

Package ‘rxode2lincmt’

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Version 0.1.0

Title Linear Compartment Model Solutions and Gradients for 'rxode2'

Maintainer Matthew L. Fidler <matthew.fidler@gmail.com>

Depends R (>= 4.1.0)

Imports Rcpp (>= 1.0.8), checkmate

Suggests covr, testthat (>= 3.0.0)

Description Analytic one, two and three compartment linear pharmacokinetic solutions with their parameter gradients from 'stan' automatic differentiation (Carpenter et al (2015) <[doi:10.48550/arXiv.1509.07164](https://doi.org/10.48550/arXiv.1509.07164)>), eigen decompositions and derived-parameter conversions used by 'rxode2' (Wang, Hallow and James (2016) <[doi:10.1002/psp4.12052](https://doi.org/10.1002/psp4.12052)>). Split out of 'rxode2' so its installation does not compile 'stan' AD items which made it take too long to compile by itself.
The closed-form solutions follow the idea of the 'wnl' package (Bae, <<https://CRAN.R-project.org/package=wnl>>), though the implementation here is different.

BugReports <https://github.com/nlmixr2/rxode2lincmt/issues/>

NeedsCompilation yes

License GPL (>= 3)

URL <https://nlmixr2.github.io/rxode2lincmt/>,
<https://github.com/nlmixr2/rxode2lincmt/>

Biarch true

LinkingTo Rcpp (>= 1.0.8), RcppEigen (>= 0.3.3.9.2), StanHeaders (>= 2.21.0.7), BH, RcppParallel

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Author Matthew L. Fidler [aut, cre] (ORCID:
<<https://orcid.org/0000-0001-8538-6691>>),
Richard Upton [ctb]

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linCmtMicros	<i>Micro-constants of a linear compartment model</i>
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Description

Converts one parameter set, in any of the linCmt() parameterizations, to the central volume and micro-constants that the analytic solutions use.

Usage

```
linCmtMicros(p1, v1, p2 = 0, p3 = 0, p4 = 0, p5 = 0, ncmt, trans = 1L)
```

Arguments

- p1 first parameter (for example clearance or k)
- v1 central volume (or its parameterization-specific counterpart)
- p2 second parameter (two and three compartments)
- p3 third parameter (two and three compartments)
- p4 fourth parameter (three compartments)
- p5 fifth parameter (three compartments)
- ncmt number of compartments, 1 to 3
- trans parameterization number (see Details)

Details

Supported trans values: one compartment 1 (c1, v), 2 (k, v), 10 (alpha, A with v1 holding A), 11 (alpha, v); two compartments 1 (c1, v, q, vp), 2 (k, v, k12, k21), 3 (c1, v, q, vss), 4 (alpha, beta, k21), 5 (alpha, beta, aob), 10, 11; three compartments 1 (c1, v, q, vp, q2, vp2), 2 (k, v, k12, k21, k13, k31), 10, 11.

Value

named numeric vector: v, k, and for two or more compartments k12, k21, and for three compartments k13, k31

Author(s)

Matthew L. Fidler

Examples

```
linCmtMicros(p1 = 2, v1 = 20, ncmt = 1)
linCmtMicros(p1 = 2, v1 = 20, p2 = 3, p3 = 40, ncmt = 2)
```

linCmtModelDouble	<i>Advance a linear compartment model by one step</i>
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Description

Advances the amounts of a one, two or three compartment linear model by dt and returns the central concentration, optionally with its derivatives. This is the per-row kernel behind rxode2's `linCmt()`.

Usage

```
linCmtModelDouble(
  dt,
  p1,
  v1,
  p2,
  p3,
  p4,
  p5,
  ka,
  alastNV,
  rateNV,
  ncmt,
  oral0,
  trans,
  deriv,
  type,
  tau,
  tinf,
  amt,
  bolusCmt,
  ndiff,
  sensType = 3L,
  sensH = 0.001
)
```

Arguments

dt	time step
p1, v1, p2, p3, p4, p5	parameters in the trans parameterization (see linCmtMicros())
ka	absorption rate constant (used when oral0 is 1)
alastNV	amounts at the start of the step (depot first when oral0 is 1, then central and peripherals); with deriv = TRUE followed by their parameter sensitivities
rateNV	zero-order rates into each compartment, in the same order
ncmt	number of compartments, 1 to 3
oral0	1 when the model has a depot compartment, otherwise 0
trans	parameterization number
deriv	logical; also return the derivatives
type	0 for a regular step; 1 and 2 steady-state infusion, 3 steady-state bolus
tau	steady-state dosing interval
tinf	steady-state infusion duration
amt	steady-state bolus amount
bolusCmt	steady-state bolus compartment
ndiff	differentiation bit mask as used by rxode2 (ka 1, p1 2, v1 4, p2 8, p3 16, p4 32, p5 64)
sensType	derivative method: 3 or 30 forward-mode automatic differentiation, 32 all directions in one forward-mode pass, 31 reverse mode, 100 automatic choice, 1 and 2 forward and central differences with the kernel's own step, 10 and 20 forward and central differences with step sensH
sensH	finite-difference step for sensType 10 and 20

Value

list with val (central concentration) and Alast (carried state after the step); with deriv = TRUE also J (Jacobian of the amounts) and Jg (gradient of val)

Examples

```
linCmtModelDouble(1, 2, 20, 0, 0, 0, 0, 0, 100, 0, 1L, 0L, 1L, FALSE,
                  0L, 0, 0, 0, 0L, 0L)
```

solComp2

*Eigenvalues and coefficients of the two compartment model***Description**

Computes the exponents (L) and coefficient matrices (C1, C2) of the two compartment linear system from its micro-constants. The idea comes from the 'wnl' package by Kyun-Seop Bae; the implementation is different.

Usage

```
solComp2(k10, k12, k21)
```

Arguments

k10	elimination rate
k12	rate from central to peripheral compartment
k21	rate from peripheral to central compartment

Value

List with L vector and matrices C1 and C2

Author(s)

Matthew L. Fidler, based on the idea in the 'wnl' package

Examples

```
solComp2(k10 = 0.1, k12 = 3, k21 = 1)
```

solComp3

*Eigenvalues and coefficients of the three compartment model***Description**

Eigenvalues and coefficients of the three compartment model

Usage

```
solComp3(k10, k12, k21, k13, k31)
```

Arguments

k10	elimination rate
k12	rate from central to peripheral compartment
k21	rate from peripheral to central compartment
k13	rate from central to peripheral compartment #2
k31	rate from peripheral compartment #2 to central

Value

List with L vector and matrices C1, C2 and C3

Author(s)

Matthew L. Fidler, based on the idea in the 'wnl' package

Examples

```
solComp3(k10 = 0.1, k12 = 3, k21 = 1, k13 = 2, k31 = 0.5)
```

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