MLM and LSF Fitting

Maximum Likelihood Method (MLM)

The maximum likelihood method determines a parameter λ that maximizes (or respectively minimizes) a function of given measurements. This method revolves around the likelihood function, which can be formalized in one of two ways (depending on what the scenario calls for):

$$L = \prod_{i=1}^{n} f\,(x_i,\,\lambda) \text{ or } \ln(L) = \prod_{i=1}^{n} \ln\,(f(x_i,\,\lambda))$$

To solve for the maximum/minimum λ, we simply use the first derivative test: $\frac{\partial L}{\partial \lambda}\,|_{\lambda=\lambda^*} = 0$.

In[181]:=

```
L[f_, xi_] := Product[f[x, λ], {x, xi}];
```

In[177]:=

```
Param[L_] := Solve[∂λ L == 0, λ];
```

Example

In[182]:=

```
f[x_, λ_] := 1 + λ x;
L[f, {1, 2, 3}]
Param[L[f, {1, 2, 3}]]
```

Out[183]=

$(1+\lambda)\ (1+2\,\lambda)\ (1+3\,\lambda)$

Out[184]=

$\left\{\left\{\lambda \to \frac{1}{18}\left(-11-\sqrt{13}\right)\right\},\left\{\lambda \to \frac{1}{18}\left(-11+\sqrt{13}\right)\right\}\right\}$

Least Squares Fitting (LSF)

Least squares fitting is a method for finding a linear fit from a given set of data. This fit depends on summations of the x data, y data, x data squared, and x times y data. On top of that, if each measurement has a different uncertainty, then that can be taken into account as well.

The form of the linear fit for the data is: $y = \alpha + \beta\,x$, where:

$$\alpha = \frac{\sum_{i=1}^{n} \frac{y_i}{\sigma_i^2} \sum_{i=1}^{n} \frac{x_i^2}{\sigma_i^2} - \sum_{i=1}^{n} \frac{x_i\, y_i}{\sigma_i^2} \sum_{i=1}^{n} \frac{x_i}{\sigma_i^2}}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2} \sum_{i=1}^{n} \frac{x_i^2}{\sigma_i^2} - \left(\sum_{i=1}^{n} \frac{x_i}{\sigma_i^2}\right)^2}$$

$$\beta = \frac{\sum_{i=1}^{n} \frac{1}{\sigma_i^2} \sum_{i=1}^{n} \frac{x_i\, y_i}{\sigma_i^2} - \sum_{i=1}^{n} \frac{x_i}{\sigma_i^2} \sum_{i=1}^{n} \frac{y_i}{\sigma_i^2}}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2} \sum_{i=1}^{n} \frac{x_i^2}{\sigma_i^2} - \left(\sum_{i=1}^{n} \frac{x_i}{\sigma_i^2}\right)^2}$$

If all the uncertainties, σ_i, are the same, then the forms for these simplify down to:

$$\alpha = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i\, y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\beta = \frac{n \sum_{i=1}^{n} x_i\, y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

In[161]:=

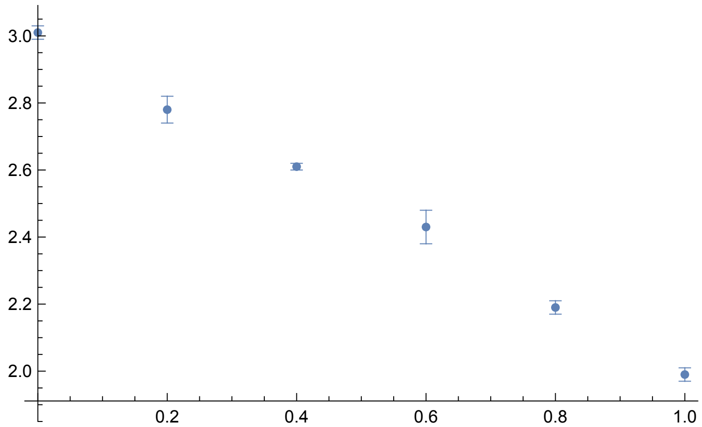
```
Δ[xi_, σi_] := Sum[1 / s^2, {s, σi}] × Sum[x[[i]]^2 / s[[i]]^2, {i, 1, Length[s]}] -
    (Sum[x[[i]] / s[[i]]^2, {i, 1, Length[s]}])^2;
α[xi_, yi_, σi_] := 1/Δ[xi, σi]
    (Sum[y[[i]] / s[[i]]^2, {i, 1, Length[s]}] × Sum[x[[i]]^2 / s[[i]]^2, {i, 1, Length[s]}] -
      Sum[x[[i]] × y[[i]] / s[[i]]^2, {i, 1, Length[s]}] × Sum[x[[i]] / s[[i]]^2, {i, 1, Length[s]}]);
β[xi_, yi_, σi_] :=
   1/Δ[xi, σi] (Sum[1 / s^2, {s, σi}] × Sum[x[[i]] × y[[i]] / s[[i]]^2, {i, 1, Length[s]}] -
      Sum[x[[i]] / s[[i]]^2, {i, 1, Length[s]}] × Sum[y[[i]] / s[[i]]^2, {i, 1, Length[s]}]);
```

Example

In[136]:=

```
x = {0, 0.2, 0.4, 0.6, 0.8, 1};
y = {3.01, 2.78, 2.61, 2.43, 2.19, 1.99};
s = {0.02, 0.04, 0.01, 0.05, 0.02, 0.02};
ListPlot[Table[{x⟦n⟧, Around[y⟦n⟧, s⟦n⟧]}, {n, 1, 6}]]
```

Out[139]=



In[160]:=

```
a = α[x, y, s]
```

Out[160]=

```
3.0146
```

In[164]:=

```
b = β[x, y, s]
```

Out[164]=

```
-1.0221
```

In[169]:=

```
f[x_] := a + b x;
p1 = ListPlot[Table[{x⟦n⟧, Around[y⟦n⟧, s⟦n⟧]}, {n, 1, 6}]];
p2 = Plot[f[x], {x, 0, 1}, PlotStyle → Red];
Show[p1, p2]
```

Out[172]=