Package 'rTPC'

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Type Package

Title Fitting and Analysing Thermal Performance Curves

Version 1.0.4

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Description Helps to fit thermal performance curves (TPCs). 'rTPC' contains 26 model formulations previously used to fit TPCs and has helper functions to set sensible start parameters, upper and lower parameter limits and estimate parameters useful in downstream analyses, such as cardinal temperatures, maximum rate and optimum temperature. See Padfield et al. (2021) <doi:10.1111/2041-210X.13585>.

License GPL-3

URL https://github.com/padpadpad/rTPC

BugReports https://github.com/padpadpadpad/rTPC/issues

Depends R (>= 2.10)

Imports stats

Suggests boot, broom, car, forcats, ggplot2, ggrepel, knitr, minpack.lm, MuMIn, nls.multstart, nlstools, patchwork, progress, RColorBrewer, rmarkdown, stringr, testthat, tidyverse

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bacteria_tpc

Example thermal performance curves of bacterial growth

Description

A dataset containing example data of growth rates of the bacteria Pseudomonas fluorescens in the presence and absence of its phage, phi2. Growth rates were measured across a range of assay temperatures to incorporate the entire thermal performance of the bacteria The dataset is the cleaned version so some data points have been omitted. There are multiple independent measurements per temperature for each treatment.

Usage

```
data("bacteria_tpc")
```

Format

A data frame with 649 rows and 7 variables:

phage whether the bacteria was grown with or without phagetemp the assay temperature at which the growth rate was measured (degrees centigrade)rate estimated growth rate per hour

Source

Daniel Padfield

References

Padfield, D., Castledine, M., & Buckling, A. (2020). Temperature-dependent changes to host–parasite interactions alter the thermal performance of a bacterial host. The ISME Journal, 14(2), 389-398.

```
data("bacteria_tpc")
library(ggplot2)
ggplot(bacteria_tpc) +
  geom_point(aes(temp, rate, col = phage))
```

beta_2012

beta_2012

Beta model for fitting thermal performance curves

Description

Beta model for fitting thermal performance curves

Usage

```
beta_2012(temp, a, b, c, d, e)
```

Arguments

temp	temperature in degrees centigrade
a	dimensionless parameter
b	dimensionless parameter
С	dimensionless parameter
d	dimensionless parameter
е	dimensionless parameter

Details

Equation:

$$rate = \frac{a\left(\frac{temp - b + \frac{c(d-1)}{d+e-2}}{c}\right)^{d-1} \cdot \left(1 - \frac{temp - b + \frac{c(d-1)}{d+e-2}}{c}\right)^{e-1}}{\left(\frac{d-1}{d+e-2}\right)^{d-1} \cdot \left(\frac{e-1}{d+e-2}\right)^{e-1}}$$

Start values in get_start_vals are derived from the data or sensible values from the literature.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model difficult to fit.

Author(s)

Daniel Padfield

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References

Niehaus, Amanda C., et al. Predicting the physiological performance of ectotherms in fluctuating thermal environments. Journal of Experimental Biology 215.4: 694-701 (2012)

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'beta_2012')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~beta_2012(temp = temp, a, b, c, d, e),</pre>
data = d,
iter = c(7,7,7,7,7),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'beta_2012'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'beta_2012'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

boatman_2017

Boatman model for fitting thermal performance curves

Description

Boatman model for fitting thermal performance curves

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Usage

```
boatman_2017(temp, rmax, tmin, tmax, a, b)
```

Arguments

temp	temperature in degrees centigrade
rmax	the rate at optimum temperature
tmin	low temperature (°C) at which rates become negative
tmax	high temperature (°C) at which rates become negative
a	shape parameter to adjust the skewness of the curve
b	shape parameter to adjust the kurtosis of the curve

Details

Equation:

$$rate = r_{max} \cdot \left(sin \left(\pi \left(\frac{temp - t_{min}}{t_{max} - t_{min}} \right)^{a} \right) \right)^{b}$$

Start values in get_start_vals are derived from the data or sensible values from the literature.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Boatman, T. G., Lawson, T., & Geider, R. J. A key marine diazotroph in a changing ocean: The interacting effects of temperature, CO2 and light on the growth of Trichodesmium erythraeum IMS101. PLoS ONE, 12, e0168796 (2017)

```
# load in ggplot
library(ggplot2)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'boatman_2017')</pre>
```

briere2_1999 7

```
# fit model
mod <- nls.multstart::nls_multstart(rate~boatman_2017(temp = temp, rmax, tmin, tmax, a, b),</pre>
data = d,
iter = c(4,4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'boatman_2017'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'boatman_2017'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

briere2_1999

Briere2 model for fitting thermal performance curves

Description

Briere2 model for fitting thermal performance curves

Usage

```
briere2_1999(temp, tmin, tmax, a, b)
```

Arguments

temp	temperature in degrees centigrade
tmin	low temperature (°C) at which rates become negative
tmax	high temperature (°C) at which rates become negative
a	scale parameter to adjust maximum rate of the curve
b	shape parameter to adjust the asymmetry of the curve

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Details

Equation:

$$rate = a \cdot temp \cdot (temp - t_{min}) \cdot (t_{max} - temp)^{\frac{1}{b}}$$

Start values in get_start_vals are derived from the data or sensible values from the literature.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Brière, J.F., Pracros, P., Le Roux, A.Y., Pierre, J.S., A novel rate model of temperature-dependent development for arthropods. Environmental Entomololgy, 28, 22–29 (1999)

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'briere2_1999')
mod <- nls.multstart::nls_multstart(rate~briere2_1999(temp = temp, tmin, tmax, a, b),</pre>
data = d,
iter = c(4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'briere2_1999'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'briere2_1999'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
```

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```
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

calc_params

Calculate extra parameters of a thermal performance curve

Description

Calculate extra parameters of a thermal performance curve

Usage

```
calc_params(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Currently estimates:

- maximum rate (rmax) using get_rmax()
- optimum temperature (topt) using get_topt()
- critical thermal maximum (ctmax) using get_ctmax()
- critical thermal minimum (ctmin) using get_ctmin()
- activation energy (e) using get_e()
- deactivation energy (eh) using get_eh()
- q10 value using get_q10()
- thermal safety margin using get_thermalsafetymargin()
- thermal tolerance using get_thermaltolerance()
- thermal performance breadth using get_breadth()
- skewness using get_skewness()

Value

a dataframe containing the estimates of key TPC traits for a given model object. If any parameters cannot be calculated for a thermal performance curve, they will return NA.

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chlorella_tpc

Example metabolic thermal performance curves

Description

A dataset containing example data of rates of photosynthesis and respiration of the phytoplankton Chlorella vulgaris. Instantaneous rates of metabolism were made across a range of assay temperatures to incorporate the entire thermal performance of the populations. The dataset is the cleaned version so some datapoints have been omitted.

Usage

```
data("chlorella_tpc")
```

Format

A data frame with 649 rows and 7 variables:

curve_id a unique value for each separate curve

growth_temp the growth temperature that the culture was maintained at before measurements were taken (degrees centigrade)

process whether the cultures had been kept for a long time at their growth temperature (adaptation/~100 generations) or a short time (a measure of acclimation/~10 generations)

flux whether the curve depicts respiration or gross photosynthesis

temp the assay temperature at which the metabolic rate was measured (degrees centigrade)

rate the metabolic rate measured (micro mol O2 micro gram C-1 hr-1)

Source

Daniel Padfield

References

Padfield, D., Yvon-durocher, G., Buckling, A., Jennings, S. & Yvon-durocher, G. (2015). Rapid evolution of metabolic traits explains thermal adaptation in phytoplankton, Ecology Letters, 19, 133-142.

```
data("chlorella_tpc")
library(ggplot2)
ggplot(chlorella_tpc) +
  geom_point(aes(temp, rate, col = process)) +
  facet_wrap(~ growth_temp + flux)
```

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delong_2017	DeLong enzyme-assisted Arrhenius model for fitting thermal performance curves

Description

DeLong enzyme-assisted Arrhenius model for fitting thermal performance curves

Usage

```
delong_2017(temp, c, eb, ef, tm, ehc)
```

Arguments

temp	temperature in degrees centigrade
С	potential reaction rate
eb	baseline energy needed for the reaction to occur (eV)
ef	temperature dependence of folding the enzymes used in the metabolic reaction, relative to the melting temperature (eV)
tm	melting temperature in degrees centigrade
ehc	temperature dependence of the heat capacity between the folded and unfolded state of the enzymes, relative to the melting temperature (eV)

Details

Equation:

$$rate = c \cdot exp \frac{-\left(e_b - \left(e_f\left(1 - \frac{temp + 273.15}{t_m}\right) + e_{hc} \cdot \left(\left(temp + 273.15\right) - t_m - \left(temp + 273.15\right) \cdot ln(\frac{temp + 273.15}{t_m})\right)\right)\right)}{k \cdot \left(temp + 273.15\right)}$$

where k is Boltzmann's constant with a value of 8.62e-05 and tm is actually tm - 273.15

Start values in get_start_vals are derived from the data or sensible values from the literature.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

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References

DeLong, John P., et al. The combined effects of reactant kinetics and enzyme stability explain the temperature dependence of metabolic rates. Ecology and evolution 7.11 (2017): 3940-3950.

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'delong_2017')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~delong_2017(temp = temp, c, eb, ef, tm,ehc),</pre>
data = d,
iter = c(4,4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'delong_2017'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'delong_2017'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

deutsch_2008

Modified deutsch model for fitting thermal performance curves

Description

Modified deutsch model for fitting thermal performance curves

Usage

```
deutsch_2008(temp, rmax, topt, ctmax, a)
```

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Arguments

temp	temperature in degrees centigrade
rmax	maximum rate at optimum temperature
topt	optimum temperature (°C)
ctmax	critical thermal maximum (°C)
а	related to the full curve width

Details

Equation:

$$\text{if} \quad temp < t_{opt} : rate = r_{max} \cdot exp^{-\left(\frac{temp - t_{opt}}{2a}\right)^2}$$

$$\text{if} \quad temp > t_{opt} : rate = r_{max} \cdot \left(1 - \left(\frac{temp - t_{opt}}{t_{opt} - ct_{max}}\right)^2\right)$$

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Deutsch, C. A., Tewksbury, J. J., Huey, R. B., Sheldon, K. S., Ghalambor, C. K., Haak, D. C., & Martin, P. R. Impacts of climate warming on terrestrial ectotherms across latitude. Proceedings of the National Academy of Sciences, 105(18), 6668-6672. (2008)

```
# load in ggplot
library(ggplot2)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'deutsch_2008')
# fit model
mod <- nls.multstart::nls_multstart(rate~deutsch_2008(temp = temp, rmax, topt, ctmax, a),</pre>
```

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```
data = d,
iter = c(4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'deutsch_2008'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'deutsch_2008'),
supp\_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

flinn_1991

Flinn model for fitting thermal performance curves

Description

Flinn model for fitting thermal performance curves

Usage

```
flinn_1991(temp, a, b, c)
```

Arguments

temp	temperature in degrees centigrade
a	parameter that controls the height of the curve
b	parameter that controls the slope of the initial increase of the curve
С	parameter that controls the position and steepness of the decline of the curve

Details

Equation:

$$rate = \frac{1}{1 + a + b \cdot temp + c \cdot temp^2}$$

Start values in get_start_vals are derived from previous methods from the literature.

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

flinn_1991

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Flinn PW Temperature-dependent functional response of the parasitoid Cephalonomia waterstoni (Gahan) (Hymenoptera, Bethylidae) attacking rusty grain beetle larvae (Coleoptera, Cucujidae). Environmental Entomology, 20, 872–876, (1991)

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'flinn_1991')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~flinn_1991(temp = temp, a, b, c),</pre>
data = d,
iter = c(4,4,4),
start_lower = start_vals - 1,
start_upper = start_vals + 1,
lower = get_lower_lims(d$temp, d$rate, model_name = 'flinn_1991'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'flinn_1991'),
supp\_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

gaussian_1987

gaussian_1987

Gaussian model for fitting thermal performance curves

Description

Gaussian model for fitting thermal performance curves

Usage

```
gaussian_1987(temp, rmax, topt, a)
```

Arguments

temp temperature in degrees centigrade

rmax maximum rate at optimum temperature

topt optimum temperature (°C)

a related to the full curve width

Details

Equation:

$$rate = r_{max} \cdot exp^{\left(-0.5\left(\frac{|temp-t_{opt}|}{a}\right)^{2}\right)}$$

Start values in get_start_vals are derived from the data

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Lynch, M., Gabriel, W., Environmental tolerance. The American Naturalist. 129, 283-303. (1987)

get_breadth 17

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'gaussian_1987')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~gaussian_1987(temp = temp,rmax, topt,a),</pre>
data = d,
iter = c(4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'gaussian_1987'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'gaussian_1987'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

get_breadth

Estimate thermal performance breadth of a thermal performance curve

Description

Estimate thermal performance breadth of a thermal performance curve

Usage

```
get_breadth(model, level = 0.8)
```

18 get_ctmax

Arguments

model nls model object that contains a model of a thermal performance curve

level proportion of maximum rate over which thermal performance breadth is calcu-

lated

Details

Thermal performance breadth is calculated as the range of temperatures over which a curve's rate is at least 0.8 of peak. This defaults to a proportion of 0.8 but can be changed using the level argument.

Value

Numeric estimate of thermal performance breadth (in °C)

Description

Estimate the critical thermal maximum of a thermal performance curve

Usage

```
get_ctmax(model)
```

Arguments

model nls model object that contains a model of a thermal performance curve

Details

Critical thermal maximum is calculated by predicting over a temperature range 50 °C beyond the maximum value in the dataset. The predicted rate value closest to 0 is then extracted. When this is impossible due to the curve formula (i.e the Sharpe-Schoolfield model), the temperature where the rate is 5 percent of the maximum rate is estimated. Predictions are done every 0.001 °C so the estimate of the critical thermal maximum should be accurate up to 0.001 °C.

Value

Numeric estimate of critical thermal maximum (°C)

get_ctmin 19

get_ctmin

Estimate the critical thermal minimum of a thermal performance curve

Description

Estimate the critical thermal minimum of a thermal performance curve

Usage

```
get_ctmin(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Optimum temperature is calculated by predicting over a temperature range 50 degrees lower than the minimum value in the dataset. The predicted rate value closest to 0 is then extracted. When this is impossible due to the curve formula (i.e the Sharpe-Schoolfield model), the temperature where the rate is 5 percent of the maximum rate is estimated. Predictions are done every 0.001 °C value so the estimate of the critical thermal minimum should be accurate up to 0.001 °C.

Value

Numeric estimate of critical thermal minimum (°C)

get_e

Estimate the activation energy of a thermal performance curve

Description

Estimate the activation energy of a thermal performance curve

Usage

```
get_e(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Fits a modified-Boltzmann equation to all raw data below the optimum temperature (°C; as estimated by get_topt).

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Value

Numeric estimate of activation energy (eV)

get_eh

Estimate the deactivation energy of a thermal performance curve

Description

Estimate the deactivation energy of a thermal performance curve

Usage

```
get_eh(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Fits a modified-Boltzmann equation to all raw data beyond the optimum temperature (°C; as estimated by get_topt).

Value

Numeric estimate of activation energy (eV)

get_lower_lims

Set broad lower limits on parameter values

Description

Sets wide lower limits on parameter values for each TPC model

Usage

```
get_lower_lims(x, y, model_name)
```

Arguments

x vector of temperature values

y vector of rate values

model_name the name of the model being fitted

get_model_names 21

Value

Named list of lower limits given the data and model being fitted

Author(s)

Daniel Padfield

get_model_names

Lists the models available in rTPC

Description

Lists the models available in rTPC

Usage

```
get_model_names()
```

Value

character vector of thermal performance curves available in rTPC

Examples

```
get_model_names()
```

get_q10

Estimate the q10 value of a thermal performance curve

Description

Estimate the q10 value of a thermal performance curve

Usage

```
get_q10(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Fits the q10 portion of rezende_2019 to all raw data below the optimum temperature (°C; as estimated by get_topt).

Value

Numeric estimate of q10 value

22 get_skewness

get_rmax

Estimate maximum rate of a thermal performance curve

Description

Estimate maximum rate of a thermal performance curve

Usage

```
get_rmax(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Maximum rate is calculated by predicting over the temperature range using the previously estimated parameters and picking the maximum rate value. Predictions are done every 0.001 °C.

Value

Numeric estimate of maximum rate

get_skewness

Estimates skewness of a thermal performance curve

Description

Estimates skewness of a thermal performance curve

Usage

```
get_skewness(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Skewness is calculated from the values of activation energy (e) and deactivation energy (eh) as: skewness = e - eh. A negative skewness indicates the TPC is left skewed, the drop after the optimum is steeper than the rise up to the optimum. A positive skewness means that the TPC is right skewed and a value of 0 would mean the curve is symmetrical around the optimum.

get_start_vals 23

Value

Numeric estimate of skewness

get_start_vals

Estimate start values for TPC fitting

Description

Estimates sensible start values for fitting thermal performance curves

Usage

```
get_start_vals(x, y, model_name)
```

Arguments

x vector of temperature values

y vector of rate values

model_name the name of the model being fitted

Value

Named list of start parameters given the data and model being fitted

Author(s)

Daniel Padfield

```
get_thermalsafetymargin
```

Estimate thermal safety margin of a thermal performance curve

Description

Estimate thermal safety margin of a thermal performance curve

Usage

```
get_thermalsafetymargin(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

24 get_topt

Details

Thermal safety margin is calculated as: CTmax - Topt. This is calculated using the functions get_ctmax and get_topt.

Value

Numeric estimate of thermal safety margin (in °C)

Description

Estimate thermal tolerance of a thermal performance curve

Usage

```
get_thermaltolerance(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

Details

Thermal tolerance is calculated as: CTmax - CTmin. This is calculated using the functions get_ctmax and get_ctmin.

Value

Thermal tolerance (in °C)

get_topt

Estimate optimum temperature of a thermal performance curve

Description

Estimate optimum temperature of a thermal performance curve

Usage

```
get_topt(model)
```

Arguments

model

nls model object that contains a model of a thermal performance curve

get_upper_lims 25

Details

Optimum temperature (°C) is calculated by predicting over the temperature range using the previously estimated parameters and keeping the temperature where the largest rate value occurs. Predictions are done every 0.001 °C so the estimate of optimum temperature should be accurate up to 0.001 °C.

Value

Numeric estimate of optimum temperature (in °C)

get_upper_lims

Set broad upper limits on parameter values

Description

Sets wide upper limits on parameter values for each TPC model

Usage

```
get_upper_lims(x, y, model_name)
```

Arguments

x vector of temperature values

y vector of rate values

model_name the name of the model being fitted

Value

Named list of upper limits given the data and model being fitted

Author(s)

Daniel Padfield

26 hinshelwood_1947

hinshelwood_1947

Hinshelwood model for fitting thermal performance curves

Description

Hinshelwood model for fitting thermal performance curves

Usage

```
hinshelwood_1947(temp, a, e, b, eh)
```

Arguments

temp	temperature in degrees centigrade
a	pre-exponential constant for the activation energy
е	activation energy (eV)
b	pre-exponential constant for the deactivation energy
eh	de-activation energy (eV)

Details

Equation:

$$rate = a \cdot exp^{\frac{-e}{k \cdot (temp + 273.15)}} - b \cdot exp^{\frac{-e_h}{k \cdot (temp + 273.15)}}$$

where k is Boltzmann's constant with a value of 8.62e-05

Start values in get_start_vals are taken from the literature.

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model difficult to fit.

References

Hinshelwood C.N. The Chemical Kinetics of the Bacterial Cell. Oxford University Press. (1947)

joehnk_2008 27

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'hinshelwood_1947')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~hinshelwood_1947(temp = temp,a, e, b, eh),</pre>
data = d,
iter = c(5,5,5,5),
start_lower = start_vals - 1,
start_upper = start_vals + 1,
lower = get_lower_lims(d$temp, d$rate, model_name = 'hinshelwood_1947'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'hinshelwood_1947'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

joehnk_2008

Jöhnk model for fitting thermal performance curves

Description

Jöhnk model for fitting thermal performance curves

Usage

```
joehnk_2008(temp, rmax, topt, a, b, c)
```

Arguments

temp

temperature in degrees centigrade

28 joehnk_2008

rmax	the rate at optimum temperature
topt	optimum temperatute (°C)
a	parameter with no biological meaning
b	parameter with no biological meaning
С	parameter with no biological meaning

Details

Equation:

$$rate = r_{max} \left(1 + a \left(\left(b^{temp - t_{opt}} - 1 \right) - \frac{ln(b)}{ln(c)} (c^{temp - t_{opt}} - 1) \right) \right)$$

Start values in get_start_vals are derived from the data or sensible values from the literature.

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Joehnk, Klaus D., et al. Summer heatwaves promote blooms of harmful cyanobacteria. Global change biology 14.3: 495-512 (2008)

```
# load in ggplot
library(ggplot2)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'joehnk_2008')

# fit model
mod <- nls.multstart::nls_multstart(rate~joehnk_2008(temp = temp, rmax, topt, a, b, c),
data = d,
iter = c(3,3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'joehnk_2008'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'joehnk_2008'),</pre>
```

johnsonlewin_1946 29

```
supp_errors = 'Y',
convergence_count = FALSE)

# look at model fit
summary(mod)

# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))
preds <- broom::augment(mod, newdata = preds)

# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()</pre>
```

johnsonlewin_1946

Johnson-Lewin model for fitting thermal performance curves

Description

Johnson-Lewin model for fitting thermal performance curves

Usage

```
johnsonlewin_1946(temp, r0, e, eh, topt)
```

Arguments

temp	temperature in degrees centigrade
r0	scaling parameter
е	activation energy (eV)
eh	high temperature de-activation energy (eV)
topt	optimum temperature (°C)

Details

Equation:

$$rate = \frac{r_0 \cdot exp^{\frac{-e}{k \cdot (temp + 273.15)}}}{1 + exp^{-\frac{e_h - \left(\frac{e_h}{(topt + 273.15)} + k \cdot ln\left(\frac{e}{e_h - e}\right)\right) \cdot (temp + 273.15)}{k \cdot (temp + 273.15)}}$$

where k is Boltzmann's constant with a value of 8.62e-05.

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

johnsonlewin_1946

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model difficult to fit.

References

Johnson, Frank H., and Isaac Lewin. The growth rate of E. coli in relation to temperature, quinine and coenzyme. Journal of Cellular and Comparative Physiology 28.1 (1946): 47-75.

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'johnsonlewin_1946')</pre>
# fit model
mod <- suppressWarnings(</pre>
nls.multstart::nls_multstart(rate~johnsonlewin_1946(temp = temp, r0, e, eh, topt),
data = d,
iter = c(5,5,5,5),
start_lower = start_vals - 1,
start_upper = start_vals + 1,
lower = get_lower_lims(d$temp, d$rate, model_name = 'johnsonlewin_1946'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'johnsonlewin_1946'),
supp\_errors = 'Y',
convergence_count = FALSE)
)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

kamykowski_1985 31

kamykowski_1	985
--------------	-----

Kamykowski model for fitting thermal performance curves

Description

Kamykowski model for fitting thermal performance curves

Usage

```
kamykowski_1985(temp, tmin, tmax, a, b, c)
```

Arguments

temp	temperature in degrees centigrade
tmin	low temperature (°C) at which rates become negative
tmax	high temperature (°C) at which rates become negative
а	parameter with no biological meaning
b	parameter with no biological meaning
С	parameter with no biological meaning

Details

Equation:

$$rate = a \cdot \left(1 - exp^{-b \cdot \left(temp - t_{min}\right)}\right) \cdot \left(1 - exp^{-c \cdot \left(t_{max} - temp\right)}\right)$$

Start values in get_start_vals are derived from the data or sensible values from the literature.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Kamykowski, Daniel. A survey of protozoan laboratory temperature studies applied to marine dinoflagellate behaviour from a field perspective. Contributions in Marine Science. (1985).

32 lactin2_1995

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'kamykowski_1985')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~kamykowski_1985(temp = temp, tmin, tmax, a, b, c),</pre>
data = d,
iter = c(3,3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'kamykowski_1985'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'kamykowski_1985'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

lactin2_1995

Lactin2 model for fitting thermal performance curves

Description

Lactin2 model for fitting thermal performance curves

Usage

```
lactin2_1995(temp, a, b, tmax, delta_t)
```

Arguments

temp

temperature in degrees centigrade

lactin2_1995 33

a	constant that determines the steepness of the rising portion of the curve
b	constant that determines the height of the overall curve
tmax	the temperature at which the curve begins to decelerate beyond the optimum $({}^{\circ}\!C)$
delta_t	thermal safety margin (°C)

Details

Equation:

$$rate = exp^{a \cdot temp} - exp^{a \cdot t_{max} - \left(\frac{t_{max} - temp}{\delta_t}\right)} + b$$

Start values in get_start_vals are derived from the data or sensible values from the literature.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Lactin, D.J., Holliday, N.J., Johnson, D.L. & Craigen, R. Improved rate models of temperature-dependent development by arthropods. Environmental Entomology 24, 69-75 (1995)

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'lactin2_1995')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~lactin2_1995(temp = temp, a, b, tmax, delta_t),</pre>
data = d,
iter = c(3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'lactin2_1995'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'lactin2_1995'),
supp_errors = 'Y',
```

34 lrf_1991

```
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))
preds <- broom::augment(mod, newdata = preds)
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()</pre>
```

lrf_1991

Lobry-Rosso-Flandros (LRF) model for fitting thermal performance curves

Description

Lobry-Rosso-Flandros (LRF) model for fitting thermal performance curves

Usage

```
lrf_1991(temp, rmax, topt, tmin, tmax)
```

Arguments temp

rmax	maximum rate at optimum temperature
topt	optimum temperature (°C)
tmin	low temperature (°C) at which rates become negative
tmax	high temperature (°C) at which rates become negative

temperature in degrees centigrade

Details

Equation:

$$rate = rmax \cdot \frac{(temp - t_{max}) \cdot (temp - t_{min})^2}{(t_{opt} - t_{min}) \cdot ((t_{opt} - t_{min}) \cdot (temp - t_{opt}) - (t_{opt} - t_{max}) \cdot (t_{opt} + t_{min} - 2 \cdot temp))}$$

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

lrf_1991 35

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

Author(s)

Daniel Padfield

References

Rosso, L., Lobry, J. R., & Flandrois, J. P. An unexpected correlation between cardinal temperatures of microbial growth highlighted by a new model. Journal of Theoretical Biology, 162(4), 447-463. (1993)

```
# load in ggplot
library(ggplot2)
library(nls.multstart)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'sharpeschoolhigh_1981')</pre>
# fit model
mod <- nls_multstart(rate~lrf_1991(temp = temp, rmax, topt, tmin, tmax),</pre>
data = d,
iter = c(3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'lrf_1991'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'lrf_1991'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
```

```
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

modifiedgaussian_2006 Modified gaussian model for fitting thermal performance curves

Description

Modified gaussian model for fitting thermal performance curves

Usage

```
modifiedgaussian_2006(temp, rmax, topt, a, b)
```

Arguments

temp	temperature in degrees centigrade
rmax	maximum rate at optimum temperature
topt	optimum temperature
а	related to full curve width
b	allows for asymmetry in the curve fit

Details

Equation:

$$rate = r_{max} \cdot exp^{\left[-0.5\left(\frac{|temp-t_{opt}|}{a}\right)^{b}\right]}$$

Start values in get_start_vals are derived from the data and gaussian_1987

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model difficult to fit.

References

Angilletta Jr, M. J. (2006). Estimating and comparing thermal performance curves. Journal of Thermal Biology, 31(7), 541-545.

oneill_1972 37

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'modifiedgaussian_2006')
# fit model
mod <- nls.multstart::nls_multstart(rate~modifiedgaussian_2006(temp = temp, rmax, topt, a, b),</pre>
data = d,
iter = c(3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'modifiedgaussian_2006'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'modifiedgaussian_2006'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

oneill_1972

O'Neill model for fitting thermal performance curves

Description

O'Neill model for fitting thermal performance curves

Usage

```
oneill_1972(temp, rmax, ctmax, topt, q10)
```

Arguments

temp

temperature in degrees centigrade

38 oneill_1972

rmax	maximum rate at optimum temperature
ctmax	high temperature (°C) at which rates become negative
topt	optimum temperature (°C)
q10	defines the fold change in performance as a result of increasing the temperature by 10 $^{\circ}\mathrm{C}$

Details

Equation:

$$rate = r_{max} \cdot \left(\frac{ct_{max} - temp}{ct_{max} - t_{opt}}\right)^{x} \cdot exp^{x \cdot \frac{temp - t_{opt}}{ct_{max} - t_{opt}}}$$

$$where : x = \frac{w^{2}}{400} \cdot \left(1 + \sqrt{1 + \frac{40}{w}}\right)^{2}$$

$$and : w = (q_{10} - 1) \cdot (ct_{max} - t_{opt})$$

Start values in get_start_vals are derived from the data and previous values in the literature Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

O'Neill, R.V., Goldstein, R.A., Shugart, H.H., Mankin, J.B. Terrestrial Ecosystem Energy Model. Eastern Deciduous Forest Biome Memo Report Oak Ridge. The Environmental Sciences Division of the Oak Ridge National Laboratory. (1972)

```
# load in ggplot
library(ggplot2)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'oneill_1972')
# fit model
mod <- nls.multstart::nls_multstart(rate~oneill_1972(temp = temp, rmax, ctmax, topt, q10),
data = d,</pre>
```

pawar_2018 39

```
iter = c(4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'oneill_1972'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'oneill_1972'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

pawar_2018

Pawar model for fitting thermal performance curves

Description

Pawar model for fitting thermal performance curves

Usage

```
pawar_2018(temp, r_tref, e, eh, topt, tref)
```

Arguments

temp	temperature in degrees centigrade
r_tref	rate at the standardised temperature, tref
e	activation energy (eV)
eh	high temperature de-activation energy (eV)
topt	optimum temperature (°C)
tref	standardisation temperature in degrees centigrade. Temperature at which rates are not inactivated by high temperatures

40 pawar_2018

Details

This model is a modified version of sharpeschoolhigh_1981 that explicitly models the optimum temperature. Equation:

$$rate = \frac{r_{tref} \cdot exp^{\frac{-e}{k}(\frac{1}{temp+273.15} - \frac{1}{t_{ref}+273.15})}}{1 + (\frac{e}{eh - e}) \cdot exp^{\frac{e_h}{k}(\frac{1}{t_{opt+273.15}} - \frac{1}{temp+273.15})}}$$

where k is Boltzmann's constant with a value of 8.62e-05.

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

Author(s)

Daniel Padfield

References

Kontopoulos, Dimitrios - Georgios, Bernardo García-Carreras, Sofía Sal, Thomas P. Smith, and Samraat Pawar. Use and Misuse of Temperature Normalisation in Meta-Analyses of Thermal Responses of Biological Traits. PeerJ. 6 (2018),

```
# load in ggplot
library(ggplot2)
library(nls.multstart)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'pawar_2018')
# fit model
mod <- nls_multstart(rate~pawar_2018(temp = temp, r_tref, e, eh, topt, tref = 20),
data = d,
iter = c(3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,</pre>
```

quadratic_2008 41

```
lower = get_lower_lims(d$temp, d$rate, model_name = 'pawar_2018'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'pawar_2018'),
supp_errors = 'Y',
convergence_count = FALSE)

# look at model fit
summary(mod)

# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))
preds <- broom::augment(mod, newdata = preds)

# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()</pre>
```

quadratic_2008

Quadratic model for fitting thermal performance curves

Description

Quadratic model for fitting thermal performance curves

Usage

```
quadratic_2008(temp, a, b, c)
```

Arguments

temp	temperature in degrees centigrade
а	parameter that defines the rate at 0 ${\rm ^oC}$
b	parameter with no biological meaning
С	parameter with no biological meaning

Details

Equation:

$$rate = a + b \cdot temp + c \cdot temp^2$$

Start values in get_start_vals are derived from the data using previous methods in the literature Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

42 quadratic_2008

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Montagnes, David JS, et al. Short-term temperature change may impact freshwater carbon flux: a microbial perspective. Global Change Biology 14.12: 2823-2838. (2008)

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'quadratic_2008')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~quadratic_2008(temp = temp, a, b, c),</pre>
data = d,
iter = c(4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'quadratic_2008'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'quadratic_2008'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

ratkowsky_1983 43

ratkowsky_1983	Ratkowsky model for fitting thermal performance curves	

Description

Ratkowsky model for fitting thermal performance curves

Usage

```
ratkowsky_1983(temp, tmin, tmax, a, b)
```

Arguments

temp	temperature in degrees centigrade
tmin	low temperature (°C) at which rates become negative
tmax	high temperature (°C) at which rates become negative
а	parameter defined as sqrt(rate)/(temp - tmin)
b	empirical parameter needed to fit the data for temperatures beyond the optimum temperature

Details

Equation:

$$rate = (a \cdot (temp - t_{min}))^2 \cdot (1 - exp(b \cdot (temp - t_{max})))^2$$

 $Start\ values\ in\ {\tt get_start_vals}\ are\ derived\ from\ the\ data\ and\ previous\ values\ in\ the\ literature.$

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Ratkowsky, D.A., Lowry, R.K., McMeekin, T.A., Stokes, A.N., Chandler, R.E., Model for bacterial growth rate throughout the entire biokinetic temperature range. J. Bacteriol. 154: 1222–1226 (1983)

44 rezende_2019

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'ratkowsky_1983')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~ratkowsky_1983(temp = temp, tmin, tmax, a, b),</pre>
data = d,
iter = c(4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'ratkowsky_1983'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'ratkowsky_1983'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

rezende_2019

Rezende model for fitting thermal performance curves

Description

Rezende model for fitting thermal performance curves

Usage

```
rezende_2019(temp, q10, a, b, c)
```

Arguments

temp

temperature in degrees centigrade

rezende_2019 45

q10	defines the fold change in performance as a result of increasing the temperature by 10 $^{\circ}\text{C}$
а	parameter describing shifts in rate
b	parameter threshold temperature (°C) beyond which the downward curve starts
С	parameter controlling the rate of decline beyond the threshold temperature, b

Details

Equation:

$$\begin{split} &\text{if} \quad temp < b: rate = a \cdot 10^{\frac{\log_{10}(q_{10})}{(\frac{10}{temp})}} \\ &\text{if} \quad temp > b: rate = a \cdot 10^{\frac{\log_{10}(q_{10})}{(\frac{10}{temp})}} \cdot \left(1 - c \cdot (b - temp)^2\right) \end{split}$$

Start values in get_start_vals are derived from the data and previous values in the literature.

Limits in get_lower_lims and get_upper_lims are based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Rezende, Enrico L., and Francisco Bozinovic. Thermal performance across levels of biological organization. Philosophical Transactions of the Royal Society B 374.1778 (2019): 20180549.

```
# load in ggplot
library(ggplot2)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'rezende_2019')
# fit model
mod <- nls.multstart::nls_multstart(rate~rezende_2019(temp = temp, q10, a, b, c),
data = d,
iter = c(4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'rezende_2019'),</pre>
```

```
upper = get_upper_lims(d$temp, d$rate, model_name = 'rezende_2019'),
supp_errors = 'Y',
convergence_count = FALSE)

# look at model fit
summary(mod)

# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))
preds <- broom::augment(mod, newdata = preds)

# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()</pre>
```

sharpeschoolfull_1981 Full Sharpe-Schoolfield model for fitting thermal performance curves

Description

Full Sharpe-Schoolfield model for fitting thermal performance curves

Usage

```
sharpeschoolfull_1981(temp, r_tref, e, el, tl, eh, th, tref)
```

Arguments

temp	temperature in degrees centigrade
r_tref	rate at the standardised temperature, tref
е	activation energy (eV)
el	low temperature de-activation energy (eV)
tl	temperature (°C) at which enzyme is $1/2$ active and $1/2$ suppressed due to low temperatures
eh	high temperature de-activation energy (eV)
th	temperature (°C) at which enzyme is 1/2 active and 1/2 suppressed due to high temperatures
tref	standardisation temperature in degrees centigrade. Temperature at which rates are not inactivated by either high or low temperatures

Details

Equation:

$$rate = \frac{r_{tref} \cdot exp^{\frac{-e}{k}(\frac{1}{temp+273.15} - \frac{1}{t_{ref}+273.15})}}{1 + exp^{\frac{e_{l}}{k}(\frac{1}{t_{l}} - \frac{1}{temp+273.15})} + exp^{\frac{e_{h}}{k}(\frac{1}{t_{h}} - \frac{1}{temp+273.15})}}$$

where k is Boltzmann's constant with a value of 8.62e-05.

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

Author(s)

Daniel Padfield

References

Schoolfield, R. M., Sharpe, P. J. & Magnuson, C. E. Non-linear regression of biological temperature-dependent rate models based on absolute reaction-rate theory. Journal of Theoretical Biology 88, 719-731 (1981)

```
# load in ggplot
library(ggplot2)
library(nls.multstart)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'sharpeschoolfull_1981')</pre>
# fit model
mod <- nls_multstart(rate~sharpeschoolfull_1981(temp = temp, r_tref, e, el, tl, eh, th, tref = 20),</pre>
data = d,
iter = c(3,3,3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'sharpeschoolfull_1981'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'sharpeschoolfull_1981'),
supp_errors = 'Y',
```

```
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))
preds <- broom::augment(mod, newdata = preds)
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()</pre>
```

sharpeschoolhigh_1981 Sharpe-Schoolfield model (high temperature inactivation only) for fitting thermal performance curves

Description

Sharpe-Schoolfield model (high temperature inactivation only) for fitting thermal performance curves

Usage

```
sharpeschoolhigh_1981(temp, r_tref, e, eh, th, tref)
```

Arguments

temp	temperature in degrees centigrade
r_tref	rate at the standardised temperature, tref
е	activation energy (eV)
eh	high temperature de-activation energy (eV)
th	temperature (°C) at which enzyme is 1/2 active and 1/2 suppressed due to high temperatures
tref	standardisation temperature in degrees centigrade. Temperature at which rates are not inactivated by high temperatures

Details

Equation:

$$rate = \frac{r_{tref} \cdot exp^{\frac{-e}{k}(\frac{1}{temp+273.15} - \frac{1}{t_{ref}+273.15})}}{1 + exp^{\frac{e_h}{k}(\frac{1}{t_h} - \frac{1}{temp+273.15})}}$$

where k is Boltzmann's constant with a value of 8.62e-05.

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

Author(s)

Daniel Padfield

References

Schoolfield, R. M., Sharpe, P. J. & Magnuson, C. E. Non-linear regression of biological temperature-dependent rate models based on absolute reaction-rate theory. J. Theor. Biol. 88, 719-731 (1981)

```
# load in ggplot
library(ggplot2)
library(nls.multstart)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'sharpeschoolhigh_1981')</pre>
# fit model
mod <- nls_multstart(rate~sharpeschoolhigh_1981(temp = temp, r_tref, e, eh, th, tref = 20),</pre>
data = d,
iter = c(3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'sharpeschoolhigh_1981'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'sharpeschoolhigh_1981'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

sharpeschoollow_1981 Sharpe-Schoolfield model (low temperature inactivation only) for fitting thermal performance curves

Description

Sharpe-Schoolfield model (low temperature inactivation only) for fitting thermal performance curves

Usage

```
sharpeschoollow_1981(temp, r_tref, e, el, tl, tref)
```

Arguments

temp	temperature in degrees centigrade
r_tref	rate at the standardised temperature, tref
е	activation energy (eV)
el	low temperature de-activation energy (eV)
tl	temperature (°C) at which enzyme is 1/2 active and 1/2 suppressed due to low temperatures
tref	standardisation temperature in degrees centigrade. Temperature at which rates are not inactivated by high temperatures

Details

Equation:

$$rate = \frac{r_{tref} \cdot exp^{\frac{-e}{k}(\frac{1}{temp+273.15} - \frac{1}{t_{ref}+273.15})}}{1 + exp^{\frac{e_{l}}{k}(\frac{1}{t_{l}} - \frac{1}{temp+273.15})}}$$

where k is Boltzmann's constant with a value of 8.62e-05.

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

spain_1982 51

Author(s)

Daniel Padfield

References

Schoolfield, R. M., Sharpe, P. J. & Magnuson, C. E. Non-linear regression of biological temperature-dependent rate models based on absolute reaction-rate theory. J. Theor. Biol. 88, 719-731 (1981)

```
# load in ggplot
library(ggplot2)
library(nls.multstart)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'sharpeschoollow_1981')
mod <- nls_multstart(rate~sharpeschoollow_1981(temp = temp, r_tref, e, el, tl, tref = 20),</pre>
data = d,
iter = c(3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'sharpeschoollow_1981'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'sharpeschoollow_1981'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

52 spain_1982

Description

Spain model for fitting thermal performance curves

Usage

```
spain_1982(temp, a, b, c, r0)
```

Arguments

temp	temperature in degrees centigrade
а	constant that determines the steepness of the rising portion of the curve
b	constant that determines the position of topt
С	constant that determines the steepness of the decreasing part of the curve
r0	the apparent rate at 0 °C

Details

Equation:

$$rate = r_0 \cdot exp^{a \cdot temp} \cdot (1 - b \cdot exp^{c \cdot temp})$$

Start values in get_start_vals are derived from the data or plucked from thin air.

Limits in get_lower_lims and get_upper_lims are derived from the data or plucked from thin air.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

BASIC Microcomputer Models in Biology. Addison-Wesley, Reading, MA. 1982

```
# load in ggplot
library(ggplot2)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'spain_1982')
# fit model</pre>
```

thomas_2012 53

```
mod <- nls.multstart::nls_multstart(rate~spain_1982(temp = temp, a, b, c, r0),</pre>
data = d,
iter = c(3,3,3,3),
start_lower = start_vals - 1,
start_upper = start_vals + 1,
lower = get_lower_lims(d$temp, d$rate, model_name = 'spain_1982'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'spain_1982'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

thomas_2012

Thomas model (2012) for fitting thermal performance curves

Description

Thomas model (2012) for fitting thermal performance curves

Usage

```
thomas_2012(temp, a, b, c, topt)
```

Arguments

temp	temperature in degrees centigrade
а	arbitrary constant
b	arbitrary constant
С	the range of temperatures over which growth rate is positive, or the thermal niche width (°C) $$
topt	determines the location of the maximum of the quadratic portion of this function. When $b=0$, tref would equal topt

54 thomas_2012

Details

Equation:

$$rate = a \cdot exp^{b \cdot temp} \left(1 - \left(\frac{temp - t_{opt}}{c} \right)^2 \right)$$

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Thomas, Mridul K., et al. A global pattern of thermal adaptation in marine phytoplankton. Science 338.6110, 1085-1088 (2012)

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'thomas_2012')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~thomas_2012(temp = temp, a, b, c, topt),</pre>
data = d,
iter = c(4,4,4,4),
start_lower = start_vals - 1,
start_upper = start_vals + 2,
lower = get_lower_lims(d$temp, d$rate, model_name = 'thomas_2012'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'thomas_2012'),
supp_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
```

thomas_2017 55

```
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

thomas_2017

Thomas model (2017) for fitting thermal performance curves

Description

Thomas model (2017) for fitting thermal performance curves

Usage

```
thomas_2017(temp, a, b, c, d, e)
```

Arguments

temp	temperature in degrees centigrade
a	birth rate at 0 °C
b	describes the exponential increase in birth rate with increasing temperature
С	temperature-independent mortality term
d	along with e controls the exponential increase in mortality rates with temperature
е	along with d controls the exponential increase in mortality rates with temperature

Details

Equation:

$$rate = a \cdot exp^{b \cdot temp} - (c + d \cdot exp^{e \cdot temp})$$

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based on extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

56 weibull_1995

References

Thomas, Mridul K., et al. Temperature–nutrient interactions exacerbate sensitivity to warming in phytoplankton. Global change biology 23.8 (2017): 3269-3280.

Examples

```
# load in ggplot
library(ggplot2)
# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)</pre>
# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'thomas_2017')</pre>
# fit model
mod <- nls.multstart::nls_multstart(rate~thomas_2017(temp = temp, a, b, c, d, e),</pre>
data = d,
iter = c(3,3,3,3,3),
start_lower = start_vals - 10,
start_upper = start_vals + 10,
lower = get_lower_lims(d$temp, d$rate, model_name = 'thomas_2017'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'thomas_2017'),
supp\_errors = 'Y',
convergence_count = FALSE)
# look at model fit
summary(mod)
# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))</pre>
preds <- broom::augment(mod, newdata = preds)</pre>
# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()
```

weibull_1995

Weibull model for fitting thermal performance curves

Description

Weibull model for fitting thermal performance curves

Usage

```
weibull_1995(temp, a, topt, b, c)
```

weibull_1995 57

Arguments

temp	temperature in degrees centigrade
а	scale the height of the curve
topt	optimum temperature
b	defines the breadth of the curve
С	defines the curve shape

Details

Equation:

$$rate = a \cdot \left(\frac{c-1}{c}\right)^{\frac{1-c}{c}} \left(\frac{temp - t_{opt}}{b} + \left(\frac{c-1}{c}\right)^{\frac{1}{c}}\right)^{c-1} exp^{-\left(\frac{temp - t_{opt}}{b} + \left(\frac{c-1}{c}\right)^{\frac{1}{c}}\right)^{c}} + \frac{c-1}{c}$$

Start values in get_start_vals are derived from the data.

Limits in get_lower_lims and get_upper_lims are derived from the data or based extreme values that are unlikely to occur in ecological settings.

Value

a numeric vector of rate values based on the temperatures and parameter values provided to the function

Note

Generally we found this model easy to fit.

References

Angilletta Jr, Michael J. Estimating and comparing thermal performance curves. Journal of Thermal Biology 31.7 (2006): 541-545.

```
# load in ggplot
library(ggplot2)

# subset for the first TPC curve
data('chlorella_tpc')
d <- subset(chlorella_tpc, curve_id == 1)

# get start values and fit model
start_vals <- get_start_vals(d$temp, d$rate, model_name = 'weibull_1995')
# fit model
mod <- nls.multstart::nls_multstart(rate~weibull_1995(temp = temp, a, topt, b, c),
data = d,
iter = c(4,4,4,4),
start_lower = start_vals - 10,
start_upper = start_vals + 10,</pre>
```

58 weibull_1995

```
lower = get_lower_lims(d$temp, d$rate, model_name = 'weibull_1995'),
upper = get_upper_lims(d$temp, d$rate, model_name = 'weibull_1995'),
supp_errors = 'Y',
convergence_count = FALSE)

# look at model fit
summary(mod)

# get predictions
preds <- data.frame(temp = seq(min(d$temp), max(d$temp), length.out = 100))
preds <- broom::augment(mod, newdata = preds)

# plot
ggplot(preds) +
geom_point(aes(temp, rate), d) +
geom_line(aes(temp, .fitted), col = 'blue') +
theme_bw()</pre>
```

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