

# Constructing hyperprior for hierarchical co-demographic model

## Description

`build.dice` builds a hyperprior across  $\Psi/\psi$  and  $\zeta/\zeta_s$  according to: 1) uniform distribution for  $\Psi/\psi$ , for  $\zeta_T$  within each discrete  $\Psi/\psi$  value, and across all combinations of the vector  $\zeta/\zeta_s$  within each discrete  $\zeta_T$  value; 2) Dirichlet-process that weighs all allowable combinations of  $\Psi/\psi$  and  $\zeta/\zeta_s$  according to possible combinations of taxa assignment; 3) customized distribution(s).

## Usage

```
build.dice(num.taxa, num.partitions=1, tau.psi.prior=NULL,
epsilon.psi.prior=NULL, NE.psi.prior=NULL, tau.zeta.prior=NULL,
tau2.zeta.prior=NULL, epsilon.zeta.prior=NULL, epsilon2.zeta.prior=NULL,
NE.zeta.prior=NULL, tau.zeta.total.prior=NULL, tau2.zeta.total.prior=NULL,
epsilon.zeta.total.prior=NULL, epsilon2.zeta.total.prior=NULL,
NE.zeta.total.prior=NULL, dirichlet.process=F, idiosyncratic=T,
min.net.tau.zeta.total=NULL, min.net.tau2.zeta.total=NULL,
min.net.epsilon.zeta.total=NULL, min.net.epsilon2.zeta.total=NULL,
min.net.NE.zeta.total=NULL, max.net.tau.zeta.total=NULL,
max.net.tau2.zeta.total=NULL, max.net.epsilon.zeta.total=NULL,
max.net.epsilon2.zeta.total=NULL, max.net.NE.zeta.total=NULL,
min.net.tau.zeta.per.pulse=NULL, min.net.tau2.zeta.per.pulse=NULL,
min.net.epsilon.zeta.per.pulse=NULL, min.net.epsilon2.zeta.per.pulse=NULL,
min.net.NE.zeta.per.pulse=NULL, max.net.tau.zeta.per.pulse=NULL,
max.net.tau2.zeta.per.pulse=NULL, max.net.epsilon.zeta.per.pulse=NULL,
max.net.epsilon2.zeta.per.pulse=NULL, max.net.NE.zeta.per.pulse=NULL)
```

## Arguments

### DATA

`num.taxa`

List, vector of length = `num.partitions`, or positive integer.  
Number of taxa per partition. Total sum across partitions equals the total number of taxa  $n$  in dataset. See also `Details`. Required.

`num.partitions`

Positive integer. Number of partitions for taxa in dataset. Allows differential data and model specifications across user-specified taxa groupings, including sampling size of individuals, generation times, demographic syndrome, and taxon-specific nuisance parameter prior distributions. See also `Details`.

## PRIORS

`tau.psi.prior,`  
`epsilon.psi.prior, NE.psi.prior`

List, vector, or non-negative integer. Hyperprior distribution for  $\Psi/\psi$  of  $\tau$ ,  $\varepsilon$ , and  $N_E$ , respectively. For  $\tau$  and  $\varepsilon$ , if list of length = 2, then the first list element applies to the first more recent size change event (e.g.  $\tau_1$ ,  $\varepsilon_1$ ) and the second list element applies to the second more ancient size change event (e.g.  $\tau_2$ ,  $\varepsilon_2$ ), per taxon. The argument(s) specified here and their according list lengths activate which taxon-specific demographic parameters are to be hyperparameterized via  $\Psi/\psi$  as well as  $\zeta/\zeta_s/\zeta_T$  downstream. See also `Details`. At least one is required.

`tau.zeta.prior, tau2.zeta.prior,`  
`epsilon.zeta.prior,`  
`epsilon2.zeta.prior,`  
`NE.zeta.prior`

List of length = `num.partitions` or 1, vector, or non-negative proportion (i.e.  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_j$  of  $\tau_1$ ,  $\tau_2$ ,  $\varepsilon_1$ ,  $\varepsilon_2$ , and  $N_E$ , respectively, for each  $j$ th pulse from 1 to  $\Psi/\psi$ , as specified by the corresponding `psi.prior`, and per partition. See also `Details`. Required for each corresponding `psi.prior` specified, unless the maximum value in the corresponding `psi.prior` = 0.

`tau.zeta.total.prior,`  
`tau2.zeta.total.prior,`  
`epsilon.zeta.total.prior,`  
`epsilon2.zeta.total.prior,`  
`NE.zeta.total.prior`

List of length = 1, vector, or non-negative proportion (i.e.  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_T$  of  $\tau_1$ ,  $\tau_2$ ,  $\varepsilon_1$ ,  $\varepsilon_2$ , and  $N_E$ , respectively. Activates a uniform hyperprior such that each discrete  $\Psi/\psi$  value, as specified by the corresponding `psi.prior`, is first weighted with equal hyperprior probability, then all discrete  $\zeta_T$  values are weighted equally per  $\Psi/\psi$  value, and finally every possible associated vector  $\zeta/\zeta_s$  is weighted equally per  $\zeta_T$  value. See also `Details`.

## MODEL SPECIFICATIONS

`dirichlet.process`

Logical value. Activates a Dirichlet-process hyperprior that weighs all allowable combinations of  $\Psi/\psi$  and  $\zeta/\zeta_s$  according to possible combinations of taxa assignment. See also `Details`.

`idiosyncratic`

Logical value. Allows idiosyncratic taxa that freely vary i.e. are ungrouped from any of the pulses, as specified by the `psi.prior` arguments. See also `Details`.

`min.net.tau.zeta.total,`  
`min.net.tau2.zeta.total,`  
`min.net.epsilon.zeta.total,`  
`min.net.epsilon2.zeta.total,`  
`min.net.NE.zeta.total,`  
`max.net.tau.zeta.total,`  
`max.net.tau2.zeta.total,`

Non-negative proportion (i.e.  $\leq 1$  and  $\geq 0$ ). Rule for the minimum/maximum  $\zeta_T$  value, across all pulses (as specified by the corresponding `psi.prior`) and partitions, for  $\tau_1$ ,  $\tau_2$ ,  $\varepsilon_1$ ,  $\varepsilon_2$ , and  $N_E$ , respectively. See also `Details`.

max.net.epsilon.zeta.total,  
max.net.epsilon2.zeta.total,  
max.net.NE.zeta.total

min.net.tau.zeta.per.pulse,  
min.net.tau2.zeta.per.pulse,  
min.net.epsilon.zeta.per.pulse,  
min.net.epsilon2.zeta.per.pulse,  
min.net.NE.zeta.per.pulse,  
max.net.tau.zeta.per.pulse,  
max.net.tau2.zeta.per.pulse,  
max.net.epsilon.zeta.per.pulse,  
max.net.epsilon2.zeta.per.pulse,  
max.net.NE.zeta.per.pulse

List, vector of length = maximum value in corresponding `psi.prior`, or non-negative proportion (*i.e.*  $\leq 1$  and  $\geq 0$ ). Rule for the minimum/maximum  $\zeta_j$  value of  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively, for each  $j$ th pulse from 1 to  $\Psi/\psi$  (as specified by the corresponding `psi.prior`) across all partitions. See also Details.

Arguments from other Multi-DICE functions may be included here and are ignored if not applicable.

## Details

For more information, see Multi-DICE Manual.

Multi-DICE cannot currently accommodate models with more than one population per taxon, events aside from population size change, and more than two size change events.

For  $\tau_1$  and  $\tau_2$ , units are in numbers of generations, and thus may only be positive integers. For  $\epsilon_1$  and  $\epsilon_2$ , units are in ratio of size change from the ancestral effective population size to current effective population size, such that expansions are  $< 1$  and contractions are  $> 1$ , and thus may only be positive values. For  $N_E$ , unit is in number of effective haploid individuals, and thus may only be positive integers.

For `num.taxa`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, `max.net.tau.zeta.per.pulse`, `max.net.tau2.zeta.per.pulse`, `max.net.epsilon.zeta.per.pulse`, `max.net.epsilon2.zeta.per.pulse`, and `max.net.NE.zeta.per.pulse`, if list, then all list elements are concatenated to form a single vector, with the ordering within list elements and then between list elements preserved (*e.g.* for list of length = 2, with first list element of length = 2 and second list element of length = 1, the order from first to last is: 1) first vector element in first list element; 2) second vector element in first list element; 3) sole vector element in second list element).

For `tau.psi.prior`, `epsilon.psi.prior`, `NE.psi.prior`, `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, `NE.zeta.prior`, `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior`, each list element contains an entire individual discrete distribution; if vector, then converted to list of length = 1 with all vector elements comprising the entirety of a single discrete distribution. Per list element, vector elements within (*i.e.* the discrete distribution) do not need to be in any particular order. Relatedly, each vector

element is treated as an independent value, thus weighted distributions (*i.e.* not uniform) may be employed by duplicating values (e.g. a distribution of  $c(0, 1, 1, 1)$  signifies 75% probability of drawing “1” and 25% probability of drawing “0”), allowing the specification of any discretized distribution (e.g. gamma, beta, log-uniform). Accordingly, a uniform distribution with no gaps for integer values would be of length = range of distribution.

For `num.taxa`, the order of vector elements corresponds to the order of partitions, and for `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, and `NE.zeta.prior`, the order of list elements corresponds to the order of partitions. Additionally, if `length = 1` and `num.partitions > 1`, then the sole element is used for all partitions. Similarly, if `length < num.partitions`, then the first element is used for all partitions while ignoring any remaining elements, and if `length > num.partitions`, then the remaining elements beyond `length = num.partitions` are ignored; a caution is provided when the length does not equal 1 or `num.partitions`.

For `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, `max.net.tau.zeta.per.pulse`, `max.net.tau2.zeta.per.pulse`, `max.net.epsilon.zeta.per.pulse`, `max.net.epsilon2.zeta.per.pulse`, and `max.net.NE.zeta.per.pulse`, the order of vector elements corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding `psi.prior`). Additionally, if `length = 1` and maximum value in corresponding `psi.prior > 1`, then the sole element is used for all pulses. Similarly, if `length < maximum value in corresponding psi.prior`, then the first element is used for all pulses while ignoring any remaining elements, and if `length > maximum value in corresponding psi.prior`, then the remaining elements beyond `length = maximum value in corresponding psi.prior` are ignored; a caution is provided when the length does not equal 1 or maximum value in corresponding `psi.prior`.

If `num.partitions = n`, then rearrangement of bins across taxa within allele frequency classes based on descending order of the relative SNP proportions is not performed to construct the aSFS and taxon-specific inference of demographic parameters is possible. However, in general, more partitions results in more parameter space with respect to taxa samples that must be explored due to a decrease in order-independence and assumed exchangeability, thus multiple-fold more simulations must be conducted to achieve comparable accuracy in hyperparameter estimation as without partitioning.

For `tau.psi.prior`, `epsilon.psi.prior`, and `NE.psi.prior`, distinguishing between  $\Psi$  and  $\psi$  is accomplished via the corresponding `zeta.prior`, `zeta.total.prior`, `idiosyncratic` setting, and/or `min/max.net.zeta.total/per.pulse`, except for values of 0, which are explicitly for  $\psi = 0$  and thus indicate full idiosyncrasy. If list length  $> 2$  for  $\tau$  and  $\epsilon$  or list length  $> 1$  for  $N_E$ , then a caution is provided and the remaining elements beyond `length = 2` for  $\tau$  and  $\epsilon$  and `length = 1` for  $N_E$  are ignored. Applies across all partitions, such that it is regardless of partitioning.

For `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, and `NE.zeta.prior`, if `num.partitions > 1`, may be necessary to include “0.0” as a value, but can control  $\zeta_s$  and  $\zeta_T$  across partitions via corresponding `zeta.total.prior` and/or `min/max.net.zeta.total/per.pulse`. Attributes to each partition individually, but proportion values are out of the entirety of taxa dataset, thus if `num.partitions > 1`, then the upper bound for each partition should be the number of taxa within that partition divided by  $n$ . When  $\psi = \{0, 1\}$ , equivalent to hyperprior distribution for  $\zeta_T$ . If identical across all partitions, it is more computationally efficient to specify only one *i.e.* list of length = 1, or a vector.

For `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior`, if length > 1, then remaining elements beyond the first are ignored and a caution is provided.

To build a hyperprior, Multi-DICE first looks if the corresponding `zeta.total.prior` is specified, then if `dirichlet.process=T`, and if neither is such case, then all possible combinations of corresponding `psi.prior` and `zeta.prior` draws are equally weighted. Therefore, if `num.partitions=1`, corresponding `psi.prior=1`, and `dirichlet.process=F`, then `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior` equivalent to corresponding `zeta.prior` and thus unnecessary to specify.

When  $\psi = 0$  *i.e.* full idiosyncrasy, the arguments `idiosyncratic`, `min.net.tau.zeta.total`, `min.net.tau2.zeta.total`, `min.net.epsilon.zeta.total`, `min.net.epsilon2.zeta.total`, `min.net.NE.zeta.total`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, and `min.net.NE.zeta.per.pulse` are ignored.

Multi-DICE proceeds only if a valid draw is allowed given corresponding `num.taxa`, `psi.prior`, `zeta.prior` (*e.g.* minimum value in `psi.prior` \* minimum value in `zeta.prior`  $\leq$  minimum value in `num.taxa`), `zeta.total.prior`, `idiosyncratic` setting, and `min/max.net.zeta.total/per.pulse`. Importantly, there is no check on if all values in `psi.prior` have a valid draw, only if there is a valid draw among any of the values.

## Value

Returned value is a list object with each element attributed to a hyperparameterized demographic parameter and accordingly named (*i.e.* `tau`, `tau2`, `epsilon`, `epsilon2`, `NE`). Each of these list elements contain the following components:

<code>draws</code>	List of matrices. The order of list elements/matrices corresponds to the order of partitions. Per matrix, each row represents a valid draw, with rows across matrices corresponding to each other ( <i>i.e.</i> the same row number across matrices refers to the same individual draw). The first column is the $\Psi/\psi$ drawn value as specified by the
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corresponding `psi.prior`. The second column is a row index number corresponding to the matrices in the `combos` component, which contains information about the  $\zeta/\zeta_s$  drawn value(s).

`combos` List of list of matrices. The order of list elements corresponds to the order of partitions. Each of these list elements contain another list of matrices, with these list elements/matrices corresponding to the different unique  $\Psi/\psi$  values in the corresponding `psi.prior`, in ascending order of  $\Psi/\psi$  values, and accordingly named with the prefix “pulse” concatenated with  $\Psi/\psi$  value as a suffix (e.g. “pulse1”, “pulse2”). Per matrix, each row represents a possible per-partition draw, each cell is a  $S$  drawn value, and the order of columns corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding `psi.prior`).

`hyperprior` Vector. Contains constructed hyperprior distribution, with each element an indexed draw referring to the row numbers in `draws`.

## Author(s)

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## References

- Chan YL, Schanzenbach D, Hickerson MJ (2014) Detecting concerted demographic response across community assemblages using hierarchical approximate Bayesian computation. *Molecular Biology and Evolution*, **31**, 2501–2515.
- Hickerson MJ, Stahl E, Takebayashi N (2007) msBayes: Pipeline for testing comparative phylogeographic histories using hierarchical approximate Bayesian computation. *BMC bioinformatics*, **8**, 268.
- Huang W, Takebayashi N, Qi Y, Hickerson MJ (2011) MTML-msBayes: approximate Bayesian comparative phylogeographic inference from multiple taxa and multiple loci with rate heterogeneity. *BMC bioinformatics*, **12**, 1.
- Xue AT (2017) Multi-DICE Manual.
- Xue AT, Hickerson MJ (2015) The aggregate site frequency spectrum for comparative population genomic inference. *Molecular Ecology*, **24**, 6223–6240.
- Xue AT, Hickerson MJ (*submitted*) Multi-DICE: R package for comparative population genomic inference under multi-taxa hierarchical co-demographic models.

## See Also

`roll.dice`, `play.dice`, `dice.sims`, `dice.aSFS`, `dice.sumstats`

## Examples

#simplest execution akin to approach in Xue and Hickerson (2015)

```
build.dice(num.taxa=10, tau.psi.prior=c(1), tau.zeta.prior=c(1:10)/10)

#simplest execution akin to approach in software package msBayes
build.dice(num.taxa=10, tau.psi.prior=c(1:10), tau.zeta.prior=c(1:10)/10,
idiosyncratic=F)
```

# Hyperprior and parameter summary prior draws for hierarchical co-demographic model

## Description

`roll.dice` conducts random draws from the hyperprior distribution constructed in `build.dice`, as well as from user-specified prior distributions for shared pulse values. These shared pulse values (e.g.  $\tau_{1s}$ ,  $\tau_{2s}$ ,  $\epsilon_{1s}$ ,  $\epsilon_{2s}$ ,  $N_s$ ) are parameter summaries of the taxon-specific demographic parameter values for the shared pulses, as specified by the `psi.prior` arguments. `build.dice` is embedded here and is automatically deployed if `build.object` is not specified.

## Usage

```
roll.dice(num.sims, num.taxa, num.partitions=1, tau.psi.prior=NULL,
epsilon.psi.prior=NULL, NE.psi.prior=NULL, tau.zeta.prior=NULL,
tau2.zeta.prior=NULL, epsilon.zeta.prior=NULL, epsilon2.zeta.prior=NULL,
NE.zeta.prior=NULL, tau.zeta.total.prior=NULL, tau2.zeta.total.prior=NULL,
epsilon.zeta.total.prior=NULL, epsilon2.zeta.total.prior=NULL,
NE.zeta.total.prior=NULL, tau.shared.prior=NULL, tau2.shared.prior=NULL,
epsilon.shared.prior=NULL, epsilon2.shared.prior=NULL,
NE.shared.prior=NULL, dirichlet.process=F, idiosyncratic=T,
min.net.tau.zeta.total=NULL, min.net.tau2.zeta.total=NULL,
min.net.epsilon.zeta.total=NULL, min.net.epsilon2.zeta.total=NULL,
min.net.NE.zeta.total=NULL, max.net.tau.zeta.total=NULL,
max.net.tau2.zeta.total=NULL, max.net.epsilon.zeta.total=NULL,
max.net.epsilon2.zeta.total=NULL, max.net.NE.zeta.total=NULL,
min.net.tau.zeta.per.pulse=NULL, min.net.tau2.zeta.per.pulse=NULL,
min.net.epsilon.zeta.per.pulse=NULL, min.net.epsilon2.zeta.per.pulse=NULL,
min.net.NE.zeta.per.pulse=NULL, max.net.tau.zeta.per.pulse=NULL,
max.net.tau2.zeta.per.pulse=NULL, max.net.epsilon.zeta.per.pulse=NULL,
max.net.epsilon2.zeta.per.pulse=NULL, max.net.NE.zeta.per.pulse=NULL,
tau.buffer=0, tau2.buffer=0, epsilon.buffer=0, epsilon2.buffer=0,
NE.buffer=0, build.object=NULL)
```

## Arguments

`num.sims` Positive integer. Number of simulations. Required.

## DATA

`num.taxa` List, vector of length = `num.partitions`, or positive integer.  
Number of taxa per partition. Total sum across partitions



equals the total number of taxa  $n$  in dataset. See also [Details](#). Required.

`num.partitions`

Positive integer. Number of partitions for taxa in dataset. Allows differential data and model specifications across user-specified taxa groupings, including sampling size of individuals, generation times, demographic syndrome, and taxon-specific nuisance parameter prior distributions. See also [Details](#).

## PRIORS

`tau.psi.prior,`  
`epsilon.psi.prior, NE.psi.prior`

List, vector, or non-negative integer. Hyperprior distribution for  $\Psi/\psi$  of  $\tau$ ,  $\epsilon$ , and  $N_E$ , respectively. For  $\tau$  and  $\epsilon$ , if list of length = 2, then the first list element applies to the first more recent size change event (e.g.  $\tau_1$ ,  $\epsilon_1$ ) and the second list element applies to the second more ancient size change event (e.g.  $\tau_2$ ,  $\epsilon_2$ ), per taxon. The argument(s) specified here and their according list lengths activate which taxon-specific demographic parameters are to be hyperparameterized via  $\Psi/\psi$  as well as  $\zeta/\zeta_s/\zeta_T$  downstream. See also [Details](#). At least one is required.

`tau.zeta.prior, tau2.zeta.prior,`  
`epsilon.zeta.prior,`  
`epsilon2.zeta.prior,`  
`NE.zeta.prior`

List of length = `num.partitions` or 1, vector, or non-negative proportion (i.e.  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_j$  of  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively, for each  $j$ th pulse from 1 to  $\Psi/\psi$ , as specified by the corresponding `psi.prior`, and per partition. See also [Details](#). Required for each corresponding `psi.prior` specified, unless the maximum value in the corresponding `psi.prior` = 0.

`tau.zeta.total.prior,`  
`tau2.zeta.total.prior,`  
`epsilon.zeta.total.prior,`  
`epsilon2.zeta.total.prior,`  
`NE.zeta.total.prior`

List of length = 1, vector, or non-negative proportion (i.e.  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_T$  of  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively. Activates a uniform hyperprior such that each discrete  $\Psi/\psi$  value, as specified by the corresponding `psi.prior`, is first weighted with equal hyperprior probability, then all discrete  $\zeta_T$  values are weighted equally per  $\Psi/\psi$  value, and finally every possible associated vector  $\zeta/\zeta_s$  is weighted equally per  $\zeta_T$  value. See also [Details](#).

`tau.shared.prior,`  
`tau2.shared.prior,`  
`epsilon.shared.prior,`  
`epsilon2.shared.prior,`  
`NE.shared.prior`

List, vector, or positive value. Prior distribution for the demographic parameter summaries  $\tau_{1s}$ ,  $\tau_{2s}$ ,  $\epsilon_{1s}$ ,  $\epsilon_{2s}$ , and  $N_s$ , respectively (or  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N$ , respectively, if corresponding `psi.prior` specifies  $\Psi$ ). See also [Details](#). Required for each corresponding `psi.prior` specified, unless the maximum value in the corresponding `psi.prior` = 0.

## MODEL SPECIFICATIONS

<code>dirichlet.process</code>	Logical value. Activates a Dirichlet-process hyperprior that weighs all allowable combinations of $\Psi/\psi$ and $\zeta/\zeta_s$ according to possible combinations of taxa assignment. See also <code>Details</code> .
<code>idiosyncratic</code>	Logical value. Allows idiosyncratic taxa that freely vary <i>i.e.</i> are ungrouped from any of the pulses, as specified by the <code>psi.prior</code> arguments. See also <code>Details</code> .
<code>min.net.tau.zeta.total,</code> <code>min.net.tau2.zeta.total,</code> <code>min.net.epsilon.zeta.total,</code> <code>min.net.epsilon2.zeta.total,</code> <code>min.net.NE.zeta.total,</code> <code>max.net.tau.zeta.total,</code> <code>max.net.tau2.zeta.total,</code> <code>max.net.epsilon.zeta.total,</code> <code>max.net.epsilon2.zeta.total,</code> <code>max.net.NE.zeta.total</code>	Non-negative proportion ( <i>i.e.</i> $\leq 1$ and $\geq 0$ ). Rule for the minimum/maximum $\zeta_T$ value, across all pulses (as specified by the corresponding <code>psi.prior</code> ) and partitions, for $\tau_1$ , $\tau_2$ , $\epsilon_1$ , $\epsilon_2$ , and $N_E$ , respectively. See also <code>Details</code> .
<code>min.net.tau.zeta.per.pulse,</code> <code>min.net.tau2.zeta.per.pulse,</code> <code>min.net.epsilon.zeta.per.pulse,</code> <code>min.net.epsilon2.zeta.per.pulse,</code> <code>min.net.NE.zeta.per.pulse,</code> <code>max.net.tau.zeta.per.pulse,</code> <code>max.net.tau2.zeta.per.pulse,</code> <code>max.net.epsilon.zeta.per.pulse,</code> <code>max.net.epsilon2.zeta.per.pulse,</code> <code>max.net.NE.zeta.per.pulse</code>	List, vector of length = maximum value in corresponding <code>psi.prior</code> , or non-negative proportion ( <i>i.e.</i> $\leq 1$ and $\geq 0$ ). Rule for the minimum/maximum $\zeta_j$ value of $\tau_1$ , $\tau_2$ , $\epsilon_1$ , $\epsilon_2$ , and $N_E$ , respectively, for each $j$ th pulse from 1 to $\Psi/\psi$ (as specified by the corresponding <code>psi.prior</code> ) across all partitions. See also <code>Details</code> .
<code>tau.buffer,</code> <code>tau2.buffer,</code> <code>epsilon.buffer,</code> <code>epsilon2.buffer,</code> <code>NE.buffer</code>	Non-negative value or function. Pulse buffer $\beta$ of the demographic parameter summaries $\tau_{1s}$ , $\tau_{2s}$ , $\epsilon_{1s}$ , $\epsilon_{2s}$ , and $N_s$ , respectively. See also <code>Details</code> .

## OBJECTS FROM PRECEDING FUNCTIONS

<code>build.object</code>	Output from function <code>build.dice</code> . See also <code>Details</code> .
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Arguments from other `Multi-DICE` functions may be included here and are ignored if not applicable.

### **Details**

For more information, see `Multi-DICE Manual`.

`Multi-DICE` cannot currently accommodate models with more than one population per taxon, events aside from population size change, and more than two size change events.

For  $\tau_1$  and  $\tau_2$ , units are in numbers of generations, and thus may only be positive integers. For  $\epsilon_1$  and  $\epsilon_2$ , units are in ratio of size change from the ancestral effective population size to current effective population size, such that expansions are  $< 1$  and contractions are  $> 1$ , and thus may only be positive values. For  $N_E$ , unit is in number of effective haploid individuals, and thus may only be positive integers.

For `num.taxa`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, `max.net.tau.zeta.per.pulse`, `max.net.tau2.zeta.per.pulse`, `max.net.epsilon.zeta.per.pulse`, `max.net.epsilon2.zeta.per.pulse`, and `max.net.NE.zeta.per.pulse`, if `list`, then all list elements are concatenated to form a single vector, with the ordering within list elements and then between list elements preserved (e.g. for list of length = 2, with first list element of length = 2 and second list element of length = 1, the order from first to last is: 1) first vector element in first list element; 2) second vector element in first list element; 3) sole vector element in second list element).

For `tau.psi.prior`, `epsilon.psi.prior`, `NE.psi.prior`, `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, `NE.zeta.prior`, `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, `NE.zeta.total.prior`, `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, and `NE.shared.prior`, each list element contains an entire individual discrete distribution; if vector, then converted to list of length = 1 with all vector elements comprising the entirety of a single discrete distribution. Per list element, vector elements within (i.e. the discrete distribution) do not need to be in any particular order. Relatedly, each vector element is treated as an independent value, thus weighted distributions (i.e. not uniform) may be employed by duplicating values (e.g. a distribution of  $c(0, 1, 1, 1)$  signifies 75% probability of drawing “1” and 25% probability of drawing “0”), allowing the specification of any discretized distribution (e.g. gamma, beta, log-uniform). Accordingly, a uniform distribution with no gaps for integer values would be of length = range of distribution.

For `num.taxa`, the order of vector elements corresponds to the order of partitions, and for `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, and `NE.zeta.prior`, the order of list elements corresponds to the order of partitions. Additionally, if `length = 1` and `num.partitions > 1`, then the sole element is used for all partitions. Similarly, if `length < num.partitions`, then the first element is used for all partitions while ignoring any remaining elements, and if `length > num.partitions`, then the remaining elements beyond `length = num.partitions` are ignored; a caution is provided when the length does not equal 1 or `num.partitions`.

For `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, `max.net.tau.zeta.per.pulse`, `max.net.tau2.zeta.per.pulse`, `max.net.epsilon.zeta.per.pulse`, `max.net.epsilon2.zeta.per.pulse`, and `max.net.NE.zeta.per.pulse`, if `list`, then all list elements are concatenated to form a single vector, with the ordering within list elements and then between list elements preserved (e.g. for list of length = 2, with first list element of length = 2 and second list element of length = 1, the order from first to last is: 1) first vector element in first list element; 2) second vector element in first list element; 3) sole vector element in second list element).

`max.net.epsilon2.zeta.per.pulse`, and `max.net.NE.zeta.per.pulse`, the order of vector elements corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding `psi.prior`), and for `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, and `NE.shared.prior`, the order of list elements corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding `psi.prior`). Additionally, if `length = 1` and maximum value in corresponding `psi.prior > 1`, then the sole element is used for all pulses. Similarly, if `length < maximum value in corresponding psi.prior`, then the first element is used for all pulses while ignoring any remaining elements, and if `length > maximum value in corresponding psi.prior`, then the remaining elements beyond `length = maximum value in corresponding psi.prior` are ignored. A caution is provided when the length does not equal 1 or maximum value in corresponding `psi.prior`, except for the `shared.prior` arguments, which provide a caution if `length > 1` and `length < maximum value in corresponding psi.prior`, but may have additional list elements for idiosyncratic distributions (not utilized here; see `play.dice`).

If `num.partitions=n`, then rearrangement of bins across taxa within allele frequency classes based on descending order of the relative SNP proportions is not performed to construct the aSFS and taxon-specific inference of demographic parameters is possible. However, in general, more partitions results in more parameter space with respect to taxa samples that must be explored due to a decrease in order-independence and assumed exchangeability, thus multiple-fold more simulations must be conducted to achieve comparable accuracy in hyperparameter estimation as without partitioning.

For `tau.psi.prior`, `epsilon.psi.prior`, and `NE.psi.prior`, distinguishing between  $\Psi$  and  $\psi$  is accomplished via the corresponding `zeta.prior`, `zeta.total.prior`, `idiosyncratic` setting, and/or `min/max.net zeta.total/per.pulse`, except for values of 0, which are explicitly for  $\psi = 0$  and thus indicate full idiosyncrasy. If list length  $> 2$  for  $\tau$  and  $\epsilon$  or list length  $> 1$  for  $N_E$ , then a caution is provided and the remaining elements beyond length = 2 for  $\tau$  and  $\epsilon$  and length = 1 for  $N_E$  are ignored. Applies across all partitions, such that it is regardless of partitioning.

For `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, and `NE.zeta.prior`, if `num.partitions > 1`, may be necessary to include “0.0” as a value, but can control  $\zeta_s$  and  $\zeta_T$  across partitions via corresponding `zeta.total.prior` and/or `min/max.net zeta.total/per.pulse`. Attributes to each partition individually, but proportion values are out of the entirety of taxa dataset, thus if `num.partitions > 1`, then the upper bound for each partition should be the number of taxa within that partition divided by  $n$ . When  $\psi = \{0, 1\}$ , equivalent to hyperprior distribution for  $\zeta_T$ . If identical across all partitions, it is more computationally efficient to specify only one *i.e.* list of length = 1, or a vector.

For `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior`, if `length > 1`, then remaining elements beyond the first are ignored and a caution is provided.

To build a hyperprior, Multi-DICE first looks if the corresponding `zeta.total.prior` is specified, then if `dirichlet.process=T`, and if neither is such case, then all possible combinations of corresponding `psi.prior` and `zeta.prior` draws are equally weighted. Therefore, if `num.partitions=1`, corresponding `psi.prior=1`, and `dirichlet.process=F`, then `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior` equivalent to corresponding `zeta.prior` and thus unnecessary to specify.

For `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, and `NE.shared.prior`, each successive list element/distribution must have a greater minimum and maximum value than its preceding list elements/distributions. If multiple distributions are utilized for every potential pulse and these distributions overlap in their bounds, running time may slow since, in this case, draws are made from all the distributions independently and then checked if abiding by ordering and buffering, with re-draws if not.

When  $\psi = 0$  i.e. full idiosyncrasy, the arguments `idiosyncratic`, `min.net.tau.zeta.total`, `min.net.tau2.zeta.total`, `min.net.epsilon.zeta.total`, `min.net.epsilon2.zeta.total`, `min.net.NE.zeta.total`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, and `min.net.NE.zeta.per.pulse` are ignored.

Multi-DICE proceeds only if a valid draw is allowed given corresponding `num.taxa`, `psi.prior`, `zeta.prior` (e.g. minimum value in `psi.prior` \* minimum value in `zeta.prior`  $\leq$  minimum value in `num.taxa`), `zeta.total.prior`, `shared.prior`, `idiosyncratic` setting, `min/max.net.zeta.total/per.pulse`, and `buffer`. Importantly, there is no check on if all values in `psi.prior` have a valid draw, only if there is a valid draw among any of the values. Additionally, the range of a `shared.prior` argument must be greater than its corresponding  $(\Psi/\psi - 1)(2\beta + 1)$ . For `tau2.shared.prior`, consideration must also be given to any overlap with `tau.shared.prior`.

## Value

Returned value is a list object with the following components:

<code>draws.psi</code>	List of matrices. Each list element/matrix is attributed to a hyperparameterized demographic parameter and accordingly named (i.e. <code>tau</code> , <code>tau2</code> , <code>epsilon</code> , <code>epsilon2</code> , <code>NE</code> ). Per matrix, there is a single column and each cell is the $\Psi/\psi$ value drawn from the corresponding <code>psi.prior</code> for that simulation.
<code>draws.zeta</code>	List of list of matrices. Each list element is attributed to a hyperparameterized demographic parameter and accordingly named (i.e. <code>tau</code> , <code>tau2</code> , <code>epsilon</code> , <code>epsilon2</code> , <code>NE</code> ). Each of these list elements contain another list of matrices, with the order of these list elements/matrices corresponding to the order of partitions. Per matrix, each cell is the $S$ value drawn from the corresponding

`zeta.prior` for that simulation.

`draws.pulse.values` List of matrices. Each list element/matrix is attributed to a hyperparameterized demographic parameter and accordingly named (*i.e.* `tau`, `tau2`, `epsilon`, `epsilon2`, `NE`). Per matrix, each cell is the shared pulse value drawn from the corresponding `shared.prior` for that simulation.

Each row across matrices in `draws.psi`, `draws.zeta`, and `draws.pulse.values` represents an individual simulation and these rows correspond to each other *i.e.* the same row number across matrices refers to the same simulation. For matrices in `draws.zeta` and `draws.pulse.values`, the number of columns is the maximum value in the corresponding `psi.prior` that allows a valid draw, the order of columns corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding `psi.prior`), and non-applicable cells (*i.e.* columns beyond the corresponding `draws.psi` value) contain the value 0.

## Author(s)

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## References

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- Hickerson MJ, Stahl E, Takebayashi N (2007) msBayes: Pipeline for testing comparative phylogeographic histories using hierarchical approximate Bayesian computation. *BMC bioinformatics*, **8**, 268.
- Huang W, Takebayashi N, Qi Y, Hickerson MJ (2011) MTML-msBayes: approximate Bayesian comparative phylogeographic inference from multiple taxa and multiple loci with rate heterogeneity. *BMC bioinformatics*, **12**, 1.
- Xue AT (2017) Multi-DICE Manual.
- Xue AT, Hickerson MJ (2015) The aggregate site frequency spectrum for comparative population genomic inference. *Molecular Ecology*, **24**, 6223–6240.
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## See Also

`build.dice`, `play.dice`, `dice.sims`, `dice.aSFS`, `dice.sumstats`

## Examples

```
#simplest execution akin to approach in Xue and Hickerson (2015)
roll.dice(num.sims=5, num.taxa=10, tau.psi.prior=c(1),
tau.zeta.prior=c(1:10)/10, tau.shared.prior=c(1000:1000000))
```

```

#simplest execution akin to approach in Xue and Hickerson (2015); ln U
distribution applied on tau.shared.prior, with 100,000 intervals
discretized uniformly across ln(tau.shared.prior)
roll.dice(num.sims=5, num.taxa=10, tau.psi.prior=c(1),
tau.zeta.prior=c(1:10)/10,
tau.shared.prior=exp(c((log(1000)*100000):(log(1000000)*100000))/100000))

#simplest execution akin to approach in Xue and Hickerson (2015); assuming
build.dice was previously performed and the output was directed to object
build.object
roll.dice(num.sims=5, tau.psi.prior=c(1),
tau.shared.prior=c(1000:1000000), build.object=build.object)

#simplest execution akin to approach in software package msBayes
roll.dice(num.sims=5, num.taxa=10, tau.psi.prior=c(1:10),
tau.zeta.prior=c(1:10)/10, tau.shared.prior=c(1000:1000000),
idiosyncratic=F)

```

# Idiosyncratic/nuisance prior draws for hierarchical co-demographic model

## Description

`play.dice` conducts random draws from user-specified prior distributions for idiosyncratic and nuisance values, as well as determine parameter summary values. Nuisance values are for taxon-specific demographic parameters that are not hyperparameterized (*i.e.* not specified in the corresponding `psi.prior` argument and therefore values are not grouped into shared pulses) and are therefore drawn independently across taxa, similar to idiosyncratic draws. `build.dice` and `roll.dice` are embedded here and are automatically deployed if `build.object/roll.object` and `roll.object`, respectively, are not specified.

## Usage

```
play.dice(num.sims, num.taxa, num.partitions=1, tau.psi.prior=NULL,
epsilon.psi.prior=NULL, NE.psi.prior=NULL, tau.zeta.prior=NULL,
tau2.zeta.prior=NULL, epsilon.zeta.prior=NULL, epsilon2.zeta.prior=NULL,
NE.zeta.prior=NULL, tau.zeta.total.prior=NULL, tau2.zeta.total.prior=NULL,
epsilon.zeta.total.prior=NULL, epsilon2.zeta.total.prior=NULL,
NE.zeta.total.prior=NULL, tau.shared.prior=NULL, tau2.shared.prior=NULL,
epsilon.shared.prior=NULL, epsilon2.shared.prior=NULL,
NE.shared.prior=NULL, tau.idio.prior=NULL, tau2.idio.prior=NULL,
epsilon.idio.prior=NULL, epsilon2.idio.prior=NULL, NE.idio.prior=NULL,
linked.param=NULL, attached.hyper=NULL, linked.param.partition=NULL,
attached.hyper.pulse=NULL, linked.param.prior=NULL,
linked.param.fixed=NULL, anchor.prior=NULL, change.prior=NULL,
exponential.growth.rate.prior=NULL, exponential.growth.rate.prior2=NULL,
dirichlet.process=F, idiosyncratic=T, min.net.tau.zeta.total=NULL,
min.net.tau2.zeta.total=NULL, min.net.epsilon.zeta.total=NULL,
min.net.epsilon2.zeta.total=NULL, min.net.NE.zeta.total=NULL,
max.net.tau.zeta.total=NULL, max.net.tau2.zeta.total=NULL,
max.net.epsilon.zeta.total=NULL, max.net.epsilon2.zeta.total=NULL,
max.net.NE.zeta.total=NULL, min.net.tau.zeta.per.pulse=NULL,
min.net.tau2.zeta.per.pulse=NULL, min.net.epsilon.zeta.per.pulse=NULL,
min.net.epsilon2.zeta.per.pulse=NULL, min.net.NE.zeta.per.pulse=NULL,
max.net.tau.zeta.per.pulse=NULL, max.net.tau2.zeta.per.pulse=NULL,
max.net.epsilon.zeta.per.pulse=NULL, max.net.epsilon2.zeta.per.pulse=NULL,
max.net.NE.zeta.per.pulse=NULL, tau.buffer=0, tau2.buffer=0,
epsilon.buffer=0, epsilon2.buffer=0, NE.buffer=0,
tau.idiosyncratic.buffer=NULL, tau2.idiosyncratic.buffer=NULL,
epsilon.idiosyncratic.buffer=NULL, epsilon2.idiosyncratic.buffer=NULL,
NE.idiosyncratic.buffer=NULL, idiosyncratic.rule='none', num.changes=1,
flip=F, net.zeta.total=F, net.zeta.per.pulse=F, mean.tau.shared=F,
```



```
mean.tau2.shared=F, mean.epsilon.shared=F, mean.epsilon2.shared=F,
mean.NE.shared=F, mean.tau=F, mean.tau2=F, mean.epsilon=F,
mean.epsilon2=F, mean.NE=F, disp.index.tau.shared=F,
disp.index.tau2.shared=F, disp.index.epsilon.shared=F,
disp.index.epsilon2.shared=F, disp.index.NE.shared=F, disp.index.tau=F,
disp.index.tau2=F, disp.index.epsilon=F, disp.index.epsilon2=F,
disp.index.NE=F, build.object=NULL, roll.object=NULL)
```

## Arguments

`num.sims` Positive integer. Number of simulations. Required.

## DATA

`num.taxa` List, vector of length = `num.partitions`, or positive integer. Number of taxa per partition. Total sum across partitions equals the total number of taxa  $n$  in dataset. See also [Details](#). Required.

`num.partitions` Positive integer. Number of partitions for taxa in dataset. Allows differential data and model specifications across user-specified taxa groupings, including sampling size of individuals, generation times, demographic syndrome, and taxon-specific nuisance parameter prior distributions. See also [Details](#).

## PRIORS

`tau.psi.prior,`  
`epsilon.psi.prior, NE.psi.prior` List, vector, or non-negative integer. Hyperprior distribution for  $\Psi/\psi$  of  $\tau$ ,  $\epsilon$ , and  $N_E$ , respectively. For  $\tau$  and  $\epsilon$ , if list of length = 2, then the first list element applies to the first more recent size change event (e.g.  $\tau_1$ ,  $\epsilon_1$ ) and the second list element applies to the second more ancient size change event (e.g.  $\tau_2$ ,  $\epsilon_2$ ), per taxon. The argument(s) specified here and their according list lengths activate which taxon-specific demographic parameters are to be hyperparameterized via  $\Psi/\psi$  as well as  $\zeta/\zeta_S/\zeta_T$  downstream. See also [Details](#). At least one is required.

`tau.zeta.prior, tau2.zeta.prior,`  
`epsilon.zeta.prior,`  
`epsilon2.zeta.prior,`  
`NE.zeta.prior` List of length = `num.partitions` or 1, vector, or non-negative proportion (i.e.  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_j$  of  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively, for each  $j$ th pulse from 1 to  $\Psi/\psi$ , as specified by the corresponding `psi.prior`, and per partition. See also [Details](#). Required for each corresponding `psi.prior` specified, unless the maximum value in the corresponding `psi.prior` = 0.

tau.zeta.total.prior,  
tau2.zeta.total.prior,  
epsilon.zeta.total.prior,  
epsilon2.zeta.total.prior,  
NE.zeta.total.prior

List of length = 1, vector, or non-negative proportion (*i.e.*  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_T$  of  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively. Activates a uniform hyperprior such that each discrete  $\Psi/\psi$  value, as specified by the corresponding `psi.prior`, is first weighted with equal hyperprior probability, then all discrete  $\zeta_T$  values are weighted equally per  $\Psi/\psi$  value, and finally every possible associated vector  $\zeta/\zeta_s$  is weighted equally per  $\zeta_T$  value. See also `Details`.

tau.shared.prior,  
tau2.shared.prior,  
epsilon.shared.prior,  
epsilon2.shared.prior,  
NE.shared.prior

List, vector, or positive value. Prior distribution for the demographic parameter summaries  $\tau_{1s}$ ,  $\tau_{2s}$ ,  $\epsilon_{1s}$ ,  $\epsilon_{2s}$ , and  $N_s$ , respectively (or  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N$ , respectively, if corresponding `psi.prior` specifies  $\Psi$ ). See also `Details`. Required for each corresponding `psi.prior` specified, unless the maximum value in the corresponding `psi.prior` = 0.

tau.idio.prior, tau2.idio.prior,  
epsilon.idio.prior,  
epsilon2.idio.prior,  
NE.idio.prior

List of length = `num.partitions` or 1, vector, or positive value. Prior distribution for the taxon-specific demographic parameters  $\tau_{1i}$ ,  $\tau_{2i}$ ,  $\epsilon_{1i}$ ,  $\epsilon_{2i}$ , and  $N_i$ , respectively for idiosyncratic values, and  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N$ , respectively for nuisance values. See also `Details`.

linked.param, attached.hyper

List, vector, or character string, with possible values being the names of the demographic parameters (*i.e.* "tau", "tau2", "epsilon", "epsilon2", "NE"). Activates nuisance parameters in `linked.param` to have prior distributions be linked to hyperparameterized demographic parameters in `attached.hyper`, such that prior distributions may differentiate across pulses and idiosyncratic taxa with respect to the hyperparameterized demographic parameter in `attached.hyper`. See also `Details`.

linked.param.partition,  
attached.hyper.pulse

List of length = length of `linked.param` or 1, vector, or positive integer. The partitions in the linked nuisance parameter, and the pulses in the attached hyperparameterized demographic parameter, for which each element in `linked.param` and `attached.hyper`, respectively, applies. Each list element may contain multiple partitions/pulses, respectively. See also `Details`.

linked.param.prior

List of length = length of `linked.param` or 1, vector, or positive value. Prior distribution for the nuisance demographic parameter in each element of `linked.param`. See also `Details`.

<code>linked.param.fixed</code>	List, vector of length = length of <code>linked.param</code> , or logical value. Activates a fixed nuisance demographic parameter value for all taxa to which the corresponding elements in <code>linked.param.partition</code> and <code>attached.hyper.pulse</code> apply. See also Details.
<code>anchor.prior, change.prior</code>	List, vector, or positive integer. Prior distribution for $\tau_2$ based on its difference $\delta$ with $\tau_1$ . This difference value can be assigned to synchronous/shared pulses in $\tau_{1s}$ , as specified by <code>tau.psi.prior</code> , and accordingly inferred as a parameter summary vector $\delta_s$ ( <code>anchor.prior</code> ), or applied independently across taxa as an idiosyncratic or nuisance value ( <code>change.prior</code> ). See also Details.
<code>exponential.growth.rate.prior, exponential.growth.rate.prior2</code>	List of length = <code>num.partitions</code> or 1, vector, or double value. Prior distribution for the nuisance taxon-specific parameters $r_1$ and $r_2$ , respectively. Activates exponential growth model $N_t = N_0 * e^{(r * t)}$ for the first and second event, respectively, instead of instantaneous growth. Negative values indicate expansion and positive values indicate contraction. See also Details.

## MODEL SPECIFICATIONS

<code>dirichlet.process</code>	Logical value. Activates a Dirichlet-process hyperprior that weighs all allowable combinations of $\Psi/\psi$ and $\zeta/\zeta_s$ according to possible combinations of taxa assignment. See also Details.
<code>idiosyncratic</code>	Logical value. Allows idiosyncratic taxa that freely vary <i>i.e.</i> are ungrouped from any of the pulses, as specified by the <code>psi.prior</code> arguments. See also Details.
<code>min.net.tau.zeta.total, min.net.tau2.zeta.total, min.net.epsilon.zeta.total, min.net.epsilon2.zeta.total, min.net.NE.zeta.total, max.net.tau.zeta.total, max.net.tau2.zeta.total, max.net.epsilon.zeta.total, max.net.epsilon2.zeta.total, max.net.NE.zeta.total</code>	Non-negative proportion ( <i>i.e.</i> $\leq 1$ and $\geq 0$ ). Rule for the minimum/maximum $\zeta_T$ value, across all pulses (as specified by the corresponding <code>psi.prior</code> ) and partitions, for $\tau_1$ , $\tau_2$ , $\epsilon_1$ , $\epsilon_2$ , and $N_E$ , respectively. See also Details.
<code>min.net.tau.zeta.per.pulse, min.net.tau2.zeta.per.pulse, min.net.epsilon.zeta.per.pulse,</code>	List, vector of length = maximum value in corresponding <code>psi.prior</code> , or non-negative proportion ( <i>i.e.</i> $\leq 1$ and $\geq 0$ ). Rule for the minimum/maximum $\zeta_j$ value of $\tau_1$ , $\tau_2$ , $\epsilon_1$ , $\epsilon_2$ , and $N_E$ ,

min.net.epsilon2.zeta.per.pulse,  
min.net.NE.zeta.per.pulse,  
max.net.tau.zeta.per.pulse,  
max.net.tau2.zeta.per.pulse,  
max.net.epsilon.zeta.per.pulse,  
max.net.epsilon2.zeta.per.pulse,  
max.net.NE.zeta.per.pulse

respectively, for each  $j$ th pulse from 1 to  $\Psi/\psi$  (as specified by the corresponding `psi.prior`) across all partitions. See also [Details](#).

tau.buffer, tau2.buffer,  
epsilon.buffer, epsilon2.buffer,  
NE.buffer

Non-negative value or function. Pulse buffer  $\beta$  of the demographic parameter summaries  $\tau_{1s}$ ,  $\tau_{2s}$ ,  $\epsilon_{1s}$ ,  $\epsilon_{2s}$ , and  $N_s$ , respectively. See also [Details](#).

tau.idiosyncratic.buffer,  
tau2.idiosyncratic.buffer,  
epsilon.idiosyncratic.buffer,  
epsilon2.idiosyncratic.buffer,  
NE.idiosyncratic.buffer

Non-negative value or function. Idiosyncratic buffer  $\beta_i$  of the idiosyncratic taxon-specific demographic parameters  $\tau_{1i}$ ,  $\tau_{2i}$ ,  $\epsilon_{1i}$ ,  $\epsilon_{2i}$ , and  $N_i$ , respectively. See also [Details](#).

idiosyncratic.rule

Character string with possible values “recent” and “ancient”. Activates rule forcing all idiosyncratic taxa to have values less than the first shared pulse, or values greater than the last shared pulse, respectively. Any other values results in no such rules being placed on idiosyncratic taxa. See also [Details](#).

num.changes

List, vector of length = `num.partitions`, or value of 1 or 2. Number of demographic change events per taxon. See also [Details](#).

flip

List, vector of length = `num.partitions`, or logical value. Activates  $\tau_2$  to be more recent than  $\tau_1$ . See also [Details](#).

## PARAMETER SUMMARIES

net.zeta.total,  
net.zeta.per.pulse

Logical value. Activates output of  $\zeta_T$  and the vector  $\zeta/\zeta_s$  across partitions, respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value.

mean.tau.shared,  
mean.tau2.shared,  
mean.epsilon.shared,  
mean.epsilon2.shared,  
mean.NE.shared

Logical value. Activates output of  $E(\tau_{1s})$ ,  $E(\tau_{2s})$ ,  $E(\epsilon_{1s})$ ,  $E(\epsilon_{2s})$ , and  $E(N_s)$  weighted by the vector  $\zeta/\zeta_s$ , respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows

of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value. See also [Details](#).

`mean.tau, mean.tau2,`  
`mean.epsilon, mean.epsilon2,`  
`mean.NE`

Logical value. Activates output of  $E(\tau_1)$ ,  $E(\tau_2)$ ,  $E(\varepsilon_1)$ ,  $E(\varepsilon_2)$ , and  $E(N)$ , respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value.

`disp.index.tau.shared,`  
`disp.index.tau2.shared,`  
`disp.index.epsilon.shared,`  
`disp.index.epsilon2.shared,`  
`disp.index.NE.shared`

Logical value. Activates output of  $\Omega(\tau_{1s})$ ,  $\Omega(\tau_{2s})$ ,  $\Omega(\varepsilon_{1s})$ ,  $\Omega(\varepsilon_{2s})$ , and  $\Omega(N_s)$  weighted by the vector  $\zeta/\zeta_s$ , respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value. See also [Details](#).

`disp.index.tau, disp.index.tau2,`  
`disp.index.epsilon,`  
`disp.index.epsilon2,`  
`disp.index.NE`

Logical value. Activates output of  $\Omega(\tau_1)$ ,  $\Omega(\tau_2)$ ,  $\Omega(\varepsilon_1)$ ,  $\Omega(\varepsilon_2)$ , and  $\Omega(N)$ , respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value. See also [Details](#).

## OBJECTS FROM PRECEDING FUNCTIONS

`build.object`

Output from function `build.dice`. See also [Details](#).

`roll.object`

Output from function `roll.dice`. See also [Details](#).

Arguments from other `Multi-DICE` functions may be included here and are ignored if not applicable.

## **Details**

For more information, see `Multi-DICE Manual`.

`Multi-DICE` cannot currently accommodate models with more than one population per taxon, events aside from population size change, and more than two size change events.

For  $\tau_1$  and  $\tau_2$ , units are in numbers of generations, and thus may only be positive integers. For  $\epsilon_1$  and  $\epsilon_2$ , units are in ratio of size change from the ancestral effective population size to current effective population size, such that expansions are  $< 1$  and contractions are  $> 1$ , and thus may only be positive values. For  $N_E$ , unit is in number of effective haploid individuals, and thus may only be positive integers.

For `num.taxa`, `linked.param`, `attached.hyper`, `linked.param.fixed`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, `max.net.tau.zeta.per.pulse`, `max.net.tau2.zeta.per.pulse`, `max.net.epsilon.zeta.per.pulse`, `max.net.epsilon2.zeta.per.pulse`, `max.net.NE.zeta.per.pulse`, `num.changes`, and `flip`, if list, then all list elements are concatenated to form a single vector, with the ordering within list elements and then between list elements preserved (e.g. for list of length = 2, with first list element of length = 2 and second list element of length = 1, the order from first to last is: 1) first vector element in first list element; 2) second vector element in first list element; 3) sole vector element in second list element).

For `tau.psi.prior`, `epsilon.psi.prior`, `NE.psi.prior`, `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, `NE.zeta.prior`, `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, `NE.zeta.total.prior`, `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, `NE.shared.prior`, `tau.idio.prior`, `tau2.idio.prior`, `epsilon.idio.prior`, `epsilon2.idio.prior`, `NE.idio.prior`, `linked.param.prior`, `anchor.prior`, `change.prior`, `exponential.growth.rate.prior`, and `exponential.growth.rate.prior2`, each list element contains an entire individual discrete distribution; if vector, then converted to list of length = 1 with all vector elements comprising the entirety of a single discrete distribution. Per list element, vector elements within (*i.e.* the discrete distribution) do not need to be in any particular order. Relatedly, each vector element is treated as an independent value, thus weighted distributions (*i.e.* not uniform) may be employed by duplicating values (e.g. a distribution of `c(0, 1, 1, 1)` signifies 75% probability of drawing “1” and 25% probability of drawing “0”), allowing the specification of any discretized distribution (e.g. gamma, beta, log-uniform). Accordingly, a uniform distribution with no gaps for integer values would be of length = range of distribution.

For `num.taxa`, `num.changes`, and `flip`, the order of vector elements corresponds to the order of partitions, and for `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, `NE.zeta.prior`, `tau.idio.prior`, `tau2.idio.prior`, `epsilon.idio.prior`, `epsilon2.idio.prior`, `NE.idio.prior`, `change.prior`, `exponential.growth.rate.prior`, and `exponential.growth.rate.prior2`, the order of list elements corresponds to the order of partitions. Additionally, if length = 1 and `num.partitions` > 1, then the sole element is used for all partitions. Similarly, if length < `num.partitions`, then the first element is used for all partitions while ignoring any remaining elements, and if length >

num.partitions, then the remaining elements beyond length = num.partitions are ignored; a caution is provided when the length does not equal 1 or num.partitions.

For min.net.tau.zeta.per.pulse, min.net.tau2.zeta.per.pulse, min.net.epsilon.zeta.per.pulse, min.net.epsilon2.zeta.per.pulse, min.net.NE.zeta.per.pulse, max.net.tau.zeta.per.pulse, max.net.tau2.zeta.per.pulse, max.net.epsilon.zeta.per.pulse, max.net.epsilon2.zeta.per.pulse, and max.net.NE.zeta.per.pulse, the order of vector elements corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding psi.prior), and for tau.shared.prior, tau2.shared.prior, epsilon.shared.prior, epsilon2.shared.prior, NE.shared.prior, and anchor.prior, the order of list elements corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding psi.prior). Additionally, if length = 1 and maximum value in corresponding psi.prior > 1, then the sole element is used for all pulses. Similarly, if length < maximum value in corresponding psi.prior, then the first element is used for all pulses while ignoring any remaining elements. For the zeta.per.pulse arguments, if length > maximum value in corresponding psi.prior, then the remaining elements beyond length = maximum value in corresponding psi.prior are ignored; a caution is provided when the length does not equal 1 or maximum value in corresponding psi.prior. For the shared.prior arguments and anchor.prior, there may be additional list elements for idiosyncratic distributions, such that any total length = 1, maximum value in corresponding psi.prior, maximum value in corresponding psi.prior + 1, or maximum value in corresponding psi.prior + num.partitions, are allowed; for any other lengths, a caution is provided and excess elements beyond the highest acceptable length are ignored. See below for more information about adding idiosyncratic distributions to these arguments.

If num.partitions= $n$ , then rearrangement of bins across taxa within allele frequency classes based on descending order of the relative SNP proportions is not performed to construct the aSFS and taxon-specific inference of demographic parameters is possible. However, in general, more partitions results in more parameter space with respect to taxa samples that must be explored due to a decrease in order-independence and assumed exchangeability, thus multiple-fold more simulations must be conducted to achieve comparable accuracy in hyperparameter estimation as without partitioning.

For tau.psi.prior, epsilon.psi.prior, and NE.psi.prior, distinguishing between  $\Psi$  and  $\psi$  is accomplished via the corresponding zeta.prior, zeta.total.prior, idiosyncratic setting, and/or min/max.net zeta.total/per.pulse, except for values of 0, which are explicitly for  $\psi = 0$  and thus indicate full idiosyncrasy. If list length > 2 for  $\tau$  and  $\varepsilon$  or list length > 1 for  $N_E$ , then a caution is provided and the remaining elements beyond length = 2 for  $\tau$  and  $\varepsilon$  and length = 1 for  $N_E$  are ignored. Applies across all partitions, such that it is regardless of partitioning.

For tau.zeta.prior, tau2.zeta.prior, epsilon.zeta.prior, epsilon2.zeta.prior, and NE.zeta.prior, if num.partitions > 1, may be necessary to include "0.0" as a value, but can control  $\zeta_s$  and  $\zeta_T$  across partitions via corresponding zeta.total.prior and/or min/max.net

`zeta.total/per.pulse`. Attributes to each partition individually, but proportion values are out of the entirety of taxa dataset, thus if `num.partitions > 1`, then the upper bound for each partition should be the number of taxa within that partition divided by  $n$ . When  $\psi = \{0, 1\}$ , equivalent to hyperprior distribution for  $\zeta_T$ . If identical across all partitions, it is more computationally efficient to specify only one *i.e.* list of length = 1, or a vector.

For `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior`, if length > 1, then remaining elements beyond the first are ignored and a caution is provided.

To build a hyperprior, Multi-DICE first looks if the corresponding `zeta.total.prior` is specified, then if `dirichlet.process=T`, and if neither is such case, then all possible combinations of corresponding `psi.prior` and `zeta.prior` draws are equally weighted. Therefore, if `num.partitions=1`, corresponding `psi.prior=1`, and `dirichlet.process=F`, then `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior` equivalent to corresponding `zeta.prior` and thus unnecessary to specify.

For `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, and `NE.shared.prior`, each successive list element/distribution must have a greater minimum and maximum value than its preceding list elements/distributions. If multiple distributions are utilized for every potential pulse and these distributions overlap in their bounds, running time may slow since, in this case, draws are made from all the distributions independently and then checked if abiding by ordering and buffering, with re-draws if not.

For each of `tau`, `tau2`, `epsilon`, `epsilon2`, and `NE`, if hyperparameterized via its corresponding `psi.prior` while `idiosyncratic=T` or a 0 value is in said `psi.prior`, then a corresponding idiosyncratic prior is required. Multi-DICE first looks in `change.prior` (for  $\tau_2$  only), then the corresponding `idio.prior`, and finally the corresponding `shared.prior`. If a `shared.prior` argument is utilized, the additional list elements beyond length = maximum value in corresponding `psi.prior` are considered; if the number of list elements is  $\leq$  maximum value in corresponding `psi.prior`, then only the first list element is considered. These list elements undergo the same specifications as aforementioned for the corresponding `idio.prior`.

For each of `tau`, `tau2`, `epsilon`, `epsilon2`, and `NE`, if not hyperparameterized yet part of the specified model (*i.e.* `tau`, `epsilon`, and `NE` are always part of the model, and `tau2` and `epsilon2` are part of the model when `num.changes = 2`), then a corresponding nuisance prior is required. A nuisance prior differs from an idiosyncratic prior in that variation in the respective nuisance parameter is being considered while not of interest with respect to hyperparameterization (*i.e.* variability in values across taxa governed hierarchically), whereas an idiosyncratic prior is still governed by hyperparameters in coordination with the corresponding shared prior. Multi-DICE first looks in `anchor.prior` (for  $\tau_2$  only), next `change.prior` (for  $\tau_2$  only), afterward `linked.param.prior` (if applicable; see below for more information), then the corresponding `idio.prior`, and finally the



corresponding `shared.prior`. If `linked.param.prior` is utilized for a particular nuisance parameter, either the corresponding `idio.prior` or `shared.prior` must still be specified even if all taxa are always covered by `linked.param.prior` across all simulations. If a `shared.prior` argument is utilized, it undergoes the same specifications as aforementioned for the corresponding `idio.prior`.

It is highly recommended that prior distribution bounds are as far apart as possible between  $\tau_1$  and  $\tau_2$ , ideally mutually exclusive/non-overlapping. Otherwise, there could be a stop of operation due to an invalid/incompatible draw, computational lag, and/or statistical bias on prior distributions.

For `tau.buffer`, `tau2.buffer`, `epsilon.buffer`, `epsilon2.buffer`, and `NE.buffer`,  $\beta$  buffers are applied to draws of shared pulse values, thus affecting the corresponding shared prior; the corresponding idiosyncratic prior, from which draws are subsequently made, is accordingly affected by the shared pulse buffers. For `tau.idiosyncratic.buffer`, `tau2.idiosyncratic.buffer`, `epsilon.idiosyncratic.buffer`, `epsilon2.idiosyncratic.buffer`, and `NE.idiosyncratic.buffer`,  $\beta_i$  idiosyncratic buffers are then applied to idiosyncratic draws, which additionally affect the corresponding idiosyncratic prior that had already been initially transformed by the shared pulse buffers. In other words,  $\beta$  buffers idiosyncratic taxa from shared pulse values, and  $\beta_i$  buffers idiosyncratic taxa from each other. For example, if  $n = 10$ ,  $\psi_{\tau_1} = 2$ ,  $\zeta_{\tau_1,T} = 0.8$ ,  $\beta = 10,000$ ,  $\beta_i = 1,000$ ,  $\tau_1 \sim U(1,000, 100,000)$ ,  $\tau_{1s} = \{11,000, 12,001\}$ , and  $\tau_{1i} = \{99,000\}$  after the first idiosyncratic draw, then given that the synchronous/shared pulse buffers result in invalid draws from  $\sim U(1,000, 13,001)$  and the first idiosyncratic draw buffer results in invalid draws from  $\sim U(98,000, 100,000)$ , the remaining second idiosyncratic draw would be from the resulting transformed prior distribution  $\tau_{1i} \sim U(13,002, 97,999)$ . A caution is provided if an `idiosyncratic.buffer` corresponding to a specified `psi.prior` is not specified. Buffers cannot be deployed for nuisance draws (though see below when  $\psi = 0$ ).

For `num.changes`, only necessary if there are nuisance demographic parameters for a second event, since one event is the default and demographic parameters for the second event that are hyperparameterized by the corresponding `psi.prior` are already activated. If  $< 1$ , then there is a stop of operation, and if  $> 2$ , then it is converted to `num.changes=2` and a caution is provided.

If `flip=T`,  $\tau_2$  and  $\epsilon_2$  still refers to the second specified event, which in this case is the more recent one.

When  $\psi = 0$  i.e. full idiosyncrasy, the arguments `idiosyncratic`, `min.net.tau.zeta.total`, `min.net.tau2.zeta.total`, `min.net.epsilon.zeta.total`, `min.net.epsilon2.zeta.total`, `min.net.NE.zeta.total`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, and `idiosyncratic.rule` are ignored, and the arguments `tau.idiosyncratic.buffer`, `tau2.idiosyncratic.buffer`, `epsilon.idiosyncratic.buffer`, `epsilon2.idiosyncratic.buffer`, and `NE.idiosyncratic.buffer` are activated (even if `idiosyncratic=F`).

Multi-DICE proceeds only if a valid draw is allowed given corresponding `num.taxa`, `psi.prior`, `zeta.prior` (e.g. minimum value in `psi.prior` \* minimum value in `zeta.prior`  $\leq$  minimum value in `num.taxa`), `zeta.total.prior`, shared prior, idiosyncratic prior, idiosyncratic setting, `min/max.net zeta.total/per.pulse`, `buffer`, and `idiosyncratic.buffer`. Importantly, there is no check on if all values in `psi.prior` have a valid draw, only if there is a valid draw among any of the values. Additionally, the range of a shared prior must be greater than its corresponding  $(\Psi/\psi - 1)(2\beta + 1)$ , and the range of an idiosyncratic prior ought to be greater than its corresponding  $(\Psi/\psi)(2\beta + 1) + (\sigma - 1)(2\beta_i + 1)$  across every possible combination of  $\Psi/\psi$  and  $\sigma$  and with consideration given to `idiosyncratic.rule`. For `tau2.shared.prior` and `tau2.idio.prior`, consideration must also be given to any overlap with `tau.shared.prior` and `tau.idio.prior`, respectively.

## Value

Returned value is a list object with two elements, `roll.object` and `sim.specs`. The list element `roll.object` is similar to the output of the function `roll.dice`, except parameter summaries derived here are added (e.g.  $\Omega$ ,  $E()$ ,  $\delta_s$ ; see above for more information); these represent values of interest for estimation. The list element `sim.specs` contains a list of matrices, with each list element/matrix attributed to a taxon-specific parameter and accordingly named (i.e. `tau`, `tau2`, `epsilon`, `epsilon2`, `NE`, `exponential.growth.rate.prior`, `exponential.growth.rate.prior2`). Per matrix, each row represents an individual simulation, each column represents an independent taxon to be simulated, and each cell is the according demographic parameter value to be used for simulation. Rows and columns across matrices correspond to each other i.e. across matrices, the same row number refers to the same simulation and the same column number refers to the same simulated independent taxon.

## Author(s)

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## References

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- Hickerson MJ, Stahl E, Takebayashi N (2007) msBayes: Pipeline for testing comparative phylogeographic histories using hierarchical approximate Bayesian computation. *BMC bioinformatics*, **8**, 268.
- Huang W, Takebayashi N, Qi Y, Hickerson MJ (2011) MTML-msBayes: approximate Bayesian comparative phylogeographic inference from multiple taxa and multiple loci with rate heterogeneity. *BMC bioinformatics*, **12**, 1.
- Xue AT (2017) Multi-DICE Manual.
- Xue AT, Hickerson MJ (2015) The aggregate site frequency spectrum for comparative population genomic inference. *Molecular Ecology*, **24**, 6223–6240.
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inference under multi-taxa hierarchical co-demographic models.

## See Also

`build.dice`, `roll.dice`, `dice.sims`, `dice.aSFS`, `dice.sumstats`

## Examples

```
#simplest execution akin to approach in Xue and Hickerson (2015)
play.dice(num.sims=5, num.taxa=10, tau.psi.prior=c(1),
tau.zeta.prior=c(1:10)/10, tau.shared.prior=c(1000:1000000),
epsilon.idio.prior=c(1000:10000)/100000, NE.idio.prior=c(1000:100000))
```

```
#simplest execution akin to approach in Xue and Hickerson (2015); ln U
distribution applied on tau.shared.prior, with 100,000 intervals
discretized uniformly across ln(tau.shared.prior)
play.dice(num.sims=5, num.taxa=10, tau.psi.prior=c(1),
tau.zeta.prior=c(1:10)/10,
tau.shared.prior=exp(c((log(1000)*100000):(log(1000000)*100000))/100000),
epsilon.idio.prior=c(1000:10000)/100000, NE.idio.prior=c(1000:100000))
```

```
#simplest execution akin to approach in Xue and Hickerson (2015); assuming
roll.dice was previously performed and the output was directed to object
roll.object
play.dice(num.sims=5, num.taxa=10, tau.psi.prior=c(1),
tau.idio.prior=c(1000:1000000), epsilon.idio.prior=c(1000:10000)/100000,
NE.idio.prior=c(1000:100000)), roll.object=roll.object)
```

```
#simplest execution akin to approach in software package msBayes
play.dice(num.sims=5, num.taxa=10, tau.psi.prior=c(1:10),
tau.zeta.prior=c(1:10)/10, tau.shared.prior=c(1000:1000000),
epsilon.idio.prior=c(1000:10000)/100000, NE.idio.prior=c(1000:100000),
idiosyncratic=F)
```

## Simulating under hierarchical co-demographic model

### Description

`dice.sims` is a wrapper function for the command-line program `fastsimcoal2` that performs multi-taxa coalescent simulation of per-taxon summary statistics under a unified hierarchical co-demographic model as specified by `build.dice`, `roll.dice`, and `play.dice`, which are also embedded here and are automatically deployed if `build.object/roll.object/play.object`, `roll.object/play.object`, and `play.object`, respectively, are not specified. `fastsimcoal2` must be separately user-installed. `bash` commands are called upon here, thus `dice.sims` can run only within a `bash` terminal environment (e.g. Mac, Linux).

### Usage

```
dice.sims(num.sims, num.taxa, num.partitions=1, num.haploid.samples,
num.ind.sites=NULL, num.SNPs=NULL, length.seq=NULL, folded=T,
sampling.times=NULL, gen.times=NULL, tau.psi.prior=NULL,
epsilon.psi.prior=NULL, NE.psi.prior=NULL, tau.zeta.prior=NULL,
tau2.zeta.prior=NULL, epsilon.zeta.prior=NULL, epsilon2.zeta.prior=NULL,
NE.zeta.prior=NULL, tau.zeta.total.prior=NULL, tau2.zeta.total.prior=NULL,
epsilon.zeta.total.prior=NULL, epsilon2.zeta.total.prior=NULL,
NE.zeta.total.prior=NULL, tau.shared.prior=NULL, tau2.shared.prior=NULL,
epsilon.shared.prior=NULL, epsilon2.shared.prior=NULL,
NE.shared.prior=NULL, tau.idio.prior=NULL, tau2.idio.prior=NULL,
epsilon.idio.prior=NULL, epsilon2.idio.prior=NULL, NE.idio.prior=NULL,
linked.param=NULL, attached.hyper=NULL, linked.param.partition=NULL,
attached.hyper.pulse=NULL, linked.param.prior=NULL,
linked.param.fixed=NULL, anchor.prior=NULL, change.prior=NULL,
exponential.growth.rate.prior=NULL, exponential.growth.rate.prior2=NULL,
mut.rate.prior=NULL, dirichlet.process=F, idiosyncratic=T,
min.net.tau.zeta.total=NULL, min.net.tau2.zeta.total=NULL,
min.net.epsilon.zeta.total=NULL, min.net.epsilon2.zeta.total=NULL,
min.net.NE.zeta.total=NULL, max.net.tau.zeta.total=NULL,
max.net.tau2.zeta.total=NULL, max.net.epsilon.zeta.total=NULL,
max.net.epsilon2.zeta.total=NULL, max.net.NE.zeta.total=NULL,
min.net.tau.zeta.per.pulse=NULL, min.net.tau2.zeta.per.pulse=NULL,
min.net.epsilon.zeta.per.pulse=NULL, min.net.epsilon2.zeta.per.pulse=NULL,
min.net.NE.zeta.per.pulse=NULL, max.net.tau.zeta.per.pulse=NULL,
max.net.tau2.zeta.per.pulse=NULL, max.net.epsilon.zeta.per.pulse=NULL,
max.net.epsilon2.zeta.per.pulse=NULL, max.net.NE.zeta.per.pulse=NULL,
tau.buffer=0, tau2.buffer=0, epsilon.buffer=0, epsilon2.buffer=0,
NE.buffer=0, tau.idiosyncratic.buffer=NULL,
tau2.idiosyncratic.buffer=NULL, epsilon.idiosyncratic.buffer=NULL,
```

```
epsilon2.idiosyncratic.buffer=NULL, NE.idiosyncratic.buffer=NULL,
idiosyncratic.rule='none', num.changes=1, flip=F, net.zeta.total=F,
net.zeta.per.pulse=F, mean.tau.shared=F, mean.tau2.shared=F,
mean.epsilon.shared=F, mean.epsilon2.shared=F, mean.NE.shared=F,
mean.tau=F, mean.tau2=F, mean.epsilon=F, mean.epsilon2=F, mean.NE=F,
disp.index.tau.shared=F, disp.index.tau2.shared=F,
disp.index.epsilon.shared=F, disp.index.epsilon2.shared=F,
disp.index.NE.shared=F, disp.index.tau=F, disp.index.tau2=F,
disp.index.epsilon=F, disp.index.epsilon2=F, disp.index.NE=F, fsc2path,
messages.sims=NULL, output.directory, append.sims=F, keep.taxa.draws=F,
output.hyper.draws=T, output.taxa.draws=F, keep.fsc2.files=F,
build.object=NULL, roll.object=NULL, play.object=NULL)
```

## Arguments

`num.sims` Positive integer. Number of simulations. Required.

## DATA

`num.taxa` List, vector of length = `num.partitions`, or positive integer. Number of taxa per partition. Total sum across partitions equals the total number of taxa  $n$  in dataset. See also `Details`. Required.

`num.partitions` Positive integer. Number of partitions for taxa in dataset. Allows differential data and model specifications across user-specified taxa groupings, including sampling size of individuals, generation times, demographic syndrome, and taxon-specific nuisance parameter prior distributions. See also `Details`.

`num.haploid.samples` List, vector of length = `num.partitions`, or positive integer. Number of haploid samples per partition. See also `Details`. Required.

`num.ind.sites`, `num.SNPs`, `length.seq` List, vector of length = `num.partitions`, or positive integer. Data sampling level per partition, in number of independent sites/SNPs using the `fastsimcoal2` `FREQ` simulation model, in number of independent SNPs using the `fastsimcoal2` `SNP` simulation model, and in sequence length using the `fastsimcoal2` `SNP` simulation model, respectively. For each taxon, the former two simulate the SFS based on independent sites, while the latter one simulates single-sequence summary statistics. See also `Details`. At least one is required.

`folded` List, vector of length = `num.partitions`, or logical value.

Activates folding of the SFS per partition; ignored if single-sequence summary statistics are simulated. See also [Details](#).

`sampling.times`

List, vector of length = `num.partitions`, or non-negative integer. Sampling times per partition. Allows simulation of time-series or ancient data. Unnecessary if all data are collected simultaneously and in present-day, since this is assumed by default. See also [Details](#).

`gen.times`

List, vector of length = `num.partitions` or  $n$ , or positive value. Generation times per partition or per taxon, in units of years per generation. If including multiple generation times within a partition (*i.e.* vector of length =  $n$ ), generation times are randomly assigned to sets of parameter draws, though the order of output simulation files corresponds to the user-specified order (*i.e.* `dice.simulations1` corresponds to the first element, `dice.simulations2` to the second, etc.). See also [Details](#).

## PRIORS

`tau.psi.prior,`  
`epsilon.psi.prior, NE.psi.prior`

List, vector, or non-negative integer. Hyperprior distribution for  $\Psi/\psi$  of  $\tau$ ,  $\epsilon$ , and  $N_E$ , respectively. For  $\tau$  and  $\epsilon$ , if list of length = 2, then the first list element applies to the first more recent size change event (*e.g.*  $\tau_1$ ,  $\epsilon_1$ ) and the second list element applies to the second more ancient size change event (*e.g.*  $\tau_2$ ,  $\epsilon_2$ ), per taxon. The arguments(s) specified here and their according list lengths activate which taxon-specific demographic parameters are to be hyperparameterized via  $\Psi/\psi$  as well as  $\zeta/\zeta_j/\zeta_T$  downstream. See also [Details](#). At least one is required.

`tau.zeta.prior, tau2.zeta.prior,`  
`epsilon.zeta.prior,`  
`epsilon2.zeta.prior,`  
`NE.zeta.prior`

List of length = `num.partitions` or 1, vector, or non-negative proportion (*i.e.*  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_j$  of  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively, for each  $j$ th pulse from 1 to  $\Psi/\psi$ , as specified by the corresponding `psi.prior`, and per partition. See also [Details](#). Required for each corresponding `psi.prior` specified, unless the maximum value in the corresponding `psi.prior` = 0.

`tau.zeta.total.prior,`  
`tau2.zeta.total.prior,`  
`epsilon.zeta.total.prior,`  
`epsilon2.zeta.total.prior,`  
`NE.zeta.total.prior`

List of length = 1, vector, or non-negative proportion (*i.e.*  $\leq 1$  and  $\geq 0$ ). Hyperprior distribution for  $\zeta_T$  of  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively. Activates a uniform hyperprior such that each discrete  $\Psi/\psi$  value, as specified by the corresponding

`psi.prior`, is first weighted with equal hyperprior probability, then all discrete  $\zeta_T$  values are weighted equally per  $\Psi/\psi$  value, and finally every possible associated vector  $\zeta/\zeta_s$  is weighted equally per  $\zeta_T$  value. See also [Details](#).

`tau.shared.prior,`  
`tau2.shared.prior,`  
`epsilon.shared.prior,`  
`epsilon2.shared.prior,`  
`NE.shared.prior`

List, vector, or positive value. Prior distribution for the demographic parameter summaries  $\tau_{1s}$ ,  $\tau_{2s}$ ,  $\epsilon_{1s}$ ,  $\epsilon_{2s}$ , and  $N_s$ , respectively (or  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N$ , respectively, if corresponding `psi.prior` specifies  $\Psi$ ). See also [Details](#). Required for each corresponding `psi.prior` specified, unless the maximum value in the corresponding `psi.prior` = 0.

`tau.idio.prior, tau2.idio.prior,`  
`epsilon.idio.prior,`  
`epsilon2.idio.prior,`  
`NE.idio.prior`

List of length = `num.partitions` or 1, vector, or positive value. Prior distribution for the taxon-specific demographic parameters  $\tau_{1i}$ ,  $\tau_{2i}$ ,  $\epsilon_{1i}$ ,  $\epsilon_{2i}$ , and  $N_i$ , respectively for idiosyncratic values, and  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N$ , respectively for nuisance values. See also [Details](#).

`linked.param, attached.hyper`

List, vector, or character string, with possible values being the names of the demographic parameters (*i.e.* "tau", "tau2", "epsilon", "epsilon2", "NE"). Activates nuisance parameters in `linked.param` to have prior distributions be linked to hyperparameterized demographic parameters in `attached.hyper`, such that prior distributions may differentiate across pulses and idiosyncratic taxa with respect to the hyperparameterized demographic parameter in `attached.hyper`. See also [Details](#).

`linked.param.partition,`  
`attached.hyper.pulse`

List of length = length of `linked.param` or 1, vector, or positive integer. The partitions in the linked nuisance parameter, and the pulses in the attached hyperparameterized demographic parameter, for which each element in `linked.param` and `attached.hyper`, respectively, applies. Each list element may contain multiple partitions/pulses, respectively. See also [Details](#).

`linked.param.prior`

List of length = length of `linked.param` or 1, vector, or positive value. Prior distribution for the nuisance demographic parameter in each element of `linked.param`. See also [Details](#).

`linked.param.fixed`

List, vector of length = length of `linked.param`, or logical value. Activates a fixed nuisance demographic parameter value for all taxa to which the corresponding elements in

`linked.param.partition` and `attached.hyper.pulse` apply. See also `Details`.

`anchor.prior`, `change.prior`

List, vector, or positive integer. Prior distribution for  $\tau_2$  based on its difference  $\delta$  with  $\tau_1$ . This difference value can be assigned to synchronous/shared pulses in  $\tau_{1s}$ , as specified by `tau.psi.prior`, and accordingly inferred as a parameter summary vector  $\delta_s$  (`anchor.prior`), or applied independently across taxa as an idiosyncratic or nuisance value (`change.prior`). See also `Details`.

`exponential.growth.rate.prior`,  
`exponential.growth.rate.prior2`

List of length = `num.partitions` or 1, vector, or double value. Prior distribution for the nuisance taxon-specific parameters  $r_1$  and  $r_2$ , respectively. Activates exponential growth model  $N_t = N_0 * e^{(r * t)}$  for the first and second event, respectively, instead of instantaneous growth. Negative values indicate expansion and positive values indicate contraction. See also `Details`.

`mut.rate.prior`

List of length = `num.partitions` or 1, vector, or positive value. Prior distribution for mutation rate  $\mu$ . See also `Details`. Required if `length.seq` is specified.

## MODEL SPECIFICATIONS

`dirichlet.process`

Logical value. Activates a Dirichlet-process hyperprior that weighs all allowable combinations of  $\Psi/\psi$  and  $\zeta/\zeta_s$  according to possible combinations of taxa assignment. See also `Details`.

`idiosyncratic`

Logical value. Allows idiosyncratic taxa that freely vary *i.e.* are ungrouped from any of the pulses, as specified by the `psi.prior` arguments. See also `Details`.

`min.net.tau.zeta.total`,  
`min.net.tau2.zeta.total`,  
`min.net.epsilon.zeta.total`,  
`min.net.epsilon2.zeta.total`,  
`min.net.NE.zeta.total`,  
`max.net.tau.zeta.total`,  
`max.net.tau2.zeta.total`,  
`max.net.epsilon.zeta.total`,  
`max.net.epsilon2.zeta.total`,  
`max.net.NE.zeta.total`

Non-negative proportion (*i.e.*  $\leq 1$  and  $\geq 0$ ). Rule for the minimum/maximum  $\zeta_T$  value, across all pulses (as specified by the corresponding `psi.prior`) and partitions, for  $\tau_1$ ,  $\tau_2$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and  $N_E$ , respectively. See also `Details`.

`min.net.tau.zeta.per.pulse`,  
`min.net.tau2.zeta.per.pulse`,  
`min.net.epsilon.zeta.per.pulse`,

List, vector of length = maximum value in corresponding `psi.prior`, or non-negative proportion (*i.e.*  $\leq 1$  and  $\geq 0$ ). Rule



<code>min.net.epsilon2.zeta.per.pulse,</code> <code>min.net.NE.zeta.per.pulse,</code> <code>max.net.tau.zeta.per.pulse,</code> <code>max.net.tau2.zeta.per.pulse,</code> <code>max.net.epsilon.zeta.per.pulse,</code> <code>max.net.epsilon2.zeta.per.pulse,</code> <code>max.net.NE.zeta.per.pulse</code>	for the minimum/maximum $\zeta_j$ value of $\tau_1$ , $\tau_2$ , $\varepsilon_1$ , $\varepsilon_2$ , and $N_E$ , respectively, for each $j$ th pulse from 1 to $\Psi/\psi$ (as specified by the corresponding <code>psi.prior</code> ) across all partitions. See also <code>Details</code> .
<code>tau.buffer,</code> <code>tau2.buffer,</code> <code>epsilon.buffer,</code> <code>epsilon2.buffer,</code> <code>NE.buffer</code>	Non-negative value or function. Pulse buffer $\beta$ of the demographic parameter summaries $\tau_{1s}$ , $\tau_{2s}$ , $\varepsilon_{1s}$ , $\varepsilon_{2s}$ , and $N_s$ , respectively. See also <code>Details</code> .
<code>tau.idiosyncratic.buffer,</code> <code>tau2.idiosyncratic.buffer,</code> <code>epsilon.idiosyncratic.buffer,</code> <code>epsilon2.idiosyncratic.buffer,</code> <code>NE.idiosyncratic.buffer</code>	Non-negative value or function. Idiosyncratic buffer $\beta_i$ of the idiosyncratic taxon-specific demographic parameters $\tau_{1i}$ , $\tau_{2i}$ , $\varepsilon_{1i}$ , $\varepsilon_{2i}$ , and $N_i$ , respectively. See also <code>Details</code> .
<code>idiosyncratic.rule</code>	Character string with possible values “recent” and “ancient”. Activates rule forcing all idiosyncratic taxa to have values less than the first shared pulse, or values greater than the last shared pulse, respectively. Any other values results in no such rules being placed on idiosyncratic taxa. See also <code>Details</code> .
<code>num.changes</code>	List, vector of length = <code>num.partitions</code> , or value of 1 or 2. Number of demographic change events per taxon. See also <code>Details</code> .
<code>flip</code>	List, vector of length = <code>num.partitions</code> , or logical value. Activates $\tau_2$ to be more recent than $\tau_1$ . See also <code>Details</code> .

## PARAMETER SUMMARIES

<code>net.zeta.total,</code> <code>net.zeta.per.pulse</code>	Logical value. Activates output of $\zeta_T$ and the vector $\zeta/\zeta_s$ across partitions, respectively, as a list element/matrix in the <code>roll.object</code> list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the <code>roll.object</code> list element of the final output, and each cell is the aforementioned value.
<code>mean.tau.shared,</code> <code>mean.tau2.shared,</code> <code>mean.epsilon.shared,</code> <code>mean.epsilon2.shared,</code> <code>mean.NE.shared</code>	Logical value. Activates output of $E(\tau_{1s})$ , $E(\tau_{2s})$ , $E(\varepsilon_{1s})$ , $E(\varepsilon_{2s})$ , and $E(N_s)$ weighted by the vector $\zeta/\zeta_s$ , respectively, as a list element/matrix in the <code>roll.object</code> list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows

of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value. See also [Details](#).

`mean.tau, mean.tau2,`  
`mean.epsilon, mean.epsilon2,`  
`mean.NE`

Logical value. Activates output of  $E(\tau_1)$ ,  $E(\tau_2)$ ,  $E(\varepsilon_1)$ ,  $E(\varepsilon_2)$ , and  $E(N)$ , respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value.

`disp.index.tau.shared,`  
`disp.index.tau2.shared,`  
`disp.index.epsilon.shared,`  
`disp.index.epsilon2.shared,`  
`disp.index.NE.shared`

Logical value. Activates output of  $\Omega(\tau_{1s})$ ,  $\Omega(\tau_{2s})$ ,  $\Omega(\varepsilon_{1s})$ ,  $\Omega(\varepsilon_{2s})$ , and  $\Omega(N_s)$  weighted by the vector  $\zeta/\zeta_s$ , respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value. See also [Details](#).

`disp.index.tau, disp.index.tau2,`  
`disp.index.epsilon,`  
`disp.index.epsilon2,`  
`disp.index.NE`

Logical value. Activates output of  $\Omega(\tau_1)$ ,  $\Omega(\tau_2)$ ,  $\Omega(\varepsilon_1)$ ,  $\Omega(\varepsilon_2)$ , and  $\Omega(N)$ , respectively, as a list element/matrix in the `roll.object` list element of the final output, for downstream estimation. Rows of the matrix correspond to individual simulations, which correspond to rows of other matrices in the `roll.object` list element of the final output, and each cell is the aforementioned value. See also [Details](#).

## SIMULATION SPECIFICATIONS

`fsc2path`

Character string of path for `fastsimcoal2` executable file. Must include name of `fastsimcoal2` executable file. May be absolute path (*i.e.* beginning with `"/"`) or relative path from `output.directory`. Required.

`messages.sims`

Positive integer. Interval length in number of completed simulations for each cycle of messages (*e.g.* if = 10,000, a message is given when 10,000, 20,000, 30,000, etc. simulations are completed). Regardless of value or whether specified, a message is always given when the last simulation is completed.

`output.directory`

Character string of path for directory where output simulation

files are deposited, as well as from where `fastsimcoal2` is run (*i.e.* working directory changes to `output.directory` when running `fastsimcoal2`, but returns to current working directory). May or may not end with `"/"`. May be absolute path (*i.e.* beginning with `"/"`) or relative path from current working directory. See also `Details`. Required.

`append.sims`

Logical value. Allows output to be added to existing files with the same filename that are located within `output.directory`. See also `Details`.

`keep.taxa.draws,`  
`output.hyper.draws,`  
`output.taxa.draws,`  
`keep.fsc2.files`

Logical value. Activates whether taxon-specific parameter draws (*i.e.* `sim.specs` list elements) are outputted in R (not activating this may increase performance speed and decrease memory usage), whether hyperparameter and parameter summary values (*i.e.* `roll.object` list elements) are outputted to a simple text file within `output.directory`, whether taxon-specific parameter draws are outputted to a simple text file within `output.directory`, and whether the `fastsimcoal2` outputs `seed.txt` and `.lhood` are kept in simple text files per simulated independent taxon with respective filename suffixes `.seed` and `.fsc2` within `output.directory`, respectively.

## OBJECTS FROM PRECEDING FUNCTIONS

`build.object`

Output from function `build.dice`.

`roll.object`

Output from function `roll.dice`.

`play.object`

Output from function `play.dice`. See also `Details`.

Arguments from other `Multi-DICE` functions may be included here and are ignored if not applicable.

## **Details**

For more information, see `Multi-DICE Manual`.

`Multi-DICE` cannot currently accommodate models with more than one population per taxon, events aside from population size change, and more than two size change events.

For  $\tau_1$  and  $\tau_2$ , units are in numbers of generations, and thus may only be positive integers. For  $\epsilon_1$  and  $\epsilon_2$ , units are in ratio of size change from the ancestral effective population size to current effective population size, such that expansions are  $< 1$  and contractions are  $> 1$ , and thus may only be positive

values. For  $N_E$ , unit is in number of effective haploid individuals, and thus may only be positive integers.

For `num.taxa`, `num.haploid.samples`, `num.ind.sites`, `num.SNPs`, `length.seq`, `folded`, `sampling.times`, `gen.times`, `linked.param`, `attached.hyper`, `linked.param.fixed`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, `max.net.tau.zeta.per.pulse`, `max.net.tau2.zeta.per.pulse`, `max.net.epsilon.zeta.per.pulse`, `max.net.epsilon2.zeta.per.pulse`, `max.net.NE.zeta.per.pulse`, `num.changes`, and `flip`, if list, then all list elements are concatenated to form a single vector, with the ordering within list elements and then between list elements preserved (e.g. for list of length = 2, with first list element of length = 2 and second list element of length = 1, the order from first to last is: 1) first vector element in first list element; 2) second vector element in first list element; 3) sole vector element in second list element).

For `tau.psi.prior`, `epsilon.psi.prior`, `NE.psi.prior`, `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, `NE.zeta.prior`, `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, `NE.zeta.total.prior`, `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, `NE.shared.prior`, `tau.idio.prior`, `tau2.idio.prior`, `epsilon.idio.prior`, `epsilon2.idio.prior`, `NE.idio.prior`, `linked.param.prior`, `anchor.prior`, `change.prior`, `exponential.growth.rate.prior`, `exponential.growth.rate.prior2`, and `mut.rate.prior`, each list element contains an entire individual discrete distribution; if vector, then converted to list of length = 1 with all vector elements comprising the entirety of a single discrete distribution. Per list element, vector elements within (i.e. the discrete distribution) do not need to be in any particular order. Relatedly, each vector element is treated as an independent value, thus weighted distributions (i.e. not uniform) may be employed by duplicating values (e.g. a distribution of  $c(0, 1, 1, 1)$  signifies 75% probability of drawing “1” and 25% probability of drawing “0”), allowing the specification of any discretized distribution (e.g. gamma, beta, log-uniform). Accordingly, a uniform distribution with no gaps for integer values would be of length = range of distribution.

For `num.taxa`, `num.haploid.samples`, `num.ind.sites`, `num.SNPs`, `length.seq`, `folded`, `sampling.times`, `gen.times` (except when vector of length =  $n$ ), `num.changes`, and `flip`, the order of vector elements corresponds to the order of partitions, and for `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, `NE.zeta.prior`, `tau.idio.prior`, `tau2.idio.prior`, `epsilon.idio.prior`, `epsilon2.idio.prior`, `NE.idio.prior`, `change.prior`, `exponential.growth.rate.prior`, `exponential.growth.rate.prior2`, and `mut.rate.prior`, the order of list elements corresponds to the order of partitions. Additionally, if length = 1 and `num.partitions` > 1, then the sole element is used for all partitions. Similarly, if length < `num.partitions`, then the first element is used for all partitions while ignoring any remaining elements. Except for `gen.times`, if length >

`num.partitions`, then the remaining elements beyond `length = num.partitions` are ignored; a caution is provided when the length does not equal 1 or `num.partitions`. For `gen.times`, if `length > num.partitions` and `length < n`, then the remaining elements beyond `length = num.partitions` are ignored, and if `length > n`, then the remaining elements beyond `length = n` are ignored; a caution is provided when the length does not equal 1, `num.partitions`, or `n`.

For `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, `max.net.tau.zeta.per.pulse`, `max.net.tau2.zeta.per.pulse`, `max.net.epsilon.zeta.per.pulse`, `max.net.epsilon2.zeta.per.pulse`, and `max.net.NE.zeta.per.pulse`, the order of vector elements corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding `psi.prior`), and for `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, `NE.shared.prior`, and `anchor.prior`, the order of list elements corresponds to the temporal order, from most recent to most ancient, of pulses (as specified by the corresponding `psi.prior`). Additionally, if `length = 1` and maximum value in corresponding `psi.prior > 1`, then the sole element is used for all pulses. Similarly, if `length < maximum value in corresponding psi.prior`, then the first element is used for all pulses while ignoring any remaining elements. For the `zeta.per.pulse` arguments, if `length > maximum value in corresponding psi.prior`, then the remaining elements beyond `length = maximum value in corresponding psi.prior` are ignored; a caution is provided when the length does not equal 1 or maximum value in corresponding `psi.prior`. For the `shared.prior` arguments and `anchor.prior`, there may be additional list elements for idiosyncratic distributions, such that any total `length = 1`, maximum value in corresponding `psi.prior`, maximum value in corresponding `psi.prior + 1`, or maximum value in corresponding `psi.prior + num.partitions`, are allowed; for any other lengths, a caution is provided and excess elements beyond the highest acceptable length are ignored. See below for more information about adding idiosyncratic distributions to these arguments.

If `num.partitions=n`, then rearrangement of bins across taxa within allele frequency classes based on descending order of the relative SNP proportions is not performed to construct the aSFS and taxon-specific inference of demographic parameters is possible. However, in general, more partitions results in more parameter space with respect to taxa samples that must be explored due to a decrease in order-independence and assumed exchangeability, thus multiple-fold more simulations must be conducted to achieve comparable accuracy in hyperparameter estimation as without partitioning.

For `num.ind.sites`, `num.SNPs`, and `length.seq`, Multi-DICE first looks in `num.ind.sites`, then `num.SNPs`, and finally `length.seq`. For `num.ind.sites`, specified values equate to the number of genealogies simulated by the `FREQ` simulation model in `fastsimcoal2`. For `num.SNPs`, specified values equate to the number of independent loci (chromosomal structure is not considered) simulated by the `SNP` simulation model in `fastsimcoal2`. For `length.seq`, specified values equate to the number of loci within a linkage block (*i.e.* sites, or length of sequence; recombination is

not considered) simulated by the SNP simulation model in `fastsimcoal2`; to utilize `length.seq`, `mut.rate.prior` must also be specified. For both the `FREQ` and `SNP` simulation models, infinite sites are assumed by `fastsimcoal2`. Both `num.SNPs` and `length.seq` may be specified to simulate monomorphic sites and linked SNPs for the SFS, *i.e.* derive aSFS from genomic-scale whole-sequence information.

If `gen.times` is specified, output  $\tau$  values are in units of years. If generation times are equivalent across all  $n$  taxa, then it is not critical to specify `gen.times`, since output  $\tau$  values may be multiplied by the generation time scalar to covert units to years if `gen.times` is not specified. Hence, if generation time is 1 year, then output  $\tau$  values are in units of years as well.

For `tau.psi.prior`, `epsilon.psi.prior`, and `NE.psi.prior`, distinguishing between  $\Psi$  and  $\psi$  is accomplished via the corresponding `zeta.prior`, `zeta.total.prior`, `idiosyncratic` setting, and/or `min/max.net zeta.total/per.pulse`, except for values of 0, which are explicitly for  $\psi = 0$  and thus indicate full idiosyncrasy. If list length  $> 2$  for  $\tau$  and  $\epsilon$  or list length  $> 1$  for  $N_E$ , then a caution is provided and the remaining elements beyond length = 2 for  $\tau$  and  $\epsilon$  and length = 1 for  $N_E$  are ignored. Applies across all partitions, such that it is regardless of partitioning.

For `tau.zeta.prior`, `tau2.zeta.prior`, `epsilon.zeta.prior`, `epsilon2.zeta.prior`, and `NE.zeta.prior`, if `num.partitions`  $> 1$ , may be necessary to include “0.0” as a value, but can control  $\zeta_s$  and  $\zeta_T$  across partitions via corresponding `zeta.total.prior` and/or `min/max.net zeta.total/per.pulse`. Attributes to each partition individually, but proportion values are out of the entirety of taxa dataset, thus if `num.partitions`  $> 1$ , then the upper bound for each partition should be the number of taxa within that partition divided by  $n$ . When  $\psi = \{0, 1\}$ , equivalent to hyperprior distribution for  $\zeta_T$ . If identical across all partitions, it is more computationally efficient to specify only one *i.e.* list of length = 1, or a vector.

For `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior`, if length  $> 1$ , then remaining elements beyond the first are ignored and a caution is provided.

To build a hyperprior, Multi-DICE first looks if the corresponding `zeta.total.prior` is specified, then if `dirichlet.process=T`, and if neither is such case, then all possible combinations of corresponding `psi.prior` and `zeta.prior` draws are equally weighted. Therefore, if `num.partitions=1`, corresponding `psi.prior=1`, and `dirichlet.process=F`, then `tau.zeta.total.prior`, `tau2.zeta.total.prior`, `epsilon.zeta.total.prior`, `epsilon2.zeta.total.prior`, and `NE.zeta.total.prior` equivalent to corresponding `zeta.prior` and thus unnecessary to specify.

For `tau.shared.prior`, `tau2.shared.prior`, `epsilon.shared.prior`, `epsilon2.shared.prior`, and `NE.shared.prior`, each successive list element/distribution must have a greater minimum and maximum value than its preceding list elements/distributions. If multiple distributions are utilized for every potential pulse and these distributions overlap in their bounds,

running time may slow since, in this case, draws are made from all the distributions independently and then checked if abiding by ordering and buffering, with re-draws if not.

For each of `tau`, `tau2`, `epsilon`, `epsilon2`, and `NE`, if hyperparameterized via its corresponding `psi.prior` while `idiosyncratic=T` or a 0 value is in said `psi.prior`, then a corresponding idiosyncratic prior is required. Multi-DICE first looks in `change.prior` (for  $\tau_2$  only), then the corresponding `idio.prior`, and finally the corresponding `shared.prior`. If a `shared.prior` argument is utilized, the additional list elements beyond `length = maximum value in corresponding psi.prior` are considered; if the number of list elements is  $\leq$  maximum value in corresponding `psi.prior`, then only the first list element is considered. These list elements undergo the same specifications as aforementioned for the corresponding `idio.prior`.

For each of `tau`, `tau2`, `epsilon`, `epsilon2`, and `NE`, if not hyperparameterized yet part of the specified model (*i.e.* `tau`, `epsilon`, and `NE` are always part of the model, and `tau2` and `epsilon2` are part of the model when `num.changes = 2`), then a corresponding nuisance prior is required. A nuisance prior differs from an idiosyncratic prior in that variation in the respective nuisance parameter is being considered while not of interest with respect to hyperparameterization (*i.e.* variability in values across taxa governed hierarchically), whereas an idiosyncratic prior is still governed by hyperparameters in coordination with the corresponding shared prior. Multi-DICE first looks in `anchor.prior` (for  $\tau_2$  only), next `change.prior` (for  $\tau_2$  only), afterward `linked.param.prior` (if applicable; see below for more information), then the corresponding `idio.prior`, and finally the corresponding `shared.prior`. If `linked.param.prior` is utilized for a particular nuisance parameter, either the corresponding `idio.prior` or `shared.prior` must still be specified even if all taxa are always covered by `linked.param.prior` across all simulations. If a `shared.prior` argument is utilized, it undergoes the same specifications as aforementioned for the corresponding `idio.prior`.

It is highly recommended that prior distribution bounds are as far apart as possible between  $\tau_1$  and  $\tau_2$ , ideally mutually exclusive/non-overlapping. Otherwise, there could be a stop of operation due to an invalid/incompatible draw, computational lag, and/or statistical bias on prior distributions.

For `mut.rate.prior`, utilized only if `length.seq` is utilized as well. Values of 0 may technically be included, though this results in all polymorphic sites. If `keep.taxa.draws=T`, draws are outputted as a list element/matrix named `mut.rate` in the `sim.specs` list element of the final output. Each row represents an individual simulation, each column represents a simulated independent taxon, and each cell is the according mutation rate value used for simulation. Rows and columns correspond to other matrices *i.e.* the same row number refers to the same simulation and the same column number refers to the same simulated independent taxon.

For `tau.buffer`, `tau2.buffer`, `epsilon.buffer`, `epsilon2.buffer`, and `NE.buffer`,  $\beta$  buffers are applied to draws of shared pulse values, thus affecting the corresponding shared prior; the corresponding idiosyncratic prior, from which draws are subsequently made, is accordingly affected by the shared pulse buffers. For `tau.idiosyncratic.buffer`, `tau2.idiosyncratic.buffer`, `epsilon.idiosyncratic.buffer`, `epsilon2.idiosyncratic.buffer`, and

`NE.idiosyncratic.buffer`,  $\beta_i$  idiosyncratic buffers are then applied to idiosyncratic draws, which additionally affect the corresponding idiosyncratic prior that had already been initially transformed by the shared pulse buffers. In other words,  $\beta$  buffers idiosyncratic taxa from shared pulse values, and  $\beta_i$  buffers idiosyncratic taxa from each other. For example, if  $n = 10$ ,  $\psi_{\tau_1} = 2$ ,  $\zeta_{\tau_1, T} = 0.8$ ,  $\beta = 10,000$ ,  $\beta_i = 1,000$ ,  $\tau_1 \sim U(1,000, 100,000)$ ,  $\tau_{1s} = \{11,000, 12,001\}$ , and  $\tau_{1i} = \{99,000\}$  after the first idiosyncratic draw, then given that the synchronous/shared pulse buffers result in invalid draws from  $\sim U(1,000, 13,001)$  and the first idiosyncratic draw buffer results in invalid draws from  $\sim U(98,000, 100,000)$ , the remaining second idiosyncratic draw would be from the resulting transformed prior distribution  $\tau_{1i} \sim U(13,002, 97,999)$ . A caution is provided if an `idiosyncratic.buffer` corresponding to a specified `psi.prior` is not specified. Buffers cannot be deployed for nuisance draws (though see below when  $\psi = 0$ ).

For `num.changes`, only necessary if there are nuisance demographic parameters for a second event, since one event is the default and demographic parameters for the second event that are hyperparameterized by the corresponding `psi.prior` are already activated. If  $< 1$ , then there is a stop of operation, and if  $> 2$ , then it is converted to `num.changes=2` and a caution is provided.

If `flip=T`,  $\tau_2$  and  $\epsilon_2$  still refers to the second specified event, which in this case is the more recent one.

There cannot be a filename of “dice.sims.fsc2.template” within `output.directory`; `output.directory='.'` to specify current working directory.

If `append.sims=F`, then cannot have a filename of “seed.txt”, “MRCAs.txt”, “dice.log”, “dice.simulations” with a numerical suffix of “1” through  $n$ , or anything with the prefix “dice.sims” within `output.directory`. If `append.sims=T`, temporary intermediate files may cause files that have the prefix “dice.sims” within `output.directory` to be deleted.

When  $\psi = 0$  i.e. full idiosyncrasy, the arguments `idiosyncratic`, `min.net.tau.zeta.total`, `min.net.tau2.zeta.total`, `min.net.epsilon.zeta.total`, `min.net.epsilon2.zeta.total`, `min.net.NE.zeta.total`, `min.net.tau.zeta.per.pulse`, `min.net.tau2.zeta.per.pulse`, `min.net.epsilon.zeta.per.pulse`, `min.net.epsilon2.zeta.per.pulse`, `min.net.NE.zeta.per.pulse`, and `idiosyncratic.rule` are ignored, and the arguments `tau.idiosyncratic.buffer`, `tau2.idiosyncratic.buffer`, `epsilon.idiosyncratic.buffer`, `epsilon2.idiosyncratic.buffer`, and `NE.idiosyncratic.buffer` are activated (even if `idiosyncratic=F`).

Multi-DICE proceeds only if a valid draw is allowed given corresponding `num.taxa`, `psi.prior`, `zeta.prior` (e.g. minimum value in `psi.prior` \* minimum value in `zeta.prior`  $\leq$  minimum value in `num.taxa`), `zeta.total.prior`, shared prior, idiosyncratic prior, idiosyncratic setting, `min/max.net.zeta.total/per.pulse`, `buffer`, and `idiosyncratic.buffer`. Importantly, there is no check on if all values in `psi.prior` have a valid draw, only if there is a valid draw among any of the values. Additionally, the range of a shared prior must be greater than its corresponding



$(\Psi/\psi - 1)(2\beta + 1)$ , and the range of an idiosyncratic prior ought to be greater than its corresponding  $(\Psi/\psi)(2\beta + 1) + (\sigma - 1)(2\beta_i + 1)$  across every possible combination of  $\Psi/\psi$  and  $\sigma$  and with consideration given to `idiosyncratic.rule`. For `tau2.shared.prior` and `tau2.idio.prior`, consideration must also be given to any overlap with `tau.shared.prior` and `tau.idio.prior`, respectively.

## Value

Returned value is identical to that of `play.dice`, except if `keep.taxa.draws=F`, in which case the list element `sim.specs` is omitted, or if `keep.taxa.draws=T` and both `length.seq` and `mut.rate.prior` are utilized, in which case  $\mu$  draws are also added to `sim.specs` (see above for more information). Additionally, output simulation files in simple text format are deposited into `output.directory`: the filenames of `"dice.simulations"` with a numerical suffix of 1 through  $n$  (*i.e.* `"dice.simulations1"`, `"dice.simulations2"`, etc.) contain per-taxon summary statistics, tab delimited; the filenames of `"dice.sims.hyper.draws."` with a suffix corresponding to the names of hyperparameters and parameter summaries (*i.e.* names of `roll.object` list elements *e.g.* `"psi.tau"` for  $\Psi_{\tau 1}/\psi_{\tau 1}$  as specified by `tau.psi.prior`, `"zeta.tau.1"` for  $\zeta_{\tau 1}/\zeta_{\tau 1,s}$  of the first partition  $\zeta_{\tau 1,1}/\zeta_{\tau 1,s,1}$ , `"net.zeta.total.tau"` for  $\zeta_{\tau 1,T}$ , `"net.zeta.per.pulse.tau"` for  $\zeta_{\tau 1}/\zeta_{\tau 1,s}$ , `"pulse.values.tau"` for  $\tau_{1s}$  (or  $\tau_1$  if `tau.psi.prior` specifies  $\Psi_{\tau 1}$ ), `"disp.index.tau"` for  $\Omega(\tau_1)$ , etc.) contain the according values of interest for estimation, space delimited; the filenames of `"dice.sims.taxa.draws."` with a suffix corresponding to the names of taxon-specific parameters (*i.e.* names of `sim.specs` list elements: `tau`, `tau2`, `epsilon`, `epsilon2`, `NE`, `exponential.growth.rate.prior`, `exponential.growth.rate.prior2`, `mut.rate`) contain the according nuisance values used for simulation across taxa, space delimited; if `keep.fsc2.files=T`, the filenames of `"dice.sims"` with a suffix of 1 through  $n$  attached to either `.seed` and `.fsc2` (*i.e.* `"dice.sims1.seed"`, `"dice.sims1.fsc2"`, `"dice.sims2.seed"`, `"dice.sims2.fsc2"`, etc.) contain, per simulated independent taxon, the `fastsimcoal2` outputs `seed.txt` and `.lhood`, respectively. Each row per file represents an individual simulation, and rows across files correspond to each other *i.e.* the same row number refers to the same simulation across files. For `"dice.sims.taxa.draws."` files, each column per file represents each simulated independent taxon, and column order across these files and the numeric order implied by the names of the `"dice.simulations"`, `.seed`, and `.fsc2` files correspond to each other *i.e.* the same column number and filename number refer to the same simulated independent taxon. For `"dice.simulations"` files, each column per file represents an SFS allele frequency class bin (in the order described by the manual for `fastsimcoal2`) or single-sequence summary statistic (in the order of number of haplotypes, haplotype diversity, nucleotide diversity, and Tajima's  $D$ ), depending on data type simulated, for that respective simulated independent taxon.

## Author(s)

Alexander T. Xue

## References

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community assemblages using hierarchical approximate Bayesian computation. *Molecular Biology and Evolution*, **31**, 2501–2515.

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Xue AT, Hickerson MJ (*submitted*) Multi-DICE: R package for comparative population genomic inference under multi-taxa hierarchical co-demographic models.

## See Also

`build.dice`, `roll.dice`, `play.dice`, `dice.aSFS`, `dice.sumstats`

## Examples

```
#simplest execution akin to approach in Xue and Hickerson (2015)
dice.sims(num.sims=5, num.taxa=10, num.haploid.samples=10,
num.ind.sites=2000, tau.psi.prior=c(1), tau.zeta.prior=c(1:10)/10,
tau.shared.prior=c(1000:1000000), epsilon.idio.prior=c(1000:10000)/100000,
NE.idio.prior=c(1000:100000), fsc2path='example', output.directory='.')

#simplest execution akin to approach in Xue and Hickerson (2015); ln U
distribution applied on tau.shared.prior, with 100,000 intervals
discretized uniformly across ln(tau.shared.prior)
dice.sims(num.sims=5, num.taxa=10, num.haploid.samples=10,
num.ind.sites=2000, tau.psi.prior=c(1), tau.zeta.prior=c(1:10)/10,
tau.shared.prior=exp(c((log(1000)*100000):(log(1000000)*100000))/100000),
epsilon.idio.prior=c(1000:10000)/100000, NE.idio.prior=c(1000:100000),
fsc2path='example', output.directory='.')

#simplest execution akin to approach in Xue and Hickerson (2015); assuming
play.dice was previously performed and the output was directed to object
play.object
dice.sims(num.sims=5, num.taxa=10, num.haploid.samples=10,
num.ind.sites=2000, fsc2path='example', output.directory='.',
play.object=play.object)

#simplest execution akin to approach in software package msBayes
```

```
dice.sims(num.sims=5, num.taxa=10, num.haploid.samples=10,  
num.ind.sites=2000, tau.psi.prior=c(1:10), tau.zeta.prior=c(1:10)/10,  
tau.shared.prior=c(1000:1000000), epsilon.idio.prior=c(1000:10000)/100000,  
NE.idio.prior=c(1000:100000), idiosyncratic=F, fsc2path='example',  
output.directory='.')
```

## Constructing aSFS from per-taxon SFS simulations/data

### Description

`dice.aSFS` transforms per-taxon SFS, either simulated by `dice.sims` or empirically produced (*i.e.* observed/collected data), into the aSFS, following the procedure described in Xue and Hickerson (2015).

### Usage

```
dice.aSFS(num.sims, num.taxa, num.partitions=1, num.haploid.samples,  
folded=T, remove.afclasses=NULL, output.directory='.',  
input.directory=NULL, input.base=NULL, input.files=NULL)
```

### Arguments

<code>num.sims</code>	Positive integer. Number of simulations. Required. See also <code>Details</code> .
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### DATA

<code>num.taxa</code>	List, vector of length = <code>num.partitions</code> , or positive integer. Number of taxa per partition. Total sum across partitions equals the total number of taxa $n$ in dataset. See also <code>Details</code> . Required.
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<code>num.partitions</code>	Positive integer. Number of partitions for taxa in dataset. Allows differential data and model specifications across user-specified taxa groupings, including sampling size of individuals, generation times, demographic syndrome, and taxon-specific nuisance parameter prior distributions. See also <code>Details</code> .
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<code>num.haploid.samples</code>	List, vector of length = <code>num.partitions</code> , or positive integer. Number of haploid samples per partition. See also <code>Details</code> . Required.
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<code>folded</code>	List, vector of length = <code>num.partitions</code> , or logical value. Activates folding of the SFS per partition. See also <code>Details</code> .
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<code>remove.afclasses</code>	List of length = <code>num.partitions</code> or 1, vector, or non-negative integer. Allele frequency classes to be removed from the SFS per partition prior to aSFS construction, with 0 referring to
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monomorphic bins, 1 referring to singleton bins, 2 referring to doubleton bins, etc. By default, monomorphic bins are removed. See also `Details`.

## SIMULATION SPECIFICATIONS

`output.directory,`  
`input.directory`

Character string of path(s) for directory where SFS files are located. May or may not end with “/”. May be absolute path (*i.e.* beginning with “/”) or relative path from current working directory. If `output.directory` is specified, then it is assumed that there is only one directory with output SFS filenames as produced by `dice.sims`. To specify multiple directories or different filenames, `input.directory` must be specified, which may be a list or vector. See also `Details`.

`input.base`

Character string of prefix for SFS filenames. Assumed all SFS files within `input.directory` begin with prefix and end with a numerical suffix of 1 through  $n$ . See also `Details`.

`input.files`

List, vector =  $n$ , or character string of SFS filenames within `input.directory`. See also `Details`.

Arguments from other `Multi-DICE` functions may be included here and are ignored if not applicable.

### **Details**

For more information, see `Multi-DICE Manual`.

`Multi-DICE` cannot currently accommodate data for more than one population per taxon.

For `num.taxa`, `num.haploid.samples`, `folded`, `input.directory`, and `input.files`, if list, then all list elements are concatenated to form a single vector, with the ordering within list elements and then between list elements preserved (*e.g.* for list of length = 2, with first list element of length = 2 and second list element of length = 1, the order from first to last is: 1) first vector element in first list element; 2) second vector element in first list element; 3) sole vector element in second list element).

For `remove.afclasses`, if vector, then converted to list of length = 1. Per list element, vector elements within do not need to be in any particular order. Relatedly, only unique vector elements are considered, with duplicated values ignored.

For `num.taxa` and `folded`, the order of vector elements corresponds to the order of partitions, and for `remove.afclasses`, the order of list elements corresponds to the order of partitions. Additionally, if length = 1 and `num.partitions` > 1, then the sole element is used for all partitions. Similarly, if length < `num.partitions`, then the first element is used for all partitions while ignoring

any remaining elements, and if `length > num.partitions`, then the remaining elements beyond `length = num.partitions` are ignored; a caution is provided when the length does not equal 1 or `num.partitions`.

If empirical data are converted to aSFS format, then `num.sims` = number of multi-taxa comparative datasets (most likely 1). SFS files must be in similar format to output SFS files produced by `dice.sims`, such that each taxon SFS is within a separate tab-delimited file, number of rows = `num.sims`, number of columns = number of SFS allele frequency classes (*i.e.* number of haploid samples + 1 (number of haploid samples – 1 if monomorphic bins are already removed), or if folded, then may be (number of haploid samples/2) + 1, rounded up, with + 1 omitted if monomorphic bins are already removed), and no headers or labels. Values are converted to proportions out of the total of polymorphic bins by default, thus values do not need to be user-converted.

If `num.partitions=n`, then rearrangement of bins across taxa within allele frequency classes based on descending order of the relative SNP proportions is not performed to construct the aSFS and taxon-specific inference of demographic parameters is possible. However, in general, more partitions results in more parameter space with respect to taxa samples that must be explored due to a decrease in order-independence and assumed exchangeability, thus multiple-fold more simulations must be conducted to achieve comparable accuracy in hyperparameter estimation as without partitioning.

For `remove.afclasses`, monomorphic bins are not removed by default if specified, thus 0 must be included if desired to be removed. To include the monomorphic frequency class without removing any bins, the integer of `num.haploid.samples + 1` (or any value(s) > `num.haploid.samples`) must be specified.

To determine input directory, Multi-DICE first looks in `input.directory`, then `output.directory`. If `input.directory` is utilized, may be of any length, with order corresponding to arrangement of output aSFS matrix rows. Filenames are assumed to be consistent across `input.directory` directories. To determine filename format, Multi-DICE first looks in `input.base`, then `input.files`. If `input.base` is list or vector of length > 1, then only first vector element is considered. For `input.files`, length must be  $\geq n$ ; if >  $n$ , then the remaining elements beyond `length = n` are ignored and a caution is provided. If neither `input.files` nor `input.base` is specified, or if `output.directory` is utilized, then filenames assumed to follow the same format as output SFS files produced by `dice.sims` (*i.e.* "dice.simulations1", "dice.simulations2", etc.). To accommodate parallelized runs across multiple directories, `input.directory` ought to be utilized.

## Value

Returned value is aSFS matrix, with each row representing an individual simulation and in the same order as input files (followed then by the user-specified order of input directories if applicable), and each column representing an aSFS bin.

## Author(s)

Alexander T. Xue

## References

Xue AT (2017) Multi-DICE Manual.

Xue AT, Hickerson MJ (2015) The aggregate site frequency spectrum for comparative population genomic inference. *Molecular Ecology*, **24**, 6223–6240.

Xue AT, Hickerson MJ (*submitted*) Multi-DICE: R package for comparative population genomic inference under multi-taxa hierarchical co-demographic models.

## See Also

`build.dice`, `roll.dice`, `play.dice`, `dice.sims`

## Examples

```
#simplest execution
dice.aSFS(num.sims=5, num.taxa=10, num.haploid.samples=10,
output.directory='example')
```

# Constructing multi-taxa single-sequence summary statistic vector from per-taxon summary statistics simulations/data

## Description

`dice.sumstats` transforms per-taxon single-sequence summary statistics, either simulated by `dice.sims` or empirically produced (*i.e.* observed/collected data), into the multi-taxa single-sequence summary statistic vector, following the procedure described in Chan *et al.* (2015). Empirical sequence data may also be inputted. If `convert.sequences=T`, then `bash` commands are called upon here and `dice.sumstats` can run only within a `bash` terminal environment (e.g. Mac, Linux).

## Usage

```
dice.sumstats(num.sims, num.taxa, num.partitions=1, num.haploid.samples,  
convert.sequences=F, output.directory='.', input.directory=NULL,  
input.base=NULL, input.files=NULL)
```

## Arguments

`num.sims` Positive integer. Number of simulations. Required. See also [Details](#).

## DATA

`num.taxa` List, vector of length = `num.partitions`, or positive integer. Number of taxa per partition. Total sum across partitions equals the total number of taxa  $n$  in dataset. See also [Details](#). Required.

`num.partitions` Positive integer. Number of partitions for taxa in dataset. Allows differential data and model specifications across user-specified taxa groupings, including sampling size of individuals, generation times, demographic syndrome, and taxon-specific nuisance parameter prior distributions. See also [Details](#).

`num.haploid.samples` List, vector of length = `num.partitions`, or positive integer. Number of haploid samples per partition. See also [Details](#). Required.

`convert.sequences` Logical value. Activates sequence data input. See also [Details](#).



## SIMULATION SPECIFICATIONS

`output.directory,`  
`input.directory`

Character string of path(s) for directory where SFS files are located. May or may not end with "/". May be absolute path (*i.e.* beginning with "/") or relative path from current working directory. If `output.directory` is specified, then it is assumed that there is only one directory with output SFS filenames as produced by `dice.sims`. To specify multiple directories or different filenames, `input.directory` must be specified, which may be a list or vector. See also `Details`.

`input.base`

Character string of prefix for SFS filenames. Assumed all SFS files within `input.directory` begin with prefix and end with a numerical suffix of 1 through  $n$ . See also `Details`.

`input.files`

List, vector =  $n$ , or character string of SFS filenames within `input.directory`. See also `Details`.

Arguments from other `Multi-DICE` functions may be included here and are ignored if not applicable.

### **Details**

For more information, see `Multi-DICE Manual`.

`Multi-DICE` cannot currently accommodate data for more than one population per taxon.

For `num.taxa`, `num.haploid.samples`, `input.directory`, and `input.files`, if list, then all list elements are concatenated to form a single vector, with the ordering within list elements and then between list elements preserved (*e.g.* for list of length = 2, with first list element of length = 2 and second list element of length = 1, the order from first to last is: 1) first vector element in first list element; 2) second vector element in first list element; 3) sole vector element in second list element).

For `num.taxa`, the order of vector elements corresponds to the order of partitions. Additionally, if `length = 1` and `num.partitions > 1`, then the sole element is used for all partitions. Similarly, if `length < num.partitions`, then the first element is used for all partitions while ignoring any remaining elements, and if `length > num.partitions`, then the remaining elements beyond `length = num.partitions` are ignored; a caution is provided when the length does not equal 1 or `num.partitions`.

If empirical data are converted, then `num.sims` = number of multi-taxa comparative datasets (most likely 1). If `convert.sequences=F`, files must be in similar format to output simulation files produced by `dice.sims`, such that each taxon single-sequence summary statistics are within a separate tab-delimited file, number of rows = `num.sims`, number of columns = 4, no headers or

labels, and columns are in order of: number of haplotypes, haplotype diversity, nucleotide diversity, Tajima's *D*.

If `num.partitions=n`, then distribution moments (*i.e.* transforming into multi-taxa single-sequence summary statistic vector) are irrelevant (mean = per-taxon value; variance, skewness, kurtosis set to 0) and taxon-specific inference of demographic parameters is possible. However, in general, more partitions results in more parameter space with respect to taxa samples that must be explored due to a decrease in order-independence and assumed exchangeability, thus multiple-fold more simulations must be conducted to achieve comparable accuracy in hyperparameter estimation as without partitioning.

If `convert.sequences=T`, assumed that: each taxon single-sequence data are within a separate file; sequence format is in 1/0 (with missing data = 9), AGTC (with missing data = N or -), or IUPAC (with missing data = N or -); each row corresponds to a haploid (diploid for IUPAC format) sample such that number of rows = `num.haploid.samples`; no headers or labels; each multi-taxa comparative dataset is within a separate directory such that length of directories = `num.sims` and `num.sims=1` if `output.directory` is utilized; sequence format is consistent across all directories. To calculate number of haplotypes per taxon, missing data in otherwise monomorphic sites are converted to the according monomorphic base and sites that are missing across all samples are removed, then unique haplotypes are discovered (while ignoring missing sites) from the sequences in order from least to most missing data (ties result in original user-specified order). Additionally, there cannot be a filename of "dice.sims.fsc2.template" within any directory.

To determine input directory, Multi-DICE first looks in `input.directory`, then `output.directory`. If `input.directory` is utilized, may be of any length, with order corresponding to arrangement of output matrix rows. Filenames are assumed to be consistent across `input.directory` directories. To determine filename format, Multi-DICE first looks in `input.base`, then `input.files`. If `input.base` is list or vector of length > 1, then only first vector element is considered. For `input.files`, length must be  $\geq n$ ; if >  $n$ , then the remaining elements beyond length =  $n$  are ignored and a caution is provided. If neither `input.files` nor `input.base` is specified, or if `output.directory` is utilized, then filenames assumed to follow the same format as output files produced by `dice.sims` (*i.e.* "dice.simulations1", "dice.simulations2", etc.). To accommodate parallelized runs across multiple directories, `input.directory` ought to be utilized.

## Value

Returned value is matrix of multi-taxa single-sequence summary statistic vectors, with each row representing an individual simulation and in the same order as input files (followed then by the user-specified order of input directories if applicable), and each column representing an element of the multi-taxa single-sequence summary statistic vector and in the order of mean, variance, skewness, and kurtosis, per single-taxon summary statistic (following same order as before: number of haplotypes, haplotype diversity, nucleotide diversity, Tajima's *D*), per partition.

## Author(s)

Alexander T. Xue

## References

Chan YL, Schanzenbach D, Hickerson MJ (2014) Detecting concerted demographic response across community assemblages using hierarchical approximate Bayesian computation. *Molecular Biology and Evolution*, **31**, 2501–2515.

Xue AT (2017) Multi-DICE Manual.

Xue AT, Hickerson MJ (*submitted*) Multi-DICE: R package for comparative population genomic inference under multi-taxa hierarchical co-demographic models.

## See Also

`build.dice`, `roll.dice`, `play.dice`, `dice.sims`

## Examples

```
#simplest execution
dice.sumstats(num.sims=5, num.taxa=10, num.haploid.samples=10,
output.directory='example')
```