

Package ‘paramGUI’

July 23, 2025

Title A Shiny GUI for some Parameter Estimation Examples

Version 2.2.0

Description Allows specification and fitting of some parameter estimation examples inspired by time-resolved spectroscopy via a Shiny GUI.

URL <https://github.com/glotaran/paramGUI/>

License GPL (>= 2)

Depends R (>= 3.0.0)

Imports shiny, shinydashboard, TIMP, fields

BugReports <https://github.com/glotaran/paramGUI/issues>

Encoding UTF-8

Language en-US

LazyData true

RoxygenNote 7.2.3

NeedsCompilation no

Author Joris Snellenburg [cre, aut],
Katharine Mullen [aut],
Ivo van Stokkum [aut]

Maintainer Joris Snellenburg <j.snellenburg@vu.nl>

Repository CRAN

Date/Publication 2023-01-08 15:00:07 UTC

Contents

calcE	2
example_dataset	2
is_compressed	3
is_rdata	3
kroneckercol	4
linlogtics	4
paramGUI	5

plotterforGUI	5
runGUI	6
simndecay_gen_paramGUI	6
spectemp	8
startGUI	9

Index	10
--------------	-----------

calcE	<i>Calculates a matrix in which each column is a skewed Gaussian</i>
-------	--

Description

Calculates a matrix in which each column is a skewed Gaussian. Like calcEhiergaus from TIMP package but uses a vector not a list of parameter estimates.

Usage

```
calcE(theta, lambda)
```

Arguments

theta	vector of parameter estimates
lambda	wavelengths at which to calculate model

Value

matrix

example_dataset	<i>This is an example dataset included in this package</i>
-----------------	--

Description

Dispersion corrected time-resolved transient-absorption data of the peridinin chlorophyll protein (PCP) excited with 490 nm laser light from the publication of Stokkum et.al. (2009)

Author(s)

Ivo van Stokkum <i.h.m.van.stokkum@vu.nl>

References

[doi:10.1016/j.chemphys.2008.10.005](https://doi.org/10.1016/j.chemphys.2008.10.005)

is_compressed	<i>is_compressed</i>
---------------	----------------------

Description

Helper function for `is_rdata`, checks if the file is a compressed (gzip) file. Does not (yet) check for bzip2 or xz compression.

Usage

```
is_compressed(filename, magic.number = as.raw(c("0x1f", "0x8b")))
```

Arguments

<code>filename</code>	The filename of the file to test for magic compression codes
<code>magic.number</code>	The magic numbers in as a vector of strings with the hexadecimal numbers (e.g. "0x1f")

Value

boolean, TRUE if the file is compressed

is_rdata	<i>is_rdata</i>
----------	-----------------

Description

Checks a file is a rdata file by inspecting the file for so called magic bytes

Usage

```
is_rdata(filename)
```

Arguments

<code>filename</code>	The filename of the file to test if it is an rdata file
-----------------------	---

Value

boolean, TRUE if the file is an rdata file

kroneckercol	<i>kroneckercol: column-wise kronecker product</i>
--------------	--

Description

The column-wise kronecker product is also called the Khatri–Rao product

Usage

```
kroneckercol(A, B)
```

Arguments

A	numerical matrix
B	numerical matrix

Value

column-wise kronecker product of A and B

linlogtics	<i>Generate linlog tics for a linear-logarithmic axis</i>
------------	---

Description

Generate linlog tics for a linear-logarithmic axis

Usage

```
linlogtics(x, mu, alpha)
```

Arguments

x	values for which to calculate a linlog axis
mu	center of axis in the original x axis
alpha	linear part

Value

Returns matrix with new x values in first column and the corresponding labels in the second column.

paramGUI

*paramGUI***Description**

Allows specification and fitting of some parameter estimation examples inspired by time-resolved spectroscopy via a Shiny GUI.

plotterforGUI

*Master plot function for paramGUI***Description**

Master plot function for paramGUI

Usage

```
plotterforGUI(
  modtype = "kin",
  X = matrix(),
  data,
  model,
  theta = vector(),
  result,
  lin = NA,
  mu = 0,
  guessIRF = FALSE
)
```

Arguments

modtype	either 'kin', 'spec' or 'spectemp'
X	matrix of conditionally linear parameters, if any
data	object of class <code>dat</code> containing data
model	object of class <code>dat</code> containing data
theta	object of class <code>theta</code> containing parameters
result	object returned by <code>fitModel</code> or in the case <code>modtype=='spectemp'</code> , by <code>nls</code>
lin	The linear range for the concentration plot
mu	The center of the lin-log axis is <code>lin</code> is specified
guessIRF	Boolean to indicate whether to try and guess the location of the IRF

Value

graphics

runGUI	<i>Run paramGUI</i>
--------	---------------------

Description

Runs the shiny paramGUI app.

Usage

```
runGUI()
```

Examples

```
## Not run:
runGUI()

## End(Not run)
```

simndecay_gen_paramGUI	<i>Simulate data</i>
------------------------	----------------------

Description

Calculates an object of class 'kin'. <TODO>

Usage

```
simndecay_gen_paramGUI(
  kinpar,
  tmax,
  deltat,
  specpar = vector(),
  lmin,
  lmax,
  deltal,
  sigma,
  irf = FALSE,
  irfpar = vector(),
  seqmod = FALSE,
  dispmu = FALSE,
  nocolsums = FALSE,
  disptau = FALSE,
  parmu = list(),
  partau = vector(),
```

```

    lambdac = 0,
    fullk = FALSE,
    kmat = matrix(),
    jvec = vector(),
    specfun = "gaus",
    nupow = 1,
    irffun = "gaus",
    kinscal = vector(),
    lightregimespec = list(),
    specdisp = FALSE,
    specdispar = list(),
    parmufunc = "exp",
    specdispindex = list(),
    amplitudes = vector(),
    specref = 0,
    nosiminfo = TRUE
)

```

Arguments

kinpar	vector of rate constants
tmax	last time point
deltat	time step
specpar	vector of spectral parameters for location, width, skewness
lmin	minimum wavelength (nm)
lmax	maximum wavelength (nm)
deltal	wavelength step
sigma	noise level
irf	logical for IRF usage
irfpar	vector of IRF parameters for location, width
seqmod	logical for sequential model
dispmu	logical for dispersion of IRF location mu
nocolsums	logical for <TODO>
disptau	logical for dispersion of IRF width tau
parmu	vector of dispersion parameters for IRF location mu
partau	vector of dispersion parameters for IRF width tau
lambdac	center wavelength for dispersion
fullk	logical for full K matrix
kmat	K matrix
jvec	input vector
specfun	function for spectral shape
nupow	power of nu in spectral model

irffun	function for IRF
kinscal	vector of kinetic scaling parameters
lightregimespec	<TODO>
specdisp	logical for dispersion parameters of spectral parameters
specdispar	vector of dispersion parameters of spectral parameters
parmufunc	<TODO>
specdispindex	<TODO>
amplitudes	amplitudes of components
specref	<TODO>
nosiminfo	logical for hiding simulation information

Value

an object of class 'kin'

Author(s)

Katharine M. Mullen
Ivo H. M. van Stokkum

spectemp	<i>Spectrotemporal model</i>
----------	------------------------------

Description

Spectrotemporal model

Usage

```
spectemp(sim, model, iter, kroncol = FALSE, lin = NA, l_posk = FALSE)
```

Arguments

sim	object of class dat representing data
model	object of class dat representing a model
iter	integer number of iterations
kroncol	object of class logical that is TRUE if the kroneckcol function should be used to formulate the model and FALSE if the standard kronecker is to be used instead
lin	defines the range to plot linearly (from -lin to +lin)
l_posk	object of class logical indicating whether positivity-constraints are enforced on the rate parameters

`startGUI`*Start paramGUI*

Description

The same as `runGUI()`, starts the shiny paramGUI app.

Usage

```
startGUI()
```

Index

- * **GUI**
 - runGUI, [6](#)
- * **data**
 - example_dataset, [2](#)
- * **shiny**
 - runGUI, [6](#)
- calcE, [2](#)
- datamat (example_dataset), [2](#)
- example_dataset, [2](#)
- is_compressed, [3](#)
- is_rdata, [3](#)
- kroneckercol, [4](#)
- linlogtics, [4](#)
- paramGUI, [5](#)
- plotterforGUI, [5](#)
- runGUI, [6](#)
- simndecay_gen_paramGUI, [6](#)
- spectemp, [8](#)
- startGUI, [9](#)
- times (example_dataset), [2](#)
- waves (example_dataset), [2](#)