Package ‘NRAIA’

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Title Data sets from ‘‘Nonlinear Regression Analysis and Its Applications’’

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Description Datasets from Bates and Watts (1988) ‘‘Nonlinear Regression Analysis and Its Applications’’ with sample code.

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R topics documented:

BOD2 *Biochemical Oxygen Demand*

Description

The BOD2 data frame has 8 rows and 2 columns giving the biochemical oxygen demand versus time in an evaluation of water quality.

Format

This data frame contains the following columns:

Time A numeric vector giving the time of the measurement (days).

demand A numeric vector giving the biochemical oxygen demand (mg/l).

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley, (Appendix A4.1).

Originally from Marske (1967), M.Sc. Thesis, University of Wisconsin - Madison.

Examples

```
str(BOD2)
# simplest form of fitting a first-order model to these data
(fm1 <- nls(demand ~ A*(1-exp(-exp(lrc)*Time)), data = BOD2,
   start = c(A = 2.2, lrc = log(0.25))))
coef(fm1)
# using the plinear algorithm
(fm2 <- nls(demand ~ (1-exp(-exp(lrc)*Time)), data = BOD2,
   start = c(lrc = log(0.25)), algorithm = "plinear", trace = TRUE))
# using a self-starting model
(fm3 <- nls(demand ~ SSasympOrig(Time, A, lrc), data = BOD2))
plotfit(fm3, xlab = "Time (days)",
        ylab = "Biochemical Oxygen Demand")
```

Chloride *Chloride ion concentrations*

Description

The Chloride data frame has 54 rows and 2 columns representing measurements of the chloride ion concentration in blood cells suspended in a salt solution.

Format

This data frame contains the following columns:

conc A numeric vector giving the chloride ion concentration (%).

Time A numeric vector giving the time of the concentration measurement (min).

Details

There is a noticeable serial correlation in the residuals from a fit of a simple asymptotic regression model to these data, as described in section 3.8 of Bates and Watts (Wiley, 1988). We can either use a modified model with nls, as described in the reference, or model it directly with the gnls function.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A4.1).

Originally from Sredni (1970), Ph.D. Thesis, University of Wisconsin - Madison.

Examples

```
## Fit nonlinear regression model
(fm1 <- nls(conc ~ Asym*(1 - prop*exp(-exp(lrc)*Time)), data = Chloride,
           start = c(Asym = 50, prop = 0.6, lrc = log(0.25)), trace = TRUE))
plotfit(fm1, xlab = "Time (min)", ylab = "Chloride ion concentration (%)")
plot(resid(fm1) ~ fitted(fm1),  # plot shows patterns in the residuals
     xlab = "Least squares fitted values",
     ylab = "Least squares residuals",
     main = "Residuals from least squares fit")
abline(h = 0, lty = 2, lwd = 0)
plot(resid(fm1)[-1], resid(fm1)[-length(resid(fm1))],  # lag plot
     xlab = "Least squares residual",
     ylab = "Lagged least squares residual",
     main = "Lag plot of least squares residuals")
abline(h = 0, lty = 2, lwd = 0)
abline(v = 0, lty = 2, lwd = 0)
## Use conditional linearity in another formulation of the model
(fm2 <- nls(conc ~ cbind(1, exp(-exp(lrc)*Time)), data = Chloride,
           start = c(lrc = log(0.25)), algorithm = "plinear", trace = TRUE))
## Using a self-Starting model in yet another formulation
(fm3 <- nls(conc ~ SSasympOff(Time, Asym, c0, lrc), data = Chloride))
```

`Coal` *Coal liquefaction data*

Description

The `Coal` data frame has 23 rows and 20 columns of data on a coal liquefaction process.

Format

This data frame contains the following columns:

Time the time of the observation, measured from the beginning of the run (min).

temp the temperature of the run (K).

pressure the pressure at which the run was performed (MPa).

fe2o3 iron oxide? (Fe2 O3) concentration in the run (wt% maf).

tr transfer rate of the feed (wt% maf).

x1 inlet composition of unconverted coal (wt %).

x2 inlet composition of thermal residuals (wt %).

x3 inlet composition of C4-822K (wt %).

x4 inlet composition of C1-C3 gases (wt %).

x5 inlet composition of byproduct gases (wt %).

x6 inlet composition of water (wt %).

x7 inlet composition of hydrogen (wt %).

x8 inlet composition of Coal (wt %).

y1 outlet composition of unconverted coal (wt %).

y2 outlet composition of thermal residuals (wt %).

y3 outlet composition of C4-822K (wt %).

y4 outlet composition of C1-C3 gases (wt %).

y5 outlet composition of byproduct gases (wt %).

y6 outlet composition of water (wt %).

y7 outlet composition of hydrogen (wt %).

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A4.7).

Originally from Lythgoe (1986), M.Sc. Thesis, Queen's University at Kingston.

Examples

```
str(Coal)
x8s <- with(Coal, equal.count(x8))
xyplot( y1 ~ x1 | x8s * Time, Coal, type = c("g","p"))
xyplot( y2 ~ x2 | x8s * Time, Coal, type = c("g","p"))
xyplot( y3 ~ x3 | x8s * Time, Coal, type = c("g","p"))
xyplot( y4 ~ x4 | x8s * Time, Coal, type = c("g","p"))
xyplot( y5 ~ x5 | x8s * Time, Coal, type = c("g","p"))
xyplot( y6 ~ x6 | x8s * Time, Coal, type = c("g","p"))
xyplot( y7 ~ x7 | x8s * Time, Coal, type = c("g","p"))
```

`Ethyl` *Ethyl Acrylate data*

Description

The `Ethyl` data frame has 12 rows and 3 columns of ethyl acrylate concentrations in exhalate of a rat.

Format

This data frame contains the following columns:

start start of collection period, measured from the start of the experiment (hr).

length duration of the collection period (hr).

CO2 exhaled radioactively tagged CO_2 (g).

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.10).

Originally from Watts, deBethizy, and Stiratelli (1986), Technical Report, Rohm and Haas Co.

Examples

```
str(Ethyl)
xyplot(cumsum(CO2) ~ I(start + length), # compare to Figure 3.10, page 97
     data = Ethyl, type = c("g","S"), scales=list(x=list(log =2)),
     xlab = "Time (hr)",
     ylab = expression(plain("Normalized cumulative CO")[2]*(g)))
```

Isom *Isomerization data*

Description

The Isom data frame has 24 rows and 4 columns from an isomerization experiment.

Format

This data frame contains the following columns:

hyd partial pressure of hydrogen (psia).

n.pent partial pressure of n-pentane (psia).

iso.pen partial pressure of isopentane (psia).

rate reaction rate for isomerization of n-pentane to isopentane (1/hr).

Details

These are data on the reaction rate of catalytic isomerization of n-pentane to isopentane.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Originally from Carr (1960), *Industrial and Engineering Chemistry*, 52, pp. 391-396.

Examples

```
str(Isom)
splom(Isom, main = "Isom data")
xyplot(rate ~ hyd, data = Isom, type = c("g", "p"),
     xlab = "Hydrogen partial pressure (psia)",
     ylab = expression(plain("Reaction rate (hr")^{-1}*plain(")")))
xyplot(rate ~ n.pent, data = Isom, type = c("g", "p"),
     xlab = "n-pentane partial pressure (psia)",
     ylab = expression(plain("Reaction rate (hr")^{-1}*plain(")")))
xyplot(rate ~ iso.pen, data = Isom, type = c("g", "p"),
     xlab = "iso-pentane partial pressure (psia)",
     ylab = expression(plain("Reaction rate (hr")^{-1}*plain(")")))
## Note - the model is mis-stated on page 272, x2 and x3 are reversed
fm1 <-
 nls(rate ~ b3*(n.pent - iso.pen/1.632)/(1+b2*hyd+b3*n.pent+b4*iso.pen),
         data = Isom, start = c(b2 = 0.1, b3 = 0.1, b4 = 0.1),
         algorithm = "plinear", trace = TRUE)
summary(fm1)        # compare to Table 2.2, page 56
```

Leaves *Growth of Leaves*

Description

The `Leaves` data frame has 15 rows and 2 columns of leaf length over time.

Format

This data frame contains the following columns:

Time time from initial emergence (days).

Length leaf length (cm).

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A4.5).

Originally from Heyes and Brown (1956) in F.L. Milthorpe (ed), *The Growth of Leaves*, London: Butterworth.

Examples

```
options(show.signif.stars = FALSE)
## first fit a logistic model
fm1 <- nls(Length ~ SSlogis(Time, Asym, xmid, scal), data = Leaves)
summary(fm1)
plotfit(fm1, xlab = "Time from initial emergence (days)",
        ylab = "Leaf length (cm)", main = "Logistic growth model")
## compare with Richards growth model
fm2 <- nls(Length ~ Asym/(1+exp(-(Time - xmid)/scal))^exp(-lpow), Leaves,
           c(coef(fm1),c(lpow = 0)))
summary(fm2)
anova(fm1, fm2)
plotfit(fm2, xlab = "Time from initial emergence (days)",
        ylab = "Leaf length (cm)", main = "Richards growth model")
pm1 <- profile(fm1)
plot(pm1, aspect = ’xy’, layout = c(3,1))
plot(pm1, absVal = FALSE, aspect = ’xy’, layout = c(3,1))
pm2 <- profile(fm2, alpha = 0.05)
plot(pm2, aspect = ’xy’, layout = c(4,1))
plot(pm2, absVal = FALSE, aspect = ’xy’, layout = c(4,1))
```

Lipo *Lipoprotein concentrations*

Description

The Lipo data frame has 12 rows and 2 columns of lipoprotein concentrations over time.

Format

This data frame contains the following columns:

time a numeric vector giving the time of the concentration measurement (hr)

conc a numeric vector of concentrations.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A4.1).

Examples

```
plot(conc ~ time, data = Lipo,
     xlab = "Time since drug administration (hr)",
     ylab = "Lipoprotein concentration",
     main = "Lipo data and fitted curve", las = 1)
fm1 <- nls(conc ~ SSbiexp(time, A1, lrc1, A2, lrc2), data = Lipo)
summary(fm1)
usr <- par("usr")
xx <- seq(usr[1], usr[2], len = 51)
lines(xx, predict(fm1, list(time = xx)))
title(sub = deparse(fm1$call$formula))
```

Lubricant *Viscosity of lubricants*

Description

The Lubricant data frame has 53 rows and 3 columns on the viscosity of a lubricant at different pressures and temperatures.

Format

This data frame contains the following columns:

pressure a numeric vector of pressures (stokes).

viscos a numeric vector of observed log(kinematic viscosity).

tempC a numeric vector of temperatures (degrees Celsius).

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
str(Lubricant)
tempf <- as.factor(Lubricant$tempC)
levels(tempf) <- paste(c(0.0,25.0,37.8,98.9),"C")
xyplot(viscos ~ pressure, Lubricant, groups = tempf,
     xlab = "Pressure (atm)", type = c("g", "p"),
     ylab = "kinematic viscosity (stokes)",
     scales = list(y = list(log = 2)),
     auto.key = list(space = "top", columns = 4))
rm(tempf)
```

`Nitren` *Nitrendipene data*

Description

The `Nitren` data frame has 26 rows and 5 columns from an experiment in cardiology.

Format

This data frame contains the following columns:

log.NIF a numeric vector giving the log of the NIF concentration

tiss1 a numeric vector giving the reaction in tissue 1.

tiss2 a numeric vector giving the reaction in tissue 2.

tiss3 a a numeric vector giving the reaction in tissue 3.

tiss4 a numeric vector giving the reaction in tissue 4.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
matplot(Nitren[, 1], Nitren[, -1], las = 1,
    xlab = "log(NIF concentration)",
    ylab = "reaction level",
    main = paste("Nitren data and fitted curves,",
         "omitting zero concentration data"))
## without the data at NIF concentration of zero
options(na.action = na.omit)
fm1 <- nls(tiss1 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
```

```
fm1
fm2 <- nls(tiss2 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
fm2
fm3 <- nls(tiss3 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
fm3
fm4 <- nls(tiss4 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
fm4
usr <- par("usr")
xx <- seq(usr[1], usr[2], len = 50)
lines(xx, predict(fm1, list(log.NIF = xx)), col = 1, lty = 2)
lines(xx, predict(fm2, list(log.NIF = xx)), col = 2, lty = 2)
lines(xx, predict(fm3, list(log.NIF = xx)), col = 3, lty = 2)
lines(xx, predict(fm4, list(log.NIF = xx)), col = 4, lty = 2)
title(sub = deparse(fm1$call$formula))
## replacing the data at NIF concentration of zero by a very small value
log.NIF <- Nitren[, 1]
log.NIF[ is.na(log.NIF) ] <- -18
Nitren[, 1] <- log.NIF
matplot(Nitren[, 1], Nitren[, -1], las = 1,
    xlab = "log(NIF concentration)",
    ylab = "reaction level",
    main = paste("Nitren data and fitted curves",
       "- zero concentration recoded as -18"))
fm1 <- nls(tiss1 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
fm1
fm2 <- nls(tiss2 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
fm2
fm3 <- nls(tiss3 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
fm3
fm4 <- nls(tiss4 ~ SSfpl(log.NIF, A, B, xmid, scal), Nitren)
fm4
usr <- par("usr")
xx <- seq(usr[1], usr[2], len = 50)
lines(xx, predict(fm1, list(log.NIF = xx)), col = 1, lty = 2)
lines(xx, predict(fm2, list(log.NIF = xx)), col = 2, lty = 2)
lines(xx, predict(fm3, list(log.NIF = xx)), col = 3, lty = 2)
lines(xx, predict(fm4, list(log.NIF = xx)), col = 4, lty = 2)
title(sub = deparse(fm1$call$formula))
```

Nitrite *Nitrite utilization by bean leaves*

Description

The Nitrite data frame has 48 rows and 3 columns giving nitrite utilization by bean leaves under different light conditions on two different days.

Format

This data frame contains the following columns:

light a numeric vector of light intensities.

utilization a numeric vector of nitrite utilizations.

day a factor with levels `1` `2`

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.10).

Examples

```
str(Nitrite)
xyplot(utilization ~ light, Nitrite, groups = day,
     xlab = "Light intensity", type = c("a", "g", "p"),
     ylab = "Nitrite utilization",
     auto.key = list(space = "top", columns = 2))
```

`O.xylene` *O-xylene reaction data*

Description

The `O.xylene` data frame has 57 rows and 4 columns of data on a chemical engineering experiment.

Format

This data frame contains the following columns:

oxygen a numeric vector giving the oxygen partial pressure.

o.xyl a numeric vector giving the O.xylene partial pressure.

temp a numeric vector giving the temperature (Kelvins).

rate a numeric vector giving the rate of reaction.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.6).

Examples

```
str(O.xylene)
tempf <- with(O.xylene, ordered(temp))
levels(tempf) <- paste(levels(tempf), "K")
Oxygen <- with(O.xylene, equal.count(oxygen))
O.xyl <- with(O.xylene, equal.count(o.xyl))
xyplot(rate ~ o.xyl | Oxygen * tempf, O.xylene,
       type = c("g", "p"), aspect = 'xy',
       xlab = "O.xylene partial pressure",
       ylab = "Reaction rate")
xyplot(rate ~ o.xyl | Oxygen, O.xylene, groups = tempf,
       type = c("g", "p"), aspect = 2.5,
       xlab = "O.xylene partial pressure",
       ylab = "Reaction rate",
       auto.key = list(space = "right"))
xyplot(rate ~ oxygen | O.xyl, O.xylene, groups = tempf,
       type = c("g", "p"), aspect = 2.5,
       xlab = "Oxygen partial pressure",
       ylab = "Reaction rate",
       auto.key = list(space = "right"))
```

Oilshale *Pyrolysis of Oil Shale*

Description

The Oilshale data frame has 64 rows and 4 columns from an experiment on the pyrolysis of oil shale.

Format

This data frame contains the following columns:

time a numeric vector giving the time since the beginning of the experiment.

bitumen a numeric vector giving the proportion of bitumen.

oil a numeric vector giving the proportion of oil.

temp a numeric vector giving the temperature of the run.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
str(Oilshale)
```

PCB *PCB concentrations in Lake Cayuga fish*

Description

The PCB data frame has 28 rows and 2 columns giving the concentration of polychlorinated biphenyls (PCB's) in fish caught in Lake Cayuga in northern New York state. The fish had been tagged as yearlings so their ages could be accurately determined.

Format

This data frame contains the following columns:

age a numeric vector giving the age of the fish in years.

conc a numeric vector giving the concentration of PCB's in the fish.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.1).

Examples

```
str(PCB)
# compare to Figure 1.1 (p. xxx)
xyplot(conc ~ age, PCB, aspect = 'xy',
     type = c("g", "p"), xlab = "Age of fish (yr)",
     ylab = "PCB concentration")
# compare to Figure 1.2 (p. xxx)
xyplot(conc ~ age, PCB, scales = list(y = list(log = 2)),
     aspect = 'xy', type = c("g", "p", "smooth"),
     xlab = "Age of fish (yr)",
     ylab = "PCB concentration")
# linear model in cube root of age
summary(fm1 <- lm(log(conc) ~ I(age^(1/3)), data = PCB))
xyplot(log(conc) ~ I(age^(1/3)), data = PCB, aspect = 'xy',
     xlab = "Cube root of age (yr)", type = c("g", "p", "r"),
     ylab = "log(PCB concentration)",
     main = "Transformed PCB data and fitted line",
     sub = deparse(fm1$call$formula))
# diagnostic plots
opar <- par(mfrow = c(2, 2))
plot(fm1, which = 1:4, las = 1)
par(opar)
```

Pinene *Alpha-pinene and by-products*

Description

The Pinene data frame has 8 rows and 6 columns giving the proportion of alpha-pinene and four of its by-products over time.

Format

This data frame contains the following columns:

time a numeric vector giving the time at which the observation is made. (hours)

a.pin a numeric vector giving the alpha-pinene proportion. (%)

dipen a numeric vector giving the dipene proportion. (%)

alloo a numeric vector giving the allo-ocimene proportion. (%)

pyron a numeric vector giving the pyronene proportion. (%)

dimer a numeric vector giving the dimer proportion. (%)

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.6).

Examples

```
str(Pinene)
xyplot(a.pin + dipen + alloo + pyron + dimer ~ time, Pinene,
  type = c("b", "g"), aspect = 'xy',
  xlab = "Time (hr)", ylab = "Proportion (%)",
  auto.key = list(space = "right", lines = TRUE))
```

Pinene2 *Alpha-pinene and by-products*

Description

The Pinene data frame has 8 rows and 6 columns giving the proportion of alpha-pinene and four of its by-products over time from a second experiment.

Format

This data frame contains the following columns:

time a numeric vector giving the time at which the observation is made. (hr)

a.pin a numeric vector giving the alpha-pinene proportion. (%)

dipen a numeric vector giving the dipene proportion. (%)

alloo a numeric vector giving the allo-ocimene proportion. (%)

pyron a numeric vector giving the pyronene proportion. (%)

dimer a numeric vector giving the dimer proportion. (%)

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.6).

See Also

`Pinene`

Examples

```
str(Pinene2)
xyplot(a.pin + dipen + alloo + pyron + dimer ~ time, Pinene2,
  type = c("b", "g"), aspect = 'xy',
  xlab = "Time (hr)", ylab = "Proportion (%)",
  auto.key = list(space = "right", lines = TRUE))
```

`plotfit` *Plot x-y data and a fitted model*

Description

Extract the original data from a fitted model and plot these data along with a smooth curve of the fitted model function. The fitted model must be for one covariate only.

Usage

```
plotfit(fm, ...)
## S3 method for class 'nls'
plotfit(fm, ...)
```

Arguments

`fm`	A fitted model object, typically a `nls` fitted model.
`...`	Arguments to be passed to `xyplot` or `panel.curve`.

Value

A lattice object.

See Also

xyplot, panel.curve

Examples

```
fm1 <- nls(rate ~ conc/(K + conc), Puromycin, c(K = 0.05),
           subset = state == "treated", alg = "plinear")
plotfit(fm1, from = 0)
```

Rumford *Count Rumford's cooling data*

Description

The Rumford data frame has 13 rows and 2 columns from an experiment by Count Rumford on the rate of cooling.

Format

This data frame contains the following columns:

time a numeric vector giving the time since the beginning of the experiment (hr).

temp a numeric vector giving the temperature (degrees Fahrenheit) of the cannon.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
plot(temp ~ time, Rumford, las = 1,
     xlab = "Time since beginning of experiment (hr)",
     ylab = "Temperature of cannon (degrees F)",
     main = "Rumford data and fitted curve")
fm1 <- nls(temp ~ 60 + 70 * exp(tc * time), data = Rumford,
           start = c(tc = -0.01))
summary(fm1)
usr <- par("usr")
xx <- seq(usr[1], usr[2], len = 50)
lines(xx, predict(fm1, list(time = xx)))
```

Sacch2 *Pharmacokinetics of saccharin*

Description

The Sacch2 data frame has 10 rows and 2 columns from an experiment on the pharmacokinetics of saccharin.

Format

This data frame contains the following columns:

time a numeric vector giving the time since drug administration (min).

conc a numeric vector giving the observed concentration of saccharin.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
str(Sacch2)
xyplot(conc ~ time, Sacch2, type = c("g", "b"),
     xlab = "Time since drug administration (min)",
     ylab = "Saccharin concentration", aspect = "xy")
xyplot(conc ~ time, data = Sacch2, type = c("g", "b"),
     scales = list(y = list(log = 2)), aspect = 'xy',
     xlab = "Time since drug administration (min)",
     ylab = "Saccharin concentration")
## Not run:
fm1 <- nls(conc ~ SSfol(1.0, time, lKe, lKa, lCl), data = Sacch2)
summary(fm1)
xpred <- seq(0, 140, len = 51)
ypred <- predict(fm1, list(time = xpred, Dose = rep(1.0, length(xpred))))
lines(xpred, ypred)

## End(Not run)
```

Saccharin *Elimination of saccharin*

Description

The Saccharin data frame has 9 rows and 3 columns from an experiment on the elimination of saccharin.

Format

This data frame contains the following columns:

start start of collection period, measured from the start of the experiment (hr).

length duration of the collection period (hr).

sacch exhaled radioactively tagged CO2 (g).

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
xyplot(cumsum(sacch) ~ I(start + length), Saccharin,
     type = c("g", "S"), scales = list(x = list(log = 2)),
     xlab = "Time (hr)", ylab = "Cumulative saccharin")
```

---

sPMMA *syndiotactic poly-methyl-methacrylate*

Description

The sPMMA data frame has 23 rows and 3 columns from an experiment on the dielectric response of a sample of syndiotactic poly-methyl-methacrylate (sPMMA).

Format

This data frame contains the following columns:

freq a numeric vector giving the frequency of the driving signal (Hz).

real a numeric vector giving the real component of the dielectric response.

imag a numeric vector giving the imaginary component of the dielectric response.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
str(sPMMA)
xyplot(imag ~ real, data = sPMMA, xlab = "Real component",
     ylab = "Imaginary component", type = c("p", "g"))
xyplot(real + imag ~ freq, data = sPMMA, xlab = "Frequency (Hz)",
     ylab = "Component of dielectric response",
     main = "sPMMA data", type = c("g", "p"), aspect = 'xy',
     auto.key = list(space = "right"))
```

SSRichards *Richards Growth Model*

Description

This `selfStart` model evaluates the Richards growth model function and its gradient. It has an `initial` attribute that creates initial estimates of the parameters `Asym`, `xmid`, `scal` and `lpow`.

Usage

```
SSRichards(input, Asym, xmid, scal, lpow)
```

Arguments

`input` a numeric vector of values at which to evaluate the model.

`Asym` a numeric parameter representing the asymptote.

`xmid` a numeric parameter representing the `x` value at the inflection point of the curve. The value of `SSlogis` will be `Asym/2` at `xmid`.

`scal` a numeric scale parameter on the `input` axis.

`lpow` the natural logarithm of the inverse of the power to which the denominator is raised.

Value

a numeric vector of the same length as `input`. It is the value of the expression `Asym*(1+exp((xmid-input)/scal))^(-exp(` If all of the arguments `Asym`, `xmid`, `scal` and `lpow` are names of objects, the gradient matrix with respect to these names is attached as an attribute named `gradient`.

See Also

`nls`, `selfStart`

Examples

```
summary(fm1 <- nls(Length ~ SSRichards(Time, Asym, xmid, scal, lpow), Leaves))
```

Sulfi *Pharmacokinetics of sulfisoxazole*

Description

The Sulfi data frame has 12 rows and 2 columns from an experiment on the pharmacokinetics of sulfisoxazole.

Format

This data frame contains the following columns:

time a numeric vector giving the time since drug administration (min).

conc a numeric vector giving the observed concentration of sulfisoxazole (μg/ml).

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
plot(conc ~ time, data = Sulfi, las = 1,
     xlab = "Time since drug administration (min)",
     ylab = expression(plain("Sulfisoxazole concentration (")
               *mu*plain("g/ml)")),
     main = "Sulfisoxazole data and fitted curve")
fm1 <- nls(conc ~ SSbiexp(time, A1, lrc1, A2, lrc2),
    data = Sulfi)
summary(fm1)
usr <- par("usr")
xx <- seq(usr[1], usr[2], len = 50)
lines(xx, predict(fm1, list(time = xx)))
plot(conc ~ time, data = Sulfi, las = 1, log = "y",
     xlab = "Time since drug administration (min)",
     ylab = expression(plain("Sulfisoxazole concentration (")
               *mu*plain("g/ml)")),
     main = "Sulfisoxazole data (log scale)")
lines(xx, predict(fm1, list(time = xx)))
```

Tetra *Tetracycline concentrations*

Description

The Tetra data frame has 9 rows and 2 columns from an experiment on the pharmacokinetics of tetracycline.

Format

This data frame contains the following columns:

time a numeric vector of time since drug administration (hr).

conc a numeric vector of tetracycline concentrations.

Source

Bates and Watts (1998), *Nonlinear Regression Analysis and Its Applications*, Wiley (Appendix A1.5).

Examples

```
plot(conc ~ time, data = Tetra, las = 1,
     xlab = "Time since drug administration (hr)",
     ylab = "concentration",
     main = "Tetracycline data with fitted curve")
fm1 <- nls(conc ~ SSfol(1.0, time, lKe, lKa, lCl), Tetra)
summary(fm1)
usr <- par("usr")
xx <- seq(usr[1], usr[2], len = 101)
lines(xx, predict(fm1, list(time = xx)))
```

Index