

Package: nlsMicrobio (via r-universe)

August 18, 2024

Version 1.0-0

Title Nonlinear Regression in Predictive Microbiology

Depends stats, nlstools

Suggests knitr

Description Data sets and nonlinear regression models dedicated to predictive microbiology.

URL <https://github.com/lbbe-software/nlsMicrobio>

BugReports <https://github.com/lbbe-software/nlsMicrobio/issues>

License GPL-3

LazyLoad yes

LazyData yes

NeedsCompilation no

VignetteBuilder knitr

BuildVignettes true

Repository <https://lbbe-software.r-universe.dev>

RemoteUrl <https://github.com/lbbe-software/nlsmicrobio>

RemoteRef HEAD

RemoteSha b85e82be1a84e9e8e5d387f269360c96c93a98dd

Contents

competitioncurve	2
competitionmodels	3
growthcurve	5
growthmodels	6
ross	8
secondary	9
survivalcurve	11
survivalmodels	12

Index	15
--------------	-----------

`competitioncurve`*Growth kinetics of two competitive bacterial flora*

Description

Kinetics of simultaneous growth of *Escherichia coli* O157:H7 and ground beef background microflora in enrichment broth

Usage

```
data(competition1)
data(competition2)
```

Format

Data frames with 3 columns (t: time, flora : 1 for the first flora and 2 for the second one, LOG10N: decimal logarithm of bacterial density)

Source

Two of the kinetics used in Vimont et al. (2006)

References

Vimont A, Vernozy-Rozand C, Montet MP, Lazizzera C, Bavai C and Delignette-Muller ML (2006) Modeling and predicting the simultaneous growth of *Escherichia coli* O157:H7 and ground beef background microflora in various enrichment protocols. *Applied and Environmental Microbiology* **72**, 261-268.

Examples

```
data(competition1)
data(competition2)
def.par <- par(no.readonly = TRUE)
par(mfrow = c(1,2))
twocolors <- c("red", "blue")
plot(competition1$t, competition1$LOG10N, col=twocolors[competition1$flora])
plot(competition2$t, competition2$LOG10N, col=twocolors[competition2$flora])
par(def.par)
```

competitionmodels

Competition models for simultaneous growth of two bacterial flora

Description

Formulas of primary growth models used in predictive microbiology to model the simultaneous growth of two competitive bacterial flora assuming a Jameson effect

Usage

```
jameson_buchanan  
jameson_baranyi  
jameson_without_lag
```

Details

These models describe the simultaneous evolution of the decimal logarithm of the microbial counts of two flora (LOG10N) as a function of the time (t) and of the flora (flora) coded as 1 for counts of flora 1 and 2 for counts of flora 2. These three models assume independent lag and growth parameters for flora 1 and 2, except for the saturation which is supposed to be governed by the Jameson effect and modelled by a common parameter (tmax) which represents the time at which both flora stop to multiply. Modelling the simultaneous saturation by this way enables the model to be fitted by nls, as an analytical form of the model is available.

jameson_buchanan is based on the model of Buchanan et al. (1997) for lag phase modelling and is characterized by seven parameters (LOG10N0_1, mumax_1, lag_1, LOG10N0_2, mumax_2, lag_2 and the common saturation time tmax). This model was described and used in Vimont et al. (2006).

jameson_baranyi is based on the model of Baranyi and Roberts (1994) for lag phase modelling and is characterized by seven parameters (LOG10N0_1, mumax_1, lag_1, LOG10N0_2, mumax_2, lag_2 and the common saturation time tmax)

jameson_without_lag is based on the exponential model without lag phase and is thus characterized by five parameters (LOG10N0_1, mumax_1, LOG10N0_2, mumax_2 and the common saturation time tmax)

Value

A formula

Author(s)

Florent Baty, Marie-Laure Delignette-Muller

References

Baranyi J and Roberts, TA (1994) A dynamic approach to predicting bacterial growth in food, *International Journal of Food Microbiology*, **23**, 277-294.

Buchanan RL, Whiting RC, Damert WC (1997) When is simple good enough: a comparison of the Gompertz, Baranyi, and three-phase linear models for fitting bacterial growth curves. *Food Microbiology*, **14**, 313-326.

Vimont A, Vernozy-Rozand C, Montet MP, Lazizzera C, Bavai C and Delignette-Muller ML (2006) Modeling and predicting the simultaneous growth of *Escherichia coli* O157:H7 and ground beef background microflora in various enrichment protocols. *Applied and Environmental Microbiology* **72**, 261-268.

Examples

```
options(digits = 3)

### Example 1: fit of model jameson_buchanan
data(competition1)
nls1 <- nls(jameson_buchanan, competition1,
            list(lag_1 = 2, mumax_1 = 1, LOG10N0_1 = 1, tmax = 12,
                 lag_2 = 2, mumax_2 = 1, LOG10N0_2 = 4))

overview(nls1)

# Plot of theoretical curves with data
twocolors <- c("red", "blue")
npoints <- 100
seq.t <- seq(0, max(competition1$t), length.out=npoints)
prednls1.1 <- predict(nls1, data.frame(t=seq.t, flora=rep(1, npoints)))
prednls1.2 <- predict(nls1, data.frame(t=seq.t, flora=rep(2, npoints)))
plot(competition1$t, competition1$LOG10N, col=twocolors[competition1$flora], xlab="t", ylab="LOG10N")
lines(seq.t, prednls1.1, col=twocolors[1])
lines(seq.t, prednls1.2, col=twocolors[2])

### Example 2 : fit of model jameson_baranyi
data(competition1)
nls2 <- nls(jameson_baranyi, competition1,
            list(lag_1 = 2, mumax_1 = 1, LOG10N0_1 = 1, tmax = 12,
                 lag_2 = 2, mumax_2 = 1, LOG10N0_2 = 4))

overview(nls2)
plotfit(nls2)

# Plot of theoretical curves with data
twocolors <- c("red", "blue")
npoints <- 100
seq.t <- seq(0, max(competition1$t), length.out=npoints)
prednls2.1 <- predict(nls2, data.frame(t=seq.t, flora=rep(1, npoints)))
prednls2.2 <- predict(nls2, data.frame(t=seq.t, flora=rep(2, npoints)))
```

```
plot(competition1$t,competition1$LOG10N,col=twocolors[competition1$flora],xlab="t",ylab="LOG10N")
lines(seq.t,prednls2.1,col=twocolors[1])
lines(seq.t,prednls2.2,col=twocolors[2])

### Example 3: fit of model jameson_without_lag
data(competition2)
nls3 <- nls(jameson_without_lag, competition2,
            list(mumax_1 = 1, LOG10N0_1 = 1, tmax = 12,
                 mumax_2 = 1, LOG10N0_2 = 4))

overview(nls3)
plotfit(nls3)

# Plot of theoretical curves with data
twocolors <- c("red","blue")
npoints <- 100
seq.t <- seq(0,max(competition2$t),length.out=npoints)
prednls3.1 <- predict(nls3,data.frame(t=seq.t,flora=rep(1,npoints)))
prednls3.2 <- predict(nls3,data.frame(t=seq.t,flora=rep(2,npoints)))
plot(competition2$t,competition2$LOG10N,col=twocolors[competition2$flora],xlab="t",ylab="LOG10N")
lines(seq.t,prednls3.1,col=twocolors[1])
lines(seq.t,prednls3.2,col=twocolors[2])
```

growthcurve

Bacterial kinetics data sets

Description

Bacterial kinetics data sets

Usage

```
data(growthcurve1)
data(growthcurve2)
data(growthcurve3)
data(growthcurve4)
```

Format

Data frames with 2 columns (t: time, LOG10N: decimal logarithm of bacterial density)

Source

Data obtained by Florent Baty and Marie-Laure Delignette-Muller

Examples

```
data(growthcurve1)
data(growthcurve2)
data(growthcurve3)
data(growthcurve4)
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2,2))
plot(growthcurve1)
plot(growthcurve2)
plot(growthcurve3)
plot(growthcurve4)
par(def.par)
```

growthmodels

Bacterial growth models

Description

Formulas of primary growth models commonly used in predictive microbiology

Usage

```
baranyi
baranyi_without_Nmax
baranyi_without_lag
buchanan
buchanan_without_Nmax
buchanan_without_lag
gompertz
```

Details

These models describe the evolution of the decimal logarithm of the microbial count (LOG₁₀N) as a function of the time (t).

baranyi is the model of Baranyi and Roberts (1994) with four parameters (LOG₁₀N₀, μ_{max}, lag, LOG₁₀N_{max})

baranyi_without_Nmax is the model of Baranyi and Roberts (1994) with three parameters (LOG₁₀N₀, μ_{max}, lag), without braking

baranyi_without_lag is the model of Baranyi and Roberts (1994) with three parameters (LOG₁₀N₀, μ_{max}, LOG₁₀N_{max}), without lag

buchanan is the three-phase linear model proposed by Buchanan et al. (1997)

buchanan_without_Nmax is the two-phase linear model with three parameters (LOG₁₀N₀, μ_{max}, lag), without braking

buchanan_without_lag is the two-phase linear model with three parameters (LOG10N0, mumax, LOG10Nmax), without lag

gompertzgm is the modified Gompertz model introduced by Gibson et al. (1988) and reparameterized by Zwietering et al. (1990)

Value

A formula

Author(s)

Florent Baty, Marie-Laure Delignette-Muller

References

Baranyi J and Roberts, TA (1994) A dynamic approach to predicting bacterial growth in food, *International Journal of Food Microbiology*, **23**, 277-294.

Buchanan RL, Whiting RC, Damert WC (1997) When is simple good enough: a comparison of the Gompertz, Baranyi, and three-phase linear models for fitting bacterial growth curves. *Food Microbiology*, **14**, 313-326.

Gibson AM, Bratchell N, Roberts TA (1988) Predicting microbial growth: growth responses of salmonellae in a laboratory medium as affected by pH, sodium chloride and storage temperature. *International Journal of Food Microbiology*, **6**, 155 -178.

Zwietering MH, Jongenburger I, Rombouts FM, Van't Riet K (1990) Modeling of the bacterial growth curve. *Applied and Environmental Microbiology*, **56**, 1875-1881.

Examples

```
# Example 1

data(growthcurve1)
nls1 <- nls(baranyi, growthcurve1,
  list(lag=4, mumax=1, LOG10N0 = 4, LOG10Nmax = 9))
nls2 <- nls(gompertzgm, growthcurve1,
  list(lag = 4, mumax = 1, LOG10N0 = 4, LOG10Nmax = 9))
nls3 <- nls(buchanan, growthcurve1,
  list(lag = 4, mumax = 1, LOG10N0 = 4, LOG10Nmax = 9))
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2,2))
plotfit(nls1, smooth = TRUE)
plotfit(nls2, smooth = TRUE)
plotfit(nls3, smooth = TRUE)
par(def.par)
```

```

# Example 2

data(growthcurve2)
nls4 <- nls(baranyi_without_Nmax, growthcurve2,
  list(lag = 2, mumax = 0.4, LOG10N0 = 7.4))
nls5 <- nls(buchanan_without_Nmax, growthcurve2,
  list(lag = 2, mumax = 0.4, LOG10N0 = 7.4))
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2,1))
plotfit(nls4, smooth = TRUE)
plotfit(nls5, smooth = TRUE)
par(def.par)

# Example 3

data(growthcurve3)
nls6 <- nls(baranyi_without_lag, growthcurve3,
  list(mumax = 1, LOG10N0 = 0, LOG10Nmax = 5))
nls7 <- nls(buchanan_without_lag, growthcurve3,
  list(mumax = 1, LOG10N0 = 0, LOG10Nmax = 5))
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2,1))
plotfit(nls6, smooth = TRUE)
plotfit(nls7, smooth = TRUE)
par(def.par)

```

ross

Secondary growth curves

Description

A data frames describing the specific growth rate of *Escherichia coli* as a function of various environmental factors

Usage

```
data(ross)
```

Format

A data frame with five columns (author: the author of the paper from which the data was extracted, T: the temperature in Celsius, aw: the water activity, pH: the pH value, sqrtmumax: the square root of the maximum specific growth rate)

Source

Ross T, Ratkowsky DA, Mellefont LA, McMeekin TA (2003) Modelling the effects of temperature, water activity, pH and lactic acid concentration on the growth rate of *Escherichia coli*. *International of Food Microbiology*, **82**, 33-43.

Examples

```

data(ross)
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2, 2))
plot(ross[c("T", "sqrtmumax")])
plot(ross[c("pH", "sqrtmumax")])
plot(ross[c("aw", "sqrtmumax")])
par(def.par)

```

secondary

*Secondary growth models***Description**

Formulas of secondary growth models commonly used in predictive microbiology

Usage

```

cpm_T
cpm_pH_4p
cpm_pH_3p
cpm_aw_3p
cpm_aw_2p
cpm_T_pH_aw

```

Details

All the models describe the evolution of the square root of the maximum specific growth rate (sqrtmumax) as a function of one or more environmental factors among temperature (T), pH (pH) and water activity (aw). Each model must be fitted to a data frame including at least two columns, the last one named "sqrtmumax" and the first ones named "T", "pH" or "aw" according to the model.

cpm_T is the cardinal temperature model with inflection (Rosso et al., 1993) with four parameters (Tmin, Topt, Tmax, muopt)

cpm_pH_4p is the cardinal pH model (Rosso et al., 1995) with four parameters (pHmin, pHopt, pHmax, muopt)

cpm_pH_3p is a symmetric cardinal pH model with three parameters (pHmin, pHopt, muopt), obtained by fixing pHmax to 2pHopt-pHmin in the cpm_pH_4p model

cpm_aw_3p is the cardinal aw model (Rosso and Robinson, 2001) with three parameters (awmin, awopt, muopt)

cpm_aw_2p is a simplified cardinal aw model (Rosso and Robinson, 2001) with two parameters (awmin, muopt) obtained by fixing awopt to 1 in the cpm_aw_3p model

cpm_T_pH_aw is the cardinal model based on the gamma concept (Pinon et al., 2004) with 9 parameters (Tmin, Topt, Tmax, pHmin, pHopt, pHmax, awmin, awopt, muopt)

Value

A formula

Author(s)

Florent Baty, Marie-Laure Delignette-Muller

References

Pinon A, Zwietering M, Perrier L, Membrève J, Leporq B, Mettler E, Thuault D, Coroller L, Stahl V, Vialette M (2004) Development and validation of experimental protocols for use of cardinal models for prediction of microorganism growth in food products. *Applied Environmental Microbiology*, **70**, 1081-1087.

Rosso L, Robinson TP (2001) A cardinal model to describe the effect of water activity on the growth of moulds. *International Journal of Food Microbiology*, **63**, 265-273.

Rosso L, Lobry JR, Bajard S, Flandrois JP (1995) Convenient model to describe the combined effects of temperature and pH on microbial growth. *Applied Environmental Microbiology*, **61**, 610-616.

Rosso L, Lobry JR, Flandrois JP (1993) An unexpected correlation between cardinal temperatures of microbial growth highlighted by a new model. *Journal of Theoretical Biology* **162**, 447-463.

Examples

```
data(ross)

# Example for the cpm_T model

d1 <- subset(ross, author == "salter" & aw == 0.997,
  select = c(T, sqrtmumax))
nls1 <- nls(cpm_T, d1, list(muopt = 1.7, Tmin = 4, Topt = 40, Tmax = 47))
plotfit(nls1, smooth = TRUE)
overview(nls1)

# Example for the cpm_pH_4p model

d2 <- subset(ross, author == "presser" & aw > 0.99,
  select = c(pH, sqrtmumax))
nls2 <- nls(cpm_pH_4p, d2, list(muopt = 0.5, pHmin = 4,
  pHopt = 6.5, pHmax = 9))
plotfit(nls2, smooth = TRUE)
overview(nls2)
```

```
# Example for the cpm_pH_3p model

d3 <- subset(ross, author == "presser" & aw == 0.997,
  select = c(pH, sqrtmumax))
nls3 <- nls(cpm_pH_3p, d3, list(muopt = 0.5, pHmin = 4, pHopt = 6.5))
plotfit(nls3, smooth = TRUE)
overview(nls3)

# Example for the cpm_aw_3p model

d4<-subset(ross, author == "mellefont", select = c(aw, sqrtmumax))
nls4 <- nls(cpm_aw_3p, d4, list(muopt = 0.6, awmin = 0.95, awopt = 0.995))
plotfit(nls4, smooth = TRUE)
overview(nls4)

# Example for the cpm_aw_2p model

d5 <- subset(ross, author == "mellefont" & aw < 0.99,
  select = c(aw, sqrtmumax))
nls5 <- nls(cpm_aw_2p, d5, list(muopt = 0.6, awmin = 0.95))
plotfit(nls5, smooth = TRUE)
overview(nls5)

# Examples for the cpm_T_pH_aw model

d6 <- subset(ross, select = c(T, pH, aw, sqrtmumax))
nls6 <- nls(cpm_T_pH_aw, d6, list(muopt = 2, Tmin = 4, Topt = 40, Tmax = 49,
  pHmin = 4, pHopt = 6.5, pHmax = 9, awmin = 0.95, awopt = 0.995))
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2, 2))
plotfit(nls6, variable = 1)
plotfit(nls6, variable = 2)
plotfit(nls6, variable = 3)
overview(nls6)
par(def.par)
```

survivalcurve

Bacterial survival data sets

Description

Bacterial kinetics data sets

Usage

```
data(survivalcurve1)
data(survivalcurve2)
data(survivalcurve3)
```

Format

Data frames with 2 columns (t: time, LOG10N: decimal logarithm of bacterial density)

Source

Data obtained by Florent Baty and Marie-Laure Delignette-Muller

Examples

```
data(survivalcurve1)
data(survivalcurve2)
data(survivalcurve3)
def.par <- par(no.readonly = TRUE)
par(mfrow=c(2,2))
plot(survivalcurve1, type="b")
plot(survivalcurve2, type="b")
plot(survivalcurve3, type="b")
par(def.par)
```

survivalmodels

Bacterial survival models

Description

Formulas of primary survival models commonly used in predictive microbiology

Usage

```
geeraerd
geeraerd_without_Nres
geeraerd_without_Sl
mafart
albert
trilinear
bilinear_without_Nres
bilinear_without_Sl
```

Details

These models describe the evolution of the decimal logarithm of the microbial count (LOG10N) as a function of the time (t).

geeraerd is the model of Geeraerd et al. (2005) with four parameters (LOG10N0, kmax, Sl, LOG10Nres)

geeraerd_without_Nres is the model of Geeraerd et al. (2005) with three parameters (LOG10N0, kmax, Sl), without tail

geeraerd_without_Sl is the model of Geeraerd et al. (2005) with three parameters (LOG10N0,

kmax, Nres), without shoulder

mafart is the Weibull model as parameterized by Mafart et al. (2002) with three parameters (p, delta, LOG10N0)

albert is the modified Weibull model proposed by Albert and Mafart (2005) with four parameters (p, delta, LOG10N0, LOG10Nres)

trilinear is the three-phase linear model with four parameters (LOG10N0, kmax, Sl, LOG10Nres)

bilinear_without_Nres is the two-phase linear model with three parameters (LOG10N0, kmax, Sl), without tail

bilinear_without_Sl is the two-phase linear model with three parameters (LOG10N0, kmax, LOG10Nres), without shoulder

Value

A formula

Author(s)

Florent Baty, Marie-Laure Delignette-Muller

References

Albert I, Mafart P (2005) A modified Weibull model for bacterial inactivation. *International Journal of Food Microbiology*, **100**, 197-211.

Geeraerd AH, Valdramidis VP, Van Impe JF (2005) GInaFiT, a freeware tool to assess non-log-linear microbial survivor curves. *International Journal of Food Microbiology*, **102**, 95-105.

Mafart P, Couvert O, Gaillard S, Leguerinel I (2002) On calculating sterility in thermal preservation methods : application of the Weibull frequency distribution model. *International Journal of Food Microbiology*, **72**, 107-113.

Examples

```
# Example 1

data(survivalcurve1)
nls1a <- nls(geeraerd, survivalcurve1,
  list(Sl = 5, kmax = 1.5, LOG10N0 = 7, LOG10Nres = 1))
nls1b <- nls(trilinear, survivalcurve1,
  list(Sl = 5, kmax = 1.5, LOG10N0 = 7, LOG10Nres = 1))
nls1c <- nls(albert, survivalcurve1,
  list(p = 1.2, delta = 4, LOG10N0 = 7, LOG10Nres = 1))
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2,2))
overview(nls1a)
```

```
plotfit(nls1a, smooth = TRUE)
overview(nls1b)
plotfit(nls1b, smooth = TRUE)
overview(nls1c)
plotfit(nls1c, smooth = TRUE)
par(def.par)

# Example 2

data(survivalcurve2)
nls2a <- nls(geeraerd_without_Nres, survivalcurve2,
  list(S1 = 10, kmax = 1.5, LOG10N0 = 7.5))
nls2b <- nls(bilinear_without_Nres, survivalcurve2,
  list(S1 = 10, kmax = 1.5, LOG10N0 = 7.5))
nls2c <- nls(mafart, survivalcurve2,
  list(p = 1.5, delta = 8, LOG10N0 = 7.5))
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2,2))
overview(nls2a)
plotfit(nls2a, smooth = TRUE)
overview(nls2b)
plotfit(nls2b, smooth = TRUE)
overview(nls2c)
plotfit(nls2c, smooth = TRUE)
par(def.par)

# Example 3

data(survivalcurve3)
nls3a <- nls(geeraerd_without_S1, survivalcurve3,
  list(kmax = 4, LOG10N0 = 7.5, LOG10Nres = 1))
nls3b <- nls(bilinear_without_S1, survivalcurve3,
  list(kmax = 4, LOG10N0 = 7.5, LOG10Nres = 1))
nls3c <- nls(mafart, survivalcurve3,
  list(p = 0.5, delta = 0.2, LOG10N0 = 7.5))
def.par <- par(no.readonly = TRUE)
par(mfrow = c(2,2))
overview(nls3a)
plotfit(nls3a, smooth = TRUE)
overview(nls3b)
plotfit(nls3b, smooth = TRUE)
overview(nls3c)
plotfit(nls3c, smooth = TRUE)
par(def.par)
```

Index

* datasets

competitioncurve, 2
growthcurve, 5
ross, 8
survivalcurve, 11

* models

competitionmodels, 3
growthmodels, 6
secondary, 9
survivalmodels, 12

albert (survivalmodels), 12

baranyi (growthmodels), 6
baranyi_without_lag (growthmodels), 6
baranyi_without_Nmax (growthmodels), 6
bilinear_without_Nres (survivalmodels),
12
bilinear_without_Sl (survivalmodels), 12
buchanan (growthmodels), 6
buchanan_without_lag (growthmodels), 6
buchanan_without_Nmax (growthmodels), 6

competition1 (competitioncurve), 2
competition2 (competitioncurve), 2
competitioncurve, 2
competitionmodels, 3
cpm_aw_2p (secondary), 9
cpm_aw_3p (secondary), 9
cpm_pH_3p (secondary), 9
cpm_pH_4p (secondary), 9
cpm_T (secondary), 9
cpm_T_pH_aw (secondary), 9

geeraerd (survivalmodels), 12
geeraerd_without_Nres (survivalmodels),
12
geeraerd_without_Sl (survivalmodels), 12
gompertz (growthmodels), 6
growthcurve, 5

growthcurve1 (growthcurve), 5
growthcurve2 (growthcurve), 5
growthcurve3 (growthcurve), 5
growthcurve4 (growthcurve), 5
growthmodels, 6

jameson_baranyi (competitionmodels), 3
jameson_buchanan (competitionmodels), 3
jameson_without_lag
(competitionmodels), 3

mafart (survivalmodels), 12

ross, 8

secondary, 9
survivalcurve, 11
survivalcurve1 (survivalcurve), 11
survivalcurve2 (survivalcurve), 11
survivalcurve3 (survivalcurve), 11
survivalmodels, 12

trilinear (survivalmodels), 12