# Package 'NISTnls'

October 12, 2022

<b>Version</b> 0.9-13
<b>Date</b> 2012-09-05
Title Nonlinear least squares examples from NIST
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Author original from National Institutes for Standards and Technology (NIST) http://www.itl.nist.gov/div898/strd/nls/nls_main.shtml R port by Douglas Bates <bates@stat.wisc.edu></bates@stat.wisc.edu>
<b>Description</b> Datasets for testing nonlinear regression routines.
<b>Depends</b> stats, R (>= $2.14.0$ )
LazyData yes
License GPL (>= 2)
<b>LicenseDetails</b> The original data sets and descriptions are from the NIST web site and were not covered by an explicit copyright. Modifications for R data sets are covered by GPL (>= 2).
Repository CRAN
<b>Date/Publication</b> 2012-09-06 05:18:31
NeedsCompilation no
R topics documented:
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Bennett5

Magentization modelling

# Description

The Bennett5 data frame has 154 rows and 2 columns of data from a magnetism study

# **Format**

This data frame contains the following columns:

- y A numeric vector of magnetism values.
- **x** A numeric vector of log(time).

# **Details**

These data are the result of a NIST study involving superconductivity magnetization modeling. The response variable is magnetism, and the predictor variable is the log of time in minutes.

# **Source**

Bennett, L., L. Swartzendruber, and H. Brown, NIST (1994). Superconductivity Magnetization Modeling.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val plot(y ~ x, data = Bennett5)  
Try(fm1 <- nls(y ~ b1*(b2+x)**(-1/b3), data = Bennett5, start = c(b1 = -2000, b2 = 50, b3 = 0.8), trace = TRUE))  
Try(fm1a <- nls(y ~ b1*(b2+x)**(-1/b3), data = Bennett5, start = c(b1 = -2000, b2 = 50, b3 = 0.8),
```

Chwirut1 3

```
trace = TRUE, alg = "port"))
Try(fm2 <- nls(y \sim b1*(b2+x)**(-1/b3), data = Bennett5, \\ start = c(b1 = -1500, b2 = 45, b3 = 0.85), trace = TRUE))
Try(fm2a <- nls(y \sim b1*(b2+x)**(-1/b3), data = Bennett5, \\ start = c(b1 = -1500, b2 = 45, b3 = 0.85), \\ trace = TRUE, alg = "port"))
Try(fm3 <- nls(y \sim (b2+x)**(-1/b3), data = Bennett5, alg = "plinear", \\ start = c(b2 = 50, b3 = 0.8), trace = TRUE))
Try(fm4 <- nls(y \sim (b2+x)**(-1/b3), data = Bennett5, alg = "plinear", \\ start = c(b2 = 45, b3 = 0.8), trace = TRUE))
```

Chwirut1

Ultrasonic calibration study 1

# **Description**

The Chwirut1 data frame has 214 rows and 2 columns giving

#### **Format**

This data frame contains the following columns:

- y A numeric vector of ultrasonic response values
- x A numeric vector or metal distance values

## **Details**

These data are the result of a NIST study involving ultrasonic calibration. The response variable is ultrasonic response, and the predictor variable is metal distance.

# Source

Chwirut, D., NIST (197?). Ultrasonic Reference Block Study.

4 Chwirut2

Chwirut2

Ultrasonic calibration data 2

# **Description**

The Chwirut2 data frame has nr rows and nc columns giving

## **Format**

This data frame contains the following columns:

- y A numeric vector of ultrasonic response values.
- **x** A numeric vector of metal distance values.

## **Details**

These data are the result of a NIST study involving ultrasonic calibration. The response variable is ultrasonic response, and the predictor variable is metal distance.

## Source

Chwirut, D., NIST (197?). Ultrasonic Reference Block Study.

DanielWood 5

DanielWood

Radiated energy

# **Description**

The DanielWood data frame has 6 rows and 2 columns giving the energy radiated from a carbon filament versus the absolute temperature of the filament.

#### **Format**

This data frame contains the following columns:

- **y** A numeric vector of the energy radiated from a carbon filament lamp.
- **x** A numeric vector of the temperature of the filament (1000 K).

## **Details**

These data and model are described in Daniel and Wood (1980), and originally published in E.S.Keeping, "Introduction to Statistical Inference," Van Nostrand Company, Princeton, NJ, 1962, p. 354. The response variable is energy radiated from a carbon filament lamp per cm\*\*2 per second, and the predictor variable is the absolute temperature of the filament in 1000 degrees Kelvin.

#### Source

Daniel, C. and F. S. Wood (1980). Fitting Equations to Data, Second Edition. New York, NY: John Wiley and Sons, pp. 428-431.

6 Eckerle4

Eckerle4

Circular interference data

# Description

The Eckerle4 data frame has 35 rows and 2 columns giving transmittance as a function of wavelength.

## **Format**

This data frame contains the following columns:

- y A numeric vector of transmittance values.
- **x** A numeric vector of wavelengths.

#### **Details**

These data are the result of a NIST study involving circular interference transmittance. The response variable is transmittance, and the predictor variable is wavelength.

## **Source**

Eckerle, K., NIST (197?). Circular Interference Transmittance Study.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Eckerle4)
## should fail - ridiculous starting value for b3
Try(fm1 \leftarrow nls(y \sim (b1/b2) * exp(-0.5*((x-b3)/b2)**2), Eckerle4,
                trace = TRUE,
                start = c(b1 = 1, b2 = 10, b3 = 500))
Try(fm1a \leftarrow nls(y \sim (b1/b2) * exp(-0.5*((x-b3)/b2)**2), Eckerle4,
                   trace = TRUE, alg = "port",
                   start = c(b1 = 1, b2 = 10, b3 = 500))
Try(fm2 <- nls(y \sim (b1/b2) * exp(-0.5*((x-b3)/b2)**2),
            Eckerle4, trace = TRUE,
            start = c(b1 = 1.5, b2 = 5, b3 = 450))
Try(fm2a <- nls(y \sim (b1/b2) * exp(-0.5*((x-b3)/b2)**2),
            Eckerle4, trace = TRUE, alg = "port",
            start = c(b1 = 1.5, b2 = 5, b3 = 450))
## should fail - ridiculous starting value for b3
Try(fm3 <- nls(y \sim (1/b2) * exp(-0.5*((x-b3)/b2)**2),
               Eckerle4, trace = TRUE,
                start = c(b2 = 10, b3 = 500), algorithm = "plinear"))
Try(fm4 <- nls(y \sim (1/b2) * exp(-0.5*((x-b3)/b2)**2), Eckerle4, trace = TRUE,
           start = c(b2 = 5, b3 = 450), algorithm = "plinear"))
```

ENSO 7

**ENSO** 

Atmospheric pressure differences

# **Description**

The ENSO data frame has 168 rows and 2 columns giving atmospheric pressure differences over time.

#### **Format**

This data frame contains the following columns:

- y A numeric vector of monthly averaged atmospheric pressure differences between Easter Island and Darwin, Australia.
- x A numeric vector of time values.

## **Details**

The data are monthly averaged atmospheric pressure differences between Easter Island and Darwin, Australia. This difference drives the trade winds in the southern hemisphere. Fourier analysis of the data reveals 3 significant cycles. The annual cycle is the strongest, but cycles with periods of approximately 44 and 26 months are also present. These cycles correspond to the El Nino and the Southern Oscillation. Arguments to the SIN and COS functions are in radians.

## Source

Kahaner, D., C. Moler, and S. Nash, (1989). Numerical Methods and Software. Englewood Cliffs, NJ: Prentice Hall, pp. 441-445.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = ENSO)
plot(y \sim x, data = ENSO, type = "1") # to see the pattern more clearly
Try(fm1 <- nls(y \sim b1 + b2*cos(2*pi*x/12) + b3*sin(2*pi*x/12)
                   + b5*cos( 2*pi*x/b4 ) + b6*sin( 2*pi*x/b4 )
                   + b8*cos(2*pi*x/b7) + b9*sin(2*pi*x/b7),
            data = ENSO, trace = TRUE,
            start = c(b1 = 11.0, b2 = 3.0, b3 = 0.5, b4 = 40.0, b5 = -0.7,
                      b6 = -1.3, b7 = 25.0, b8 = -0.3, b9 = 1.4)))
Try(fm1a \leftarrow nls(y \sim b1 + b2*cos(2*pi*x/12) + b3*sin(2*pi*x/12)
                    + b5*cos( 2*pi*x/b4 ) + b6*sin( 2*pi*x/b4 )
                    + b8*cos( 2*pi*x/b7 ) + b9*sin( 2*pi*x/b7 ),
             data = ENSO, trace = TRUE, alg = "port",
             start = c(b1 = 11.0, b2 = 3.0, b3 = 0.5, b4 = 40.0, b5 = -0.7,
                       b6 = -1.3, b7 = 25.0, b8 = -0.3, b9 = 1.4)))
Try(fm2 <- nls(y \sim b1 + b2*cos(2*pi*x/12) + b3*sin(2*pi*x/12)
                   + b5*cos( 2*pi*x/b4 ) + b6*sin( 2*pi*x/b4 )
                   + b8*cos(2*pi*x/b7) + b9*sin(2*pi*x/b7),
```

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```
data = ENSO, trace = TRUE,
            start = c(b1 = 10.0, b2 = 3.0, b3 = 0.5, b4 = 44.0, b5 = -1.5,
                     b6 = 0.5, b7 = 26.0, b8 = -0.1, b9 = 1.5)))
Try(fm2a \leftarrow nls(y \sim b1 + b2*cos(2*pi*x/12) + b3*sin(2*pi*x/12)
                    + b5*cos( 2*pi*x/b4 ) + b6*sin( 2*pi*x/b4 )
                    + b8*cos( 2*pi*x/b7 ) + b9*sin( 2*pi*x/b7 ),
             data = ENSO, trace = TRUE, alg = "port",
             start = c(b1 = 10.0, b2 = 3.0, b3 = 0.5, b4 = 44.0, b5 = -1.5,
                     b6 = 0.5, b7 = 26.0, b8 = -0.1, b9 = 1.5)))
Try(fm3 <- nls(y \sim cbind(1, cos(2*pi*x/12), sin(2*pi*x/12), cos(2*pi*x/b4),
                      sin( 2*pi*x/b4 ), cos( 2*pi*x/b7 ), sin( 2*pi*x/b7 )),
            data = ENSO, trace = TRUE,
            start = c(b4 = 40.0, b7 = 25.0), algorithm = "plinear"))
Try(fm4 \leftarrow nls(y \sim cbind(1, cos(2*pi*x/12), sin(2*pi*x/12), cos(2*pi*x/b4),
                    sin( 2*pi*x/b4 ), cos( 2*pi*x/b7 ), sin( 2*pi*x/b7 )),
            data = ENSO, trace = TRUE,
            start = c(b4 = 44.0, b7 = 26.0), algorithm = "plinear"))
```

Gauss1

Generated data

# Description

The Gauss1 data frame has 250 rows and 2 columns of generated data.

# Format

This data frame contains the following columns:

- y A numeric vector of generated responses.
- **x** A numeric vector of generated input values.

# **Details**

The data are generated data with two well-separated Gaussians on a decaying exponential baseline plus normally distributed zero-mean noise with variance = 6.25.

#### Source

```
Rust, B., NIST (1996).
```

Gauss2

```
+ b6*exp(-(x-b7)**2 / b8**2), data = Gauss1, trace = TRUE,
             start = c(b1 = 97.0, b2 = 0.009, b3 = 100.0, b4 = 65.0, b5 = 20.0,
                     b6 = 70.0, b7 = 178., b8 = 16.5), alg = "port"))
Try(fm2 <- nls(y \sim b1*exp(-b2*x) + b3*exp(-(x-b4)**2 / b5**2)
               + b6*exp(-(x-b7)**2 / b8**2), data = Gauss1, trace = TRUE,
           start = c(b1 = 94.0, b2 = 0.0105, b3 = 99.0, b4 = 63.0, b5 = 25.0,
                     b6 = 71.0, b7 = 180.0, b8 = 20.0))
Try(fm2a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-(x-b4)**2 / b5**2)
              + b6*exp(-(x-b7)**2 / b8**2), data = Gauss1, trace = TRUE,
           start = c(b1 = 94.0, b2 = 0.0105, b3 = 99.0, b4 = 63.0, b5 = 25.0,
                     b6 = 71.0, b7 = 180.0, b8 = 20.0), alg = "port"))
Try(fm3 <- nls(y \sim cbind(exp(-b2*x), exp(-(x-b4)**2/b5**2), exp(-(x-b7)**2/b8**2)),
           data = Gauss1, trace = TRUE,
           start = c(b2 = 0.009, b4 = 65.0, b5 = 20.0, b7 = 178., b8 = 16.5),
           algorithm = "plinear"))
Try(fm4 <- nls(y \sim cbind(exp(-b2*x), exp(-(x-b4)**2/b5**2), exp(-(x-b7)**2/b8**2)),
           data = Gauss1, trace = TRUE,
           start = c(b2 = 0.0105, b4 = 63.0, b5 = 25.0, b7 = 180., b8 = 20.0),
           algorithm = "plinear"))
```

Gauss2

Generated data

## **Description**

The Gauss2 data frame has 250 rows and 2 columns giving

# Format

This data frame contains the following columns:

- y A numeric vector of generated response values.
- **x** A numeric vector of generated input values.

# **Details**

The data are two slightly-blended Gaussians on a decaying exponential baseline plus normally distributed zero-mean noise with variance = 6.25.

#### Source

```
Rust, B., NIST (1996)
```

10 Gauss3

```
b6 = 72, b7 = 151, b8 = 18)))
Try(fm1a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-(x-b4)**2 / b5**2)
               + b6*exp(-(x-b7)**2 / b8**2), data = Gauss2, trace = TRUE,
             start = c(b1 = 96, b2 = 0.009, b3 = 103, b4 = 106, b5 = 18,
                       b6 = 72, b7 = 151, b8 = 18), alg = "port"))
Try(fm2 <- nls(y \sim b1*exp( -b2*x ) + b3*exp( -(x-b4)**2 / b5**2 )
               + b6*exp(-(x-b7)**2 / b8**2), data = Gauss2, trace = TRUE,
           start = c(b1 = 98, b2 = 0.0105, b3 = 103, b4 = 105, b5 = 20,
                     b6 = 73, b7 = 150, b8 = 20)))
Try(fm2a \leftarrow nls(y \sim b1*exp(-b2*x) + b3*exp(-(x-b4)**2 / b5**2)
               + b6*exp(-(x-b7)**2 / b8**2), data = Gauss2, trace = TRUE,
           start = c(b1 = 98, b2 = 0.0105, b3 = 103, b4 = 105, b5 = 20,
                     b6 = 73, b7 = 150, b8 = 20), alg = "port"))
Try(fm3 <- nls(y \sim cbind(exp(-b2*x), exp(-(x-b4)**2/b5**2), exp(-(x-b7)**2/b8**2)),
           data = Gauss2, trace = TRUE,
           start = c(b2 = 0.009, b4 = 106, b5 = 18, b7 = 151, b8 = 18),
           algorithm = "plinear"))
Try(fm4 \leftarrow nls(y \sim cbind(exp(-b2*x), exp(-(x-b4)**2/b5**2), exp(-(x-b7)**2/b8**2)),
           data = Gauss2, trace = TRUE,
           start = c(b2 = 0.0105, b4 = 105, b5 = 20, b7 = 150, b8 = 20),
           algorithm = "plinear"))
```

Gauss3

Generated data

# Description

The Gauss3 data frame has 250 rows and 2 columns giving generated data of Gaussian peaks with a decaying exponential background.

#### **Format**

This data frame contains the following columns:

- y A numeric vector of generated responses.
- **x** A numeric vector of generated inputs.

## **Details**

The data are two strongly-blended Gaussians on a decaying exponential baseline plus normally distributed zero-mean noise with variance = 6.25.

#### Source

Rust, B., NIST (1996).

Hahn1 11

# **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val
plot(y \sim x, data = Gauss3)
Try(fm1 \leftarrow nls(y \sim b1*exp(-b2*x) + b3*exp(-(x-b4)**2 / b5**2)
               + b6*exp(-(x-b7)**2 / b8**2), data = Gauss3, trace = TRUE,
           start = c(b1 = 94.9, b2 = 0.009, b3 = 90.1, b4 = 113, b5 = 20,
                     b6 = 73.8, b7 = 140, b8 = 20)))
Try(fm1a <- nls(y \sim b1*exp( -b2*x ) + b3*exp( -(x-b4)**2 / b5**2 )
                + b6*exp(-(x-b7)**2 / b8**2), data = Gauss3, trace = TRUE,
            start = c(b1 = 94.9, b2 = 0.009, b3 = 90.1, b4 = 113, b5 = 20,
                      b6 = 73.8, b7 = 140, b8 = 20), alg = "port"))
Try(fm2 <- nls(y \sim b1*exp( -b2*x ) + b3*exp( -(x-b4)**2 / b5**2 )
               + b6*exp(-(x-b7)**2 / b8**2), data = Gauss3, trace = TRUE,
           start = c(b1 = 96, b2 = 0.0096, b3 = 80, b4 = 110, b5 = 25,
                     b6 = 74, b7 = 139, b8 = 25)))
Try(fm2a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-(x-b4)**2 / b5**2)
               + b6*exp(-(x-b7)**2 / b8**2), data = Gauss3, trace = TRUE,
           start = c(b1 = 96, b2 = 0.0096, b3 = 80, b4 = 110, b5 = 25,
                     b6 = 74, b7 = 139, b8 = 25), alg = "port"))
Try(fm3 \leftarrow nls(y \sim cbind(exp(-b2*x), exp(-(x-b4)**2/b5**2), exp(-(x-b7)**2/b8**2)),
           data = Gauss3, trace = TRUE,
           start = c(b2 = 0.009, b4 = 113, b5 = 20, b7 = 140, b8 = 20),
           algorithm = "plinear"))
Try(fm4 \leftarrow nls(y \sim cbind(exp(-b2*x), exp(-(x-b4)**2/b5**2), exp(-(x-b7)**2/b8**2)),
           data = Gauss3, trace = TRUE,
           start = c(b2 = 0.0096, b4 = 110, b5 = 25, b7 = 139, b8 = 25),
           algorithm = "plinear"))
```

Hahn1

Thermal expansion data

# **Description**

The Hahn1 data frame has 236 rows and 2 columns of data from a study on the thermal expansion of copper.

# **Format**

This data frame contains the following columns:

- y A numeric vector of values of the coefficient of thermal expansion.
- **x** A numeric vector of temperatures (K).

# **Details**

These data are the result of a NIST study involving the thermal expansion of copper. The response variable is the coefficient of thermal expansion, and the predictor variable is temperature in degrees Kelvin.

12 Kirby2

#### Source

Hahn, T., NIST (197?). Copper Thermal Expansion Study.

## **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val
plot(y \sim x, data = Hahn1)
Try(fm1 <- nls(y \sim (b1+b2*x+b3*x**2+b4*x**3) \ / \ (1+b5*x+b6*x**2+b7*x**3),
           data = Hahn1, trace = TRUE,
           start = c(b1 = 10, b2 = -1, b3 = 0.05,
             b4 = -0.00001, b5 = -0.05, b6 = 0.001, b7 = -0.000001)))
Try(fm1a <- nls(y \sim (b1+b2*x+b3*x**2+b4*x**3) / (1+b5*x+b6*x**2+b7*x**3),
           data = Hahn1, trace = TRUE, alg = "port",
           start = c(b1 = 10, b2 = -1, b3 = 0.05,
             b4 = -0.00001, b5 = -0.05, b6 = 0.001, b7 = -0.000001)))
Try(fm2 \leftarrow nls(y \sim (b1+b2*x+b3*x**2+b4*x**3) / (1+b5*x+b6*x**2+b7*x**3),
           data = Hahn1, trace = TRUE,
           start = c(b1 = 1, b2 = -0.1, b3 = 0.005, b4 = -0.000001,
              b5 = -0.005, b6 = 0.0001, b7 = -0.0000001)))
Try(fm2a \leftarrow nls(y \sim (b1+b2*x+b3*x**2+b4*x**3) / (1+b5*x+b6*x**2+b7*x**3),
             data = Hahn1, trace = TRUE, alg = "port",
           start = c(b1 = 1, b2 = -0.1, b3 = 0.005, b4 = -0.000001,
              b5 = -0.005, b6 = 0.0001, b7 = -0.0000001)))
Try(fm3 \leftarrow nls(y \sim cbind(1, x, x^2, x^3)/(1+x*(b5+x*(b6+x*b7))),
           data = Hahn1, trace = TRUE, algorithm = "plinear",
           start = c(b5 = -0.05, b6 = 0.001, b7 = -0.000001)))
Try(fm4 \leftarrow nls(y \sim cbind(1, x, x^2, x^3)/(1+x*(b5+x*(b6+x*b7))),
           data = Hahn1, trace = TRUE, algorithm = "plinear",
           start = c(b5 = -0.005, b6 = 0.0001, b7 = -0.0000001)))
```

Kirby2

Microscope line width standards

# **Description**

The Kirby2 data frame has 151 rows and 2 columns of data from an NIST study on scanning electron microscope line width standards.

# **Format**

This data frame contains the following columns:

- y A numeric vector of response values.
- **x** A numeric vector of input values.

## **Details**

These data are the result of a NIST study involving scanning electron microscope line with standards.

Lanczos1 13

## Source

Kirby, R., NIST (197?). Scanning electron microscope line width standards.

## **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Kirby2)
Try(fm1 <- nls(y \sim (b1 + b2*x + b3*x**2) / (1 + b4*x + b5*x**2),
           data = Kirby2, trace = TRUE,
           start = c(b1 = 2, b2 = -0.1, b3 = 0.003,
                      b4 = -0.001, b5 = 0.00001))
Try(fm1a <- nls(y \sim (b1 + b2*x + b3*x**2) / (1 + b4*x + b5*x**2),
           data = Kirby2, trace = TRUE, alg = "port",
           start = c(b1 = 2, b2 = -0.1, b3 = 0.003,
                      b4 = -0.001, b5 = 0.00001))
Try(fm2 \leftarrow nls(y \sim (b1 + b2*x + b3*x**2) / (1 + b4*x + b5*x**2),
           data = Kirby2, trace = TRUE,
           start = c(b1 = 1.5, b2 = -0.15, b3 = 0.0025,
                      b4 = -0.0015, b5 = 0.00002)))
Try(fm2a <- nls(y \sim (b1 + b2*x + b3*x**2) / (1 + b4*x + b5*x**2),
             data = Kirby2, trace = TRUE, alg = "port",
             start = c(b1 = 1.5, b2 = -0.15, b3 = 0.0025,
                        b4 = -0.0015, b5 = 0.00002)))
Try(fm3 \leftarrow nls(y \sim cbind(1, x, x**2)/(1 + x*(b4 + b5*x)),
           data = Kirby2, trace = TRUE, algorithm = "plinear",
           start = c(b4 = -0.001, b5 = 0.00001))
Try(fm4 <- nls(y \sim cbind(1, x, x**2)/(1 + x*(b4 + b5*x)),
           data = Kirby2, trace = TRUE, algorithm = "plinear",
           start = c(b4 = -0.0015, b5 = 0.00002)))
```

Lanczos1

Generated data

# Description

The Lanczos1 data frame has 24 rows and 2 columns of generated data.

# Format

This data frame contains the following columns:

- y A numeric vector of generated responses.
- x A numeric vector of generated input values

# **Details**

These data are taken from an example discussed in Lanczos (1956). The data were generated to 14-digits of accuracy using  $f(x) = 0.0951 \times exp(-x) + 0.8607 \times exp(-3*x) + 1.5576 \times exp(-5*x)$ .

14 Lanczos2

#### Source

Lanczos, C. (1956). Applied Analysis. Englewood Cliffs, NJ: Prentice Hall, pp. 272-280.

# **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Lanczos1)
## plot on log scale to see the apparent number of exponential terms
plot(y \sim x, data = Lanczos1, log = "y")
## data are an exact fit so the convergence criterion fails
Try(fm1 <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos1, trace = TRUE,
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
Try(fm1a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
                data = Lanczos1, trace = TRUE, alg = "port",
                start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6,
                          b4 = 5.5, b5 = 6.5, b6 = 7.6)))
## data are an exact fit so the convergence criterion fails
Try(fm2 <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos1, trace = TRUE,
           start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6, b4 = 4.2,
                     b5 = 4, b6 = 6.3))
Try(fm2a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
                data = Lanczos1, trace = TRUE, alg = "port",
                start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6,
                          b4 = 4.2, b5 = 4, b6 = 6.3))
## data are an exact fit so the convergence criterion fails
Try(fm3 <- nls(y \sim exp(outer(x, -c(b2, b4, b6))),
               data = Lanczos1, trace = TRUE, algorithm = "plinear",
               start = c(b2 = 0.3, b4 = 5.5, b6 = 7.6))
## data are an exact fit so the convergence criterion fails
Try(fm4 <- nls(y \sim exp(outer(x,-c(b2, b4, b6))),
               data = Lanczos1, trace = TRUE, algorithm = "plinear",
               start = c(b2 = 0.7, b4 = 4.2, b6 = 6.3))
```

Lanczos2

Generated data

## **Description**

The Lanczos2 data frame has 24 rows and 2 columns of generated data.

## **Format**

This data frame contains the following columns:

- y A numeric vector of generated responses.
- **x** A numeric vector of generated input values.

Lanczos2 15

## **Details**

These data are taken from an example discussed in Lanczos (1956). The data were generated to 6-digits of accuracy using  $f(x) = 0.0951 \times \exp(-x) + 0.8607 \times \exp(-3 \times x) + 1.5576 \times \exp(-5 \times x)$ .

#### Source

Lanczos, C. (1956). Applied Analysis. Englewood Cliffs, NJ: Prentice Hall, pp. 272-280.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Lanczos2)
## plot log response to see the number of exponential terms
plot(y \sim x, data = Lanczos2, log = "y")
## Numerical derivatives do not produce sufficient accuracy to converge
Try(fm1 <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos2, trace = TRUE,
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
Try(fm1a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos2, trace = TRUE, alg = "port",
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
## Numerical derivatives do not produce sufficient accuracy to converge
Try(fm2 <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos2, trace = TRUE,
           start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6, b4 = 4.2,
                     b5 = 4, b6 = 6.3))
Try(fm2a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos2, trace = TRUE, alg = "port",
           start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6, b4 = 4.2,
                     b5 = 4, b6 = 6.3))
## Numerical derivatives do not produce sufficient accuracy to converge
Try(fm3 <- nls(y \sim exp(outer(x,-c(b2, b4, b6))),
           data = Lanczos2, trace = TRUE, algorithm = "plinear",
           start = c(b2 = 0.3, b4 = 5.5, b6 = 7.6)))
## Numerical derivatives do not produce sufficient accuracy to converge
Try(fm4 <- nls(y \sim exp(outer(x,-c(b2, b4, b6))),
           data = Lanczos2, trace = TRUE, algorithm = "plinear",
           start = c(b2 = 0.7, b4 = 4.2, b6 = 6.3))
## Use analytic derivatives
Lanczos <- deriv(~b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
                 paste("b", 1:6, sep = ""),
                 function(x, b1, b2, b3, b4, b5, b6){})
Try(fm5 <- nls(y \sim Lanczos(x, b1, b2, b3, b4, b5, b6),
           data = Lanczos2, trace = TRUE,
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
Try(fm5a <- nls(y \sim Lanczos(x, b1, b2, b3, b4, b5, b6),
           data = Lanczos2, trace = TRUE, alg = "port",
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6)))
```

16 Lanczos3

```
\label{eq:transformation} \begin{split} & \text{Try}(\text{fm6} < - \text{ nls}(\text{y} \sim \text{Lanczos}(\text{x}, \text{ b1}, \text{ b2}, \text{ b3}, \text{ b4}, \text{ b5}, \text{ b6}), \\ & \text{data} = \text{Lanczos2}, \text{ trace} = \text{TRUE}, \\ & \text{start} = \text{c}(\text{b1} = 0.5, \text{ b2} = 0.7, \text{ b3} = 3.6, \text{ b4} = 4.2, \\ & \text{b5} = 4, \text{ b6} = 6.3))) \end{split} \text{Try}(\text{fm6a} < - \text{ nls}(\text{y} \sim \text{Lanczos}(\text{x}, \text{ b1}, \text{ b2}, \text{ b3}, \text{ b4}, \text{ b5}, \text{ b6}), \\ & \text{data} = \text{Lanczos2}, \text{ trace} = \text{TRUE}, \text{ alg} = \text{"port"}, \\ & \text{start} = \text{c}(\text{b1} = 0.5, \text{ b2} = 0.7, \text{ b3} = 3.6, \text{ b4} = 4.2, \\ & \text{b5} = 4, \text{ b6} = 6.3))) \end{split}
```

Lanczos3

Generated data

# **Description**

The Lanczos3 data frame has 24 rows and 2 columns of generated data.

#### **Format**

This data frame contains the following columns:

- y A numeric vector of generated responses.
- **x** A numeric vector of generated input values.

## **Details**

These data are taken from an example discussed in Lanczos (1956). The data were generated to 5-digits of accuracy using  $f(x) = 0.0951 \times exp(-x) + 0.8607 \times exp(-3*x) + 1.5576 \times exp(-5*x)$ .

## Source

Lanczos, C. (1956). Applied Analysis. Englewood Cliffs, NJ: Prentice Hall, pp. 272-280.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Lanczos3)
## plot log response to see the number of exponential terms
plot(y \sim x, data = Lanczos3, log = "y")
Try(fm1 <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos3, trace = TRUE,
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
Try(fm1a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos3, trace = TRUE, alg = "port",
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
Try(fm2 <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos3, trace = TRUE,
           start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6, b4 = 4.2,
                     b5 = 4, b6 = 6.3))
```

MGH09 17

```
Try(fm2a <- nls(y \sim b1*exp(-b2*x) + b3*exp(-b4*x) + b5*exp(-b6*x),
           data = Lanczos3, trace = TRUE, alg = "port",
           start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6, b4 = 4.2,
                     b5 = 4, b6 = 6.3))
Try(fm3 <- nls(y \sim exp(outer(x, -c(b2, b4, b6))),
           data = Lanczos3, trace = TRUE, algorithm = "plinear",
           start = c(b2 = 0.3, b4 = 5.5, b6 = 7.6))
Try(fm4 <- nls(y \sim exp(outer(x, -c(b2, b4, b6))),
           data = Lanczos3, trace = TRUE, algorithm = "plinear",
           start = c(b2 = 0.7, b4 = 4.2, b6 = 6.3))
## Use analytic derivatives
Lanczos <- deriv(^{b1*exp(-b2*x)} + b3*exp(-b4*x) + b5*exp(-b6*x),
                 paste("b", 1:6, sep = ""),
                 function(x, b1, b2, b3, b4, b5, b6){})
Try(fm5 \leftarrow nls(y \sim Lanczos(x, b1, b2, b3, b4, b5, b6),
           data = Lanczos3, trace = TRUE,
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
Try(fm5a <- nls(y \sim Lanczos(x, b1, b2, b3, b4, b5, b6),
           data = Lanczos3, trace = TRUE, alg = "port",
           start = c(b1 = 1.2, b2 = 0.3, b3 = 5.6, b4 = 5.5,
                     b5 = 6.5, b6 = 7.6))
Try(fm6 \leftarrow nls(y \sim Lanczos(x, b1, b2, b3, b4, b5, b6),
           data = Lanczos3, trace = TRUE,
           start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6, b4 = 4.2,
                     b5 = 4, b6 = 6.3))
Try(fm6a <- nls(y \sim Lanczos(x, b1, b2, b3, b4, b5, b6),
           data = Lanczos3, trace = TRUE, alg = "port",
           start = c(b1 = 0.5, b2 = 0.7, b3 = 3.6, b4 = 4.2,
                     b5 = 4, b6 = 6.3))
```

MGH09

More, Gabrow and Hillstrom example 9

## Description

The MGH09 data frame has 11 rows and 2 columns giving

#### **Format**

This data frame contains the following columns:

- y A numeric vector of response values.
- x A numeric vector of input values.

## **Details**

This problem was found to be difficult for some very good algorithms. There is a local minimum at (+inf, -14.07..., -inf, -inf) with final sum of squares 0.00102734....

See More, J. J., Garbow, B. S., and Hillstrom, K. E. (1981). *Testing unconstrained optimization software*. **ACM Transactions on Mathematical Software**. 7(1): pp. 17–41.

18 MGH10

## **Source**

Kowalik, J.S., and M. R. Osborne, (1978). Methods for Unconstrained Optimization Problems. New York, NY: Elsevier North-Holland.

# **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = MGH09)
## starting values for this attempt are ridiculous
Try(fm1 <- nls(y \sim b1*(x**2+x*b2) / (x**2+x*b3+b4),
           data = MGH09, trace = TRUE,
           start = c(b1 = 25, b2 = 39, b3 = 41.5, b4 = 39)))
Try(fm1a <- nls(y \sim b1*(x**2+x*b2) / (x**2+x*b3+b4),
           data = MGH09, trace = TRUE, alg = "port";
           start = c(b1 = 25, b2 = 39, b3 = 41.5, b4 = 39)))
Try(fm2 <- nls(y \sim b1*(x**2+x*b2) / (x**2+x*b3+b4),
           data = MGH09, trace = TRUE,
           start = c(b1 = 0.25, b2 = 0.39, b3 = 0.415, b4 = 0.39)))
Try(fm2a <- nls(y \sim b1*(x**2+x*b2) / (x**2+x*b3+b4),
           data = MGH09, trace = TRUE, alg = "port",
           start = c(b1 = 0.25, b2 = 0.39, b3 = 0.415, b4 = 0.39)))
Try(fm3 <- nls(y \sim cbind(x, x**2) / (x**2+x*b3+b4),
           data = MGH09, trace = TRUE, algorithm = "plinear",
           start = c(b3 = 41.5, b4 = 39))
Try(fm4 <- nls(y \sim cbind(x, x**2) / (x**2+x*b3+b4),
           data = MGH09, trace = TRUE, algorithm = "plinear",
           start = c(b3 = 0.415, b4 = 0.39)))
```

MGH10

More, Gabrow and Hillstrom example 10

## **Description**

The MGH10 data frame has 16 rows and 2 columns.

## **Format**

This data frame contains the following columns:

- y A numeric vector of response values.
- **x** A numeric vector of input values.

# **Details**

This problem was found to be difficult for some very good algorithms.

See More, J. J., Garbow, B. S., and Hillstrom, K. E. (1981). *Testing unconstrained optimization software*. **ACM Transactions on Mathematical Software**. 7(1): pp. 17-41.

MGH17 19

## **Source**

Meyer, R. R. (1970). Theoretical and computational aspects of nonlinear regression. In Nonlinear Programming, Rosen, Mangasarian and Ritter (Eds). New York, NY: Academic Press, pp. 465-486.

# **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = MGH10)
## check plot on log scale for shape
plot(y \sim x, data = MGH10, log = "y")
## starting values for this run are ridiculous
Try(fm1 \leftarrow nls(y \sim b1 * exp(b2/(x+b3)), data = MGH10, trace = TRUE,
           start = c(b1 = 2, b2 = 400000, b3 = 25000)))
Try(fm1a <- nls(y \sim b1 * exp(b2/(x+b3)), data = MGH10,
                 trace = TRUE, alg = "port",
                 start = c(b1 = 2, b2 = 400000, b3 = 25000)))
Try(fm2 \leftarrow nls(y \sim b1 * exp(b2/(x+b3)), data = MGH10, trace = TRUE,
           start = c(b1 = 0.02, b2 = 4000, b3 = 250))
Try(fm2a <- nls(y \sim b1 * exp(b2/(x+b3)), data = MGH10,
                 trace = TRUE, alg = "port",
                 start = c(b1 = 0.02, b2 = 4000, b3 = 250))
Try(fm3 <- nls(y \sim exp(b2/(x+b3)), data = MGH10, trace = TRUE,
                start = c(b2 = 400000, b3 = 25000),
                algorithm = "plinear"))
Try(fm4 \leftarrow nls(y \sim exp(b2/(x+b3)), data = MGH10, trace = TRUE,
           start = c(b2 = 4000, b3 = 250),
            algorithm = "plinear"))
```

MGH17

More, Gabrow and Hillstrom example 17

# **Description**

The MGH17 data frame has 33 rows and 2 columns

## **Format**

This data frame contains the following columns:

- y A numeric vector of response values.
- **x** A numeric vector of input values.

## **Details**

This problem was found to be difficult for some very good algorithms.

See More, J. J., Garbow, B. S., and Hillstrom, K. E. (1981). *Testing unconstrained optimization software*. **ACM Transactions on Mathematical Software**. 7(1): pp. 17-41.

20 Misra1a

## **Source**

Osborne, M. R. (1972). Some aspects of nonlinear least squares calculations. In Numerical Methods for Nonlinear Optimization, Lootsma (Ed). New York, NY: Academic Press, pp. 171-189.

## **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = MGH17)
## Starting values here are ridiculous
Try(fm1 <- nls(y \sim b1 + b2*exp(-x*b4) + b3*exp(-x*b5),
           data = MGH17, trace = TRUE,
           start = c(b1 = 50, b2 = 150, b3 = -100, b4 = 1, b5 = 2)))
Try(fm1a <- nls(y \sim b1 + b2*exp(-x*b4) + b3*exp(-x*b5),
           data = MGH17, trace = TRUE, alg = "port",
           start = c(b1 = 50, b2 = 150, b3 = -100, b4 = 1, b5 = 2)))
Try(fm2 <- nls(y \sim b1 + b2*exp(-x*b4) + b3*exp(-x*b5),
           data = MGH17, trace = TRUE,
           start = c(b1 = 0.5, b2 = 1.5, b3 = -1, b4 = 0.01, b5 = 0.02)))
Try(fm2a <- nls(y \sim b1 + b2*exp(-x*b4) + b3*exp(-x*b5),
           data = MGH17, trace = TRUE, alg = "port",
           start = c(b1 = 0.5, b2 = 1.5, b3 = -1, b4 = 0.01, b5 = 0.02)))
Try(fm3 <- nls(y \sim cbind(1, exp(-x*b4), exp(-x*b5)),
           data = MGH17, trace = TRUE, algorithm = "plinear",
           start = c(b4 = 1, b5 = 2))
Try(fm4 <- nls(y \sim cbind(1, exp(-x*b4), exp(-x*b5)),
           data = MGH17, trace = TRUE, algorithm = "plinear",
           start = c(b4 = 0.01, b5 = 0.02))
```

Misra1a

Monomolecular Absorption Data

# **Description**

The Misrala data frame has 14 rows and 2 columns.

## **Format**

This data frame contains the following columns:

- y A numeric vector of volume values.
- **x** A numeric vector of pressure values.

## **Details**

These data are the result of a NIST study regarding dental research in monomolecular adsorption. The response variable is volume, and the predictor variable is pressure.

Misra1b 21

## Source

Misra, D., NIST (1978). Dental Research Monomolecular Adsorption Study.

# **Examples**

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Misra1a)
Try(fm1 \leftarrow nls(y \sim b1*(1-exp(-b2*x)), data = Misra1a, trace = TRUE,
           start = c(b1 = 500, b2 = 0.0001))
Try(fm1a \leftarrow nls(y \sim b1*(1-exp(-b2*x)), data = Misra1a, trace = TRUE,
           alg = "port", start = c(b1 = 500, b2 = 0.0001)))
Try(fm2 <- nls(y \sim b1*(1-exp(-b2*x)), data = Misra1a, trace = TRUE,
           start = c(b1 = 250, b2 = 0.0005)))
Try(fm2a <- nls(y \sim b1*(1-exp(-b2*x)), data = Misra1a, trace = TRUE,
           alg = "port", start = c(b1 = 250, b2 = 0.0005)))
Try(fm3 <- nls(y \sim 1-exp(-b2*x)), data = Misra1a, trace = TRUE,
           start = c(b2 = 0.0001), algorithm = "plinear" ))
Try(fm4 \leftarrow nls(y \sim 1-exp(-b2*x), data = Misra1a, trace = TRUE,
           start = c(b2 = 0.0005), algorithm = "plinear"))
## Using a self-starting model
Try(fm5 <- nls(y ~ SSasympOrig(x, Asym, lrc), data = Misra1a))</pre>
```

Misra<sub>1</sub>b

Monomolecular Absorption Data

# **Description**

The Misra1b data frame has 14 rows and 2 columns. It is the same data as Misra1a but a different model is fit.

# Format

This data frame contains the following columns:

- y A numeric vector of volume values.
- **x** A numeric vector of pressure values.

## **Details**

These data are the result of a NIST study regarding dental research in monomolecular adsorption. The response variable is volume, and the predictor variable is pressure.

## Source

Misra, D., NIST (1978). Dental Research Monomolecular Adsorption Study.

22 Misra1c

## **Examples**

Misra1c

Monomolecular Absorption data

#### **Description**

The Misra1c data frame has 14 rows and 2 columns. This is the same data as Misra1a but a different model is fit.

## Format

This data frame contains the following columns:

- y A numeric vector of volume values.
- **x** A numeric vector of pressure values.

# **Details**

These data are the result of a NIST study regarding dental research in monomolecular adsorption. The response variable is volume, and the predictor variable is pressure.

#### Source

Misra, D., NIST (1978). Dental Research Monomolecular Adsorption Study.

Misra1d 23

```
start = c(b1 = 600, \ b2 = 0.0002) \ )) Try(fm2a <- \ nls(y \sim b1*(1-(1+2*b2*x)**(-.5)), \ data = Misra1c, \ trace = TRUE, \ alg = "port", \ start = c(b1 = 600, \ b2 = 0.0002) \ )) Try(fm3 <- \ nls(y \sim 1-(1+2*b2*x)**(-.5), \ data = Misra1c, \ trace = TRUE, \ start = c(b2 = 0.0001), \ algorithm = "plinear" \ )) Try(fm4 <- \ nls(y \sim 1-(1+2*b2*x)**(-.5), \ data = Misra1c, \ trace = TRUE, \ start = c(b2 = 0.0002), \ algorithm = "plinear" \ ))
```

Misra1d

Monomolecular Absorption data

# **Description**

The Misrald data frame has 14 rows and 2 columns. This is the same data as Misrala but a different model is fit.

#### **Format**

This data frame contains the following columns:

- y A numeric vector of volume values.
- **x** A numeric vector of pressure values.

# Details

These data are the result of a NIST study regarding dental research in monomolecular adsorption. The response variable is volume, and the predictor variable is pressure.

## Source

Misra, D., NIST (1978). Dental Research Monomolecular Adsorption Study.

24 Nelson

Nelson

Dialectric breakdown data

# **Description**

The Nelson data frame has 128 rows and 3 columns of data from an accelerated test of dialectric breakdown.

## **Format**

This data frame contains the following columns:

- y A numeric vector of dialectric breakdown strength values.
- **x1** A numeric vector of time values.
- **x2** A numeric vector of temperature values.

## **Details**

These data are the result of a study involving the analysis of performance degradation data from accelerated tests, published in IEEE Transactions on Reliability. The response variable is dialectric breakdown strength in kilo-volts, and the predictor variables are time in weeks and temperature in degrees Celsius.

## Source

Nelson, W. (1981). Analysis of Performance-Degradation Data. IEEE Transactions on Reliability. Vol. 2, R-30, No. 2, pp. 149-155.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val
plot(y \sim x1, data = Nelson, log = "y")
plot(y \sim x2, data = Nelson, log = "y")
coplot(y \sim x1 \mid x2, data = Nelson)
coplot(y \sim x2 \mid x1, data = Nelson)
Try(fm1 <- nls(log(y) \sim b1 - b2*x1 * exp(-b3*x2), data = Nelson,
           start = c(b1 = 2, b2 = 0.0001, b3 = -0.01), trace = TRUE))
Try(fm1a <- nls(log(y) \sim b1 - b2*x1 * exp(-b3*x2), data = Nelson,
            trace = TRUE, alg = "port",
            start = c(b1 = 2, b2 = 0.0001, b3 = -0.01)))
Try(fm2 <- nls(log(y) \sim b1 - b2*x1 * exp(-b3*x2), data = Nelson,
           start = c(b1 = 2.5, b2 = 0.000000005, b3 = -0.05), trace = TRUE))
Try(fm2 \leftarrow nls(log(y) \sim b1 - b2*x1 * exp(-b3*x2), data = Nelson,
           trace = TRUE, alg = "port",
           start = c(b1 = 2.5, b2 = 0.000000005, b3 = -0.05)))
Try(fm3 <- nls(log(y) \sim cbind(1, -x1 * exp(-b3*x2)), data = Nelson,
```

Ratkowsky2 25

```
start = c(b3 = -0.01), trace = TRUE, algorithm = "plinear"))
Try(fm4 <- nls(log(y) \sim cbind(1, -x1 * exp(-b3*x2)), data = Nelson,
start = c(b3 = -0.05), trace = TRUE, algorithm = "plinear"))
```

Ratkowsky2

Pasture yield data

## **Description**

The Ratkowsky2 data frame has 9 rows and 2 columns.

## **Format**

This data frame contains the following columns:

- y A numeric vector of pasture yields.
- x A numeric vector of growing times.

## **Details**

This model and data are an example of fitting sigmoidal growth curves taken from Ratkowsky (1983). The response variable is pasture yield, and the predictor variable is growing time.

#### Source

Ratkowsky, D.A. (1983). Nonlinear Regression Modeling. New York, NY: Marcel Dekker, pp. 61 and 88.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Ratkowsky2)
Try(fm1 <- nls(y \sim b1 / (1+exp(b2-b3*x)), data = Ratkowsky2, trace = TRUE,
           start = c(b1 = 100, b2 = 1, b3 = 0.1)))
Try(fm1a <- nls(y \sim b1 / (1+exp(b2-b3*x)), data = Ratkowsky2,
            trace = TRUE, alg = "port",
            start = c(b1 = 100, b2 = 1, b3 = 0.1))
Try(fm2 <- nls(y \sim b1 / (1+exp(b2-b3*x)), data = Ratkowsky2, trace = TRUE,
           start = c(b1 = 75, b2 = 2.5, b3 = 0.07))
Try(fm2a <- nls(y \sim b1 / (1+exp(b2-b3*x))), data = Ratkowsky2,
            trace = TRUE, alg = "port",
            start = c(b1 = 75, b2 = 2.5, b3 = 0.07))
Try(fm3 \leftarrow nls(y \sim 1 / (1+exp(b2-b3*x)), data = Ratkowsky2, trace = TRUE,
           start = c(b2 = 1, b3 = 0.1), alg = "plinear"))
Try(fm4 \leftarrow nls(y \sim 1 / (1+exp(b2-b3*x)), data = Ratkowsky2, trace = TRUE,
           start = c(b2 = 2.5, b3 = 0.07), alg = "plinear"))
```

26 Ratkowsky3

```
## Using a self-starting model
Try(fm5 <- nls(y ~ SSlogis(x, Asym, xmid, scal), data = Ratkowsky2))
summary(fm5)</pre>
```

Ratkowsky3

Onion growth data

# **Description**

The Ratkowsky3 data frame has 15 rows and 2 columns.

# **Format**

This data frame contains the following columns:

- y A numeric vector of dry weights of onion bulbs and tops.
- x A numeric vector of growing times.

## **Details**

This model and data are an example of fitting sigmoidal growth curves taken from Ratkowsky (1983). The response variable is the dry weight of onion bulbs and tops, and the predictor variable is growing time.

#### Source

Ratkowsky, D.A. (1983). Nonlinear Regression Modeling. New York, NY: Marcel Dekker, pp. 62 and 88.

Roszman1 27

Roszman1

Quantum defects in iodine

# **Description**

The Roszman1 data frame has 25 rows and 2 columns of data on the number of quantum defects in iodine atoms at different energy states.

#### **Format**

This data frame contains the following columns:

- y A numeric vector of number of quantum defects.
- **x** A numeric vector of the excited energy state.

## **Details**

These data are the result of a NIST study involving quantum defects in iodine atoms. The response variable is the number of quantum defects, and the predictor variable is the excited energy state. The argument to the ARCTAN function is in radians.

## Source

Roszman, L., NIST (19??). Quantum Defects for Sulfur I Atom.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val plot(y ~ x, data = Roszman1)  
Try(fm1 <- nls(y ~ b1 - b2*x - atan(b3/(x-b4))/pi, data = Roszman1, start = c(b1 = 0.1, b2 = -0.00001, b3 = 1000, b4 = -100), trace = TRUE))  
Try(fm1a <- nls(y ~ b1 - b2*x - atan(b3/(x-b4))/pi, data = Roszman1, start = c(b1 = 0.1, b2 = -0.00001, b3 = 1000, b4 = -100), alg = "port", trace = TRUE))  
Try(fm2 <- nls(y ~ b1 - b2*x - atan(b3/(x-b4))/pi, data = Roszman1, start = c(b1 = 0.2, b2 = -0.0000015, b3 = 1200, b4 = -150), trace = TRUE))  
Try(fm2a <- nls(y ~ b1 - b2*x - atan(b3/(x-b4))/pi, data = Roszman1, start = c(b1 = 0.2, b2 = -0.0000015, b3 = 1200, b4 = -150), alg = "port", trace = TRUE))
```

28 Thurber

Thurber

Electron mobility data

# **Description**

The Thurber data frame has 37 rows and 2 columns.

# **Format**

This data frame contains the following columns:

- y A numeric vector of electron mobility values.
- x A numeric vector of logs of electron density values.

## **Details**

These data are the result of a NIST study involving semiconductor electron mobility. The response variable is a measure of electron mobility, and the predictor variable is the natural log of the density.

## **Source**

Thurber, R., NIST (197?). Semiconductor electron mobility modeling.

```
Try <- function(expr) if (!inherits(val <- try(expr), "try-error")) val</pre>
plot(y \sim x, data = Thurber)
Try(fm1 \leftarrow nls(y \sim (b1+x*(b2+x*(b3+b4*x))) / (1+x*(b5+x*(b6+x*b7))),
           data = Thurber, trace = TRUE,
           start = c(b1 = 1000, b2 = 1000, b3 = 400, b4 = 40,
                      b5 = 0.7, b6 = 0.3, b7 = 0.03)))
Try(fm1a \leftarrow nls(y \sim (b1+x*(b2+x*(b3+b4*x))) / (1+x*(b5+x*(b6+x*b7))),
           data = Thurber, trace = TRUE, alg = "port",
           start = c(b1 = 1000, b2 = 1000, b3 = 400, b4 = 40,
                      b5 = 0.7, b6 = 0.3, b7 = 0.03))
Try(fm2 <- nls(y \sim (b1+x*(b2+x*(b3+b4*x))) / (1+x*(b5+x*(b6+x*b7))),
           data = Thurber, trace = TRUE,
           start = c(b1 = 1300, b2 = 1500, b3 = 500, b4 = 75,
                      b5 = 1, b6 = 0.4, b7 = 0.05))
Try(fm2a <- nls(y \sim (b1+x*(b2+x*(b3+b4*x))) / (1+x*(b5+x*(b6+x*b7))),
           data = Thurber, trace = TRUE, alg = "port",
           start = c(b1 = 1300, b2 = 1500, b3 = 500, b4 = 75,
                      b5 = 1, b6 = 0.4, b7 = 0.05))
Try(fm3 \leftarrow nls(y \sim outer(x, 0:3, "^")/(1+x*(b5+x*(b6+x*b7))),
           data = Thurber, trace = TRUE,
           start = c(b5 = 0.7, b6 = 0.3, b7 = 0.03), alg = "plinear"))
Try(fm4 <- nls(y \sim outer(x, 0:3, "^")/(1+x*(b5+x*(b6+x*b7))),
           data = Thurber, trace = TRUE,
           start = c(b5 = 1, b6 = 0.4, b7 = 0.05), alg = "plinear"))
```

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