Package 'branchCorr'

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Cor_xyFrom1

Model-based correlation from HSC

Description

This function computes the model-based correlation between two mature cell types given that the process begins with one HSC. The function is basically a wrapper around those used to compute variance and covariances.

Usage

```
Cor_xyFrom1(t, rates, progType1, progType2, type1, type2, progStructure)
```

Arguments

t	The length of time
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,, deathMature1, deathMature2,)
progType1	An index indicating the progenitor type that mature cell 1 can descend from
progType2	An index indicating the progenitor type that mature cell 2 can descend from
type1	An index indicating the type of mature cell 1
type2	An index indicating the type of mature cell 2
progStructur	e
	A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Correlation between specified mature type compartments at time t

Cor_xyFrom2 3

Cor_xyFrom2 Model-based correlation from progenitor

Description

This function computes the model-based correlation between two mature cell types given that the process begins with one progenitor. The function is basically a wrapper around those used to compute variance and covariances.

Usage

```
Cor_xyFrom2(t, rates, progType1, progType2, type1, type2, progStructure)
```

Arguments

t	The length of time
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,)
progType1	An index indicating the progenitor type that mature cell 1 can descend from
progType2	An index indicating the progenitor type that mature cell 2 can descend from
type1	An index indicating the type of mature cell 1
type2	An index indicating the type of mature cell 2
progStructur	re
	A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Correlation between specified mature type compartments at time t

Cov_xyFrom1 Model-based covariance from HSC

Description

This function computes the model-based covariance between two mature cell types given that the process begins with one HSC. The function simply converts the raw moments U, M into the corresponding covariance expression.

```
Cov_xyFrom1(t, rates, progType1, progType2, type1, type2, progStructure)
```

Cov_xyFrom2

Arguments

t	The length of time
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,)
progType1	An index indicating the progenitor type that mature cell 1 can descend from
progType2	An index indicating the progenitor type that mature cell 2 can descend from
type1	An index indicating the type of mature cell 1
type2	An index indicating the type of mature cell 2
progStructu	re
	A vector of length equal to number of mature types whose i'th entry contains

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Covariance between specified mature type compartments at time t

Description

This function computes the model-based covariance between two mature cell types given that the process begins with one progenitor. The function simply converts the raw moments U, M into the corresponding covariance expression.

Usage

```
Cov_xyFrom2(t, rates, progType1, progType2, type1, type2, progStructure)
```

Arguments

t	The length of time
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,)
progType1	An index indicating the progenitor type that mature cell 1 can descend from
progType2	An index indicating the progenitor type that mature cell 2 can descend from
type1	An index indicating the type of mature cell 1
type2	An index indicating the type of mature cell 2
progStructur	re
	A vector of length equal to number of mature types whose i'th entry contains

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends expit 5

Value

Covariance between specified mature type compartments at time t

expit

Expit function

Description

Evaluates the expit function

Usage

```
expit(x)
```

Arguments

Х

A number or vector

Value

The value of expit(x)

Examples

```
x = .25; expit(x)
x = 1:5; expit(x)
```

getObsCorr

Compute observed pairwise correlations

Description

Returns the empirical pairwise correlations between each pair of types, given a dataset of observed counts and a vector containing the corresponding observation times. The data matrix should be in the same format as returned by simCompObserved with vecOutput=TRUE

Usage

```
getObsCorr(data, obsTimes)
```

Arguments

data A matrix of mature cell type counts, in format produced by simCompObserved

with vecOutput=TRUE

obsTimes A vector of corresponding observation times

Value

Matrix containing pairwise correlations at each observation time

ample Hypergeometric sampling

Description

Samples hypergeometrically from a matrix containing discretely observed data from a stochastic compartmental model.

Usage

```
hyperGeoSample(data, sampSize, constantPopulation = FALSE, N = 10000)
```

Arguments

Ν

data	A matrix containing discretely observed data, in the format returned by simCompObserved	
sampSize	The sample size or number of draws n in a hypergeometric distribution	
constantPopulation		
	Logical whether to sample from equal total population, N, for all compartments	

The fixed total population if constantPopulation=TRUE

inferNLMINBSamplingCorr

Optimize correlation loss function

Description

This function uses the generic optimization package nlminb to optimize the objective function given by samplingCorrObjective. Takes additional initial guess parameter and allows specification of true death rates, which are often known and can be fixed throughout optimization.

Usage

```
inferNLMINBSamplingCorr(initGuess, obsTimes, obsCorr, nSample, nTotal,
    trueDeaths, progStructure, max = 5000)
```

Arguments

initGuess	Vector containing initial guess for par
obsTimes	A vector of observation times
obsCorr	Matrix of empirical correlations returned by getObsCorr
nSample	A vector containing the sample sizes of each mature type as arguments to hypergeometric sampling; this is the number of draws n
nTotal	A vector containing the total sizes of each mature population; this is the total population N in hypergeometric sampling
trueDeaths	Vector containing the true death rates to be fixed
progStructure	
	A vector of length equal to number of mature types whose i'th entry contains

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

max Max iterations, default to 5000

marginalizedCor_xy 7

Value

An nlminb object containing optimal parameters

marginalizedCor_xy Marginalized model-based correlations

Description

Computes the marginalized correlation between two mature cell types, given the initial probability distribution.

Usage

```
marginalizedCor_xy(t, rates, initProb, type1, type2, progStructure)
```

Arguments

t	The time length
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,)
initProb	vector containing initial probabilities of beginning in HSC comparatent and each progenitor compartment
type1	Index of mature type 1
type2	Index of mature type 2
progStructur	

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

The model-based marginalized correlation between types at time t

M_1x Mean population starting from HSC

Description

This function computes the model-based mean of a mature cell type compartment, given rates and that the process begins with one initial hematopoietic stem cell (compartment 1).

```
M_1x(t, rates, progType, type, progStructure)
```

8 M_2x

Arguments

t The length of time rates A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1, diffMature2, ..., deathMature1, deathMature2, ...)

An index indicating the progenitor type that the mature cell type can descend

from

An index indicating the mature cell type type

progStructure

progType

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

The mean population of compartment 'type' after time t

M_2x	This function computes the model-based mean of a mature cell type compartment, given rates and that the process begins with one initial
	progenitor.

Description

This function computes the model-based mean of a mature cell type compartment, given rates and that the process begins with one initial progenitor.

Usage

```
M_2x(t, rates, progType, type, progStructure)
```

Arguments

The length of time t rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

An index indicating the initial progenitor type progType An index indicating the mature cell type type

progStructure

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

The mean population of compartment 'type' after time t

NLMINBtrycatch 9

NLMINBtrycatch	Infer optimal rates via correlation loss function with error handling

Description

This function is a wrapper for optimizeSamplingCorrNLMINB that checks for any error codes using tryCatch

Usage

NLMINBtrycatch(data, numInits, initMean, obsTimes, nSample, nTotal, trueDeaths, progStructure)

Arguments

data	$A\ matrix\ of\ observed\ counts\ in\ the\ same\ format\ as\ produced\ by\ \verb simCompObserved $	
numInits	Number of random restarts	
initMean	The mean for the random initial parameters	
obsTimes	A vector of observation times	
nSample	A vector containing the sample sizes of each mature type as arguments to hypergeometric sampling; this is the number of draws n	
nTotal	A vector containing the total sizes of each mature population; this is the total population N in hypergeometric sampling	
trueDeaths	Vector containing the true death rates to be fixed	
progStructure		
	A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends	

optimizeSamplingCorrNLMINB

Infer optimal rates via correlation loss function

Description

This function is a wrapper for inferNLMINBSamplingCorr that takes a dataset in the format produced by simCompObserved and infers its most likely parameters. Computes the empirical correlations and optimizes the correlation loss function over many random initializations, and returns the best estimate in terms of lowest objective function value.

Usage

optimizeSamplingCorrNLMINB(data, numInits, initMean, obsTimes, nSample, nTotal, trueDeaths, progStructure) 10 randInit

Arguments

data	$A\ matrix\ of\ observed\ counts\ in\ the\ same\ format\ as\ produced\ by\ \verb simCompObserved $	
numInits	Number of random restarts	
initMean	The mean for the random initial parameters	
obsTimes	A vector of observation times	
nSample	A vector containing the sample sizes of each mature type as arguments to hypergeometric sampling; this is the number of draws n	
nTotal	A vector containing the total sizes of each mature population; this is the total population N in hypergeometric sampling	
trueDeaths	Vector containing the true death rates to be fixed	
progStructure		
	A vector of length equal to number of mature types whose i'th entry contains	

the corresponding hidden progenitor type from which mature type i descends

Value

Vector containing the best fitting parameters

randInit	Generate random initial population vector
Landinit	Generale random initial роришной vector

Description

This function converts an initial distribution to an initial population indicator vector. It samples from the initial distribution, and returns an initial population vector with an indicator of 1 in the compartment from which the process will begin, with zeros elsewhere.

Usage

```
randInit(initProbs, totalTypes)
```

Arguments

initProbs The initial distribution vector
totalTypes The total number of compartments or types

Value

A vector of zeros in all but one entry, indicating the initial type

samplingCorrObjective

Correlation loss function objective

Description

Computes the objective function of the correlation-matching loss function estimator. Takes in model parameters and a matrix of empirical correlations in the format produced by getObsCorr. This can then be plugged into a generic optimization routine such as nlminb. Natural constraints such as positivity of parameters are enforced via a log-barrier penalty.

Usage

samplingCorrObjective(par, obsTimes, obsCorr, nSample, nTotal, progStructure)

Arguments

par	A vector containing the process rates followed by all but the first component of the initial distribution vector. The rates should be ordered as before, beginning with self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diff-ProgB,, deathProgA, deathProgB, diffMature1, diffMature2,, deathMature1, deathMature2,)	
obsTimes	A vector of observation times	
obsCorr	Matrix of empirical correlations returned by getObsCorr	
nSample	A vector containing the sample sizes of each mature type as arguments to hypergeometric sampling; this is the number of draws n	
nTotal	A vector containing the total sizes of each mature population; this is the total population N in hypergeometric sampling	
progStructure		
	A vector of length equal to number of mature types whose i'th entry contains	

A vector of length equal to number of mature types whose i th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Objective value

samplingCor_xy

Marginalized model-based correlations with sampling

Description

Computes the marginalized correlation between two mature cell types, given the initial probability distribution, incorporating the effect of hypergeometric sampling.

sim.once

Usage

```
samplingCor_xy(t, rates, initProb, type1, type2, pop1, pop2, total1, total2,
    progStructure)
```

Arguments

t	The time length	
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,, deathMature1, deathMature2,)	
initProb	vector containing initial probabilities of beginning in HSC comparatent and each progenitor compartment	
type1	Index of mature type 1	
type2	Index of mature type 2	
pop1	Sample size of mature type 1	
pop2	Sample size of mature type 2	
total1	Total population of mature type 1 cells	
total2	Total population of mature type 2 cells	
progStructure		
	A vector of length equal to number of mature types whose i'th entry contains	

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Correlation between types at time t after marginalizing over sampling distribution and initial distribution

imulate discretely observed data from a stochastic compartmental nodel with error check

Description

Wrapper for simCompObserved that checks for no error code

```
sim.once(t.end, initPopulation, rates, progStructure, obsTimes,
   vecOutput = FALSE, maxEvents = 99999999999)
```

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Arguments

t.end The total time until end of simulation

initPopulation

A vector of length equal to total number of compartments/types; entries contain

the initial population of each type

rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

progStructure

A vector of length equal to number of mature types whose i'th entry contains

the corresponding hidden progenitor type from which mature type i descends

 $\hbox{\tt obsTimes} \qquad \quad A \ vector \ containing \ the \ observation \ times$

vecOutput Logical, whether to return a vectorized representation of the matrix of observa-

tion times by population counts

maxEvents The maximum number of events to simulate

simCompartments

Forward simulate from a stochastic compartmental model

Description

Uses Gillespie forward simulation from a stochastic compartmental model, i.e. representing a hematopoietic tree.

Usage

```
simCompartments(t.end, initPopulation, rates, progStructure,
maxEvents = 99999999999)
```

Arguments

t.end The total time until end of simulation

initPopulation

A vector of length equal to total number of compartments/types; entries contain

the initial population of each type

rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

progStructure

A vector of length equal to number of mature types whose i'th entry contains

the corresponding hidden progenitor type from which mature type i descends

maxEvents The maximum number of events to simulate

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Value

A vector containing the mature type populations at end of simulation period (time t=t.end).

Examples

```
progStructure <- c(1,1,1,2,2)
initPopulation <- c(10,0,0,0,0,0,0,0)
rates <- c(.3,.2,.5,.06,.03,2,4,5,3,1,.15,.5,.8,.1,.05)
simCompartments(5, initPopulation, rates,progStructure)
```

simCompObserved

Simulate discretely observed data from a stochastic compartmental model

Description

This code simulates data analogously to simCompartments, but records populations at a specified list of observation times.

Usage

```
simCompObserved(t.end, initPopulation, rates, progStructure, obsTimes,
  vecOutput = FALSE, maxEvents = 99999999999)
```

Arguments

t.end The total time until end of simulation

initPopulation

A vector of length equal to total number of compartments/types; entries contain

the initial population of each type

rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

progStructure

A vector of length equal to number of mature types whose i'th entry contains

the corresponding hidden progenitor type from which mature type i descends

obsTimes A vector containing the observation times

vecOutput Logical, whether to return a vectorized representation of the matrix of observa-

tion times by population counts

maxEvents The maximum number of events to simulate

Value

A matrix of population sizes of each compartment at each observation time. Rows index cell type; columns index observation times. Returns the vectorized form of thie matrix if vecOutput=TRUE.

 $U_{\perp}xx$

Examples

```
progStructure <- c(1,1,1,2,2)
initPopulation <- c(10,0,0,0,0,0,0,0)
obsTimes <- 1:5
rates <- c(.3,.2,.5,.06,.03,2,4,5,3,1,.15,.5,.8,.1,.05)
simCompObserved(5, initPopulation, rates, progStructure, obsTimes)
```

 U_xx

Second moments starting from HSC

Description

This function computes the model-based second moments, denoted U_mml0 in the manuscript, of a mature cell type, given rates and that the process begins with one initial hematopoietic stem cell (compartment 1).

Usage

```
U_xx(t, rates, progType, type, progStructure)
```

Arguments

t	The length of time
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,, deathMature1, deathMature2,)
progType	An index indicating the progenitor type that the mature cell type can descend from
type	An index indicating the mature cell type
progStructure	
	A vector of length equal to number of mature types whose i'th entry contains

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Value of second moment at time t

16 Var_xFrom1

U	X	V

Second cross-moments starting from HSC

Description

This function computes the model-based second cross-moments, denoted U_mnl0 in the manuscript, between two mature cell types, given rates and that the process begins with one initial hematopoietic stem cell (compartment 1).

Usage

```
U_xy(t, rates, progType1, progType2, type1, type2, progStructure)
```

Arguments

t	The length of time	
rates	A rate vector containing self-renewal rates of first compartment, followed by differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB,, deathProgA, deathProgB, diffMature1, diffMature2,)	
progType1	An index indicating the progenitor type that mature cell 1 can descend from	
progType2	An index indicating the progenitor type that mature cell 2 can descend from	
type1	An index indicating the type of mature cell 1	
type2	An index indicating the type of mature cell 2	
progStructure		
	A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends	

Value

Value of second cross-moment at time t

|--|

Description

This function computes the model-based variance of a mature cell type given that the process begins with one HSC. The function simply converts the raw moments U, M into the corresponding variance expression.

```
Var_xFrom1(t, rates, progType, type, progStructure)
```

Var_xFrom2

Arguments

t The length of time

rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

progType An index indicating the progenitor type that the mature cell type can descend

from

type An index indicating the mature cell type

progStructure

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Variance of specified mature cell compartment at time t

Var_xFrom2 Model-based variance from progenitor

Description

This function computes the model-based variance of a mature cell type given that the process begins with one progenitor. The function simply converts the raw moments U, M into the corresponding variance expression.

Usage

```
Var_xFrom2(t, rates, progType, type, progStructure)
```

Arguments

t The length of time

rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

progType An index indicating the initial progenitor type

type An index indicating the mature cell type

progStructure

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Variance of specified mature cell compartment at time t

 $V_{-}xy$

V	XX

Second moments starting from progenitor

Description

This function computes the model-based second moments, denoted U_mmla in the manuscript, of a mature cell type, given rates and that the process begins with one initial progenitor cell.

Usage

```
V_xx(t, rates, progType, type, progStructure)
```

Arguments

t The length of time

rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

progType An index indicating the initial progenitor type

type An index indicating the mature cell type

progStructure

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Value of second moment at time t

V_xy

Second cross-moments starting from progenitor

Description

This function computes the model-based second cross-moments, denoted U_mnla in the manuscript, between two mature cell types, given rates and that the process begins with one progenitor cell.

```
V_xy(t, rates, progType1, progType2, type1, type2, progStructure)
```

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Arguments

t The length of time

rates A rate vector containing self-renewal rates of first compartment, followed by

differentiation rates of intermediate types, death rates of intermediate types, differentiation rates of mature types, and death rates of mature types, i.e. (renewHSC, diffProgA, diffProgB, ..., deathProgA, deathProgB, ... diffMature1,

diffMature2, ..., deathMature1, deathMature2, ...)

progType1 An index indicating the progenitor type that mature cell 1 can descend from progType2 An index indicating the progenitor type that mature cell 2 can descend from

type1 An index indicating the type of mature cell 1 type2 An index indicating the type of mature cell 2

progStructure

A vector of length equal to number of mature types whose i'th entry contains the corresponding hidden progenitor type from which mature type i descends

Value

Value of second cross-moment at time t