# Package 'biogrowth'

August 19, 2023

Type Package
Title Modelling of Population Growth
Version 1.0.3
<b>Description</b> Modelling of population growth under static and dynamic environmental conditions. Includes functions for model fitting and making prediction under isothermal and dynamic conditions. The methods (algorithms & models) are based on predictive microbiology (See Perez-Rodriguez and Valero (2012, ISBN:978-1-4614-5519-6)).
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approx_env

calculate_gammas_secondary check_growth_guess check_primary_pars check_secondary_pars check_secondary_pars check_stochastic_pars compare_growth_fits comditions_pH_temperature CPM_model dBaranyi distribution_to_logcount DynamicGrowth example_cardinal example_dynamic_growth example_env_conditions extract_primary_pars extract_secondary_pars FitDynamicGrowth FitDynamicGrowth FitDynamicGrowth FitMultipleDynamicGrowth FitMultipleDynamicGrowth FitMultipleDynamicGrowth fit_growth fit_growth fit_growth fit_growth fit_moultiple_growth fit_multiple_growth fit_multiple_gr	ors	
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multiple_experiments
predictMCMC92
predict_dynamic_growth
predict_growth
predict_growth_uncertainty
predict_isothermal_growth
predict_MCMC_growth
predict_stochastic_growth
primary_model_data
Q0_to_lambda
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SecondaryComparison
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4 arabian\_tractors

approx_env	Generates functions for linear interpolation of environmental conditions

# Description

Generates functions for linear interpolation of environmental conditions

### Usage

```
approx_env(env_conditions)
```

# Arguments

env\_conditions A tibble describing the variation of the environmental conditions through the storage time. Must contain a column named time and as many additional columns

as environmental factors.

#### Value

A list of functions that return the value of each environmental condition for some storage time

arabian\_tractors

Number of tractors in the Arab World according to the World Bank

# Description

A dataset showing the increase in tractors in the Arab World. It was retrieved from https://data.worldbank.org/indicator/AG.Al

# Usage

```
arabian_tractors
```

## **Format**

A tibble with 40 rows (each corresponding to one year) and 7 columns:

year Year for the recording

tractors Number of tractors

calculate\_gammas 5

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calculate gammas	Calcui
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Calculates every gamma factor

#### **Description**

A helper function for predict\_dynamic\_growth() that calculates the value of every gamma factor corresponding to some storage time.

# Usage

```
calculate_gammas(this_t, env_func, sec_models)
```

#### **Arguments**

this\_t Storage time

env\_func A list of functions (generated using approxfun) that give the value of each en-

vironmental function for some storage time.

sec\_models A nested list describing the secondary models.

#### Value

A vector of gamma factors (one per environmental factor).

```
calculate_gammas_secondary
```

Gamma factors for fitting secondary models

## **Description**

A helper for fitting the secondary gamma models. Calculates the gamma factors corresponding to the models defined and the experimental conditions. In order for it to work, the environmental factors must be named identically in the 3 arguments.

#### **Usage**

```
calculate_gammas_secondary(sec_model_names, my_data, secondary_models)
```

# **Arguments**

sec\_model\_names

named character vector defining the type of secondary model. Its names correspond to the environmental conditions and its values define the corresponding

type of secondary model.

my\_data Tibble of experimental conditions.

secondary\_models

A list defining the parameters of the secondary models.

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# Value

a numeric vector of length nrow(my\_data) with the gamma factor for each experimental condition.

check\_growth\_guess

Visual check of an initial guess of the model parameters

# Description

# [Stable]

Generates a plot comparing a set of data points against the model prediction corresponding to an initial guess of the model parameters

# Usage

```
check_growth_guess(
  fit_data,
  model_keys,
  guess,
  environment = "constant",
  env_conditions = NULL,
  approach = "single",
  logbase_mu = 10,
  formula = logN ~ time
)
```

# Arguments

fit_data	Tibble (or data.frame) of data for the fit. It must have two columns, one with the elapsed time (time by default) and another one with the decimal logarithm of the population size (logN by default). Different column names can be defined using the formula argument.
model_keys	Named the equations of the secondary model as in fit_growth()
guess	Named vector with the initial guess of the model parameters as in $fit\_growth()$
environment	type of environment. Either "constant" (default) or "dynamic" (see below for details on the calculations for each condition) $\frac{1}{2}$
env_conditions	Tibble describing the variation of the environmental conditions for dynamic experiments. See fit_growth(). Ignored when environment = "constant"
approach	whether "single" (default) or "global". Please see fit_growth() for details."
logbase_mu	Base of the logarithm the growth rate is referred to. By default, 10 (i.e. $\log 10$ ). See vignette about units for details.
formula	an object of class "formula" describing the $x$ and $y$ variables. $logN \sim time$ as a default.

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#### Value

A ggplot() comparing the model prediction against the data

# **Examples**

```
## Examples under constant environmental conditions ------
## We need some data
my_data <- data.frame(time = 0:9,
                     logN = c(2, 2.1, 1.8, 2.5, 3.1, 3.4, 4, 4.5, 4.8, 4.7)
## We can directly plot the comparison for some values
check_growth_guess(my_data, list(primary = "modGompertz"),
                  c(logN0 = 1.5, mu = .8, lambda = 4, C = 3)
## Ot it can be combined with the automatic initial guess
check_growth_guess(my_data, list(primary = "modGompertz"),
                  make_guess_primary(my_data, "modGompertz")
## Examples under dynamic environmental conditions ------
## We will use the datasets included in the package
data("example_dynamic_growth")
data("example_env_conditions")
## Model equations are assigned as in fit_growth
sec_models <- list(temperature = "CPM", aw = "CPM")</pre>
## Guesses of model parameters are also defined as in fit_growth
guess \leftarrow list(Nmax = 1e4,
             N0 = 1e0, Q0 = 1e-3,
             mu_opt = 4,
             temperature_n = 1,
             aw_xmax = 1, aw_xmin = .9, aw_n = 1,
             temperature_xmin = 25, temperature_xopt = 35,
             temperature_xmax = 40, aw_xopt = .95
## We can now check our initial guess
check_growth_guess(example_dynamic_growth, sec_models, guess,
                   "dynamic",
```

example\_env\_conditions)

check\_primary\_pars

Basic check of parameters for primary models

# **Description**

Checks that: the model name is correct, the right number of model parameters have been defined and that the parameters have the right names

## Usage

```
check_primary_pars(model_name, pars)
```

## **Arguments**

model\_name

Model identifier

pars

A named list of model parameters

#### Value

If there is no error, the model function.

check\_secondary\_pars Basic checks of secondary parameters

# **Description**

Checks that the model names are correct, that no parameter is defined twice, that every parameter is defined and that no unknown parameter has been defined. Raises an error if any of these conditions is not met.

```
check_secondary_pars(
  starting_point,
  known_pars,
  sec_model_names,
  primary_pars = "mu_opt"
)
```

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# **Arguments**

starting\_point Named vector with initial values for the model parameters to estimate from the

data. The growth rate under optimum conditions must be named mu\_opt. The rest must be called 'env\_factor'+'\_'+'parameter'. For instance, the minimum

pH for growth is 'pH\_xmin'.

known\_pars Named vector of fixed model parameters. Must be named using the same con-

vention as starting\_point.

sec\_model\_names

Named character vector defining the secondary model for each environmental

factor.

primary\_pars Character vector with the parameter names of the primary model.

check\_stochastic\_pars Model definition checks for predict\_stochastic\_growth

#### Description

Does several checks of the model parameters. Besides those by check\_primary\_pars, it checks that corr\_matrix is square, that pars and corr\_matrix have compatible dimensions, and that pars has the correct names.

### Usage

```
check_stochastic_pars(model_name, pars, corr_matrix)
```

#### **Arguments**

model\_name Character describing the primary growth model.

pars A tibble describing the parameter uncertainty (see details).

corr\_matrix Correlation matrix of the model parameters. Defined in the same order as in

pars. An identity matrix by default (uncorrelated parameters).

 ${\tt compare\_growth\_fits} \qquad {\tt \textit{Model comparison and selection for growth models}}$ 

# Description

#### [Experimental]

This function is a constructor for GrowthComparison or GlobalGrowthComparison, a class that provides several functions for model comparison and model selection for growth models fitted using fit\_growth(). Please see the help pages for GrowthComparison or GlobalGrowthComparison for further details.

Although it is not necessary, we recommend passing the models as a named list, as these names will later be kept in plots and tables.

#### Usage

```
compare_growth_fits(models)
```

#### **Arguments**

models

a (we recommend named) list of models fitted using fit\_growth(). Every model should be of the same class. Otherwise, some functions may give unexpected results.

#### **Examples**

```
## Example 1 - Fitting under static environmental conditions -------
## We will use the data on growth of Salmonella included in the package
data("growth_salmonella")
## We will fit 3 different models to the data
fit1 <- fit_growth(growth_salmonella,</pre>
                   list(primary = "Baranyi"),
                   start = c(lambda = 0, logNmax = 8, mu = .1, logN0 = 2),
                   known = c(),
                   environment = "constant",
fit2 <- fit_growth(growth_salmonella,</pre>
                   list(primary = "Baranyi"),
                   start = c(logNmax = 8, mu = .1, logN0 = 2),
                   known = c(lambda = 0),
                   environment = "constant",
                   )
fit3 <- fit_growth(growth_salmonella,</pre>
                   list(primary = "modGompertz"),
                   start = c(C = 8, mu = .1, logN0 = 2),
                   known = c(lambda = 0),
                   environment = "constant",
## We can now put them in a (preferably named) list
my_models <- list(`Baranyi` = fit1,</pre>
                  'Baranyi no lag' = fit2,
                  'Gompertz no lag' = fit3)
## And pass them to compare_growth_fits
model_comparison <- compare_growth_fits(my_models)</pre>
## The instance of GrowthComparison has useful S3 methods
```

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```
print(model_comparison)
plot(model_comparison)
plot(model_comparison, type = 2)
plot(model_comparison, type = 3)
## The statistical indexes can be accessed through summary and coef
summary(model_comparison)
coef(model_comparison)
## Example 2 - Fitting under dynamic environmental conditions ------
## We will use one of the example datasets
data("example_dynamic_growth")
data("example_env_conditions")
## First model fitted
sec_models <- list(temperature = "CPM", aw = "CPM")</pre>
known_pars <- list(Nmax = 1e4,</pre>
                   N0 = 1e0, Q0 = 1e-3,
                   mu_opt = 4,
                   temperature_n = 1,
                   aw_xmax = 1, aw_xmin = .9, aw_n = 1
my_start <- list(temperature_xmin = 25, temperature_xopt = 35,</pre>
                 temperature_xmax = 40, aw_xopt = .95)
dynamic_fit <- fit_growth(example_dynamic_growth,</pre>
                           sec_models,
                           my_start, known_pars,
                           environment = "dynamic",
                           env_conditions = example_env_conditions
## Second model (different secondary model for temperature)
sec_models <- list(temperature = "Zwietering", aw = "CPM")</pre>
known_pars <- list(Nmax = 1e4,</pre>
                   N0 = 1e0, Q0 = 1e-3,
                   mu_opt = 4,
                   temperature_n = 1,
                   aw_xmax = 1, aw_xmin = .9, aw_n = 1
my_start <- list(temperature_xmin = 25, temperature_xopt = 35,</pre>
                 aw\_xopt = .95)
```

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```
dynamic_fit2 <- fit_growth(example_dynamic_growth,</pre>
                           sec_models,
                           my_start, known_pars,
                           environment = "dynamic",
                           env_conditions = example_env_conditions
## Once both models have been fitted, we can call the function
dynamic_comparison <- compare_growth_fits(list(m1 = dynamic_fit, m2 = dynamic_fit2))</pre>
## Which also returns an instance of GrowthComparison with the same S3 methods
print(dynamic_comparison)
plot(dynamic_comparison)
plot(dynamic_comparison, type = 2)
plot(dynamic_comparison, type = 3)
## The statistical indexes can be accessed through summary and coef
summary(dynamic_comparison)
coef(dynamic_comparison)
## Example 3 - Global fitting ------
## We use the example data
data("multiple_counts")
data("multiple_conditions")
## We need to fit (at least) two models
sec_models <- list(temperature = "CPM", pH = "CPM")</pre>
known_pars <- list(Nmax = 1e8, N0 = 1e0, Q0 = 1e-3,
                   temperature_n = 2, temperature_xmin = 20,
                   temperature\_xmax = 35,
                   pH_n = 2, pH_xmin = 5.5, pH_xmax = 7.5, pH_xopt = 6.5)
my_start <- list(mu_opt = .8, temperature_xopt = 30)</pre>
global_fit <- fit_growth(multiple_counts,</pre>
                         sec_models,
                         my_start,
                         known_pars,
                         environment = "dynamic",
                         algorithm = "regression",
                         approach = "global",
                         env_conditions = multiple_conditions
```

```
sec_models <- list(temperature = "CPM", pH = "CPM")</pre>
known_pars <- list(Nmax = 1e8, N0 = 1e0, Q0 = 1e-3,
                   temperature_n = 1, temperature_xmin = 20,
                   temperature\_xmax = 35,
                   pH_n = 2, pH_xmin = 5.5, pH_xmax = 7.5, pH_xopt = 6.5)
my_start <- list(mu_opt = .8, temperature_xopt = 30)</pre>
global_fit2 <- fit_growth(multiple_counts,</pre>
                           sec_models,
                           my_start,
                           known_pars,
                           environment = "dynamic",
                           algorithm = "regression",
                           approach = "global",
                           env_conditions = multiple_conditions
## We can now pass both models to the function as a (named) list
global_comparison <- compare_growth_fits(list(`n=2` = global_fit,</pre>
                                                `n=1` = global_fit2)
## The residuals and model fits plots are divided by experiments
plot(global_comparison)
plot(global_comparison, type = 3)
## The remaining S3 methods are the same as before
print(global_comparison)
plot(global_comparison, type = 2)
summary(global_comparison)
coef(global_comparison)
```

compare\_secondary\_fits

Model comparison and selection for secondary growth models

# **Description**

# [Experimental]

This function is a constructor for SecondaryComparison a class that provides several functions for model comparison and model selection for growth models fitted using fit\_secondary\_growth(). Please see the help pages for SecondaryComparison for further details.

Although it is not necessary, we recommend passing the models as a named list, as these names will later be kept in plots and tables.

#### Usage

```
compare_secondary_fits(models)
```

#### **Arguments**

models a (we recommend named) list of models fitted using fit\_secondary\_growth().

#### **Examples**

```
## We first need to fit some models
data("example_cardinal")
sec_model_names <- c(temperature = "Zwietering", pH = "CPM")</pre>
known_pars <- list(mu_opt = 1.2, temperature_n = 1,</pre>
                    pH_n = 2, pH_xmax = 6.8, pH_xmin = 5.2)
my_start <- list(temperature_xmin = 5, temperature_xopt = 35,</pre>
                  pH\_xopt = 6.5)
fit1 <- fit_secondary_growth(example_cardinal, my_start, known_pars, sec_model_names)</pre>
known_pars <- list(mu_opt = 1.2, temperature_n = 2,</pre>
                    pH_n = 2, pH_xmax = 6.8, pH_xmin = 5.2)
 fit2 <- fit_secondary_growth(example_cardinal, my_start, known_pars, sec_model_names)</pre>
 ## We can now pass the models to the constructor
 comparison <- compare_secondary_fits(list(`n=1` = fit1,</pre>
                                             n=2 = fit2)
 ## The function includes several S3 methods for model selection and comparison
 print(comparison)
 plot(comparison)
 plot(comparison, type = 2)
 ## The numerical indexes can be accessed using coef and summary
 coef(comparison)
 summary(comparison)
```

 $conditions\_pH\_temperature$ 

Conditions during a dynamic growth experiment

# **Description**

A dataset to demonstrate the use of fit\_dynamic\_growth. The observations environmental conditions are described in conditions\_pH\_temperature.

# Usage

```
conditions\_pH\_temperature
```

# **Format**

A tibble with 4 rows and 3 columns:

time elapsed timetemperature temperaturepH pH

CPM\_model

Secondary Cardinal Parameter (CPM) model

# Description

Secondary cardinal parameter model as defined by Rosso et al. (1995).

# Usage

```
CPM_model(x, xmin, xopt, xmax, n)
```

# Arguments

X	Value of the environmental factor.
xmin	Minimum value for growth.
xopt	Optimum value for growth.
xmax	Maximum value for growth.
n	Order of the CPM model.

## Value

The corresponding gamma factor.

dBaranyi	Baranyi growth model
ubai aiiyi	Daranyi growin moaci

#### **Description**

Microbial growth model as defined in Baranyi and Roberts (1994). It has been implemented according to the requirements of ode(). For consistency in the function for isothermal growth, calculations are done assuming the user input for mu is in log10 scale. In other words, the input is multiplied by ln(10).

#### Usage

```
dBaranyi(time, state, pars, env_func, sec_models)
```

#### **Arguments**

time numeric vector (length 1) of storage time

state named numeric vector with two components: Q and N

pars named numeric vector of model parameters (Nmax and mu\_opt)

env\_func named list of functions returning the values of the environmental conditions for

time (t)

sec\_models named list of parameters of the secondary model

#### Value

A numeric vector of two components according to the requirements of ode().

```
distribution_to_logcount
```

Distribution of times to reach a certain microbial count

# Description

#### [Superseded]

The function distribution\_to\_logcount() has been superseded by function time\_to\_size(), which provides more general interface.

Returns the probability distribution of the storage time required for the microbial count to reach log\_count according to the predictions of a stochastic model. Calculations are done using linear interpolation of the individual model predictions.

```
distribution_to_logcount(model, log_count)
```

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#### **Arguments**

model An instance of StochasticGrowth or MCMCgrowth. log\_count The target microbial count.

#### Value

An instance of TimeDistribution().

# **Examples**

DynamicGrowth

 $Dynamic Growth\ class$ 

# **Description**

#### [Superseded]

The class DynamicGrowth has been superseded by the top-level class GrowthPrediction, which provides a unified approach for growth modelling.

Still, it is returned if the superseded predict\_dynamic\_growth() is called.

A subclass of list with items:

- simulation: A tibble with the model prediction
- gammas: A tibble with the value of each gamma factor for each value of times.
- env\_conditions: A list of functions interpolating the environmental conditions.
- primary\_pars: A list with the model parameters of the primary model.
- sec\_models: A nested list defining the secondary models.

DynamicGrowth

# Usage

```
## S3 method for class 'DynamicGrowth'
print(x, ...)
## S3 method for class 'DynamicGrowth'
plot(
 х,
 y = NULL,
 add_factor = NULL,
 ylims = NULL,
  label_y1 = "logN",
  label_y2 = add_factor,
 line_col = "black",
  line_size = 1,
  line_type = "solid",
  line_col2 = "black",
  line\_size2 = 1,
 line_type2 = "dashed",
  label_x = "time"
)
## S3 method for class 'DynamicGrowth'
coef(object, ...)
```

# Arguments

X	The object of class DynamicGrowth to plot.
	ignored
У	ignored
add_factor	whether to plot also one environmental factor. If NULL (default), no environmental factor is plotted. If set to one character string that matches one entry of $x$ env_conditions, that condition is plotted in the secondary axis
ylims	A two dimensional vector with the limits of the primary y-axis.
label_y1	Label of the primary y-axis.
label_y2	Label of the secondary y-axis.
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
line_col2	Same as lin_col, but for the environmental factor.
line_size2	Same as line_size, but for the environmental factor.
line_type2	Same as lin_type, but for the environmental factor.

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label\_x Label of the x-axis.

object an instance of DynamicGrowth

# Methods (by generic)

- print(DynamicGrowth): print of the model
- plot(DynamicGrowth): predicted growth curve under dynamic conditions.
- coef(DynamicGrowth): coefficients of the model

example\_cardinal

Growth rates obtained for several growth experiments

# Description

An example dataset illustrating the requirements of the fit\_secondary\_growth() function.

#### Usage

```
example_cardinal
```

#### **Format**

A data frame with 64 rows and 3 variables:

```
temperature \ \ storage \ temperature \ (^{o}C)
```

**pH** pH of the media

mu specific growth rate (log10 CFU/h)

example\_dynamic\_growth

Microbial growth under dynamic conditions

# **Description**

An example dataset illustrating the requirements of the fit\_dynamic\_growth() function.

#### Usage

```
example_dynamic_growth
```

# **Format**

A data frame with 30 rows and 2 variables:

```
time elapsed time (h)
```

logN log population size (log10 CFU)

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```
example_env_conditions
```

Environmental conditions during a dynamic experiment

## **Description**

An example dataset illustrating the requirements of the fit\_dynamic\_growth() function.

# Usage

```
example_env_conditions
```

#### **Format**

A data frame with 3 rows and 3 variables:

```
time elapsed time (h)
```

**temperature** storage temperature (°C)

aw water activity

extract\_primary\_pars A helper to build the primary models

# **Description**

Most of the functions for fitting mix in the vectors parameters for the primary and secondary models, but the functions for making predictions need that they are separated. This one extracts the parameters of the primary model.

#### Usage

```
extract_primary_pars(this_p, known_pars)
```

# **Arguments**

this\_p A named vector of model parameters (usually, the ones fitted).

known\_pars Another named vector of model parameters (usually the known ones).

### Value

A list with the parameters of the primary model

extract\_secondary\_pars

extract\_secondary\_pars

A helper to build the secondary models

# **Description**

Most of the functions for fitting mix in the vectors parameters for the primary and secondary models, but the functions for making predictions need that they are separated. This one extracts the parameters of the secondary model.

#### Usage

```
extract_secondary_pars(this_p, known_pars, sec_model_names)
```

#### **Arguments**

this\_p A named vector of model parameters (usually, the ones fitted).

known\_pars Another named vector of model parameters (usually the known ones).

sec\_model\_names

A named character vector defining for each environmental factor (vector names)

the type of secondary model (vector values).

#### Value

A nested list defining the secondary models.

FitDynamicGrowth

FitDynamicGrowth class

# Description

#### [Superseded]

The class FitDynamicGrowth has been superseded by the top-level class GrowthFit, which provides a unified approach for growth modelling.

Still, it is still returned if the superseded fit\_dynamic\_growth() is called.

It is a subclass of list with the items:

- fit\_results: the object returned by modFit.
- best\_prediction: the model prediction for the fitted parameters.
- env conditions: environmental conditions for the fit.
- data: data used for the fit.
- starting: starting values for model fitting
- known: parameter values set as known.
- sec\_models: a named vector with the secondary model for each environmental factor

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```
## S3 method for class 'FitDynamicGrowth'
print(x, ...)
## S3 method for class 'FitDynamicGrowth'
plot(
  Х,
 y = NULL
  . . . ,
  add_factor = NULL,
 ylims = NULL,
  label_y1 = "logN",
  label_y2 = add_factor,
  line_col = "black",
  line_size = 1,
  line_type = 1,
  point_col = "black",
  point_size = 3,
  point_shape = 16,
  line_col2 = "black",
  line\_size2 = 1,
  line_type2 = "dashed"
)
## S3 method for class 'FitDynamicGrowth'
summary(object, ...)
## S3 method for class 'FitDynamicGrowth'
residuals(object, ...)
## S3 method for class 'FitDynamicGrowth'
coef(object, ...)
## S3 method for class 'FitDynamicGrowth'
vcov(object, ...)
## S3 method for class 'FitDynamicGrowth'
deviance(object, ...)
## S3 method for class 'FitDynamicGrowth'
fitted(object, ...)
## S3 method for class 'FitDynamicGrowth'
predict(object, times = NULL, newdata = NULL, ...)
## S3 method for class 'FitDynamicGrowth'
logLik(object, ...)
```

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```
## S3 method for class 'FitDynamicGrowth'
AIC(object, ..., k = 2)
```

# Arguments

Χ	The object of class FitDynamicGrowth to plot.
• • •	ignored
у	ignored
add_factor	whether to plot also one environmental factor. If NULL (default), no environmental factor is plotted. If set to one character string that matches one entry of x\$env_conditions, that condition is plotted in the secondary axis
ylims	A two dimensional vector with the limits of the primary y-axis.
label_y1	Label of the primary y-axis.
label_y2	Label of the secondary y-axis.
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
point_col	Aesthetic parameter to change the colour of the point geom, see: geom_point()
<pre>point_size</pre>	Aesthetic parameter to change the size of the point geom, see: geom_point()
point_shape	Aesthetic parameter to change the shape of the point geom, see: geom_point()
line_col2	Same as lin_col, but for the environmental factor.
line_size2	Same as line_size, but for the environmental factor.
line_type2	Same as lin_type, but for the environmental factor.
object	an instance of FitDynamicGrowth
times	A numeric vector with the time points for the simulations. NULL by default (using the same time points as those for the simulation).
newdata	a tibble describing the environmental conditions (as env_conditions) in predict_dynamic_growth(). If NULL (default), uses the same conditions as those for fitting.
k	penalty for the parameters (k=2 by default)

# Methods (by generic)

- print(FitDynamicGrowth): comparison between the fitted model and the data.
- plot(FitDynamicGrowth): comparison between the fitted model and the data.
- summary(FitDynamicGrowth): statistical summary of the fit.
- residuals(FitDynamicGrowth): residuals of the model.
- coef(FitDynamicGrowth): vector of fitted parameters.
- vcov(FitDynamicGrowth): (unscaled) variance-covariance matrix of the model, calculated as 1/(0.5\*Hessian)

- deviance(FitDynamicGrowth): deviance of the model.
- fitted(FitDynamicGrowth): fitted values.
- predict(FitDynamicGrowth): model predictions.
- logLik(FitDynamicGrowth): loglikelihood of the model
- AIC(FitDynamicGrowth): Akaike Information Criterion

FitDynamicGrowthMCMC FitDynamicGrowthMCMC class

# Description

### [Superseded]

The class FitDynamicGrowthMCMC has been superseded by the top-level class GrowthFit, which provides a unified approach for growth modelling.

Still, it is returned if the superseded fit\_MCMC\_growth() is called.

It is a subclass of list with the items:

- fit\_results: the object returned by modMCMC.
- best\_prediction: the model prediction for the fitted parameters.
- env\_conditions: environmental conditions for the fit.
- data: data used for the fit.
- starting: starting values for model fitting
- known: parameter values set as known.
- sec\_models: a named vector with the secondary model for each environmental factor

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

## S3 method for class 'FitDynamicGrowthMCMC'
plot(
    x,
    y = NULL,
    ...,
    add_factor = NULL,
    ylims = NULL,
    label_y1 = "logN",
    label_y2 = add_factor,
    line_col = "black",
    line_type = 1,
    point_col = "black",
```

```
point_size = 3,
  point_shape = 16,
  line_col2 = "black",
  line\_size2 = 1,
  line_type2 = "dashed"
## S3 method for class 'FitDynamicGrowthMCMC'
summary(object, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
residuals(object, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
coef(object, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
vcov(object, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
deviance(object, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
fitted(object, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
predict(object, times = NULL, newdata = NULL, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
logLik(object, ...)
## S3 method for class 'FitDynamicGrowthMCMC'
AIC(object, ..., k = 2)
## S3 method for class 'FitDynamicGrowthMCMC'
predictMCMC(
 model,
  times,
  env_conditions,
 niter,
  newpars = NULL,
  formula = . \sim time
)
```

# Arguments

```
x The object of class FitDynamicGrowthMCMC to plot.... ignored
```

у	ignored
add_factor	whether to plot also one environmental factor. If NULL (default), no environmenta factor is plotted. If set to one character string that matches one entry of x\$env_conditions, that condition is plotted in the secondary axis
ylims	A two dimensional vector with the limits of the primary y-axis.
label_y1	Label of the primary y-axis.
label_y2	Label of the secondary y-axis.
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
point_col	Aesthetic parameter to change the colour of the point geom, see: geom_point()
<pre>point_size</pre>	Aesthetic parameter to change the size of the point geom, see: geom_point()
point_shape	Aesthetic parameter to change the shape of the point geom, see: geom_point()
line_col2	Same as lin_col, but for the environmental factor.
line_size2	Same as line_size, but for the environmental factor.
line_type2	Same as lin_type, but for the environmental factor.
object	an instance of FitDynamicGrowthMCMC
times	Numeric vector of storage times for the predictions.
newdata	a tibble describing the environmental conditions (as env_conditions) in predict_dynamic_growth(). If NULL (default), uses the same conditions as those for fitting.
k	penalty for the parameters (k=2 by default)
model	An instance of FitDynamicGrowthMCMC
env_conditions	Tibble with the (dynamic) environmental conditions during the experiment. It must have one column named 'time' with the storage time and as many columns as required with the environmental conditions.
niter	Number of iterations.
newpars	A named list defining new values for the some model parameters. The name must be the identifier of a model already included in the model. These parameters do not include variation, so defining a new value for a fitted parameters "fixes" it. NULL by default (no new parameters).
formula	A formula stating the column named defining the elapsed time in env_conditions.

# Value

An instance of MCMCgrowth().

By default, . ~ time.

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### Methods (by generic)

- print(FitDynamicGrowthMCMC): print of the model
- plot(FitDynamicGrowthMCMC): compares the model fitted against the data.
- summary(FitDynamicGrowthMCMC): statistical summary of the fit.
- residuals(FitDynamicGrowthMCMC): model residuals.
- coef(FitDynamicGrowthMCMC): vector of fitted model parameters.
- vcov(FitDynamicGrowthMCMC): variance-covariance matrix of the model, estimated as the variance of the samples from the Markov chain.
- deviance(FitDynamicGrowthMCMC): deviance of the model, calculated as the sum of squared residuals for the parameter values resulting in the best fit.
- fitted(FitDynamicGrowthMCMC): vector of fitted values.
- predict(FitDynamicGrowthMCMC): vector of model predictions.
- logLik(FitDynamicGrowthMCMC): loglikelihood of the model
- AIC(FitDynamicGrowthMCMC): Akaike Information Criterion
- predictMCMC(FitDynamicGrowthMCMC): prediction including parameter uncertainty

FitIsoGrowth

FitIsoGrowth class

# **Description**

#### [Superseded]

The class FitIsoGrowth has been superseded by the top-level class GrowthFit, which provides a unified approach for growth modelling.

Still, it is still returned if the superseded fit\_isothermal\_growth() is called.

It is a subclass of list with the items:

- data: data used for model fitting
- model: name of the primary inactivation model
- starting\_point: initial value of the model parameters
- known: fixed model parameters
- fit: object returned by modFit()
- best\_prediction: model prediction for the model fitted.

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### Usage

```
## S3 method for class 'FitIsoGrowth'
print(x, ...)
## S3 method for class 'FitIsoGrowth'
plot(
  Х,
 y = NULL,
  line_col = "black",
  line_size = 1,
  line_type = 1,
  point_col = "black",
 point_size = 3,
  point_shape = 16
## S3 method for class 'FitIsoGrowth'
summary(object, ...)
## S3 method for class 'FitIsoGrowth'
residuals(object, ...)
## S3 method for class 'FitIsoGrowth'
coef(object, ...)
## S3 method for class 'FitIsoGrowth'
vcov(object, ...)
## S3 method for class 'FitIsoGrowth'
deviance(object, ...)
## S3 method for class 'FitIsoGrowth'
fitted(object, ...)
## S3 method for class 'FitIsoGrowth'
predict(object, times = NULL, ...)
## S3 method for class 'FitIsoGrowth'
logLik(object, ...)
## S3 method for class 'FitIsoGrowth'
AIC(object, ..., k = 2)
```

#### **Arguments**

```
x The object of class FitIsoGrowth to plot.
```

... ignored

У	ignored
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
point_col	Aesthetic parameter to change the colour of the point geom, see: geom_point()
point_size	Aesthetic parameter to change the size of the point geom, see: geom_point()
point_shape	Aesthetic parameter to change the shape of the point geom, see: geom_point()
object	an instance of FitIsoGrowth
times	numeric vector describing the time points for the prediction. If NULL (default), uses the same points as those used for fitting.
k	penalty for the parameters (k=2 by default)

# Methods (by generic)

- print(FitIsoGrowth): print of the model
- plot(FitIsoGrowth): compares the fitted model against the data.
- summary(FitIsoGrowth): statistical summary of the fit.
- residuals(FitIsoGrowth): vector of model residuals.
- coef(FitIsoGrowth): vector of fitted model parameters.
- vcov(FitIsoGrowth): variance-covariance matrix of the model, estimated as 1/(0.5\*Hessian)
- deviance(FitIsoGrowth): deviance of the model.
- fitted(FitIsoGrowth): vector of fitted values.
- predict(FitIsoGrowth): vector of model predictions.
- logLik(FitIsoGrowth): loglikelihood of the model
- AIC(FitIsoGrowth): Akaike Information Criterion

### **Description**

#### [Superseded]

The class FitMultipleDynamicGrowth has been superseded by the top-level class GlobalGrowthFit, which provides a unified approach for growth modelling.

Still, it is still returned if the superseded fit\_multiple\_growth() is called.

It is a subclass of list with the items:

- fit\_results: the object returned by modFit.
- best\_prediction: a list with the models predictions for each condition.
- data: a list with the data used for the fit.
- starting: starting values for model fitting
- known: parameter values set as known.
- sec\_models: a named vector with the secondary model for each environmental factor.

```
## S3 method for class 'FitMultipleDynamicGrowth'
print(x, ...)
## S3 method for class 'FitMultipleDynamicGrowth'
plot(
  Х,
 y = NULL
  add_factor = NULL,
  ylims = NULL,
  label_x = "time"
  label_y1 = "logN",
  label_y2 = add_factor,
  line_col = "black",
  line_size = 1,
  line_type = "solid",
  line_col2 = "black",
  line\_size2 = 1,
  line_type2 = "dashed",
  point_size = 3,
  point_shape = 16,
  subplot_labels = "AUTO"
)
## S3 method for class 'FitMultipleDynamicGrowth'
summary(object, ...)
## S3 method for class 'FitMultipleDynamicGrowth'
residuals(object, ...)
```

```
## S3 method for class 'FitMultipleDynamicGrowth'
coef(object, ...)

## S3 method for class 'FitMultipleDynamicGrowth'
vcov(object, ...)

## S3 method for class 'FitMultipleDynamicGrowth'
deviance(object, ...)

## S3 method for class 'FitMultipleDynamicGrowth'
fitted(object, ...)

## S3 method for class 'FitMultipleDynamicGrowth'
predict(object, env_conditions, times = NULL, ...)

## S3 method for class 'FitMultipleDynamicGrowth'
logLik(object, ...)

## S3 method for class 'FitMultipleDynamicGrowth'
logLik(object, ...)
```

# **Arguments** ×

	1 7
	ignored
у	ignored
add_factor	whether to plot also one environmental factor. If NULL (default), no environmental factor is plotted. If set to one character string that matches one entry of $x$ env_conditions, that condition is plotted in the secondary axis
ylims	A two dimensional vector with the limits of the primary y-axis.
label_x	label of the x-axis
label_y1	Label of the primary y-axis.
label_y2	Label of the secondary y-axis.
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
line_col2	Same as lin_col, but for the environmental factor.
line_size2	Same as line_size, but for the environmental factor.
line_type2	Same as lin_type, but for the environmental factor.
point_size	Size of the data points
point_shape	shape of the data points

an instance of FitMultipleDynamicGrowth.

subplot\_labels labels of the subplots according to plot\_grid.

object an instance of FitMultipleDynamicGrowth

env\_conditions a tibble describing the environmental conditions (as in fit\_multiple\_growth().

times A numeric vector with the time points for the simulations. NULL by default (using the same time points as the ones defined in env\_conditions).

k penalty for the parameters (k=2 by default)

### Methods (by generic)

- print(FitMultipleDynamicGrowth): print of the model
- plot(FitMultipleDynamicGrowth): comparison between the fitted model and the experimental data.
- summary(FitMultipleDynamicGrowth): statistical summary of the fit.
- residuals(FitMultipleDynamicGrowth): calculates the model residuals. Returns a tibble with 4 columns: time (storage time), logN (observed count), exp (name of the experiment) and res (residual).
- coef(FitMultipleDynamicGrowth): vector of fitted parameters.
- vcov(FitMultipleDynamicGrowth): (unscaled) variance-covariance matrix, estimated as 1/(0.5\*Hessian).
- deviance(FitMultipleDynamicGrowth): deviance of the model.
- fitted(FitMultipleDynamicGrowth): fitted values. They are returned as a tibble with 3 columns: time (storage time), exp (experiment identifier) and fitted (fitted value).
- predict(FitMultipleDynamicGrowth): vector of model predictions
- logLik(FitMultipleDynamicGrowth): loglikelihood of the model
- AIC(FitMultipleDynamicGrowth): Akaike Information Criterion

FitMultipleGrowthMCMC  $\it FitMultipleGrowthMCMC \it class$ 

#### **Description**

#### [Superseded]

The class FitMultipleGrowthMCMC has been superseded by the top-level class GlobalGrowthFit, which provides a unified approach for growth modelling.

Still, it is still returned if the superseded fit\_multiple\_growth\_MCMC() is called.

It is a subclass of list with the items:

- fit\_results: the object returned by modFit.
- best\_prediction: a list with the models predictions for each condition.
- data: a list with the data used for the fit.
- starting: starting values for model fitting
- known: parameter values set as known.
- sec\_models: a named vector with the secondary model for each environmental factor.

```
## S3 method for class 'FitMultipleGrowthMCMC'
print(x, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
plot(
  х,
 y = NULL
  . . . ,
  add_factor = NULL,
 ylims = NULL,
  label_x = "time",
  label_y1 = "logN",
  label_y2 = add_factor,
  line_col = "black",
  line_size = 1,
  line_type = "solid",
  line_col2 = "black",
  line\_size2 = 1,
  line_type2 = "dashed",
  point_size = 3,
  point_shape = 16,
  subplot_labels = "AUTO"
)
## S3 method for class 'FitMultipleGrowthMCMC'
summary(object, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
residuals(object, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
coef(object, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
vcov(object, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
deviance(object, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
fitted(object, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
predict(object, env_conditions, times = NULL, ...)
## S3 method for class 'FitMultipleGrowthMCMC'
logLik(object, ...)
```

```
## S3 method for class 'FitMultipleGrowthMCMC'
AIC(object, ..., k = 2)

## S3 method for class 'FitMultipleGrowthMCMC'
predictMCMC(
   model,
   times,
   env_conditions,
   niter,
   newpars = NULL,
   formula = . ~ time
)
```

#### **Arguments**

an instance of FitMultipleGrowthMCMC. Х ignored У ignored add\_factor whether to plot also one environmental factor. If NULL (default), no environmental factor is plotted. If set to one character string that matches one entry of x\$env\_conditions, that condition is plotted in the secondary axis ylims A two dimensional vector with the limits of the primary y-axis. label\_x label of the x-axis label\_y1 Label of the primary y-axis. label\_y2 Label of the secondary y-axis. line col Aesthetic parameter to change the colour of the line geom in the plot, see: geom\_line() line\_size Aesthetic parameter to change the thickness of the line geom in the plot, see: geom\_line() Aesthetic parameter to change the type of the line geom in the plot, takes numline\_type bers (1-6) or strings ("solid") see: geom\_line() line\_col2 Same as lin\_col, but for the environmental factor. line\_size2 Same as line\_size, but for the environmental factor. line\_type2 Same as lin\_type, but for the environmental factor. point\_size Size of the data points point\_shape shape of the data points subplot\_labels labels of the subplots according to plot\_grid. an instance of FitMultipleGrowthMCMC object env\_conditions Tibble with the (dynamic) environmental conditions during the experiment. It must have one column named 'time' with the storage time and as many columns as required with the environmental conditions. times Numeric vector of storage times for the predictions.

k penalty for the parameters (k=2 by default)

model An instance of FitMultipleGrowthMCMC

niter Number of iterations.

newpars A named list defining new values for the some model parameters. The name

must be the identifier of a model already included in the model. These parameters do not include variation, so defining a new value for a fitted parameters

"fixes" it. NULL by default (no new parameters).

formula A formula stating the column named defining the elapsed time in env\_conditions.

By default, . ~ time.

#### Value

An instance of MCMCgrowth().

#### Methods (by generic)

- print(FitMultipleGrowthMCMC): print of the model
- plot(FitMultipleGrowthMCMC): comparison between the model fitted and the data.
- summary(FitMultipleGrowthMCMC): statistical summary of the fit.
- residuals(FitMultipleGrowthMCMC): model residuals. They are returned as a tibble with 4 columns: time (storage time), logN (observed count), exp (name of the experiment) and res (residual).
- coef(FitMultipleGrowthMCMC): vector of fitted model parameters.
- vcov(FitMultipleGrowthMCMC): variance-covariance matrix of the model, estimated as the variance of the samples from the Markov chain.
- deviance(FitMultipleGrowthMCMC): deviance of the model, calculated as the sum of squared residuals of the prediction with the lowest standard error.
- fitted(FitMultipleGrowthMCMC): fitted values of the model. They are returned as a tibble with 3 columns: time (storage time), exp (experiment identifier) and fitted (fitted value).
- predict(FitMultipleGrowthMCMC): model predictions. They are returned as a tibble with 3 columns: time (storage time), logN (observed count), and exp (name of the experiment).
- logLik(FitMultipleGrowthMCMC): loglikelihood of the model
- AIC(FitMultipleGrowthMCMC): Akaike Information Criterion
- predictMCMC(FitMultipleGrowthMCMC): prediction including parameter uncertainty

36 FitSecondaryGrowth

FitSecondaryGrowth

FitSecondaryGrowth class

# **Description**

The FitSecondaryGrowth class contains a model fitted to a set of growth rates gathered under a variety of static conditions. Its constructor is fit\_secondary\_growth().

It is a subclass of list with the items:

- fit\_results: object returned by modFit().
- secondary\_model: secondary model fitted to the data.
- mu\_opt\_fit: estimated growth rate under optimum conditions.
- data: data used for the fit.
- transformation: type of transformation of mu for the fit.

```
## S3 method for class 'FitSecondaryGrowth'
print(x, ...)
## S3 method for class 'FitSecondaryGrowth'
plot(x, y = NULL, ..., which = 1, add_trend = FALSE, add_segment = FALSE)
## S3 method for class 'FitSecondaryGrowth'
summary(object, ...)
## S3 method for class 'FitSecondaryGrowth'
residuals(object, ...)
## S3 method for class 'FitSecondaryGrowth'
coef(object, ...)
## S3 method for class 'FitSecondaryGrowth'
vcov(object, ...)
## S3 method for class 'FitSecondaryGrowth'
deviance(object, ...)
## S3 method for class 'FitSecondaryGrowth'
fitted(object, ...)
## S3 method for class 'FitSecondaryGrowth'
predict(object, newdata = NULL, ...)
## S3 method for class 'FitSecondaryGrowth'
logLik(object, ...)
```

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```
## S3 method for class 'FitSecondaryGrowth'
AIC(object, ..., k = 2)
```

#### **Arguments**

x An instance of FitSecondaryGrowth.

ignoredignored.

which A numeric with the type of plot. 1 for obs versus predicted (default), 2 for

gamma curve

add\_trend Whether to add a trend line (only for which=2)

add\_segment Whether to join the observed and fitted points (only for which=2)

object an instance of FitSecondaryGrowth

newdata A tibble describing the environmental conditions as in fit\_secondary\_growth().

If NULL, it uses the same conditions as for model fitting (default).

k penalty for the parameters (k=2 by default)

#### Methods (by generic)

- print(FitSecondaryGrowth): print of the model
- plot(FitSecondaryGrowth): plots to evaluate the goodness of the fit.
- summary(FitSecondaryGrowth): statistical summary of the fit.
- residuals(FitSecondaryGrowth): vector of model residuals.
- coef(FitSecondaryGrowth): vector of fitted model parameters.
- vcov(FitSecondaryGrowth): variance-covariance matrix of the model, estimated as 1/(0.5\*Hessian)
- deviance(FitSecondaryGrowth): deviance of the model.
- fitted(FitSecondaryGrowth): vector of fitted values.
   The fitted values are returned in the same scale as the one used for the fitting (sqrt, log or none).
- predict(FitSecondaryGrowth): vector of model predictions.
- logLik(FitSecondaryGrowth): loglikelihood of the model
- AIC(FitSecondaryGrowth): Akaike Information Criterion

38 fit\_dynamic\_growth

fit\_dynamic\_growth

Fit dynamic growth models

## **Description**

## [Superseded]

The function fit\_dynamic\_growth() has been superseded by the top-level function fit\_growth(), which provides a unified approach for growth modelling.

Nonetheless, it can still fit a growth model to data obtained under dynamic conditions using the one-step approach (non-linear regression).

# Usage

```
fit_dynamic_growth(
  fit_data,
  env_conditions,
  starting_point,
  known_pars,
  sec_model_names,
  . . . ,
  check = TRUE,
  logbase_mu = logbase_logN,
  logbase_logN = 10,
  formula = logN ~ time
)
```

#### **Arguments**

fit\_data

Tibble with the data to use for model fit. It must contain a column with the elapsed time (named "time" by default) and another one with the decimal logarithm of the observed population size (named "logN" by default). Different column names can be specified using the "formula" argument.

env\_conditions

Tibble with the (dynamic) environmental conditions during the experiment. It must have one column with the elapsed time (named "time" by default) and as many columns as required with the environmental conditions. A different column name can be specified using the "formula" argument, although it must be the same one as in "fit\_data". Note that only those defined in "sec\_model\_names" will be considered for the model fit.

starting\_point A named vector of starting values for the model parameters. Parameters for the primary model must be named in the usual way. Parameters for the secondary model are named as env\_factor+'\_'+parameter. For instance, the maximum growth temperature shall be named 'temperature\_xmax'.

known\_pars

A named vector of known model parameters (i.e. not fitted). They must be named using the same convention as for starting\_point.

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sec\_model\_names

A named character vector defining the secondary model for each environmental factor. The names define the factor and the value the type of model. Names must metab columns in fit data and any conditions.

match columns in fit\_data and env\_conditions.

... Additional arguments passed to modFit.

check Whether to check model parameters (TRUE by default).

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

formula an object of class "formula" describing the x and y variables. logN ~ time as a

default.

#### Value

An instance of FitDynamicGrowth().

# **Examples**

```
## We use the datasets included in the package
data("example_dynamic_growth")
data("example_env_conditions")
## Define the secondary models
sec_model_names <- c(temperature = "CPM", aw= "CPM")</pre>
## Any model parameter can be fixed
known_pars <- list(Nmax = 1e4, # Primary model</pre>
   N0 = 1e0, Q0 = 1e-3, # Initial values of the primary model
   mu_opt = 4, # mu_opt of the gamma model
   temperature_n = 1, # Secondary model for temperature
    aw_xmax = 1, aw_xmin = .9, aw_n = 1 # Secondary model for water activity
## The remaining parameters need initial values
my_start <- list(temperature_xmin = 25, temperature_xopt = 35,</pre>
    temperature_xmax = 40, aw_xopt = .95)
## We can now call the fitting function
my_dyna_fit <- fit_dynamic_growth(example_dynamic_growth, example_env_conditions,</pre>
   my_start, known_pars, sec_model_names)
summary(my_dyna_fit)
```

```
## We can compare the data and the fitted curve
plot(my_dyna_fit)
## We can plot any environmental condition using add_factor
plot(my_dyna_fit, add_factor = "aw",
    label_y1 = "Log count (log CFU/ml)",
    label_y2 = "Water activity")
```

fit\_growth

Fitting microbial growth

## **Description**

## [Stable]

This function provides a top-level interface for fitting growth models to data describing the variation of the population size through time, either under constant or dynamic environment conditions. See below for details on the calculations.

#### Usage

```
fit_growth(
  fit_data,
  model_keys,
  start,
  known,
  environment = "constant",
  algorithm = "regression",
  approach = "single",
  env_conditions = NULL,
  niter = NULL,
  . . . ,
  check = TRUE,
  logbase_mu = logbase_logN,
  logbase_logN = 10,
  formula = logN ~ time
)
```

## **Arguments**

fit\_data observed microbial growth. The format varies depending on the type of model fit. See the relevant sections (and examples) below for details.

model\_keys a named list assigning equations for the primary and secondary models. See the relevant sections (and examples) below for details.

start	a named numeric vector assigning initial guesses to the model parameters to estimate from the data. See relevant section (and examples) below for details.
known	named numeric vector of fixed model parameters, using the same conventions as for "start".
environment	type of environment. Either "constant" (default) or "dynamic" (see below for details on the calculations for each condition)
algorithm	either "regression" (default; Levenberg-Marquard algorithm) or "MCMC" (Adaptive Monte Carlo algorithm).
approach	approach for model fitting. Either "single" (the model is fitted to a unique experiment) or "global" (the model is fitted to several dynamic experiments).
env_conditions	Tibble describing the variation of the environmental conditions for dynamic experiments. See the relevant sections (and examples) below for details. Ignored for environment="constant".
niter	number of iterations of the MCMC algorithm. Ignored when algorithm!="MCMC"
	Additional arguments for modFit().
check	Whether to check the validity of the models. TRUE by default.
logbase_mu	Base of the logarithm the growth rate is referred to. By default, the same as logbase_logN. See vignette about units for details.
logbase_logN	Base of the logarithm for the population size. By default, 10 (i.e. log10). See vignette about units for details.
formula	An object of class "formula" defining the names of the $x$ and $y$ variables in the data. logN $\sim$ time as a default.

## Value

If approach="single, an instance of GrowthFit. If approach="multiple", an instance of GlobalGrowthFit

Please check the help pages of each class for additional information.

#### Fitting under constant conditions

When environment="constant", the functions fits a primary growth model to the population size observed during an experiment. In this case, the data has to be a tibble (or data.frame) with two columns:

- time: the elapsed time
- logN: the logarithm of the observed population size Nonetheless, the names of the columns can be modified with the formula argument.

The model equation is defined through the model\_keys argument. It must include an entry named "primary" assigned to a model. Valid model keys can be retrieved calling primary\_model\_data().

The model is fitted by non-linear regression (using modFit()). This algorithm needs initial guesses for every model parameter. This are defined as a named numeric vector. The names must be valid model keys, which can be retrieved using primary\_model\_data() (see example below). Apart from that, any model parameter can be fixed using the "known" argument. This is a named numeric vector, with the same convenctions as "start".

## Fitting under dynamic conditions to a single experiment

When environment="constant" and approach="single", a dynamic growth model combining the Baranyi primary growth model with the gamma approach for the effect of the environmental conditions on the growth rate is fitted to an experiment gathered under dynamic conditions. In this case, the data is similar to fitting under constant conditions: a tibble (or data.frame) with two columns:

- time: the elapsed time
- logN: the logarithm of the observed population size Note that these default names can be changed using the formula argument.

The values of the experimental conditions during the experiment are defined using the "env\_conditions" argument. It is a tibble (or data.frame) with one column named ("time") defining the elapsed time. Note that this default name can be modified using the formula argument of the function. The tibble needs to have as many additional columns as environmental conditions included in the model, providing the values of the environmental conditions.

The model equations are defined through the model\_keys argument. It must be a named list where the names match the column names of "env\_conditions" and the values are model keys. These can be retrieved using secondary\_model\_data().

The model can be fitted using regression (modFit()) or an adaptive Monte Carlo algorithm (modMCMC()). Both algorithms require initial guesses for every model parameter to fit. These are defined through the named numeric vector "start". Each parameter must be named as *factor+"\_"+parameter*, where *factor* is the name of the environmental factor defined in "model\_keys". The *parameter* is a valid key that can be retrieved from secondary\_model\_data(). For instance, parameter Xmin for the factor temperature would be defined as "temperature\_xmin".

Note that the argument ... allows passing additional arguments to the fitting functions.

#### Fitting under dynamic conditions to multiple experiments (global fitting)

When environment="constant" and approach="global", fit\_growth tries to find the vector of model parameters that best describe the observations of several growth experiments.

The input requirements are very similar to the case when approach="single". The models (equations, initial guesses, known parameters, algorithms...) are identical. The only difference is that "fit\_data" must be a list, where each element describes the results of an experiment (using the same conventions as when approach="single"). In a similar fashion, "env\_conditions" must be a list describing the values of the environmental factors during each experiment. Although it is not mandatory, it is recommended that the elements of both lists are named. Otherwise, the function assigns automatically-generated names, and matches them by order.#'

## **Examples**

```
## Example 1 - Fitting a primary model -----
## A dummy dataset describing the variation of the population size

my_{data} \leftarrow data.frame(time = c(0, 25, 50, 75, 100), logN = c(2, 2.5, 7, 8, 8))
```

```
## A list of model keys can be gathered from
primary_model_data()
## The primary model is defined as a list
models <- list(primary = "Baranyi")</pre>
## The keys of the model parameters can also be gathered from primary_model_data
primary_model_data("Baranyi")$pars
## Any model parameter can be fixed
known <- c(mu = .2)
## The remaining parameters need initial guesses
start <- c(logNmax = 8, lambda = 25, logN0 = 2)
primary_fit <- fit_growth(my_data, models, start, known,</pre>
                          environment = "constant",
## The instance of FitIsoGrowth includes several useful methods
print(primary_fit)
plot(primary_fit)
coef(primary_fit)
summary(primary_fit)
## time_to_size can be used to calculate the time for some concentration
time_to_size(primary_fit, 4)
## Example 2 - Fitting under dynamic conditions-----
## We will use the example data included in the package
data("example_dynamic_growth")
## And the example environmental conditoins (temperature & aw)
data("example_env_conditions")
## Valid keys for secondary models can be retrived from
secondary_model_data()
## We need to assign a model equation (secondary model) to each environmental factor
sec_models <- list(temperature = "CPM", aw = "CPM")</pre>
```

```
## The keys of the model parameters can be gathered from the same function
secondary_model_data("CPM")$pars
## Any model parameter (of the primary or secondary models) can be fixed
known_pars <- list(Nmax = 1e4,  # Primary model</pre>
                   N0 = 1e0, Q0 = 1e-3, # Initial values of the primary model
                   mu_opt = 4, # mu_opt of the gamma model
                   temperature_n = 1, # Secondary model for temperature
                 aw_xmax = 1, aw_xmin = .9, aw_n = 1 # Secondary model for water activity
## The rest, need initial guesses (you know, regression)
my_start <- list(temperature_xmin = 25, temperature_xopt = 35,</pre>
                 temperature_xmax = 40, aw_xopt = .95)
## We can now fit the model
dynamic_fit <- fit_growth(example_dynamic_growth,</pre>
                          sec_models,
                          my_start, known_pars,
                          environment = "dynamic",
                          env_conditions = example_env_conditions
## The instance of FitDynamicGrowth has several S3 methods
plot(dynamic_fit, add_factor = "temperature")
summary(dynamic_fit)
## We can use time_to_size to calculate the time required to reach a given size
time_to_size(dynamic_fit, 3)
## Example 3- Fitting under dynamic conditions using MCMC --------
## We can reuse most of the arguments from the previous example
## We just need to define the algorithm and the number of iterations
set.seed(12421)
MCMC_fit <- fit_growth(example_dynamic_growth,</pre>
                       sec_models,
                       my_start, known_pars,
                       environment = "dynamic",
                       env_conditions = example_env_conditions,
                       algorithm = "MCMC",
                       niter = 1000
```

## The instance of FitDynamicGrowthMCMC has several S3 methods plot(MCMC\_fit, add\_factor = "aw") summary(MCMC\_fit) ## We can use time\_to\_size to calculate the time required to reach a given size time\_to\_size(MCMC\_fit, 3) ## It can also make growth predictions including uncertainty uncertain\_growth <- predictMCMC(MCMC\_fit,</pre> seq(0, 10, length = 1000),example\_env\_conditions, niter = 1000)## The instance of MCMCgrowth includes several nice S3 methods plot(uncertain\_growth) print(uncertain\_growth) ## time\_to\_size can calculate the time to reach some count time\_to\_size(uncertain\_growth, 2) time\_to\_size(uncertain\_growth, 2, type = "distribution") ## Example 4 - Fitting a unique model to several dynamic experiments ------## We will use the data included in the package data("multiple\_counts") data("multiple\_conditions") ## We need to assign a model equation for each environmental factor sec\_models <- list(temperature = "CPM", pH = "CPM")</pre> ## Any model parameter (of the primary or secondary models) can be fixed  $known_pars <- list(Nmax = 1e8, N0 = 1e0, Q0 = 1e-3,$ temperature\_n = 2, temperature\_xmin = 20,  $temperature\_xmax = 35,$  $pH_n = 2$ ,  $pH_xmin = 5.5$ ,  $pH_xmax = 7.5$ ,  $pH_xopt = 6.5$ ) ## The rest, need initial guesses my\_start <- list(mu\_opt = .8, temperature\_xopt = 30)</pre>

## We can now fit the model

```
global_fit <- fit_growth(multiple_counts,</pre>
                         sec_models,
                         my_start,
                         known_pars,
                         environment = "dynamic",
                         algorithm = "regression",
                         approach = "global",
                         env_conditions = multiple_conditions
                         )
## The instance of FitMultipleDynamicGrowth has nice S3 methods
plot(global_fit)
summary(global_fit)
print(global_fit)
## We can use time_to_size to calculate the time to reach a given size
time_to_size(global_fit, 4.5)
## Example 5 - MCMC fitting a unique model to several dynamic experiments ---
## Again, we can re-use all the arguments from the previous example
## We just need to define the right algorithm and the number of iterations
## On top of that, we will also pass upper and lower bounds to modMCMC
set.seed(12421)
global_MCMC <- fit_growth(multiple_counts,</pre>
                         sec_models,
                         my_start,
                         known_pars,
                         environment = "dynamic",
                         algorithm = "MCMC",
                         approach = "global",
                         env_conditions = multiple_conditions,
                         niter = 1000,
                         lower = c(.2, 29), # lower limits of the model parameters
                         upper = c(.8, 34) # upper limits of the model parameters
                         )
## The instance of FitMultipleDynamicGrowthMCMC has nice S3 methods
plot(global_MCMC)
summary(global_MCMC)
print(global_MCMC)
## We can use time_to_size to calculate the time to reach a given size
```

fit\_isothermal\_growth 47

fit\_isothermal\_growth Fit primary growth models

## **Description**

## [Superseded]

The function fit\_isothermal\_growth() has been superseded by the top-level function fit\_growth(), which provides a unified approach for growth modelling.

Nonetheless, it can still fit a primary growth model to data obtained under static environmental conditions.

```
fit_isothermal_growth(
   fit_data,
   model_name,
   starting_point,
   known_pars,
   ...,
   check = TRUE,
   formula = logN ~ time,
   logbase_mu = logbase_logN,
   logbase_logN = 10
)
```

## **Arguments**

fit\_data Tibble of data for the fit. It must have two columns, one with the elapsed time

(time by default) and another one with the decimal logarithm of the populatoin size (logN by default). Different column names can be defined using the

formula argument.

model\_name Character defining the primary growth model

starting\_point Named vector of initial values for the model parameters.

known\_pars Named vector of known model parameters (not fitted).

... Additional arguments passed to modFit().

check Whether to do some basic checks (TRUE by default).

formula an object of class "formula" describing the x and y variables. logN ~ time as a

default.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

#### Value

An instance of FitIsoGrowth().

## **Examples**

```
## Some dummy data
library(tibble)

my_data <- tibble(time = c(0, 25, 50, 75, 100),
        logN = c(2, 2.5, 7, 8, 8))

## Choose the model

my_model <- "Baranyi"

## Initial values for the model parameters

start = c(logNmax = 8, lambda = 25, logN0 = 2)

## Any model parameter can be fixed

known <- c(mu = .2)

## Now, we can call the function

static_fit <- fit_isothermal_growth(my_data, my_model, start, known)

summary(static_fit)</pre>
```

49 fit\_MCMC\_growth

```
## We can plot the fitted model against the observations
plot(static_fit)
```

fit\_MCMC\_growth

Fit growth models using MCMC

## **Description**

## [Superseded]

The function fit\_MCMC\_growth() has been superseded by the top-level function fit\_growth(), which provides a unified approach for growth modelling.

But, it can still fit a growth model to a data obtained under dynamic conditions using the one-step approach (MCMC algorithm).

## **Usage**

```
fit_MCMC_growth(
  fit_data,
  env_conditions,
  starting_point,
  known_pars,
  sec_model_names,
  niter,
  . . . ,
  check = TRUE,
  formula = logN \sim time,
  logbase_mu = logbase_logN,
  logbase_logN = 10
)
```

#### **Arguments**

fit\_data

Tibble with the data to use for model fit. It must contain a column with the elapsed time (named "time" by default) and another one with the decimal logarithm of the observed population size (named "logN" by default). Different column names can be specified using the "formula" argument.

env\_conditions Tibble with the (dynamic) environmental conditions during the experiment. It must have one column with the elapsed time (named "time" by default) and as many columns as required with the environmental conditions. A different column name can be specified using the "formula" argument, although it must be the same one as in "fit\_data". Note that only those defined in "sec\_model\_names" will be considered for the model fit.

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starting\_point A named vector of starting values for the model parameters. Parameters for the primary model must be named in the usual way. Parameters for the secondary model are named as env\_factor+'\_'+parameter. For instance, the maximum growth temperature shall be named 'temperature\_xmax'.

known\_pars A named vector of known model parameters (i.e. not fitted). They must be named using the same convention as for starting\_point.

sec\_model\_names

A named character vector defining the secondary model for each environmental factor. The names define the factor and the value the type of model. Names must

match columns in fit\_data and env\_conditions.

niter number of iterations of the MCMC algorithm.

... Additional arguments passed to modFit.

check Whether to check model parameters (TRUE by default).

formula an object of class "formula" describing the x and y variables. logN ~ time as a

default.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

#### Value

An instance of FitDynamicGrowthMCMC().

## **Examples**

```
## We use the example data included in the package

data("example_dynamic_growth")
data("example_env_conditions")

## Definition of the secondary models
sec_model_names <- c(temperature = "CPM", aw= "CPM")

## Any model parameter can be fixed
known_pars <- list(Nmax = 1e4, # Primary model
    N0 = 1e0, Q0 = 1e-3, # Initial values of the primary model
    mu_opt = 4, # mu_opt of the gamma model
    temperature_n = 1, # Secondary model for temperature
    aw_xmax = 1, aw_xmin = .9, aw_n = 1 # Secondary model for water activity
)

## We need starting values for the remaining parameters

my_start <- list(temperature_xmin = 25, temperature_xopt = 35,
    temperature_xmax = 40,
    aw_xopt = .95)</pre>
```

fit\_multiple\_growth 51

fit\_multiple\_growth

Fitting growth models to multiple dynamic experiments

# Description

# [Superseded]

The function fit\_multiple\_growth() has been superseded by the top-level function fit\_growth(), which provides a unified approach for growth modelling.

But, if you so wish, this function still enables fitting a growth model using a dataset comprised of several experiments with potentially different dynamic experimental conditions. Note that the definition of secondary models must comply with the secondary\_model\_data function.

```
fit_multiple_growth(
    starting_point,
    experiment_data,
    known_pars,
    sec_model_names,
    ...,
    check = TRUE,
    formula = logN ~ time,
    logbase_mu = logbase_logN,
    logbase_logN = 10
)
```

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#### **Arguments**

starting\_point a named vector of starting values for the model parameters. experiment\_data

a nested list with the experimental data. Each entry describes one experiment as a list with two elements: data and conditions. data is a tibble with a column giving the elapsed time (named "time" by default) and another one with the decimal logarithm of the population size (named "logN" by default). conditions is a tibble with one column giving the elapsed time (using the same name as data) and as many additional columns as environmental factors. The default column names can be changed with the formula argument.

known\_pars named vector of known model parameters

sec\_model\_names

named character vector with names of the environmental conditions and values

of the secondary model (see secondary\_model\_data).

... additional arguments for modFit().

check Whether to check the validity of the models. TRUE by default.

formula an object of class "formula" describing the x and y variables. logN ~ time as a

default.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

## Value

An instance of FitMultipleDynamicGrowth().

# Examples

```
## We can now call the fitting function
global_fit <- fit_multiple_growth(start, multiple_experiments, known, sec_names)
## Parameter estimates can be retrieved with summary
summary(global_fit)
## We can compare fitted model against observations
plot(global_fit)
## Any single environmental factor can be added to the plot using add_factor
plot(global_fit, add_factor = "temperature")</pre>
```

fit\_multiple\_growth\_MCMC

Fitting growth models to multiple dynamic experiments using MCMC

## **Description**

## [Superseded]

The function fit\_multiple\_growth\_MCMC() has been superseded by the top-level function fit\_growth(), which provides a unified approach for growth modelling.

However, this functions can still be used to fit a growth model using a dataset comprised of several experiments with potentially different dynamic experimental conditions.

```
fit_multiple_growth_MCMC(
    starting_point,
    experiment_data,
    known_pars,
    sec_model_names,
    niter,
    ...,
    check = TRUE,
    formula = logN ~ time,
    logbase_mu = logbase_logN,
    logbase_logN = 10
)
```

#### **Arguments**

starting\_point a named vector of starting values for the model parameters. experiment\_data

a nested list with the experimental data. Each entry describes one experiment as a list with two elements: data and conditions. data is a tibble with a column giving the elapsed time (named "time" by default) and another one with the decimal logarithm of the population size (named "logN" by default). conditions is a tibble with one column giving the elapsed time (using the same name as data) and as many additional columns as environmental factors. The default column names can be changed with the formula argument.

known\_pars named vector of known model parameters

sec\_model\_names

named character vector with names of the environmental conditions and values

of the secondary model (see secondary\_model\_data).

niter number of samples of the MCMC algorithm.

... additional arguments for modMCMC (e.g. upper and lower bounds).

check Whether to check the validity of the models. TRUE by default.

formula an object of class "formula" describing the x and y variables. logN ~ time as a

default.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

#### Value

An instance of FitMultipleGrowthMCMC().

# Examples

fit\_secondary\_growth 55

```
start <- list(mu_opt = .8, temperature_xopt = 30)
## We can now call the fitting function
set.seed(12412)
global_MCMC <- fit_multiple_growth_MCMC(start, multiple_experiments, known, sec_names, niter = 1000,
    lower = c(.2, 29),  # lower limits of the model parameters
    upper = c(.8, 34))  # upper limits of the model parameters

## Parameter estimates can be retrieved with summary
summary(global_MCMC)

## We can compare fitted model against observations
plot(global_MCMC)

## Any single environmental factor can be added to the plot using add_factor
plot(global_MCMC, add_factor = "temperature")</pre>
```

fit\_secondary\_growth Fit secondary growth models

## **Description**

## [Stable]

Fits a secondary growth model to a set of growth rates obtained experimentally. Modelling is done according to the gamma concept proposed by Zwietering (1992) and cardinal parameter models.

#### Usage

```
fit_secondary_growth(
  fit_data,
  starting_point,
  known_pars,
  sec_model_names,
  transformation = "sq",
  ...,
  check = TRUE,
  formula = mu ~ .
)
```

#### **Arguments**

fit\_data

Tibble with the data used for the fit. It must have one column with the observed growth rate (named mu by default; can be changed using the "formula" argument) and as many columns as needed with the environmental factors.

starting\_point Named vector with initial values for the model parameters to estimate from the

data. The growth rate under optimum conditions must be named mu\_opt. The rest must be called 'env\_factor'+'\_'+'parameter'. For instance, the minimum

pH for growth is 'pH\_xmin'.

known\_pars Named vector of fixed model parameters. Must be named using the same con-

vention as starting\_point.

sec\_model\_names

Named character vector defining the secondary model for each environmental

factor.

transformation Character defining the transformation of mu for model fitting. One of sq (square

root; default), log (log-transform) or none (no transformation).

... Additional arguments passed to modFit().

check Whether to do some basic checks (TRUE by default).

formula an object of class "formula" describing the y variable. The right hand side must

be ".". By default mu ~ ..

## Value

An instance of FitSecondaryGrowth().

## **Examples**

full\_Ratkowski 57

```
plot(fit_cardinal)

## Passing which = 2, generates a different kind of plot

plot(fit_cardinal, which = 2)
plot(fit_cardinal, which = 2, add_trend = TRUE)
plot(fit_cardinal, which = 2, add_segment = TRUE)
```

full\_Ratkowski

Full Ratkowsky model

## **Description**

Gamma model adapted from the one by Ratkowsky et al. (1983).

## **Usage**

```
full_Ratkowski(x, xmin, xmax, c)
```

# Arguments

x Value of the environmental factor.xmin Minimum value for growthxmax Maximum value for growth

c Parameter defining the speed of the decline

get\_all\_predictions A helper for making the plots

## **Description**

A helper for making the plots

## Usage

```
get_all_predictions(model)
```

## **Arguments**

model

An instance of FitMultipleDynamicGrowth

58 get\_dyna\_residuals

## **Description**

Function for calculating residuals of a dynamic prediction according to the requirements of modFit().

## Usage

```
get_dyna_residuals(
  this_p,
  fit_data,
  env_conditions,
  known_pars,
  sec_model_names,
  cost = NULL,
  logbase_mu = logbase_logN,
  logbase_logN = 10
)
```

## **Arguments**

this\_p named vector of model parameters

fit\_data tibble with the data for the fit

env\_conditions tibble with the environmental conditions known\_pars named vector of known model parameters

sec\_model\_names

named character vector with names the environmental conditions and values the

secondary model (e.g. 'CPM').

an instance of modCost to be combined (to fit multiple models).

logbase\_mu Base of the logarithm of the growthrate. By default, the same as logbase\_logN.

See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

#### Value

An instance of modCost().

get\_iso\_residuals 59

get_iso_residuals Residua	als of	f isothermal	prediction
---------------------------	--------	--------------	------------

## **Description**

Residuals of isothermal prediction

# Usage

```
get_iso_residuals(
  this_p,
  fit_data,
  model_name,
  known_pars,
  logbase_mu = logbase_logN,
  logbase_logN = 10
)
```

# Arguments

this\_p named vector of model parameters to fit

fit\_data tibble with the data for the fit

model\_name character defining the primary growth model

known\_pars named vector of fixed model parameters

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See vignette about units for details.

## Value

An instance of modCost.

# Description

Function for calculating residuals of dynamic predictions under different conditions for the same model parameters according to the requirements of modFit().

## Usage

```
get_multi_dyna_residuals(
   this_p,
   experiment_data,
   known_pars,
   sec_model_names,
   logbase_mu = logbase_logN,
   logbase_logN = 10
)
```

## **Arguments**

this\_p named vector of model parameters

experiment\_data

a nested list with the experimental data. Each entry describes one experiment as a list with two elements: data and conditions. data is a tibble with two columns: time and logN. conditions is a tibble with one column named time and as many additional solumns as a programmental factors.

additional columns as environmental factors.

known\_pars named vector of known model parameters

sec\_model\_names

named character vector with names of the environmental conditions and values

of the secondary model (see secondary\_model\_data).

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

#### Value

an instance of modCost.

```
get_secondary_residuals
```

Residuals of secondary models

## **Description**

Residual function for fit\_secondary\_growth().

```
get_secondary_residuals(
  this_p,
  my_data,
  known_pars,
  sec_model_names,
  transformation
)
```

## **Arguments**

this\_p Named vector of model parameter values.

my\_data Tibble with the data used for the fit.

known\_pars Named vector of fixed model paramaters.

sec\_model\_names

Named character vector defining the secondary model for each environmental

factor.

transformation Character defining the tranformation of mu for model fitting. One of sq (square

root), log (log-transform) or none (no transformation).

## Value

A numeric vector of residuals.

GlobalGrowthComparison

GlobalGrowthComparison class

## **Description**

The GlobalGrowthComparison class contains several functions for model comparison and model selection of growth models. It should not be instanced directly. Instead, it should be constructed using compare\_growth\_fits(). It is similar to GrowthComparison, although with specific tools to deal with several experiments.

It includes two type of tools for model selection and comparison: statistical indexes and visual analyses. Please check the sections below for details.

Note that all these tools use the names defined in compare\_growth\_fits(), so we recommend passing a named list to that function.

```
## S3 method for class 'GlobalGrowthComparison'
coef(object, ...)

## S3 method for class 'GlobalGrowthComparison'
summary(object, ...)

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

## S3 method for class 'GlobalGrowthComparison'
plot(x, y, ..., type = 1, add_trend = TRUE)
```

#### **Arguments**

object an instance of GlobalGrowthComparison

... ignored

x an instance of GlobalGrowthComparison

y ignored

type if type==1, the plot compares the model predictions. If type ==2, the plot compares the parameter estimates. If type==3, the plot shows the residuals

add\_trend should a trend line of the residuals be added for type==3? TRUE by default

## Methods (by generic)

• coef(GlobalGrowthComparison): table of parameter estimates

• summary(GlobalGrowthComparison): summary table for the comparison

• print(GlobalGrowthComparison): print of the model comparison

• plot(GlobalGrowthComparison): illustrations comparing the fitted models

#### Statistical indexes

 ${\sf GlobalGrowthComparison}$  implements two  ${\sf S3}$  methods to obtain numerical values to facilitate model comparison and selection.

- the coef method returns a tibble with the values of the parameter estimates and their corresponding standard errors for each model.
- the summary returns a tibble with the AIC, number of degrees of freedom, mean error and root mean squared error for each model.

## Visual analyses

The S3 plot method can generate three types of plots:

- when type = 1, the plot compares the fitted growth curves against the experimental data used to fit the model.
- when type = 2, the plot compares the parameter estimates using error bars, where the limits of the error bars are the expected value +/- one standard error. In case one model does not has some model parameter (i.e. either because it is not defined or because it was fixed), the parameter is not included in the plot.
- when type=3, the plot shows the tendency of the residuals for each model. This plot can be used to detect deviations from independence.

These plots are divided by facets for each experiment.

GlobalGrowthFit 63

GlobalGrowthFit

GlobalGrowthFit class

## **Description**

## [Stable]

The GlobalGrowthFit class contains a growth model fitted to data using a global approach. Its constructor is fit\_growth().

It is a subclass of list with the items:

- algorithm: type of algorithm as in fit\_growth()
- data: data used for model fitting
- start: initial guess of the model parameters
- known: fixed model parameters
- primary\_model: a character describing the primary model
- fit\_results: an instance of modFit or modMCMC with the results of the fit
- best\_prediction: Instance of GrowthPrediction with the best growth fit
- sec\_models: a named vector with the secondary models assigned for each environmental factor. NULL for environment="constant"
- env\_conditions: a list with the environmental conditions used for model fitting. NULL for environment="constant"
- niter: number of iterations of the Markov chain. NULL if algorithm != "MCMC"
- logbase\_mu: base of the logarithm for the definition of parameter mu (check the relevant vignette)
- logbase\_logN: base of the logarithm for the definition of the population size (check the relevant vignette)
- environment: "dynamic". Always

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

## S3 method for class 'GlobalGrowthFit'
coef(object, ...)

## S3 method for class 'GlobalGrowthFit'
summary(object, ...)

## S3 method for class 'GlobalGrowthFit'
predict(object, env_conditions, times = NULL, ...)

## S3 method for class 'GlobalGrowthFit'
```

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```
residuals(object, ...)
## S3 method for class 'GlobalGrowthFit'
vcov(object, ...)
## S3 method for class 'GlobalGrowthFit'
deviance(object, ...)
## S3 method for class 'GlobalGrowthFit'
fitted(object, ...)
## S3 method for class 'GlobalGrowthFit'
logLik(object, ...)
## S3 method for class 'GlobalGrowthFit'
AIC(object, ..., k = 2)
## S3 method for class 'GlobalGrowthFit'
plot(
  Х,
 y = NULL,
  add_factor = NULL,
  ylims = NULL,
  label_x = "time",
  label_y1 = NULL,
  label_y2 = add_factor,
  line_col = "black",
  line_size = 1,
  line_type = "solid",
  line_col2 = "black",
  line\_size2 = 1,
  line_type2 = "dashed",
  point_size = 3,
  point_shape = 16,
  subplot_labels = "AUTO"
)
## S3 method for class 'GlobalGrowthFit'
predictMCMC(
 model,
  times,
  env_conditions,
 niter,
 newpars = NULL,
  formula = . \sim time
)
```

GlobalGrowthFit 65

#### **Arguments**

x an instance of GlobalGrowthFit

... ignored

object an instance of GlobalGrowthFit

env\_conditions Tibble with the (dynamic) environmental conditions during the experiment. It

must have one column named 'time' with the storage time and as many columns

as required with the environmental conditions.

times Numeric vector of storage times for the predictions.

k penalty for the parameters (k=2 by default)

y ignored

add\_factor whether to plot also one environmental factor. If NULL (default), no environ-

mental factor is plotted. If set to one character string that matches one entry of

x\$env\_conditions, that condition is plotted in the secondary axis

ylims A two dimensional vector with the limits of the primary y-axis.

label\_x label of the x-axis

label\_y1 Label of the primary y-axis.label\_y2 Label of the secondary y-axis.

line\_col Aesthetic parameter to change the colour of the line geom in the plot, see:

geom\_line()

line\_size Aesthetic parameter to change the thickness of the line geom in the plot, see:

geom\_line()

line\_type Aesthetic parameter to change the type of the line geom in the plot, takes num-

bers (1-6) or strings ("solid") see: geom\_line()

line\_col2 Same as lin\_col, but for the environmental factor.

line\_size2 Same as line\_size, but for the environmental factor.

line\_type2 Same as lin\_type, but for the environmental factor.

point\_size Size of the data points
point\_shape shape of the data points

subplot\_labels labels of the subplots according to plot\_grid.

model An instance of GlobalGrowthFit

niter Number of iterations.

newpars A named list defining new values for the some model parameters. The name

must be the identifier of a model already included in the model. These parameters do not include variation, so defining a new value for a fitted parameters

"fixes" it. NULL by default (no new parameters).

formula A formula stating the column named defining the elapsed time in env\_conditions.

By default, . ~ time.

#### Value

An instance of MCMCgrowth.

66 greek\_tractors

## Methods (by generic)

- print(GlobalGrowthFit): print of the model
- coef(GlobalGrowthFit): vector of fitted model parameters.
- summary(GlobalGrowthFit): statistical summary of the fit.
- predict(GlobalGrowthFit): vector of model predictions
- residuals (GlobalGrowthFit): model residuals. They are returned as a tibble with 4 columns: time (storage time), logN (observed count), exp (name of the experiment) and res (residual).
- vcov(GlobalGrowthFit): variance-covariance matrix of the model, estimated as 1/(0.5\*Hessian) for regression and as the variance-covariance of the draws for MCMC
- deviance(GlobalGrowthFit): deviance of the model.
- fitted(GlobalGrowthFit): fitted values. They are returned as a tibble with 3 columns: time (storage time), exp (experiment identifier) and fitted (fitted value).
- logLik(GlobalGrowthFit): loglikelihood of the model
- AIC(GlobalGrowthFit): Akaike Information Criterion
- plot(GlobalGrowthFit): comparison between the fitted model and the experimental data.
- predictMCMC(GlobalGrowthFit): prediction including parameter uncertainty

greek\_tractors

Number of tractors in Greece according to the World Bank

# Description

A dataset showing the increase in tractors in Greece. It was retrieved from https://data.worldbank.org/indicator/AG.AGR.TRA

## Usage

greek\_tractors

## **Format**

A tibble with 46 rows (each corresponding to one year) and 7 columns:

year Year for the recording

tractors Number of tractors

GrowthComparison 67

## Description

The GrowthComparison class contains several functions for model comparison and model selection of growth models. It should not be instanced directly. Instead, it should be constructed using compare\_growth\_fits().

It includes two type of tools for model selection and comparison: statistical indexes and visual analyses. Please check the sections below for details.

Note that all these tools use the names defined in compare\_growth\_fits(), so we recommend passing a named list to that function.

# Usage

```
## S3 method for class 'GrowthComparison'
plot(x, y, ..., type = 1, add_trend = TRUE)
## S3 method for class 'GrowthComparison'
coef(object, ...)
## S3 method for class 'GrowthComparison'
print(x, ...)
## S3 method for class 'GrowthComparison'
summary(object, ...)
```

## **Arguments**

X	an instance of GrowthComparison
у	ignored
	ignored
type	if type==1, the plot compares the model predictions. If type ==2, the plot compares the parameter estimates. If type==3, the plot shows the residuals
add_trend	should a trend line of the residuals be added for type==3? TRUE by default
object	an instance of GrowthComparison

## Methods (by generic)

- plot(GrowthComparison): illustrations comparing the fitted models
- $\bullet \ \ \mathsf{coef}(\mathsf{GrowthComparison}) \colon \mathsf{table} \ \mathsf{of} \ \mathsf{parameter} \ \mathsf{estimates}$
- print(GrowthComparison): print of the model comparison
- summary(GrowthComparison): summary table for the comparison

#### Statistical indexes

GrowthComparison implements two S3 methods to obtain numerical values to facilitate model comparison and selection.

- the coef method returns a tibble with the values of the parameter estimates and their corresponding standard errors for each model.
- the summary returns a tibble with the AIC, number of degrees of freedom, mean error and root mean squared error for each model.

#### Visual analyses

The S3 plot method can generate three types of plots:

- when type = 1, the plot compares the fitted growth curves against the experimental data used to fit the model.
- when type = 2, the plot compares the parameter estimates using error bars, where the limits of the error bars are the expected value +/- one standard error. In case one model does not have some model parameter (i.e. either because it is not defined or because it was fixed), the parameter is not included in the plot.
- when type=3, the plot shows the tendency of the residuals for each model. This plot can be used to detect deviations from independence.

GrowthFit

GrowthFit class

## **Description**

## [Stable]

The GrowthFit class contains a growth model fitted to data under static or dynamic conditions. Its constructor is fit\_growth().

It is a subclass of list with the items:

- environment: type of environment as in fit\_growth()
- algorithm: type of algorithm as in fit\_growth()
- data: data used for model fitting
- · start: initial guess of the model parameters
- known: fixed model parameters
- primary\_model: a character describing the primary model
- fit\_results: an instance of modFit or modMCMC with the results of the fit
- best\_prediction: Instance of GrowthPrediction with the best growth fit
- sec\_models: a named vector with the secondary models assigned for each environmental factor. NULL for environment="constant"
- env\_conditions: a tibble with the environmental conditions used for model fitting. NULL for environment="constant"

- niter: number of iterations of the Markov chain. NULL if algorithm != "MCMC"
- logbase\_mu: base of the logarithm for the definition of parameter mu (check the relevant vignette)
- logbase\_logN: base of the logarithm for the definition of the population size (check the relevant vignette)

```
## S3 method for class 'GrowthFit'
print(x, ...)
## S3 method for class 'GrowthFit'
coef(object, ...)
## S3 method for class 'GrowthFit'
summary(object, ...)
## S3 method for class 'GrowthFit'
predict(object, times = NULL, env_conditions = NULL, ...)
## S3 method for class 'GrowthFit'
residuals(object, ...)
## S3 method for class 'GrowthFit'
vcov(object, ...)
## S3 method for class 'GrowthFit'
deviance(object, ...)
## S3 method for class 'GrowthFit'
fitted(object, ...)
## S3 method for class 'GrowthFit'
logLik(object, ...)
## S3 method for class 'GrowthFit'
AIC(object, ..., k = 2)
## S3 method for class 'GrowthFit'
plot(
  Х,
 y = NULL,
  ...,
  add_factor = NULL,
  line_col = "black",
  line_size = 1,
  line_type = 1,
  point_col = "black",
```

```
point_size = 3,
 point_shape = 16,
 ylims = NULL,
  label_y1 = NULL,
 label_y2 = add_factor,
 label_x = "time",
 line_col2 = "black",
 line\_size2 = 1,
 line_type2 = "dashed"
)
## S3 method for class 'GrowthFit'
predictMCMC(
 model,
  times,
  env_conditions,
 niter,
 newpars = NULL,
  formula = . \sim time
```

# **Arguments** ×

	ignored.
object	an instance of GrowthFit
times	Numeric vector of storage times for the predictions.
env_conditions	Tibble with the (dynamic) environmental conditions during the experiment. It must have one column named 'time' with the storage time and as many columns as required with the environmental conditions.
k	penalty for the parameters (k=2 by default)
У	ignored
add_factor	whether to plot also one environmental factor. If NULL (default), no environmental factor is plotted. If set to one character string that matches one entry of x\$env_conditions, that condition is plotted in the secondary axis. Ignored if environment="constant"
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
point_col	Aesthetic parameter to change the colour of the point geom, see: geom_point()
point_size	Aesthetic parameter to change the size of the point geom, see: geom_point()
point_shape	Aesthetic parameter to change the shape of the point geom, see: geom_point()

The object of class GrowthFit to plot.

ylims	A two dimensional vector with the limits of the primary y-axis. NULL by default
label_y1	Label of the primary y-axis.
label_y2	Label of the secondary y-axis. Ignored if environment="constant"
label_x	Label of the x-axis
line_col2	$Same \ as \ lin\_col, \ but \ for \ the \ environmental \ factor. \ Ignored \ if \ environment="constant"$
line_size2	Same as line_size, but for the environmental factor. Ignored if environment="constant"
line_type2	$Same \ as \ lin\_type, \ but \ for \ the \ environmental \ factor. \ Ignored \ if \ environment="constant"$
model	An instance of GrowthFit
niter	Number of iterations.
newpars	A named list defining new values for the some model parameters. The name must be the identifier of a model already included in the model. These parameters do not include variation, so defining a new value for a fitted parameters "fixes" it. NULL by default (no new parameters).
formula	A formula stating the column named defining the elapsed time in env_conditions. By default, . ~ time.

## Value

An instance of MCMCgrowth.

# Methods (by generic)

- print(GrowthFit): print of the model
- coef(GrowthFit): vector of fitted model parameters.
- summary (GrowthFit): statistical summary of the fit.
- predict(GrowthFit): vector of model predictions.
- residuals(GrowthFit): vector of model residuals.
- vcov(GrowthFit): variance-covariance matrix of the model, estimated as 1/(0.5\*Hessian) for regression and as the variance-covariance of the draws for MCMC
- deviance(GrowthFit): deviance of the model.
- fitted(GrowthFit): vector of fitted values.
- logLik(GrowthFit): loglikelihood of the model
- AIC(GrowthFit): Akaike Information Criterion
- plot(GrowthFit): compares the fitted model against the data.
- predictMCMC(GrowthFit): prediction including parameter uncertainty

72 GrowthPrediction

GrowthPrediction

GrowthPrediction class

#### **Description**

#### [Stable]

The GrowthPrediction class contains the results of a growth prediction. Its constructor is predict\_growth(). It is a subclass of list with the items:

- simulation: a tibble with the model simulation
- primary model: a list describing the primary model as in predict\_growth()
- environment: a character describing the type of environmental conditions as in predict\_growth()
- env\_conditions: a named list with the functions used to approximate the (dynamic) environmental conditions. NULL if environment="constant".
- sec\_models: a named list describing the secondary models as in predict\_growth(). NULL if environment="constant".
- gammas: a tibble describing the variation of the gamma factors through the experiment. NUll if environment="constant".
- logbase\_mu: the log-base for the definition of parameter mu (see the relevant vignette)
- logbase\_logN: the log-base for the definition of the logarithm of the population size

```
## S3 method for class 'GrowthPrediction'
print(x, ...)
## S3 method for class 'GrowthPrediction'
summary(object, ...)
## S3 method for class 'GrowthPrediction'
plot(
  х,
 y = NULL
  add_factor = NULL,
  ylims = NULL,
  label_y1 = NULL,
  label_y2 = add_factor,
  line_col = "black",
  line_size = 1,
  line_type = "solid",
  line_col2 = "black",
  line_size2 = 1,
  line_type2 = "dashed",
```

GrowthPrediction 73

```
label_x = "time"
)
## S3 method for class 'GrowthPrediction'
coef(object, ...)
```

# Arguments

x	The object of class GrowthPrediction to plot.
	ignored
object	an instance of GrowthPrediction
У	ignored
add_factor	whether to plot also one environmental factor. If NULL (default), no environmental factor is plotted. If set to one character string that matches one entry of x\$env_conditions, that condition is plotted in the secondary axis. Ignored for environment="constant".
ylims	A two dimensional vector with the limits of the primary y-axis.
label_y1	Label of the primary y-axis.
label_y2	Label of the secondary y-axis.
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
line_col2	Same as lin_col, but for the environmental factor.
line_size2	Same as line_size, but for the environmental factor.
line_type2	Same as lin_type, but for the environmental factor.
label_x	Label of the x-axis.

# Methods (by generic)

- print(GrowthPrediction): print of the model
- summary(GrowthPrediction): summary of the model
- plot(GrowthPrediction): predicted growth curve.
- coef(GrowthPrediction): coefficients of the model

74 GrowthUncertainty

GrowthUncertainty

GrowthUncertainty class

# **Description**

#### [Stable]

The GrowthUncertainty class contains the results of a growth prediction under isothermal conditions considering parameter uncertainty. Its constructor is predict\_growth\_uncertainty().

It is a subclass of list with the items:

- sample: parameter sample used for the calculations.
- simulations: growth curves predicted for each parameter.
- quantiles: limits of the credible intervals (5%, 10%, 50%, 90%, 95%) for each time point.
- model: Model used for the calculations.
- mus: Mean parameter values used for the simulations.
- sigma: Variance-covariance matrix used for the simulations.

#### Usage

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

## S3 method for class 'GrowthUncertainty'
plot(
    x,
    y = NULL,
    ...,
    line_col = "black",
    line_size = 0.5,
    line_type = "solid",
    ribbon80_fill = "grey",
    ribbon90_fill = "grey",
    alpha80 = 0.5,
    alpha90 = 0.4
)
```

#### **Arguments**

line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
ribbon80_fill	fill colour for the space between the 10th and 90th quantile, see: geom_ribbon()
ribbon90_fill	fill colour for the space between the 5th and 95th quantile, see: <pre>geom_ribbon()</pre>
alpha80	transparency of the ribbon aesthetic for the space between the 10th and 90th quantile. Takes a value between 0 (fully transparant) and 1 (fully opaque)
alpha90	transparency of the ribbon aesthetic for the space between the 5th and 95th quantile. Takes a value between 0 (fully transparant) and 1 (fully opaque).

# Methods (by generic)

- print(GrowthUncertainty): print of the model
- plot(GrowthUncertainty): Growth prediction (prediction band) considering parameter uncertainty.

 ${\tt growth\_pH\_temperature} \ \ \textit{Example of dynamic growth}$ 

# Description

A dataset to demonstrate the use of fit\_dynamic\_growth. The values of the environmental conditions are described in conditions\_pH\_temperature.

# Usage

```
growth_pH_temperature
```

# **Format**

A tibble with 20 rows and 2 columns:

time elapsed time

logN decimal logarithm of the population size

76 is.DynamicGrowth

growth\_salmonella

Growth of Salmonella spp in broth

# Description

An example dataset to illustrate fit\_isothermal\_growth(). It describes the growth of Salmonella spp. in broth. It was retrieved from ComBase (ID: B092\_10).

# Usage

```
growth_salmonella
```

#### **Format**

A tibble with 21 rows and 2 columns:

time elapsed time in hours.

**logN** observed population size (log CFU/g).

is.DynamicGrowth

Test of DynamicGrowth object

# Description

Tests if an object is of class DynamicGrowth.

# Usage

```
is.DynamicGrowth(x)
```

## **Arguments**

Χ

object to be checked.

#### Value

A boolean specifying whether x is of class DynamicGrowth

is.FitDynamicGrowth 77

is.FitDynamicGrowth

Test of FitDynamicGrowth object

# Description

Tests if an object is of class FitDynamicGrowth.

## Usage

```
is.FitDynamicGrowth(x)
```

# Arguments

Χ

object to be checked.

## Value

A boolean specifying whether x is of class FitDynamicGrowth

```
\verb"is.FitDynamicGrowthMCMC"
```

Test of FitDynamicGrowthMCMC object

# Description

Tests if an object is of class FitDynamicGrowthMCMC.

# Usage

```
is.FitDynamicGrowthMCMC(x)
```

## **Arguments**

Χ

object to be checked.

## Value

A boolean specifying whether x is of class FitDynamicGrowthMCMC

is.FitIsoGrowth

Test of FitIsoGrowth object

# Description

Tests if an object is of class FitIsoGrowth.

## Usage

```
is.FitIsoGrowth(x)
```

# Arguments

Χ

object to be checked.

## Value

A boolean specifying whether x is of class FitIsoGrowth

```
is. Fit {\tt Multiple Dynamic Growth}
```

Test of FitMultipleDynamicGrowth object

# Description

Tests if an object is of class FitMultipleDynamicGrowth.

# Usage

```
is.FitMultipleDynamicGrowth(x)
```

## **Arguments**

Х

object to be checked.

## Value

A boolean specifying whether  $\boldsymbol{x}$  is of class FitMultipleDynamicGrowth

is.FitMultipleDynamicGrowthMCMC

 $Test\ of\ Fit Multiple Dynamic Growth MCMC\ object$ 

# Description

Tests if an object is of class FitMultipleDynamicGrowthMCMC.

## Usage

```
is.FitMultipleDynamicGrowthMCMC(x)
```

# Arguments

x object to be checked.

# Value

A boolean specifying whether x is of class FitMultipleDynamicGrowthMCMC

 ${\tt is.FitSecondaryGrowth}\ \ \textit{Test of FitSecondaryGrowth object}$ 

## **Description**

Tests if an object is of class FitSecondaryGrowth.

# Usage

```
is.FitSecondaryGrowth(x)
```

## **Arguments**

x object to be checked.

## Value

A boolean specifying whether x is of class FitSecondaryGrowth

80 is.GrowthFit

is.GlobalGrowthFit

Test of GlobalGrowthFit object

# Description

Tests if an object is of class GlobalGrowthFit

# Usage

```
is.GlobalGrowthFit(x)
```

## **Arguments**

Χ

object to be checked.

#### Value

A boolean specifying whether x is of class GlobalGrowthFit

is.GrowthFit

Test of GrowthFit object

# Description

Tests if an object is of class GrowthFit

## Usage

```
is.GrowthFit(x)
```

# Arguments

Х

object to be checked.

## Value

A boolean specifying whether x is of class GrowthFit

is.GrowthPrediction 81

is.GrowthPrediction

Test of GrowthPrediction object

# Description

Tests if an object is of class GrowthPrediction

# Usage

```
is.GrowthPrediction(x)
```

## **Arguments**

Х

object to be checked.

#### Value

A boolean specifying whether x is of class GrowthPrediction

# Description

Tests if an object is of class GrowthUncertainty

## Usage

```
is.GrowthUncertainty(x)
```

# Arguments

Х

object to be checked.

# Value

A boolean specifying whether x is of class GrowthUncertainty

is.MCMCgrowth

is.IsothermalGrowth Tes

Test of IsothermalGrowth object

# Description

Tests if an object is of class IsothermalGrowth.

# Usage

```
is.IsothermalGrowth(x)
```

## **Arguments**

Х

object to be checked.

#### Value

A boolean specifying whether x is of class IsothermalGrowth

 $is. {\tt MCMCgrowth}$ 

Test of MCMCgrowth object

# Description

Tests if an object is of class MCMCgrowth.

## Usage

```
is.MCMCgrowth(x)
```

# Arguments

Х

object to be checked.

## Value

A boolean specifying whether x is of class MCMCgrowth

is.StochasticGrowth 83

is.StochasticGrowth Test

Test of StochasticGrowth object

## **Description**

Tests if an object is of class StochasticGrowth.

# Usage

```
is.StochasticGrowth(x)
```

## **Arguments**

Χ

object to be checked.

#### Value

A boolean specifying whether x is of class StochasticGrowth

IsothermalGrowth

IsothermalGrowth class

### **Description**

### [Superseded]

The class IsothermalGrowth has been superseded by the top-level class GrowthPrediction, which provides a unified approach for growth modelling.

Still, it is still returned if the superseded predict\_isothermal\_growth() is called.

It is a subclass of list with the items:

- simulation: A tibble with the model simulation.
- model: The name of the model used for the predictions.
- pars: A list with the values of the model parameters.

## Usage

```
## S3 method for class 'IsothermalGrowth'
print(x, ...)
## S3 method for class 'IsothermalGrowth'
plot(
    x,
    y = NULL,
```

84 iso\_Baranyi

```
line_col = "black",
line_size = 1,
line_type = "solid",
ylims = NULL,
label_y = NULL,
label_x = "time"
)

## S3 method for class 'IsothermalGrowth'
coef(object, ...)
```

# Arguments

X	The object of class IsothermalGrowth to plot.
	ignored
У	ignored
line_col	Aesthetic parameter to change the colour of the line, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line, see: geom_line()
line_type	Aesthetic parameter to change the type of the line, takes numbers (1-6) or strings ("solid") see: geom_line()
ylims	Two-dimensional numeric vector with the limits of the y-axis (or NULL, which is the default)
label_y	Title of the y-axis
label_x	Title of the x-axis
object	an instance of IsothermalGrowth

# Methods (by generic)

- print(IsothermalGrowth): print of the model
- plot(IsothermalGrowth): plot of the predicted growth curve.
- coef(IsothermalGrowth): coefficients of the model

iso_Baranyi Isothermal Baranyi model	iso_Baranyi
--------------------------------------	-------------

# Description

Baranyi growth model as defined by Baranyi and Roberts (1994). We use the solution calculated by Poschet et al. (2005, doi: https://doi.org/10.1016/j.ijfoodmicro.2004.10.008) after log-transformation according to MONTE CARLO ANALYSIS FOR MICROBIAL GROWTH CURVES, by Oksuz and Buzrul.

### Usage

```
iso_Baranyi(times, logN0, mu, lambda, logNmax)
```

iso\_repGompertz 85

## **Arguments**

times Numeric vector of storage times

logN0 Initial log microbial count

mu Maximum specific growth rate (in ln CFU/t)

lambda Lag phase duration

logNmax Maximum log microbial count

#### Value

Numeric vector with the predicted microbial count.

iso\_repGompertz Reparameterized Gompertz model

# Description

Reparameterized Gompertz growth model defined by Zwietering et al. (1990).

## Usage

```
iso_repGompertz(times, logN0, C, mu, lambda)
```

# **Arguments**

times Numeric vector of storage times

logN0 Initial log microbial count

C Difference between logN0 and the maximum log-count.

mu Maximum specific growth rate (in ln CFU/t)

lambda Lag phase duration

# Value

Numeric vector with the predicted microbial count.

86 logistic\_model

lambda_to_Q0 Q0 from lag p	pnase a	uration
----------------------------	---------	---------

# Description

## [Stable]

Convenience function to calculate the value of Q0 for the Baranyi model from the duration of the lag phase

#### Usage

```
lambda_to_Q0(lambda, mu, logbase_mu = 10)
```

## Arguments

lambda Duration of the lag phase.

mu Specific growth rate in the exponential phase.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, 10 (i.e. log10).

See vignette about units for details.

## **Description**

Logistic growth model

# Usage

```
logistic_model(times, logN0, mu, lambda, C)
```

## **Arguments**

times Numeric vector of storage times logN0 Initial log microbial count

mu Maximum specific growth rate (in ln CFU/t)

lambda Lag phase duration

C Difference between logN0 and the maximum log-count.

#### Value

Numeric vector with the predicted microbial count

make\_guess\_factor 87

make_guess_f	fac	tor
--------------	-----	-----

Initial guesses for the secondary model of one factor

#### **Description**

Initial guesses for the secondary model of one factor

### Usage

```
make_guess_factor(fit_data, sec_model, factor)
```

#### **Arguments**

fit\_data Tibble with the data used for the fit. It must have one column with the observed

growth rate (named mu by default; can be changed using the "formula" argument)

and as many columns as needed with the environmental factors.

sec\_model character defining the secondary model equation according to secondary\_model\_data()

factor character defining the environmental factor

make\_guess\_primary

*Initial guesses for fitting primary growth models* 

#### **Description**

#### [Experimental]

The function uses some heuristics to provide initial guesses for the parameters of the growth model selected that can be used with fit\_growth().

#### Usage

```
make_guess_primary(
  fit_data,
  primary_model,
  logbase_mu = 10,
  formula = logN ~ time
)
```

### **Arguments**

fit\_data the experimental data. A tibble (or data.frame) with a column named time with

the elapsed time and one called logN with the logarithm of the population size

primary\_model a string defining the equation of the primary model, as defined in primary\_model\_data()

logbase\_mu Base of the logarithm the growth rate is referred to. By default, 10 (i.e. log10).

See vignette about units for details.

formula an object of class "formula" describing the x and y variables. logN ~ time as a

default.

### Value

A named numeric vector of initial guesses for the model parameters

#### **Examples**

## **Description**

# [Experimental]

Uses some heuristic rules to generate an initial guess of the model parameters of secondary growth models that can be used for model fitting with fit\_secondary\_growth().

#### Usage

```
make_guess_secondary(fit_data, sec_model_names)
```

MCMCgrowth 89

#### **Arguments**

fit\_data

Tibble with the data used for the fit. It must have one column with the observed growth rate (named mu by default; can be changed using the "formula" argument) and as many columns as needed with the environmental factors.

sec\_model\_names

Named character vector defining the secondary model for each environmental factor.

#### **Examples**

MCMCgrowth

MCMCgrowth class

### **Description**

#### [Stable]

The MCMCgrowth class contains the results of a growth prediction consider parameter variability based on a model fitted using an MCMC algorithm.

It is a subclass of list with items:

- sample: Parameter sample used for the calculations.
- simulations: Individual growth curves calculated based on the parameter sample.
- quantiles: Tibble with the limits of the credible intervals (5%, 10%, 50%, 90% and 95%) for each time point.
- model: Instance of FitDynamicGrowthMCMC used for predictions.
- env\_conditions: A tibble with the environmental conditions of the simulation.

90 MCMCgrowth

# Usage

```
## S3 method for class 'MCMCgrowth'
print(x, ...)
## S3 method for class 'MCMCgrowth'
plot(
  х,
  y = NULL,
  add_factor = NULL,
  alpha_80 = 0.5,
  fill_80 = "grey",
  alpha_90 = 0.5,
  fill_90 = "grey",
  label_y1 = "logN",
  label_y2 = add_factor,
  line_col = "black",
  line_type = 1,
  line_size = 1,
  line_type2 = 2,
  line_col2 = "black",
  line\_size2 = 1,
  ylims = NULL
)
```

# Arguments

x	The object of class MCMCgrowth to plot.
	ignored.
у	ignored
add_factor	Includes the variation of one environmental factor in the plot. It must be one of the column names in x\$env_conditions.
alpha_80	transparency of the ribbon for the 80th posterior5 by default.
fill_80	fill colour of the ribbon for the 80th posterior. "grey" by default.
alpha_90	transparency of the ribbon for the 90th posterior5 by default.
fill_90	fill colour of the ribbon for the 90th posterior. "grey" by default.
label_y1	label of the primary y axis. "logN" by default.
label_y2	label of the secondary y axis. The name of the environmental factor by default.
line_col	colour of the line representing the median. "black" by default.
line_type	linetype for the line representing the median. solid by default.
line_size	size of the line representing the median. 1 by default.
line_type2	linetype for the line representing the environmental condition. Dashed by default.
line_col2	colour of the line representing the environmental condition. "black" by default.

multiple\_conditions 91

line\_size2 size of the line representing the environmental condition. 1 by default. ylims limits of the primary y-axis. NULL by default (let ggplot choose).

# Methods (by generic)

- print(MCMCgrowth): print of the model
- plot(MCMCgrowth): plot of predicted growth (prediction band).

#### **Description**

This dataset is paired with multiple\_counts to illustrate the global fitting of fit\_growth().

#### Usage

```
multiple_conditions
```

#### **Format**

A nested list with two elements, each one corresponding to one experiment. Each element is a data.frame with three columns:

• time: elapsed time

• temperature: observed temperature

• pH: observed pH

multiple\_counts

Population growth observed in several dynamic experiments

# Description

This dataset is paired with multiple\_conditions to illustrate the global fitting of fit\_growth().

#### Usage

```
multiple_counts
```

#### **Format**

A nested list with two elements, each one corresponding to one experiment. Each element is a data.frame with two columns:

• time: elapsed time

• logN: log10 of the microbial concentration

92 predictMCMC

multiple\_experiments A set of growth experiments under dynamic conditions

## **Description**

An example dataset illustrating the requirements of  $fit_multiple_growth()$  and  $fit_multiple_growth_MCMC()$ .

## Usage

```
multiple_experiments
```

#### **Format**

A nested list with two elements. Each element corresponds to one experiment and is described by a list with two data frames:

data a tibble describing the microbial counts. It has 2 columns: time (elapsed time) and logN (logarithm of the microbial count).

**conditions** a tibble describing the environmental conditions. It has 3 columns: time (elapsed time), temperature (storage temperature) and pH (pH of the media).

predictMCMC

Generic for calculating predictions with uncertainty from fits

## **Description**

Generic for calculating predictions with uncertainty from fits

## Usage

```
predictMCMC(
  model,
  times,
  env_conditions,
  niter,
  newpars = NULL,
  formula = . ~ time
)
```

### Arguments

model Fit object

times see specific methods for each class env\_conditions see specific methods for each class niter see specific methods for each class newpars see specific methods for each class

formula A formula stating the column named defining the elapsed time in env\_conditions.

By default, . ~ time.

predict\_dynamic\_growth

Growth under dynamic conditions

# **Description**

# [Superseded]

The function predict\_dynamic\_growth() has been superseded by the top-level function predict\_growth(), which provides a unified approach for growth modelling.

Regardless on that, it can still predict population growth under dynamic conditions based on the Baranyi model (Baranyi and Roberts, 1994) and secondary models based on the gamma concept (Zwietering et al. 1992).

Model predictions are done by linear interpolation of the environmental conditions defined in env\_conditions.

#### **Usage**

```
predict_dynamic_growth(
   times,
   env_conditions,
   primary_pars,
   secondary_models,
   ...,
   check = TRUE,
   logbase_logN = 10,
   logbase_mu = logbase_logN,
   formula = . ~ time
)
```

# Arguments

times Numeric vector of storage times to make the predictions

env\_conditions Tibble (or data.frame) describing the variation of the environmental conditions

during storage. It must have with the elapsed time (named time by default; can be changed with the "formula" argument), and as many additional columns as

environmental factors.

primary\_pars A named list defining the parameters of the primary model and the initial values of the model variables. That is, with names mu\_opt, Nmax, N0, Q0.

secondary\_models

A nested list describing the secondary models.

... Additional arguments for ode().

check Whether to check the validity of the models. TRUE by default.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

formula An object of class "formula" describing the x variable. . ~ time as a default.

#### Value

An instance of DynamicGrowth().

## **Examples**

```
## Definition of the environmental conditions
library(tibble)
my\_conditions <- tibble(time = c(0, 5, 40),
    temperature = c(20, 30, 35),
    pH = c(7, 6.5, 5)
## Definition of the model parameters
my_primary <- list(mu_opt = 2,</pre>
    Nmax = 1e8, N0 = 1e0,
    Q0 = 1e-3
sec_temperature <- list(model = "Zwietering",</pre>
    xmin = 25, xopt = 35, n = 1)
sec_pH = list(model = "CPM",
    xmin = 5.5, xopt = 6.5,
    xmax = 7.5, n = 2)
my_secondary <- list(</pre>
    temperature = sec_temperature,
    pH = sec_pH
my_times < - seq(0, 50, length = 1000)
## Do the simulation
```

predict\_growth

Prediction of microbial growth

## **Description**

#### [Stable]

This function provides a top-level interface for predicting population growth. Predictions can be made either under constant or dynamic environmental conditions. See below for details on the calculations.

#### Usage

```
predict_growth(
   times,
   primary_model,
   environment = "constant",
   secondary_models = NULL,
   env_conditions = NULL,
   ...,
   check = TRUE,
   logbase_mu = logbase_logN,
   logbase_logN = 10,
   formula = . ~ time
)
```

#### **Arguments**

times numeric vector of time points for making the predictions

primary\_model named list defining the values of the parameters of the primary growth model

environment type of environment. Either "constant" (default) or "dynamic" (see below for details on the calculations for each condition)

secondary\_models

a nested list describing the secondary models. See below for details

env\_conditions Tibble describing the variation of the environmental conditions for dynamic ex-

periments. It must have with the elapsed time (named time by default; can be changed with the "formula" argument), and as many additional columns as

environmental factors. Ignored for "constant" environments.

... Additional arguments for ode().

check Whether to check the validity of the models. TRUE by default.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

formula An object of class "formula" describing the x variable for predictions under

dynamic conditions. . ~ time as a default.

#### **Details**

To ease data input, the functions can convert between parameters defined in different scales. Namely, for predictions in constant environments (environment="constant"):

- "logN0" can be defined as "N0". The function automatically calculates the log-transformation.
- "logNmax" can be defined as "Nmax". The function automatically calculates the log-transformation.
- "mu" can be defined as "mu\_opt". The function assumes the prediction is under optimal growth conditions.
- "lambda" can be defined by "Q0". The duration of the lag phase is calculated using  $Q0_{to_1}$

And, for predictions in dynamic environments (environment="dynamic"):

- "N0" can be defined as "N0". The function automatically calculates the antilog-transformation.
- "Nmax" can be defined as "logNmax". The function automatically calculates the antilogtransformation.
- "mu" can be defined as "mu\_opt". The function assumes mu was calculated under optimal growth conditions.
- "Q0" can be defined by the value of "lambda" under dynamic conditions. Then, the value of Q0 is calculated using lambda\_to\_Q0().

#### Value

An instance of GrowthPrediction.

#### **Predictions in constant environments**

Predictions under constant environments are calculated using only primary models. Consequently, the arguments "secondary\_models" and "env\_conditions" are ignored. If these were passed, the function would return a warning. In this case, predictions are calculated using the algebraic form of the primary model (see vignette for details).

The growth model is defined through the "primary\_model" argument using a named list. One of the list elements must be named "model" and must take take one of the valid keys returned by primary\_model\_data(). The remaining entries of the list define the values of the parameters of the selected model. A list of valid keys can be retrieved using primary\_model\_data() (see example below). Note that the functions can do some operations to facilitate the compatibility between constant and dynamic environments (see Details).

#### Predictions in dynamic environments

Predictions under dynamic environments are calculated by solving numerically the differential equation of the Baranyi growth model. The effect of changes in the environmental conditions in the growth rate are calculated according to the gamma approach. Therefore, one must define both primary and secondary models.

The dynamic environmental conditions are defined using a tibble (or data.frame) through the "env\_conditions" argument. It must include one column named "time" stating the elapsed time and as many additional columns as environmental conditions included in the prediction. For values of time not included in the tibble, the values of the environmental conditions are calculated by linear interpolation.

Primary models are defined as a named list through the "primary\_model" argument. It must include the following elements:

- N0: initial population size
- Nmax: maximum population size in the stationary growth phase
- mu\_opt: growth rate under optimal growth conditions
- Q0: value defining the duration of the lag phase Additional details on these parameters can be found in the package vignettes.

Secondary models are defined as a nested list through the "secondary\_models" argument. The list must have one entry per environmental condition, whose name must match those used in the "env\_conditions" argument. Each of these entries must be a named list defining the secondary model for each environmental condition. The model equation is defined in an entry named "model" (valid keys can be retrieved from secondary\_model\_data()). Then, additional entries defined the values of each model parameters (valid keys can be retrieved from secondary\_model\_data())

For additional details on how to define the secondary models, please see the package vignettes (and examples below).

#### **Examples**

```
## Example 1 - Growth under constant conditions ------
## Valid model keys can be retrieved calling primary_model_data()
primary_model_data()

my_model <- "modGompertz" # we will use the modified-Gompertz

## The keys of the model parameters can also be obtained from primary_model_data()
primary_model_data(my_model)$pars</pre>
```

```
## We define the primary model as a list
my_model <- list(model = "modGompertz", logN0 = 0, C = 6, mu = .2, lambda = 20)
## We can now make the predictions
my_time <- seq(0, 100, length = 1000) # Vector of time points for the calculations
my_prediction <- predict_growth(my_time, my_model, environment = "constant")</pre>
## The instance of IsothermalGrowth includes several S3 methods
print(my_prediction)
plot(my_prediction)
coef(my_prediction)
## Example 2 - Growth under dynamic conditions ------
## We will consider the effect of two factors: temperature and pH
my\_conditions \leftarrow data.frame(time = c(0, 5, 40),
                            temperature = c(20, 30, 35),
                            pH = c(7, 6.5, 5)
## The primary model is defined as a named list
my_primary <- list(mu = 2, Nmax = 1e7, N0 = 1, Q0 = 1e-3)
## The secondary model is defined independently for each factor
sec_temperature <- list(model = "Zwietering",</pre>
    xmin = 25, xopt = 35, n = 1)
sec_pH = list(model = "CPM",
   xmin = 5.5, xopt = 6.5,
   xmax = 7.5, n = 2)
## Then, they are assigned to each factor using a named list
my_secondary <- list(</pre>
    temperature = sec_temperature,
    pH = sec_pH
## We can call the function now
my\_times <- seq(0, 50, length = 1000) # Where the output is calculated
dynamic_prediction <- predict_growth(environment = "dynamic",</pre>
                                     my_times, my_primary, my_secondary,
                                     my_conditions
```

```
## The instance of DynamicGrowth includes several useful S3 methods
print(dynamic_prediction)
plot(dynamic_prediction)
plot(dynamic_prediction, add_factor = "pH")
coef(dynamic_prediction)
## The time_to_size function can predict the time to reach a population size
```

time\_to\_size(my\_prediction, 3)

predict\_growth\_uncertainty

Isothermal growth with parameter uncertainty

### **Description**

#### [Stable]

Simulation of microbial growth considering uncertianty in the model parameters. Calculations are based on Monte Carlo simulations, considering the parameters follow a multivariate normal distribution.

#### Usage

```
predict_growth_uncertainty(
  model_name,
  times,
  n_sims,
  pars,
  corr_matrix = diag(nrow(pars)),
  check = TRUE
)
```

#### **Arguments**

model\_name Character describing the primary growth model.

times Numeric vector of storage times for the simulations.

n\_sims Number of simulations.

pars A tibble describing the parameter uncertainty (see details).

corr\_matrix Correlation matrix of the model parameters. Defined in the same order as in

pars. An identity matrix by default (uncorrelated parameters).

check Whether to do some tests. FALSE by default.

#### **Details**

The distributions of the model parameters are defined in the pars argument using a tibble with 4 columns:

- par: identifier of the model parameter (according to primary\_model\_data()),
- mean: mean value of the model parameter.,
- sd: standard deviation of the model parameter.,
- scale: scale at which the model parameter is defined. Valid values are 'original' (no transformation), 'sqrt' square root or 'log' log-scale. The parameter sample is generated considering the parameter follows a marginal normal distribution at this scale, and is later converted to the original scale for calculations.

#### Value

An instance of GrowthUncertainty().

### **Examples**

```
## Definition of the simulation settings
my_model <- "Baranyi"</pre>
my\_times \leftarrow seq(0, 30, length = 100)
n_sims <- 3000
library(tibble)
pars <- tribble(</pre>
    ~par, ~mean, ~sd, ~scale,
    "logN0", 0, .2, "original",
    "mu", 2, .3, "sqrt",
    "lambda", 4, .4, "sqrt",
    "logNmax", 6, .5, "original"
)
## Calling the function
stoc_growth <- predict_growth_uncertainty(my_model, my_times, n_sims, pars)</pre>
## We can plot the results
plot(stoc_growth)
## Adding parameter correlation
my\_cor <- matrix(c(1, 0, 0, 0,
    0, 1, 0.7, 0,
    0, 0.7, 1, 0,
    0, 0, 0, 1),
    nrow = 4)
```

```
stoc_growth2 <- predict_growth_uncertainty(my_model, my_times, n_sims, pars, my_cor)
plot(stoc_growth2)
## The time_to_size function can calculate the median growth curve to reach a size
time_to_size(stoc_growth, 4)
## Or the distribution of times
dist <- time_to_size(stoc_growth, 4, type = "distribution")
plot(dist)</pre>
```

predict\_isothermal\_growth

Isothermal microbial growth

# Description

## [Superseded]

The function predict\_isothermal\_growth() has been superseded by the top-level function predict\_growth(), which provides a unified approach for growth modelling.

Regardless of that, it can still be used to predict population growth under static environmental conditions (i.e. using primary models).

## Usage

```
predict_isothermal_growth(
  model_name,
  times,
  model_pars,
  check = TRUE,
  logbase_mu = 10,
  logbase_logN = 10
)
```

### **Arguments**

model\_name Character defining the growth model.

times Numeric vector of storage times for the predictions.

model\_pars Named vector or list defining the values of the model parameters.

check Whether to do basic checks (TRUE by default).

logbase\_mu Base of the logarithm the growth rate is referred to. By default, the same as

logbase\_logN. See vignette about units for details.

logbase\_logN Base of the logarithm for the population size. By default, 10 (i.e. log10). See

vignette about units for details.

# Value

An instance of IsothermalGrowth().

# **Examples**

```
## Define the simulations parameters

my_model <- "modGompertz"

my_pars <- list(logN0 = 2, C = 6, mu = .2, lambda = 25)

my_time <- seq(0, 100, length = 1000)

## Do the simulation

static_prediction <- predict_isothermal_growth(my_model, my_time, my_pars)

## Plot the results

plot(static_prediction)</pre>
```

predict\_MCMC\_growth

Stochastic growth of MCMC fit

## Description

### [Superseded]

The function predict\_MCMC\_growth() has been superseded by predictMCMC() S3 methods of the relevant classes.

Nonetheless, it can still make a prediction of microbial growth including parameter uncertainty based on a growth model fitted using fit\_MCMC\_growth() or fit\_multiple\_growth\_MCMC(). This function predicts growth curves for niter samples (with replacement) of the samples of the MCMC algorithm. Then, credible intervals are calculated based on the quantiles of the model predictions at each time point.

# Usage

```
predict_MCMC_growth(
   MCMCfit,
   times,
   env_conditions,
   niter,
```

```
newpars = NULL,
formula = . ~ time
)
```

#### **Arguments**

MCMCfit An instance of FitDynamicGrowthMCMC or FitMultipleGrowthMCMC.

times Numeric vector of storage times for the predictions.

env\_conditions Tibble with the (dynamic) environmental conditions during the experiment. It

must have one column named 'time' with the storage time and as many columns

as required with the environmental conditions.

niter Number of iterations.

newpars A named list defining new values for the some model parameters. The name

must be the identifier of a model already included in the model. These parameters do not include variation, so defining a new value for a fitted parameters

"fixes" it. NULL by default (no new parameters).

formula A formula stating the column named defining the elapsed time in env\_conditions.

By default, . ~ time.

#### Value

An instance of MCMCgrowth().

#### **Examples**

```
## We need a FitDynamicGrowthMCMC object
data("example_dynamic_growth")
data("example_env_conditions")
sec_model_names <- c(temperature = "CPM", aw= "CPM")</pre>
known_pars <- list(Nmax = 1e4, # Primary model</pre>
   N0 = 1e0, Q0 = 1e-3, # Initial values of the primary model
   mu_opt = 4, # mu_opt of the gamma model
    temperature_n = 1, # Secondary model for temperature
    aw_xmax = 1, aw_xmin = .9, aw_n = 1 # Secondary model for water activity
my_start <- list(temperature_xmin = 25, temperature_xopt = 35,</pre>
    temperature\_xmax = 40,
    aw\_xopt = .95)
set.seed(12124) # Setting seed for repeatability
my_MCMC_fit <- fit_MCMC_growth(example_dynamic_growth, example_env_conditions,</pre>
    my_start, known_pars, sec_model_names, niter = 3000)
## Define the conditions for the simulation
```

predict\_stochastic\_growth

Deprecated isothermal growth with parameter uncertainty

# Description

# [Deprecated]

predict\_stochastic\_growth() was renamed predict\_growth\_uncertainty() because the original function name may be misleading, as this is not a stochastic differential equation

## Usage

```
predict_stochastic_growth(
  model_name,
  times,
  n_sims,
  pars,
  corr_matrix = diag(nrow(pars)),
  check = TRUE
)
```

primary\_model\_data 105

# Arguments

model\_name Character describing the primary growth model.

times Numeric vector of storage times for the simulations.

n\_sims Number of simulations.

pars A tibble describing the parameter uncertainty (see details).

corr\_matrix Correlation matrix of the model parameters. Defined in the same order as in

pars. An identity matrix by default (uncorrelated parameters).

check Whether to do some tests. FALSE by default.

primary\_model\_data

Metainformation of primary growth models

## **Description**

## [Stable]

Provides different types of meta-data about the primary growth models included in biogrowth. This information is the basis of the automatic checks, and can also help in the definition of models for predict\_growth() and fit\_growth().

## Usage

```
primary_model_data(model_name = NULL)
```

# **Arguments**

model\_name The name of the model or NULL (default).

#### Value

If model\_name is NULL, returns a character string with the available models. If is a valid identifier, it returns a list with metainformation about the model. If model\_name name is not a valid identifier, raises an error.

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Q0_to_lambda	
--------------	--

#### **Description**

#### [Stable]

Convenience function to calculate the lag phase duration (lambda) of the Baranyi model from the maximum specific growth rate and the initial value of the variable Q.

Note that this function uses the unit system of biogrowth (i.e. log10). Care must be taken when using parameters obtained from other sources.

# Usage

```
Q0_to_lambda(q0, mu, logbase_mu = 10)
```

#### Arguments

q0 Initial value of the variable Q.

mu Specific growth rate in the exponential phase.

logbase\_mu Base of the logarithm the growth rate is referred to. By default, 10 (i.e. log10).

See vignette about units for details.

refrigeratorSpain Temperature recorded in refrigerators

# Description

This dataset includes the temperature recorded in refrigerators in households of the Catalonia region. The data was published as part of Jofre et al. (2019) Domestic refrigerator temperatures in Spain: Assessment of its impact on the safety and shelf-life of cooked meat products. Food Research International, 126, 108578. And was kindly provided by the original authors of the study.

### Usage

refrigeratorSpain

#### **Format**

A tibble with three columns:

- time: elapsed time in hours
- A1: temperature observed in refrigerator "1"
- A2: temperature observed in refrigerator "2"

richards\_model 107

richards_model	Richards growth model	

## Description

Richards growth model

## Usage

```
richards_model(times, logN0, mu, lambda, C, nu)
```

## **Arguments**

times	Numeric vector of storage times
logN0	Initial log microbial count
mu	Maximum specific growth rate (in ln CFU/t)

lambda Lag phase duration

C Difference between logN0 and the maximum log-count.

nu Parameter describing the transition between growth phases

SecondaryComparison SecondaryComparison class

# Description

The SecondaryComparison class contains several functions for model comparison and model selection of growth models. It should not be instanced directly. Instead, it should be constructed using compare\_secondary\_fits().

It includes two type of tools for model selection and comparison: statistical indexes and visual analyses. Please check the sections below for details.

Note that all these tools use the names defined in compare\_secondary\_fits(), so we recommend passing a named list to that function.

## Usage

```
## S3 method for class 'SecondaryComparison'
coef(object, ...)
## S3 method for class 'SecondaryComparison'
summary(object, ...)
## S3 method for class 'SecondaryComparison'
print(x, ...)
## S3 method for class 'SecondaryComparison'
plot(x, y, ..., type = 1, add_trend = TRUE)
```

### **Arguments**

object	an instance of SecondaryComparison
	ignored
x	an instance of SecondaryComparison
У	ignored
type	if type==1, the plot compares the model predictions. If type ==2, the plot compares the parameter estimates.
add_trend	should a trend line of the residuals be added for type==3? TRUE by default

## Methods (by generic)

- coef(SecondaryComparison): table of parameter estimates
- summary(SecondaryComparison): summary table for the comparison
- print(SecondaryComparison): print of the model comparison
- plot(SecondaryComparison): illustrations comparing the fitted models

#### Statistical indexes

SecondaryComparison implements two S3 methods to obtain numerical values to facilitate model comparison and selection.

- the coef method returns a tibble with the values of the parameter estimates and their corresponding standard errors for each model.
- the summary returns a tibble with the AIC, number of degrees of freedom, mean error and root mean squared error for each model.

### Visual analyses

The S3 plot method can generate three types of plots:

- when type = 1, the plot compares the observations against the model predictions for each model. The plot includes a linear model fitted to the residuals. In the case of a perfect fit, the line would have slope=1 and intercept=0 (shown as a black, dashed line).
- when type = 2, the plot compares the parameter estimates using error bars, where the limits of the error bars are the expected value +/- one standard error. In case one model does not has some model parameter (i.e. either because it is not defined or because it was fixed), the parameter is not included in the plot.

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# Description

## [Stable]

Provides different types of meta-data about the secondary growth models included in biogrowth. This information is the basis of the automatic checks, and can also help in the definition of models for predict\_growth() and fit\_growth().

#### Usage

```
secondary_model_data(model_name = NULL)
```

## **Arguments**

model\_name

The name of the model or NULL (default).

#### Value

If model\_name is NULL, returns a character string with the available models. If is a valid identifier, it returns a list with metainformation about the model. If model\_name name is not a valid identifier, raises an error.

show\_guess\_dynamic

Plot of the initial guess for growth under dynamic environmental conditions

## **Description**

Compares the prediction corresponding to a guess of the parameters of the model against experimental data

# Usage

```
show_guess_dynamic(
  fit_data,
  model_keys,
  guess,
  env_conditions,
  logbase_mu = 10,
  formula = logN ~ time
)
```

show\_guess\_primary

## **Arguments**

fit\_data Tibble (or data.frame) of data for the fit. It must have two columns, one with the elapsed time (time by default) and another one with the decimal logarithm of the populatoin size (logN by default). Different column names can be defined using the formula argument. Named the equations of the secondary model as in fit\_growth() model\_keys Named vector with the initial guess of the model parameters as in fit\_growth() guess env\_conditions Tibble describing the variation of the environmental conditions for dynamic experiments. See fit\_growth(). logbase\_mu Base of the logarithm the growth rate is referred to. By default, 10 (i.e. log10). See vignette about units for details. formula an object of class "formula" describing the x and y variables. logN ~ time as a

#### Value

A ggplot() comparing the model prediction against the data

default.

 ${\tt show\_guess\_primary} \qquad \textit{Plot of the initial guess for growth under constant environmental conditions}$ 

## **Description**

Compares the prediction corresponding to a guess of the parameters of the primary model against experimental data

#### Usage

```
show_guess_primary(
  fit_data,
  model_name,
  guess,
  logbase_mu = 10,
  formula = logN ~ time
)
```

#### **Arguments**

Tibble (or data.frame) of data for the fit. It must have two columns, one with the elapsed time (time by default) and another one with the decimal logarithm of the population size (logN by default). Different column names can be defined using the formula argument.

Model\_name

Character defining the primary growth model as per primary\_model\_data()

Named vector with the initial guess of the model parameters

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logbase_mu	Base of the logarithm the growth rate is referred to. By default, 10 (i.e. log10). See vignette about units for details.
formula	an object of class "formula" describing the $x$ and $y$ variables. $logN \sim time$ as a default.

#### Value

A ggplot() comparing the model prediction against the data

StochasticGrowth StochasticGrowth class

## **Description**

#### [Deprecated]

The class StochasticGrowth has been deprecated by class GrowthUncertainty, which provides less misleading name.

Still, it is still returned if the deprecated predict\_stochastic\_growth() is called.

The StochasticGrowth class contains the results of a growth prediction under isothermal conditions considering parameter unceratinty. Its constructor is predict\_stochastic\_growth().

It is a subclass of list with the items:

- sample: parameter sample used for the calculations.
- simulations: growth curves predicted for each parameter.
- quantiles: limits of the credible intervals (5%, 10%, 50%, 90%, 95%) for each time point.
- model: Model used for the calculations.
- mus: Mean parameter values used for the simulations.
- sigma: Variance-covariance matrix used for the simulations.

## Usage

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

## S3 method for class 'StochasticGrowth'
plot(
    x,
    y = NULL,
    ...,
    line_col = "black",
    line_size = 0.5,
    line_type = "solid",
    ribbon80_fill = "grey",
    ribbon90_fill = "grey",
    alpha80 = 0.5,
    alpha90 = 0.4
)
```

TimeDistribution

## **Arguments**

X	The object of class StochasticGrowth to plot.
	ignored.
у	ignored
line_col	Aesthetic parameter to change the colour of the line geom in the plot, see: geom_line()
line_size	Aesthetic parameter to change the thickness of the line geom in the plot, see: geom_line()
line_type	Aesthetic parameter to change the type of the line geom in the plot, takes numbers (1-6) or strings ("solid") see: geom_line()
ribbon80_fill	fill colour for the space between the 10th and 90th quantile, see: geom_ribbon()
ribbon90_fill	fill colour for the space between the 5th and 95th quantile, see: geom_ribbon()
alpha80	transparency of the ribbon aesthetic for the space between the 10th and 90th quantile. Takes a value between 0 (fully transparant) and 1 (fully opaque)
alpha90	transparency of the ribbon aesthetic for the space between the 5th and 95th quantile. Takes a value between 0 (fully transparant) and 1 (fully opaque).

## **Details**

FitIsoGrowth class

# Methods (by generic)

- print(StochasticGrowth): print of the model
- plot(StochasticGrowth): Growth prediction (prediction band) considering parameter uncertainty.

TimeDistribution	TimeDistribution class	
------------------	------------------------	--

# Description

The TimeDistribution class contains an estimate of the probability distribution of the time to reach a given microbial count. Its constructor is distribution\_to\_logcount().

It is a subclass of list with the items:

- distribution Sample of the distribution of times to reach log\_count.
- summary Summary statistics of distribution (mean, sd, median, q10 and q90).

time\_to\_logcount 113

## Usage

```
## S3 method for class 'TimeDistribution'
print(x, ...)
## S3 method for class 'TimeDistribution'
summary(object, ...)
## S3 method for class 'TimeDistribution'
plot(x, y = NULL, ..., bin_width = NULL)
```

#### **Arguments**

x The object of class TimeDistribution to plot.

... ignored.

object An instance of TimeDistribution.

y ignored.

bin\_width A number that specifies the width of a bin in the histogram, see: geom\_histogram().

NULL by default.

## Methods (by generic)

• print(TimeDistribution): print of the model

• summary(TimeDistribution): summary of the model

• plot(TimeDistribution): plot of the distribution of the time to reach a microbial count.

time\_to\_logcount

Time to reach a given microbial count

## **Description**

#### [Superseded]

The function time\_to\_logcount() has been superseded by function time\_to\_size(), which provides a more general interface.

But it still returns the storage time required for the microbial count to reach log\_count according to the predictions of model. Calculations are done using linear interpolation of the model predictions.

## Usage

```
time_to_logcount(model, log_count)
```

# Arguments

model An instance of IsothermalGrowth or DynamicGrowth.

log\_count The target log microbial count.

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## Value

The predicted time to reach log\_count.

#### **Examples**

```
## First of all, we will get an IsothermalGrowth object

my_model <- "modGompertz"

my_pars <- list(logN0 = 2, C = 6, mu = .2, lambda = 25)

my_time <- seq(0, 100, length = 1000)

static_prediction <- predict_isothermal_growth(my_model, my_time, my_pars)

plot(static_prediction)

## And now we calculate the time to reach a microbial count

time_to_logcount(static_prediction, 2.5)

## If log_count is outside the range of the predicted values, NA is returned

time_to_logcount(static_prediction, 20)</pre>
```

time\_to\_size

Time for the population to reach a given size

## **Description**

# [Experimental]

Calculates the elapsed time required for the population to reach a given size (in log scale)

## Usage

```
time_to_size(model, size, type = "discrete", logbase_logN = NULL)
```

## **Arguments**

model	An instance of GrowthPrediction, GrowthFit, GlobalGrowthFit, GrowthUncertainty or MCMCgrowth.
size	Target population size (in log scale)
type	Tye of calculation, either "discrete" (default) or "distribution"
logbase_logN	Base of the logarithm for the population size. By default, 10 (i.e. log10). See vignette about units for details.

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#### **Details**

The calculation method differs depending on the value of type. If type="discrete" (default), the function calculates by linear interpolation a discrete time to reach the target population size. If type="distribution", this calculation is repeated several times, generating a distribution of the time. Note that this is only possible for instances of GrowthUncertainty or MCMCgrowth.

#### Value

If type="discrete", a number. If type="distribution", an instance of TimeDistribution.

#### **Examples**

```
## Example 1 - Growth predictions ------
## The model is defined as usual with predict_growth
my_model <- list(model = "modGompertz", logN0 = 0, C = 6, mu = .2, lambda = 20)</pre>
my_time <- seq(0, 100, length = 1000) # Vector of time points for the calculations
my_prediction <- predict_growth(my_time, my_model, environment = "constant")</pre>
plot(my_prediction)
## We just have to pass the model and the size (in log10)
time_to_size(my_prediction, 3)
## If the size is not reached, it returns NA
time_to_size(my_prediction, 8)
## By default, it considers the population size is defined in the same log-base
## as the prediction. But that can be changed using logbase_logN
time_to_size(my_prediction, 3)
time_to_size(my_prediction, 3, logbase_logN = 10)
time_to_size(my_prediction, log(100), logbase_logN = exp(1))
## Example 2 - Model fit -------
my_{data} \leftarrow data.frame(time = c(0, 25, 50, 75, 100),
                     logN = c(2, 2.5, 7, 8, 8))
models <- list(primary = "Baranyi")</pre>
known <- c(mu = .2)
start <- c(logNmax = 8, lambda = 25, logN0 = 2)
primary_fit <- fit_growth(my_data, models, start, known,</pre>
```

trilinear\_model

```
environment = "constant",
plot(primary_fit)
time_to_size(primary_fit, 4)
## Example 3 - Global fitting -----
## We need a model first
data("multiple_counts")
data("multiple_conditions")
sec_models <- list(temperature = "CPM", pH = "CPM")</pre>
known_pars <- list(Nmax = 1e8, N0 = 1e0, Q0 = 1e-3,
                  temperature_n = 2, temperature_xmin = 20,
                  temperature\_xmax = 35,
                  temperature_xopt = 30,
                  pH_n = 2, pH_xmin = 5.5, pH_xmax = 7.5, pH_xopt = 6.5)
my_start <- list(mu_opt = .8)
global_fit <- fit_growth(multiple_counts,</pre>
                        sec_models,
                        my_start,
                        known_pars,
                        environment = "dynamic",
                        algorithm = "regression",
                        approach = "global",
                        env_conditions = multiple_conditions
plot(global_fit)
## The function calculates the time for each experiment
time_to_size(global_fit, 3)
## It returns NA for the particular experiment if the size is not reached
time_to_size(global_fit, 4.5)
```

trilinear\_model

*Trilinear growth model* 

### **Description**

Trilinear growth model defined by Buchanan et al. (1997).

zwietering\_gamma 117

#### Usage

```
trilinear_model(times, logN0, mu, lambda, logNmax)
```

## **Arguments**

times Numeric vector of storage times logN0 Initial log microbial count

mu Maximum specific growth rate (in ln CFU/t)

lambda Lag phase duration

logNmax Maximum log microbial count

#### Value

Numeric vector with the predicted microbial count.

zwietering\_gamma model

## **Description**

Gamma model as defined by Zwietering et al. (1992). To avoid unreasonable predictions, it has been modified setting gamma=0 for values of x outside (xmin, xopt)

# Usage

```
zwietering_gamma(x, xmin, xopt, n)
```

# **Arguments**

x Value of the environmental factor.

xmin Minimum value of the environmental factor for growth.

xopt Maximum value for growth

n Exponent of the secondary model

## Value

The corresponding gamma factor.

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