# Package: simmr (via r-universe)

September 8, 2024

```
Title A Stable Isotope Mixing Model
Version 0.5.1.216
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URL https://github.com/andrewcparnell/simmr,
     https://andrewcparnell.github.io/simmr/
BugReports https://github.com/andrewcparnell/simmr/issues
Language en-US
Description Fits Stable Isotope Mixing Models (SIMMs) and is meant as
     a longer term replacement to the previous widely-used package
     SIAR. SIMMs are used to infer dietary proportions of organisms
     consuming various food sources from observations on the stable
     isotope values taken from the organisms' tissue samples.
     However SIMMs can also be used in other scenarios, such as in
     sediment mixing or the composition of fatty acids. The main
     functions are simmr_load() and simmr_mcmc(). The two vignettes
     contain a quick start and a full listing of all the features.
     The methods used are detailed in the papers Parnell et al 2010
     <doi:10.1371/journal.pone.0009672>, and Parnell et al 2013
     <doi:10.1002/env.2221>.
Depends R (>= 3.5.0), R2jags, ggplot2
Imports compositions, boot, reshape2, graphics, stats, viridis,
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Type Package

2 combine\_sources

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# Description

This function takes in an object of class simmr\_output and combines two of the food sources. It works for single and multiple group data.

combine\_sources 3

## Usage

```
combine_sources(
  simmr_out,
  to_combine = NULL,
  new_source_name = "combined_source"
)
```

# **Arguments**

simmr\_out An object of class simmr\_output created from simmr\_mcmc or simmr\_ffvb
to\_combine The names of exactly two sources. These should match the names given to
simmr\_load.
new\_source\_name

A name to give to the new combined source.

#### **Details**

Often two sources either (1) lie in similar location on the iso-space plot, or (2) are very similar in phylogenetic terms. In case (1) it is common to experience high (negative) posterior correlations between the sources. Combining them can reduce this correlation and improve precision of the estimates. In case (2) we might wish to determine the joint amount eaten of the two sources when combined. This function thus combines two sources after a run of simmr\_mcmc or simmr\_ffvb (known as a posteriori combination). The new object can then be called with plot.simmr\_input or plot.simmr\_output to produce iso-space plots of summaries of the output after combination.

## Value

A new simmr\_output object

#### Author(s)

Andrew Parnell <andrew.parnell@mu.ie>, Emma Govan

#### See Also

See simmr\_mcmc and simmr\_ffvb and the associated vignette for examples.

```
# The data
data(geese_data)

# Load into simmr
simmr_1 <- with(
   geese_data_day1,
   simmr_load(
     mixtures = mixtures,
     source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,</pre>
```

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```
correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# Plot
plot(simmr_1)
# Print
simmr_1
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
# Print it
print(simmr_1_out)
# Summary
summary(simmr_1_out)
summary(simmr_1_out, type = "diagnostics")
summary(simmr_1_out, type = "correlations")
summary(simmr_1_out, type = "statistics")
ans <- summary(simmr_1_out, type = c("quantiles", "statistics"))</pre>
# Plot
plot(simmr_1_out)
plot(simmr_1_out, type = "boxplot")
plot(simmr_1_out, type = "histogram")
plot(simmr_1_out, type = "density")
plot(simmr_1_out, type = "matrix")
simmr_out_combine <- combine_sources(simmr_1_out,</pre>
  to_combine = c("U.lactuca", "Enteromorpha"),
  new_source_name = "U.lac+Ent"
)
plot(simmr_out_combine$input)
plot(simmr_out_combine, type = "boxplot", title = "simmr output: combined sources")
```

compare\_groups

Compare dietary proportions for a single source across different groups

# **Description**

This function takes in an object of class simmr\_output and creates probabilistic comparisons for a given source and a set of at least two groups.

compare\_groups 5

## Usage

```
compare_groups(
  simmr_out,
  source_name = simmr_out$input$source_names[1],
  groups = 1:2,
  plot = TRUE
)
```

#### **Arguments**

simmr\_out An object of class simmr\_output created from simmr\_mcmc or simmr\_ffvb.

The name of a source. This should match the names exactly given to simmr\_load.

The integer values of the group numbers to be compared. At least two groups must be specified.

A logical value specifying whether plots should be produced or not.

#### **Details**

When two groups are specified, the function produces a direct calculation of the probability that one group is bigger than the other. When more than two groups are given, the function produces a set of most likely probabilistic orderings for each combination of groups. The function produces boxplots by default and also allows for the storage of the output for further analysis if required.

## Value

If there are two groups, a vector containing the differences between the two groups proportions for that source. If there are multiple groups, a list containing the following fields:

Ordering The different possible orderings of the dietary proportions across groups
out\_all The dietary proportions for this source across the groups specified as columns
in a matrix

#### Author(s)

Andrew Parnell <andrew.parnell@mu.ie>

## See Also

See simmr\_mcmc for complete examples.

```
## Not run:
data(geese_data)
simmr_in <- with(
   geese_data,
   simmr_load(
     mixtures = mixtures,
     source_names = source_names,</pre>
```

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```
source_means = source_means,
    source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
   concentration_means = concentration_means,
   group = groups
)
# Print
simmr_in
# Plot
plot(simmr_in,
 group = 1:8, xlab = expression(paste(delta^13, "C (per mille)", sep = "")),
 ylab = expression(paste(delta^15, "N (per mille)", sep = "")),
 title = "Isospace plot of Inger et al Geese data"
)
# Run MCMC for each group
simmr_out <- simmr_ffvb(simmr_in)</pre>
# Print output
simmr_out
# Summarise output
summary(simmr_out, type = "quantiles", group = 1)
summary(simmr_out, type = "quantiles", group = c(1, 3))
summary(simmr_out, type = c("quantiles", "statistics"), group = c(1, 3))
# Plot - only a single group allowed
plot(simmr_out, type = "boxplot", group = 2, title = "simmr output group 2")
plot(simmr_out, type = c("density", "matrix"), grp = 6, title = "simmr output group 6")
# Compare groups
compare_groups(simmr_out, source = "Zostera", groups = 1:2)
compare_groups(simmr_out, source = "Zostera", groups = 1:3)
compare_groups(simmr_out, source = "U.lactuca", groups = c(4:5, 7, 2))
## End(Not run)
```

compare\_sources

Compare dietary proportions between multiple sources

# **Description**

This function takes in an object of class simmr\_output and creates probabilistic comparisons between the supplied sources. The group number can also be specified.

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## Usage

```
compare_sources(
  simmr_out,
  source_names = simmr_out$input$source_names,
  group = 1,
 plot = TRUE
)
```

## **Arguments**

simmr\_out An object of class simmr\_output created from simmr\_mcmc or simmr\_ffvb. The names of at least two sources. These should match the names exactly given source\_names to simmr\_load. group The integer values of the group numbers to be compared. If not specified as-

sumes the first or only group

A logical value specifying whether plots should be produced or not. plot

#### **Details**

When two sources are specified, the function produces a direct calculation of the probability that the dietary proportion for one source is bigger than the other. When more than two sources are given, the function produces a set of most likely probabilistic orderings for each combination of sources. The function produces boxplots by default and also allows for the storage of the output for further analysis if required.

## Value

If there are two sources, a vector containing the differences between the two dietary proportion proportions for these two sources. If there are multiple sources, a list containing the following fields:

**Ordering** The different possible orderings of the dietary proportions across sources out\_all The dietary proportions for these sources specified as columns in a matrix

## Author(s)

Andrew Parnell <andrew.parnell@mu.ie>

#### See Also

See simmr\_mcmc for complete examples.

```
data(geese_data_day1)
simmr_1 <- with(
 geese_data_day1,
 simmr_load(
   mixtures = mixtures,
```

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```
source_names = source_names,
    source_means = source_means,
    source_sds = source_sds,
    correction_means = correction_means,
   correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# Plot
plot(simmr_1)
# Print
simmr_1
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
# Print it
print(simmr_1_out)
# Summary
summary(simmr_1_out)
summary(simmr_1_out, type = "diagnostics")
summary(simmr_1_out, type = "correlations")
summary(simmr_1_out, type = "statistics")
ans <- summary(simmr_1_out, type = c("quantiles", "statistics"))</pre>
# Plot
plot(simmr_1_out, type = "boxplot")
plot(simmr_1_out, type = "histogram")
plot(simmr_1_out, type = "density")
plot(simmr_1_out, type = "matrix")
# Compare two sources
compare_sources(simmr_1_out, source_names = c("Zostera", "Grass"))
# Compare multiple sources
compare_sources(simmr_1_out)
```

geese\_data

Geese stable isotope mixing data set

# **Description**

A real Geese data set with 251 observations on 2 isotopes, with 4 sources, and with corrections/trophic enrichment factors (TEFs or TDFs), and concentration dependence means. Taken from Inger et al (2016). See link for paper

geese\_data\_day1

## Usage

geese\_data

#### **Format**

A list with the following elements

mixtures A two column matrix containing delta 13C and delta 15N values respectively

source names A character vector of the food source names

tracer names A character vector of the tracer names (d13C, d15N, d34S)

source\_means A matrix of source mean values for the tracers in the same order as mixtures above

source\_sds A matrix of source sd values for the tracers in the same order as mixtures above

**correction\_means** A matrix of TEFs mean values for the tracers in the same order as mixtures above

correction\_sds A matrix of TEFs sd values for the tracers in the same order as mixtures above concentration\_means A matrix of concentration dependence mean values for the tracers in the same order as mixtures above ...

@seealso simmr\_mcmc for an example where it is used

#### Source

<doi:10.1111/j.1365-2656.2006.01142.x>

geese\_data\_day1

A smaller version of the Geese stable isotope mixing data set

# Description

A real Geese data set with 9 observations on 2 isotopes, with 4 sources, and with corrections/trophic enrichment factors (TEFs or TDFs), and concentration dependence means. Taken from Inger et al (2016). See link for paper

## Usage

```
geese_data_day1
```

# **Format**

A list with the following elements

mixtures A two column matrix containing delta 13C and delta 15N values respectively

source\_names A character vector of the food source names

tracer\_names A character vector of the tracer names (d13C, d15N, d34S)

source\_means A matrix of source mean values for the tracers in the same order as mixtures above

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source\_sds A matrix of source sd values for the tracers in the same order as mixtures above
correction\_means A matrix of TEFs mean values for the tracers in the same order as mixtures above

correction\_sds A matrix of TEFs sd values for the tracers in the same order as mixtures above concentration\_means A matrix of concentration dependence mean values for the tracers in the same order as mixtures above ...

@seealso simmr\_mcmc for an example where it is used

# **Source**

```
<doi:10.1111/j.1365-2656.2006.01142.x>
```

plot.simmr\_input

Plot the simmr\_input data created from simmr\_load

# Description

This function creates iso-space (AKA tracer-space or delta-space) plots. They are vital in determining whether the data are suitable for running in a SIMM.

# Usage

```
## $3 method for class 'simmr_input'
plot(
    x,
    tracers = c(1, 2),
    title = "Tracers plot",
    xlab = colnames(x$mixtures)[tracers[1]],
    ylab = colnames(x$mixtures)[tracers[2]],
    sigmas = 1,
    group = 1:x$n_groups,
    mix_name = "Mixtures",
    ggargs = NULL,
    colour = TRUE,
    ...
)
```

# **Arguments**

Х	An object of class simmr_input created via the function simmr_load
tracers	The choice of tracers to plot. If there are more than two tracers, it is recommended to plot every pair of tracers to determine whether the mixtures lie in the mixing polygon defined by the sources
title	A title for the graph
xlab	The x-axis label. By default this is assumed to be delta-13C but can be made richer if required. See examples below.

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ylab	The y-axis label. By default this is assumed to be delta-15N in per mil but can be changed as with the x-axis label
sigmas	The number of standard deviations to plot on the source values. Defaults to 1.
group	Which groups to plot. Can be a single group or multiple groups
mix_name	A optional string containing the name of the mixture objects, e.g. Geese.
ggargs	Extra arguments to be included in the ggplot (e.g. axis limits)
colour	If TRUE (default) creates a plot. If not, puts the plot in black and white
	Not used

#### **Details**

It is desirable to have the vast majority of the mixture observations to be inside the convex hull defined by the food sources. When there are more than two tracers (as in one of the examples below) it is recommended to plot all the different pairs of the food sources. See the vignette for further details of richer plots.

#### Value

isospace plot

## Author(s)

Andrew Parnell <andrew.parnell@mu.ie>

#### See Also

See plot.simmr\_output for plotting the output of a simmr run. See simmr\_mcmc for running a simmr object once the iso-space is deemed acceptable.

```
# A simple example with 10 observations, 4 food sources and 2 tracers
data(geese_data_day1)
simmr_1 <- with(
 geese_data_day1,
 simmr_load(
   mixtures = mixtures,
   source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
    concentration_means = concentration_means
 )
)
# Plot
plot(simmr_1)
```

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```
### A more complicated example with 30 obs, 3 tracers and 4 sources
data(simmr_data_2)
simmr_3 <- with(
  simmr_data_2,
  simmr_load(
   mixtures = mixtures,
    source_names = source_names,
    source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# Plot 3 times - first default d13C vs d15N
plot(simmr_3)
# Now plot d15N vs d34S
plot(simmr_3, tracers = c(2, 3))
# and finally d13C vs d34S
plot(simmr_3, tracers = c(1, 3))
# See vignette('simmr') for fancier x-axis labels
# An example with multiple groups - the Geese data from Inger et al 2006
data(geese_data)
simmr_4 <- with(
  geese_data,
  simmr_load(
   mixtures = mixtures,
    source_names = source_names,
    source_means = source_means,
    source_sds = source_sds,
    correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means,
    group = groups
)
# Print
simmr_4
# Plot
plot(simmr_4,
  xlab = expression(paste(delta^13, "C (per mille)", sep = "")),
  ylab = expression(paste(delta^15, "N (per mille)", sep = "")),
  title = "Isospace plot of Inger et al Geese data"
) #'
```

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# **Description**

This function allows for 4 different types of plots of the simmr output created from simmr\_mcmc or simmr\_ffvb. The types are: histogram, kernel density plot, matrix plot (most useful) and boxplot. There are some minor customisation options.

# Usage

```
## S3 method for class 'simmr_output'
plot(
    x,
    type = c("isospace", "histogram", "density", "matrix", "boxplot"),
    group = 1,
    binwidth = 0.05,
    alpha = 0.5,
    title = if (length(group) == 1) {
        "simmr output plot"
} else {
        paste("simmr output plot: group", group)
},
        ggargs = NULL,
        ...
)
```

# **Arguments**

Х	An object of class simmr_output created via simmr_mcmc or simmr_ffvb.
type	The type of plot required. Can be one or more of 'histogram', 'density', 'matrix', or 'boxplot'
group	Which group(s) to plot.
binwidth	The width of the bins for the histogram. Defaults to 0.05
alpha	The degree of transparency of the plots. Not relevant for matrix plots
title	The title of the plot.
ggargs	Extra arguments to be included in the ggplot (e.g. axis limits)
	Currently not used

## **Details**

The matrix plot should form a necessary part of any SIMM analysis since it allows the user to judge which sources are identifiable by the model. Further detail about these plots is provided in the vignette. Some code from https://stackoverflow.com/questions/14711550/is-there-a-way-to-change-the-color-palette-for-ggallyggpairs-using-ggplot accessed March 2023

## Value

```
one or more of 'histogram', 'density', 'matrix', or 'boxplot'
```

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## Author(s)

Andrew Parnell <andrew.parnell@mu.ie>, Emma Govan

## See Also

See simmr\_mcmc and simmr\_ffvb for creating objects suitable for this function, and many more examples. See also simmr\_load for creating simmr objects, plot.simmr\_input for creating isospace plots, summary.simmr\_output for summarising output.

```
# A simple example with 10 observations, 2 tracers and 4 sources
# The data
data(geese_data)
# Load into simmr
simmr_1 <- with(
  geese_data_day1,
  simmr_load(
   mixtures = mixtures,
   source_names = source_names,
   source_means = source_means,
    source_sds = source_sds,
    correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means
)
# Plot
plot(simmr_1)
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
plot(simmr_1_out) # Creates all 4 plots
plot(simmr_1_out, type = "boxplot")
plot(simmr_1_out, type = "histogram")
plot(simmr_1_out, type = "density")
plot(simmr_1_out, type = "matrix")
```

posterior\_predictive 15

# **Description**

This function takes the output from simmr\_mcmcand plots the posterior predictive distribution to enable visualisation of model fit. The simulated posterior predicted values are returned as part of the object and can be saved for external use

# Usage

```
posterior_predictive(simmr_out, group = 1, prob = 0.5, plot_ppc = TRUE)
```

# Arguments

simmr\_out A run of the simmr model from simmr\_mcmc

group Which group to run it for (currently only numeric rather than group names)

The probability interval for the posterior predictives. The default is 0.5 (i.e. 50pc intervals)

plot\_ppc Whether to create a bayesplot of the posterior predictive or not.

#### Value

plot of posterior predictives and simulated values

```
data(geese_data_day1)
simmr_1 <- with(
  geese_data_day1,
  simmr_load(
    mixtures = mixtures,
    source_names = source_names,
    source_means = source_means,
    source_sds = source_sds,
    correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# Plot
plot(simmr_1)
# Print
simmr_1
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
# Prior predictive
post_pred <- posterior_predictive(simmr_1_out)</pre>
```

print.simmr\_output

print.simmr\_input

Print simmr input object

# **Description**

Print simmr input object

# Usage

```
## S3 method for class 'simmr_input'
print(x, ...)
```

# Arguments

x An object of class simmr\_input
... Other arguments (not supported)

# Value

A neat presentation of your simmr object.

print.simmr\_output

Print simmr output object

# **Description**

Print simmr output object

# Usage

```
## S3 method for class 'simmr_output' print(x, ...)
```

# **Arguments**

x An object of class simmr\_output... Other arguments (not supported)

# Value

Returns a neat summary of the object

#### See Also

```
simmr_mcmc and simmr_ffvb for creating simmr_output objects
```

prior\_viz 17

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Plot the prior distribution for a simmr run

# **Description**

This function takes the output from simmr\_mcmc or simmr\_ffvb and plots the prior distribution to enable visual inspection. This can be used by itself or together with posterior\_predictive to visually evaluate the influence of the prior on the posterior distribution.

## Usage

```
prior_viz(
    simmr_out,
    group = 1,
    plot = TRUE,
    include_posterior = TRUE,
    n_sims = 10000,
    scales = "free"
)
```

# **Arguments**

simmr\_out A run of the simmr model from simmr\_mcmc or simmr\_ffvb
group Which group to run it for (currently only numeric rather than group names)
plot Whether to create a density plot of the prior or not. The simulated prior values are returned as part of the object
include\_posterior
Whether to include the posterior distribution on top of the priors. Defaults to TRUE

n\_sims The number of simulations from the prior distribution
scales The type of scale from facet\_wrap allowing for fixed, free, free\_x, free\_y

# Value

A list containing plot: the ggplot object (useful if requires customisation), and sim: the simulated prior values which can be compared with the posterior densities

```
data(geese_data_day1)
simmr_1 <- with(
  geese_data_day1,
  simmr_load(
    mixtures = mixtures,
    source_names = source_names,
    source_means = source_means,</pre>
```

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```
source_sds = source_sds,
    correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# Plot
plot(simmr_1)
# Print
simmr_1
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
# Prior predictive
prior <- prior_viz(simmr_1_out)</pre>
head(prior$p_prior_sim)
summary(prior$p_prior_sim)
```

simmr

simmr: A package for fitting stable isotope mixing models via JAGS and FFVB in R

# Description

This package runs a simple Stable Isotope Mixing Model (SIMM) and is meant as a longer term replacement to the previous function SIAR.. These are used to infer dietary proportions of organisms consuming various food sources from observations on the stable isotope values taken from the organisms' tissue samples. However SIMMs can also be used in other scenarios, such as in sediment mixing or the composition of fatty acids. The main functions are simmr\_load, simmr\_mcmc, and simmr\_ffvb. The help files contain examples of the use of this package. See also the vignette for a longer walkthrough.

#### **Details**

An even longer term replacement for properly running SIMMs is MixSIAR, which allows for more detailed random effects and the inclusion of covariates.

# Author(s)

Andrew Parnell <andrew.parnell@mu.ie>

#### References

Andrew C. Parnell, Donald L. Phillips, Stuart Bearhop, Brice X. Semmens, Eric J. Ward, Jonathan W. Moore, Andrew L. Jackson, Jonathan Grey, David J. Kelly, and Richard Inger. Bayesian stable isotope mixing models. Environmetrics, 24(6):387–399, 2013.

simmr\_data\_1

Andrew C Parnell, Richard Inger, Stuart Bearhop, and Andrew L Jackson. Source partitioning using stable isotopes: coping with too much variation. PLoS ONE, 5(3):5, 2010.

# **Examples**

```
# A first example with 2 tracers (isotopes), 10 observations, and 4 food sources
data(geese_data_day1)
simmr_in <- with(</pre>
  geese_data_day1,
  simmr_load(
    mixtures = mixtures,
    source_names = source_names,
    source_means = source_means,
    source_sds = source_sds,
    correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# Plot
plot(simmr_in)
# MCMC run
simmr_out <- simmr_mcmc(simmr_in)</pre>
# Check convergence - values should all be close to 1
summary(simmr_out, type = "diagnostics")
# Look at output
summary(simmr_out, type = "statistics")
# Look at influence of priors
prior_viz(simmr_out)
# Plot output
plot(simmr_out, type = "histogram")
```

simmr\_data\_1

A simple fake stable isotope mixing data set

#### **Description**

A simple fake data set with 10 observations on 2 isotopes, with 4 sources, and with corrections/trophic enrichment factors (TEFs or TDFs), and concentration dependence means

# Usage

```
simmr_data_1
```

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#### **Format**

A list with the following elements

mixtures A two column matrix containing delta 13C and delta 15N values respectively

source\_names A character vector of the food source names

tracer\_names A character vector of the tracer names (d13C and d15N)

**source\_means** A matrix of source mean values for the tracers in the same order as mixtures above

source\_sds A matrix of source sd values for the tracers in the same order as mixtures above

correction\_means A matrix of TEFs mean values for the tracers in the same order as mixtures above

correction\_sds A matrix of TEFs sd values for the tracers in the same order as mixtures above concentration\_means A matrix of concentration dependence mean values for the tracers in the same order as mixtures above ...

@seealso simmr\_mcmc for an example where it is used

simmr\_data\_2

A 3-isotope fake stable isotope mixing data set

#### **Description**

A fake data set with 30 observations on 3 isotopes, with 4 sources, and with corrections/trophic enrichment factors (TEFs or TDFs), and concentration dependence means

# Usage

simmr\_data\_2

#### **Format**

A list with the following elements

**mixtures** A three column matrix containing delta 13C, delta 15N, and delta 34S values respectively **source\_names** A character vector of the food source names

tracer\_names A character vector of the tracer names (d13C, d15N, d34S)

source\_means A matrix of source mean values for the tracers in the same order as mixtures above
source\_sds A matrix of source sd values for the tracers in the same order as mixtures above

**correction\_means** A matrix of TEFs mean values for the tracers in the same order as mixtures above

correction\_sds A matrix of TEFs sd values for the tracers in the same order as mixtures above concentration\_means A matrix of concentration dependence mean values for the tracers in the same order as mixtures above ...

@seealso simmr\_mcmc for an example where it is used

simmr\_elicit 21

simmr_elicit Function to allow informative prior distribution to be incl simmr	luded in	
-----------------------------------------------------------------------------------	----------	--

# **Description**

The main simmr\_mcmc function allows for a prior distribution to be set for the dietary proportions. The prior distribution is specified by transforming the dietary proportions using the centralised log ratio (CLR). The simmr\_elicit and simmr\_elicit functions allows the user to specify prior means and standard deviations for each of the dietary proportions, and then finds CLR-transformed values suitable for input into simmr\_mcmc.

## Usage

```
simmr_elicit(
  n_sources,
  proportion_means = rep(1/n_sources, n_sources),
  proportion_sds = rep(0.1, n_sources),
  n_sims = 1000
)
```

#### **Arguments**

n\_sources

The number of sources required

proportion\_means

The desired prior proportion means. These should sum to 1. Should be a vector of length n\_sources

proportion\_sds

The desired prior proportions standard deviations. These have no restricted sum but should be reasonable estimates for a proportion.

n\_sims

The number of simulations for which to run the optimisation routine.

## Details

The function takes the desired proportion means and standard deviations, and fits an optimised least squares to the means and standard deviations in turn to produced CLR-transformed estimates for use in simmr\_mcmc. Using prior information in SIMMs is highly desirable given the restricted nature of the inference. The prior information might come from previous studies, other experiments, or other observations of e.g. animal behaviour.

Due to the nature of the restricted space over which the dietary proportions can span, and the fact that this function uses numerical optimisation, the procedure will not match the target dietary proportion means and standard deviations exactly. If this problem is severe, try increasing the n\_sims value.

#### Value

A list object with two components

mean The best estimates of the mean to use in control.prior in simmr\_mcmc

sd The best estimates of the standard deviations to use in control.prior in simmr\_mcmc

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## Author(s)

Andrew Parnell <andrew.parnell@mu.ie>

```
# Data set: 10 observations, 2 tracers, 4 sources
data(geese_data_day1)
simmr_1 <- with(
  geese_data_day1,
  simmr_load(
   mixtures = mixtures,
   source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
# Look at the prior influence
prior_viz(simmr_1_out)
# Summary
summary(simmr_1_out, "quantiles")
# A bit vague:
            2.5% 25% 50% 75% 97.5%
# Source A 0.029 0.115 0.203 0.312 0.498
# Source B 0.146 0.232 0.284 0.338 0.453
# Source C 0.216 0.255 0.275 0.296 0.342
# Source D 0.032 0.123 0.205 0.299 0.465
# Now suppose I had prior information that:
# proportion means = 0.5, 0.2, 0.2, 0.1
\# proportion sds = 0.08,0.02,0.01,0.02
prior <- simmr_elicit(4, c(0.5, 0.2, 0.2, 0.1), c(0.08, 0.02, 0.01, 0.02))
simmr_1a_out <- simmr_mcmc(simmr_1, prior_control =</pre>
list(means = prior$mean,
      sd = prior$sd,
      sigma_shape = c(3,3),
      sigma_rate = c(3/50, 3/50))
#' # Look at the prior influence now
prior_viz(simmr_1a_out)
summary(simmr_1a_out, "quantiles")
# Much more precise:
          2.5% 25% 50% 75% 97.5%
```

```
# Source A 0.441 0.494 0.523 0.553 0.610
# Source B 0.144 0.173 0.188 0.204 0.236
# Source C 0.160 0.183 0.196 0.207 0.228
# Source D 0.060 0.079 0.091 0.105 0.135
```

simmr\_ffvb

Run a simmr\_input object through the Fixed Form Variational Bayes(FFVB) function

# **Description**

This is the main function of simmr. It takes a simmr\_input object created via simmr\_load, runs it in fixed form Variational Bayes to determine the dietary proportions, and then outputs a simmr\_output object for further analysis and plotting via summary.simmr\_output and plot.simmr\_output.

# Usage

```
simmr_ffvb(
    simmr_in,
    prior_control = list(mu_0 = rep(0, simmr_in$n_sources), sigma_0 = 1),
    ffvb_control = list(n_output = 3600, S = 100, P = 10, beta_1 = 0.9, beta_2 = 0.9, tau =
    100, eps_0 = 0.0225, t_W = 50)
)
```

#### **Arguments**

simmr\_in An object created via the function simmr\_load

prior\_control A list of values including arguments named mu\_0 (prior for mu), and sigma\_0

(prior for sigma).

ffvb\_control A list of values including arguments named n\_output (number of rows in theta

output), S (number of samples taken at each iteration of the algorithm), P (patience parameter), beta\_1 and beta\_2 (adaptive learning weights), tau (threshold for exploring learning space), eps\_0 (fixed learning rate), t\_W (rolling win-

dow size)

#### Value

An object of class simmr\_output with two named top-level components:

input The simmr\_input object given to the simmr\_ffvb function

output A set of outputs produced by the FFVB function. These can be analysed using

the summary.simmr\_output and plot.simmr\_output functions.

# Author(s)

Andrew Parnell <andrew.parnell@mu.ie>, Emma Govan

## References

Andrew C. Parnell, Donald L. Phillips, Stuart Bearhop, Brice X. Semmens, Eric J. Ward, Jonathan W. Moore, Andrew L. Jackson, Jonathan Grey, David J. Kelly, and Richard Inger. Bayesian stable isotope mixing models. Environmetrics, 24(6):387–399, 2013.

Andrew C Parnell, Richard Inger, Stuart Bearhop, and Andrew L Jackson. Source partitioning using stable isotopes: coping with too much variation. PLoS ONE, 5(3):5, 2010.

## See Also

simmr\_load for creating objects suitable for this function, plot.simmr\_input for creating isospace
plots, summary.simmr\_output for summarising output, and plot.simmr\_output for plotting output.

```
## Not run:
## See the package vignette for a detailed run through of these 4 examples
# Data set 1: 10 obs on 2 isos, 4 sources, with tefs and concdep
data(geese_data_day1)
simmr_1 <- with(
 geese_data_day1,
 simmr_load(
   mixtures = mixtures,
   source_names = source_names,
    source_means = source_means,
    source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
    concentration_means = concentration_means
)
# Plot
plot(simmr_1)
# Print
simmr_1
# FFVB run
simmr_1_out <- simmr_ffvb(simmr_1)</pre>
# Print it
print(simmr_1_out)
# Summary
summary(simmr_1_out, type = "correlations")
summary(simmr_1_out, type = "statistics")
ans <- summary(simmr_1_out, type = c("quantiles", "statistics"))</pre>
# Plot
```

```
plot(simmr_1_out, type = "boxplot")
plot(simmr_1_out, type = "histogram")
plot(simmr_1_out, type = "density")
plot(simmr_1_out, type = "matrix")
# Compare two sources
compare_sources(simmr_1_out, source_names = c("Zostera", "Enteromorpha"))
# Compare multiple sources
compare_sources(simmr_1_out)
# A version with just one observation
data(geese_data_day1)
simmr_2 <- with(
 geese_data_day1,
 simmr_load(
   mixtures = mixtures[1, , drop = FALSE],
   source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
   concentration_means = concentration_means
)
# Plot
plot(simmr_2)
# FFVB run - automatically detects the single observation
simmr_2_out <- simmr_ffvb(simmr_2)</pre>
# Print it
print(simmr_2_out)
# Summary
summary(simmr_2_out)
ans <- summary(simmr_2_out, type = c("quantiles"))</pre>
# Plot
plot(simmr_2_out)
plot(simmr_2_out, type = "boxplot")
plot(simmr_2_out, type = "histogram")
plot(simmr_2_out, type = "density")
plot(simmr_2_out, type = "matrix")
# Data set 2: 3 isotopes (d13C, d15N and d34S), 30 observations, 4 sources
data(simmr_data_2)
simmr_3 <- with(
```

```
simmr_data_2,
 simmr_load(
   mixtures = mixtures,
   source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
   concentration_means = concentration_means
)
# Get summary
print(simmr_3)
# Plot 3 times
plot(simmr_3)
plot(simmr_3, tracers = c(2, 3))
plot(simmr_3, tracers = c(1, 3))
# See vignette('simmr') for fancier axis labels
# FFVB run
simmr_3_out <- simmr_ffvb(simmr_3)</pre>
# Print it
print(simmr_3_out)
# Summary
summary(simmr_3_out)
summary(simmr_3_out, type = "quantiles")
summary(simmr_3_out, type = "correlations")
# Plot
plot(simmr_3_out)
plot(simmr_3_out, type = "boxplot")
plot(simmr_3_out, type = "histogram")
plot(simmr_3_out, type = "density")
plot(simmr_3_out, type = "matrix")
# Data set 5 - Multiple groups Geese data from Inger et al 2006
# Do this in raw data format - Note that there's quite a few mixtures!
data(geese_data)
simmr_5 <- with(
 geese_data,
 simmr_load(
   mixtures = mixtures,
   source_names = source_names,
   source_means = source_means,
    source_sds = source_sds,
   correction_means = correction_means,
```

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```
correction_sds = correction_sds,
   concentration_means = concentration_means,
   group = groups
 )
)
# Plot
plot(simmr_5,
 xlab = expression(paste(delta^13, "C (per mille)", sep = "")),
 ylab = expression(paste(delta^15, "N (per mille)", sep = "")),
 title = "Isospace plot of Inger et al Geese data"
# Run MCMC for each group
simmr_5_out <- simmr_ffvb(simmr_5)</pre>
# Summarise output
summary(simmr_5_out, type = "quantiles", group = 1)
summary(simmr_5_out, type = "quantiles", group = c(1, 3))
summary(simmr_5_out, type = c("quantiles", "statistics"), group = c(1, 3))
# Plot - only a single group allowed
plot(simmr_5_out, type = "boxplot", group = 2, title = "simmr output group 2")
plot(simmr_5_out, type = c("density", "matrix"), grp = 6, title = "simmr output group 6")
# Compare sources within a group
compare_sources(simmr_5_out, source_names = c("Zostera", "U.lactuca"), group = 2)
compare_sources(simmr_5_out, group = 2)
# Compare between groups
compare_groups(simmr_5_out, source = "Zostera", groups = 1:2)
compare_groups(simmr_5_out, source = "Zostera", groups = 1:3)
compare_groups(simmr_5_out, source = "U.lactuca", groups = c(4:5, 7, 2))
## End(Not run)
```

simmr\_load

Function to load in simmr data and check for errors

# Description

This function takes in the mixture data, food source means and standard deviations, and (optionally) correction factor means and standard deviations, and concentration proportions. It performs some (non-exhaustive) checking of the data to make sure it will run through simmr. It outputs an object of class simmr\_input.

# Usage

```
simmr_load(
```

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```
mixtures,
  source_names,
  source_means,
  source_sds,
  correction_means = NULL,
  correction_sds = NULL,
  concentration_means = NULL,
  group = NULL
```

## **Arguments**

mixtures The mixture data given as a matrix where the number of rows is the number

of observations and the number of columns is the number of tracers (usually

isotopes)

source\_names The names of the sources given as a character string

source\_means The means of the source values, given as a matrix where the number of rows is

the number of sources and the number of columns is the number of tracers

source\_sds The standard deviations of the source values, given as a matrix where the number

of rows is the number of sources and the number of columns is the number of

tracers

correction\_means

The means of the correction values, given as a matrix where the number of rows is the number of sources and the number of columns is the number of tracers. If

not provided these are set to 0.

correction\_sds The standard deviations of the correction values, given as a matrix where the

number of rows is the number of sources and the number of columns is the

number of tracers. If not provided these are set to 0.

concentration\_means

The means of the concentration values, given as a matrix where the number of rows is the number of sources and the number of columns is the number of tracers. These should be between 0 and 1. If not provided these are all set to 1.

group A grouping variable. These can be a character or factor variable

#### **Details**

For standard stable isotope mixture modelling, the mixture matrix will contain a row for each individual and a column for each isotopic value. simmr will allow for any number of isotopes and any number of observations, within computational limits. The source means/sds should be provided for each food source on each isotope. The correction means (usually trophic enrichment factors) can be set as zero if required, and should be of the same shape as the source values. The concentration dependence means should be estimated values of the proportion of each element in the food source in question and should be given in proportion format between 0 and 1. At present there is no means to include concentration standard deviations.

## Value

An object of class simmr\_input with the following elements:

simmr\_load 29

mixtures The mixture data source\_neams Source means

sources\_sds Source standard deviations

correction\_means

Correction means

correction\_sds Correction standard deviations

concentration\_means

Concentration dependence means

n\_obs The number of observations

n\_tracers The number of tracers/isotopes

n\_sources The number of sources
n\_groups The number of groups

# Author(s)

Andrew Parnell <andrew.parnell@mu.ie>

#### See Also

See simmr\_mcmc for complete examples.

```
# A simple example with 10 observations, 2 tracers and 4 sources
data(geese_data_day1)
simmr_1 <- with(
    geese_data_day1,
    simmr_load(
        mixtures = mixtures,
        source_names = source_names,
        source_means = source_means,
        source_sds = source_sds,
        correction_means = correction_means,
        correction_sds = correction_sds,
        concentration_means = concentration_means
)
)
print(simmr_1)</pre>
```

simmr_mcmc	Run a simmr_input object through the main simmr Markov chain
	Monte Carlo (MCMC) function

# **Description**

This is the main function of simmr. It takes a simmr\_input object created via simmr\_load, runs an MCMC to determine the dietary proportions, and then outputs a simmr\_output object for further analysis and plotting via summary.simmr\_output and plot.simmr\_output.

## Usage

```
simmr_mcmc(
  simmr_in,
  prior_control = list(means = rep(0, simmr_in$n_sources), sd = rep(1,
    simmr_in$n_sources), sigma_shape = rep(3, simmr_in$n_tracers), sigma_rate = rep(3/50,
    simmr_in$n_tracers)),
  mcmc_control = list(iter = 10000, burn = 1000, thin = 10, n.chain = 4)
)
```

## **Arguments**

simmr\_in An object created via the function simmr\_load

prior\_control A list of values including arguments named: means and sd which represent the

prior means and standard deviations of the dietary proportions in centralised log-ratio space; shape and rate which represent the prior distribution on the residual standard deviation. These can usually be left at their default values unless you wish to include to include prior information, in which case you should

use the function simmr\_elicit.

mcmc\_control A list of values including arguments named iter (number of iterations), burn

(size of burn-in), thin (amount of thinning), and n. chain (number of MCMC

chains).

#### **Details**

If, after running simmr\_mcmc the convergence diagnostics in summary.simmr\_output are not satisfactory, the values of iter, burn and thin in mcmc\_control should be increased by a factor of 10.

# Value

An object of class simmr\_output with two named top-level components:

input The simmr\_input object given to the simmr\_mcmc function

output A set of MCMC chains of class mcmc.list from the coda package. These can

be analysed using the summary.simmr\_output and plot.simmr\_output func-

tions.

#### Author(s)

Andrew Parnell <andrew.parnell@mu.ie>

#### References

Andrew C. Parnell, Donald L. Phillips, Stuart Bearhop, Brice X. Semmens, Eric J. Ward, Jonathan W. Moore, Andrew L. Jackson, Jonathan Grey, David J. Kelly, and Richard Inger. Bayesian stable isotope mixing models. Environmetrics, 24(6):387–399, 2013.

Andrew C Parnell, Richard Inger, Stuart Bearhop, and Andrew L Jackson. Source partitioning using stable isotopes: coping with too much variation. PLoS ONE, 5(3):5, 2010.

## See Also

simmr\_load for creating objects suitable for this function, plot.simmr\_input for creating isospace
plots, summary.simmr\_output for summarising output, and plot.simmr\_output for plotting output.

```
## See the package vignette for a detailed run through of these 4 examples
# Data set 1: 10 obs on 2 isos, 4 sources, with tefs and concdep
data(geese_data_day1)
simmr_1 <- with(
  geese_data_day1,
  simmr_load(
   mixtures = mixtures,
   source_names = source_names,
   source_means = source_means,
    source_sds = source_sds,
    correction_means = correction_means,
    correction_sds = correction_sds,
    concentration_means = concentration_means
  )
)
# Plot
plot(simmr_1)
# Print
simmr_1
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
# Print it
print(simmr_1_out)
# Summary
summary(simmr_1_out, type = "diagnostics")
```

```
summary(simmr_1_out, type = "correlations")
summary(simmr_1_out, type = "statistics")
ans <- summary(simmr_1_out, type = c("quantiles", "statistics"))</pre>
# Plot
plot(simmr_1_out, type = "boxplot")
plot(simmr_1_out, type = "histogram")
plot(simmr_1_out, type = "density")
plot(simmr_1_out, type = "matrix")
# Compare two sources
\verb|compare_sources(simmr_1_out, source_names = c("Zostera", "Enteromorpha"))| \\
# Compare multiple sources
compare_sources(simmr_1_out)
# A version with just one observation
data(geese_data_day1)
simmr_2 <- with(
 geese_data_day1,
 simmr_load(
   mixtures = mixtures[1, , drop = FALSE],
   source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
   concentration_means = concentration_means
 )
)
# Plot
plot(simmr_2)
# MCMC run - automatically detects the single observation
simmr_2_out <- simmr_mcmc(simmr_2)</pre>
# Print it
print(simmr_2_out)
# Summary
summary(simmr_2_out)
summary(simmr_2_out, type = "diagnostics")
ans <- summary(simmr_2_out, type = c("quantiles"))</pre>
# Plot
plot(simmr_2_out)
plot(simmr_2_out, type = "boxplot")
plot(simmr_2_out, type = "histogram")
plot(simmr_2_out, type = "density")
plot(simmr_2_out, type = "matrix")
```

```
# Data set 2: 3 isotopes (d13C, d15N and d34S), 30 observations, 4 sources
data(simmr_data_2)
simmr_3 <- with(
 simmr_data_2,
 simmr_load(
   mixtures = mixtures,
   source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
   concentration_means = concentration_means
 )
)
# Get summary
print(simmr_3)
# Plot 3 times
plot(simmr_3)
plot(simmr_3, tracers = c(2, 3))
plot(simmr_3, tracers = c(1, 3))
# See vignette('simmr') for fancier axis labels
# MCMC run
simmr_3_out <- simmr_mcmc(simmr_3)</pre>
# Print it
print(simmr_3_out)
# Summary
summary(simmr_3_out)
summary(simmr_3_out, type = "diagnostics")
summary(simmr_3_out, type = "quantiles")
summary(simmr_3_out, type = "correlations")
# Plot
plot(simmr_3_out)
plot(simmr_3_out, type = "boxplot")
plot(simmr_3_out, type = "histogram")
plot(simmr_3_out, type = "density")
plot(simmr_3_out, type = "matrix")
# Data set 5 - Multiple groups Geese data from Inger et al 2006
# Do this in raw data format - Note that there's quite a few mixtures!
data(geese_data)
simmr_5 <- with(
```

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```
geese_data,
 simmr_load(
   mixtures = mixtures,
    source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
   concentration_means = concentration_means,
    group = groups
)
# Plot
plot(simmr_5,
 xlab = expression(paste(delta^13, "C (per mille)", sep = "")),
 ylab = expression(paste(delta^15, "N (per mille)", sep = "")),
 title = "Isospace plot of Inger et al Geese data"
)
# Run MCMC for each group
simmr_5_out <- simmr_mcmc(simmr_5)</pre>
# Summarise output
summary(simmr_5_out, type = "quantiles", group = 1)
summary(simmr_5_out, type = "quantiles", group = c(1, 3))
summary(simmr_5_out, type = c("quantiles", "statistics"), group = c(1, 3))
# Plot - only a single group allowed
plot(simmr_5_out, type = "boxplot", group = 2, title = "simmr output group 2")
plot(simmr_5_out, type = c("density", "matrix"), grp = 6, title = "simmr output group 6")
# Compare sources within a group
compare_sources(simmr_5_out, source_names = c("Zostera", "U.lactuca"), group = 2)
compare_sources(simmr_5_out, group = 2)
# Compare between groups
compare_groups(simmr_5_out, source = "Zostera", groups = 1:2)
compare_groups(simmr_5_out, source = "Zostera", groups = 1:3)
compare_groups(simmr_5_out, source = "U.lactuca", groups = c(4:5, 7, 2))
## End(Not run)
```

square\_data

An artificial data set used to indicate effect of priors

## **Description**

A fake box data set identified by Fry (2014) as a failing of SIMMs See the link for more interpretation of these data and the output

summary.simmr\_output 35

## Usage

```
square_data
```

#### **Format**

A list with the following elements

mixtures A two column matrix containing delta 13C and delta 15N values respectively

source\_names A character vector of the food source names

tracer\_names A character vector of the tracer names (d13C, d15N)

source\_means A matrix of source mean values for the tracers in the same order as mixtures above

source\_sds A matrix of source sd values for the tracers in the same order as mixtures above

**correction\_means** A matrix of TEFs mean values for the tracers in the same order as mixtures above

correction\_sds A matrix of TEFs sd values for the tracers in the same order as mixtures above concentration\_means A matrix of concentration dependence mean values for the tracers in the same order as mixtures above ...

@seealso simmr\_mcmc for an example where it is used

#### **Source**

```
<doi:10.3354/meps10535>
```

summary.simmr\_output Summarises the output created with simmr\_mcmc or simmr\_ffvb

# Description

Produces textual summaries and convergence diagnostics for an object created with simmr\_mcmc or simmr\_ffvb. The different options are: 'diagnostics' which produces Brooks-Gelman-Rubin diagnostics to assess MCMC convergence, 'quantiles' which produces credible intervals for the parameters, 'statistics' which produces means and standard deviations, and 'correlations' which produces correlations between the parameters.

## Usage

```
## S3 method for class 'simmr_output'
summary(
  object,
  type = c("diagnostics", "quantiles", "statistics", "correlations"),
  group = 1,
  ...
)
```

# **Arguments**

object	An object of class simmr_output produced by the function $simmr\_mcmc$ or $simmr\_ffvb$
type	The type of output required. At least none of 'diagnostics', 'quantiles', 'statistics', or 'correlations'.
group	Which group or groups the output is required for.
	Not used

#### **Details**

The quantile output allows easy calculation of 95 per cent credible intervals of the posterior dietary proportions. The correlations, along with the matrix plot in plot.simmr\_output allow the user to judge which sources are non-identifiable. The Gelman diagnostic values should be close to 1 to ensure satisfactory convergence.

When multiple groups are included, the output automatically includes the results for all groups.

#### Value

A list containing the following components:

gelman The convergence diagnostics
quantiles The quantiles of each parameter from the posterior distribution
statistics The means and standard deviations of each parameter
correlations The posterior correlations between the parameters

Note that this object is reported silently so will be discarded unless the function is called with an object as in the example below.

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## See Also

See simmr\_mcmc and simmr\_ffvbfor creating objects suitable for this function, and many more examples. See also simmr\_load for creating simmr objects, plot.simmr\_input for creating isospace plots, plot.simmr\_output for plotting output.

```
# A simple example with 10 observations, 2 tracers and 4 sources
# The data
data(geese_data_day1)
simmr_1 <- with(
   geese_data_day1,
   simmr_load(
      mixtures = mixtures,</pre>
```

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```
source_names = source_names,
   source_means = source_means,
   source_sds = source_sds,
   correction_means = correction_means,
   correction_sds = correction_sds,
   concentration_means = concentration_means
  )
)
# Plot
plot(simmr_1)
# MCMC run
simmr_1_out <- simmr_mcmc(simmr_1)</pre>
# Summarise
summary(simmr_1_out) # This outputs all the summaries
summary(simmr_1_out, type = "diagnostics") # Just the diagnostics
# Store the output in an
ans <- summary(simmr_1_out,</pre>
  type = c("quantiles", "statistics")
```

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