⊞— Plot Utilities

⊞— ListCollect

⊞—Levenberg Marquardt's second algorithm

$$ft(x) := \beta_2 + \frac{\beta_1 - \beta_2}{1 + \left(\frac{x}{\beta_3}\right)^{\beta_4}} - \frac{\beta_1 - \beta_2}{\left(1 + \left(\frac{x}{\beta_3}\right)^{\beta_4}\right)^2} \cdot \left(\frac{x}{\beta_3}\right)^{\beta_4} \cdot \beta_4$$

$\varepsilon := 10^{-12}$ clear ln0 undefined

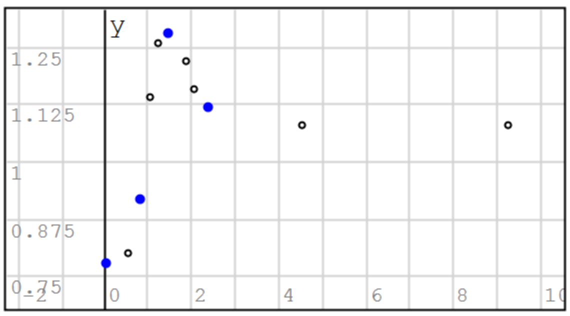
Point solve equalities

$$XY := \begin{bmatrix} \varepsilon & 0.78 \\ 0.51 & 0.8 \\ 0.82 & 0.92 \\ 1.02 & 1.14 \\ 1.23 & 1.26 \\ 1.43 & 1.28 \\ 1.85 & 1.22 \\ 2.05 & 1.16 \\ 2.36 & 1.12 \\ 4.52 & 1.08 \\ 9.22 & 1.08 \end{bmatrix}$$

$\left\{ \begin{array}{l} list := [\,1\ 3\ 6\ 9\,] \\ xy := ListCollect(XY, list) \end{array} \right.$

1. selct the support points
2. collect for al_nleqsolve

raw := plot(XY, "o", 5, "black")
support := plot(xy, ".", 14, "blue")



$\left\{ \begin{array}{l} support \\ raw \end{array} \right.$

$$xy = \begin{bmatrix} 0 & 0.78 \\ 0.82 & 0.92 \\ 1.43 & 1.28 \\ 2.36 & 1.12 \end{bmatrix}$$

4 DATA

$\left\{ \begin{array}{l} x := \mathrm{col}(xy, 1) \\ y := \mathrm{col}(xy, 2) \end{array} \right.$

$t0 := \mathrm{time}(1)$

JEAN

$\beta := [\,0.5\ 1\ 1\ 1\,]^T$

$Tol := 0.00000001$

$$LMSA(x, y, \beta, Tol, \beta s) = \begin{bmatrix} 0.7800 \\ 1.063 \\ 1.317 \\ 4.850 \end{bmatrix} \qquad \begin{bmatrix} 0.78 \\ 1.06345 \\ 1.3168 \\ 4.85016 \end{bmatrix}$$

$\mathrm{time}(1) - t0 = 0.723\ \mathrm{s}$

automated ... either NUMERIC/SYMBOLIC

$$\Phi(x, \alpha) := \alpha_2 + \frac{\alpha_1 - \alpha_2}{1 + \left(\frac{x}{\alpha_3}\right)^{\alpha_4}} - \frac{\alpha_1 - \alpha_2}{\left(1 + \left(\frac{x}{\alpha_3}\right)^{\alpha_4}\right)^2} \cdot \left(\frac{x}{\alpha_3}\right)^{\alpha_4} \cdot \alpha_4$$

```
f(α) := | ct := 1
        | for j ∈ [1..rows(x)]
        |   | Ω_ct := Φ(x_j, α) − y_j
        |   | ct := ct + 1
        | Ω
```

$$\alpha := \beta s = \begin{bmatrix} 0.77999 \\ 1.06345 \\ 1.31681 \\ 4.84968 \end{bmatrix}$$

Original version

$$f(\alpha) = \begin{bmatrix} \Phi(x_1, \alpha) - y_1 \\ \Phi(x_2, \alpha) - y_2 \\ \Phi(x_3, \alpha) - y_3 \\ \Phi(x_4, \alpha) - y_4 \end{bmatrix}$$

Notes...

1. solves a system of [n equalities = n parameters.
2. The order of equalities is immaterial.
3. Guess wisely the best support equalities !

JEAN

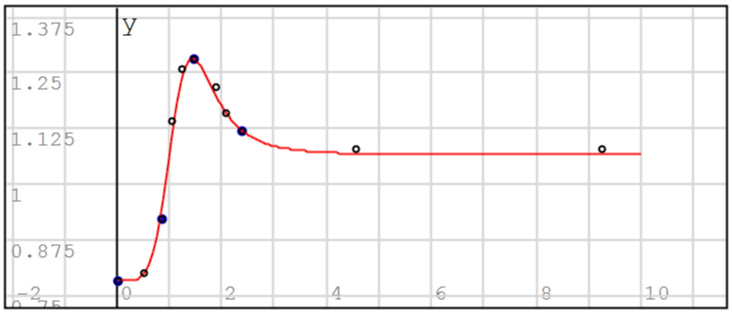
$$sanity := \begin{bmatrix} \Phi(0, \alpha) \\ \Phi(1, \alpha) \\ \Phi(2, \alpha) \\ \Phi(3, \alpha) \end{bmatrix} = \begin{bmatrix} 0.78 \\ 1.066 \\ 1.172 \\ 1.083 \end{bmatrix} \quad \begin{bmatrix} 0.78 \\ 1.066 \\ 1.172 \\ 1.083 \end{bmatrix}$$

$$f(\alpha) = \begin{bmatrix} -0.000010553698 \\ 0.000007914683 \\ -0.000015697896 \\ 0.000016568730 \end{bmatrix}$$

Clear $(x) = 1$

$u := (0 \le x) \cdot (x \le 10)$

Fit " a la carte"



$$\begin{cases} raw \\ \dfrac{\Phi(x, \alpha)}{u} \\ support \end{cases}$$

Clear $(x, y) = 1.000$

ALL DATA

$$\begin{cases} X := \mathrm{col}(XY, 1) \\ Y := \mathrm{col}(XY, 2) \end{cases}$$

$Tol := 10^{-16}$

data := plot (XY, "o", 5, "black")

$t0 := \mathrm{time}(1)$

JEAN

$$LMSA(X, Y, \beta, Tol, \beta s) = \begin{bmatrix} 0.7773 \\ 1.0727 \\ 1.2781 \\ 4.8008 \end{bmatrix} \quad \begin{bmatrix} 0.778997 \\ 1.072526 \\ 1.281669 \\ 4.824839 \end{bmatrix}$$

$\mathrm{time}(1) - t0 = 3.545\ s$

Minimize Conjugate-Gradient

$$f(x, \beta s) := \beta s_2 + \frac{\beta s_1 - \beta s_2}{1 + \left(\frac{x}{\beta s_3}\right)^{\beta s_4}} - \frac{\beta s_1 - \beta s_2}{\left(1 + \left(\frac{x}{\beta s_3}\right)^{\beta s_4}\right)^2} \cdot \left(\frac{x}{\beta s_3}\right)^{\beta s_4} \cdot \beta s_4$$

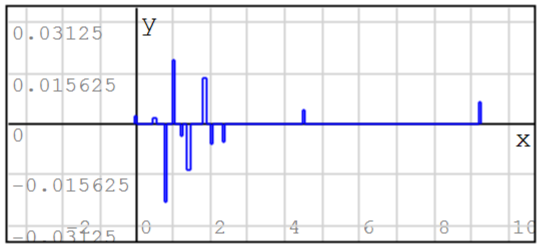
$SSD = 0.0015$ $\quad$ $corr = 1.0794$

Absolute residuals

$$\delta := \left| \begin{array}{l} \text{for } j \in [1..\text{rows}(XY)] \\ \quad \Delta_j := \text{eval}\left(Y_j - f\left(X_j, \beta\right)\right) \\ \text{augment}(X, \Delta) \end{array} \right.$$

$$FIT := \left| \begin{array}{l} U := [0, 0.025..10] \\ \text{for } i \in [1..\text{rows}(U)] \\ \quad vy_i := \text{eval}\left(f\left(U_i, \beta\right)\right) \\ \text{augment}(U, vy) \end{array} \right.$$

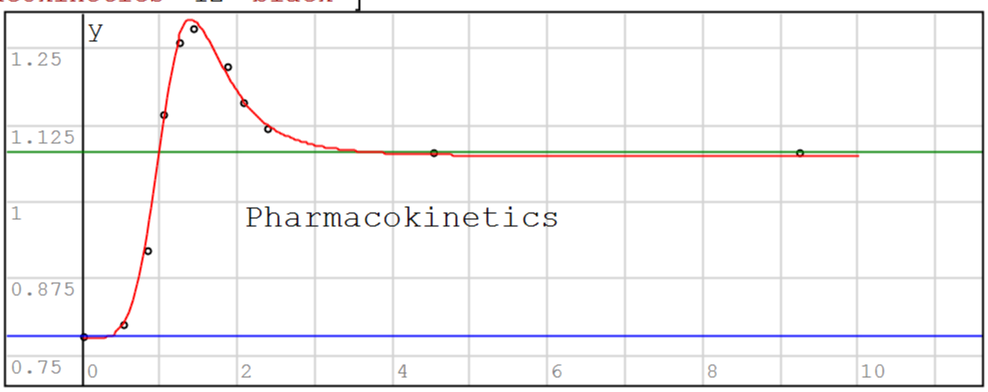
$bar := (BarSize(\delta, 0.0375))$



bar

$Title := [\,2\ 1\ \text{"Pharmacokinetics"}\ 12\ \text{"black"}\,]$

$$collect := \begin{cases} 0.78 \\ FIT \\ 1.08 \\ data \\ Title \end{cases}$$



$\text{Clear}(x, \beta) = 1.000$

FUNCTION

$$ft(x) := \beta_1 \cdot \beta_2 \cdot x^{\beta_2 - 1} \cdot \exp\left(-\beta_1 \cdot x^{\beta_2}\right)$$

$$x := \begin{bmatrix} 0.132 \\ 0.322 \\ 0.511 \\ 0.701 \\ 0.891 \\ 1.082 \\ 1.27 \\ 1.46 \\ 1.65 \\ 1.839 \\ 2.029 \\ 2.219 \end{bmatrix} \qquad y := \begin{bmatrix} 0.1 \\ 0.258 \\ 0.543 \\ 0.506 \\ 0.606 \\ 0.622 \\ 0.569 \\ 0.453 \\ 0.438 \\ 0.316 \\ 0.29 \\ 0.195 \end{bmatrix} \qquad \beta := \begin{bmatrix} 0.8 \\ 1 \end{bmatrix}$$

$Tol := 0.0000000001$

$t0 := \text{time}(1)$

$$LMSA(x, y, \beta, Tol, \beta s) = \begin{bmatrix} 0.5022 \\ 2.0004 \end{bmatrix}$$

FUNCTION

$\text{time}(1) - t0 = 1.042\ \text{s}$

$$ft(t, \beta s) := \beta s_1 \cdot \beta s_2 \cdot t^{\beta s_2 - 1} \cdot \exp\left(-\beta s_1 \cdot t^{\beta s_2}\right)$$

$t := x \qquad m := \text{rows}(x)$

Relative residuals

$$Residuals := \left| \begin{array}{l} \text{for } i \in [1..\text{rows}(t)] \\ \quad \Delta_i := \text{eval}\left(1 - \dfrac{y_i}{ft\left(t_i, \beta s\right)}\right) \\ \text{augment}(t, \Delta) \end{array} \right.$$

SSD = "Sum Square Differences"

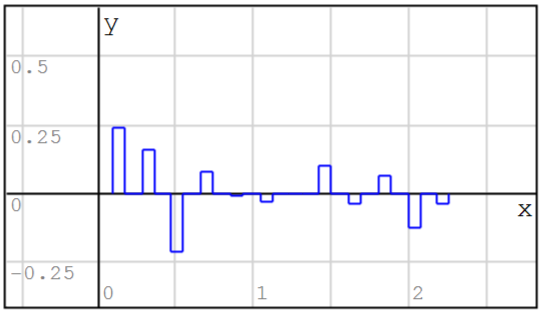
$$SSD := \sum_{i=1}^{m} \left(\left(y_i - ft\left(t_i, \beta s\right)\right)^2\right) = 0.0186$$

RMS difference

$$RMSD := \sqrt{\frac{SSD}{m}}$$

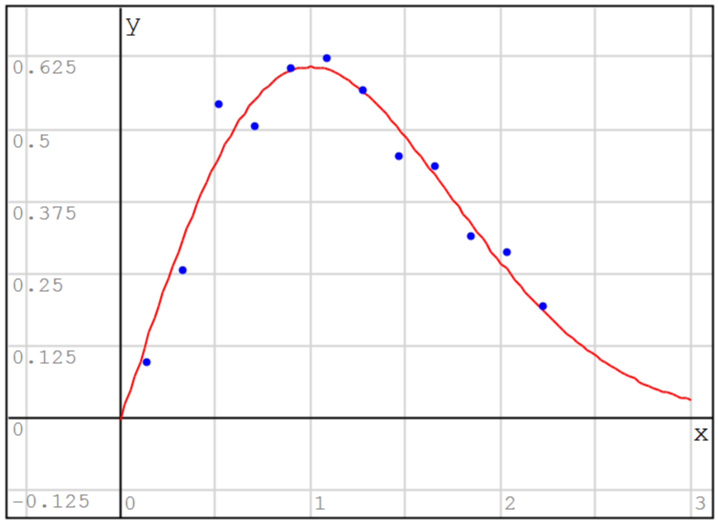
$$\sqrt{\frac{SSD}{m}} = 0.0394$$

Relative residuals



{BarSize(Residuals, RMSD)

```
data := plotG(x, y, ".", 12, "blue")
FIT := | "range, populate"
       | U := [0, 0.025..3]
       | for i ∈ [1..rows(U)]
       |   vy_i := eval(ft(U_i, βs))
       | augment(U, vy)
```



{data
FIT

D2 ... D3

XY := D2

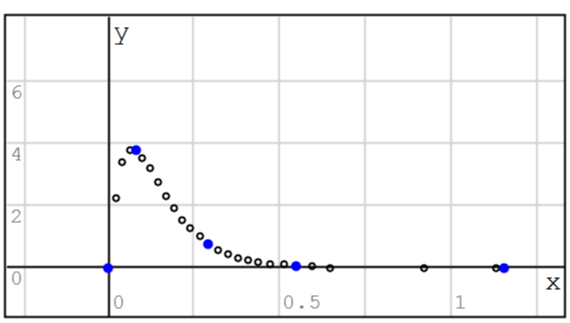
Point solve equalities

rows(D2) = 27

```
{list := [1 5 14 22 27]
{xy := ListCollect(XY, list)
```

1. selct the support points
2. collect for al_nleqsolve

```
raw := plot(XY, "o", 5, "black")
support := plot(xy, ".", 14, "blue")
```



{support
raw

Clear$(x, \beta) = 1$

$$ft(x) := x \cdot \left(\beta_1 + \beta_2 \cdot \exp\left(-\frac{x}{\beta_4}\right) + \beta_3 \cdot \exp\left(-\frac{x}{\beta_5}\right)\right)$$

model to D2(x)

$$xy = \begin{bmatrix} 0 & 0 \\ 0.079 & 3.782 \\ 0.29 & 0.77 \\ 0.545 & 0.068 \\ 1.154 & 0 \end{bmatrix}$$

$$\beta := \begin{bmatrix} 10^{-12} & 10 & -5 & 0.1 & -5 \end{bmatrix}^T$$

vector of guesses ...
from robust2crucifying !

$$\begin{cases} x := \text{col}(xy, 1) \\ y := \text{col}(xy, 2) \end{cases}$$

$Tol := 10^{-16}$

$t0 := \text{time}(1)$

$$LMSA(x, y, \beta, Tol, \beta s) = \begin{bmatrix} 2.1283 \\ 142.4114 \\ -2.0372 \\ 0.0723 \\ -26.376 \end{bmatrix}$$

Jean Solution

$$\begin{bmatrix} 1.1077 \\ 142.40751 \\ -1.01751 \\ 0.07235 \\ -13.58616 \end{bmatrix}$$

$\text{time}(1) - t0 = 0\ \text{s}$

$\alpha := \beta s$

$$\Phi(x, \alpha) := x \cdot \left(\alpha_1 + \alpha_2 \cdot \exp\left(-\frac{x}{\alpha_4}\right) + \alpha_3 \cdot \exp\left(-\frac{x}{\alpha_5}\right)\right)$$

model to D2(x)

Implicit equalities = 0

$$f(\alpha) := \begin{bmatrix} \Phi(x_1, \alpha) - y_1 \\ \Phi(x_2, \alpha) - y_2 \\ \Phi(x_3, \alpha) - y_3 \\ \Phi(x_4, \alpha) - y_4 \\ \Phi(x_5, \alpha) - y_5 \end{bmatrix} \qquad \alpha = \begin{bmatrix} 2.12827 \\ 142.41144 \\ -2.03717 \\ 0.07235 \\ -26.37602 \end{bmatrix}$$

Notes . . . Smath 7251

1. solves a system of [n equalities = n parameters.

2. The order of equalities is immaterial.

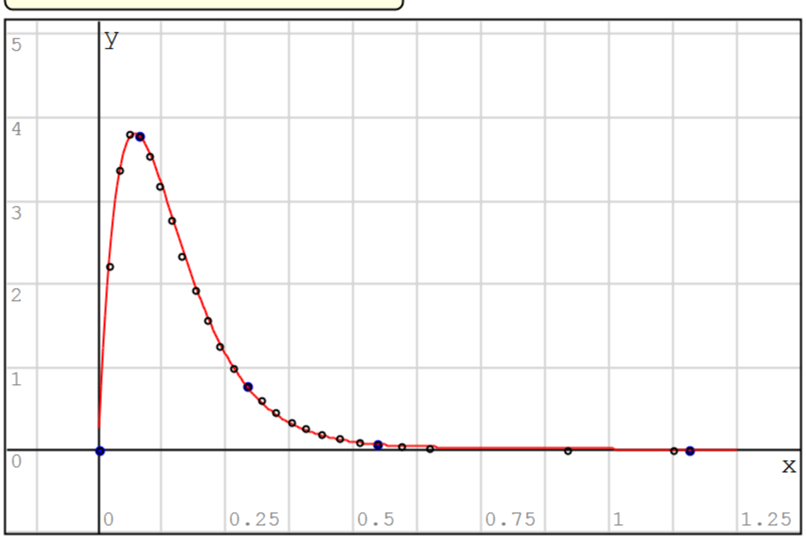
3. Guess wisely the best support equalities **!**

$$f(\alpha) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{cases} \left[X := \text{col}(XY, 1) \quad Y := \text{col}(XY, 2) \right] \\ data := plot(XY, \text{"o"}, 5, \text{"black"}) \end{cases}$$

$$c(x) := \begin{cases} 1 & \text{if } (0 \le x) \wedge (x \le 1.25) \\ \text{""} & \text{otherwise} \end{cases}$$

Fit " a la carte" from LMA



$$\begin{cases} data \\ \Phi(x, \alpha) \cdot c(x) \\ support \end{cases}$$

Support points

$$xy = \begin{bmatrix} 0 & 0 \\ 0.079 & 3.782 \\ 0.29 & 0.77 \\ 0.545 & 0.068 \\ 1.154 & 0 \end{bmatrix}$$

$XY := D3$

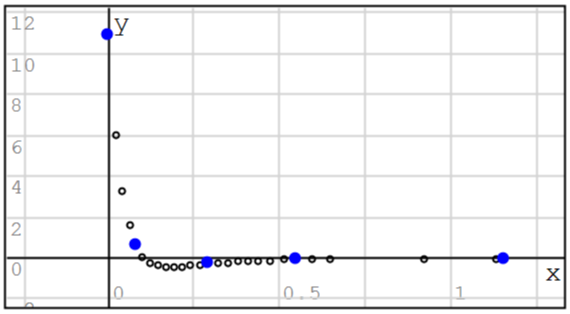
====== D3 data set ======

$\text{rows}(D3) = 27$

$list := [1\ 5\ 14\ 22\ 27]$
$xy := ListCollect(XY, list)$

1. selct the support points
2. collect for LMA

$raw := plot(XY, \text{"o"}, 5, \text{"black"})$
$support := plot(xy, \text{"."}, 15, \text{"blue"})$



support
raw

$\text{Clear}(x, \beta) = 1$

$$ft(x) := \beta_1 - \beta_2 \cdot \left(\exp\left(\frac{-x + \beta_3}{\beta_5} \right) - \exp\left((-x + \beta_3) \cdot \frac{\beta_4 + \beta_5}{\beta_4 \cdot \beta_5} \right) \right)$$

model to D3(x)

$$xy = \begin{bmatrix} 0 & 10.861 \\ 0.079 & 0.706 \\ 0.29 & -0.226 \\ 0.545 & -0.031 \\ 1.154 & 0 \end{bmatrix} \quad \begin{cases} x := \text{col}(xy, 1) \\ y := \text{col}(xy, 2) \end{cases} \quad x = \begin{bmatrix} 0.000 \\ 0.07900 \\ 0.2900 \\ 0.5450 \\ 1.154 \end{bmatrix} \quad y = \begin{bmatrix} 10.86 \\ 0.7060 \\ -0.2260 \\ -0.03100 \\ 0.000 \end{bmatrix} \begin{bmatrix} 0 & 10.861 \\ 0.079 & 0.706 \\ 0.29 & -0.226 \\ 0.545 & -0.031 \\ 1.154 & 0 \end{bmatrix}$$

$\beta := [0\ 1\ 0.1\ 0.075\ 0.1]^T$

vector of guesses ...
from robust2crucifying !

$Tol := 10^{-16}$

$t0 := \text{time}(1)$

$$LMSA(x, y, \beta, Tol, \beta s) = \begin{bmatrix} 0.00024 \\ 1.03264 \\ 0.1063 \\ 0.06231 \\ 0.12544 \end{bmatrix}$$

Jean Solution

$$\begin{bmatrix} 0.00071 \\ 1.0028 \\ 0.10647 \\ 0.06114 \\ 0.12774 \end{bmatrix}$$

$\text{time}(1) - t0 = 0\ \text{s}$

$\beta := \beta s$

$$\Phi(x, \beta) := \beta_1 - \beta_2 \cdot \left(\exp\left(\frac{-x + \beta_3}{\beta_5} \right) - \exp\left((-x + \beta_3) \cdot \frac{\beta_4 + \beta_5}{\beta_4 \cdot \beta_5} \right) \right)$$

model to D3(x)

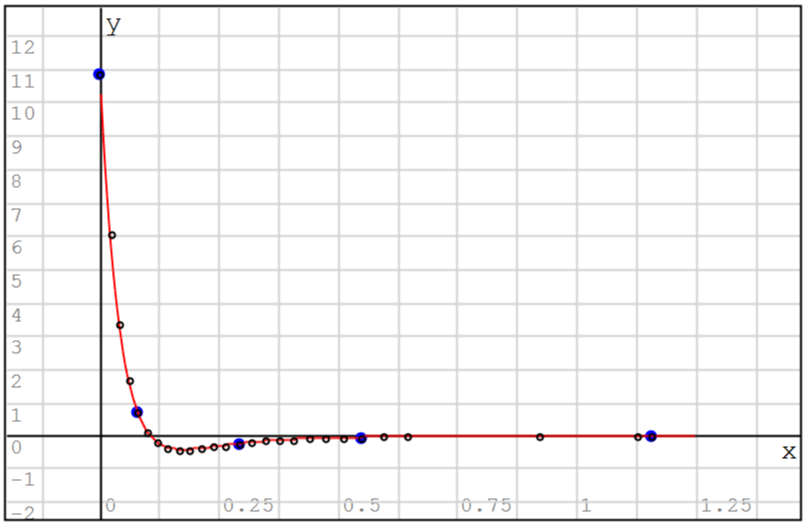
Implicit equalities = 0

$$f(\beta) := \begin{bmatrix} \Phi(x_1, \beta) - y_1 \\ \Phi(x_2, \beta) - y_2 \\ \Phi(x_3, \beta) - y_3 \\ \Phi(x_4, \beta) - y_4 \\ \Phi(x_5, \beta) - y_5 \end{bmatrix} \qquad \beta = \begin{bmatrix} 0.00024 \\ 1.03264 \\ 0.1063 \\ 0.06231 \\ 0.12544 \end{bmatrix}$$

$[X := \text{col}(XY, 1)\ Y := \text{col}(XY, 2)]$
$data := plot(XY, \text{"o"}, 5, \text{"black"})$

$$c(x) := \begin{cases} 1 & \text{if } (0 \le x) \wedge (x \le 1.25) \\ \text{""} & \text{otherwise} \end{cases}$$

Fit " a la carte" from al_nleqsolve



$$\begin{cases} data \\ \Phi(x, \beta) \cdot c(x) \\ support \end{cases}$$

$$f(\beta) = \begin{bmatrix} 5.588 \cdot 10^{-12} \\ 6.377 \cdot 10^{-13} \\ 5.117 \cdot 10^{-11} \\ -1.627 \cdot 10^{-10} \\ 1.112 \cdot 10^{-10} \end{bmatrix}$$

Jean

$$\begin{bmatrix} 2.932 \cdot 10^{-6} \\ 2.063 \cdot 10^{-6} \\ 0.0001973 \\ -0.0006440 \\ 0.0004336 \end{bmatrix}$$

XY Thurber

$$Clear(x, \beta) = 1$$

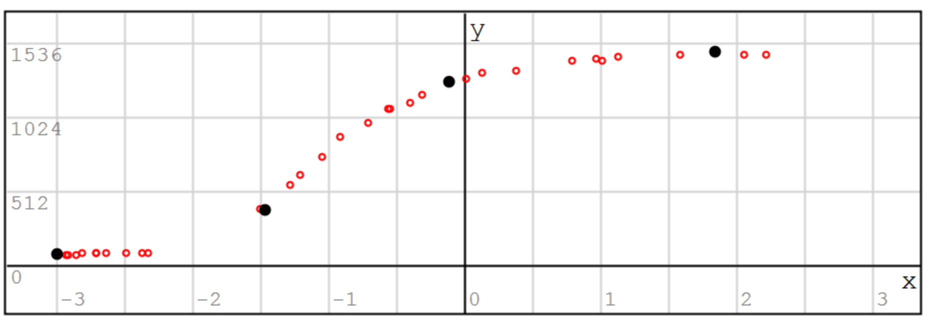
$$ft(x) := \beta_1 + \beta_2 \cdot \exp\left(-\exp\left(-\beta_3 \cdot \left(x - \beta_4\right)\right)\right)$$

SGompertz Thurber model fnct

$$\begin{cases} list := [1\ 13\ 24\ 34] \\ xy := ListCollect(XY, list) \end{cases}$$

1. selct the support points
2. collect for LMA

raw := plot(XY, "o", 5, "red")
support := plot(xy, ".", 16, "black")



$$\beta := [80\ 1400\ 1\ 0]^T$$

vector of guesses ...
from robust2crucifying !

$$Tol := 10^{-16}$$

$$xy = \begin{bmatrix} -2.981 & 84.248 \\ -1.46 & 390.724 \\ -0.109 & 1260 \\ 1.841 & 1470 \end{bmatrix}$$

$$\begin{cases} x := col(xy, 1) \\ y := col(xy, 2) \end{cases}$$

$$t0 := time(1)$$

$$LMSA(x, y, \beta, Tol, \beta s) = \begin{bmatrix} 84.24796852 \\ 1396.05301219 \\ 1.61215217 \\ -1.20180484 \end{bmatrix} \begin{bmatrix} 84.25 \\ 1396.05 \\ 1.61 \\ -1.2 \end{bmatrix}$$

$$time(1) - t0 = 1\ s$$

SGompertz…
is extremely **reflexive**, declared unfittable in Smath [L-M, CG]. Possible attempt OriginLab, Mathcad 11. As offered, and fitted by al_nleqsolve, at this point, you may want to round/refactor the coefficients. The fillet region is a bit sparse !

$$\Phi(x, m) := m_1 + m_2 \cdot \exp\left(-\exp\left(-m_3 \cdot \left(x - m_4\right)\right)\right)$$ SGompertz Thurber model fnct

Implicit equalities = 0

$$f(\mu) := \begin{bmatrix} \Phi(x_1, \mu) - y_1 \\ \Phi(x_2, \mu) - y_2 \\ \Phi(x_3, \mu) - y_3 \\ \Phi(x_4, \mu) - y_4 \end{bmatrix}$$

$$\mu := \beta s = \begin{bmatrix} 84.25 \\ 1396.05 \\ 1.61 \\ -1.2 \end{bmatrix}$$

Notes ... Smath 7251

1. solves a system of [n equalities = n parameters].

2. The order of equalities is immaterial.

3. Guess wisely the best support equalities !

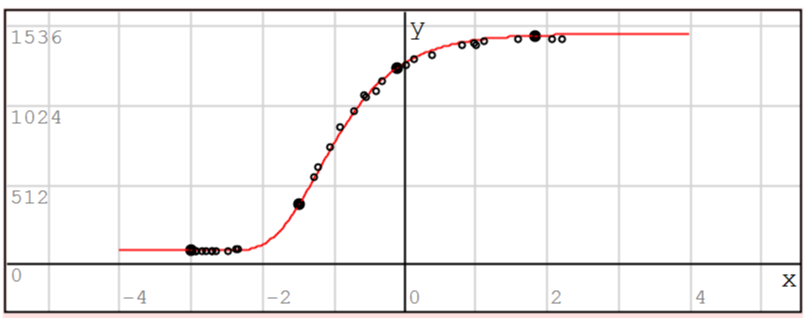
$$f(\mu) = \begin{bmatrix} 0.000000000051 \\ 0 \\ -0.00000000001 \\ -0.000000000031 \end{bmatrix} \quad \begin{bmatrix} 0.000000000000 \\ -0.000000000003 \\ 0.000000000000 \\ 0.000000000002 \end{bmatrix}$$

$$\begin{cases} \left[X := \mathrm{col}(XY, 1) \;\; Y := \mathrm{col}(XY, 2) \right] \\ data := plot(XY, \text{"o"}, 5, \text{"black"}) \end{cases}$$

$$c(x) := \begin{cases} 1 & \text{if } (-4 \le x) \wedge (x \le 4) \\ \text{""} & \text{otherwise} \end{cases}$$

$$\mu := \begin{bmatrix} \begin{bmatrix} 84.25 \\ 1396 \\ 1.61 \\ -1.2 \end{bmatrix} \end{bmatrix}$$

$$j := 1$$



$$\begin{cases} data \\ \Phi\left(x, \mu_{1\,j}\right) \cdot c(x) \\ support \end{cases}$$

Support points

$$xy = \begin{bmatrix} -2.981 & 84.248 \\ -1.46 & 390.724 \\ -0.109 & 1260 \\ 1.841 & 1470 \end{bmatrix}$$