn2D(x0 = c(0, 0), alpha = alpha, mu = mu, sigma = sigma,
                    N = 200, delta = 0.5)
b <- function(x, pars) driftWn2D(x = x, A = alphaToA(alpha = pars[1:3],</pre>
                                                       sigma = sigma),
                                  mu = pars[4:5], sigma = sigma)
sigma2 <- function(x, pars) repRow(sigma^2, nrow(x))</pre>
exactOu <- mleMou(data = data, delta = 0.5, sigma = sigma,</pre>
                  start = c(1, 1, 0, 1, 1),
                  lower = c(0.1, 0.1, -25, -25, -25),
                  upper = c(25, 25, 25, 25, 25), optMethod = "nlm")
pdeWn <- mlePde2D(data = data, delta = 0.5, b = b, sigma2 = sigma2,</pre>
                  Mx = 20, My = 20, Mt = 10, start = rbind(c(1, 1, 0, 1, 1)),
                  lower = c(0.1, 0.1, -25, -25, -25),
                  upper = c(25, 25, 25, 25, 25), verbose = 2,
                  optMethod = "nlm")
pdeWnLin <- mlePde2D(data = data, delta = 0.5, b = b, sigma2 = sigma2,</pre>
                     Mx = 20, My = 20, Mt = 10,
                     start = rbind(c(1, 1, 0, 1, 1)),
                     lower = c(0.1, 0.1, -25, -25, -25),
                     upper = c(25, 25, 25, 25, 25), verbose = 2,
                     linearBinning = TRUE)
```

head(exactOu)
head(pdeOu)
head(pdeOuLin)

periodicTrapRule1D Quadrature rules in 1D, 2D and 3D

Description

Quadrature rules for definite integrals over intervals in 1D, $\int_{x_1}^{x_2} f(x)dx$, rectangles in 2D, $\int_{x_1}^{x_2} \int_{y_1}^{y_2} f(x, y) dy dx$ and cubes in 3D, $\int_{x_1}^{x_2} \int_{y_1}^{y_2} \int_{z_1}^{z_2} f(x, y, z) dz dy dx$. The trapezoidal rules assume that the function is periodic, whereas the Simpson rules work for arbitrary functions.

Usage

```
periodicTrapRule1D(fx, endsMatch = FALSE, na.rm = TRUE,
  lengthInterval = 2 * pi)
periodicTrapRule2D(fxy, endsMatch = FALSE, na.rm = TRUE,
  lengthInterval = rep(2 * pi, 2))
periodicTrapRule3D(fxyz, endsMatch = FALSE, na.rm = TRUE,
  lengthInterval = rep(2 * pi, 3))
integrateSimp1D(fx, lengthInterval = 2 * pi, na.rm = TRUE)
integrateSimp2D(fxy, lengthInterval = rep(2 * pi, 2), na.rm = TRUE)
integrateSimp3D(fxyz, lengthInterval = rep(2 * pi, 3), na.rm = TRUE)
```

Arguments

fx	vector containing the evaluation of the function to integrate over a uniform grid in $[x_1, x_2]$.
endsMatch	flag to indicate whether the values of the last entries of fx, fxy or fxyz are the ones in the first entries (elements, rows, columns, slices). See examples for usage.
na.rm	logical. Should missing values (including NaN) be removed?
lengthInterval	vector containing the lengths of the intervals of integration.
fxy	matrix containing the evaluation of the function to integrate over a uniform grid in $[x_1, x_2] \times [y_1, y_2]$.
fxyz	three dimensional array containing the evaluation of the function to integrate over a uniform grid in $[x_1, x_2] \times [y_1, y_2] \times [z_1, z_2]$.

psMle

Details

The simple trapezoidal rule has a very good performance for periodic functions in 1D and 2D(order of error). The higher dimensional extensions are obtained by iterative usage of the 1D rules.

Value

The value of the integral.

References

Press, W. H., Teukolsky, S. A., Vetterling, W. T., Flannery, B. P. (1996). *Numerical Recipes in Fortran 77: The Art of Scientific Computing (Vol. 1 of Fortran Numerical Recipes).* Cambridge University Press, Cambridge.

Examples

```
# In 1D. True value: 3.55099937
N <- 21
grid <- seq(-pi, pi, l = N)</pre>
fx <- sin(grid)^2 * exp(cos(grid))</pre>
periodicTrapRule1D(fx = fx, endsMatch = TRUE)
periodicTrapRule1D(fx = fx[-N], endsMatch = FALSE)
integrateSimp1D(fx = fx, lengthInterval = 2 * pi)
integrateSimp1D(fx = fx[-N]) # Worse, of course
# In 2D. True value: 22.31159
fxy <- outer(grid, grid, function(x, y) (sin(x)^2 * exp(cos(x)) +
                                          sin(y)^2 * exp(cos(y))) / 2)
periodicTrapRule2D(fxy = fxy, endsMatch = TRUE)
periodicTrapRule2D(fxy = fxy[-N, -N], endsMatch = FALSE)
periodicTrapRule1D(apply(fxy[-N, -N], 1, periodicTrapRule1D))
integrateSimp2D(fxy = fxy)
integrateSimp1D(apply(fxy, 1, integrateSimp1D))
# In 3D. True value: 140.1878
fxyz <- array(fxy, dim = c(N, N, N))
for (i in 1:N) fxyz[i, , ] <- fxy</pre>
periodicTrapRule3D(fxyz = fxyz, endsMatch = TRUE)
```

psMle

integrateSimp3D(fxyz = fxyz)

Maximum pseudo-likelihood estimation by wrapped pseudo-likelihoods

Description

Maximum pseudo-likelihood using the Euler and Shoji-Ozaki pseudo-likelihoods.

Usage

```
psMle(data, delta, method = c("E", "SO", "SO2"), b, jac.b, sigma2, b1, b2,
start, lower, upper, circular = TRUE, maxK = 2, vmApprox = FALSE, ...)
```

Arguments

data	a matrix of dimension c(n, p).
delta	discretization step.
method	a string for choosing "E" (Euler), "S0" (Shoji–Ozaki) or "S02" (Shoji–Ozaki with Ito's expansion in the drift) method.
b	drift function. Must return a matrix of the same size as x.
jac.b	jacobian of the drift function.
sigma2	diagonal of the diffusion matrix (if univariate, this is the square of the diffusion coefficient). Must return an object of the same size as x.
b1	first derivative of the drift function (univariate). Must return a vector of the same length as x.
b2	second derivative of the drift function (univariate). Must return a vector of the same length as x.
start	starting values, a matrix with p columns, with each entry representing a different starting value.
lower, upper	bound for box constraints as in method "L-BFGS-B" of optim.
circular	flag to indicate circular data.
maxK	maximum absolute winding number used if circular = TRUE.
vmApprox	flag to indicate von Mises approximation to wrapped normal. See momentMatchWnVm and scoreMatchWnBvm.
	further parameters passed to mleOptimWrapper.

Details

See Section 3.2 in García-Portugués et al. (2019) for details. "S02" implements Shoji and Ozai (1998)'s expansion with for p = 1. "S0" is the same expansion, for arbitrary p, but considering null second derivatives.

Value

Output from mleOptimWrapper.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Shoji, I. and Ozaki, T. (1998) A statistical method of estimation and simulation for systems of stochastic differential equations. *Biometrika*, 85(1):240–243. doi:10.1093/biomet/85.1.240

psMle

```
# Example in 1D
delta <- 0.5
pars <- c(0.25, 0, 2)
set.seed(12345678)
samp <- rTrajWn1D(x0 = 0, alpha = pars[1], mu = pars[2], sigma = pars[3],</pre>
                  N = 100, delta = delta)
b <- function(x, pars) driftWn1D(x = x, alpha = pars[1], mu = pars[2],</pre>
                                  sigma = pars[3], maxK = 2, expTrc = 30)
b1 <- function(x, pars, h = 1e-4) {
  1 \le length(x)
  res <- b(x = c(x + h, x - h), pars = pars)
  drop(res[1:1] - res[(1 + 1):(2 * 1)])/(2 * h)
}
b2 <- function(x, pars, h = 1e-4) {
  1 \le length(x)
  res - b(x = c(x + h, x, x - h)), pars = pars)
  drop(res[1:1] - 2 * res[(1 + 1):(2 * 1)] + res[(2 * 1 + 1):(3 * 1)])/(h^2)
}
sigma2 <- function(x, pars) rep(pars[3]^2, length(x))</pre>
lower <- c(0.1, -pi, 0.1)
upper <- c(10, pi, 10)
psMle(data = samp, delta = delta, method = "E", b = b, sigma2 = sigma2,
      start = pars, lower = lower, upper = upper)
psMle(data = samp, delta = delta, method = "E", b = b, sigma2 = sigma2,
      start = pars, lower = lower, upper = upper, vmApprox = TRUE)
psMle(data = samp, delta = delta, method = "SO2", b = b, b1 = b1,
      b2 = b2, sigma2 = sigma2, start = pars, lower = lower, upper = upper)
psMle(data = samp, delta = delta, method = "SO2", b = b, b1 = b1,
      b2 = b2, sigma2 = sigma2, start = pars, lower = lower,
      upper = upper, vmApprox = TRUE)
psMle(data = samp, delta = delta, method = "SO", b = b, b1 = b1,
      lower = lower, upper = upper, sigma2 = sigma2, start = pars)
approxMleWn1D(data = samp, delta = delta, start = pars)
mlePde1D(data = samp, delta = delta, b = b, sigma2 = sigma2,
         start = pars, lower = lower, upper = upper)
# Example in 2D
delta <- 0.5
pars <- c(1, 0.5, 0, 0, 0, 1, 2)
set.seed(12345678)
samp <- rTrajWn2D(x0 = c(0, 0), alpha = pars[1:3], mu = pars[4:5],</pre>
                  sigma = pars[6:7], N = 100, delta = delta)
b <- function(x, pars) driftWn2D(x = x, A = alphaToA(alpha = pars[1:3],</pre>
                                                      sigma = pars[6:7]),
                                  mu = pars[4:5], sigma = pars[6:7], maxK = 2,
                                  expTrc = 30)
jac.b <- function(x, pars, h = 1e-4) {</pre>
  1 <- nrow(x)
```

```
res <- b(x = rbind(cbind(x[, 1] + h, x[, 2]),</pre>
                     cbind(x[, 1] - h, x[, 2]),
                     cbind(x[, 1], x[, 2] + h),
                     cbind(x[, 1], x[, 2] - h)), pars = pars)
 cbind(res[1:1, ] - res[(1 + 1):(2 * 1), ],
        res[2 * l + 1:l, ] - res[2 * l + (l + 1):(2 * l), ]) / (2 * h)
}
sigma2 <- function(x, pars) matrix(pars[6:7]^2, nrow = length(x) / 2L,</pre>
                                   ncol = 2)
lower <- c(0.01, 0.01, -25, -pi, -pi, 0.01, 0.01)
upper <- c(25, 25, 25, pi, pi, 25, 25)
psMle(data = samp, delta = delta, method = "E", b = b, sigma2 = sigma2,
      start = pars, lower = lower, upper = upper)
psMle(data = samp, delta = delta, method = "E", b = b, sigma2 = sigma2,
      start = pars, lower = lower, upper = upper, vmApprox = TRUE)
psMle(data = samp, delta = delta, method = "SO", b = b, jac.b = jac.b,
      sigma2 = sigma2, start = pars, lower = lower, upper = upper)
approxMleWn2D(data = samp, delta = delta, start = c(pars, 0))
# Set maxit = 5 to test and avoid a very long evaluation
mlePde2D(data = samp, delta = delta, b = b, sigma2 = sigma2, start = pars,
         lower = lower, upper = upper, maxit = 5)
```

rStat₩n2D

```
Simulation from the stationary density of a WN diffusion in 2D
```

Description

Simulates from the stationary density of the WN diffusion in 2D.

Usage

rStatWn2D(n, mu, alpha, sigma, rho = 0)

Arguments

n	sample size.
mu	a vector of length 2 giving the mean.
alpha	vector of length 3 parametrizing the A matrix as in alphaToA.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .

Value

A matrix of dimension c(n, 2) containing the samples from the stationary distribution.

rTpdWn2D

Examples

rTpdWn2D	Simulation from the approximated transition distribution of a WN dif-
	fusion in 2D

Description

Simulates from the approximate transition density of the WN diffusion in 2D.

Usage

```
rTpdWn2D(n, x0, t, mu, alpha, sigma, rho = 0, maxK = 2L, expTrc = 30)
```

Arguments

n	sample size.
x0	a matrix of dimension c(nx0, 2) giving the starting values.
t	vector of length nx0 containing the times between observations.
mu	a vector of length 2 giving the mean.
alpha	vector of length 3 parametrizing the A matrix as in alphaToA.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

An array of dimension c(n, 2, nx0) containing the n samples of the transition distribution, conditioned on that the process was at x0 at t instants ago. The samples are all in $[\pi, \pi)$.

Examples

```
alpha <- c(3, 2, -1)
sigma <- c(0.5, 1)
mu <- c(pi, pi)</pre>
x <- seq(-pi, pi, l = 100)
t <- 0.5
image(x, x, matrix(dTpdWou2D(x = as.matrix(expand.grid(x, x)),
                            x0 = matrix(rep(0, 100 * 2)),
                                        nrow = 100 * 100, ncol = 2),
                            t = t, mu = mu, alpha = alpha, sigma = sigma,
                            maxK = 2, expTrc = 30), nrow = 100, ncol = 100),
      zlim = c(0, 0.5))
points(rTpdWn2D(n = 500, x0 = rbind(c(0, 0)), t = t, mu = mu, alpha = alpha,
                sigma = sigma)[, , 1], col = 3)
points(stepAheadWn2D(x0 = rbind(c(0, 0)), delta = t / 500,
                     A = alphaToA(alpha = alpha, sigma = sigma),
                     mu = mu, sigma = sigma, N = 500, M = 500, maxK = 2,
                     expTrc = 30, col = 4)
```

```
rTrajLangevin
```

Simulation of trajectories of a Langevin diffusion

Description

Simulation of an arbitrary Langevin diffusion in dimension p by subsampling a fine trajectory obtained by the Euler discretization.

Usage

```
rTrajLangevin(x0, drift, SigDif, N = 100, delta = 0.01, NFine = ceiling(N
 * delta/deltaFine), deltaFine = min(delta/100, 0.001), circular = TRUE,
    ...)
```

Arguments

x0	vector of length p giving the initial point.
drift	drift for the diffusion.
SigDif	matrix of size c(p, p) giving the infinitesimal (constant) covariance matrix of the diffusion.
Ν	number of discretization steps in the resulting trajectory.
delta	discretization step.
NFine	number of discretization steps for the fine trajectory. Must be larger than N.
deltaFine	discretization step for the fine trajectory. Must be smaller than delta.
circular	whether to wrap the resulting trajectory to $[-\pi,\pi)^p$.
	parameters to be passed to drift.

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rTrajMou

Details

The fine trajectory is subsampled using the indexes seq(1, NFine + 1, by = NFine / N).

Value

A vector of length N + 1 containing x0 in the first entry and the discretized trajectory.

Examples

```
isRStudio <- identical(.Platform$GUI, "RStudio")</pre>
if (isRStudio) {
 # 1D
 manipulate::manipulate({
   x \le seq(0, N * delta, by = delta)
   plot(x, x, ylim = c(-pi, pi), type = "n",
        ylab = expression(X[t]), xlab = "t")
   linesCirc(x, rTrajLangevin(x0 = 0, drift = driftJp, SigDif = sigma,
                               alpha = alpha, mu = 0, psi = psi, N = N,
                               delta = 0.01))
    }, delta = manipulate::slider(0.01, 5.01, step = 0.1),
   N = manipulate::slider(10, 500, step = 10, initial = 200),
   alpha = manipulate::slider(0.01, 5, step = 0.1, initial = 1),
   psi = manipulate::slider(-2, 2, step = 0.1, initial = 1),
    sigma = manipulate::slider(0.01, 5, step = 0.1, initial = 1))
 # 2D
 samp <- rTrajLangevin(x0 = c(0, 0), drift = driftMvm, alpha = c(1, 1),</pre>
                        mu = c(2, -1), A = diag(rep(0, 2)),
                        SigDif = diag(rep(1, 2)), N = 1000, delta = 0.1)
 plot(samp, xlim = c(-pi, pi), ylim = c(-pi, pi), pch = 19, cex = 0.25,
       xlab = expression(X[t]), ylab = expression(Y[t]), col = rainbow(1000))
 linesTorus(samp[, 1], samp[, 2], col = rainbow(1000))
}
```

rTrajMou

Simulation of trajectories for the multivariate OU diffusion

Description

Simulation of trajectories of the multivariate Ornstein-Uhlenbeck (OU) diffusion

$$dX_{t} = A(\mu - X_{t})dt + \Sigma^{\frac{1}{2}}dW_{t}, X_{0} = x_{0}$$

using the exact transition probability density.

Usage

rTrajMou(x0, A, mu, Sigma, N = 100, delta = 0.001)

Arguments

x0	a vector of length p containing initial point.
А	the drift matrix, of size c(p, p).
mu	unconditional mean of the diffusion, a vector of length p.
Sigma	square of the diffusion matrix, a matrix of size c(p, p).
Ν	number of discretization steps in the resulting trajectory.
delta	time discretization step.

Details

The law of the discretized trajectory at *each* time step is a multivariate normal with mean meantMou and covariance matrix covtMou. See rTrajOu for the univariate case (more efficient).

solve(A) %*% Sigma has to be a covariance matrix (symmetric and positive definite) in order to have a proper transition density. For the bivariate case, this can be ensured with the alphaToA function. In the multivariate case, it is ensured if Sigma is isotropic and A is a covariance matrix.

Value

A matrix of size c(N + 1, p) containing x0 in the first row and the exact discretized trajectory on the remaining rows.

Examples

rTrajOu

Simulation of trajectories for the univariate OU diffusion

Description

Simulation of trajectories of the univariate Ornstein-Uhlenbeck (OU) diffusion

 $dX_t = \alpha(\mu - X_t)dt + \sigma dW_t, X_0 = x_0$

using the exact transition probability density.

```
rTrajOu(x0, alpha, mu, sigma, N = 100, delta = 0.001)
```

rTrajWn1D

Arguments

x0	initial point.
alpha	strength of the drift.
mu	unconditional mean of the diffusion.
sigma	diffusion coefficient.
Ν	number of discretization steps in the resulting trajectory.
delta	time discretization step.

Details

The law of the discretized trajectory is a multivariate normal with mean meantOu and covariance matrix covstOu. See rTrajMou for the multivariate case (less efficient for dimension one).

Value

A vector of length N + 1 containing x0 in the first entry and the exact discretized trajectory on the remaining elements.

Examples

```
isRStudio <- identical(.Platform$GUI, "RStudio")
if (isRStudio) {
    manipulate::manipulate({
        set.seed(345678);
        plot(seq(0, N * delta, by = delta), rTrajOu(x0 = 0, alpha = alpha, mu = 0,
            sigma = sigma, N = N, delta = delta), ylim = c(-4, 4), type = "l",
            ylab = expression(X[t]), xlab = "t")
        }, delta = manipulate::slider(0.01, 5.01, step = 0.1),
        N = manipulate::slider(10, 500, step = 10, initial = 200),
        alpha = manipulate::slider(0.01, 5, step = 0.1, initial = 1),
        sigma = manipulate::slider(0.01, 5, step = 0.1, initial = 1))
}</pre>
```

rTrajWn1D

Simulation of trajectories for the WN diffusion in 1D

Description

Simulation of the Wrapped Normal (WN) diffusion in 1D by subsampling a fine trajectory obtained by the Euler discretization.

Arguments

x0	initial point.
alpha	drift parameter.
mu	mean parameter. Must be in $[\pi, \pi)$.
sigma	diffusion coefficient.
Ν	number of discretization steps in the resulting trajectory.
delta	discretization step.
NFine	number of discretization steps for the fine trajectory. Must be larger than \ensuremath{N} .
deltaFine	discretization step for the fine trajectory. Must be smaller than delta.

Details

The fine trajectory is subsampled using the indexes seq(1, NFine + 1, by = NFine / N).

Value

A vector of length N + 1 containing x0 in the first entry and the discretized trajectory.

Examples

rTrajWn2D

Simulation of trajectories for the WN diffusion in 2D

Description

Simulation of the Wrapped Normal (WN) diffusion in 2D by subsampling a fine trajectory obtained by the Euler discretization.

```
rTrajWn2D(x0, alpha, mu, sigma, rho = 0, N = 100, delta = 0.01,
NFine = ceiling(N * delta/deltaFine), deltaFine = min(delta/100, 0.001))
```

safeSoftMax

Arguments

x0	vector of length 2 giving the initial point.
alpha	vector of length 3 parametrizing the A matrix as in alphaToA.
mu	a vector of length 2 giving the mean.
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
Ν	number of discretization steps in the resulting trajectory.
delta	discretization step.
NFine	number of discretization steps for the fine trajectory. Must be larger than N.
deltaFine	discretization step for the fine trajectory. Must be smaller than delta.

Details

The fine trajectory is subsampled using the indexes seq(1, NFine + 1, by = NFine / N).

Value

A matrix of size c(N + 1, 2) containing x0 in the first entry and the discretized trajectory.

Examples

safeSoftMax

Safe softmax function for computing weights

Description

Computes the weights $w_i = \frac{e^{p_i}}{\sum_{j=1}^k e^{p_j}}$ from $p_i, i = 1, \dots, k$ in a safe way to avoid overflows and to truncate automatically to zero low values of w_i .

Usage

safeSoftMax(logs, expTrc = 30)

Arguments

logs	matrix of logarithms where each row contains a set of p_1, \ldots, p_k to compute the weights from.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Details

The logs argument must be always a matrix.

Value

A matrix of the size as logs containing the weights for each row.

Examples

```
# A matrix
safeSoftMax(rbind(1:10, 20:11))
rbind(exp(1:10) / sum(exp(1:10)), exp(20:11) / sum(exp(20:11)))
# A row-matrix
safeSoftMax(rbind(-100:100), expTrc = 30)
exp(-100:100) / sum(exp(-100:100))
```

```
scoreMatchWnBvm
```

Score and moment matching of a univariate or bivariate wrapped normal by a von Mises

Description

Given a wrapped normal density, find the parameters of a von Mises that matches it according to two characteristics: moments and scores. Score matching estimators are available for univariate and bivariate cases and moment matching only for the former.

Usage

```
scoreMatchWnBvm(Sigma = NULL, invSigma)
```

```
scoreMatchWnVm(sigma, sigma2 = NULL)
```

```
momentMatchWnVm(sigma, sigma2 = NULL)
```

Arguments

Sigma, invSigma

covariance or precision matrix of the bivariate wrapped normal.

sigma, sigma2 standard deviation or variance of the wrapped normal.

Details

If the precision matrix is singular or if there are no solutions for the score matching estimator, c(0, 0, 0) is returned.

Value

Vector of parameters $(\kappa_1, \kappa_2, \lambda)$, where $(\kappa_1, \kappa_2, 2\lambda)$ is a suitable input for kappa in dBvm.

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sdetorus

References

Mardia, K. V., Kent, J. T., and Laha, A. K. (2016). Score matching estimators for directional distributions. *arXiv:1604.0847*. https://arxiv.org/abs/1604.08470

Examples

```
# Univariate WN approximation
sigma <- 0.5
curve(dWn1D(x = x, mu = 0, sigma = sigma), from = -pi, to = pi,
      ylab = "Density", ylim = c(0, 1))
curve(dVm(x = x, mu = 0, kappa = momentMatchWnVm(sigma = sigma)), from = -pi,
      to = pi, col = "red", add = TRUE)
curve(dVm(x = x, mu = 0, kappa = scoreMatchWnVm(sigma = sigma)), from = -pi,
      to = pi, col = "green", add = TRUE)
# Bivariate WN approximation
# WN
alpha <- c(2, 1, 1)
sigma <- c(1, 1)
mu <- c(pi / 2, pi / 2)
x <- seq(-pi, pi, l = 101)[-101]
plotSurface2D(x, x, f = function(x) dStatWn2D(x = x, alpha = alpha, mu = mu,
                                               sigma = sigma), fVect = TRUE)
A <- alphaToA(alpha = alpha, sigma = sigma)
S <- 0.5 * solve(A) %*% diag(sigma)</pre>
# Score matching
kappa <- scoreMatchWnBvm(Sigma = S)</pre>
# dBvm uses lambda / 2 in the exponent
plotSurface2D(x, x, f = function(x) dBvm(x = x, mu = mu,
                                         kappa = c(kappa[1:2], 2 * kappa[3])),
             fVect = TRUE)
# With singular Sigma
invSigma <- matrix(c(1, sqrt(0.999), sqrt(0.999), 1), nrow = 2, ncol = 2)</pre>
scoreMatchWnBvm(invSigma = invSigma)
invSigma <- matrix(1, nrow = 2, ncol = 2)</pre>
scoreMatchWnBvm(invSigma = invSigma)
```

sdetorus

sdetorus - Statistical Tools for Toroidal Diffusions

Description

Implementation of statistical methods for the estimation of toroidal diffusions. Several diffusive models are provided, most of them belonging to the Langevin family of diffusions on the torus. Specifically, the wrapped normal and von Mises processes are included, which can be seen as

toroidal analogues of the Ornstein–Uhlenbeck diffusion. A collection of methods for approximate maximum likelihood estimation, organized in four blocks, is given: (i) based on the exact transition probability density, obtained as the numerical solution to the Fokker-Plank equation; (ii) based on wrapped pseudo-likelihoods; (iii) based on specific analytic approximations by wrapped processes; (iv) based on maximum likelihood of the stationary densities. The package allows the replicability of the results in García-Portugués et al. (2019) <doi:10.1007/s11222-017-9790-2>.

Author(s)

Eduardo García-Portugués.

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

sigmaDiff

High-frequency estimate of the diffusion matrix

Description

Estimation of the Σ in the multivariate diffusion

$$dX_t = b(X_t)dt + \Sigma dW_t$$

by the high-frequency estimate

$$\hat{\Sigma} = \frac{1}{N\Delta} \sum_{i=1}^{N} (X_i - X_{i-1}) (X_i - X_{i-1})^T$$

Usage

```
sigmaDiff(data, delta, circular = TRUE, diagonal = FALSE,
isotropic = FALSE)
```

Arguments

data	vector or matrix of size c(N, p) containing the discretized process.
delta	discretization step.
circular	whether the process is circular or not.
diagonal, isotropic	
	enforce different constraints for the diffusion matrix.

Details

See Section 3.1 in García-Portugués et al. (2019) for details.

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solveTridiag

Value

The estimated diffusion matrix of size c(p, p).

References

García-Portugués, E., Sørensen, M., Mardia, K. V. and Hamelryck, T. (2019) Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, 29(2):1–22. doi:10.1007/s1122201797902

Examples

solveTridiag	Thomas algorithm for solving tridiagonal matrix systems, with op-
	tional presaving of LU decomposition

Description

Implementation of the Thomas algorithm to solve efficiently the tridiagonal matrix system

$$b_1x_1 + c_1x_2 + a_1x_n = d_1$$

$$a_2x_1 + b_2x_2 + c_2x_3 = d_2$$

$$\vdots \\ a_{n-1}x_{n-2} + b_{n-1}x_{n-1} + c_{n-1}x_n = d_{n-1}$$

$$c_nx_1 + a_nx_{n-1} + b_nx_n = d_n$$

with $a_1 = c_n = 0$ (usual tridiagonal matrix). If $a_1 \neq 0$ or $c_n \neq 0$ (circulant tridiagonal matrix), then the Sherman–Morrison formula is employed.

```
solveTridiag(a, b, c, d, LU = 0L)
solveTridiagMatConsts(a, b, c, d, LU = 0L)
solvePeriodicTridiag(a, b, c, d, LU = 0L)
forwardSweepTridiag(a, b, c)
```

forwardSweepPeriodicTridiag(a, b, c)

Arguments

a, b, c	subdiagonal (below main diagonal), diagonal and superdiagonal (above main diagonal), respectively. They all are vectors of length n.
d	vector of constant terms, of length n. For solveTridiagMatConsts, it can be a matrix with n rows.
LU	flag denoting if the forward sweep encoding the LU decomposition is supplied in vectors b and c. See details and examples.

Details

The Thomas algorithm is stable if the matrix is diagonally dominant.

For the periodic case, two non-periodic tridiagonal systems with different constant terms (but same coefficients) are solved using solveTridiagMatConsts. These two solutions are combined by the Sherman–Morrison formula to obtain the solution to the periodic system.

Note that the output of solveTridiag and solveTridiagMatConsts are independent from the values of a[1] and c[n], but solvePeriodicTridiag is not.

If LU is TRUE, then b and c must be precomputed with forwardSweepTridiag or forwardSweepPeriodicTridiag for its use in the call of the appropriate solver, which will be slightly faster.

Value

- solve* functions: the solution, a vector of length n and a matrix with n rows for solveTridiagMatConsts.
- forward* functions: the matrix cbind(b, c) creating the suitable b and c arguments for calling solve* when LU is TRUE.

References

Thomas, J. W. (1995). *Numerical Partial Differential Equations: Finite Difference Methods*. Springer, New York. doi:10.1007/9781489972781

Conte, S. D. and de Boor, C. (1980). *Elementary Numerical Analysis: An Algorithmic Approach*. Third edition. McGraw-Hill, New York. doi:10.1137/1.9781611975208

stepAheadWn1D

Examples

```
# Tridiagonal matrix
n <- 10
a <- rnorm(n, 3, 1)
b <- rnorm(n, 10, 1)
c <- rnorm(n, 0, 1)
d <- rnorm(n, 0, 1)
A \leq matrix(0, nrow = n, ncol = n)
diag(A) <- b
for (i in 1:(n - 1)) {
 A[i + 1, i] <- a[i + 1]
  A[i, i + 1] <- c[i]
}
А
# Same solutions
drop(solveTridiag(a = a, b = b, c = c, d = d))
solve(a = A, b = d)
# Presaving the forward sweep (encodes the LU factorization)
LU <- forwardSweepTridiag(a = a, b = b, c = c)
drop(solveTridiag(a = a, b = LU[, 1], c = LU[, 2], d = d, LU = 1))
# With equal coefficient matrix
solveTridiagMatConsts(a = a, b = b, c = c, d = cbind(d, d + 1))
cbind(solve(a = A, b = d), solve(a = A, b = d + 1))
LU <- forwardSweepTridiag(a = a, b = b, c = c)
solveTridiagMatConsts(a = a, b = LU[, 1], c = LU[, 2], d = cbind(d, d + 1), LU = 1)
# Periodic matrix
A[1, n] <- a[1]
A[n, 1] <- c[n]
А
# Same solutions
drop(solvePeriodicTridiag(a = a, b = b, c = c, d = d))
solve(a = A, b = d)
# Presaving the forward sweep (encodes the LU factorization)
LU <- forwardSweepPeriodicTridiag(a = a, b = b, c = c)
drop(solvePeriodicTridiag(a = a, b = LU[, 1], c = LU[, 2], d = d, LU = 1))
```

stepAheadWn1D

Multiple simulation of trajectory ends of the WN or vM diffusion in 1D

Description

Simulates M trajectories starting from different initial values x0 of the WN or vM diffusion in 1D, by the Euler method, and returns their ends.

Usage

stepAheadWn1D(x0, alpha, mu, sigma, M, N = 100L, delta = 0.01, type = 1L, maxK = 2L, expTrc = 30)

Arguments

x0	vector of length nx0 giving the initial points.
alpha	drift parameter.
mu	mean parameter. Must be in $[\pi, \pi)$.
sigma	diffusion coefficient.
М	number of Monte Carlo replicates.
Ν	number of discretization steps.
delta	discretization step.
type	integer giving the type of diffusion. Currently, only 1 for WN and 2 for vM are supported.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

A matrix of size c(nx0, M) containing the M trajectory ends for each starting value x0.

stepAheadWn2D Multiple simulation of trajectory ends of the WN or MvM diffusion in 2D

Description

Simulates M trajectories starting from different initial values x0 of the WN or MvM diffusion in 2D, by the Euler method, and returns their ends.

Usage

Arguments

x0	matrix of size $c(nx0, 2)$ giving the initial points.
mu	a vector of length 2 giving the mean.
A	drift matrix of size c(2, 2).
sigma	vector of length 2 containing the square root of the diagonal of Σ , the diffusion matrix.
rho	correlation coefficient of Σ .
М	number of Monte Carlo replicates.
Ν	number of discretization steps.
delta	discretization step.
type	integer giving the type of diffusion. Currently, only 1 for WN and 2 for vM are supported.
maxK	maximum absolute value of the windings considered in the computation of the WN.
expTrc	truncation for exponential: $exp(x)$ with $x \le -expTrc$ is set to zero. Defaults to 30.

Value

An array of size c(nx0, 2, M) containing the M trajectory ends for each starting value x0.

```
N <- 100
nx0 <- 3
x0 <- seq(-pi, pi, l = nx0 + 1)[-(nx0 + 1)]
x0 <- as.matrix(expand.grid(x0, x0))
nx0 <- nx0<sup>2</sup>
set.seed(12345678)
samp1 <- euler2D(x0 = x0, mu = c(0, 0), A = rbind(c(3, 1), 1:2),</pre>
```

toPiInt

Wrapping of radians to its principal values

Description

Utilities for transforming a reals into $[-\pi, \pi)$, $[0, 2\pi)$ or [a, b).

Usage

toPiInt(x)
to2PiInt(x)

toInt(x, a, b)

Arguments

Х	a vector, matrix or object for whom Arithmetic is defined.
a,b	the lower and upper limits of $[a, b)$.

Details

Note that b is **excluded** from the result, see examples.

Value

The wrapped vector in the chosen interval.

Examples

```
# Wrapping of angles
x <- seq(-3 * pi, 5 * pi, 1 = 100)
toPiInt(x)
to2PiInt(x)</pre>
```

Transformation to [1, 5)

torusAxis

```
x <- 1:10
toInt(x, 1, 5)
toInt(x + 1, 1, 5)
# Transformation to [1, 5]
toInt(x, 1, 6)
toInt(x + 1, 1, 6)
```

torusAxis

Draws pretty axis labels for circular variables

Description

Wrapper for drawing pretty axis labels for circular variables. To be invoked after plot with axes = FALSE has been called.

Usage

torusAxis(sides = 1:2, twoPi = FALSE, ...)

Arguments

sides	an integer vector specifying which side of the plot the axes are to be drawn on. The axes are placed as follows: $1 = below$, $2 = left$, $3 = above$, and $4 = right$.
twoPi	flag indicating that $[0, 2\pi)$ is the support, instead of $[-\pi, \pi)$.
	further parameters passed to axis.

Details

The function calls box.

Value

This function is usually invoked for its side effect, which is to add axes to an already existing plot.

torusAxis3d

Description

Wrapper for drawing pretty axis labels for circular variables. To be invoked after plot3d with axes = FALSE and box = FALSE has been called.

Usage

```
torusAxis3d(sides = 1:3, twoPi = FALSE, ...)
```

Arguments

sides	an integer vector specifying which side of the plot the axes are to be drawn on. The axes are placed as follows: $1 = x$, $2 = y$, $3 = z$.
twoPi	flag indicating that $[0, 2\pi)$ is the support, instead of $[-\pi, \pi)$.
	further parameters passed to axis3d.

Details

The function calls box3d.

Value

This function is usually invoked for its side effect, which is to add axes to an already existing plot.

unwrapCircSeries Unwrapping of circular time series

Description

Completes a circular time series to a linear one by computing the closest wind numbers. Useful for plotting circular trajectories with crossing of boundaries.

Usage

```
unwrapCircSeries(x)
```

Arguments

Х

wrapped angles. Must be a vector or a matrix, see details.

Details

If x is a matrix then the unwrapping is carried out row-wise, on each column separately.

Value

A vector or matrix containing a choice of unwrapped angles of x that maximizes linear continuity.

```
# Vectors
x <- c(-pi, -pi/2, pi - 0.1, -pi + 0.2)
u <- unwrapCircSeries(x)</pre>
max(abs(toPiInt(u) - x))
plot(toPiInt(x), ylim = c(-pi, pi))
for(k in -1:1) lines(u + 2 * k * pi)
# Matrices
N <- 100
set.seed(234567)
x <- t(euler2D(x0 = rbind(c(0, 0)), A = diag(c(1, 1)), sigma = rep(1, 2),</pre>
                 mu = c(pi, pi), N = N, delta = 1, type = 2)[1, , ])
u <- unwrapCircSeries(x)</pre>
max(abs(toPiInt(u) - x))
plot(x, xlim = c(-pi, pi), ylim = c(-pi, pi))
for(k1 in -3:3) for(k2 in -3:3) lines(u[, 1] + 2 * k1 * pi,
                                       u[, 2] + 2 * k2 * pi, col = gray(0.5))
```

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