TITE, Applied Mathematics

Ti5417700 Modelling methodology/T. Kauranne

Exercise 28.11.2006

1. Find the least squares fit for the parameters b_1, b_2 of the model $y = b_1(1-e^{-b_2 x})$ to the data $x = (1, 3, 5, 7, 9)$, $y = (0.076, 0.258, 0.369, 0.492, 0.559)$. Use the FMINSEARCH optimizer.

2. To study the chemical reaction $A + B \xrightarrow{k} C$ an experiment was performed using the initial concentrations $A(0) = 0.054, B(0) = 0.106$. The data below was measured:

```
% time  cA
  426   0.0351
  1150  0.0222
  1660  0.0186
  3120  0.0124
```

   Estimate the value for the reaction rate constant k, when the reaction is given by the expression $Re = kAB$. Would a better fit be obtained by some of the forms $Re = kA^m B^n$, where m and n may get the values 1 or 2 ?

3. The chemical reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ was started using the initial concentrations $A(0) = 1, B(0) = C(0) = 0$. Estimate the values for reaction rate constants, when the data below was measured:

```
!  time      A          B
   1.0e+00   5.04e-01   4.15e-01
   2.0e+00   1.85e-01   4.88e-01
   3.0e+00   2.17e-01   5.94e-01
   4.0e+00   2.26e-02   5.05e-01
   5.0e+00   1.01e-01   4.93e-01
   6.0e+00   5.79e-02   4.57e-01
   7.0e+00   6.45e-02   3.94e-01
   8.0e+00   0.00e+00   3.34e-01
   9.0e+00   8.20e-02   3.09e-01
```