Package ‘pCODE’

November 23, 2019

Type     Package
Title    Estimation of an Ordinary Differential Equation Model by Parameter Cascade Method
Version  0.9.3
Imports  fda, pracma, MASS, deSolve, base, stats
Depends  R (>= 3.5.0)
Description  An implementation of the parameter cascade method Ramsay, J. O., Hooker, G., Campbell, D., and Cao, J. (2007) <doi:10.1111/j.1467-9868.2007.00610.x> for estimating ordinary differential equation models with missing or complete observations. It combines smoothing method and profile estimation to estimate any non-linear dynamic system. The package also offers variance estimates for parameters of interest based on either bootstrap or Delta method.
License  GPL
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bootsvar

**Description**

Obtaining an estimate of variance for structural parameters by bootstrap method.

**Usage**

```r
bootsvar(data, time, ode.model, par.names, state.names, likelihood.fun = NULL,
         par.initial, basis.list, lambda = NULL, bootstrrep, controls = NULL)
```

**Arguments**

- **data**: A data frame or a matrix contain observations from each dimension of the ODE model.
- **time**: A vector contain observation times or a matrix if time points are different between dimensions.
- **ode.model**: An R function that computes the time derivative of the ODE model given observations of states variable and structural parameters.
- **par.names**: The names of structural parameters defined in the 'ode.model'.
- **state.names**: The names of state variables defined in the 'ode.model'.
- **likelihood.fun**: A likelihood function passed to PCODE in case of that the error terms do not have a Normal distribution.
- **par.initial**: Initial value of structural parameters to be optimized.
- **basis.list**: A list of basis objects for smoothing each dimension’s observations. Can be the same or different across dimensions.
deltavar

<table>
<thead>
<tr>
<th>lambda</th>
<th>Penalty parameter.</th>
</tr>
</thead>
<tbody>
<tr>
<td>bootsrep</td>
<td>Bootstrap sample to be used for estimating variance.</td>
</tr>
<tr>
<td>controls</td>
<td>A list of control parameters. Same as the controls in pcode.</td>
</tr>
</tbody>
</table>

**Value**

| boots.var | The bootstrap variance of each structural parameters. |

**Description**

Obtaining variance of structural parameters by Delta method.

**Usage**

```r
deltavar(data, time, ode.model, par.names, state.names, likelihood.fun, par.initial, basis.list, lambda, stepsize, y_stepsize, controls)
```

**Arguments**

- `data`: A data frame or a matrix contain observations from each dimension of the ODE model.
- `time`: A vector contain observation times or a matrix if time points are different between dimensions.
- `ode.model`: An R function that computes the time derivative of the ODE model given observations of states variable and structural parameters.
- `par.names`: The names of structural parameters defined in the `ode.model`.
- `state.names`: The names of state variables defined in the `ode.model`.
- `likelihood.fun`: A likelihood function passed to PCODE in case of that the error terms do not have a Normal distribution.
- `par.initial`: Initial value of structural parameters to be optimized.
- `basis.list`: A list of basis objects for smoothing each dimension’s observations. Can be the same or different across dimensions.
- `lambda`: Penalty parameter.
- `stepsize`: Stepsize used in estimating partial derivatives with respect to structural parameters for the Delta method.
- `y_stepsize`: Stepsize used in estimating partial derivatives with respect to observations for the Delta method.
- `controls`: A list of control parameters. Same as the controls in pcode.

**Value**

| par.var | The variance of structural parameters obtained by Delta method. |
innerobj  
*Inner objective function (Single dimension version)*

**Description**

An objective function combines the sum of squared error of basis expansion estimates and the penalty controls how those estimates fail to satisfy the ODE model.

**Usage**

```r
innerobj(basis_coef, ode.par, input, derive.model, NLS)
```

**Arguments**

- **basis_coef**: Basis coefficients for interpolating observations given a basis object.
- **ode.par**: Structural parameters of the ODE model.
- **input**: Contains dependencies for the optimization, including observations, penalty parameter lambda, and etc.
- **derive.model**: The function defines the ODE model and is the same as the ode.model in `pcode`.
- **NLS**: Default is `TRUE` so the function returns vector of residuals, and otherwise returns sum of squared errors.

**Value**

- **residual.vec**: Vector of residuals and evaluation of penalty function on quadrature points for approximating the integral.

innerobj_lkh  
*Inner objective function (likelihood and multiple dimension version)*

**Description**

An objective function combines the likelihood or loglikelihood of errors from each dimension of state variables and the penalty controls how the state estimates fail to satisfy the ODE model.

**Usage**

```r
innerobj_lkh(basis_coef, ode.par, input, derive.model, likelihood.fun)
```
**innerobj_lkh_1d**

**Arguments**

- `basis_coef`: Basis coefficients for interpolating observations given a basis object.
- `ode.par`: Structural parameters of the ODE model.
- `input`: Contains dependencies for the optimization, including observations, ode penalty, and etc..
- `derive.model`: The function defines the ODE model and is the same as the `ode.model` in `pcode`.
- `likelihood.fun`: The likelihood or loglikelihood function of the errors.

**Value**

- `obj.eval`: The evaluation of the inner objective function.

---

**innerobj_lkh_1d**

*Inner objective function (Likelihood and Single dimension version)*

**Description**

An objective function combines the likelihood or loglikelihood of errors from each dimension of state variables and the penalty controls how the state estimates fail to satisfy the ODE model.

**Usage**

```
innerobj_lkh_1d(basis_coef, ode.par, input, derive.model, likelihood.fun)
```

**Arguments**

- `basis_coef`: Basis coefficients for interpolating observations given a basis object.
- `ode.par`: Structural parameters of the ODE model.
- `input`: Contains dependencies for the optimization, including observations, ode penalty, and etc..
- `derive.model`: The function defines the ODE model and is the same as the `ode.model` in `pcode`.
- `likelihood.fun`: The likelihood or loglikelihood function of the errors.

**Value**

- `obj.eval`: The evaluation of the inner objective function.
**innerobj_multi**

*Inner objective function (multiple dimension version)*

### Description

An objective function combines the sum of squared error of basis expansion estimates and the penalty controls how those estimates fail to satisfy the ODE model.

### Usage

innerobj_multi(basis_coef, ode.par, input, derive.model, NLS)

### Arguments

- **basis_coef**: Basis coefficients for interpolating observations given a basis object.
- **ode.par**: Structural parameters of the ODE model.
- **input**: Contains dependencies for the optimization, including observations, penalty parameter lambda, and etc..
- **derive.model**: The function defines the ODE model and is the same as the `ode.model` in `pcode`.
- **NLS**: Default is `TRUE` so the function returns vector of residuals, and otherwise returns sum of squared errors.

### Value

- **residual.vec**: Vector of residuals and evaluation of penalty function on quadrature points for approximating the integral.

---

**innerobj_multi_missing**

*Inner objective function (multiple dimension version with unobserved state variables)*

### Description

An objective function combines the sum of squared error of basis expansion estimates and the penalty controls how those estimates fail to satisfy the ODE model.

### Usage

innerobj_multi_missing(basis_coef, ode.par, input, derive.model, NLS)
**nls_optimize**

**Optimizer for non-linear least square problems**

**Description**

Obtain the solution to minimize the sum of squared errors of the defined function `fun` by levenberg-marquardt method. Adapted from PRACMA package.

**Usage**

```r
nls_optimize(fun, x0, ..., options, verbal)
```

**Arguments**

- `fun` The function returns the vector of weighted residuals.
- `x0` The initial value for optimization.
- `...` Parameters to be passed for `fun`.
- `options` Additional optimization controls.
- `verbal` Default = 1 for printing iteration and other for suppressing

**Value**

- `par` The solution to the non-linear least square problem, the same size as `x0`
**nls_optimize.inner**  
*Optimizer for non-linear least square problems (for inner objective functions)*

**Description**

Obtain the solution to minimize the sum of squared errors of the defined function `fun` by levenberg-marquardt method. Adapted from PRACMA package.

**Usage**

```r
nls_optimize.inner(fun, x0, ..., options)
```

**Arguments**

- `fun` The function returns the vector of weighted residuals.
- `x0` The initial value for optimization.
- `...` Parameters to be passed for `fun`.
- `options` Additional optimization controls.

**Value**

- `par` The solution to the non-linear least square problem, the same size as `x0`.

---

**outerobj**  
*Outer objective function (Single dimension version)*

**Description**

An objective function of the structural parameter computes the measure of fit.

**Usage**

```r
outerobj(ode.parameter, basis.initial, derivative.model, inner.input, NLS)
```

**Arguments**

- `ode.parameter` Structural parameters of the ODE model.
- `basis.initial` Initial values of the basis coefficients for nonlinear least square optimization.
- `derivative.model` The function defines the ODE model and is the same as the ode.model in 'pcode'.
- `inner.input` Input that will be passed to the inner objective function. Contains dependencies for the optimization, including observations, penalty parameter lambda, and etc..
- `NLS` Default is `TRUE` so the function returns vector of residuals, and otherwise returns sum of squared errors.
Outer objective function (likelihood and multiple dimension version)

Description
An objective function of the structural parameter computes the measure of fit.

Usage
outerobj_lkh(ode.parameter, basis.initial, derivative.model, likelihood.fun, inner.input)

Arguments
- ode.parameter: Structural parameters of the ODE model.
- basis.initial: Initial values of the basis coefficients for nonlinear least square optimization.
- derivative.model: The function defines the ODE model and is the same as the ode.model in 'pcode'
- likelihood.fun: The likelihood or loglikelihood function of the errors.
- inner.input: Input that will be passed to the inner objective function. Contains dependencies for the optimization, including observations, penalty parameter lambda, and etc..

Value
neglik The negative of the likelihood or the loglikelihood function that will be passed further to the 'optim' function.

Outer objective function (likelihood and single dimension version)

Description
An objective function of the structural parameter computes the measure of fit.

Usage
outerobj_lkh_1d(ode.parameter, basis.initial, derivative.model, likelihood.fun, inner.input)
Arguments

ode.parameter Structural parameters of the ODE model.
basis.initial Initial values of the basis coefficients for nonlinear least square optimization.
derivative.model The function defines the ODE model and is the same as the ode.model in 'pcode'
likelihood.fun The likelihood or loglikelihood function of the errors.
inner.input Input that will be passed to the inner objective function. Contains dependencies for the optimization, including observations, penalty parameter lambda, and etc..

Value

neglik The negative of the likelihood or the loglikelihood function that will be passed further to the 'optim' function.

outterobj_multi_missing

Outer objective function (multiple dimension version with unobserved state variables)

Description

An objective function of the structural parameter computes the measure of fit for the basis expansion.

Usage

outterobj_multi_missing(ode.parameter, basis.initial, derivative.model, inner.input, NLS)

Arguments

ode.parameter Structural parameters of the ODE model.
basis.initial Initial values of the basis coefficients for nonlinear least square optimization.
derivative.model The function defines the ODE model and is the same as the ode.model in 'pcode'
inner.input Input that will be passed to the inner objective function. Contains dependencies for the optimization, including observations, penalty parameter lambda, and etc..
NLS Default is TRUE so the function returns vector of residuals, and otherwise returns sum of squared errors.

Value

residual Vector of residuals and evaluation of penalty function on quadrature points for approximating the integral.
outerobj_multi_nls

Outer objective function (multiple dimension version)

Description
An objective function of the structural parameter computes the measure of fit for the basis expansion.

Usage
outerobj_multi_nls(ode.parameter, basis.initial, derivative.model, inner.input, NLS)

Arguments
ode.parameter Structural parameters of the ODE model.
basis.initial Initial values of the basis coefficients for nonlinear least square optimization.
derivative.model The function defines the ODE model and is the same as the ode.model in pcode.
inner.input Input that will be passed to the inner objective function. Contains dependencies for the optimization, including observations, penalty parameter lambda, and etc..
NLS Default is TRUE so the function returns vector of residuals, and otherwise returns sum of squared errors.

Value
residual Vector of residuals and evaluation of penalty function on quadrature points for approximating the integral.

pcode
Parameter Cascade Method for Ordinary Differential Equation Models

Description
Obtain estimates of both structural and nuisance parameters of an ODE model by parameter cascade method.

Usage
pcode(data, time, ode.model, par.names, state.names, likelihood.fun, par.initial, basis.list, lambda, controls)
Arguments

data A data frame or a matrix contain observations from each dimension of the ODE model.
time A vector contain observation times or a matrix if time points are different between dimensions.
ode.model An R function that computes the time derivative of the ODE model given observations of states variable and structural parameters.
par.names The names of structural parameters defined in the 'ode.model'.
state.names The names of state variables defined in the 'ode.model'.
likelihood.fun A likelihood function passed to PCODE in case of that the error terms do not have a Normal distribution.
par.initial Initial value of structural parameters to be optimized.
basis.list A list of basis objects for smoothing each dimension’s observations. Can be the same or different across dimensions.
lambda Penalty parameter for controlling the fidelity of interpolation.
controls A list of control parameters. See Details.

Details

The controls argument is a list providing addition inputs for the nonlinear least square optimizer or general optimizer optim:

nquadpts Determine the number of quadrature points for approximating an integral. Default is 101.
smooth.lambda Determine the smoothness penalty for obtaining initial value of nuisance parameters.
tau Initial value of Marquardt parameter. Small values indicate good initial values for structural parameters.
tolx Tolerance for parameters of objective functions. Default is set at 1e-6.
tolg Tolerance for the gradient of parameters of objective functions. Default is set at 1e-6.
maxeval The maximum number of evaluation of the outer optimizer. Default is set at 20.

Value

structural.par The structural parameters of the ODE model.
nuisance.par The nuisance parameters or the basis coefficients for interpolating observations.

Examples

library(fda)
library(deSolve)
library(MASS)
library(pracma)
#Simple ode model example
#define model parameters
model.par <- c(theta = c(0.1))
#define state initial value
state <- c(X = 0.1)
#Define model for function 'ode' to numerically solve the system
ode.model <- function(t, state, parameters){
  with(as.list(c(state,parameters)),
  {
    dX <- theta*X*(1-X/10)
    return(list(dX))
  })
}
#Observation time points
times <- seq(0,100,length.out=101)
#Solve the ode model
desolve.mod <- ode(y=state,times=times,func=ode.model,parms = model.par)
#Prepare for doing parameter cascading method
#Generate basis object for interpolation and as argument of pcode
#21 knots equally spaced within [0,100]
knots <- seq(0,100,length.out=21)
#order of basis functions
norder <- 4
#number of basis functions
nbasis <- length(knots) + norder - 2
#creating Bspline basis
basis <- create.bspline.basis(c(0,100),nbasis,norder,breaks = knots)
#Add random noise to ode solution for simulating data
nobs <- length(times)
scale <- 0.1
noise <- scale*rnorm(n = nobs, mean = 0 , sd = 1)
observation <- desolve.mod[,2] + noise
#parameter estimation
pcode(data = observation, time = times, ode.model = ode.model,
  par.initial = 0.1, par.names = 'theta',state.names = 'X',
  basis.list = basis, lambda = 1e2)

---

**Description**

Obtain estiamtes of structural parameters of an ODE model by parameter cascade method.

**Usage**

pcode_1d(data, time, ode.model, par.initial, par.names, basis, lambda, controls = list())
Arguments

data A data frame or a vector contains observations from the ODE model.
time The vector contain observation times.
ode.model Defined R function that computes the time derivative of the ODE model given observations of states variable.
par.initial Initial value of structural parameters to be optimized.
par.names The names of structural parameters defined in the 'ode.model'.
basis A basis objects for smoothing observations.
lambda Penalty parameter.
controls A list of control parameters. See ‘Details’.

Value

structural.par The structural parameters of the ODE model.
nuisance.par The nuisance parameters or the basis coefficients for interpolating observations.

Description

Obtain estimates of both structural and nuisance parameters of an ODE model by parameter cascade method.

Usage

pcode_lkh(data, likelihood.fun, time, ode.model, par.names, state.names, par.initial, basis.list, lambda, controls)

Arguments

data A data frame or a matrix contain observations from each dimension of the ODE model.
likelihood.fun A function computes the likelihood or the loglikelihood of the errors.
time A vector contains observation ties or a matrix if time points are different between dimension.
ode.model An R function that computes the time derivative of the ODE model given observations of states variable and structural parameters.
par.names The names of structural parameters defined in the 'ode.model'.
state.names The names of state variables defined in the 'ode.model'.
par.initial Initial value of structural parameters to be optimized.
basis.list A list of basis objects for smoothing each dimension’s observations. Can be the same or different across dimensions.
lambda Penalty parameter.
controls A list of control parameters. See ‘Details’.
Details

The controls argument is a list providing addition inputs for the nonlinear least square optimizer:

• `nquadpts` Determine the number of quadrature points for approximating an integral. Default is 101.
• `smooth.lambda` Determine the smoothness penalty for obtaining initial value of nuisance parameters.
• `tau` Initial value of Marquardt parameter. Small values indicate good initial values for structural parameters.
• `tolx` Tolerance for parameters of objective functions. Default is set at 1e-6.
• `toly` Tolerance for the gradient of parameters of objective functions. Default is set at 1e-6.
• `maxeval` The maximum number of evaluation of the optimizer. Default is set at 20.

Value

<table>
<thead>
<tr>
<th>structural.par</th>
<th>The structural parameters of the ODE model.</th>
</tr>
</thead>
<tbody>
<tr>
<td>nuisance.par</td>
<td>The nuisance parameters or the basis coefficients for interpolating observations.</td>
</tr>
</tbody>
</table>

Description

Obtain estimates of both structural and nuisance parameters of an ODE model by parameter cascade method.

Usage

```r
pcode_lkh_1d(data, likelihood.fun, time, ode.model, par.names, state.names, par.initial, basis.list, lambda, controls)
```

Arguments

<table>
<thead>
<tr>
<th>data</th>
<th>A data frame or a matrix contain observations from each dimension of the ODE model.</th>
</tr>
</thead>
<tbody>
<tr>
<td>likelihood.fun</td>
<td>A function computes the likelihood or the loglikelihood of the errors.</td>
</tr>
<tr>
<td>time</td>
<td>A vector contains observation ties or a matrix if time points are different between dimension.</td>
</tr>
<tr>
<td>ode.model</td>
<td>An R function that computes the time derivative of the ODE model given observations of states variable and structural parameters.</td>
</tr>
<tr>
<td>par.names</td>
<td>The names of structural parameters defined in the ‘ode.model’.</td>
</tr>
<tr>
<td>state.names</td>
<td>The names of state variables defined in the ‘ode.model’.</td>
</tr>
</tbody>
</table>
par.initial: Initial value of structural parameters to be optimized.

basis.list: A list of basis objects for smoothing each dimension’s observations. Can be the same or different across dimensions.

lambda: Penalty parameter.

controls: A list of control parameters. See ‘Details’.

Details

The controls argument is a list providing additional inputs for the nonlinear least square optimizer:

- nquadpts: Determine the number of quadrature points for approximating an integral. Default is 101.
- smooth.lambda: Determine the smoothness penalty for obtaining initial value of nuisance parameters.
- tau: Initial value of Marquardt parameter. Small values indicate good initial values for structural parameters.
- tolx: Tolerance for parameters of objective functions. Default is set at 1e-6.
- tolg: Tolerance for the gradient of parameters of objective functions. Default is set at 1e-6.
- maxeval: The maximum number of evaluation of the optimizer. Default is set at 20.

Value

structural.par: The structural parameters of the ODE model.

nuisance.par: The nuisance parameters or the basis coefficients for interpolating observations.

Description

Obtain estimates of both structural and nuisance parameters of an ODE model by parameter cascade method when the dynamics are partially observed.

Usage

pcode_missing(data, time, ode.model, par.names, state.names, likelihood.fun, par.initial, basis.list, lambda, controls)
Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>data</td>
<td>A data frame or a matrix contain observations from each dimension of the ODE model.</td>
</tr>
<tr>
<td>time</td>
<td>A vector contain observation times or a matrix if time points are different between dimensions.</td>
</tr>
<tr>
<td>ode.model</td>
<td>An R function that computes the time derivative of the ODE model given observations of states variable and structural parameters.</td>
</tr>
<tr>
<td>par.names</td>
<td>The names of structural parameters defined in the 'ode.model'.</td>
</tr>
<tr>
<td>state.names</td>
<td>The names of state variables defined in the 'ode.model'.</td>
</tr>
<tr>
<td>likelihood.fun</td>
<td>A likelihood function passed to PCODE in case of that the error terms do not have a Normal distribution.</td>
</tr>
<tr>
<td>par.initial</td>
<td>Initial value of structural parameters to be optimized.</td>
</tr>
<tr>
<td>basis.list</td>
<td>A list of basis objects for smoothing each dimension’s observations. Can be the same or different across dimensions.</td>
</tr>
<tr>
<td>lambda</td>
<td>Penalty parameter.</td>
</tr>
<tr>
<td>controls</td>
<td>A list of control parameters. See Details.</td>
</tr>
</tbody>
</table>

Details

The controls argument is a list providing addition inputs for the nonlinear least square optimizer or general optimizer optim:

- nquadpts Determine the number of quadrature points for approximating an integral. Default is 101.
- smooth.lambda Determine the smoothness penalty for obtaining initial value of nuisance parameters.
- tau Initial value of Marquardt parameter. Small values indicate good initial values for structural parameters.
- tolx Tolerance for parameters of objective functions. Default is set at 1e-6.
- tolg Tolerance for the gradient of parameters of objective functions. Default is set at 1e-6.
- maxeval The maximum number of evaluation of the optimizer. Default is set at 20.

Value

- structural.par The structural parameters of the ODE model.
- nuisance.par The nuisance parameters or the basis coefficients for interpolating observations.
prepare_basis  

Evaluate basis objects over observation times and quadrature points

Description
Calculate all basis functions over observation time points and store them as columns in a single matrix for each dimension. Also include first and second order derivative. Repeat over quadrature points.

Usage
prepare_basis(basis, times, nquadpts)

Arguments
- basis: A basis object.
- times: The vector contain observation times for corresponding dimension.
- nquadpts: Number of quadrature points will be used later for approximating integrals.

Value
- Phi.mat: Evaluations of all basis functions stored as columns in the matrix.
- Qmat: Evaluations of all basis functions over quadrature points stored as columns in the matrix.
- Q.D1mat: Evaluations of first order derivative all basis functions over quadrature points stored as columns in the matrix.
- Q.D2mat: Evaluations of second order derivative all basis functions over quadrature points stored as columns in the matrix.
- quadts: Quadrature points.
- quadwts: Quadrature weights.

tunelambda  

Find optimal penalty parameter lambda by cross-validation.

Description
Obtain the optimal sparsity parameter given a search grid based on cross validation score with replications.

Usage
tunelambda(data, time, ode.model, par.names, state.names, par.initial, basis.list, lambda_grid, cv_portion, kfolds, rep, controls)
Arguments

data A data frame or matrix contain observations from each dimension of the ODE model.
time The vector contain observation times or a matrix if time points are different between dimensions.
ode.model Defined R function that computes the time derivative of the ODE model given observations of states variable.
par.names The names of structural parameters defined in the 'ode.model'.
state.names The names of state variables defined in the 'ode.model'.
par.initial Initial value of structural parameters to be optimized.
basis.list A list of basis objects for smoothing each dimension’s observations. Can be the same or different across dimensions.
lambda_grid A search grid for finding the optimal sparsity parameter lambda.
cv_portion A number indicating the proportion of data will be saved for doing cross validation. Default is set at 5 as minimum.
kfolds A number indicating the number of folds the data should be separated into.
rep A integer controls the number of replication of doing cross-validation for each penalty parameter.
controls A list of control parameters. See ‘Details’.

Value

lambda_grid The original input vector of a search grid for the optimal lambda.
cv.score The matrix contains the cross validation score for each lambda of each replication.
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