

Package ‘magi’

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Description

Provides fast and accurate inference for the parameter estimation problem in Ordinary Differential Equations, including the case when there are unobserved system components. Implements the MAGI method (MAnifold-constrained Gaussian process Inference) of Yang, Wong, and Kou (2021) <[doi:10.1073/pnas.2020397118](https://doi.org/10.1073/pnas.2020397118)>.

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calCov	<i>Calculate stationary Gaussian process kernel</i>
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Description

Covariance calculations for Gaussian process kernels. Currently supports matern, rbf, compact1, periodicMatern, generalMatern, and rationalQuadratic kernels. Can also return m_phi and other additional quantities useful for ODE inference.

Usage

```
calCov(
  phi,
  rInput,
  signrInput,
  bandsize = NULL,
  complexity = 3,
  kerneltype = "matern",
  df,
  noiseInjection = 1e-07
)
```

Arguments

phi	the kernel hyper-parameters. See details for hyper-parameter specification for each kerneltype.
rInput	the distance matrix between all time points s and t, i.e., s - t
signrInput	the sign matrix of the time differences, i.e., sign(s - t)

bandsize	size for band matrix approximation. See details.
complexity	integer value for the complexity of the kernel calculations desired: <ul style="list-style-type: none"> • 0 includes C only • 1 additionally includes Cprime, Cdoubleprime, dCdphi • 2 or above additionally includes Ceigenlover, CeigenVec, Cinv, mphi, Kphi, Keigenlover, KeigenVec, Kinv, mphiLeftHalf, dCdphiCube See details for their definitions.
kerneltype	must be one of matern, rbf, compact1, periodicMatern, generalMatern, rationalQuadratic. See details for the kernel formulae.
df	degrees of freedom, for generalMatern and rationalQuadratic kernels only. Default is df=2.01 for generalMatern and df=0.01 for rationalQuadratic.
noiseInjection	a small value added to the diagonal elements of C and Kphi for numerical stability

Details

The covariance formulae and the hyper-parameters phi for the supported kernels are as follows. Stationary kernels have $C(s, t) = C(r)$ where $r = |s - t|$ is the distance between the two time points. Generally, the hyper-parameter phi[1] controls the overall variance level while phi[2] controls the bandwidth.

matern This is the simplified Matern covariance with $df = 5/2$:

$$C(r) = \text{phi}[1] * (1 + \sqrt{5}r/\text{phi}[2] + 5r^2/(3\text{phi}[2]^2)) * \exp(-\sqrt{5}r/\text{phi}[2])$$

rbf

$$C(r) = \text{phi}[1] * \exp(-r^2/(2\text{phi}[2]^2))$$

compact1

$$C(r) = \text{phi}[1] * \max(1 - r/\text{phi}[2], 0)^4 * (4r/\text{phi}[2] + 1)$$

periodicMatern Define $r' = |\sin(r\pi/\text{phi}[3]) * 2|$. Then the covariance is given by $C(r')$ using the Matern formula.

generalMatern

$$C(r) = \text{phi}[1] * 2^{(1-df)}/\Gamma(df) * (\sqrt{(2.0*df)*r/\text{phi}[2]})^{df} * \text{besselK}(\sqrt{(2.0*df)*r/\text{phi}[2]}, df)$$

where **besselK** is the modified Bessel function of the second kind.

rationalQuadratic

$$C(r) = \text{phi}[1] * (1 + r^2/(2df\text{phi}[2]^2))^{-(df)}$$

The kernel calculations available and their definitions are as follows:

C The covariance matrix corresponding to the distance matrix rInput.

Cprime The cross-covariance matrix $dC(s, t)/ds$.

Cdoubleprime The cross-covariance matrix $d^2C(s, t)/dsdt$.

dCdphi A list with the matrices $dC/dphi$ for each element of phi.

Ceigen1over The reciprocals of the eigenvalues of C .

CeigenVec Matrix of eigenvectors of C .

Cinv The inverse of C .

mphi The matrix $C_{\text{prime}} * C_{\text{inv}}$.

Kphi The matrix $C_{\text{doubleprime}} - C_{\text{prime}} * K_{\text{inv}} * t(C_{\text{prime}})$.

Keigen1over The reciprocals of the eigenvalues of K_{phi} .

Kinv The inverse of K_{phi} .

mphiLeftHalf The matrix $C_{\text{prime}} * C_{\text{eigenVec}}$.

dCdphiCube $dC/dphi$ as a 3-D array, with the third dimension corresponding to the elements of phi .

If `bandsize` is a positive integer, additionally `CinvBand`, `mphiBand`, and `KinvBand` are provided in the return list, which are band matrix approximations to `Cinv`, `mphi`, and `Kinv` with the specified `bandsize`.

Value

A list containing the kernel calculations included by the value of `complexity`.

Examples

```
foo <- outer(0:40, t(0:40), '-')[, 1, ]
r <- abs(foo)
signr <- -sign(foo)
calCov(c(0.2, 2), r, signr, bandsize = 20, kerneltype = "generalMatern", df = 2.01)
```

FNdat

Dataset of noisy observations from the FitzHugh-Nagumo (FN) equations

Description

The classic FN equations model the spike potentials of neurons, where system components V and R are the voltage and recovery variables, respectively.

V and R are governed by the following differential equations:

$$\frac{dV}{dt} = c(V - \frac{V^3}{3} + R)$$

$$\frac{dR}{dt} = -\frac{1}{c}(V - a + bR)$$

where $\theta = (a, b, c)$ are system parameters. This dataset was generated by first numerically solving these ODEs from $t = 0$ to $t = 20$, with initial conditions $V(0) = -1$ and $R(0) = 1$ and parameters $\theta = (0.2, 0.2, 3)$. The system components were taken to be measured at 28 observation time points (as indicated in `time` column) with additive Gaussian noise (standard deviation 0.2).

Usage

```
data(FNdat)
```

Format

A data frame with 28 rows and 3 columns (time, V , R).

References

FitzHugh, R (1961). Impulses and Physiological States in Theoretical Models of Nerve Membrane. *Biophysical Journal*, 1(6), 445–466.

 fnmodelODE

The FitzHugh-Nagumo (FN) equations

Description

The classic FN equations model the spike potentials of neurons, where system components $X = (V, R)$ represent the voltage and recovery variables, respectively.

V and R are governed by the following differential equations:

$$\begin{aligned}\frac{dV}{dt} &= c\left(V - \frac{V^3}{3} + R\right) \\ \frac{dR}{dt} &= -\frac{1}{c}(V - a + bR)\end{aligned}$$

where $\theta = (a, b, c)$ are system parameters.

Usage

```
fnmodelODE(theta, x, tvec)
```

```
fnmodelDx(theta, x, tvec)
```

```
fnmodelDtheta(theta, x, tvec)
```

Arguments

`theta` vector of parameters.

`x` matrix of system states (one per column) at the time points in `tvec`.

`tvec` vector of time points

Value

`fnmodelODE` returns an array with the values of the derivatives \dot{X} .

`fnmodelDx` returns a 3-D array with the values of the gradients with respect to X .

`fnmodelDtheta` returns a 3-D array with the values of the gradients with respect to θ .

References

FitzHugh, R (1961). Impulses and Physiological States in Theoretical Models of Nerve Membrane. *Biophysical Journal*, 1(6), 445–466.

Examples

```
theta <- c(0.2, 0.2, 3)
x <- matrix(1:10, nrow = 5, ncol = 2)
tvec <- 1:5
```

```
fnmodelODE(theta, x, tvec)
```

gpsmoothing

Gaussian process smoothing

Description

Estimate hyper-parameters ϕ and noise standard deviation σ for a vector of observations using Gaussian process smoothing.

Usage

```
gpsmoothing(yobs, tvec, kerneltype = "generalMatern", sigma = NULL)
```

Arguments

yobs	vector of observations
tvec	vector of time points corresponding to observations
kerneltype	the covariance kernel, types matern, compact1, periodicMatern, generalMatern are supported. See calCov for their definitions.
sigma	the noise level (if known). By default, both ϕ and σ are estimated. If a value for σ is supplied, then σ is held fixed at the supplied value and only ϕ is estimated.

Value

A list containing the elements ϕ and σ with their estimated values.

Examples

```
# Sample data and observation times
tvec <- seq(0, 20, by = 0.5)
y <- c(-1.16, -0.18, 1.57, 1.99, 1.95, 1.85, 1.49, 1.58, 1.47, 0.96,
0.75, 0.22, -1.34, -1.72, -2.11, -1.56, -1.51, -1.29, -1.22,
-0.36, 1.78, 2.36, 1.78, 1.8, 1.76, 1.4, 1.02, 1.28, 1.21, 0.04,
-1.35, -2.1, -1.9, -1.49, -1.55, -1.35, -0.98, -0.34, 1.9, 1.99, 1.84)
```

```
gpsmoothing(y, tvec)
```

gpsmoothlik *Marginal log-likelihood for Gaussian process smoothing*

Description

Marginal log-likelihood and gradient as a function of GP hyper-parameters ϕ and observation noise standard deviation σ . For use in Gaussian process smoothing where values of ϕ and σ may be optimized.

Usage

```
gpsmoothlik(phisig, yobs, rInput, kerneltype = "generalMatern")
```

Arguments

phisig	vector containing GP hyper-parameters ϕ and observation noise SD σ . See calCov for the definitions of the hyper-parameters.
yobs	vector of observations
rInput	distance matrix between all time points of yobs
kerneltype	the covariance kernel, types matern, rbf, compact1, periodicMatern, generalMatern are supported. See calCov for their definitions.

Value

A list with elements value and grad, which are the log-likelihood value and gradient with respect to phisig, respectively.

Examples

```
# Suppose phi[1] = 0.5, phi[2] = 3, sigma = 0.1
gpsmoothlik(c(0.5, 3, 0.1), rnorm(10), abs(outer(0:9, t(0:9), '-')[, 1, ]))
```

hes1modelODE

*Hes1 equations: oscillation of mRNA and protein levels***Description**

The Hes1 equations model the oscillatory cycles of protein and messenger ribonucleic acid (mRNA) levels in cultured cells. The system components $X = (P, M, H)$ represent the concentrations of protein, mRNA, and the Hes1-interacting factor that provides a negative feedback loop.

P , M , and H are governed by the following differential equations:

$$\begin{aligned}\frac{dP}{dt} &= -aPH + bM - cP \\ \frac{dM}{dt} &= -d_M M + \frac{e}{1 + P^2} \\ \frac{dH}{dt} &= -aPH + \frac{f}{1 + P^2} - gH\end{aligned}$$

where $\theta = (a, b, c, d_M, e, f, g)$ are system parameters.

Usage

```
hes1modelODE(theta, x, tvec)
```

```
hes1modelDx(theta, x, tvec)
```

```
hes1modelDtheta(theta, x, tvec)
```

```
hes1logmodelODE(theta, x, tvec)
```

```
hes1logmodelDx(theta, x, tvec)
```

```
hes1logmodelDtheta(theta, x, tvec)
```

Arguments

theta	vector of parameters.
x	matrix of system states (one per column) at the time points in tvec.
tvec	vector of time points

Value

hes1modelODE returns an array with the values of the derivatives \dot{X} .

hes1modelDx returns a 3-D array with the values of the gradients with respect to X .

hes1modelDtheta returns a 3-D array with the values of the gradients with respect to θ .

hes1logmodelODE, hes1logmodelDx, and hes1logmodelDtheta are the log-transformed versions of hes1modelODE, hes1modelDx, and hes1modelDtheta, respectively.

References

Hirata H, Yoshiura S, Ohtsuka T, Bessho Y, Harada T, Yoshikawa K, Kageyama R (2002). Oscillatory Expression of the bHLH Factor Hes1 Regulated by a Negative Feedback Loop. *Science*, 298(5594), 840–843.

Examples

```
theta <- c(0.022, 0.3, 0.031, 0.028, 0.5, 20, 0.3)
x <- matrix(1:15, nrow = 5, ncol = 3)
tvec <- 1:5

hes1modelODE(theta, x, tvec)
```

is.magioutput	<i>MagiSolver output (magioutput) object</i>
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Description

Check for and create a magioutput object

Usage

```
is.magioutput(object)

magioutput(...)
```

Arguments

object	an R object
...	arguments required to create a magioutput object. See details.

Details

Using the core [MagiSolver](#) function returns a magioutput object as output, which is a list that contains the following elements:

theta matrix of MCMC samples for the system parameters θ , after burn-in.
xsampled array of MCMC samples for the system trajectories at each discretization time point, after burn-in.
sigma matrix of MCMC samples for the observation noise SDs σ , after burn-in.
phi matrix of estimated GP hyper-parameters, one column for each system component.
lp vector of log-posterior values at each MCMC iteration, after burn-in.

Printing a magioutput object displays a brief summary of the settings used for the MagiSolver run. The summary method for a magioutput object prints a table of parameter estimates, see [summary.magioutput](#) for more details. Plotting a magioutput object shows the inferred trajectories for each component, see [plot.magioutput](#) for more details.

Value

logical. Is the input a magioutput object?

Examples

```
# Set up odeModel list for the Fitzhugh-Nagumo equations
fnmodel <- list(
  fOde = fnmodelODE,
  fOdeDx = fnmodelDx,
  fOdeDtheta = fnmodelDtheta,
  thetaLowerBound = c(0, 0, 0),
  thetaUpperBound = c(Inf, Inf, Inf)
)

# Example FN data
data(FNdat)

# Create magioutput from a short MagiSolver run (demo only, more iterations needed for convergence)
result <- MagiSolver(FNdat, fnmodel, control = list(nstepsHmc = 5, niterHmc = 50))

is.magioutput(result)
```

magi

magi: *MANifold-Constrained Gaussian Process Inference*

Description

magi is a package that provides fast and accurate inference for the parameter estimation problem in Ordinary Differential Equations, including the case when there are unobserved system components. In the references below, please see Yang, Wong, and Kou (2021) for details of the MAGI method (MANifold-constrained Gaussian process Inference), and Wong, Yang, and Kou (2022) for a detailed user guide.

References

- Yang, S., Wong, S. W. K., & Kou, S. C. (2021). Inference of Dynamic Systems from Noisy and Sparse Data via Manifold-constrained Gaussian Processes. *Proceedings of the National Academy of Sciences*, 118 (15), e2020397118. doi:10.1073/pnas.2020397118
- Wong, S. W. K., Yang, S., & Kou, S. C. (2022). MAGI: A Package for Inference of Dynamic Systems from Noisy and Sparse Data via Manifold-constrained Gaussian Processes. <https://arxiv.org/abs/2203.06066>

MagiPosterior	<i>MAGI posterior density</i>
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Description

Computes the MAGI log-posterior value and gradient for an ODE model with the given inputs: the observations Y , the latent system trajectories X , the parameters θ , the noise standard deviations σ , and covariance kernels.

Usage

```
MagiPosterior(
  y,
  xlatent,
  theta,
  sigma,
  covAllDimInput,
  odeModel,
  priorTemperatureInput = 1,
  useBand = FALSE
)
```

Arguments

y	data matrix of observations
xlatent	matrix of system trajectory values
theta	vector of parameter values θ
sigma	vector of observation noise for each system component
covAllDimInput	list of covariance kernel objects for each system component. Covariance calculations may be carried out with calCov .
odeModel	list of ODE functions and inputs. See details.
priorTemperatureInput	vector of tempering factors for the GP prior, derivatives, and observations, in that order. Controls the influence of the GP prior relative to the likelihood. Recommended values: the total number of observations divided by the total number of discretization points for the GP prior and derivatives, and 1 for the observations.
useBand	logical: should the band matrix approximation be used? If TRUE, covAllDimInput must include CinvBand, mphiBand, and KinBand as computed by calCov .

Value

A list with elements value for the value of the log-posterior density and grad for its gradient.

Examples

```

# Trajectories from the Fitzhugh-Nagumo equations
tvec <- seq(0, 20, 2)
Vtrue <- c(-1, 1.91, 1.38, -1.32, -1.5, 1.73, 1.66, 0.89, -1.82, -0.93, 1.89)
Rtrue <- c(1, 0.33, -0.62, -0.82, 0.5, 0.94, -0.22, -0.9, -0.08, 0.95, 0.3)

# Noisy observations
Vobs <- Vtrue + rnorm(length(tvec), sd = 0.05)
Robs <- Rtrue + rnorm(length(tvec), sd = 0.1)

# Prepare distance matrix for covariance kernel calculation
foo <- outer(tvec, t(tvec), '-')[, 1, ]
r <- abs(foo)
r2 <- r^2
signr <- -sign(foo)

# Choose some hyperparameter values to illustrate
rphi <- c(0.95, 3.27)
vphi <- c(1.98, 1.12)
phiTest <- cbind(vphi, rphi)

# Covariance computations
curCovV <- calCov(phiTest[,1], r, signr, kerneltype = "generalMatern")
curCovR <- calCov(phiTest[,2], r, signr, kerneltype = "generalMatern")

# Y and X inputs to MagiPosterior
yInput <- data.matrix(cbind(Vobs, Robs))
xlatentTest <- data.matrix(cbind(Vtrue, Rtrue))

# Create odeModel list for FN equations
fnmodel <- list(
  fOde = fnmodelODE,
  fOdeDx = fnmodelDx,
  fOdeDtheta = fnmodelDtheta,
  thetaLowerBound = c(0, 0, 0),
  thetaUpperBound = c(Inf, Inf, Inf)
)

MagiPosterior(yInput, xlatentTest, theta = c(0.2, 0.2, 3), sigma = c(0.05, 0.1),
  list(curCovV, curCovR), fnmodel)

```

Description

Core function of the MAGI method for inferring the parameters and trajectories of dynamic systems governed by ordinary differential equations.

Usage

```
MagiSolver(y, odeModel, tvec, control = list())
```

Arguments

y data matrix of observations

odeModel list of ODE functions and inputs. See details.

tvec vector of discretization time points corresponding to rows of **y**. If missing, **MagiSolver** will use the column named 'time' in **y**.

control list of control variables, which may include 'sigma', 'phi', 'xInit', 'thetaInit', 'mu', 'dotmu', 'priorTemperature', 'niterHmc', 'burninRatio', 'nstepsHmc', 'stepSizeFactor', 'bandSize', 'useFixedSigma', 'verbose'. See details.

Details

The data matrix **y** has a column for each system component, and optionally a column 'time' with the discretization time points. If the column 'time' is not provided in **y**, a vector of time points must be provided via the **tvec** argument. The rows of **y** correspond to the discretization set I at which the GP is constrained to the derivatives of the ODE system. To set the desired discretization level for inference, use [setDiscretization](#) to prepare the data matrix for input into **MagiSolver**. Missing observations are indicated with NA or NaN.

The list **odeModel** is used for specification of the ODE system and its parameters. It must include five elements:

fOde function that computes the ODEs, specified with the form $f(\theta, x, t)$. See examples.

fOdeDx function that computes the gradients of the ODEs with respect to the system components. See examples.

fOdeDtheta function that computes the gradients of the ODEs with respect to the parameters θ . See examples.

thetaLowerBound a vector indicating the lower bounds of each parameter in θ .

thetaUpperBound a vector indicating the upper bounds of each parameter in θ .

Additional control variables can be supplied to **MagiSolver** via the optional list **control**, which may include the following:

sigma a vector of noise levels (observation noise standard deviations) σ for each component, at which to initialize MCMC sampling. By default, **MagiSolver** computes starting values for **sigma** via Gaussian process (GP) smoothing. If the noise levels are known, specify **sigma** together with **useFixedSigma = TRUE**.

phi a matrix of GP hyper-parameters for each component, with two rows for **phi[1]** and **phi[2]** and a column for each system component. By default, **MagiSolver** estimates **phi** via an optimization routine.

theta a vector of starting values for the parameters θ , at which to initialize MCMC sampling. By default, **MagiSolver** uses an optimization routine to obtain starting values.

xInit a matrix of values for the system trajectories of the same dimension as **y**, at which to initialize MCMC sampling. Default is linear interpolation between the observed (non-missing) values of **y** and an optimization routine for entirely unobserved components of **y**.

`mu` a matrix of values for the mean function of the GP prior, of the same dimension as `y`. Default is a zero mean function.

`dotmu` a matrix of values for the derivatives of the GP prior mean function, of the same dimension as `y`. Default is zero.

`priorTemperature` the tempering factor by which to divide the contribution of the GP prior, to control the influence of the GP prior relative to the likelihood. Default is the total number of observations divided by the total number of discretization points.

`niterHmc` MCMC sampling from the posterior is carried out via Hamiltonian Monte Carlo (HMC). `niterHmc` specifies the number of HMC iterations to run. Default is 20000 HMC iterations.

`nstepsHmc` the number of leapfrog steps per HMC iteration. Default is 200.

`burninRatio` the proportion of HMC iterations to be discarded as burn-in. Default is 0.5, which discards the first half of the MCMC samples.

`stepSizeFactor` initial leapfrog step size factor for HMC. Can be specified as a scalar (applied to all posterior dimensions) or a vector (with length corresponding to the dimension of the posterior). Default is 0.01, and the leapfrog step size is automatically tuned during burn-in to achieve an acceptance rate between 60-90%.

`bandSize` a band matrix approximation is used to speed up matrix operations, with default band size 20. Can be increased if MagiSolver returns an error indicating numerical instability.

`useFixedSigma` logical, set to TRUE if `sigma` is known. If `useFixedSigma=TRUE`, the known values of σ must be supplied via the `sigma` control variable. Default is FALSE.

`skipMissingComponentOptimization` logical, set to TRUE to skip automatic optimization for missing components. If `skipMissingComponentOptimization=TRUE`, values for `xInit` and `phi` must be supplied for all system components. Default is FALSE.

`positiveSystem` logical, set to TRUE if the system cannot be negative. Default is FALSE.

`verbose` logical, set to TRUE to output diagnostic and progress messages to the console. Default is FALSE.

Value

MagiSolver returns an object of class `magioutput` which contains the following elements:

`theta` matrix of MCMC samples for the system parameters θ , after burn-in.

`xsampled` array of MCMC samples for the system trajectories at each discretization time point, after burn-in.

`sigma` matrix of MCMC samples for the observation noise SDs σ , after burn-in.

`phi` matrix of estimated GP hyper-parameters, one column for each system component.

`lp` vector of log-posterior values at each MCMC iteration, after burn-in.

`y`, `tvec`, `odeModel` from the inputs to MagiSolver.

References

Shihao Yang, Samuel WK Wong, SC Kou (2021). Inference of Dynamic Systems from Noisy and Sparse Data via Manifold-constrained Gaussian Processes. *Proceedings of the National Academy of Sciences*, 118 (15), e2020397118.

Examples

```

# Set up odeModel list for the Fitzhugh-Nagumo equations
fnmodel <- list(
  fOde = fnmodelODE,
  fOdeDx = fnmodelDx,
  fOdeDtheta = fnmodelDtheta,
  thetaLowerBound = c(0, 0, 0),
  thetaUpperBound = c(Inf, Inf, Inf)
)

# Example noisy data observed from the FN system
data(FNdat)

# Set discretization for a total of 81 equally-spaced time points from 0 to 20
yinput <- setDiscretization(FNdat, by = 0.25)

# Run MagiSolver
# Short sampler run for demo only, more iterations needed for convergence
MagiSolver(yinput, fnmodel, control = list(nstepsHmc = 5, niterHmc = 101))

# Use 3000 HMC iterations with 100 leapfrog steps per iteration
FNres <- MagiSolver(yinput, fnmodel, control = list(nstepsHmc = 100, niterHmc = 3000))
# Summary of parameter estimates
summary(FNres)
# Plot of inferred trajectories
plot(FNres, comp.names = c("V", "R"), xlab = "Time", ylab = "Level")

```

plot.magioutput

Plot trajectories from magioutput object

Description

Plots the inferred trajectories from the output of MagiSolver

Usage

```

## S3 method for class 'magioutput'
plot(
  x,
  obs = TRUE,
  ci = TRUE,
  comp.names,
  lower = 0.025,
  upper = 0.975,
  nplotcol = 3,
  ...
)

```

Arguments

<code>x</code>	a magioutput object.
<code>obs</code>	logical; if true, points will be added on the plots for the observations.
<code>ci</code>	logical; if true, credible bands will be added to the plots.
<code>comp.names</code>	vector of system component names. If provided, should be the same length as the number of system components in X .
<code>lower</code>	the lower quantile of the credible band, default is 0.025. Only used if <code>ci = TRUE</code> .
<code>upper</code>	the upper quantile of the credible band, default is 0.975. Only used if <code>ci = TRUE</code> .
<code>nplotcol</code>	the number of subplots per row.
<code>...</code>	additional arguments to <code>plot</code> .

Details

Plots inferred trajectories (posterior means) and credible bands from the MCMC samples, one subplot for each system component. By default, `lower = 0.025` and `upper = 0.975` produces a central 95% credible band when `ci = TRUE`. Adding the observed data points (`obs = TRUE`) can provide a visual assessment of the inferred trajectories.

Examples

```
# Set up odeModel list for the Fitzhugh-Nagumo equations
fnmodel <- list(
  fOde = fnmodelODE,
  fOdeDx = fnmodelDx,
  fOdeDtheta = fnmodelDtheta,
  thetaLowerBound = c(0, 0, 0),
  thetaUpperBound = c(Inf, Inf, Inf)
)

# Example FN data
data(FNdat)
y <- setDiscretization(FNdat, by = 0.25)

# Create magioutput from a short MagiSolver run (demo only, more iterations needed for convergence)
result <- MagiSolver(y, fnmodel, control = list(nstepsHmc = 20, niterHmc = 500))

plot(result, comp.names = c("V", "R"), xlab = "Time", ylab = "Level")
```


Description

The protein transduction equations model a biochemical reaction involving a signaling protein that degrades over time. The system components $X = (S, S_d, R, S_R, R_{pp})$ represent the levels of signaling protein, its degraded form, inactive state of R , $S - R$ complex, and activated state of R .

S, S_d, R, S_R and R_{pp} are governed by the following differential equations:

$$\begin{aligned}\frac{dS}{dt} &= -k_1 \cdot S - k_2 \cdot S \cdot R + k_3 \cdot S_R \\ \frac{dS_d}{dt} &= k_1 \cdot S \\ \frac{dR}{dt} &= -k_2 \cdot S \cdot R + k_3 \cdot S_R + \frac{V \cdot R_{pp}}{K_m + R_{pp}} \\ \frac{dS_R}{dt} &= k_2 \cdot S \cdot R - k_3 \cdot S_R - k_4 \cdot S_R \\ \frac{dR_{pp}}{dt} &= k_4 \cdot S_R - \frac{V \cdot R_{pp}}{K_m + R_{pp}}\end{aligned}$$

where $\theta = (k_1, k_2, k_3, k_4, V, K_m)$ are system parameters.

Usage

```
ptransmodelODE(theta, x, tvec)
```

```
ptransmodelDx(theta, x, tvec)
```

```
ptransmodelDtheta(theta, x, tvec)
```

Arguments

theta	vector of parameters.
x	matrix of system states (one per column) at the time points in tvec.
tvec	vector of time points

Value

ptransmodelODE returns an array with the values of the derivatives \dot{X} .

ptransmodelDx returns a 3-D array with the values of the gradients with respect to X .

ptransmodelDtheta returns a 3-D array with the values of the gradients with respect to θ .

References

Vyshemirsky, V., & Girolami, M. A. (2008). Bayesian Ranking of Biochemical System Models. *Bioinformatics*, 24(6), 833-839.

Examples

```
theta <- c(0.07, 0.6, 0.05, 0.3, 0.017, 0.3)
x <- matrix(1:25, nrow = 5, ncol = 5)
tvec <- 1:5

ptransmodelODE(theta, x, tvec)
```

```
setDiscretization      Set discretization level
```

Description

Set the discretization level of a data matrix for input to [MagiSolver](#), by inserting time points where the GP is constrained to the derivatives of the ODE system.

Usage

```
setDiscretization(dat, level, by)
```

Arguments

dat	data matrix. Must include a column with name 'time'.
level	discretization level (a positive integer). $2^{\text{level}} - 1$ equally-spaced points will be inserted between existing data points in dat.
by	discretization interval. As an alternative to level, equally-spaced spaced time points will be inserted with interval by between successive points.

Details

Specify the desired discretization using level or by.

Value

Returns a data matrix with the same columns as dat, with rows added for the inserted discretization time points.

Examples

```
dat <- data.frame(time = 0:10, x = rnorm(11))
setDiscretization(dat, level = 2)
setDiscretization(dat, by = 0.2)
```

summary.magioutput *Summary of parameter estimates from magioutput object*

Description

Computes a summary table of parameter estimates from the output of MagiSolver

Usage

```
## S3 method for class 'magioutput'
summary(
  object,
  sigma = FALSE,
  par.names,
  lower = 0.025,
  upper = 0.975,
  digits = 3,
  ...
)
```

Arguments

object	a magioutput object.
sigma	logical; if true, the noise levels σ will be included in the summary.
par.names	vector of parameter names for the summary table. If provided, should be the same length as the number of parameters in θ , or the combined length of θ and σ when sigma = TRUE.
lower	the lower quantile of the credible interval, default is 0.025.
upper	the upper quantile of the credible interval, default is 0.975.
digits	integer; the number of significant digits to print.
...	additional arguments affecting the summary produced.

Details

Computes parameter estimates (posterior means) and credible intervals from the MCMC samples. By default, lower = 0.025 and upper = 0.975 produces a central 95% credible interval.

Value

Returns a matrix where rows display the posterior mean, lower credible limit, and upper credible limit of each parameter.

Examples

```
# Set up odeModel list for the Fitzhugh-Nagumo equations
fnmodel <- list(
  fOde = fnmodelODE,
  fOdeDx = fnmodelDx,
  fOdeDtheta = fnmodelDtheta,
  thetaLowerBound = c(0, 0, 0),
  thetaUpperBound = c(Inf, Inf, Inf)
)

# Example FN data
data(FNdat)

# Create magioutput from a short MagiSolver run (demo only, more iterations needed for convergence)
result <- MagiSolver(FNdat, fnmodel, control = list(nstepsHmc = 5, niterHmc = 100))

summary(result, sigma = TRUE, par.names = c("a", "b", "c", "sigmaV", "sigmaR"))
```

testDynamicalModel *Test dynamic system model specification*

Description

Given functions for the ODE and its gradients (with respect to the system components and parameters), verify the correctness of the gradients using numerical differentiation.

Usage

```
testDynamicalModel(modelODE, modelDx, modelDtheta, modelName, x, theta, tvec)
```

Arguments

modelODE	function that computes the ODEs, specified with the form $f(\theta, x, t)$. See examples.
modelDx	function that computes the gradients of the ODEs with respect to the system components. See examples.
modelDtheta	function that computes the gradients of the ODEs with respect to the parameters θ . See examples.
modelName	string giving a name for the model
x	data matrix of system values, one column for each component, at which to test the gradients
theta	vector of parameter values for θ , at which to test the gradients
tvec	vector of time points corresponding to the rows of x

Details

Calls `test_that` to test equality of the analytic and numeric gradients.

Value

A list with elements testDx and testDtheta, each with value TRUE if the corresponding gradient check passed and FALSE if not.

Examples

```
# ODE system and gradients for Fitzhugh-Nagumo equations: fnmodelODE, fnmodelDx, fnmodelDtheta

# Example of incorrect gradient with respect to parameters theta
fnmodelDthetaWrong <- function(theta, x, tvec) {
  resultDtheta <- array(0, c(nrow(x), length(theta), ncol(x)))

  V = x[, 1]
  R = x[, 2]

  resultDtheta[, 3, 1] = V - V^3 / 3.0 - R

  resultDtheta[, 1, 2] = 1.0 / theta[3]
  resultDtheta[, 2, 2] = -R / theta[3]
  resultDtheta[, 3, 2] = 1.0 / (theta[3]^2) * (V - theta[1] + theta[2] * R)

  resultDtheta
}

# Sample data for testing gradient correctness
data(FNdat)

# Correct gradients
testDynamicalModel(fnmodelODE, fnmodelDx, fnmodelDtheta,
  "FN equations", FNdat[, c("V", "R")], c(.5, .6, 2), FNdat$time)

# Incorrect theta gradient (test fails)
testDynamicalModel(fnmodelODE, fnmodelDx, fnmodelDthetaWrong,
  "FN equations", FNdat[, c("V", "R")], c(.5, .6, 2), FNdat$time)
```

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