MA/ST 810, HOMEWORK 1, FALL 2009

Due October 13, 2009

Consider the chemostat model developed in class:

$$\begin{aligned}\frac{dN}{dt} &= r(c)N - qN \\ \frac{dc}{dt} &= q(c_0 - c) - \frac{1}{y}r(c)N,\end{aligned} \qquad (1)$$

where $N(0) = N_0$, $c(0) = 0$. Moreover,

$$r(c) = \frac{R_{\max}\, c}{K_m + c}, \quad q = \frac{Q}{V}.$$

$$\theta = (V, Q, R_{\max}, K_m, c_0, y)^T,$$

(Note here that the symbol "y" represents a parameter and not a realization of an observation.) Typical values for the parameters in this model are

$$V = 20 \text{ l}, \quad c_0 = 2.5 \text{ g/l}, \quad K_m = 12.3\,\mu\text{g/ml}, \quad R_{\max} = 0.85/\text{hr}, \quad y = 10.6 \text{ l/g}$$

Take $N_0 = 0.025$ g.

1. Simulate and plot graphs of the forward solution to the system (1) using the parameter values and initial conditions given above for values of Q ranging from 14 to 16 l/hr.

2. Now take several of your simulation results from part 1. to use as data for observations at times t_j, $j = 1, \ldots, n$, and, for each, use a least squares inverse problem formulation to estimate:

   (a) $R_{\max}$, holding all other model parameters fixed at the given values.

   (b) K_m, holding all other model parameters fixed at the given values.

   (c) $R_{\max}$ and K_m (simultaneously), holding all other model parameters fixed at the given values.

   Each of (a)–(c) should be done using (i) observations of $c(t)$ only, (ii) observations of $N(t)$ only, and (iii) observations of both $c(t)$ and $N(t)$. Carry out each combination of (a)–(c) and (i)–(iii) for several different sets of time points $(t_1, \ldots, t_n)$ and discuss how the solution depends on the choice of n, the values of t_j, $j = 1, \ldots, n$, and the availability of observations of $c(t)$, $N(t)$, or both.

3. Take a typical forward simulation result from part 1. and add random noise as follows. Let $f(t_j, \theta) = \{f^{(1)}(t_j, \theta), f^{(2)}(t_j, \theta)\}^T$ be the value of the forward solution from part 1 [observations of $c(t)$ and $N(t)$ at t_j at a particular value of θ] and obtain realizations of "data" (y_j, t_j), $j = 1, \ldots, n$, according to the statistical model

$$Y_j = f(t_j, \theta) + \sigma \begin{pmatrix} f^{(1)}(t_j, \theta) & 0 \\ 0 & f^{(2)}(t_j, \theta) \end{pmatrix} \epsilon_j.$$

Create four data sets by taking $\sigma = 0.05$ and $\sigma = 0.10$ with $\epsilon_j = (\epsilon_j^{(1)}, \epsilon_j^{(2)})^T$ generated independently for each j according to:

(a) $\epsilon_j^{(k)}$ independent for $k = 1, 2,$, each uniformly distributed on $(-\sqrt{3}, \sqrt{3})$

(b) $\epsilon_j^{(k)}$ independent for $k = 1, 2$, each having a standard normal distribution (mean 0, variance 1).

For each of these four data sets, repeat part 2.