Package ‘flexFitR’

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Type Package

Title Flexible Non-Linear Least Square Model Fitting

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Description Provides tools for flexible non-linear least squares model fitting using general-purpose optimization techniques. The package supports a variety of optimization algorithms, including those provided by the 'optimx' package, making it suitable for handling complex non-linear models. Features include parallel processing support via the 'future' and 'foreach' packages, comprehensive model diagnostics, and visualization capabilities. Implements methods described in Nash and Varadhan (2011, <doi:10.18637/jss.v043.i09>).

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URL `https://apariciojohan.github.io/flexFitR/`,
`https://github.com/AparicioJohan/flexFitR`

BugReports `https://github.com/AparicioJohan/flexFitR/issues`

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Contents

`anova.modeler` *Extra Sum-of-Squares F-Test for* `modeler` *objects*

Description

Perform an extra sum-of-squares F-test to compare two nested models of class `modeler`. This test assesses whether the additional parameters in the full model significantly improve the fit compared to the reduced model.

Usage

```
## S3 method for class 'modeler'
anova(object, full_model = NULL, ...)
```

Arguments

`object`	An object of class `modeler` representing the reduced model with fewer parameters.
`full_model`	An optional object of class `modeler` representing the full model with more parameters.
`...`	Additional parameters for future functionality.

Value

A `tibble` containing columns with the F-statistic and corresponding p-values, indicating whether the full model provides a significantly better fit than the reduced model.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
dt <- data.frame(X = 1:6, Y = c(12, 16, 44, 50, 95, 100))
mo_1 <- modeler(dt, X, Y, fn = "fn_lin", param = c(m = 10, b = -5))
plot(mo_1)
mo_2 <- modeler(dt, X, Y, fn = "fn_quad", param = c(a = 1, b = 10, c = 5))
plot(mo_2)
anova(mo_1, mo_2)
```

`augment` *Augment a* `modeler` *object with influence diagnostics*

Description

This function computes various influence diagnostics, including standardized residuals, studentized residuals, and Cook's distance, for an object of class `modeler`.

Usage

```
augment(x, id = NULL, metadata = TRUE, ...)
```

Arguments

`x`	An object of class `modeler`.
`id`	Optional unique identifier to filter by a specific group. Default is `NULL`.
`metadata`	Logical. If `TRUE`, metadata is included with the predictions. Default is `FALSE`
`...`	Additional parameters for future functionality.

Value

A tibble containing the following columns:

`uid`	Unique identifier for the group.
`fn_name`	Function name associated with the model.
`x`	Predictor variable values.
`y`	Observed response values.
`.fitted`	Fitted values from the model.
`.resid`	Raw residuals (observed - fitted).
`.hat`	Leverage values for each observation.
`.cooksd`	Cook's distance for each observation.
`.std.resid`	Standardized residuals.
`.stud.resid`	Studentized residuals.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_logistic",
    parameters = c(L = 100, k = 4, t0 = 40),
    subset = 2
  )
print(mod_1)
augment(mod_1)
```

`c.modeler` *Combine objects of class* `modeler`

Description

Combine objects of class `modeler`. Use with caution, some functions might not work as expected.

Usage

```
## S3 method for class 'modeler'
c(...)
```

Arguments

`...`	Objects of class `modeler`, typically the result of calling `modeler()`.

Value

A `modeler` object.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_logistic",
    parameters = c(L = 100, k = 4, t0 = 40),
    subset = 1:2
  )
mod_2 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 100),
    subset = 1:2
  )
mod <- c(mod_1, mod_2)
print(mod)
plot(mod, id = 1:2)
```

`coef.modeler` *Coefficients for an object of class* `modeler`

Description

Extract the estimated coefficients from an object of class `modeler`.

Usage

```
## S3 method for class 'modeler'
coef(object, id = NULL, metadata = FALSE, df = FALSE, ...)
```

Arguments

`object`	An object of class `modeler`, typically the result of calling the `modeler()` function.
`id`	An optional unique identifier to filter by a specific group. Default is `NULL`.
`metadata`	Logical. If `TRUE`, metadata is included along with the coefficients. Default is `FALSE`.
`df`	Logical. If `TRUE`, the degrees of freedom for the fitted model are returned alongside the coefficients. Default is `FALSE`.
`...`	Additional parameters for future functionality.

Value

A `data.frame` containing the model's estimated coefficients, standard errors, and optional metadata or degrees of freedom if specified.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(15, 2, 45)
  )
print(mod_1)
coef(mod_1, id = 2)
```

`confint.modeler` *Confidence intervals for a modeler object*

Description

Extract confidence intervals for the estimated parameters of an object of class `modeler`.

Usage

```
## S3 method for class 'modeler'
confint(object, parm = NULL, level = 0.95, id = NULL, ...)
```

Arguments

`object`	An object of class `modeler`, typically the result of calling the `modeler()` function.
`parm`	A character vector specifying which parameters should have confidence intervals calculated. If `NULL`, confidence intervals for all parameters are returned. Default is `NULL`.
`level`	A numeric value indicating the confidence level for the intervals. Default is 0.95, corresponding to a 95% confidence interval.
`id`	An optional unique identifier to filter by a specific group. Default is `NULL`.
`...`	Additional parameters for future functionality.

Value

A `tibble` containing the lower and upper confidence limits for each specified parameter.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(15, 35, 45)
  )
print(mod_1)
confint(mod_1)
```

`dt_potato` *Drone-derived data from a potato breeding trial*

Description

Canopy and Green Leaf Index for a potato trial arranged in a p-rep design.

Usage

```
dt_potato
```

Format

A tibble with 1372 rows and 8 variables:

Trial chr trial name

Plot dbl denoting the unique plot id

Row dbl denoting the row coordinate

Range dbl denoting range coordinate

gid chr denoting the genotype id

DAP dbl denoting Days after planting

Canopy dbl Canopy UAV-Derived

GLI dbl Green Leaf Index UAV-Derived

Source

UW - Potato Breeding Program

`explorer` *Explore data*

Description

Explores data from a data frame in wide format.

Usage

```
explorer(data, x, y, id, metadata)
```

Arguments

`data`	A `data.frame` containing the input data for analysis.
`x`	The name of the column in `data` that contains x points.
`y`	The names of the columns in `data` that contain the variables to be analyzed.
`id`	The names of the columns in `data` that contains a grouping variable.
`metadata`	The names of the columns in `data` to keep across the analysis.

Details

This function helps to explore the dataset before being analyzed with `modeler()`.

Value

An object of class `explorer`, which is a list containing the following elements:

`summ_vars` A data.frame containing summary statistics for each trait at each x point, including minimum, mean, median, maximum, standard deviation, coefficient of variation, number of non-missing values, percentage of missing values, and percentage of negative values.

`summ_metadata` A data.frame summarizing the metadata.

`locals_min_max` A data.frame containing the local minima and maxima of the mean y values over x.

`dt_long` A data.frame in long format, with columns for uid, metadata, var, x, and y

`metadata` A character vector with the names of the variables to keep across.

Examples

```
library(flexFitR)
data(dt_potato)
results <- dt_potato |>
  explorer(
    x = DAP,
    y = c(Canopy, GLI),
    id = Plot,
    metadata = c(gid, Row, Range)
  )
names(results)
head(results$summ_vars)
plot(results, label_size = 4, signif = TRUE, n_row = 2)
# New data format
head(results$dt_long)
```

`fitted.modeler` *Extract fitted values from a* `modeler` *object*

Description

Extract fitted values from a `modeler` object

Usage

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

Arguments

`object`	An object of class ‘modeler‘
`...`	Additional parameters for future functionality.

Value

A numeric vector of fitted values.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(15, 2, 45)
  )
fitted(mod_1)
```

`fn_exp1_exp` *Exponential exponential function 1*

Description

Computes a value based on an exponential growth curve and exponential decay model for time.

Usage

```
fn_exp1_exp(t, t1, t2, alpha, beta)
```

Arguments

`t`	Numeric. The time value.
`t1`	Numeric. The lower threshold time. Assumed to be known.
`t2`	Numeric. The upper threshold time.
`alpha`	Numeric. The parameter for the first exponential term. Must be greater than 0.
`beta`	Numeric. The parameter for the second exponential term. Must be less than 0.

Details

Value

A numeric value based on the double exponential model. If `t` is less than `t1`, the function returns 0. If `t` is between `t1` and `t2` (inclusive), the function returns `exp(alpha * (t - t1)) - 1`. If `t` is greater than `t2`, the function returns `(exp(alpha * (t2 - t1)) - 1) * exp(beta * (t - t2))`.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_exp1_exp",
  params = c(t1 = 35, t2 = 55, alpha = 1 / 20, beta = -1 / 30),
  interval = c(0, 108),
  n_points = 2000,
  auc_label_size = 3,
  y_auc_label = 0.2
)
```

`fn_exp1_lin` *Exponential linear function 1*

Description

Computes a value based on an exponential growth curve and linear decay model for time.

Usage

```
fn_exp1_lin(t, t1, t2, alpha, beta)
```

Arguments

`t`	Numeric. The time value.
`t1`	Numeric. The lower threshold time. Assumed to be known.
`t2`	Numeric. The upper threshold time.
`alpha`	Numeric. The parameter for the exponential term. Must be greater than 0.
`beta`	Numeric. The parameter for the linear term. Must be less than 0.

Details

Value

A numeric value based on the exponential linear model. If `t` is less than `t1`, the function returns 0. If `t` is between `t1` and `t2` (inclusive), the function returns `exp(alpha * (t - t1)) - 1`. If `t` is greater than `t2`, the function returns `beta * (t - t2) + (exp(alpha * (t2 - t1)) - 1)`.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_exp1_lin",
  params = c(t1 = 35, t2 = 55, alpha = 1 / 20, beta = -1 / 40),
  interval = c(0, 108),
  n_points = 2000,
  auc_label_size = 3
)
```

`fn_exp2_exp` *Exponential exponential Function 2*

Description

Computes a value based on an exponential growth curve and exponential decay model for time.

Usage

```
fn_exp2_exp(t, t1, t2, alpha, beta)
```

Arguments

`t`	Numeric. The time value.
`t1`	Numeric. The lower threshold time. Assumed to be known.
`t2`	Numeric. The upper threshold time.
`alpha`	Numeric. The parameter for the first exponential term. Must be greater than 0.
`beta`	Numeric. The parameter for the second exponential term. Must be less than 0.

Details

Value

A numeric value based on the double exponential model. If `t` is less than `t1`, the function returns 0. If `t` is between `t1` and `t2` (inclusive), the function returns `exp(alpha * (t - t1)^2) - 1`. If `t` is greater than `t2`, the function returns `(exp(alpha * (t2 - t1)^2) - 1) * exp(beta * (t - t2))`.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_exp2_exp",
  params = c(t1 = 35, t2 = 55, alpha = 1 / 600, beta = -1 / 30),
  interval = c(0, 108),
  n_points = 2000,
```

```
  auc_label_size = 3,
  y_auc_label = 0.15
)
```

`fn_exp2_lin` *Exponential linear function 2*

Description

Computes a value based on an exponential growth curve and linear decay model for time.

Usage

```
fn_exp2_lin(t, t1, t2, alpha, beta)
```

Arguments

`t`	Numeric. The time value.
`t1`	Numeric. The lower threshold time. Assumed to be known.
`t2`	Numeric. The upper threshold time.
`alpha`	Numeric. The parameter for the exponential term. Must be greater than 0.
`beta`	Numeric. The parameter for the linear term. Must be less than 0.

Details

Value

A numeric value based on the exponential linear model. If `t` is less than `t1`, the function returns 0. If `t` is between `t1` and `t2` (inclusive), the function returns `exp(alpha * (t - t1)^2) - 1`. If `t` is greater than `t2`, the function returns `beta * (t - t2) + (exp(alpha * (t2 - t1)^2) - 1)`.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_exp2_lin",
  params = c(t1 = 35, t2 = 55, alpha = 1 / 600, beta = -1 / 80),
  interval = c(0, 108),
  n_points = 2000,
  auc_label_size = 3
)
```

`fn_lin` *Linear function*

Description

Computes a value based on a linear function.

Usage

```
fn_lin(t, m, b)
```

Arguments

`t`	Numeric value.
`m`	Numeric value for the slope coefficient.
`b`	Numeric value for the intercept coefficient.

Details

Value

A numeric value based on the linear function.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_lin",
  params = c(m = 2, b = 10),
  interval = c(0, 108),
  n_points = 2000
)
```

`fn_linear_sat` *Linear plateau function*

Description

Computes a value based on a linear growth curve reaching a plateau for time.

Usage

```
fn_linear_sat(t, t1 = 45, t2 = 80, k = 0.9)
```

Arguments

`t`	Numeric. The time value.
`t1`	Numeric. The lower threshold time. Default is 45.
`t2`	Numeric. The upper threshold time. Default is 80.
`k`	Numeric. The maximum value of the function. Default is 0.9. Assumed to be known.

Details

Value

A numeric value based on the threshold model. If `t` is less than `t1`, the function returns 0. If `t` is between `t1` and `t2` (inclusive), the function returns a value between 0 and `k` in a linear trend. If `t` is greater than `t2`, the function returns `k`.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_linear_sat",
  params = c(t1 = 34.9, t2 = 61.8, k = 100),
  interval = c(0, 108),
  n_points = 2000,
  auc_label_size = 3
)
```

`fn_lin_pl_lin` *Linear plateau linear function*

Description

Linear plateau linear function

Usage

```
fn_lin_pl_lin(t, t1, t2, t3, k, beta)
```

Arguments

`t`	Numeric. The time value.
`t1`	Numeric. The lower threshold time. Default is 45.
`t2`	Numeric. The upper threshold time before plateau. Default is 80.
`t3`	Numeric. The lower threshold time after plateau. Default is 45.
`k`	Numeric. The maximum value of the function. Default is 0.9.
`beta`	Numeric. Slope of the linear decay.

Details

Value

A numeric value based on the linear plateau linear model.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_lin_pl_lin",
  params = c(t1 = 38.7, t2 = 62, t3 = 90, k = 0.32, beta = -0.01),
  interval = c(0, 108),
  n_points = 2000,
  auc_label_size = 3
)
```

`fn_lin_pl_lin2` *Linear plateau linear with constrains*

Description

Linear plateau linear with constrains

Usage

```
fn_lin_pl_lin2(t, t1, t2, dt, k, beta)
```

Arguments

`t`	Numeric. The time value.
`t1`	Numeric. The lower threshold time.
`t2`	Numeric. The upper threshold time before plateau.
`dt`	Numeric. dt = t3 - t2.
`k`	Numeric. The maximum value of the function.
`beta`	Numeric. Slope of the linear decay.

Details

Value

A numeric value based on the linear plateau linear model.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_lin_pl_lin2",
  params = c(t1 = 38.7, t2 = 62, dt = 28, k = 0.32, beta = -0.01),
  interval = c(0, 108),
  n_points = 2000,
  auc_label_size = 3
)
```

`fn_logistic` *Logistic function*

Description

Computes a value based on a logistic function.

Usage

```
fn_logistic(t, L, k, t0)
```

Arguments

`t`	Numeric value.
`L`	Numeric value.
`k`	Numeric value.
`t0`	Numeric value.

Details

Value

A numeric value based on the logistic function.

Examples

```
library(flexFitR)
plot_fn(
  fn = "fn_logistic",
  params = c(L = 100, k = 0.199, t0 = 47.7),
  interval = c(0, 108),
  n_points = 2000
)
```

`fn_quad` *Quadratic function*

Description

Computes a value based on a quadratic function..

Usage

```
fn_quad(t, a, b, c)
```

Arguments

`t`	Numeric value.
`a`	Numeric value for coefficient a.
`b`	Numeric value for coefficient b.
`c`	Numeric value for coefficient c.

Details

Value

A numeric value based on the linear function.

Examples

```
library(flexFitR)
plot_fn(fn = "fn_quad", params = c(a = 1, b = 10, c = 5))
```

`goodness_of_fit` *Akaike's An Information Criterion for an object of class* `modeler`

Description

Generic function calculating Akaike's ‘An Information Criterion’ for fitted model object of class `modeler`.

Usage

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

## S3 method for class 'modeler'
BIC(object, ...)
```

Arguments

`object`	An object inheriting from class `modeler` resulting of executing the function `modeler()`
`...`	Further parameters. For future improvements.
`k`	Numeric, the penalty per parameter to be used; the default k = 2 is the classical AIC.

Value

A `tibble` with columns giving the corresponding AIC and BIC.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
dt <- data.frame(X = 1:6, Y = c(12, 16, 44, 50, 95, 100))
mo_1 <- modeler(dt, X, Y, fn = "fn_lin", param = c(m = 10, b = -5))
mo_2 <- modeler(dt, X, Y, fn = "fn_quad", param = c(a = 1, b = 10, c = 5))
AIC(mo_1)
AIC(mo_2)
BIC(mo_1)
BIC(mo_2)
```

`list_funs` *Print available functions in flexFitR*

Description

Print available functions in flexFitR

Usage

```
list_funs()
```

Value

A vector with available functions

Examples

```
library(flexFitR)
list_funs()
```

`list_methods` *Print available methods in flexFitR*

Description

Print available methods in flexFitR

Usage

```
list_methods(bounds = FALSE, check_package = FALSE)
```

Arguments

`bounds`	If TRUE, returns methods for box (or bounds) constraints. FALSE by default.
`check_package`	If TRUE, ensures solvers are installed. FALSE by default.

Value

A vector with available methods

Examples

```
library(flexFitR)
list_methods()
```

`logLik.modeler` *Extract Log-Likelihood for an object of class* `modeler`

Description

logLik for an object of class `modeler`

Usage

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

Arguments

`object`	An object inheriting from class `modeler` resulting of executing the function `modeler()`
`...`	Further parameters. For future improvements.

Value

A `tibble` with the Log-Likelihood for the fitted models.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
dt <- data.frame(X = 1:6, Y = c(12, 16, 44, 50, 95, 100))
mo_1 <- modeler(dt, X, Y, fn = "fn_lin", param = c(m = 10, b = -5))
plot(mo_1)
logLik(mo_1)
```

`metrics` *Metrics for an object of class* `modeler`

Description

Computes various performance metrics for a modeler object. The function calculates Sum of Squared Errors (SSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and the Coefficient of Determination (R-squared).

Usage

```
metrics(x, by_grp = TRUE)
```

Arguments

`x`	An object of class ‘modeler‘ containing the necessary data to compute the metrics.
`by_grp`	Return the metrics by id? TRUE by default.

Details

Value

A data frame containing the calculated metrics grouped by uid, metadata, and variables.

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
```

```
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(1:2)
  )
plot(mod_1, id = c(1:2))
print(mod_1)
metrics(mod_1)
```

`modeler` *Modeler: Non-linear regression for curve fitting*

Description

A versatile function for performing non-linear least squares optimization on grouped data. It supports customizable optimization methods, flexible initial/fixed parameters, and parallel processing.

Usage

```
modeler(
  data,
  x,
  y,
  grp,
  keep,
  fn = "fn_linear_sat",
  parameters = NULL,
  lower = -Inf,
  upper = Inf,
  fixed_params = NULL,
  method = c("subplex", "pracmanm", "anms"),
  subset = NULL,
  options = modeler.options(),
  control = list()
)
```

Arguments

`data`	A `data.frame` containing the input data for analysis.
`x`	The name of the column in `data` representing the independent variable (x points).
`y`	The name of the column in `data` containing the dependent variable to analyze (response variable).
`grp`	Column(s) in `data` used as grouping variable(s). Defaults to `NULL`. (Optional)
`keep`	Names of columns to retain in the output. Defaults to `NULL`. (Optional)
`fn`	A string. The name of the function used for curve fitting. Example: `"fn_lin"`. Defaults to `"fn_linear_sat"`.
`parameters`	A numeric vector, named list, or `data.frame` providing initial values for parameters:

	Numeric vector Named vector specifying initial values (e.g., `c(k = 0.5, t1 = 30)`). **Data frame** Requires a `uid` column with group IDs and parameter values for each group. **List** Named list where parameter values can be numeric or expressions (e.g., `list(k = "max(y)", t1 = 40)`). Defaults to `NULL`.
`lower`	A numeric vector specifying lower bounds for parameters. Defaults to `-Inf` for all parameters.
`upper`	A numeric vector specifying upper bounds for parameters. Defaults to `Inf` for all parameters.
`fixed_params`	A list or `data.frame` for fixing specific parameters: **List** Named list where parameter values can be numeric or expressions (e.g., `list(k = "max(y)", t1 = 40)`). **Data frame** Requires a `uid` column for group IDs and fixed parameter values. Defaults to `NULL`.
`method`	A character vector specifying optimization methods. Check available methods using `list_methods()` and their dependencies using `optimx::checkallsolvers()`. Defaults to `c("subplex", "pracmanm", "anms")`.
`subset`	A vector (optional) containing levels of `grp` to filter the data for analysis. Defaults to `NULL` (all groups are included).
`options`	A list of additional options. See `modeler.options()` `progress` Logical. If `TRUE` a progress bar is displayed. Default is `FALSE`. Try this before running the function: `progressr::handlers("progress", "beepr")`. `parallel` Logical. If `TRUE` the model fit is performed in parallel. Default is `FALSE`. `workers` The number of parallel processes to use. `parallel::detectCores()` `trace` If `TRUE` , convergence monitoring of the current fit is reported in the console. `FALSE` by default. `return_method` Logical. If `TRUE`, includes the optimization method used in the result. Default is `FALSE`.
`control`	A list of control parameters to be passed to the optimization function. For example: `list(maxit = 500)`.

Value

An object of class `modeler`, which is a list containing the following elements:

`param` Data frame containing optimized parameters and related information.

`dt` Data frame with input data, fitted values, and residuals.

`metrics` Metrics and summary of the models.

`execution` Total execution time for the analysis.

`response` Name of the response variable analyzed.

`keep` Metadata retained based on the keep argument.

`fun` Name of the curve-fitting function used.

`parallel` List containing parallel execution details (if applicable).

`fit` List of fitted models for each group.

Examples

```
library(flexFitR)
data(dt_potato)
explorer <- explorer(dt_potato, x = DAP, y = c(Canopy, GLI), id = Plot)
# Example 1
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = GLI,
    grp = Plot,
    fn = "fn_lin_pl_lin",
    parameters = c(t1 = 38.7, t2 = 62, t3 = 90, k = 0.32, beta = -0.01),
    subset = 195
  )
plot(mod_1, id = 195)
print(mod_1)
# Example 2
mod_2 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = 195
  )
plot(mod_2, id = 195)
print(mod_2)
```

`performance` *Compare performance of different models*

Description

Computes indices of model performance for different models at once and hence allows comparison of indices across models.

Usage

```
performance(..., metrics = "all", metadata = FALSE, digits = 2)
```

Arguments

`...`	Multiple model objects (only of class ‘modeler‘).
`metrics`	Can be "all" or a character vector of metrics to be computed (one or more of "logLik", "AIC", "AICc", "BIC", "Sigma", "SSE", "MAE", "MSE", "RMSE", "R2"). "all" by default.
`metadata`	Logical. If `TRUE`, metadata is included with the performance metrics. Default is `FALSE`.
`digits`	An integer. The number of decimal places to round the output. Default is 2.

Value

A data.frame with performance metrics for models in (...).

Examples

```
library(flexFitR)
data(dt_potato)
# Model 1
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 90),
    subset = 40
  )
print(mod_1)
# Model 2
mod_2 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_logistic",
    parameters = c(L = 100, k = 4, t0 = 50),
    subset = 40
  )
print(mod_2)
# Model 3
mod_3 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_lin",
    parameters = c(m = 20, b = 2),
    subset = 40
  )
print(mod_3)
performance(mod_1, mod_2, mod_3, metrics = c("AIC", "AICc", "BIC", "Sigma"))
```

`plot.explorer` *Plot an object of class* `explorer`

Description

Creates various plots for an object of class `explorer`. Depending on the specified type, the function can generate plots that show correlations between variables over x, correlations between x values for each variable, or the evolution of variables over x.

Usage

```
## S3 method for class 'explorer'
plot(
  x,
  type = "var_by_x",
  label_size = 4,
  signif = FALSE,
  method = "pearson",
  filter_var = NULL,
  id = NULL,
  n_row = NULL,
  n_col = NULL,
  base_size = 13,
  return_gg = FALSE,
  add_avg = FALSE,
  ...
)
```

Arguments

`x`	An object inheriting from class `explorer`, resulting from executing the function `explorer()`.
`type`	Character string or number specifying the type of plot to generate. Available options are: `"var_by_x"` or `1` Plots correlations between variables over x (default). `"x_by_var"` or `2` Plots correlations between x points for each variable (y). `"evolution"` or `3` Plot the evolution of the variables (y) over x. `"xy"` or `4` Scatterplot (x, y)
`label_size`	Numeric. Size of the labels in the plot. Default is 4. Only works with type 1 and 2.
`signif`	Logical. If `TRUE`, adds p-values to the correlation plot labels. Default is `FALSE`. Only works with type 1 and 2.
`method`	Character string specifying the method for correlation calculation. Available options are `"pearson"` (default), `"spearman"`, and `"kendall"`. Only works with type 1 and 2.

`filter_var`	Character vector specifying the variables to exclude from the plot.
`id`	Optional unique identifier to filter the evolution type of plot. Default is `NULL`. Only works with type 3.
`n_row`	Integer specifying the number of rows to use in `facet_wrap()`. Default is `NULL`. Only works with type 1 and 2.
`n_col`	Integer specifying the number of columns to use in `facet_wrap()`. Default is `NULL`. Only works with type 1 and 2.
`base_size`	Numeric. Base font size for the plot. Default is 13.
`return_gg`	Logical. If `TRUE`, returns the ggplot object instead of printing it. Default is `FALSE`.
`add_avg`	Logical. If `TRUE`, returns evolution plot with the average trend across groups. Default is `FALSE`.
`...`	Further graphical parameters for future improvements.

Value

A ggplot object and an invisible data.frame containing the correlation table when `type` is `"var_by_x"` or `"x_by_var"`.

Examples

```
library(flexFitR)
data(dt_potato)
results <- explorer(dt_potato, x = DAP, y = c(Canopy, GLI), id = Plot)
table <- plot(results, label_size = 4, signif = TRUE, n_row = 2)
table
plot(results, type = "x_by_var", label_size = 4, signif = TRUE)
```

`plot.modeler` *Plot an object of class* `modeler`

Description

Creates several plots for an object of class `modeler`.

Usage

```
## S3 method for class 'modeler'
plot(
  x,
  id = NULL,
  type = 1,
  label_size = 4,
  base_size = 14,
  color = "red",
  color_points = "black",
```

```
  parm = NULL,
  n_points = 1000,
  title = NULL,
  add_ci = TRUE,
  color_ci = "blue",
  color_pi = "red",
  add_ribbon_ci = FALSE,
  add_ribbon_pi = FALSE,
  color_ribbon_ci = "blue",
  color_ribbon_pi = "red",
  ...
)
```

Arguments

`x`	An object of class `modeler`, typically the result of calling `modeler()`.
`id`	An optional group ID to filter the data for plotting, useful for avoiding overcrowded plots.
`type`	Numeric value (1-6) to specify the type of plot to generate. Default is 1. `type = 1` Plot of raw data with fitted curves. `type = 2` Plot of coefficients with confidence intervals. `type = 3` Plot of fitted curves, colored by group. `type = 4` Plot of fitted curves with confidence intervals. `type = 5` Plot of first derivative with confidence intervals. `type = 6` Plot of second derivative with confidence intervals.
`label_size`	Numeric value for the size of labels. Default is 4.
`base_size`	Numeric value for the base font size in pts. Default is 14.
`color`	Character string specifying the color for the fitted line when `type = 1`. Default is "red".
`color_points`	Character string specifying the color for the raw data points when `type = 1`. Default is "black".
`parm`	Character vector specifying the parameters to plot for `type = 2`. If `NULL`, all parameters are included.
`n_points`	Numeric value specifying the number of points for interpolation along the x-axis. Default is 2000.
`title`	Optional character string to add a title to the plot.
`add_ci`	Logical value indicating whether to add confidence intervals for `type = 4, 5, 6`. Default is `TRUE`.
`color_ci`	Character string specifying the color of the confidence interval when `type = 4, 5, 6`. Default is "blue".
`color_pi`	Character string specifying the color of the prediction interval when `type = 4`. Default is "red".
`add_ribbon_ci`	Logical value indicating whether to add a ribbon for confidence intervals in `type = 4, 5, 6`. Default is `FALSE`.

`add_ribbon_pi`	Logical value indicating whether to add a ribbon for prediction intervals in `type = 4`. Default is `FALSE`.
`color_ribbon_ci`	Character string specifying the color of the ribbon (ci). Default is "blue".
`color_ribbon_pi`	Character string specifying the color of the ribbon (pi). Default is "red".
`...`	Additional graphical parameters for future extensions.

Value

A `ggplot` object representing the specified plot.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
# Example 1
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(1:3)
  )
print(mod_1)
plot(mod_1, id = 1:2)
plot(mod_1, id = 1:3, type = 2, label_size = 10)
```

`plot.performance` *Plot an object of class* `performance`

Description

Creates plots for an object of class `performance`

Usage

```
## S3 method for class 'performance'
plot(
  x,
  id = NULL,
  type = 1,
```

```
  rescale = FALSE,
  linewidth = 1,
  base_size = 12,
  return_table = FALSE,
  ...
)
```

Arguments

`x`	An object of class `performance`, typically the result of calling `performance()`.
`id`	An optional group ID to filter the data for plotting, useful for avoiding overcrowded plots. This argument is not used when type = 2.
`type`	Numeric value (1-3) to specify the type of plot to generate. Default is 1. `type = 1` Radar plot by uid `type = 2` Radar plot averaging `type = 3` Bar plot by model-metric
`rescale`	Logical. If `TRUE`, metrics in type 3 plot are (0, 1) rescaled to improve interpretation. Higher values are better models. `FALSE` by default.
`linewidth`	Numeric value specifying size of line geoms.
`base_size`	Numeric value for the base font size in pts. Default is 12
`return_table`	Logical. If `TRUE`, table to generate the plot is returned. `FALSE` by default.
`...`	Additional graphical parameters for future extensions.

Value

A `ggplot` object representing the specified plot.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
# Model 1
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 90),
    subset = 40
  )
# Model 2
mod_2 <- dt_potato |>
  modeler(
```

```
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_logistic",
    parameters = c(L = 100, k = 4, t0 = 50),
    subset = 40
  )
# Model 3
mod_3 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_lin",
    parameters = c(m = 20, b = 2),
    subset = 40
  )
plot(performance(mod_1, mod_2, mod_3), type = 1)
plot(performance(mod_1, mod_2, mod_3, metrics = c("AICc", "BIC")), type = 3)
```

`plot_fn` *Plot user-defined function*

Description

This function plots a function over a specified interval and annotates the plot with the calculated Area Under the Curve (AUC) and parameter values. The aim of ‘plot_fn‘ is to allow users to play with different starting values in their functions before fitting any models.

Usage

```
plot_fn(
  fn = "fn_linear_sat",
  params = c(t1 = 34.9, t2 = 61.8, k = 100),
  interval = c(0, 100),
  n_points = 1000,
  auc = FALSE,
  x_auc_label = NULL,
  y_auc_label = NULL,
  auc_label_size = 4,
  param_label_size = 4,
  base_size = 12,
  color = "red",
  label_color = "grey30"
)
```

Arguments

`fn`	A character string representing the name of the function to be plotted. Default is "fn_linear_sat".
`params`	A named numeric vector of parameters to be passed to the function. Default is `c(t1 = 34.9, t2 = 61.8, k = 100)`.
`interval`	A numeric vector of length 2 specifying the interval over which the function is to be plotted. Default is `c(0, 100)`.
`n_points`	An integer specifying the number of points to be used for plotting. Default is 1000.
`auc`	Print AUC in the plot? Default is `FALSE`.
`x_auc_label`	A numeric value specifying the x-coordinate for the AUC label. Default is `NULL`.
`y_auc_label`	A numeric value specifying the y-coordinate for the AUC label. Default is `NULL`.
`auc_label_size`	A numeric value specifying the size of the AUC label text. Default is 3.
`param_label_size`	A numeric value specifying the size of the parameter label text. Default is 3.
`base_size`	A numeric value specifying the base size for the plot's theme. Default is 12.
`color`	A character string specifying the color for the plot lines and area fill. Default is "red".
`label_color`	A character string specifying the color for the labels. Default is "grey30".

Value

A ggplot object representing the plot.

Examples

```
# Example usage
plot_fn(
  fn = ”fn_linear_sat”,
  params = c(t1 = 34.9, t2 = 61.8, k = 100),
  interval = c(0, 100),
  n_points = 1000
)
plot_fn(
  fn = ”fn_lin_pl_lin”,
  params <- c(t1 = 38.7, t2 = 62, t3 = 90, k = 0.32, beta = -0.01),
  interval = c(0, 100),
  n_points = 1000,
  base_size = 12
)
```

`predict.modeler` *Predict an object of class* `modeler`

Description

Generate model predictions from an object of class `modeler`. This function allows for flexible prediction types, including point predictions, area under the curve (AUC), first or second order derivatives, and functions of the parameters.

Usage

```
## S3 method for class 'modeler'
predict(
  object,
  x = NULL,
  id = NULL,
  type = c("point", "auc", "fd", "sd"),
  se_interval = c("confidence", "prediction"),
  n_points = 1000,
  formula = NULL,
  metadata = FALSE,
  ...
)
```

Arguments

`object`	An object of class `modeler`, typically the result of calling the `modeler()` function.
`x`	A numeric value or vector specifying the points at which predictions are made. For `type = "auc"`, `x` must be a vector of length 2 that specifies the interval over which to calculate the AUC.
`id`	Optional unique identifier to filter predictions by a specific group. Default is `NULL`.
`type`	A character string specifying the type of prediction. Default is "point". `"point"` Predicts the value of `y` for the given `x`. `"auc"` Calculates the area under the curve (AUC) for the fitted model over the interval specified by `x`. `"fd"` Returns the first derivative (rate of change) of the model at the given `x` value(s). `"sd"` Returns the second derivative of the model at the given `x` value(s).
`se_interval`	A character string specifying the type of interval for standard error calculation. Options are `"confidence"` (default) or `"prediction"`. Only works with "point" estimation.
`n_points`	An integer specifying the number of points used to approximate the area under the curve (AUC) when `type = "auc"`. Default is `1000`.

`formula`	A formula specifying a function of the parameters to be estimated (e.g., `~ b * 500`). Default is `NULL`.
`metadata`	Logical. If `TRUE`, metadata is included with the predictions. Default is `FALSE`.
`...`	Additional parameters for future functionality.

Value

A `data.frame` containing the predicted values, their associated standard errors, and optionally the metadata.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(15, 2, 45)
  )
print(mod_1)
# Point Prediction
predict(mod_1, x = 45, type = "point", id = 2)
# AUC Prediction
predict(mod_1, x = c(0, 108), type = "auc", id = 2)
# First Derivative
predict(mod_1, x = 45, type = "fd", id = 2)
# Second Derivative
predict(mod_1, x = 45, type = "sd", id = 2)
# Function of the parameters
predict(mod_1, formula = ~ t2 - t1, id = 2)
```

`print.modeler` *Print an object of class* `modeler`

Description

Prints information about `modeler` function.

Usage

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

Arguments

`x`	An object fitted with the function `modeler()`.
`...`	Options used by the tibble package to format the output. See 'tibble::print()' for more details.

Value

an object inheriting from class `modeler`.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(1:5)
  )
plot(mod_1, id = c(1:4))
print(mod_1)
```

`residuals.modeler` *Extract residuals from a* `modeler` *object*

Description

Extract residuals from a `modeler` object

Usage

```
## S3 method for class 'modeler'
residuals(object, ...)
```

Arguments

`object`	An object of class 'modeler'
`...`	Additional parameters for future functionality.

Value

A numeric vector of residuals

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(15, 2, 45)
  )
residuals(mod_1)
```

`series_mutate` *Transform variables in a data frame*

Description

This function performs transformations on specified columns of a data frame, including truncating maximum values, handling negative values, and adding a zero to the series. It allows for grouping and supports retaining metadata in the output.

Usage

```
series_mutate(
  data,
  x,
  y,
  grp,
  metadata,
  max_as_last = FALSE,
  check_negative = FALSE,
  add_zero = FALSE,
  interval = NULL
)
```

Arguments

`data`	A `data.frame` containing the input data for analysis.
`x`	The name of the column in `data` representing the independent variable (x points).
`y`	The name of the column(s) in `data` containing variables to transform.
`grp`	Column(s) in `data` used as grouping variable(s). Defaults to `NULL` (optional).

`metadata`	Names of columns to retain in the output. Defaults to `NULL` (optional).
`max_as_last`	Logical. If `TRUE`, appends the maximum value after reaching the maximum. Default is `FALSE`.
`check_negative`	Logical. If `TRUE`, converts negative values in the data to zero. Default is `FALSE`.
`add_zero`	Logical. If `TRUE`, adds a zero value to the series at the start. Default is `FALSE`.
`interval`	A numeric vector of length 2 (start and end) specifying the range to filter the data. Defaults to `NULL`.

Value

A transformed `data.frame` with the specified modifications applied.

Examples

```
data(dt_potato)
new_data <- series_mutate(
  data = dt_potato,
  x = DAP,
  y = GLI,
  grp = gid,
  max_as_last = TRUE,
  check_negative = TRUE
)
```

`subset.modeler` *Subset an object of class* `modeler`

Description

Subset an object of class `modeler`

Usage

```
## S3 method for class 'modeler'
subset(x, id = NULL, ...)
```

Arguments

`x`	An object of class `modeler`, typically the result of calling `modeler()`.
`id`	Unique identifier to filter a `modeler` object by a specific group. Default is `NULL`.
`...`	Additional parameters for future functionality.

Value

A `modeler` object.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_logistic",
    parameters = c(L = 100, k = 4, t0 = 40),
    subset = 1:2
  )
print(mod)
mod_new <- subset(mod, id = 2)
print(mod_new)
```

`vcov.modeler` *Variance-Covariance matrix for an object of class* `modeler`

Description

Extract the variance-covariance matrix for the parameter estimates from an object of class `modeler`.

Usage

```
## S3 method for class 'modeler'
vcov(object, id = NULL, ...)
```

Arguments

`object`	An object of class `modeler`, typically the result of calling the `modeler()` function.
`id`	An optional unique identifier to filter by a specific group. Default is `NULL`.
`...`	Additional parameters for future functionality.

Value

A list of matrices, where each matrix represents the variance-covariance matrix of the estimated parameters for each group or fit.

Author(s)

Johan Aparicio [aut]

Examples

```
library(flexFitR)
data(dt_potato)
mod_1 <- dt_potato |>
  modeler(
    x = DAP,
    y = Canopy,
    grp = Plot,
    fn = "fn_linear_sat",
    parameters = c(t1 = 45, t2 = 80, k = 0.9),
    subset = c(15, 2, 45)
  )
print(mod_1)
vcov(mod_1)
```

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