MATLAB SCRIPTS

Goto the directory containing the m-scripts and data files.

The Matlab scripts that are used to fit an equation to a set of experimental data:

- `linear_fit.m` Function used to fit a straight line to set of experimental data
- `xyData1.mat`  `xyData2.mat`  `xyData3.mat` Sample data files

CURVE FITTING - LEAST SQUARES FIT TO A STRAIGHT LINE (Linear, Power, Exponential)

A large part of physics involves taking measurements and determining a functional relationship describing the measurements so that a comparison can be made with the theoretical predictions of some model. One way to do this is by plotting the measurements and finding an equation that best fits the data. There are a number of methods that can be used to fit a theoretical curve to a set of measurements, for example, the least squares fit to a straight line.

Matlab can be used to find an equation to fit the measurements when the data is plotted in a figure window and using Tools / Basic Fitting. However, we will consider an alternative way of curve fitting by using the extrinsic function `linear_fit.m` which uses a least squares method or linear regression in which there are no uncertainties in the $X$ or $Y$ data.
The function `linear_fit.m` can be used to test whether a linear, power or exponential curve fits a set of experiment data as each relationship can be expressed in the form of a straight line $Y = mX + b$ where $X$ and $Y$ are the variables and the constants are the slope $m$ and intercept $b$.

1. **Linear relationship**

   $y = a_1 + a_2 x$
   
   $Y \equiv y \quad X \equiv x \quad b \equiv a_1 \quad m \equiv a_2$

2. **Power relationship**

   $y = a_1 x^{a_2} \Rightarrow \log_{10}(y) = \log_{10}(a_1) + a_2 \log_{10}(x)$
   
   $Y \equiv \log_{10}(y) \quad X \equiv \log_{10}(x) \quad b \equiv \log_{10}(a_1) \quad m \equiv a_2$

3. **Exponential relationship**

   $y = a_1 e^{a_2 x} \Rightarrow \log_e(y) = \log_e(a_1) + a_2 x$
   
   $Y \equiv \log_e(y) \quad X \equiv x \quad b \equiv \log_e(a_1) \quad m \equiv a_2$

The $(x,y)$ data is enter into the $n \times 2$ array, where $n$ is the number of data points, for example, `xyData`. The type of fit is selected by a variable called `flag` (1, 2 or 3). The $X$-range for the graph is determined by the values of the variables `xmin` and `xmax`. The function returns values for the coefficients $a_1$ and $a_2$ and the uncertainties in these quantities $E_{a_1}$ and $E_{a_2}$ and the correlation coefficient $r$, as shown in Fig. 1.

The uncertainties of the slope and intercept give an indication of the precision of the regression. Measurements are never perfect. In repeated measurements, there is usually some variation. To interpret the meaning of the uncertainties, consider a large set of measurements were made and in each case estimates were found for the slope and intercept. You would then expect that 68% the estimates for the slope would be in the range $(m \pm E_m)$ and 68% of the intercepts in the range $(b \pm E_b)$. Hence, the smaller the uncertainties the more consistent are the repeated measurements. The correlation coefficient $r$ is a measure of the how good the line of best fit is to the data. The value of $r$ can vary from -1 to +1. There is no linear correlation between the measurements $x$ and $y$ and if $r = 0$. If $r = +1$, all the data points lie perfectly on the straight line with positive slope, with $x$ and $y$ increasing together. When all the data points lie on the line with negative slope, $y$ decreases with increasing $x$, then $r = -1$.

Entering or changing the labeling of the graph is done within the m-script for `linear_fit.m` or changing the m-script so that the labeling is entered into the Command Window using the input command.
How to use the function \texttt{linear_fit} is outlined in Fig. 1.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Parameters describing the use of the function \texttt{linear_fit}.}
\end{figure}

Three examples are given to illustrate how to use the \texttt{linear_fit.m} function for measurements related to a mass-spring system.

\textbf{Example 1 – Linear relationship}

A spring was loaded by adding weights to it, causing an extension. The load $F$ was measured in newtons and the extension $e$ in mm. The hypothesis to be tested is that the load $F$ is proportional to the extension $e$

$$F = k e$$

where the constant of proportionality $k$ is known as the spring constant which is normally measured in N.m$^{-1}$. This relationship is known as Hooke’s Law. If the hypothesis is accepted, the value of the spring constant $k$ and its uncertainty can be estimated.

The measurements for the load $F$ and extension $e$ were

\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
$e$ (mm) & 0 & 20 & 55 & 78 & 98 & 130 & 154 & 173 & 205 \\
$F$ (N) & 0 & 0.50 & 1.00 & 1.50 & 2.00 & 2.50 & 3.00 & 3.50 & 4.00 \\
\hline
\end{tabular}

\begin{enumerate}
\item $y = a_1 + a_2 x$
\item $y = a_1 x^{a_2}$
\item $y = a_1 e^{a_2 x}$
\end{enumerate}

\begin{itemize}
\item [Flag = 1 or 2 or 3]
\item \[a1, a2, Ea1, Ea2, r] = linear_fit(xyData, xmin, xmax, flag)\]
\item $x_i, y_i$ data in a matrix of \(n\) rows by 2 columns
\item Column 1: $x_i$ data
\item Column 2: $y_i$ data
\item min $x$ value for plot
\item max $x$ value for plot
\end{itemize}

Step 1: Enter the data into the array \texttt{xyData1} in the Command Window

$X$ data: $e$ → \texttt{xyData1(:,1)} \hspace{1cm} Y data: $F$ → \texttt{xyData1(:,2)}

The data can be copied and pasted from MS EXCEL into Matlab. For example, create the array \texttt{xyData1 = zeros(9,2)} and view it using \texttt{Workspace / Variable Edit}. Then, copy the data from MS EXCEL and paste into the Variable Edit Window for the array \texttt{xyData1}.
Step 2: In the Command Window, type and execute the fitting function

```
[a1, a2, Ea1, Ea2, r] = linear_fit(xyData1, 0, 250, 1);
```

You can just type and execute `linear_fit(xyData1, 0, 250, 1)` in the Command Window but not all values will be passed to the Workspace.

The output of this function to the Command Window is

\[ y = m \cdot x + b \]

\[ n = 9 \]

slope \( m = 0.01957 \) \quad Em = 0.0003751

intercept \( b = 0.0147 \) \quad Eb = 0.04537

correlation \( r = 0.9987 \)

The plot of the data and the fitted function and the fit parameters are shown in Fig. 2.

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Fig. 2. Plot for the loaded spring showing the measurements, the straight line of best fit and values for the slope, intercept and correlation coefficient.

A straight line \( y = a_1 + a_2 \cdot x \) fits the data well with a correlation \( r > 0.998 \), therefore the hypothesis can be accepted and that the quantities \( a_1 \) and \( a_2 \) are meaningful. The uncertainty in a measurement should be quoted to only 1 or 2 significant figures, hence the final coefficients describing the straight fit should be written as

- Intercept \( a_1 = (0.01 \pm 0.04) \text{ N} \)
- Slope \( a_2 = (19.6 \pm 0.4) \text{ N.m}^{-1} \)

We can conclude within the uncertainties of the intercept that \( b = 0 \) and that the load, \( F \) and extension, \( e \) are proportional to each other \( F = k \cdot x \) and the slope of the straight line correspondence to the spring constant \( k \) is

\[ k = (19.6 \pm 0.4) \text{ N.m}^{-1} \]
Example 2 – Power relationship

A spring had a load added to it causing it to extend. The spring was then displacement from its equilibrium so that it vibrated up and down about its equilibrium position. The period $T$ of the oscillations was measured for different loads $m$. The period $T$ was measured in seconds and the load $m$ was measured in kilograms. The hypothesis is to be tested is that the period of oscillations $T$ is related to the load $m$ by the relationship

$$T = 2\pi \sqrt{\frac{m}{k}} \implies T = \frac{2\pi}{\sqrt{k}} m^{\frac{1}{2}}$$

where $k$ is the spring constant measured in N.m$^{-1}$. The measurements were entered into the array $xyData2$

<table>
<thead>
<tr>
<th>$m$ (kg)</th>
<th>0.020</th>
<th>0.050</th>
<th>0.100</th>
<th>0.150</th>
<th>0.200</th>
<th>0.250</th>
<th>0.300</th>
<th>0.350</th>
<th>0.400</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$ (s)</td>
<td>0.20</td>
<td>0.31</td>
<td>0.46</td>
<td>0.53</td>
<td>0.62</td>
<td>0.71</td>
<td>0.76</td>
<td>0.84</td>
<td>0.91</td>
</tr>
</tbody>
</table>

You can’t have any measurements entered as zero since the $\log_{10}(0) = -\infty$.

In the Command Window, type and execute the fitting function

$$[a1, a2, Ea1, Ea2, r] = \text{linear_fit}(xyData2, 0.01, 0.4, 2)$$

The output of this function to the Command Window is

$y = a1 \times ^{(a2)}$

$n = 9$

$a1 = 1.413 \quad Ea1 = 0.009916$

$a2 = 0.5016 \quad Ea2 = 0.007565$

correlation $r = 0.9992$

The graphical output for a power relationship is displayed in Fig. 3.
Fig. 3. Least squares straight line fit and the power fit to the data for a vibrating mass/spring system and the fitting parameters.

A straight line fits the data well with a correlation \( r > 0.999 \), therefore the hypothesis can be accepted that an appropriate model to describe the period of vibration of the spring is

\[
T = \frac{2\pi}{\sqrt{k}} m^{1/2}
\]

The coefficient describing the fit should be expressed to the correct number of significant figures

\[
a_1 = (1.41 \pm 0.01) \text{ s.kg}^{1/2} \\
a_2 = (0.50 \pm 0.01)
\]

which confirms the hypothesis that \( T \propto \sqrt{m} \) or \( T \propto m^{1/2} \).

The value of the spring constant \( k \) is determined from the coefficient \( a_1 \)

\[
a_1 = \frac{2\pi}{\sqrt{k}} \\
k = \frac{4\pi^2}{a_1^2} \\
\frac{E_k}{k} = 2 \frac{E_{a_1}}{a_1}
\]

\[
k = (19.7 \pm 0.3) \text{ N.m}^{-1}
\]

which agrees with the value of \( k \) from the data in Example 1, \( k = (19.6 \pm 0.4) \text{ N.m}^{-1} \).
Example 3 – Exponential relationship

A spring had a load added to it causing it to extend. The spring was then displacement from its equilibrium so that it vibrated up and down about its equilibrium position. The amplitude $A$ of the vibration slowly decreased. The amplitude $A$ of the vibration was measured in millimeters and the time $t$ in seconds. The hypothesis is to be tested is that the amplitude of vibration $A$ decreases exponentially with time $t$

$$A = A_0 e^{-\beta t}$$

where $\beta$ is the decay constant. The measurements were entered into the matrix $xyData3$.

<table>
<thead>
<tr>
<th>$t$ (s)</th>
<th>0</th>
<th>10</th>
<th>20</th>
<th>30</th>
<th>40</th>
<th>50</th>
<th>60</th>
<th>70</th>
<th>80</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ (mm)</td>
<td>20.0</td>
<td>12.5</td>
<td>8.0</td>
<td>5.0</td>
<td>3.5</td>
<td>2.5</td>
<td>1.5</td>
<td>1.0</td>
<td>05</td>
</tr>
</tbody>
</table>

In the Command Window, the following was entered and the fitting function was executed

$[a1, a2, Ea1, Ea2, r] = \text{linear_fit}(xyData3, 0, 80, 3)$

The output of this function to the Command Window is

$y = a1 \exp(a2 \times x)$  
$n = 9$

$a1 = 19.9$  
$a2 = -0.04396$

$E(a1) = 1.127$  
$E(a2) = 0.001189$

$\text{correlation} r = -0.9974$

The graphical output for the exponential fit is shown in a power relationship is displayed in Fig. 4.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{example3_exp_fit.png}
\caption{Least squares straight line fit and the exponential fit to the data for a vibrating mass/spring system and the fitting parameters.}
\end{figure}
A straight line fits the data well with a correlation $r > 0.997$, therefore the hypothesis can be accepted that an appropriate model to describe the decay in the amplitude is of the form

$$A = A_0 e^{-\beta t}$$

The initial amplitude $A_0$ is given by the coefficient $a_1$ and the decay constant $\beta$ by the coefficient $a_2$

$$A_0 = (19.9 \pm 1.1) \text{ m}$$
$$\beta = (-0.0440 \pm 0.0012) \text{ s}^{-1}$$
Method of Least Squares or Regression Analysis

To avoid individual judgments in approximating the curves to fit a set of data in which any uncertainties are ignored, it is necessary to agree on a definition of ‘best fit’. One way to do this is that all the curves approximating a given set of experimental data, have the property that

$$\sum (y_i - f_i)^2$$

is a minimum

where \((y_i - f_i)\) is the deviation between the value of the measurements \((x_i, y_i)\) and the fitted values \(f_i = f(x_i)\). This approach of finding the curve of best fit is known as the Method of Least Squares or Regression Analysis.

A straight line fit is the simplest and most common curve fitted to a set of measurements. The equation of a straight line is

$$f(x) = y = mx + b$$

where the constants \(m\) and \(b\) are the slope or gradient of the straight line and the intercept (value of \(y\) when \(x = 0\)) respectively. If a straight line fits the data, we say that there is a linear relationship between the measurements \(x\) and \(y\) and if the intercept \(b = 0\) then \(y\) is said to be proportional to \(x\) (\(y \propto x\) or \(y = mx\)) where the slope \(m\) corresponds to the constant of proportionality.

Using the method of least squares for a set of \(n\) measurements \((x_i, y_i)\), estimates of the slope \(m\), intercept \(b\) and the uncertainties in the slope \(E_m\) and intercept \(E_b\) for the line of best fit are

slope

$$m = \frac{n \sum (x_i y_i) - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$$

intercept

$$b = \frac{1}{n} \left( \sum y_i - m \sum x_i \right)$$

standard error in slope

$$E_m = s \sqrt{\frac{n}{n \sum x_i^2 - (\sum x_i)^2}}$$

standard error in intercept

$$E_b = s \sqrt{\frac{(\sum x_i)^2}{n \sum x_i^2 - (\sum x_i)^2}}$$
where

\[
S = \sqrt{\frac{\sum y_i^2 - \frac{1}{n} \left( \sum y_i \right)^2 - m \left( \sum x_i y_i - \frac{1}{n} \sum x_i \sum y_i \right)}{(n - 2)}}
\]

correlation coefficient

\[
r = \frac{\sum x_i y_i - \frac{1}{n} \sum x_i \sum y_i}{\sqrt{\left( \sum x_i^2 - \frac{1}{n} \left( \sum x_i \right)^2 \right) \left( \sum y_i^2 - \frac{1}{n} \left( \sum y_i \right)^2 \right)}}
\]

Simply quoting the values of the slope \( m \) and intercept \( b \) is not very useful, it is always best to give measures of the ‘goodness of the fit’ - the correlation coefficient \( r \), and the uncertainties of the slope \( E_m \) and intercept \( E_b \).

Often the relationship between the \( x \) and \( y \) data is non-linear but of a form that can be easily reduced to one which is linear. Two very common relationships of this form are the power and exponential relationships

- **Power relationship**
  \[ y = a_1 x^{a_2} \]
- **Exponential relationship**
  \[ y = a_1 e^{a_2 x} \]

**Power relationship**

\[
y = a_1 x^{a_2}; \quad \log_{10} y = \log_{10} a_1 + a_2 \log_{10} x
\]

\[ Y = \log_{10} y \quad X = \log_{10} x \quad m = a_2 \quad b = \log_{10} a_1 \quad a_1 = 10^b \]

\[ Y = mX + b \]

The \( X \) and \( Y \) data is used to determine the slope \( m \) and intercept \( b \) and hence the coefficients \( a_1 \) and \( a_2 \). The uncertainty in the power is \( E_{a_2} = E_m \) and the uncertainty \( E_b \) in the intercept \( b \) is determined by

\[
E_{a_1} = \left( \frac{\partial a_1}{\partial b} \right) E_b
\]

\[
\log_{10} a_1 = b \quad \Rightarrow \quad \frac{1}{a_1} \left( \frac{\partial a_1}{\partial b} \right) = 1 \quad \Rightarrow \quad \left( \frac{\partial a_1}{\partial b} \right) = a_1 = 10^b
\]

\[ E_{a_1} = 10^b E_b \]
Exponential relationship

\[ y = a_1 e^{a_2 x} \]

\[ \log_e y = \log_e a_1 + a_2 x \]

\[ Y = \log_e y \quad X = x \quad m = a_2 \quad b = \log_e a_1 \quad a_1 = e^b \]

\[ Y = mX + b \]

The \( X \) and \( Y \) data is used to determine the slope \( m \) and intercept \( b \) and hence the coefficients \( a_1 \) and \( a_2 \). The uncertainty in the power is \( E_{a_2} = E_m \) and the uncertainty \( E_b \) in the intercept \( b \) is determined by:

\[ \log_e a_1 = b \quad \Rightarrow \quad a_1 = e^b \quad \Rightarrow \quad \left( \frac{\partial a_1}{\partial b} \right) = e^b \quad \Rightarrow \quad E_{a_1} = e^b E_b \]