Monomolecular curve for simulated data

Contents

1. Introduction

In this example we consider the fitting of a monomolecular curve to simulated longitudinal data. Values were simulated for 20 time points and 80 cases. Data are given in **modexponen.lsf** and the data for the first case are shown below.

modexponen.lsf

	id2	id1	y	time
1	1.00	1.00	685.64	1.00
2	1.00	2.00	569.82	2.00
3	1.00	3.00	486.43	3.00
4	1.00	4.00	413.64	4.00
5	1.00	5.00	364.24	5.00
6	1.00	6.00	322.72	6.00
7	1.00	7.00	282.27	7.00
8	1.00	8.00	256.26	8.00
9	1.00	9.00	233.31	9.00
10	1.00	10.00	223.29	10.00
11	1.00	11.00	211.04	11.00
12	1.00	12.00	198.38	12.00
13	1.00	13.00	192.83	13.00
14	1.00	14.00	180.65	14.00
15	1.00	15.00	173.32	15.00
16	1.00	16.00	177.05	16.00
17	1.00	17.00	171.41	17.00
18	1.00	18.00	162.10	18.00
19	1.00	19.00	164.61	19.00
20	1.00	20.00	165.57	20.00

The model is defined as

$$y = b_1 * [1 + s * \exp(b_2 - b_3 * Time)] + e$$

with b_1 = 160.0, b_2 = 1.50, and b_3 = 0.25 used for simulation, where

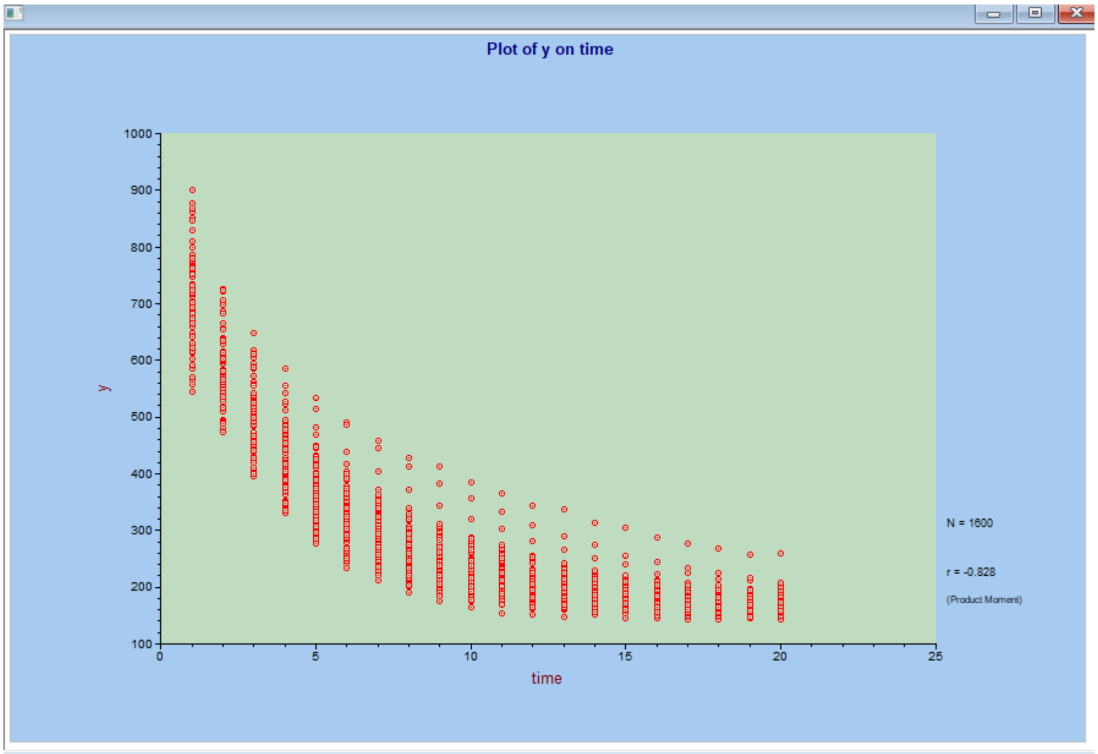
$$b_1 = \beta_1 + u_1$$
$$b_2 = \beta_2 + u_2$$
$$b_3 = \beta_3 + u_3$$

The covariance matrix of the parameters b_1, b_2, and b_3 used for simulation was

$$\begin{bmatrix} 85.000 & & \\ -1.000 & 0.050 & \\ 0.060 & 0.008 & 0.005 \end{bmatrix}$$

along with a value of 15for σ^2.

A scatterplot of the *y* measurements over time is shown below. The relationship between *y* and time is nonlinear. When function values decrease monotonically over time as is the case here, s = 1.



2. Monomolecular curve

We now fit a monomolecular curve to the data in order to examine how the estimated and simulated coefficients compare. The syntax file for this model is shown in the syntax file **modexpon.prl**. The variable ID2 is used as level-2 identifier.

MODEXPON.prl

```
OPTIONS METHOD = ML CONVERGE = 0.00001 MAXITER =20 QUADPTS= 93;
TITLE = Simulated data modified exponential function ;
SY=modexponen.lsf;
ID1 = id1;
ID2 = id2;
RESPONSE = y;
FIXED = time;
MODEL = Monomolecular;
```

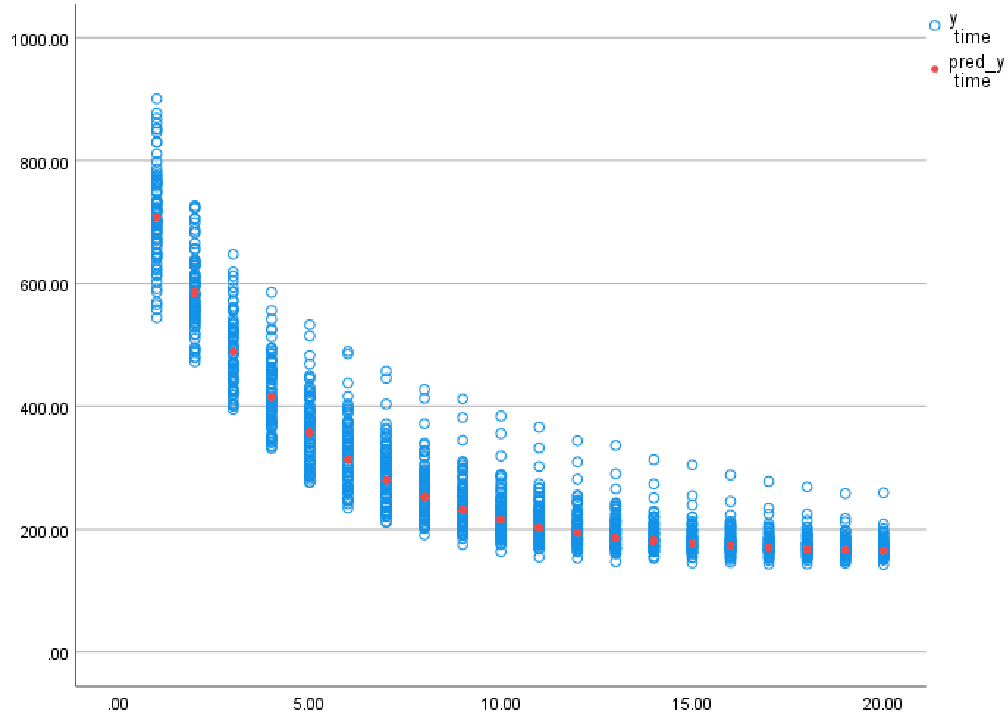
The ML solution is as follows.

MODEXPON.OUT

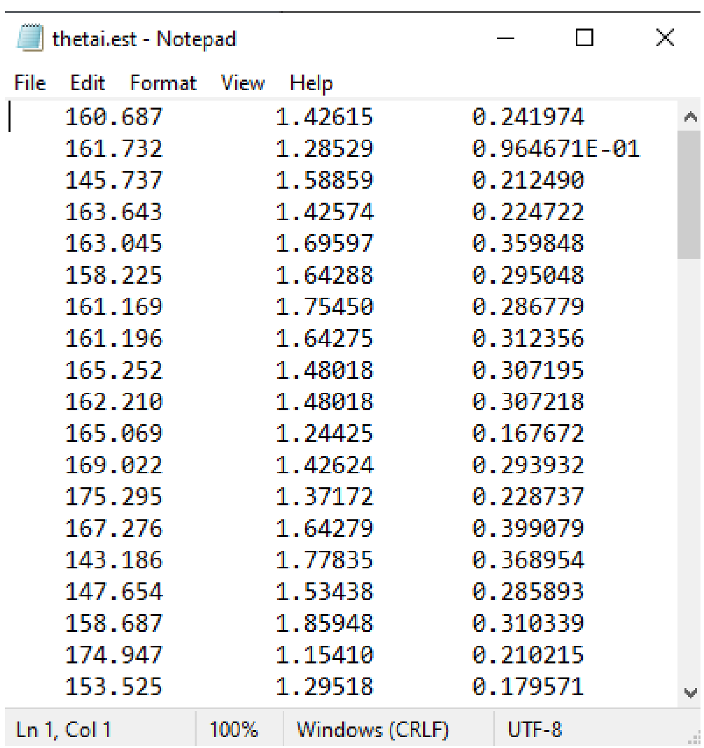
```
Maximum Likelihood Solution



  ---------------------------------------------------------------------------
   Coefficients          Beta          Std.Err.      Z-value        P > |z|
  ---------------------------------------------------------------------------
               b1      160.75768       0.75635     212.54540        0.00000
               b2        1.48017       0.01528      96.85824        0.00000
               b3        0.25525       0.00538      47.44247        0.00000


  ---------------------------------------------------------------------------
   Variance estimate     Level 1       Std.Err.      Z-value        P > |z|
  ---------------------------------------------------------------------------
    Sigma**2            16.37343       0.40653      40.27582        0.00000



  ---------------------------------------------------------------------------
   Covariances           Level 2       Std.Err.      Z-value        P > |z|
  ---------------------------------------------------------------------------
            u1,u1       86.57256      10.19262       8.49365        0.00000
            u2,u1       -0.89759       0.16346      -5.49119        0.00000
            u2,u2        0.03712       0.00418       8.88571        0.00000
            u3,u1        0.09816       0.05212       1.88351        0.05963
            u3,u2        0.00579       0.00114       5.09686        0.00000
            u3,u3        0.00462       0.00052       8.91245        0.00000

   Note: ML estimates of individual coefficients written to file THETAI.EST
```

The estimated beta coefficients are very close in value to those used in the simulation. This is also true of the estimated variance-covariance components.

A scatterplot of the predicted outcome and the simulated outcome over time is given below.



The program also writes the estimated parameters for each level-2 unit to an external text file named **thetai.est**. The contents of this file for the first few cases are as follows:

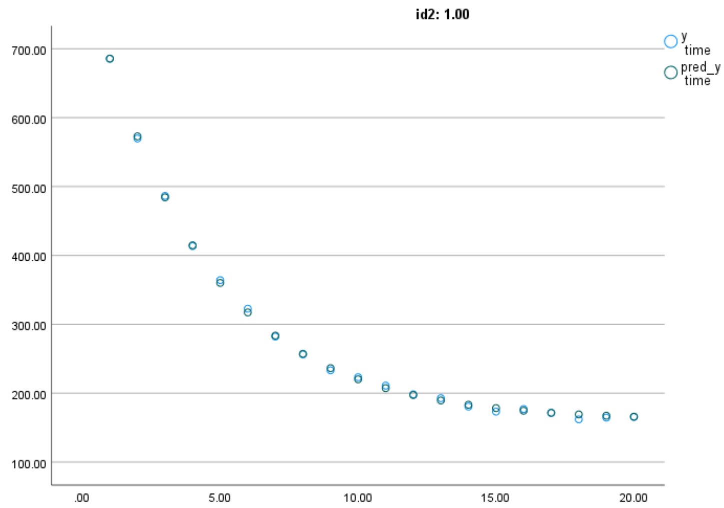


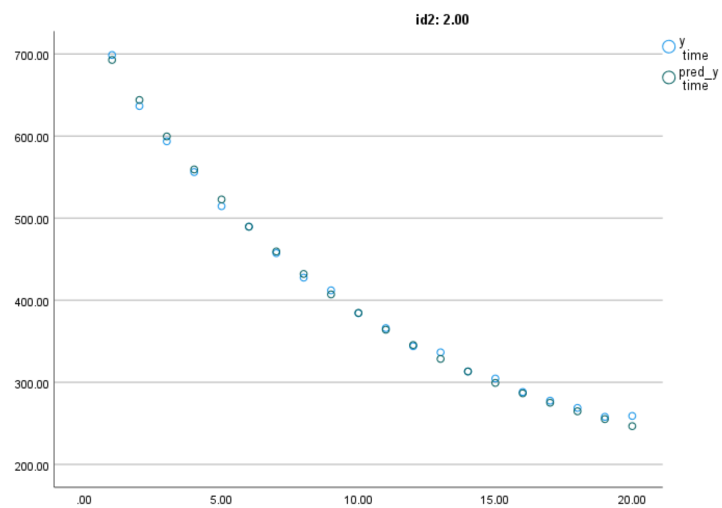
160.687	1.42615	0.241974
161.732	1.28529	0.964671E-01
145.737	1.58859	0.212490
163.643	1.42574	0.224722
163.045	1.69597	0.359848
158.225	1.64288	0.295048
161.169	1.75450	0.286779
161.196	1.64275	0.312356
165.252	1.48018	0.307195
162.210	1.48018	0.307218
165.069	1.24425	0.167672
169.022	1.42624	0.293932
175.295	1.37172	0.228737
167.276	1.64279	0.399079
143.186	1.77835	0.368954
147.654	1.53438	0.285893
158.687	1.85948	0.310339
174.947	1.15410	0.210215
153.525	1.29518	0.179571

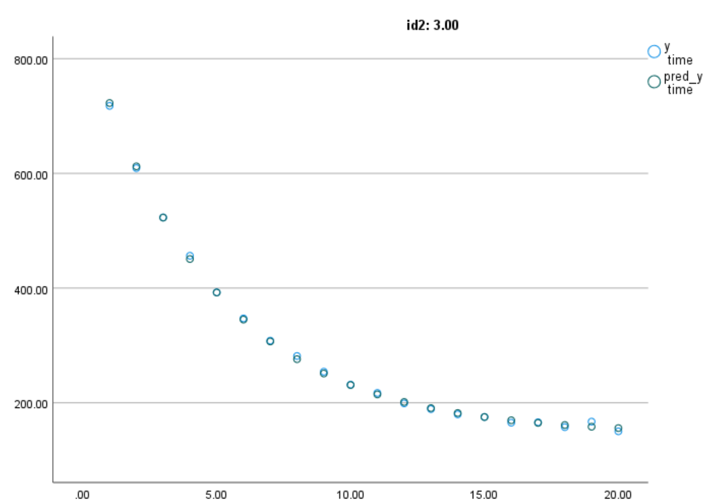
Using these results, the predicted outcome of, for example, the third case can be expressed as:

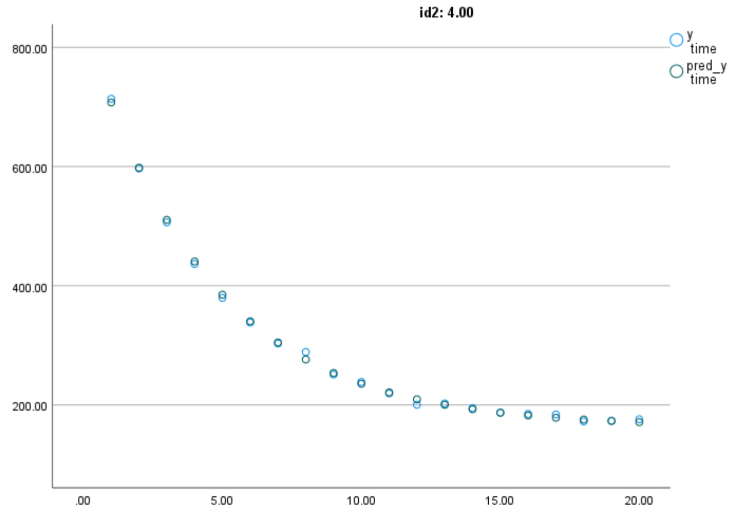
$$\hat{y} = 163.643 * [1 + \exp(1.42574 - 0.224722 * Time)]$$

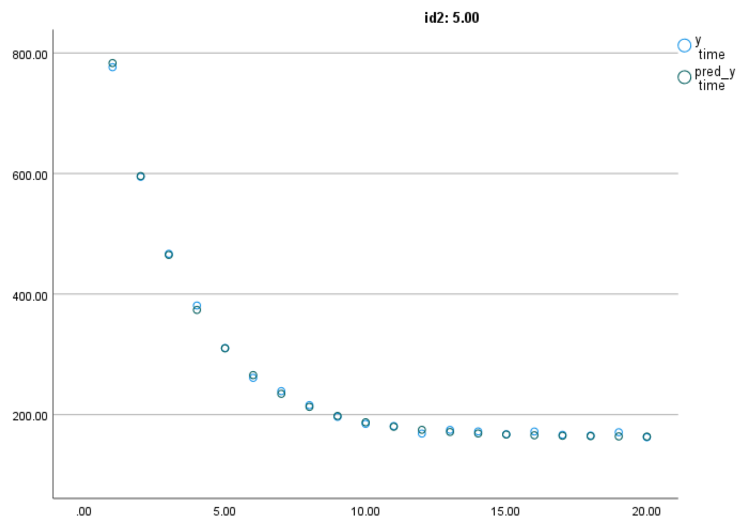
When the observed and predicted outcomes are plotted, we see that the fitted curve describes the data well, as illustrated by the plots for the first 5 cases shown below.








id2: 4.00
y
time
pred_y
time
800.00
600.00
400.00
200.00
.00
5.00
10.00
15.00
20.00


id2: 5.00
y
time
pred_y
time
800.00
600.00
400.00
200.00
.00
5.00
10.00
15.00
20.00