Computational Science:
Computational Methods in Engineering

Nonlinear Regression Examples

https://empossible.net/academics/emp4301_5301/

Lecture Outline

- Example – Fit to a Gaussian
- MATLAB Implementation
  https://empossible.net/academics/emp4301_5301/

Slide 2

Example – Fit to a Gaussian

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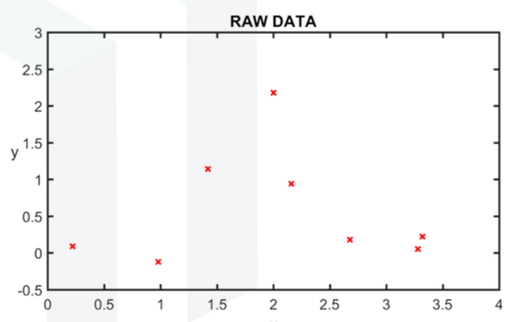
Slide 3

Example 1 – Fit to a Gaussian

Suppose it is desired to fit a set of measured data to a standard Gaussian function.

$$f(x) = A\exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right]$$




```
% MEASURED DATA
xm = [ -0.14 ; 0.22 ;  0.98 ; 1.42 ; 2.00 ; 2.16 ; 2.68 ; 3.28 ; 3.32  ];
fm = [  0.01 ; 0.09 ; -0.12 ; 1.14 ; 2.18 ; 0.94 ; 0.18 ; 0.05 ; 0.22  ];
```

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Example 1 – Fit to a Gaussian

Formulation Step 1 – Identify the unknown parameters.

$$f(x) = A\exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right]$$

In this case, there are 3 unknown parameters: A, x_0, and σ.

$$[a] = \begin{bmatrix} A \\ x_0 \\ \sigma \end{bmatrix}$$

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Example 1 – Fit to a Gaussian

Formulation Step 2 – Derive terms in $[Z]$ matrix.

$$\frac{\partial f(x)}{\partial A} \quad \frac{\partial f(x)}{\partial x_0} \quad \frac{\partial f(x)}{\partial \sigma}$$

$$[Z] = \begin{bmatrix} \frac{\partial f(x_1)}{\partial A} & \frac{\partial f(x_1)}{\partial x_0} & \frac{\partial f(x_1)}{\partial \sigma} \\ \frac{\partial f(x_2)}{\partial A} & \frac{\partial f(x_2)}{\partial x_0} & \frac{\partial f(x_2)}{\partial \sigma} \\ & \vdots & \\ \frac{\partial f(x_M)}{\partial A} & \frac{\partial f(x_M)}{\partial x_0} & \frac{\partial f(x_M)}{\partial \sigma} \end{bmatrix}$$

$$\frac{\partial f(x)}{\partial A} = \exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right] = \frac{f(x)}{A}$$

$$\frac{\partial f(x)}{\partial x_0} = A\exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right]\cdot\left\{-\frac{2}{\sigma^2}(x-x_0)\cdot(-1)\right\} = \frac{2(x-x_0)}{\sigma^2}f(x)$$

$$\frac{\partial f(x)}{\partial \sigma} = A\exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right]\cdot\left\{-(x-x_0)^2\cdot\left(-\frac{2}{\sigma^3}\right)\right\} = \frac{2(x-x_0)^2}{\sigma^3}f(x)$$

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Example 1 – Fit to a Gaussian

The $[Z]$ matrix is

$$[Z]=\begin{bmatrix} \frac{f(x_1)}{A} & \frac{2(x_1-x_0)}{\sigma^2}f(x_1) & \frac{2(x_1-x_0)^2}{\sigma^3}f(x_1) \\ \frac{f(x_2)}{A} & \frac{2(x_2-x_0)}{\sigma^2}f(x_2) & \frac{2(x_2-x_0)^2}{\sigma^3}f(x_2) \\ & \vdots & \\ \frac{f(x_M)}{A} & \frac{2(x_M-x_0)}{\sigma^2}f(x_M) & \frac{2(x_M-x_0)^2}{\sigma^3}f(x_M) \end{bmatrix}$$

$$=\begin{bmatrix} \frac{1}{A}f(\mathbf{x}) & \frac{2(\mathbf{x}-x_0)}{\sigma^2}f(\mathbf{x}) & \frac{2(\mathbf{x}-x_0)^2}{\sigma^3}f(\mathbf{x}) \end{bmatrix}$$

← $[Z]$ will be calculated this way.

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Example 1 – Fit to a Gaussian

An example of a more intelligent initial guess…

$$f(x)=A\exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right]$$

$A_1 \leftarrow \max[f_i]$

Consider finding the maximum value of f_i in the measured points as the initial guess for A.

$x_{0,1} \leftarrow \text{average}[x_i]$

Consider using the average value of x_i as the initial guess for x_0.

$\sigma \leftarrow s(\max[x_i]-\min[x_i])$

The standard deviation will likely be on the same order of magnitude as the range of values of x_i. Maybe choose $s = 0.5$?

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Example 1 – Fit to a Gaussian

The main loop…

Step a – Calculate $[f_i]$

$$[f]_i = \left[f_i(x_1) \quad f_i(x_2) \quad f_i(x_3) \quad \cdots \quad f_i(x_{M-1}) \quad f_i(x_M) \right]^T$$

Here is $[f]$ over ten iterations…

0.6452	0.0393	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.9780	0.1218	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.7707	0.6366	0.0160	0.2244	0.0088	0.0234	0.0131	0.0141	0.0141	0.0141
2.0931	1.0530	0.4043	1.7341	0.7211	1.2323	1.1202	1.1358	1.1357	1.1357
2.1414	1.2289	1.5594	1.3029	2.3184	2.0714	2.1838	2.1829	2.1833	2.1833
2.0714	1.1582	1.2653	0.6630	1.2660	0.9323	0.9277	0.9363	0.9361	0.9362
1.6520	0.7047	0.1130	0.0124	0.0111	0.0042	0.0026	0.0028	0.0028	0.0028
1.0165	0.2228	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.9757	0.2018	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

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Example 1 – Fit to a Gaussian

The main loop…

Step b – Calculate error term $[d_i]$

$$[d]_i = [y] - [f]_i$$

Here is $[d]$ over ten iterations…

-0.6352	-0.0293	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100
-0.8880	-0.0318	0.0900	0.0899	0.0900	0.0900	0.0900	0.0900	0.0900	0.0900
-1.8907	-0.7566	-0.1360	-0.3444	-0.1288	-0.1434	-0.1331	-0.1341	-0.1341	-0.1341
-0.9531	0.0870	0.7357	-0.5941	0.4189	-0.0923	0.0198	0.0042	0.0043	0.0043
0.0386	0.9511	0.6206	0.8771	-0.1384	0.1086	-0.0038	-0.0029	-0.0033	-0.0033
-1.1314	-0.2182	-0.3253	0.2770	-0.3260	0.0077	0.0123	0.0037	0.0039	0.0038
-1.4720	-0.5247	0.0670	0.1676	0.1689	0.1758	0.1774	0.1772	0.1772	0.1772
-0.9665	-0.1728	0.0497	0.0500	0.0500	0.0500	0.0500	0.0500	0.0500	0.0500
-0.7557	0.0182	0.2198	0.2200	0.2200	0.2200	0.2200	0.2200	0.2200	0.2200

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Example 1 – Fit to a Gaussian

The main loop…

Step c – Build $[Z_i]$

$$\mathbf{z}_1 = \frac{1}{A} f(\mathbf{x}) \qquad \mathbf{z}_2 = \frac{2(\mathbf{x}-x_0)}{\sigma^2} f(\mathbf{x})$$

$$\mathbf{z}_3 = \frac{2(\mathbf{x}-x_0)^2}{\sigma^3} f(\mathbf{x})$$

$$\mathbf{Z}_i = [\mathbf{z}_1 \quad \mathbf{z}_2 \quad \mathbf{z}_3]$$

$$\mathbf{Z}_1 = \begin{bmatrix} 0.2960 & -0.8230 & 0.9081 \\ 0.4486 & -1.0123 & 0.9063 \\ 0.8123 & -0.9335 & 0.4257 \\ 0.9601 & -0.4880 & 0.0984 \\ 0.9823 & 0.3307 & 0.0442 \\ 0.9502 & 0.5414 & 0.1224 \\ 0.7578 & 1.0058 & 0.5297 \\ 0.4663 & 1.0265 & 0.8966 \\ 0.4476 & 1.0114 & 0.9068 \end{bmatrix} \qquad \mathbf{Z}_{10} = \begin{bmatrix} 0.0000 & -0.0000 & 0.0000 \\ 0.0000 & -0.0000 & 0.0000 \\ 0.0042 & -0.1944 & 0.4552 \\ 0.3352 & -6.9938 & 7.3115 \\ 0.6445 & 8.5245 & 5.6503 \\ 0.2763 & 6.2539 & 7.0924 \\ 0.0008 & 0.0436 & 0.1163 \\ 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 \end{bmatrix}$$

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Example 1 – Fit to a Gaussian

The main loop…

Step d – Solve for $[\Delta a]_i$

$$[\Delta a]_i = \left([Z]_i^T [Z]_i\right)^{-1} \left([Z]_i^T [d]_i\right)$$

Here is $[\Delta a]$ over ten iterations…

-0.9316	0.3327	0.7433	0.5188	0.3549	0.2022	-0.0135	0.0010	-0.0000	0.0000
0.0958	0.0823	-0.2859	0.1775	-0.0723	0.0092	-0.0006	0.0000	-0.0000	0.0000
-0.6519	-0.6268	-0.0058	-0.0881	-0.0027	-0.0172	0.0022	-0.0001	0.0000	-0.0000

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Example 1 – Fit to a Gaussian

The main loop…

Step e – Update coefficients $[a]_i$

$$[a]_{i+1} = [a]_i + [\Delta a]_i$$

Here is $[a] = [A \;\; x_0 \;\; \sigma]^T$ over ten iterations…

1.2484	1.5810	2.3244	2.8432	3.1981	3.4003	3.3868	3.3878	3.3878	3.3878
1.8647	1.9470	1.6611	1.8386	1.7663	1.7755	1.7749	1.7750	1.7750	1.7750
1.0781	0.4513	0.4454	0.3574	0.3546	0.3374	0.3396	0.3395	0.3395	0.3395

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Example 1 – Fit to a Gaussian

The main loop…

Step f – Calculate error and check for convergence

$$\varepsilon = \max\left[\left|\frac{a_{n,i+1} - a_{n,i}}{a_{n,i+1}}\right|\right]$$

Here is `err` over ten iterations…

0.7463	1.3889	0.3198	0.2465	0.1110	0.0595	0.0065	0.0003	0.0000	0.0000

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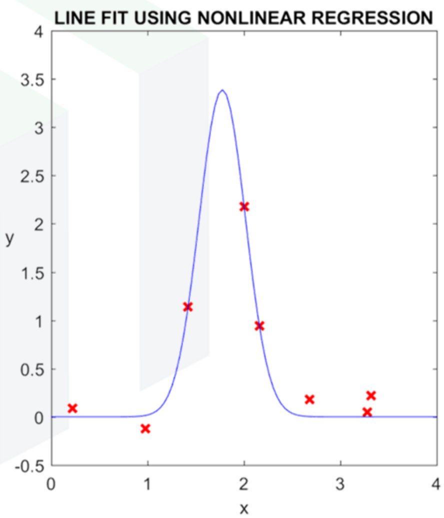
Example 1 – Fit to a Gaussian

The final answer is…

$$A = 3.3878$$
$$x_0 = 1.7750$$
$$\sigma = 0.3395$$

$$f(x) = A\exp\left[-\left(\frac{x-x_0}{\sigma}\right)^2\right] = 3.3878\exp\left[-\left(\frac{x-1.7750}{0.3395}\right)^2\right]$$



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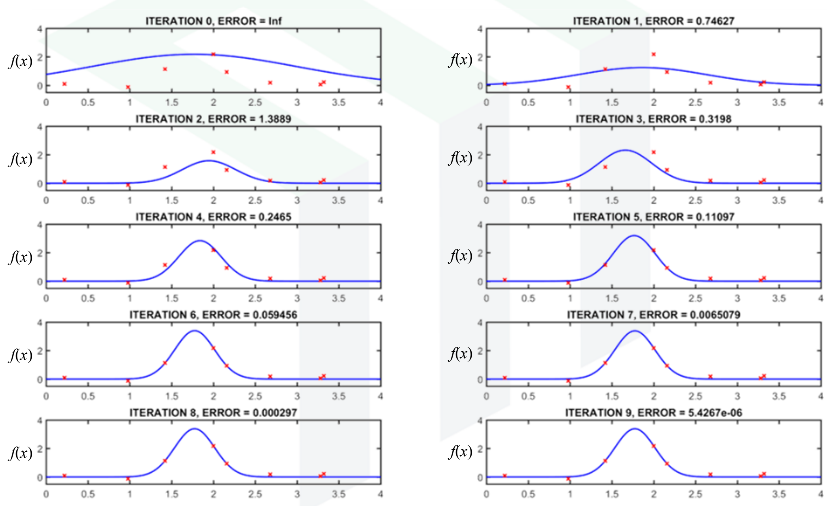
Example 1 – Fit to a Gaussian

Here are the first 10 iterations of the algorithm visualized…



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