Exponential least-squares, part I

From our virtual experiments on dropping weights (lecture 18), we have learned that we can estimate the parameters of a model (in that case, g, v_0 and H) with the help of a least-squares fit to measured data. In this assignment and the next one, you will try the same approach for an exponential (instead of quadratic) dependence.

Many processes in nature, like the growth of a bacterial culture in the abundance of nutrition or the intensity of light travelling through a medium, are exponential in nature. If a is the quantity we are interested in and x is the variable it depends on (in the examples time and distance travelled, respectively), then we expect that

$$a(x) = c\exp(\lambda x)$$

for some c, $\lambda \in \mathbb{R}$. When measuring a in an experiment, at discrete values of x, we necessarily incur some error and uncertainty. Assume we are given a list of measurements (x_j, y_j) where y_j is close to, but differs from, the model value $a(x_j)$.

(a) Find an expression for the sum of squares of the errors $a(x_j) - y_j$ as a function of c and λ.

$$E(c,\lambda) = \sum_{j=0}^{n}(a(x_j) - y_j)^2 = \sum_{j=0}^{n}\left(c\exp(\lambda x_j) - y_j\right)^2$$

(b) Find the system of equations that is satisfied at each maximum or minimum of the error function you found at (a).

$$\frac{\partial E}{\partial c} = 2\sum_{j=0}^{n}\left(c\exp(\lambda x_j) - y_j\right)\exp(\lambda x_j) = 0$$

$$\frac{\partial E}{\partial \lambda} = 2\sum_{j=0}^{n}\left(c\exp(\lambda x_j) - y_j\right)cx_j\exp(\lambda x_j) = 0$$

(c) You have found two coupled, nonlinear equations. We can find an approximate solution with Newton-Raphson iteration. One necessary ingredient for Newton-Raphson iteration is the Jacobian matrix

$$J = \begin{bmatrix} \frac{\partial^2 E}{\partial c^2} & \frac{\partial^2 E}{\partial \lambda \partial c} \\ \frac{\partial^2 E}{\partial c \partial \lambda} & \frac{\partial^2 E}{\partial \lambda^2} \end{bmatrix}$$

compute the elements of this matrix.

$$J = \begin{bmatrix} 2\sum_{j=0}^{n}\exp(2\lambda x_j) & 2\sum_{j=0}^{n}\left(2c\exp(\lambda x_j) - y_j\right)x_j\exp(\lambda x_j) \\ 2\sum_{j=0}^{n}\left(2c\exp(\lambda x_j) - y_j\right)x_j\exp(\lambda x_j) & 2\sum_{j=0}^{n}\left(2c\exp(\lambda x_j) - y_j\right)cx_j^2\exp(\lambda x_j) \end{bmatrix}$$

(d) The last ingredient you need to implement the least-squares fit to approximately exponential data is an initial guess for c and λ. Find a way to set reasonable initial values for both that is based on the input data and is easily and quickly computed.

There are many ways to do this. One is to pick the first and last data point and ignore the other data. This leads to

$$ce^{\lambda x_0} = y_0$$
$$ce^{\lambda x_n} = y_n$$

with solution

$$\lambda = \frac{\ln y_0 - \ln y_n}{x_0 - x_n}$$
$$c = y_0 e^{-\lambda x_0}$$

I am curious to see what you came up with!