Least-Squares Fitting

Introduction

It is often assumed that at constant density the thermal conductivity of a mineral is inversely proportional to the temperature:

$$k = k_0 \left(\frac{T_0}{T}\right)^a \quad (1)$$

where $k(T)$ is the thermal conductivity at any given temperature T; k_0 is a known value of the thermal conductivity at temperature T_0 and a = 1.

Imagine that, in order to test this hypothesis (i.e. that a = 1), you perform a series of experiments to determine the thermal conductivity of periclase as a function of increasing temperature, keeping the density fixed. The error in the temperature is assumed to be negligible, but that in the thermal conductivity measurements are not and all have different magnitudes. You want to use weighted least-squares fitting to fit your data and calculate the best value for a and its associated error.

Since the equation is non-linear, we first need to reformulate it:

$$\ln(k) = \ln(k_0) + a \ln\left(\frac{T_0}{T}\right) \quad (2)$$

Thus a plot of $\ln(k)$ against $\ln(T_0/T)$ should yield a straight line with a gradient a. Since you are now plotting $\ln(k)$ instead of $k(T)$ you will need to use the error in $\ln(k)$ in your fit rather than that in $k \Rightarrow \sigma_{\ln(k)} = \sigma_k/k$.

Use k_0 = 52.3 $Wm^{-1}K^{-1}$ at T_0 = 300 K.

Data File

The values have been stored in a file called `data`, which is available here:

`/nfs/ugrad-library/SOEE2250/practical_3`

Use you favorite text editor to view the contents of the file. The first column lists T values (in K), the second column lists k values (in $Wm^{-1}K^{-1}$) and the third column lists σ_k values (in $Wm^{-1}K^{-1}$).

Your Task

Your task today is to write a short MATLAB function to perform weighted, linear least-squares fitting of any set of x, y and σ_y values. The x, y and σ_y values should not be read in from a file, but passed to the function at the command line. Upon completion, the function should plot y against x (with y error bars) and the calculated fit on the same figure.

More Details

To read in the values from the file use `importdata`:

```
values = importdata('data')
```

Following this, you can load them into individual column vectors:

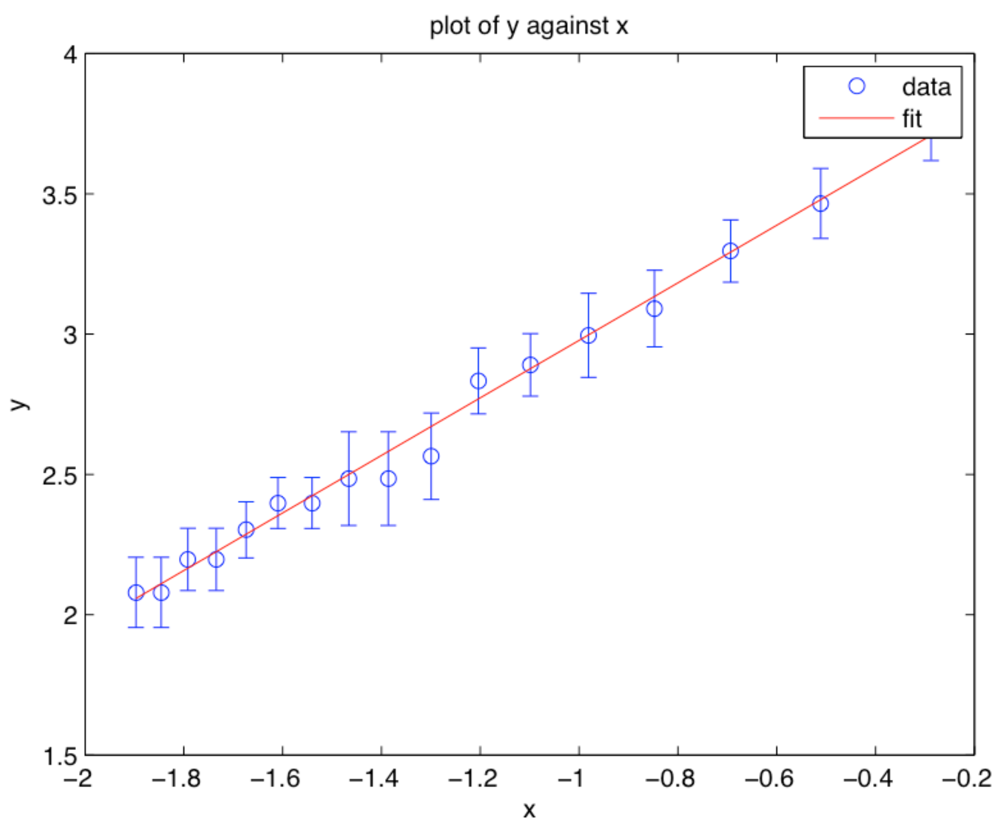
```
t = values(:,1);
k = values(:,2);
sigk = values(:,3);
```

You will need to manipulate these at the command line, in order to produce `x` $= \ln(T_0/T)$, `y` $= \ln(k)$ and `sigy` $= (\sigma_k/k)$, before passing them to the function.

Your function should be executed at the command line as:

```
[A,sigA,B,sigB] = wlsqr(x,y,sigy)
```

Use your function to calculate a and its associated error.



How does your value for a compare with the value of 1, often assumed. Is it reasonable to assume that the hypothesis is correct?

Further Work

If you have time, use your estimate of a to write a MATLAB script to plot Eq. 1 and its associated error, together with the thermal conductivity data. Read the values from the file. Plot the error in Eq. 1 as confidence bands.