# Package 'KGode'

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<b>Title</b> Kernel Based Gradient Matching for Parameter Inference in Ordinary Differential Equations
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<b>Description</b> The kernel ridge regression and the gradient matching algorithm proposed in Niu et al. (2016) <a href="https://proceedings.mlr.press/v48/niu16.html">httml</a> and the warp ing algorithm proposed in Niu et al. (2017) <a href="https://poli.org/10.1007/s00180-017-0753-z">DOI:10.1007/s00180-017-0753-z</a> are implemented for parameter inference in differential equations. Four schemes are provided for improving parameter estimation in odes by using the odes regularisation and warping.
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R topics documented:
bootstrap
crossv
diagnostic
Kernel
MLP
ode
RBF
rkg3
rkhs

2 bootstrap

	Warp	26
	warpfun	28
	warpInitLen	31
Index	3	34

bootstrap	The 'bootstrap' function
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#### **Description**

This function is used to perform bootstrap procedure to estimate parameter uncertainty.

#### Usage

```
bootstrap(kkk, y_no, ktype, K, ode_par, intp_data, www = NULL)
```

## Arguments

kkk	ode class object.
y_no	matrix(of size $n_s*n_o$ ) containing noisy observations. The row(of length $n_s$ ) represent the ode states and the column(of length $n_o$ ) represents the time points.
ktype	character containing kernel type. User can choose 'rbf' or 'mlp' kernel.
K	the number of bootstrap replicates to collect.
ode_par	a vector of ode parameters estimated using gradient matching.
intp_data	a list of interpolations produced by gradient matching for each ode state.
www	an optional warping object (if warping has been performed using warpfun).

#### **Details**

Arguments of the 'bootstrap' function are 'ode' class, noisy observation, kernel type, the set of parameters that have been estimated before using gradient matching, a list of interpolations for each of the ode state from gradient matching, and the warping object (if warping has been performed). It returns a vector of the median absolute standard deviations for each ode state, computed from the bootstrap replicates.

#### Value

return a vector of the median absolute deviation (MAD) for each ode state.

#### Author(s)

Mu Niu <mu.niu@glasgow.ac.uk>

bootstrap 3

```
## Not run:
require(mvtnorm)
noise = 0.1 ## set the variance of noise
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
  alpha=par_ode[1]
  beta=par_ode[2]
  gamma=par_ode[3]
  delta=par_ode[4]
  as.matrix( c(alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
}
## Define the gradient of ode function against ode parameters
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum( 2*( z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum(2*(z_p[2,]-grad_ode[2,])*gamma*y_p[2,])
dres[4] = sum(-2*(z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
}
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_grlNODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Add noise to the numerical solution of the ode model and use it as the noisy observation.
n_o = max(dim(kkk0\$y_ode))
t_no = kkk0$t
y_no = t(kkk0y_ode) + rmvnorm(n_o,c(0,0),noise*diag(2))
## Create a ode class object by using the simulation data we created from the ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## Set initial value of ode parameters.
init_par = rep(c(0.1),4)
init\_yode = t(y\_no)
init_t = t_no
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode)
## The following examples with CPU or elapsed time > 10s
```

4 bootstrap

```
##Use function 'rkg' to estimate the ode parameters. The standard gradient matching method is coded
##in the the 'rkg' function. The parameter estimations are stored in the returned vector of 'rkg'.
## Choose a kernel type for 'rkhs' interpolation. Two options are provided 'rbf' and 'mlp'.
ktype ='rbf'
rkgres = rkg(kkk,y_no,ktype)
## show the results of ode parameter estimation using the standard gradient matching
kkk$ode_par
## Perform bootstrap procedure to estimate the median absolute deviations of ode parameters
# here we get the resulting interpolation from gradient matching using 'rkg' for each ode state
bbb = rkgres$bbb
nst = length(bbb)
intp_data = list()
for( i in 1:nst) {
    intp_data[[i]] = bbb[[i]]$predictT(bbb[[i]]$t)$pred
K = 12 # the number of bootstrap replicates
mads = bootstrap(kkk, y_no, ktype, K, ode_par, intp_data)
## show the results of ode parameter estimation and its uncertainty
## using the standard gradient matching
ode_par
mads
########## gradient matching + ODE regularisation
crtype='i'
lam=c(10,1,1e-1,1e-2,1e-4)
lamil1 = crossv(lam,kkk,bbb,crtype,y_no)
lambdai1=lamil1[[1]]
res = third(lambdai1,kkk,bbb,crtype)
oppar = res$oppar
### do bootstrap here for gradient matching + ODE regularisation
ode_par = oppar
K = 12
intp_data = list()
for( i in 1:nst) {
    intp_data[[i]] = res$rk3$rk[[i]]$predictT(bbb[[i]]$t)$pred
mads = bootstrap(kkk, y_no, ktype, K, ode_par, intp_data)
ode_par
mads
######### gradient matching + ODE regularisation + warping
##### warp state
peod = c(6,5.3) #8#9.7
                           ## the guessing period
                ## the standard deviation of period
fixlens=warpInitLen(peod,eps,rkgres)
kkkrkg = kkk$clone()
www = warpfun(kkkrkg,bbb,peod,eps,fixlens,y_no,kkkrkg$t)
### do bootstrap here for gradient matching + ODE regularisation + warping
nst = length(bbb)
```

crossv 5

```
K = 12
ode_par = www$wkkk$ode_par
intp_data = list()
for( i in 1:nst) {
    intp_data[[i]] = www$bbbw[[i]]$predictT(www$wtime[i, ])$pred
}
mads = bootstrap(kkk, y_no, ktype, K, ode_par, intp_data,www)
ode_par
mads
## End(Not run)
```

crossv

The 'crossy' function

## Description

This function is used to estimate the weighting parameter for ode regularisation using cross validation.

## Usage

```
crossv(lam, kkk, bbb, crtype, y_no, woption, resmtest, dtilda, fold)
```

## Arguments

lam	vector containing different choices of the weighting parameter of ode regularisation.
kkk	'ode' class object containing all information about the odes.
bbb	list of 'rkhs' class object containing the interpolation for all ode states.
crtype	character containing the optimisation scheme type. User can choose 'i' or '3'. 'i' is for fast iterative scheme and '3' for optimising the ode parameters and interpolation coefficients simultaneously.
y_no	matrix(of size $n_s*n_o$ ) containing noisy observations. The row(of length $n_s$ ) represent the ode states and the column(of length $n_o$ ) represents the time points.
woption	character containing the indication of using warping. If the warping scheme is done before using the ode regularisation, user can choose 'w' otherwise just leave this option empty.
resmtest	vector(of length n_o) containing the warped time points. This variable is only used if user want to combine warping and the ode regularisation.
dtilda	vector(of length n_o) containing the gradient of warping function. This variable is only used if user want to combine warping and the ode regularisation.
fold	scalar indicating the folds of cross validation.

6 crossv

#### **Details**

Arguments of the 'crossv' function are list of weighting parameter for ode regularisation, 'ode' class objects, 'rkhs' class objects, noisy observation, type of regularisation scheme, option of warping and the gradient of warping function. It return the interpolation for each of the ode states. The ode parameters are estimated using gradient matching, and the results are stored in the 'ode' class as the ode\_par attribute.

#### Value

return list containing:

- lam scalar containing the optimised weighting parameter.
- ress -vector containing the cross validation error for all choices of weighting parameter.

#### Author(s)

Mu Niu <mu.niu@glasgow.ac.uk>

```
## Not run:
require(mvtnorm)
noise = 0.1
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
  alpha=par_ode[1]
  beta=par_ode[2]
  gamma=par_ode[3]
  delta=par_ode[4]
  as.matrix( c(alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
## Define the gradient of ode function against ode parameters
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum( 2*( z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum(2*(z_p[2,]-grad_ode[2,])*gamma*y_p[2,])
dres[4] = sum(-2*(z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_gr1NODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
```

diagnostic 7

```
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Add noise to the numerical solution of the ode model and use it as the noisy observation.
n_o = max(dim(kkk0\$y_ode))
t_no = kkk0$t
y_no = t(kkk0y_ode) + rmvnorm(n_o,c(0,0),noise*diag(2))
## create a ode class object by using the simulation data we created from the Ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## set initial value of Ode parameters.
init_par = rep(c(0.1),4)
init\_yode = t(y\_no)
init_t = t_no
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode)
## The following examples with CPU or elapsed time > 10s
## Use function 'rkg' to estimate the Ode parameters.
ktype ='rbf'
rkgres = rkg(kkk,y_no,ktype)
bbb = rkgres$bbb
########## gradient matching + third step
crtype='i'
## using cross validation to estimate the weighting parameters of the ode regularisation
lam=c(1e-4, 1e-5)
lamil1 = crossv(lam,kkk,bbb,crtype,y_no)
lambdai1=lamil1[[1]]
## End(Not run)
```

diagnostic

The 'diagnostic' function

#### Description

This function is used to perform diagnostic procedure to compute the residual and make diagnostic plots.

#### Usage

```
diagnostic(infer_list, index, type, qq_plot)
```

#### **Arguments**

infer\_list a list of inference results including ode objects and inference objects.

the index of the ode states which the user want to do the diagnostic analysis.

8 diagnostic

type character containing the type of inference methods. User can choose 'rkg', 'third', or 'warp'.

qq\_plot boolean variable, enable or disable the plotting function.

#### **Details**

Arguments of the 'diagnostic' function are inference list, inference type, a list of interpolations for each of the ode state from gradient matching, and . It returns a vector of the median absolute standard deviations for each ode state.

#### Value

return list containing:

- residual vector containing residual.
- interp vector containing interpolation.

#### Author(s)

Mu Niu <mu.niu@glasgow.ac.uk>

```
## Not run:
require(mvtnorm)
set.seed(SEED); SEED = 19537
FN_fun <- function(t, x, par_ode) {</pre>
a = par_ode[1]
b = par_ode[2]
c = par_ode[3]
as.matrix(c(c*(x[1]-x[1]^3/3 + x[2]), -1/c*(x[1]-a+b*x[2])))
solveOde = ode$new(sample=2,fun=FN_fun)
xinit = as.matrix(c(-1,-1))
tinterv = c(0,10)
solveOde$solve_ode(par_ode=c(0.2,0.2,3),xinit,tinterv)
n_o = max(dim(solveOde$y_ode))
noise = 0.01
y_no = t(solveOde\$y_ode)+rmvnorm(n_o,c(0,0),noise*diag(2))
t_no = solve0de$t
odem = ode new(fun = FN_fun, grfun = NULL, t = t_no, ode_par = rep(c(0.1), 3), y_ode = t(y_no))
ktype = 'rbf'
rkgres = rkg(odem,y_no,ktype)
rkgdiag = diagnostic( rkgres,1,'rkg',qq_plot=FALSE )
## End(Not run)
```

Kernel 9

Kernel

The 'Kernel' class object

#### **Description**

This a abstract class provide the kernel function and the 1st order derivative of rbf kernel function.

#### **Format**

R6Class object.

#### Value

an R6Class object which can be used for the rkhs interpolation.

#### Methods

kern(t1,t2) This method is used to calculate the kernel function given two one dimensional real inputs.

dkd\_kpar(t1,t2) This method is used to calculate the gradient of kernel function against the kernel hyper parameters given two one dimensional real inputs.

dkdt(t1,t2) This method is used to calculate the 1st order derivative of kernel function given two one dimensional real inputs.

#### **Public fields**

k\_par vector(of length n\_hy) containing the hyper-parameter of kernel. n\_hy is the length of kernel hyper parameters.

#### Methods

#### **Public methods:**

- Kernel\$new()
- Kernel\$greet()
- Kernel\$kern()
- Kernel\$dkd\_kpar()
- Kernel\$dkdt()
- Kernel\$clone()

#### Method new():

```
Usage:
Kernel$new(k_par = NULL)
```

## Method greet():

Usage:

10 MLP

```
Method kern():
    Usage:
    Kernel$kern(t1, t2)

Method dkd_kpar():
    Usage:
    Kernel$dkd_kpar(t1, t2)

Method dkdt():
    Usage:
    Kernel$dkdt(t1, t2)

Method clone(): The objects of this class are cloneable with this method.
    Usage:
    Kernel$clone(deep = FALSE)
    Arguments:
    deep Whether to make a deep clone.

or(s)
```

## Author(s)

Mu Niu, <mu.niu@glasgow.ac.uk>

MLP

The 'MLP' class object

## Description

This a R6 class. It inherits from 'kernel' class. It provides the mlp kernel function and the 1st order derivative of mlp kernel function.

### **Format**

R6Class object.

#### Value

an R6Class object which can be used for the rkhs interpolation.

## Super class

KGode::Kernel -> MLP

MLP 11

#### Methods

```
Public methods:
  • MLP$greet()
  • MLP$set_k_par()
  • MLP$kern()
  • MLP$dkd_kpar()
  • MLP$dkdt()
  • MLP$clone()
Method greet():
 Usage:
 MLP$greet()
Method set_k_par():
 Usage:
 MLP$set_k_par(val)
Method kern():
 Usage:
 MLP$kern(t1, t2)
Method dkd_kpar():
 Usage:
 MLP$dkd_kpar(t1, t2)
Method dkdt():
 Usage:
 MLP$dkdt(t1, t2)
Method clone(): The objects of this class are cloneable with this method.
 Usage:
 MLP$clone(deep = FALSE)
 Arguments:
 deep Whether to make a deep clone.
```

## Author(s)

Mu Niu, <mu.niu@glasgow.ac.uk>

12 ode

ode

The 'ode' class object

#### **Description**

This class provide all information about odes and methods for numerically solving odes.

#### **Format**

R6Class object.

#### Value

an R6Class object which can be used for gradient matching.

#### Methods

solve\_ode(par\_ode,xinit,tinterv) This method is used to solve ode numerically.

optim\_par(par,y\_p,z\_p) This method is used to estimate ode parameters by standard gradient matching.

lossNODE(par,y\_p,z\_p) This method is used to calculate the mismatching between gradient of interpolation and gradient from ode.

#### **Public fields**

ode\_par vector(of length n\_p) containing ode parameters. n\_p is the number of ode parameters. ode\_fun function containing the ode function.

t vector(of length n\_o) containing time points of observations. n\_o is the length of time points.

#### Methods

#### **Public methods:**

- ode\$new()
- ode\$greet()
- ode\$solve\_ode()
- ode\$rmsfun()
- ode\$gradient()
- ode\$lossNODE()
- ode\$grlNODE()
- ode\$loss32NODE()
- ode\$grl32NODE()
- ode\$optim\_par()
- ode\$clone()

### Method new():

ode 13

```
Usage:
 ode$new(
   sample = NULL,
   fun = NULL,
   grfun = NULL,
   t = NULL,
   ode_par = NULL,
   y\_ode = NULL
 )
Method greet():
 Usage:
 ode$greet()
Method solve_ode():
 Usage:
 ode$solve_ode(par_ode, xinit, tinterv)
Method rmsfun():
 Usage:
 ode$rmsfun(par_ode, state, M1, true_par)
Method gradient():
 Usage:
 ode$gradient(y_p, par_ode)
Method lossNODE():
 Usage:
 ode$lossNODE(par, y_p, z_p)
Method grlNODE():
 Usage:
 ode$grlNODE(par, y_p, z_p)
Method loss32NODE():
 Usage:
 ode$loss32NODE(par, y_p, z_p)
Method grl32NODE():
 Usage:
 ode$gr132NODE(par, y_p, z_p)
Method optim_par():
 Usage:
 ode$optim_par(par, y_p, z_p)
Method clone(): The objects of this class are cloneable with this method.
 Usage:
 ode$clone(deep = FALSE)
 Arguments:
 deep Whether to make a deep clone.
```

14 RBF

#### Author(s)

```
Mu Niu, < mu.niu@glasgow.ac.uk>
```

```
noise = 0.1 ## set the variance of noise
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
  alpha=par_ode[1]
  beta=par_ode[2]
  gamma=par_ode[3]
  delta=par_ode[4]
  as.matrix( c(alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
## Define the gradient of ode function against ode parameters
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum( 2*( z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum( 2*( z_p[2,]-grad_ode[2,])*gamma*y_p[2,] )
dres[4] = sum( -2*( z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
}
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_grlNODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Create another ode class object by using the simulation data from the ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## set initial values for ode parameters.
init_par = rep(c(0.1),4)
init_yode = kkk0$y_ode
init_t = kkk0$t
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode )
```

RBF 15

#### **Description**

This a R6 class. It inherits from 'kernel' class. It provides the rbf kernel function and the 1st order derivative of rbf kernel function.

#### **Format**

```
R6Class object.
```

#### Value

an R6Class object which can be used for the rkhs interpolation.

#### Super class

```
KGode::Kernel -> RBF
```

## Methods

#### **Public methods:**

```
• RBF$greet()
```

- RBF\$set\_k\_par()
- RBF\$kern()
- RBF\$dkd\_kpar()
- RBF\$dkdt()
- RBF\$clone()

## Method greet():

```
Usage:
RBF$greet()
```

## Method set\_k\_par():

```
Usage:
```

RBF\$set\_k\_par(val)

#### Method kern():

```
Usage:
```

RBF\$kern(t1, t2)

## Method dkd\_kpar():

Usage:

RBF\$dkd\_kpar(t1, t2)

## Method dkdt():

Usage:

RBF\$dkdt(t1, t2)

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

```
Usage:
```

RBF\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

## Author(s)

Mu Niu, <mu.niu@glasgow.ac.uk>

rkg

The 'rkg' function

#### **Description**

This function is used to create 'rkhs' class object and estimate ode parameters using standard gradient matching.

## Usage

```
rkg(kkk, y_no, ktype)
```

## **Arguments**

kkk ode class object.

y\_no matrix(of size n\_s\*n\_o) containing noisy observations. The row(of length n\_s)

represent the ode states and the column(of length n\_o) represents the time points.

ktype character containing kernel type. User can choose 'rbf' or 'mlp' kernel.

#### **Details**

Arguments of the 'rkg' function are 'ode' class, noisy observation, and kernel type. It return the interpolation for each of the ode states. The Ode parameters are estimated using gradient matching, and the results are stored in the 'ode' class as the ode\_par attribute.

## Value

return list containing:

- intp list containing interpolation for each ode state.
- bbb rkhs class objects for each ode state.

#### Author(s)

Mu Niu <mu.niu@glasgow.ac.uk>

```
## Not run:
require(mvtnorm)
noise = 0.1 ## set the variance of noise
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
  alpha=par_ode[1]
  beta=par_ode[2]
  gamma=par_ode[3]
  delta=par_ode[4]
  as.matrix( c(alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
}
## Define the gradient of ode function against ode parameters
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum( 2*( z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum(2*(z_p[2,]-grad_ode[2,])*gamma*y_p[2,])
dres[4] = sum(-2*(z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
}
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_grlNODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Add noise to the numerical solution of the ode model and use it as the noisy observation.
n_o = max(dim(kkk0\$y_ode))
t_no = kkk0$t
y_no = t(kkk0y_ode) + rmvnorm(n_o,c(0,0),noise*diag(2))
## Create a ode class object by using the simulation data we created from the ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## Set initial value of ode parameters.
init_par = rep(c(0.1),4)
init\_yode = t(y\_no)
init_t = t_no
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode)
## The following examples with CPU or elapsed time > 10s
```

```
##Use function 'rkg' to estimate the ode parameters. The standard gradient matching method is coded
##in the the 'rkg' function. The parameter estimations are stored in the returned vector of 'rkg'.
## Choose a kernel type for 'rkhs' interpolation. Two options are provided 'rbf' and 'mlp'.
ktype ='rbf'
rkgres = rkg(kkk,y_no,ktype)
## show the results of ode parameter estimation using the standard gradient matching
kkk$ode_par
## End(Not run)
```

rkg3

The 'rkg3' class object

#### **Description**

This class provides advanced gradient matching method by using the ode as a regularizer.

#### **Format**

R6Class object.

#### Value

an R6Class object which can be used for improving ode parameters estimation by using ode as a regularizer.

## Methods

iterate(iter,innerloop,lamb) Iteratively updating ode parameters and interpolation regression coefficients.

witerate(iter,innerloop,dtilda,lamb) Iteratively updating ode parameters and the warped interpolation regression coefficients.

full(par, lam) Updating ode parameters and rkhs interpolation regression coefficients simultaneously. This method is slow but guarantee convergence.

#### **Public fields**

rk the 'rkhs' class object containing the interpolation information for each state of the ode. ode\_m the 'ode' class object containing the information about the odes.

#### **Active bindings**

ode\_m the 'ode' class object containing the information about the odes.

#### Methods

```
Public methods:
  • rkg3$new()
  • rkg3$greet()
  • rkg3$add()
  • rkg3$iterate()
  • rkg3$witerate()
  • rkg3$full()
  • rkg3$wfull()
  • rkg3$opfull()
  • rkg3$wopfull()
  • rkg3$cross()
  • rkg3$fullos()
  • rkg3$clone()
Method new():
 Usage:
 rkg3$new(rk = NULL, odem = NULL)
Method greet():
 Usage:
 rkg3$greet()
Method add():
 Usage:
 rkg3$add(x)
Method iterate():
 Usage:
 rkg3$iterate(iter, innerloop, lamb)
Method witerate():
 Usage:
 rkg3$witerate(iter, innerloop, dtilda, lamb)
Method full():
 Usage:
 rkg3$full(par, lam)
Method wfull():
 Usage:
 rkg3$wfull(par, lam, dtilda)
Method opfull():
```

20 rkhs

```
Usage:
  rkg3$opfull(lam)

Method wopfull():
    Usage:
    rkg3$wopfull(lam, dtilda)

Method cross():
    Usage:
    rkg3$cross(lam, testX, testY)

Method fullos():
    Usage:
    rkg3$fullos(par)

Method clone(): The objects of this class are cloneable with this method.
    Usage:
    rkg3$clone(deep = FALSE)
    Arguments:
    deep Whether to make a deep clone.
```

Author(s)

Mu Niu, <mu.niu@glasgow.ac.uk>

rkhs

The 'rkhs' class object

#### **Description**

This class provide the interpolation methods using reproducing kernel Hilbert space.

## **Format**

R6Class object.

#### Value

an R6Class object which can be used for doing interpolation using reproducing kernel Hilbert space.

#### Methods

```
predict() This method is used to make prediction on given time points
```

skcross() This method is used to do cross-validation to estimate the weighting parameter lambda of  $L^2$  norm.

rkhs 21

#### **Public fields**

```
y matrix(of size n_s*n_o) containing observation.
```

- t vector(of length n\_o) containing time points for observation.
- b vector(of length n\_o) containing coefficients of kernel or basis functions.

lambda scalar containing the weighting parameter for L2 norm of the reproducing kernel Hilbert space.

ker kernel class object containing kernel.

#### Methods

```
Public methods:
```

```
rkhs$new()
```

- rkhs\$greet()
- rkhs\$showker()
- rkhs\$predict()
- rkhs\$predictT()
- rkhs\$lossRK()
- rkhs\$grlossRK()
- rkhs\$numgrad()
- rkhs\$skcross()
- rkhs\$mkcross()
- rkhs\$loss11()
- rkhs\$grloss11()
- rkhs\$clone()

#### Method new():

```
Usage:
  rkhs$new(y = NULL, t = NULL, b = NULL, lambda = NULL, ker = NULL)

Method greet():
  Usage:
  rkhs$greet()

Method showker():
  Usage:
  rkhs$showker()
Method predict():
```

## Method predictT():

rkhs\$predict()

Usage:

Usage:

rkhs rkhs

```
rkhs$predictT(testT)
Method lossRK():
 Usage:
 rkhs$lossRK(par, tl1, y_d, jitter)
Method grlossRK():
 Usage:
 rkhs$grlossRK(par, tl1, y_d, jitter)
Method numgrad():
 Usage:
 rkhs$numgrad(par, tl1, y_d, jitter)
Method skcross():
 Usage:
 rkhs$skcross(init, bounded)
Method mkcross():
 Usage:
 rkhs$mkcross(init)
Method loss11():
 Usage:
 rkhs$loss11(par, tl1, y_d, jitter)
Method grloss11():
 Usage:
 rkhs$grloss11(par, tl1, y_d, jitter)
Method clone(): The objects of this class are cloneable with this method.
 Usage:
 rkhs$clone(deep = FALSE)
 Arguments:
 deep Whether to make a deep clone.
```

#### Author(s)

```
Mu Niu, <mu.niu@glasgow.ac.uk>
```

rkhs 23

```
## Not run:
require(mvtnorm)
noise = 0.1 ## set the variance of noise
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
  alpha=par_ode[1]
  beta=par_ode[2]
  gamma=par_ode[3]
  delta=par_ode[4]
  as.matrix( c(alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
}
## Define the gradient of ode function against ode parameters
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum( 2*( z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum(2*(z_p[2,]-grad_ode[2,])*gamma*y_p[2,])
dres[4] = sum(-2*(z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
}
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_grlNODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Add noise to the numerical solution of the ode model and use it as the noisy observation.
n_o = max(dim(kkk0\$y_ode))
t_no = kkk0$t
y_no = t(kkk0y_ode) + rmvnorm(n_o,c(0,0),noise*diag(2))
## Create a ode class object by using the simulation data we created from the ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## Set initial value of ode parameters.
init_par = rep(c(0.1),4)
init\_yode = t(y\_no)
init_t = t_no
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode)
## The following examples with CPU or elapsed time > 5s
###### rkhs interpolation for the 1st state of ode using 'rbf' kernel
```

24 third

```
### set initial value of length scale of rbf kernel
initlen = 1
aker = RBF$new(initlen)
bbb = rkhs$new(t(y_no)[1,],t_no,rep(1,n_o),1,aker)
## optimise lambda by cross-validation
## initial value of lambda
initlam = 2
bbb$skcross( initlam )

## make prediction using the 'predict()' method of 'rkhs' class and plot against the time.
plot(t_no,bbb$predict()$pred)

## End(Not run)
```

third

The 'third' function

## **Description**

This function is used to create 'rk3g' class objects and estimate ode parameters using ode regularised gradient matching.

#### Usage

```
third(lam, kkk, bbb, crtype, woption, dtilda)
```

#### Arguments

lam	scalar containing the weighting parameter of ode regularisation.
kkk	'ode' class object containing all information about the odes.
bbb	list of 'rkhs' class object containing the interpolation for all ode states.
crtype	character containing the optimisation scheme type. User can choose 'i' or '3'. 'i' is for fast iterative scheme and '3' for optimising the ode parameters and interpolation coefficients simultaneously.
woption	character containing the indication of using warping. If the warping scheme is done before using the ode regularisation, user can choose 'w' otherwise just leave this option empty.
dtilda	vector(of length n_o) containing the gradient of warping function. This variable is only used if user want to combine warping and the ode regularisation.

#### **Details**

Arguments of the 'third' function are ode regularisation weighting parameter, 'ode' class objects, 'rkhs' class objects, noisy observation, type of regularisation scheme, option of warping and the gradient of warping function. It return the interpolation for each of the ode states. The ode parameters are estimated using gradient matching, and the results are stored in the ode\_par attribute of 'ode' class.

third 25

#### Value

return list containing:

• oppar - vector(of length n\_p) containing the ode parameters estimation. n\_p is the length of ode parameters.

• rk3 - list of 'rkhs' class object containing the updated interpolation results.

#### Author(s)

Mu Niu <mu.niu@glasgow.ac.uk>

```
## Not run:
require(mvtnorm)
noise = 0.1
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
  alpha=par_ode[1]
  beta=par_ode[2]
  gamma=par_ode[3]
  delta=par_ode[4]
  as.matrix( c( alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
## Define the gradient of ode function against ode parameters
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum(2*(z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum( 2*( z_p[2,]-grad_ode[2,])*gamma*y_p[2,] )
dres[4] = sum(-2*(z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
}
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_grlNODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Add noise to the numerical solution of the ode model and use it as the noisy observation.
n_o = max(dim(kkk0\$y_ode))
t_no = kkk0$t
```

26 Warp

```
y_no = t(kkk0\$y_ode) + rmvnorm(n_o,c(0,0),noise*diag(2))
## create a ode class object by using the simulation data we created from the ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## set initial value of Ode parameters.
init_par = rep(c(0.1),4)
init\_yode = t(y\_no)
init_t = t_no
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode)
## The following examples with CPU or elapsed time > 10s
## Use function 'rkg' to estimate the ode parameters.
ktype ='rbf'
rkgres = rkg(kkk,y_no,ktype)
bbb = rkgres$bbb
######### gradient matching + ode regularisation
crtype='i'
## using cross validation to estimate the weighting parameters of the ode regularisation
lam=c(1e-4, 1e-5)
lamil1 = crossv(lam,kkk,bbb,crtype,y_no)
lambdai1=lamil1[[1]]
## estimate ode parameters using gradient matching and ode regularisation
res = third(lambdai1,kkk,bbb,crtype)
## display the ode parameter estimation.
res$oppar
## End(Not run)
```

Warp

The 'Warp' class object

## **Description**

This class provide the warping method which can be used to warp the original signal to sinusoidal like signal.

#### **Format**

R6Class object.

#### Value

an R6Class object which can be used for doing interpolation using reproducing kernel Hilbert space.

Warp 27

#### Methods

warpsin(len ,lop,p0,eps) This method is used to warp the initial interpolation into a sinusoidal shape.

slowWarp(lens, peod, eps) This method is used to find the optimised initial hyper parameters for the sigmoid basis function for each ode states.

warpLossLen(par,lam,p0,eps) This method is used to implement the loss function for warping. It is called by the 'warpSin' function.

#### **Public fields**

- y matrix(of size n\_s\*n\_o) containing observation.
- t vector(of length n\_o) containing time points for observation.
- b vector(of length n\_o) containing coefficients of kernel or basis functions.

lambda scalar containing the weighting parameter for penalising the length of warped time span.

ker kernel class object containing sigmoid basis function.

#### Methods

#### **Public methods:**

```
• Warp$new()
```

- Warp\$greet()
- Warp\$showker()
- Warp\$warpLoss()
- Warp\$warpLossLen()
- Warp\$warpSin()
- Warp\$slowWarp()
- Warp\$clone()

### Method new():

Usage:

Warp\$warpLoss(par, len, p0, eps)

```
Usage:
Warp$new(y = NULL, t = NULL, b = NULL, lambda = NULL, ker = NULL)

Method greet():
    Usage:
    Warp$greet()

Method showker():
    Usage:
    Warp$showker()
Method warpLoss():
```

28 warpfun

```
Method warpLossLen():
    Usage:
    Warp$warpLossLen(par, lam, p0, eps)

Method warpSin():
    Usage:
    Warp$warpSin(len, lop, p0, eps)

Method slowWarp():
    Usage:
    Warp$slowWarp(lens, p0, eps)

Method clone(): The objects of this class are cloneable with this method.
    Usage:
    Warp$clone(deep = FALSE)
    Arguments:
    deep Whether to make a deep clone.
```

#### Author(s)

 $Mu\ Niu, <mu.niu@glasgow.ac.uk>$ 

warpfun

The 'warpfun' function

## Description

This function is used to produce the warping function and learning the interpolation in the warped time domain.

#### Usage

```
warpfun(kkkrkg, bbb, peod, eps, fixlens, y_no, testData, witer)
```

## Arguments

kkkrkg	'ode' class object.
bbb	list of 'rkhs' class object.
peod	vector(of length n_s) containing the period of warped signal. n_s is the length of the ode states.
eps	vector(of length n_s) containing the uncertainty level of the period. n_s is the length of the ode states.
fixlens	vector(of length n_s) containing the initial values of the hyper parameters of sigmoid basis function.

warpfun 29

y_no	matrix(of size $n_s*n_o$ ) containing noisy observations. The row(of length $n_s$ ) represent the ode states and the column(of length $n_o$ ) represents the time points.
testData	vector(of size $n_x$ ) containing user defined time points which will be warped by the warping function.
witer	scale containing the number of iterations for optimising the hyper parameters of warping.

#### **Details**

Arguments of the 'warpfun' function are 'ode' class, 'rkhs' class, period of warped signal, uncertainty level of the period, initial values of the hyper parameters for sigmoid basis function, noisy observations and the time points that user want to warped. It return the interpolation for each of the ode states. The ode parameters are estimated using gradient matching, and the results are stored in the 'ode' class as the ode\_par attribute.

#### Value

return list containing:

- dtilda vector(of length n\_x) containing the gradients of warping function at user defined time points.
- bbbw list of 'rkhs' class object containing the interpolation in warped time domain.
- wtime vector(of length n\_x) containing the warped time points.
- wfun list of 'rkhs' class object containing information about warping function.
- wkkk 'ode' class object containing the result of parameter estimation using the warped signal and gradient matching.

#### Author(s)

```
Mu Niu <mu.niu@glasgow.ac.uk>
```

```
## Not run:
require(mvtnorm)
noise = 0.1
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
    alpha=par_ode[1]
    beta=par_ode[2]
    gamma=par_ode[3]
    delta=par_ode[4]
    as.matrix( c( alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
}
## Define the gradient of ode function against ode parameters
```

30 warpfun

```
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum( 2*( z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum(2*(z_p[2,]-grad_ode[2,])*gamma*y_p[2,])
dres[4] = sum( -2*( z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
}
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_grlNODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Add noise to the numerical solution of the ode model and use it as the noisy observation.
n_o = max(dim(kkk0$y_ode))
t_no = kkk0$t
y_no = t(kkk0y_ode) + rmvnorm(n_o,c(0,0),noise*diag(2))
## create a ode class object by using the simulation data we created from the Ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## set initial value of Ode parameters.
init_par = rep(c(0.1),4)
init\_yode = t(y\_no)
init_t = t_no
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode )
## The following examples with CPU or elapsed time > 10s
## Use function 'rkg' to estimate the Ode parameters.
ktype ='rbf'
rkgres = rkg(kkk,y_no,ktype)
bbb = rkgres$bbb
###### warp all ode states
peod = c(6,5.3) ## the guessing period
eps= 1
                ## the uncertainty level of period
###### learn the initial value of the hyper parameters of the warping basis function
fixlens=warpInitLen(peod,eps,rkgres)
kkkrkg = kkk$clone() ## make a copy of ode class objects
##learn the warping function, warp data points and do gradient matching in the warped time domain.
www = warpfun(kkkrkg,bbb,peod,eps,fixlens,y_no,kkkrkg$t)
dtilda= www$dtilda ## gradient of warping function
bbbw = www$bbbw
                    ## interpolation in warped time domain
```

warpInitLen 31

```
resmtest = www$wtime ## warped time points
##display the results of parameter estimation using gradient matching in the warped time domain.
www$wkkk$ode_par
```

```
## End(Not run)
```

warpInitLen	The 'warpInitLen' function

#### **Description**

This function is used to find the optmised initial value of the hyper parameter for the sigmoid basis function which is used for warping.

#### Usage

```
warpInitLen(peod, eps, rkgres, lens)
```

## **Arguments**

peod	vector(of length n_s) containing the period of warped signal. n_s is the length of the ode states.
eps	vector(of length $n_s$ ) containing the uncertainty level of the period. $n_s$ is the length of the ode states.
rkgres	list containing interpolation and 'rkhs' class objects for all ode states.
lens	vector(of length n_l) containing a list of hyper parameters of sigmoid basis function. n_l is the length of user defined hyper parameters of the sigmoid basis function.

#### **Details**

Arguments of the 'warpfun' function are 'ode' class, 'rkhs' class, period of warped signal, uncertainty level of the period, initial values of the hyper parameters for sigmoid basis function, noisy observations and the time points that user want to warped. It return the interpolation for each of the ode states. The ode parameters are estimated using gradient matching, and the results are stored in the 'ode' class as the ode\_par attribute.

#### Value

return list containing:

 wres- vector(of length n\_s) containing the optimised initial hyper parameters of sigmoid basis function for each ode states.

#### Author(s)

```
Mu Niu <mu.niu@glasgow.ac.uk>
```

32 warpInitLen

```
## Not run:
require(mvtnorm)
noise = 0.1
SEED = 19537
set.seed(SEED)
## Define ode function, we use lotka-volterra model in this example.
## we have two ode states x[1], x[2] and four ode parameters alpha, beta, gamma and delta.
LV_fun = function(t,x,par_ode){
  alpha=par_ode[1]
  beta=par_ode[2]
  gamma=par_ode[3]
  delta=par_ode[4]
  as.matrix( c(alpha*x[1]-beta*x[2]*x[1] , -gamma*x[2]+delta*x[1]*x[2] ) )
}
## Define the gradient of ode function against ode parameters
## df/dalpha, df/dbeta, df/dgamma, df/ddelta where f is the differential equation.
LV_grlNODE= function(par,grad_ode,y_p,z_p) {
alpha = par[1]; beta= par[2]; gamma = par[3]; delta = par[4]
dres= c(0)
dres[1] = sum( -2*( z_p[1,]-grad_ode[1,])*y_p[1,]*alpha )
dres[2] = sum( 2*( z_p[1,]-grad_ode[1,])*y_p[2,]*y_p[1,]*beta)
dres[3] = sum(2*(z_p[2,]-grad_ode[2,])*gamma*y_p[2,])
dres[4] = sum(-2*(z_p[2,]-grad_ode[2,])*y_p[2,]*y_p[1,]*delta)
dres
}
## create a ode class object
kkk0 = ode$new(2,fun=LV_fun,grfun=LV_grlNODE)
## set the initial values for each state at time zero.
xinit = as.matrix(c(0.5,1))
## set the time interval for the ode numerical solver.
tinterv = c(0,6)
## solve the ode numerically using predefined ode parameters. alpha=1, beta=1, gamma=4, delta=1.
kkk0$solve_ode(c(1,1,4,1),xinit,tinterv)
## Add noise to the numerical solution of the ode model and use it as the noisy observation.
n_o = max(dim(kkk0\$y_ode))
t_no = kkk0$t
y_no = t(kkk0y_ode) + rmvnorm(n_o,c(0,0),noise*diag(2))
## create a ode class object by using the simulation data we created from the Ode numerical solver.
## If users have experiment data, they can replace the simulation data with the experiment data.
## set initial value of Ode parameters.
init_par = rep(c(0.1),4)
init\_yode = t(y\_no)
init_t = t_no
kkk = ode$new(1,fun=LV_fun,grfun=LV_grlNODE,t=init_t,ode_par= init_par, y_ode=init_yode)
## The following examples with CPU or elapsed time > 10s
```

warpInitLen 33

```
## Use function 'rkg' to estimate the Ode parameters.
ktype ='rbf'
rkgres = rkg(kkk,y_no,ktype)
bbb = rkgres$bbb

###### warp all ode states
peod = c(6,5.3) ## the guessing period
eps= 1 ## the uncertainty level of period

###### learn the initial value of the hyper parameters of the warping basis function
fixlens=warpInitLen(peod,eps,rkgres)
## End(Not run)
```

## **Index**

```
* data
     Kernel, 9
     MLP, 10
     ode, 12
     RBF, 14
     rkg3, 18
     rkhs, 20
     Warp, 26
bootstrap, 2
crossv, 5
{\tt diagnostic}, {\tt 7}
Kernel, 9
KGode::Kernel, 10, 15
MLP, 10
ode, 12
R6Class, 9, 10, 12, 15, 18, 20, 26
RBF, 14
rkg, 16
rkg3, 18
rkhs, 20
third, 24
Warp, 26
\text{warpfun}, \frac{28}{}
warpInitLen, \\ \textcolor{red}{31}
```