# *Opinionated* Lessons in Statistics

*by Bill Press*

# *#20 Nonlinear Least Squares Fitting*

**Weighted Nonlinear Least Squares Fitting**
**a.k.a. $\chi^2$ Fitting**
**a.k.a. Maximum Likelihood Estimation of Parameters (MLE)**
**a.k.a. Bayesian parameter estimation**
**(with uniform prior and maybe**
**some other normality assumptions)**

these are not all exactly identical,
but they're very close!

returned by Google for image search on "least squares fitting"!

$$y_i = y(\mathbf{x}_i|\mathbf{b}) + e_i$$

measured values supposed to be a model, plus an error term

$$e_i \sim N(0, \sigma_i)$$

the errors are Normal, either independently…

$$\mathbf{e} \sim N(0, \Sigma)$$

… or else with errors correlated in some known way (e.g., multivariate Normal)

We want to find the parameters of the model **b** from the data.

Fitting is usually presented in frequentist, MLE language.
But one can equally well think of it as Bayesian:

$$
\begin{aligned}
P(\mathbf{b}|\{y_i\}) &\propto P(\{y_i\}|\mathbf{b})P(\mathbf{b}) \\
&\propto \prod_i \exp\left[-\tfrac{1}{2}\left(\frac{y_i - y(\mathbf{x}_i|\mathbf{b})}{\sigma_i}\right)^2\right] P(\mathbf{b}) \\
&\propto \exp\left[-\tfrac{1}{2}\sum_i \left(\frac{y_i - y(\mathbf{x}_i|\mathbf{b})}{\sigma_i}\right)^2\right] P(\mathbf{b}) \\
&\propto \exp[-\tfrac{1}{2}\chi^2(\mathbf{b})]P(\mathbf{b})
\end{aligned}
$$

Now the idea is: Find (somehow!) the parameter value $\mathbf{b}_0$ that minimizes $\chi^2$ .

For linear models, you can solve linear "normal equations" or, better, use Singular Value Decomposition. See NR3 section 15.4

In the general nonlinear case, you have a general minimization problem, for which there are various algorithms, none perfect.

If $P(\mathbf{b})$ = constant, those parameters are the MLE. (So it is Bayes with uniform prior.)

So MLE and Normal errors inevitably leads to $\chi^2$. "Least squares" is not an ad hoc choice, it's the choice that maximizes the posterior probability.

$$y(x|\mathbf{b}) = b_1 \exp(-b_2 x) + b_3 \exp\left(-\frac{1}{2}\frac{(x-b_4)^2}{b_5^2}\right)$$

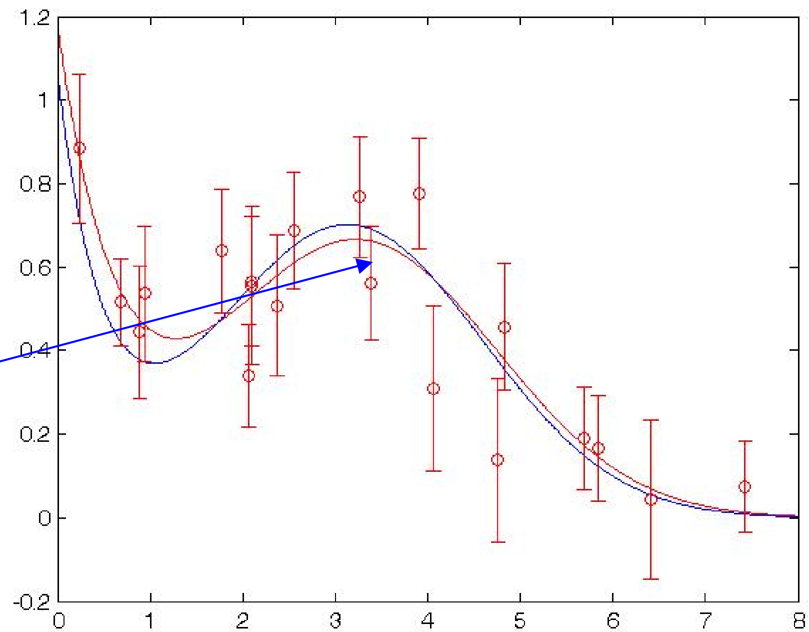
$$\chi^2 = \sum_i \left(\frac{y_i - y(x_i|\mathbf{b})}{\sigma_i}\right)^2$$

Nonlinear fits are often easy in MATLAB (or other high-level languages) **if** you can make a reasonable starting guess for the parameters.

```
ymodel = @(x,b) b(1)*exp(-b(2)*x)+b(3)*exp(-(1/2)*((x-b(4))/b(5)).^2)
chisqfun = @(b) sum(((ymodel(x,b)-y)./sig).^2)
```

```
bguess = [1 2 .5 3 1.5]
bfit = fminsearch(chisqfun,bguess)
xfit = (0:0.01:8);
yfit = ymodel(xfit,bfit);
```

*bfit = 1.1235    1.5210    0.6582*
*3.2654    1.4832*




Later, we'll suppose that what we really care about is the area of the bump, and that the other parameters are "nuisance parameters".

How accurately are the fitted parameters determined?
As Bayesians, we would **instead** say, what is their posterior distribution?

Taylor series of any function of a vector:

$$-\tfrac{1}{2}\chi^2(\mathbf{b}) \approx -\tfrac{1}{2}\chi^2_{\min} - \tfrac{1}{2}(\mathbf{b}-\mathbf{b}_0)^T \left[\frac{1}{2}\frac{\partial^2\chi^2}{\partial\mathbf{b}\partial\mathbf{b}}\right](\mathbf{b}-\mathbf{b}_0)$$

While exploring the $\chi^2$ surface to find its minimum, we can also calculate the Hessian (2nd derivative) matrix at the minimum.

Then

$$P(\mathbf{b}|\{y_i\}) \propto \exp\left[-\tfrac{1}{2}(\mathbf{b}-\mathbf{b}_0)^T \mathbf{\Sigma}_b^{-1}(\mathbf{b}-\mathbf{b}_0)\right]$$

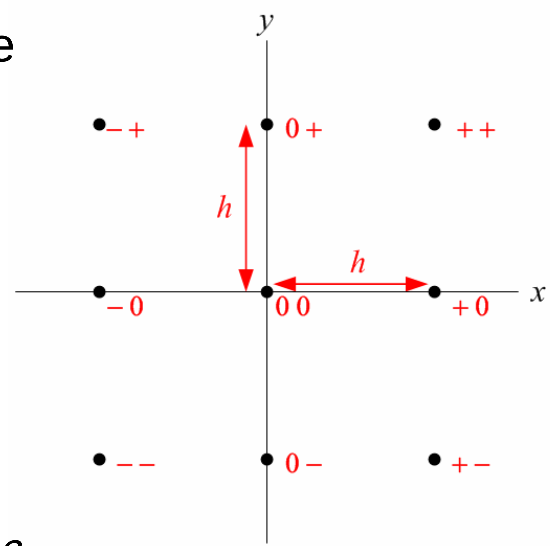
with

$$\mathbf{\Sigma}_b = \left[\frac{1}{2}\frac{\partial^2\chi^2}{\partial\mathbf{b}\partial\mathbf{b}}\right]^{-1}$$

covariance (or “standard error”) matrix of the fitted parameters

Notice that if (i) the Taylor series converges rapidly and (ii) the prior is uniform, then the posterior distribution of the $\mathbf{b}$’s is multivariate Normal, a very useful CLT-ish result!

Numerical calculation of the Hessian by finite difference




$$\frac{\partial^2 f}{\partial x \partial y} \approx \frac{1}{2h}\left(\frac{f_{++} - f_{-+}}{2h} - \frac{f_{+-} - f_{--}}{2h}\right)$$
$$= \frac{1}{4h^2}\left(f_{++} + f_{--} - f_{+-} - f_{-+}\right)$$

*bfit = 1.1235 1.5210 0.6582 3.2654 1.4832*

```
chisqfun = @(b) sum(((ymodel(x,b)-y)./sig).^2)
h = 0.1;
unit = @(i) (1:5) == i;
hess = zeros(5,5);
for i=1:5, for j=1:5,
        bpp = bfit + h*(unit(i)+unit(j));
        bmm = bfit + h*(-unit(i)-unit(j));
        bpm = bfit + h*(unit(i)-unit(j));
        bmp = bfit + h*(-unit(i)+unit(j));
        hess(i,j) = (chisqfun(bpp)+chisqfun(bmm)…
          -chisqfun(bpm)-chisqfun(bmp))./(2*h)^2;
    end
end
covar = inv(0.5*hess)
```

This also works for the diagonal components. Can you see how?

For our example, $y(x|\mathbf{b}) = b_1 \exp(-b_2 x) + b_3 \exp\left(-\frac{1}{2}\frac{(x-b_4)^2}{b_5^2}\right)$

```
bfit =
    1.1235    1.5210    0.6582    3.2654    1.4832
hess =
   64.3290  -38.3070   47.9973  -29.0683   46.0495
  -38.3070   31.8759  -67.3453   29.7140  -40.5978
   47.9973  -67.3453  723.8271  -47.5666  154.9772
  -29.0683   29.7140  -47.5666   68.6956  -18.0945
   46.0495  -40.5978  154.9772  -18.0945   89.2739
covar =
    0.1349    0.2224    0.0068   -0.0309    0.0135
    0.2224    0.6918    0.0052   -0.1598    0.1585
    0.0068    0.0052    0.0049    0.0016   -0.0094
   -0.0309   -0.1598    0.0016    0.0746   -0.0444
    0.0135    0.1585   -0.0094   -0.0444    0.0948
```

This is the covariance structure of all the parameters, and indeed (at least in CLT normal approximation) gives their entire joint distribution!

The standard errors on each parameter separately are $\sigma_i = \sqrt{C_{ii}}$

```
sigs =
    0.3672    0.8317    0.0700    0.2731    0.3079
```

But why is this, and what about two or more parameters at a time (e.g. $b_3$ and $b_5$)?