

Nonlinear Method for Least-Squared Curves

Suppose we have a data $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$ and we want to find the least square curve $y = f(x) = Ce^{Ax}$ for the data.

We minimize root mean square error $E_2(f) = \left[\frac{1}{N} \sum_{k=1}^N (f(x_k) - y_k)^2 \right]^{\frac{1}{2}}$

So, we have to minimize

$$E(f) = \sum_{k=1}^N (f(x_k) - y_k)^2$$

We minimize this.
Call it E(f).

$$E(f) = \sum_{k=1}^N (Ce^{Ax_k} - y_k)^2 \leftarrow (*)$$

We have to find A and C such that E(f) is a minimum.

For critical points, we need to set $\frac{\partial E}{\partial A} = 0$ and $\frac{\partial E}{\partial C} = 0$

$$\frac{\partial E}{\partial A} = 0 \quad (*) \Rightarrow \quad 2 \sum_{k=1}^N (Ce^{Ax_k} - y_k) \cdot (Ce^{Ax_k})(x_k) = 0$$

$$\Rightarrow \sum_{k=1}^N C^2 x_k e^{2Ax_k} - \sum_{k=1}^N C x_k y_k e^{Ax_k} = 0 \leftarrow (1)$$

$$\frac{\partial E}{\partial C} = 0 \quad (*) \Rightarrow \quad 2 \sum_{k=1}^N (Ce^{Ax_k} - y_k) \cdot (e^{Ax_k}) = 0$$

$$\Rightarrow \sum_{k=1}^N C e^{2Ax_k} - \sum_{k=1}^N y_k e^{Ax_k} = 0 \leftarrow (2)$$

(*) take the partial
derivative with
respect to
A
C

In order to find the critical points, we need to solve system of eqs (1) & (2) which is a nonlinear system.

We have seen in ch2, that solving nonlinear equations different iterative methods are used & we need to have good initial guess. We have seen one method for solving nonlinear systems in Section 3.7. There are other numerical methods to solve nonlinear systems, but they have also had problems with convergence.

So, it is not a good idea to solve the nonlinear system. **Two approaches are used to find the least squares curve $y = f(x) = Ce^{Ax}$ (& few other curves) first one** is that we transform to new variable (x_k, y_k) & find least squares line $y = Ax + B$ & then the final answer is written terms of original variables (x_k, y_k) . **The other** approach is to minimize the function $E(f)$ by using built in functions. Many software packages have a built-in minimization subroutine for functions of several variables that can be used.

Consider the data

Find the least squares curve $y = f(x) = Ce^{Ax}$ by nonlinear method using Matlab. Also calculate the root mean square error.

We have to minimize $E(f) = \sum_{k=1}^5 (Ce^{Ax_k} - y_k)^2$
 $E(f) = (Ce^0 - 1.3)^2 + (Ce^A - 2.5)^2 + (Ce^{2A} - 3.7)^2 + (Ce^{3A} - 4.9)^2 + (Ce^{4A} - 7.3)^2$

function $V = E(U)$ $\rightarrow U$ is a vector

$A = U(1);$

$C = U(2);$

$V = \text{zeros}(1, 2)$

$V = (C - 1.3) \wedge 2 + (C * \exp(A) - 2.5) \wedge 2 + (C * \exp(2 * A) - 3.7) \wedge 2$
 $+ (C * \exp(3 * A) - 4.9) \wedge 2 + (C * \exp(4 * A) - 7.3) \wedge 2;$

$\gg f_{\min\text{search}}('E', \overset{\text{initial guess}}{\underbrace{[1 \ 1]}})$
 $\text{ans} = \underbrace{0.37601}_A \quad 1.62439 \downarrow C$

(Depending on the version of Matlab/octave `fminsearch` or `fminunc` will work)

$\gg \text{fminsearch}('E', [0 \ 0])$ ^{also used} $[0 \ 1]$
 $\text{ans} = 0.3760 \quad 1.62439$

The least squares curve is $y = f(x) = Ce^{Ax} = 1.62439e^{0.37601x}$

The root mean square error is

$$\begin{aligned} E_2(f) &= \left[\frac{1}{N} \sum_{k=1}^N (f(x_k) - y_k)^2 \right]^{\frac{1}{2}} = \left[\frac{1}{5} \sum_{k=1}^5 (1.62439e^{0.37601x_k} - y_k)^2 \right]^{\frac{1}{2}} \\ &= \left[\frac{1}{5} (0.10527 + 0.01797 + 0.06457 + 0.014112 + 0.0000932) \right]^{\frac{1}{2}} \\ &= 0.201005 \end{aligned}$$