DOING PHYSICS WITH MATLAB

DATA ANALYSIS

WEIGHTED FIT

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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:

weighted.m m-script used to fit a straight line to set of experimental data which calls the following functions

fitFunction.m Function used to evaluate the fitted function

partDev.m Function to evaluate partial derivatives of the fitted function

chi2test.m Function to evaluate the χ^2 value

Sample data files: data1A.mat data1B.mat data1C.mat
wData1.mat wData2.mat wData3.mat wData4.mat

CURVE FITTING

LEAST SQUARES - UNCERTAINITES IN THE DATA

In many experiments, the functional relationship between two variables x and y is investigated by measuring a set of n values of (x_i, y_i) and their uncertainty σ_{xi}, σ_{yi}. The functional relationship between x and y can be written as

(1) $$y_f = f(a_1, a_2, \ldots, a_m; x) = f(\mathbf{a}; x)$$

The goal is to find the unknown coefficients $\mathbf{a} = \{a_1, a_2, \ldots, a_m\}$ to fit the function $f(\mathbf{a}; x)$ to the set of n measurements. For a statistical analysis, it is difficult to consider simultaneously the uncertainties in both the x and y values. In this treatment, only the uncertainties σ_{yi} in the y measurements will be considered.

For the method of least squares, to find the coefficients **a**, the best estimates are those that minimizes the χ^2 value, given by equation (2)

(2) $$\chi^2 = \sum_{i=1}^{n}\left(\frac{y_i - f(\mathbf{a}; x_i)}{\sigma_{yi}}\right)^2$$

This is simply the sum of the squared deviations of the measurements from the fitted function $f(\mathbf{a}; x)$ weighted by the uncertainties σ_{yi} in the y values.

The default m-script **weighted.m** can be used to trial any one of nine different functions to fit a set of experimental data.

1. $y = a_1 x + a_2$ (linear)
2. $y = a_1 x$ (y proportional to x)
3. $y = a_1 x^2 + a_2 x + a_3$ (parabolic)
4. $y = a_1 x^2$ (parabolic)
5. $y = a_1 x^3 + a_2 x^2 + a_3 x + a^4$ (cubic)
6. $y = a_1 x^{a_2}$ (power)
7. $y = a_1 \exp(-a_2 x)$ (exponential: $x \neq 0, y \neq 0$)
8. $y = a_1[1 - \exp(-a_2 x)]$ (exponential: $y \neq 0$)
9. $y = a_1 x^4 + a_2 x^3 + a_3 x^2 + a^4 x + a_5$ (polynomial 4th order)

This m-script calls two extrinsic functions: **fitFunction** to evaluate the fitted function and **partDev** to calculate the partial derivative of the function with respect to the coefficients, $\dfrac{\partial f(\mathbf{a}, x)}{\partial a_k}$. Also there is call to the m-script **chi2test.m** to give a measure the "goodness of the fit". An iterative procedure is used based upon the method of Marquardt where the minimum of χ^2 is found by adjusting the value of the coefficients through a damping factor u.

Details are given in the following sections so that you can modify the m-script **weighted.m** to add your own functions to fit a set of measurements. Also the m-script **chi2test.m** can be run as independent program.

CHI-SQUARED DISTRIBUTION

The **chi-squared distribution** χ^2 (χ^2 is a single entity and is not equal to $\chi\times\chi$) and is very useful for testing the **goodness-of-of fit** of a theoretical equation to a set of measurements. For a set of *n* independent random variables x_i that have a Gaussian distribution with theoretical means μ_i and standard deviations σ_i, the chi-squared distribution χ^2 defined as

(3) $$\chi^2 = \sum_i^n \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2$$

χ^2 is also a random variable because it depends upon the random variables x_i and μ_i and follows the distribution

(4) $$P(x) = \frac{\left(\frac{\chi^2}{2} \right)^{\left(\frac{\nu}{2} - 1 \right)} \exp\left(-\chi^2\right)}{2\Gamma\left(\frac{\nu}{2} \right)}$$

where $\Gamma(\ )$ is the **gamma function** and ν is the number of **degrees of freedom** and is the sole parameter related to the number of independent variables in the sum used to describe the distribution. The mean of the distribution is $\mu = \nu$ and the variance is $\sigma = 2\nu$. The **reduced chi-squared** value $\chi^2{}_{reduced}$ is defined as

(5) $$\chi^2{}_{reduced} = \frac{\chi^2}{\nu}$$

This distribution can be used to test a hypothesis that a theoretical equation fits a set of measurements.

If an improbable chi-squared value is obtained, one must question the validity of the fitted equation. Basically, we have set up a hypothesis that our measurements can be described by some analytical function $f(\mathbf{a};\, x)$. We test the hypothesis by the value of χ^2. χ^2 is a measure of the total agreement between our measurements and the hypothesis. It can be assumed that the minimum value of χ^2 is distributed according to the χ^2 distribution with $\nu = (n\text{-}m)$ degrees of freedom (*n* data points and *m* coefficients in the fitting function).

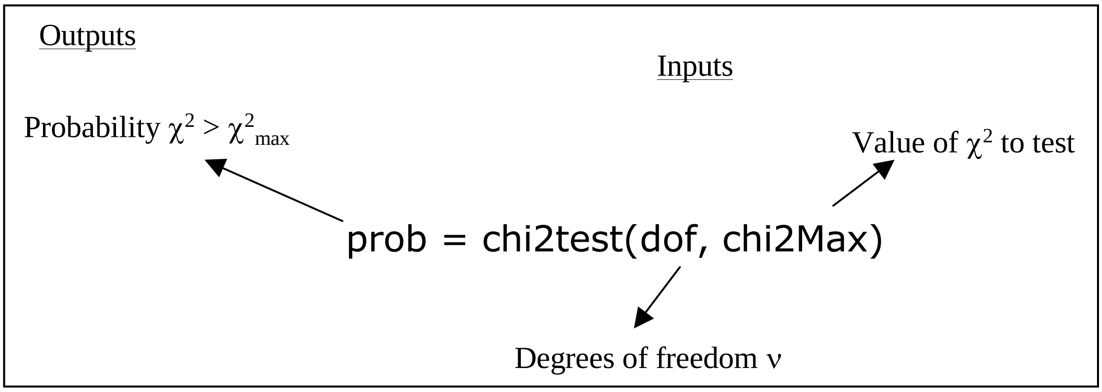
The **reduced χ^2** value$\{\chi^2{}_{\text{reduced}} = \chi^2/(n\text{-}m)\}$ is quoted as a measure of the **goodness-of-fit**

$\chi^2{}_{\text{reduced}} \sim 1$ $\Rightarrow$ hypothesis is acceptable

$\chi^2{}_{\text{reduced}} << 1$ $\Rightarrow$ the fit is much better than expected given the size of the measurement uncertainties. The hypothesis is acceptable, but the uncertainties σ_y may have been overestimated.

$\chi^2{}_{\text{reduced}} >> 1$ $\Rightarrow$ hypothesis may not be acceptable

The extrinsic function **chi2test.m** can be used to display the distribution for a given degree of freedom ν and gives the **probability** of a chi-squared value exceeding a given chi-squared value.



This function **ch12test.m** can be run independent of the m-script **weighted.m**

For example, `chi2test(6, 12)` → `prob = 6.2 %`. This would imply that the hypothesis should be **rejected** because there is only a relatively small probability that $\chi^2 = 12$ with $\nu = 6$ degrees of freedom would occur by chance. The χ^2 distribution given by equation (4) is shown in Fig. 1.

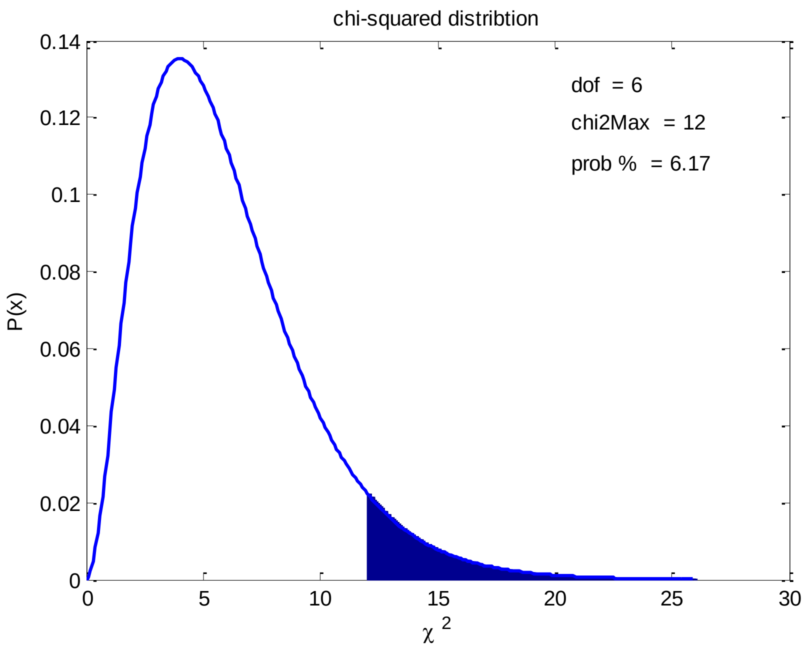


Fig. 1 Chi-squared distribution with parameters: 6 degrees of freedom, the χ^2 value = 12 and the probability = 6.17% that the χ^2 would be exceeded by chance.

A much higher value for the probability indicates it is more likely that the hypothesis is acceptable.

USING THE M-SCRIPT **weighted.m**

The measurements must be entered into a matrix called **wData** of dimension ($n \times 4$) where n is the number of data points. The analysis only uses the uncertainties σ_y associated with the y measurements. The uncertainties σ_x are only included to show any error bars when the measurements are plotted.

Measurements	Matrix
x	x = wData(:, 1)
y	y = wData(:, 2)
σ_x	dx = wData(:, 3)
σ_y	dy = wData(:, 4)

It is **necessary** to clear all variables from the Workspace using the Matlab command `clear all`.

The data (x, y, σ_x, σ_y) can be entered into the matrix `wData1` and saved to a file from the Command Window using the Matlab command **save**. To use this data at any time use the Matlab command **load** to retrieve the variable. Then let `wData = wData1` before running the m-script for **weighted.m**.

Getting started in the Command Window:

```
clear all
close all
clc
wData1 = zeros(9,4)                for 9 data points
```

Goto to the Workspace for the variable wData1 and enter data directly into the cells of the matrix displayed.

Save the data:

```
save wData1 wData1      (file name  variable)
```

Load the data:

```
load wData1
```

Assign the data to wData:

```
wData = wData1
```

Run the program fitting program:

```
weighted
```

You then will be prompted to enter:

- The minimum value for the fitted function.
- The maximum value for the fitted function.
- The title for the plot.
- The *X* axis label.
- The *Y* axis label.
- The equation to be fitted to the data by entering a number from 1 to 9
-

```
1: y = a1 * x + a2
2: y = a1 * x
3: y = a1 * x^2 + a2 * x + a3
4: y = a1 * x^2
5: y = a1 * x^3 + a2 * x^2 + a3 * x + a4
6: y = a1 * x^a2
7: y = a1 * exp(- a2 * x)            (x ≠0   y ≠ 0)
8: y = a1 * (1 - exp(-a2 * x))       (y ≠ 0)
9: y = a1 * x^4 + a2 * x^3 + a3 * x^2 + a4 * x +a5
```

After the m-script has been executed, the following information is displayed in the Command Window:

- The equation type.
- Number of measurements.
- The degrees of freedom ($n - m$) where n is the number of measurements and m is the number of coefficients (a_1, a_2, …, a_m).
- Measure s for the "good-of-fit" - χ^2 value, reduced χ^2 value, and a probability factor and a description of the fitted equation to the data.
- Coefficients in the array **a** {a_1, a_2, ... , a_m).
- The uncertainties in the coefficients in the array **sigma**.

The results are also displayed in two Figure Windows:

- The *XY* plot of the measurements and the fitted equation.
- The χ^2 distribution indicating the "good-of-fit"

Example 1 (Linear Fit `y = a1 * x + a2`)

We will consider the data concerning the extension *x* of a spring caused by a load *F*. For an ideal spring, the relationship between the applied force *F* and the extension *e* is given by **Hooke's Law**

$$F = k\,e \qquad (F \text{ directly proportional to } x)$$

where *k* is known as the spring constant. A graph of *F* vs *e* corresponds to a straight line through the origin (0,0) and the slope of the line gives the value of the spring constant *k*.

Different sets of data will be considered to illustrate the ways in which the weighted curve fitting program can be used and how we can test the hypotheses that a straight line fits the data.

wData(:,1)	wData(:,2)	wData(:,3)	wData(:,4)	wData(:,3)	wData(:,4)	wData(:,3)	wData(:,4)
x: e (mm)	y: F (N)	σ_x (mm)	σ_y (N)	σ_x (mm)	σ_y (N)	σ_x (mm)	σ_y (N)
0	0	0	0	2	0.05	0	0
20	0.50	0	0	2	0.05	1	0.03
55	1.00	0	0	2	0.05	3	0.05
78	1.50	0	0	2	0.05	4	0.07
98	2.00	0	0	2	0.05	5	0.10
130	2.50	0	0	2	0.05	6	0.13
154	3.00	0	0	2	0.05	8	0.15
173	3.50	0	0	2	0.05	9	0.17
205	4.00	0	0	2	0.05	10	0.20
data saved as		data1A		data1B		data1C	
chi-squared		0.0384772		15.3909		13.8177	
reduced chi-squared		0.00549675		2.1987		1.97395	
probability %		100		3.11		5.43	
Fit		Maybe too good ?		Acceptable		Acceptable	
slope: coefficient a_1		0.0196		0.0196		0.0195	
uncertainty in a_1		0.0051		0.0003		0.0005	
intercept: coefficient a_2		0.0147		0.0147		0.0203	
uncertainty in a_2		0.6120		0.0306		0.0346	
spring constant k (N.m^{-1})		20 ± 5		19.6 ± 0.3		19.5 ± 0.5	
intercept (N)		0.01 ± 0.6		0.01 ± 0.03		0.02 ± 0.03	

Table 1. Fitting the spring data to the linear function `y = a1 * x + a2` for three different sets of uncertainties in *x* and *y*.

For comparison, using the non-weighted linear fitting program **linear_fit.m** for the *x* and *y* data gave the following results:

Fit: $y = m\,x + b$

```
n =  9
slope m =  0.01957     Em =  0.0003751
intercept b =  0.0147   Eb =  0.04537
correlation r =  0.9987
```

$\Rightarrow$ $k = (19.57 \pm 0.04)$ N.m^{-1}

$\Rightarrow$ intercept $b = (0.01 \pm 0.04)$

By examining the results shown in Table 1, the weighted fit over-estimates the uncertainties in the coefficients when all the uncertainties in the data are zero. For the case when all the uncertainties in the data are zero, it is better to use the non-weighted linear fitting method.

Figures 2 and 3 shows the graphical output for the uncertainties given in columns 7 and 8 of Table 1.

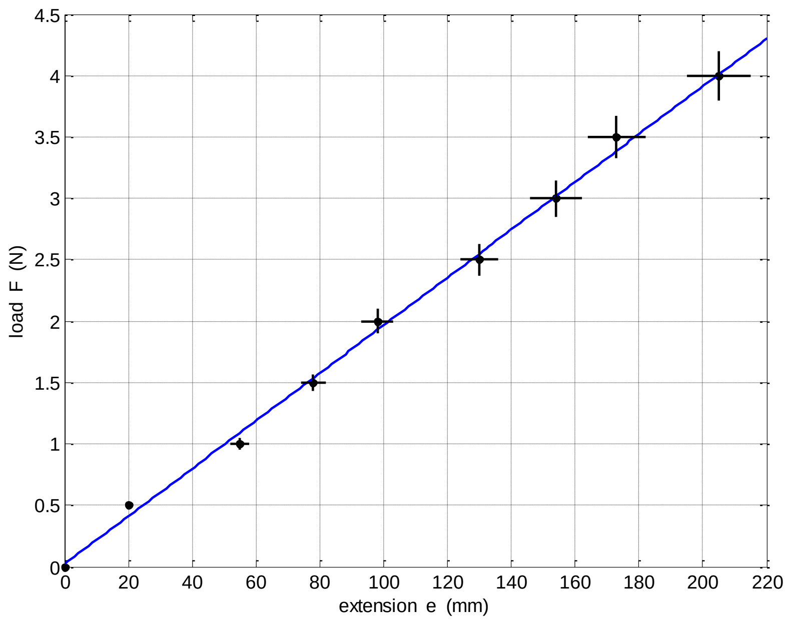


Fig. 2. Linear fit to the data `y = a1 * x + a2`. The slope of the line is (19.5 ± 0.5 N) and the intercept is (0.2 ± 0.3).

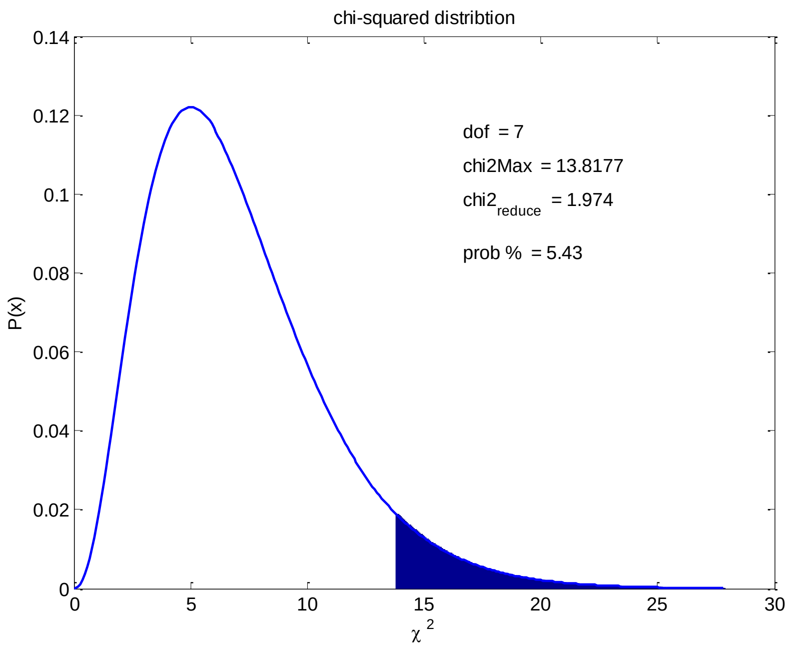


Fig. 3. Ch-squared distribution. The $\chi^2 \sim 1$, so the fit is acceptable although the probability of the weighted least squares is quite small.

Example 2 (Power relationship $y = a_1 x^{a_2}$)

The data below is used to fit a power relation $y = a_1 x^{a_2}$. Data stored as wData2.

x: m (kg)	0.02	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.50
y: T (s)	0.20	0.31	0.46	0.62	0.71	0.72	0.76	0.84	0.89	0.90
σ_x (kg)	0	0	0	0	0	0	0	0	0	0
σ_y (s)	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.10	0.10

The results of the weighted least squares fit are:

```
6: y = a1 * x^a2     power
No. measurements  =  1e+01
Degree of freedom  =  8
chi2  =  4.27503
Reduced chi2  =  0.534379
Probability =  83.1
*** Acceptable Fit   ***
Coefficients  a1, a2, ... , am
    1.3498
    0.4540
Uncertainties in coefficient
   0.0963
   0.0458
```

Hence, we can conclude the power fit $y = a_1 x^{a_2}$ is an acceptable fit to the data with coefficients: $a_1 = (1.3 \pm 0.1)$ s.kg^{-1} $a_2 = (0.45 \pm 0.05)$

The graphical outputs are shown in figures 4 and 5.

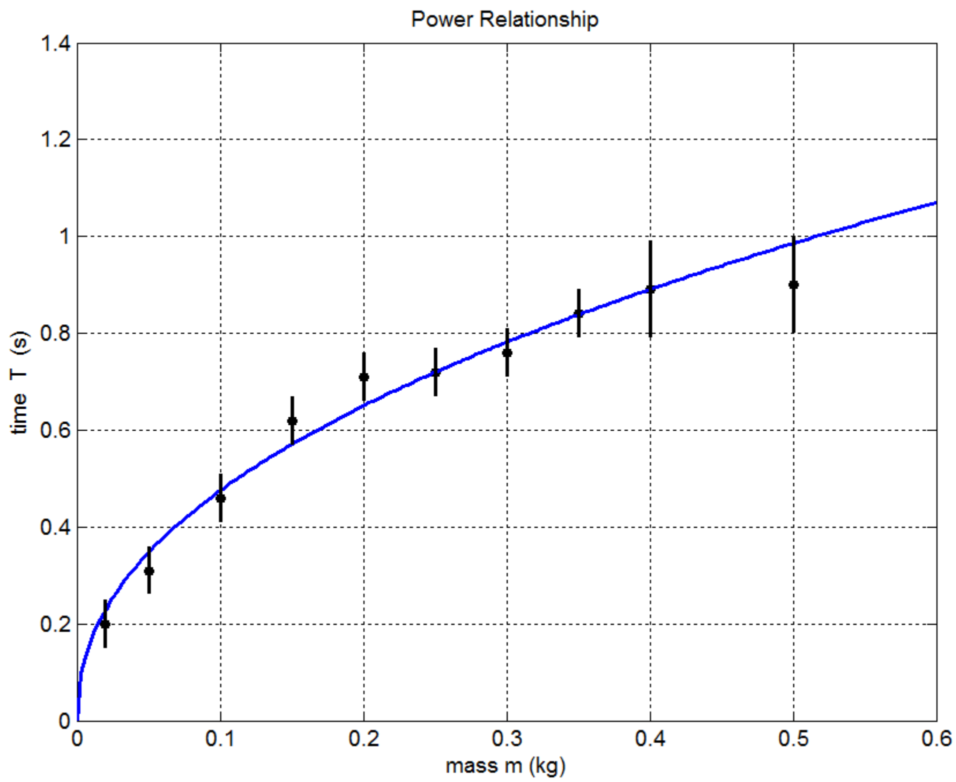


Fig. 4. Power fit $y = a_1 x^{a_2}$ to the experimental data.

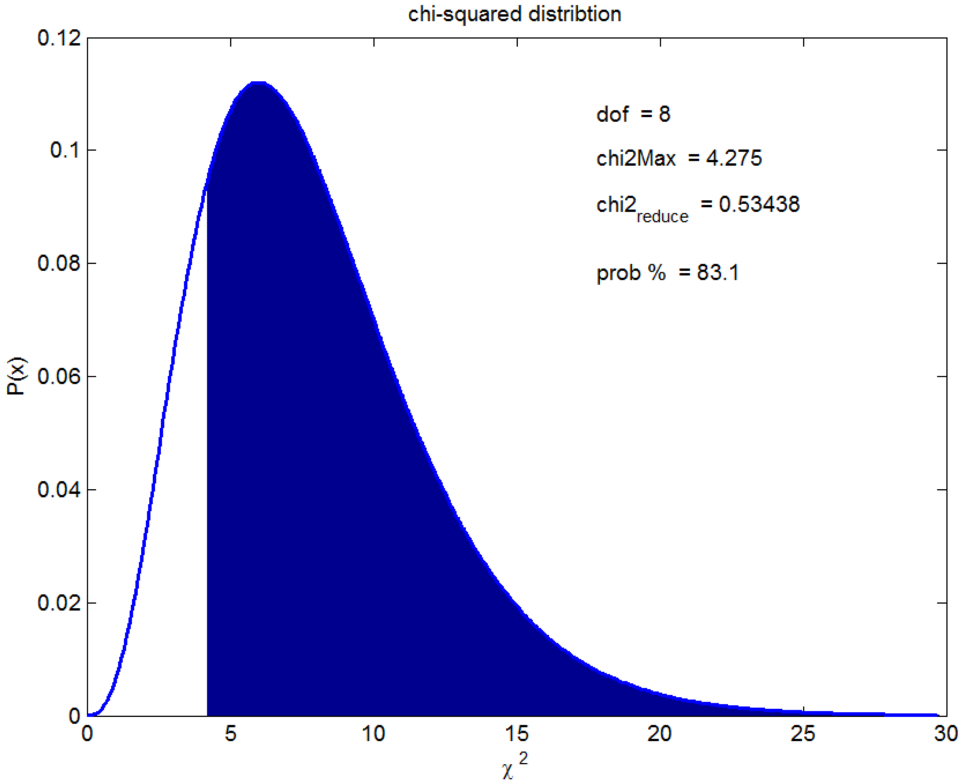


Fig.5. Plot of the chi-squared distribution showing the probability of χ^2 value being exceeded.

Example 3 (exponential decay $y = a_1 e^{-a_2 x}$)

The exponential relation $y = a_1 e^{-a_2 x}$ is used to fit to the experimental data saved as wData3.

x: t (s)	0	10	20	30	40	50	60	70	80
y: A (counts)	20	12.5	8.0	5.0	3.5	2.5	1.5	1.0	0.5
σ_x (s)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
σ_y (counts)	1.0	1.0	1.0	0.5	0.5	0.5	0.5	0.5	0.5

The results of the weighted least squares fit are:

```
7: y = a1 * exp(- a2 * x)     exponential decay
No. measurements  =  9
Degree of freedom  =  7
chi2  =  1.06625
Reduced chi2  =  0.152321
Probability =  99.3
  ? Fit may be too good ?

Coefficients  a1, a2, ... , am
  20.0000
   0.0444

Uncertainties in coefficient
   0.8857
   0.0023
```

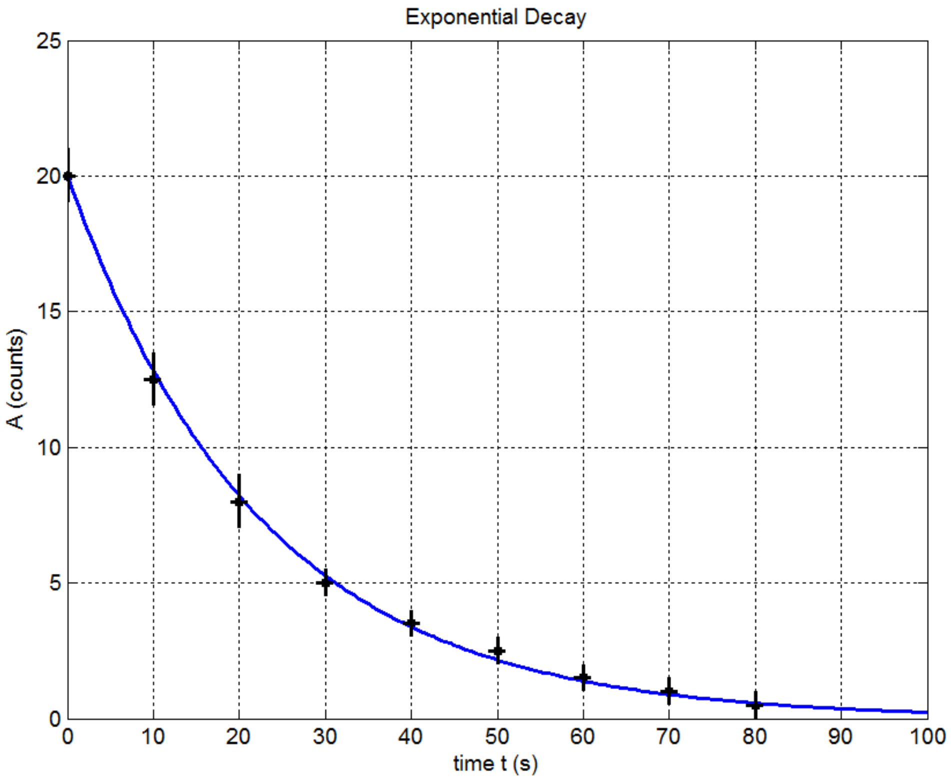


Fig. 6. Plot of data and exponential decay fit for data in Example 3.

Example 4 Interpolation

The **weighted-fit** m-script can be used for **interpolation**. For example, the viscosity η of water is a function of temperature *T* and tables give the viscosity at only fixed temperatures. By fitting a polynomial to the data, one can estimate the viscosity at a temperature between the fixed values.

x: *T* (°C)	0	10	20	30	40	50	60	80	100
y: η (mPa.s)	1.783	1.302	1.002	0.800	0.651	0.548	0.469	0.354	0.281
σ_x (°C)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
σ_y (mPa.s)	0.005	0.005	0.005	0.005	0.005	0.005	0.005	0.005	0.005

Data stored as wData4. In the Command Window type `format shorte` to display the results in scientific notation

Type of fit	**3rd order polynomial (5)**	**4th order polynomial (9)**
chi-squared	168.672	13.5519
reduced chi-squared	33.7343	3.38797
probability %	0	0.866
Fit	may not be acceptable	may not be acceptable
coefficient a_1	$-(2.68 \pm 0.07)\times10^{-6}$	$(3.4 \pm 0.3)\times10^{-8}$
coefficient a_2	$(6.0 \pm 0.1)\times10^{-4}$	$-(9.5 \pm 0.5)\times10^{-6}$
coefficient a_3	$-(4.76 \pm 0.04)\times10^{-2}$	$(1.01 \pm 0.03)\times10^{-3}$
coefficient a_4	(1.756 ± 0.004)	$-(5.56 \pm 0.08)\times10^{-2}$
coefficient a_5	---	(1.778 ± 0.005)
Table: T at 20 ^{o}C	1.002	1.002
Predicted T at 20 ^{o}C	1.021	0.996
Predicted T at 24 ^{o}C	0.9200	0.9055

The 4th order polynomial has a much lower reduced χ^2 value and gives a better fit to the data than the 3rd order polynomial.

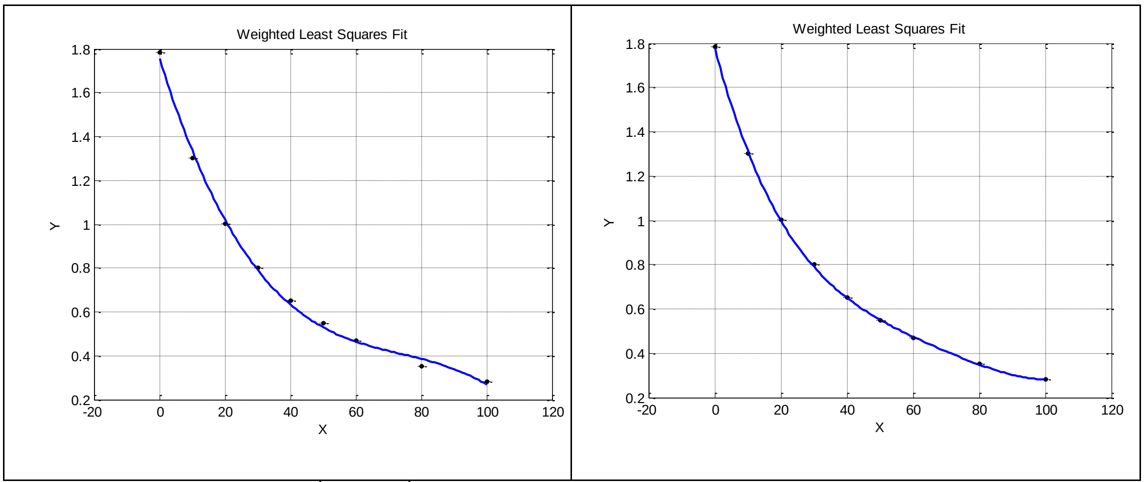


Fig. 7. 3rd and 4th order polynomial fit to viscosity data.

Step 1: Assigning the weights for finding uncertainties

Weights **w** are assigned to the uncertainties **dy** in the y measurements

w = 1/dy   if $dy_k = 0$ then $w_k = 1$ for any k

An adjustable parameter u known as the damping factor is initially set to 0.001 so that the coefficients **a** can be adjusted to minimize the χ^2 value by simply adjusting the value of u.

Step 2: Set the starting values for the coefficients **a**

To use the least squares method, we have to estimate starting values for the coefficients **a**. If the equation can be made linear in some way, then we can solve n simultaneous equations to find the unknown values of **a**. For example,

```
EqType = 5
% f = a1 * x^3 + a2 * x^2 + a3 * x + a4       cubic polynomial
xx(:,1) = x.^3;
xx(:,2) = x.^2;
xx(:,3) = x;
a = xx\y;
```

If this can't be done, a simpler method is used to set the coefficients or **a** = 1.

Step 3: Minimize χ^2 value

The counters for the number of data points n and number of coefficients m are

$i = 1, 2, \ldots, n$
$k = 1, 2, \ldots, m$
$j = 1, 2, \ldots, m$

The weighted difference matrix **D** is

$$D_i = w_i\left(y_i - f_i\right) \quad \Rightarrow \quad \mathbf{D} = w' * (y - f)$$

The value of χ^2 is then

$$\chi^2 = \mathbf{D}' * \mathbf{D}$$

where **'** gives the transpose of a matrix.

We need to adjust the coefficients by an iterative method until we find the true minimum of χ^2. For step L in the iterative procedure

$$\mathbf{a}(L+1) = \mathbf{a}(L) + \mathbf{da}$$

and our desired goal is that $\chi^2\{\mathbf{a}(L+1)\} < \chi^2\{\mathbf{a}(L)\}$.

The minimum of $\chi^2(\mathbf{a})$ is given by the condition

$$\frac{\Delta\chi^2}{\Delta a_k} = 0$$

For small variations of the coefficients, the value of $\chi^2\{\mathbf{a}(L+1)\}$ may be expanded in terms of a Taylor's series around $\chi^2\{\mathbf{a}(L)\}$ and if the expansion is truncated after the second term, we can use the approximation

$$\frac{\partial\chi^2}{\partial a_k}\Big|_{\mathbf{a}(L)} = -\sum_j^m \left\{ \left(\frac{\partial^2\chi^2}{\partial a_k\,\partial a_j}\Big|_{\mathbf{a}(L)} \right) da_j \right\}$$

This can be written in matrix form as

B = CUR * da

where $B_k = -\dfrac{1}{2}\dfrac{\partial\chi^2}{\partial a_k}\Big|_{\mathbf{a}(L)}$ and $CUR_{kj} = \dfrac{1}{2}\dfrac{\partial^2\chi^2}{\partial a_k \partial a_j}\Big|_{\mathbf{a}(L)}$

where **da** is the matrix for the increments in the coefficients, **CUR** is called the **curvature matrix** as it expresses the curvature of $\chi^2(\mathbf{a})$ with respect to **a**.

The **B** matrix, after performing the partial differentiation can be written as

$$B_k = \sum_i^n \left\{ w_i \frac{\partial f_i}{\partial a_k} w_i \left(y_i - f_i \right) \right\}$$

We need to calculate the partial derivatives of the fitted function with respect to the coefficients **a**. To make the program more general, the weighted partial derivates **pdf** are calculated numerically by the function **part_der** using the difference approximation to the derivative

$$\frac{\partial f}{\partial a_k} = \frac{f(a_k+\Delta) - f(a_k-\Delta)}{2\Delta}$$

The matrix **B** written in matrix form is

B = pdf' * D

The curvature matrix **CUR** can be approximated by

$$CUR_{kj} = \sum_{i=1}^n \left\{ \left(w_i \frac{\partial f_i}{\partial a_k} \right) \left(w_i \frac{\partial f_i}{\partial a_j} \right) \right\}$$

CUR = pdf' * pdf

The elements of the curvature matrix **CUR** may have different magnitudes. To improve the numerical stability, the elements can be scaled by the diagonal elements of the curvature matrix and the damping factor u can be added to the diagonal elements to give the modified curvature matrix **MCUR**

$$MCUR_{kj} = \frac{\left(1 + u\,\delta_{kj}\right) CUR_{kj}}{\sqrt{CUR_{kk}\,CUR_{jj}}}$$

where δ_{kj} is the Kronecker delta function ($\delta_{kj} = 1$ if $k = j$ otherwise $\delta_{kj} = 0$).

Therefore, we can approximate the incremental changes in the coefficients as

B = **MCUR** * **da**

da = (MCUR)$^{-1}$ * B = MCOV * B

where **MCOV** = **MCUR^{-1}** is the **modified covariance matrix.**

The new estimates of the coefficients and the corresponding χ^2 value can then be calculated

anew = **a** + **da**

To test the minimization χ^2 of as part of the iterative process, the following is done

If $\chi^2_{new} > \chi^2_{old}$ $\Rightarrow$ Moving away from a minimum, keep current **a** values and set u = 10 u
Repeat iteration.

If $\chi^2_{new} < \chi^2_{old}$ $\Rightarrow$ Approaching a minimum, set **a** = **anew**, *u* = *u* / 10
Repeat iteration.

$\Rightarrow$ if | $\chi^2_{new} < \chi^2_{old}$ | < 0.001
Terminate the iteration
u = 0
$\chi^2 = \chi^2_{new}$
Calculate: **CUR**, **MCUR**, **MCOV**

<u>Step 4: Output the results</u>

The square root of the diagonal elements of the covariance matrix **COV** give the **uncertainties** in the coefficients for **a**

$$sigma_k = \sqrt{COV_{kk}}$$

where

$$COV_{kj} = \frac{MCOV_{kj}}{\sqrt{CUR_{kk}\,CUR_{jj}}}$$

Basically, we have set up a hypothesis that our measurements can be described by some analytical function $f(\mathbf{a}; x)$. We need to be able to statistically test the hypothesis. This can be done using the value of χ^2. χ^2 is a measure of the total agreement between our measurements and the hypothesis. It can be assumed that the minimum value of χ^2 is distributed according to the χ^2 distribution with $(n\text{-}m)$ degrees of freedom. Often the **reduced χ^2** value{$\chi^2_{reduced} = \chi^2/(n\text{-}m)$} is quoted as a measure of the **goodness-of-fit**

$\chi^2_{reduced} \sim 1$ $\Rightarrow$ hypothesis is acceptable

$\chi^2_{reduced} << 1$ $\Rightarrow$ the fit is much better than expected given the size of the measurement uncertainties. The hypothesis is acceptable, but the uncertainties σ_y may have been overestimated.

$\chi^2_{reduced} >> 1$ $\Rightarrow$ hypothesis may not be acceptable

Also the probability of the χ^2 value being exceeded is given as another measure of the goodness-of-fit.

Finally, the measurements and fitted function are plotted together with a plot of the χ^2 distribution.

References

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