# Matrices and Eigenvectors

It might seem strange to begin a section on matrices by considering mechanics, but underlying much of matrix notation, matrix algebra and terminology is the need to describe the physical world in terms of straight lines. These straight lines may be the optimum axes for describing rotation of a rigid body or a desire to support a theory involving a relationship between two quantities such as the normal reaction force and the force of friction for a static body in contact with a surface. The former not only involves matrix notation to describe the moment of inertia of a rotating rigid body, but also involves finding eigenvalues and eigenvectors of matrices.

Matrices also appear in atomic structure calculations where approximate solutions for electronic energy levels for atoms with multiple electrons are achieved by expressing the problem in terms of matrices for which, once again, eigenvector and eigenvalues must be calculated.

Linear relationships between physical quantities are numerous, from Ohm's law relating electric current in a circuit to the Voltage, to Hooke's law relating the force exerted by a spring to the extension of the spring from the natural length of the spring. Matrix algebra and again eigenvectors for matrices are fundamental to assessing experimental data supporting these laws. An experiment performed to demonstrate the validity of either Ohm's or Hooke's law involves setting a value and measuring a response for different values. In the case of Ohm's law the value set might be the voltage applied to a copper wire and the response is measured by taking a reading for the current through the wire. Both setting the voltage and reading the current are subject to errors so although according to Ohm's law if the measured current is plotted on a graph against a range of applied voltages a straight line should result; the errors in the measurement will cause the pairs of experimental data to lie close to but not necessarily on the expected line. To verify a linear relationship between current and voltage, a line of best fit is drawn. Sixth form statistics describes a method for calculating the line of best fit in the form of a regression line without the use of matrices, however an analysis in terms of matrices motivates much of the linear algebra studied at university and used in practise in many areas of science and engineering.

All of the above examples lead to a particular type of matrix known as a symmetric matrix. A focus will therefore be placed on properties of symmetric matrices in the following discussions. Symmetric matrices have special properties which are at the basis for these discussions and solutions. The subject of symmetric matrices will now be examined using an example from linear regression.

## Statistics 1: Linear Regression and Matrices

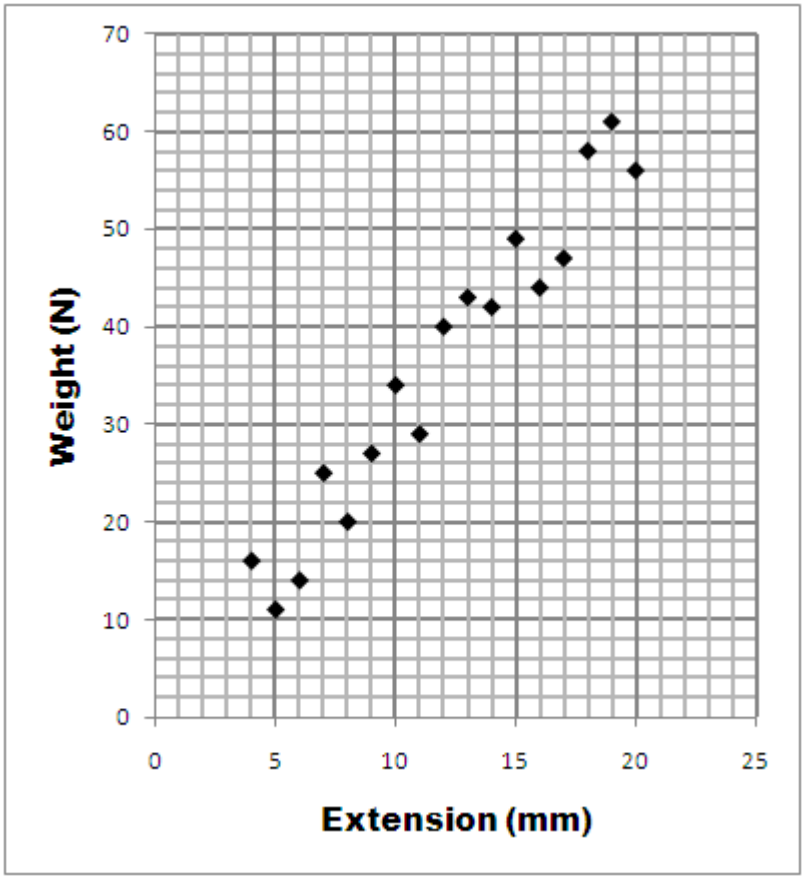
The concepts and terminology for matrices will be developed using an example from statistics. The technique for computing the line of best fit for a set of measurements provides an example where a $2 \times 2$ matrix is used to calculate the two coefficients for a straight line which approximates these two sets of data when plotted as $(x, y)$ coordinates on $2D$ Cartesian coordinate axes.

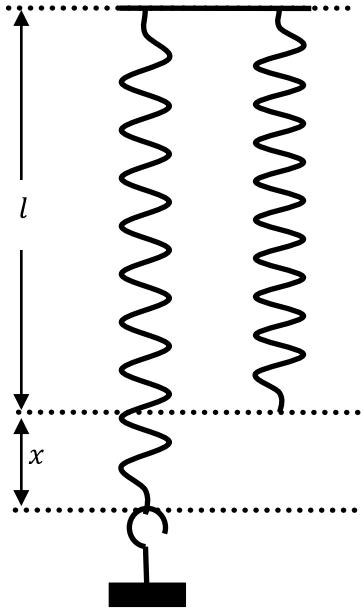
Before considering the use of matrices in linear regression, an example solved with a non-matrix approach provides an introduction to the linear regression subject and sets the context for the solution by matrices.

Example from Mechanics 3/Physics:

A class of sixth form physics students are each given a spring of equal length and same construction. Each student is provided with a weight ranging between $10\ N$ and $65\ N$. The students are asked to fix one end of the spring to a support with the spring hanging vertically below the support point, and to measure the extension of the spring from the unloaded length resulting from attaching a weight to the free end of the spring. After completion of the measurement the results for the class are tabulated and plotted as a scatter plot of weight against spring extension.

| **Extension (mm)** | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Weight (N)** | 16 | 11 | 14 | 25 | 20 | 27 | 34 | 29 | 40 | 43 | 42 | 49 | 44 | 47 | 58 | 61 | 56 |




The problem is to calculate the line of best fit and therefore verify the value of Young's modulus for the springs.

According to Hooke's law, the expected behaviour for a spring within the elastic limit is

$$T = \frac{\lambda}{l}x$$

where $\lambda\ N$ is Young's modulus, $l\ m$ is the natural length of the spring and $x\ m$ is the extension of the spring due to the tension $T\ N$.

As part of the experiment, the natural length $l = 0.1\ m$ of the spring is established before a variety of loads in the form of known weights are applied to the spring and each time a load is applied the

displacement $x\ m$ is measured from the initial position for the spring. The variation in the data points evident in the scatter plot is due to errors in determining the values for $x$ using a ruler to measure displacement, uncertainty is the true value for the weights, the uncertainty in $l$, the assumed equivalence for each of the springs used in the class experiment and potentially other factors altering the measured-value from the expected value in the experiment.

A sixth form physics student would plot the table of results on graph paper and by eye draw a line through the data points plotted on the scatter diagram. The gradient of the line would provide the information needed to calculate Young's modulus for the springs. Mathematics provides an alternative approach for determining the line of best fit based on a least squares criterion applied to the tabulated data.

## Non-Matrix Approach to Regression

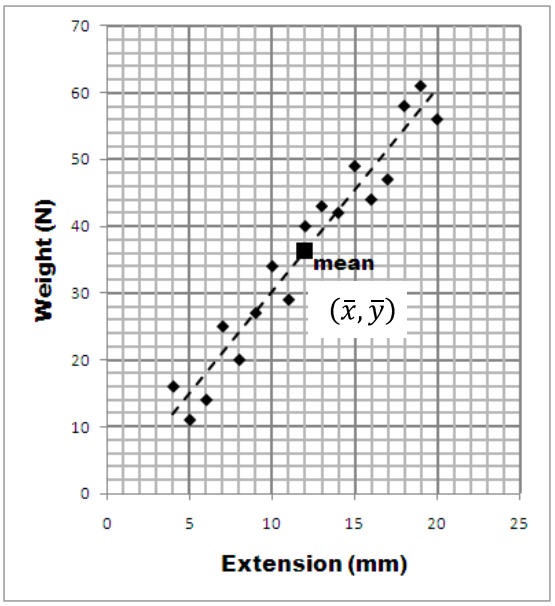
The following argument leads to a mathematical procedure for calculating the line of best fit for a set of experimental data. Consider the table of experimental results:

| **Extension (mm)** | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Weight (N)** | 16 | 11 | 14 | 25 | 20 | 27 | 34 | 29 | 40 | 43 | 42 | 49 | 44 | 47 | 58 | 61 | 56 |

The table of results is viewed as 17 pairs of coordinates $(x_i, y_i)$

| **Extension** | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ | $x_7$ | $x_8$ | $x_9$ | $x_{10}$ | $x_{11}$ | $x_{12}$ | $x_{13}$ | $x_{14}$ | $x_{15}$ | $x_{16}$ | $x_{17}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Weight** | $y_1$ | $y_2$ | $y_3$ | $y_4$ | $y_5$ | $y_6$ | $y_7$ | $y_8$ | $y_9$ | $y_{10}$ | $y_{11}$ | $y_{12}$ | $y_{13}$ | $y_{14}$ | $y_{15}$ | $y_{16}$ | $y_{17}$ |

The most common way to summarise a set of data is to offer the mean average. In this case, there are two sets of data for which two means can be calculated.




$$\bar{x} = \frac{1}{17}\sum_{i=1}^{17} x_i \text{ and } \bar{y} = \frac{1}{17}\sum_{i=1}^{17} y_i$$

If the line of best fit is defined to be of the form

$$y = a + bx$$

then the problem is that of determining the parameters $a$ and $b$ which define the intercept and gradient for the line of best fit.

It would seem reasonable to assume the line of best fit should pass through the coordinate for the mean $(\bar{x}, \bar{y})$. If it is assumed the line of best fit passes through the mean when plotted on the scatter diagram then the coordinate $(\bar{x}, \bar{y})$ must satisfy the equation $y = a + bx$ or

$$\bar{y} = a + b\bar{x}$$

$$\Rightarrow a = \bar{y} - b\bar{x} \quad \cdots \quad (1)$$

Assuming the mean coordinate lies on the line of best fit provides one equation relating the two unknowns $a$ and $b$. A second equation must be found which relates these two parameters.

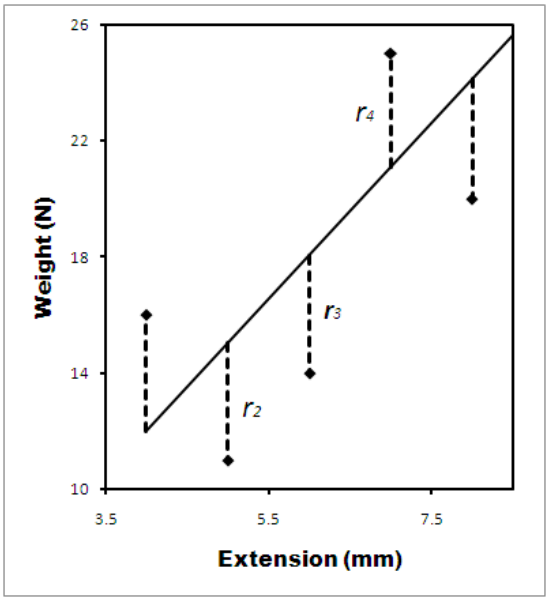
The mean for a set of values provides a number which is representative of the central value. The spread within the set of values is measured by the variance. The variance for a set of numbers such as the $y_i$ in the above table is given by

$$\sigma^2 = \frac{1}{17}\sum_{i=1}^{17}(y_i - \bar{y})^2$$

The variance is obtained by summing the squares of the differences between the values $y_i$ from the mean $\bar{y}$. Following the model for the variance, the line of best fit can be chosen so that the sum of the squares for the differences between the values $y_i$ and the corresponding point on the line of best fit is a minimum, namely,

$$\chi^2 = \sum_{i=1}^{17}(y_i - (a + bx_i))^2 \quad \cdots \quad (2)$$

If the parameters $a$ and $b$ are chosen to minimise $\chi^2$, the spread of the points in the scatter diagram from the line of best fit will be minimised.




The values $r_i = y_i - (a + bx_i)$ are called the residuals and are depicted graphically as vertical lines between the data points and the line of best fit.

$$\chi^2 = \sum_{i=1}^{17} {r_i}^2$$

The line of best fit is therefore considered to be the line which minimises the sum of the squares of the residuals.

Substituting Equation (1) into Equation (2) yields

$$\chi^2 = \sum_{i=1}^{17}(y_i - (\bar{y} - b\bar{x} + bx_i))^2$$

$$\Rightarrow \chi^2 = \sum_{i=1}^{17}((y_i - \bar{y}) - b(x_i - \bar{x}))^2$$

$$\Rightarrow \chi^2 = \sum_{i=1}^{17}((y_i - \bar{y})^2 - 2b(x_i - \bar{x})(y_i - \bar{y}) + b^2(x_i - \bar{x})^2)$$

$$\Rightarrow \chi^2 = \sum_{i=1}^{17}(y_i - \bar{y})^2 - 2b\sum_{i=1}^{17}(x_i - \bar{x})(y_i - \bar{y}) + b^2\sum_{i=1}^{17}(x_i - \bar{x})^2$$

Using the notation

$$S_{xx} = \sum_{i=1}^{17}(x_i - \bar{x})^2 \quad S_{xy} = \sum_{i=1}^{17}(x_i - \bar{x})(y_i - \bar{y}) \quad S_{yy} = \sum_{i=1}^{17}(y_i - \bar{y})^2$$

$$\Rightarrow \chi^2 = S_{yy} - 2S_{xy}b + S_{xx}b^2 \quad \cdots \quad (3)$$

Equation (3) is a quadratic in terms of $b$. The minimum for the quadratic is obtained when

$$\frac{d[\chi^2]}{db} = 0$$

$$-2S_{xy} + 2S_{xx}b = 0 \Rightarrow b = \frac{S_{xy}}{S_{xx}}$$

When calculating the quantities $S_{xx}$ and $S_{xy}$ it can be shown that

$$S_{xx} = \sum_{i=1}^{17}(x_i - \bar{x})^2 = \left[\sum_{i=1}^{17}{x_i}^2\right] - 17(\bar{x})^2$$

and

$$S_{xy} = \sum_{i=1}^{17}(x_i - \bar{x})(y_i - \bar{y}) = \left[\sum_{i=1}^{17}x_i y_i\right] - 17\bar{x}\bar{y}$$

The problem of mathematically fitting a straight line through a set of data points is therefore reduced to calculating the mean values $\bar{x}$ and $\bar{y}$, and the two summations $S_{xy}$ and $S_{xx}$ from the tabulated experimental data.

For the particular data set measured by the physics students, the line of best fit is computed from

$$\bar{x} = \frac{4+5+6+7+8+9+10+11+12+13+14+15+16+17+18+19+20}{17} = 12$$

$$\bar{y} = \frac{16+11+14+25+20+27+34+29+40+43+42+49+44+47+58+61+56}{17} = 36.24$$

$$S_{xx} = (4^2+5^2+6^2+7^2+8^2+9^2+10^2+11^2+12^2+13^2+14^2+15^2+16^2+17^2+18^2+19^2 + 20^2) - 17(12^2) = 408$$

$$S_{xy} = (16 \times 4 + 11 \times 5 + 14 \times 6 + 25 \times 7 + 20 \times 8 + 27 \times 9 + 34 \times 10 + 29 \times 11 + 40 \times 12 + 43 \times 13 + 42 \times 14 + 49 \times 15 + 44 \times 16 + 47 \times 17 + 58 \times 18 + 61 \times 19 + 56 \times 20) - 17(12)(36.24) = 1236$$

Therefore $b = \frac{S_{xy}}{S_{xx}} = \frac{1236}{408} = 3.029$ and $a = 36.24 - 3.029(12) = -0.11$. The line of best fit in a least squares sense is

$$y = -0.11 + 3.03x$$

Hooke's law ($T = \frac{\lambda}{l}x$) predicts the force in Newtons for an extension measured in metres. Since the scatter diagram plots Newtons against millimetres, the gradient for the line of best fit 3.03 is measured in $Nmm^{-1} = 1000Nm^{-1}$, therefore the value for Young's modulus for the springs is estimated by the physics students to be

$$\frac{\lambda}{0.1} = 3030 \implies \lambda = 303\ N$$

The problem of finding the line of best fit to a set of data points has so far been approached in terms of non-matrix mathematics. The same problem can and will now be investigated in terms of matrix mathematics.

## Matrix Approach to Linear Regression

If the measurements made by the physics students were without error, to calculate a straight line representative of the relationship between the force and corresponding extension would require only two measurements. Hooke's law actually assumes the line passes through the origin and therefore if Hooke's law is taken on trust then only one measurement is required. For the sake of argument it will be assumed a general equation $y = a + bx$ for a straight line is required as used in the above discussion. If two forces $y_1$ and $y_2$ with corresponding measurements for the spring extension $x_1$ and $x_2$ are used then a pair of simultaneous equations can be written as follows:

$$\begin{matrix} a + bx_1 = y_1 \\ a + bx_2 = y_2 \end{matrix} \implies \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

Assuming $\det\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix} \neq 0$ the values for $a$ and $b$ are obtained by calculating the inverse matrix for $\boldsymbol{A} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix}$, namely,

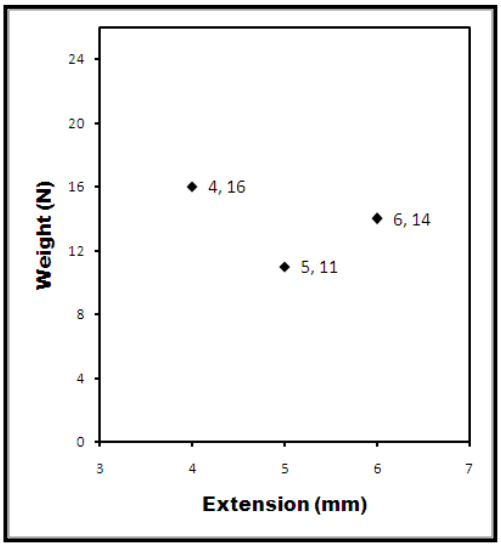
$$\boldsymbol{A^{-1}} = \frac{1}{\det(\boldsymbol{A})}\begin{bmatrix} x_2 & -x_1 \\ -1 & 1 \end{bmatrix} \implies \begin{bmatrix} a \\ b \end{bmatrix} = \boldsymbol{A^{-1}}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad \cdots \quad (4)$$

When many measurements are performed using different forces to extend the same springs the result is not two but many simultaneous equations. For example if three measurements were performed the system of equations would appear as follows.

$$\begin{matrix} a + bx_1 = y_1 \\ a + bx_2 = y_2 \\ a + bx_3 = y_3 \end{matrix} \implies \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

The problem is expressed as a $3 \times 2$ matrix for which no inverse is possible. This is mathematically stating that no one line can pass through all three points when plotted on a scatter diagram.

$$\begin{matrix} a + b4 = 16 \\ a + b5 = 11 \\ a + b6 = 14 \end{matrix} \quad \Longrightarrow \quad \begin{bmatrix} 1 & 4 \\ 1 & 5 \\ 1 & 6 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 16 \\ 11 \\ 14 \end{bmatrix}$$




The matrix corresponding to these three simultaneous equations in two unknowns can be viewed as a linear transformation $T: \mathbb{R}^2 \longrightarrow \mathbb{R}^3$. That is given a 2D vector such as $\begin{bmatrix} 2 \\ 3 \end{bmatrix}$, the matrix $\begin{bmatrix} 1 & 4 \\ 1 & 5 \\ 1 & 6 \end{bmatrix}$ provides a means of calculating a 3D vector as follows:

$$\begin{bmatrix} 1 & 4 \\ 1 & 5 \\ 1 & 6 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} (1)(2) + (4)(3) \\ (1)(2) + (5)(3) \\ (1)(2) + (6)(3) \end{bmatrix} = \begin{bmatrix} 14 \\ 17 \\ 20 \end{bmatrix}$$

The linear regression problem is to find a linear transformation $T_r: \mathbb{R}^3 \longrightarrow \mathbb{R}^2$ so that the three simultaneous equations reduce to two simultaneous equations which can be solved in principle using an inverse matrix equivalent to Equation (4).

It can be shown that the matrix for the linear transformation $T_r$ is the transpose of the matrix $\boldsymbol{A} = \begin{bmatrix} 1 & 4 \\ 1 & 5 \\ 1 & 6 \end{bmatrix}$, namely $\boldsymbol{A}^T = \begin{bmatrix} 1 & 1 & 1 \\ 4 & 5 & 6 \end{bmatrix}$, that is a $2 \times 3$ matrix formed by entering the rows of the original matrix into columns to form the transposed matrix. The transpose matrix $\begin{bmatrix} 1 & 1 & 1 \\ 4 & 5 & 6 \end{bmatrix}$ is a recipe for converting a 3D vector into a 2D vector. The transformation can be used to convert each

column of the original matrix into 2D vectors and the right-hand 3D vector into a 2D vector as follows.

$$\begin{bmatrix}1 & 1 & 1\\ 4 & 5 & 6\end{bmatrix}\begin{bmatrix}1 & 4\\ 1 & 5\\ 1 & 6\end{bmatrix} = \begin{bmatrix}3 & 15\\ 15 & 77\end{bmatrix}$$

and

$$\begin{bmatrix}1 & 1 & 1\\ 4 & 5 & 6\end{bmatrix}\begin{bmatrix}16\\ 11\\ 14\end{bmatrix} = \begin{bmatrix}41\\ 203\end{bmatrix}$$

Therefore the system of three equations in two unknowns

$$\begin{matrix}a + b4 = 16\\ a + b5 = 11\\ a + b6 = 14\end{matrix} \quad \Rightarrow \quad \begin{bmatrix}1 & 4\\ 1 & 5\\ 1 & 6\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix} = \begin{bmatrix}16\\ 11\\ 14\end{bmatrix}$$

is reduced to a 2D problem as follows.

Multiplying both sides of the matrix equation by the transpose matrix yields

$$\Rightarrow \begin{bmatrix}1 & 1 & 1\\ 4 & 5 & 6\end{bmatrix}\begin{bmatrix}1 & 4\\ 1 & 5\\ 1 & 6\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix} = \begin{bmatrix}1 & 1 & 1\\ 4 & 5 & 6\end{bmatrix}\begin{bmatrix}16\\ 11\\ 14\end{bmatrix}$$

$$\Rightarrow \begin{bmatrix}3 & 15\\ 15 & 77\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix} = \begin{bmatrix}41\\ 203\end{bmatrix}$$

The matrix $\boldsymbol{B} = \begin{bmatrix}3 & 15\\ 15 & 77\end{bmatrix}$is an example of a symmetric matrix. A matrix $\boldsymbol{B}$ is symmetric if and only if the transpose of the $\boldsymbol{B}$ is equal to $\boldsymbol{B}$, or in matrix notation, if $\boldsymbol{B} = \boldsymbol{B}^T$ then $\boldsymbol{B}$ is symmetric. Given the matrix $\boldsymbol{A} = \begin{bmatrix}a & b\\ c & d\end{bmatrix}$, the inverse matrix is $\boldsymbol{A^{-1}} = \begin{bmatrix}\frac{d}{\det(\boldsymbol{A})} & \frac{-b}{\det(\boldsymbol{A})}\\ \frac{-c}{\det(\boldsymbol{A})} & \frac{a}{\det(\boldsymbol{A})}\end{bmatrix}$. To find the inverse of $\boldsymbol{B}$ requires the calculation of the determinant for $\boldsymbol{B}$**.** Since $\det \boldsymbol{B} = (3)(77) - (15)(15) = 6$, the inverse is given by

$\boldsymbol{B^{-1}} = \frac{1}{6}\begin{bmatrix}77 & -15\\ -15 & 3\end{bmatrix}$ and is such that $\boldsymbol{B^{-1}B} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$. Hence

$$\begin{bmatrix}3 & 15\\ 15 & 77\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix} = \begin{bmatrix}41\\ 203\end{bmatrix}$$

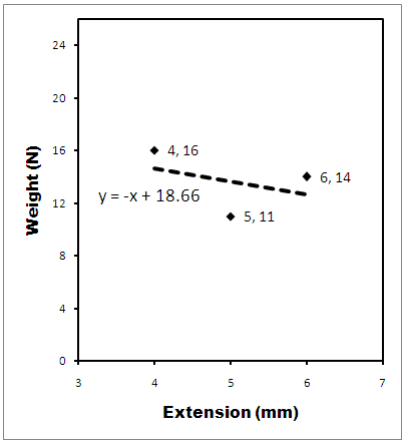
$$\Rightarrow \boldsymbol{B^{-1}B}\begin{bmatrix}a\\ b\end{bmatrix} = \boldsymbol{B^{-1}}\begin{bmatrix}41\\ 203\end{bmatrix} \text{ and } \boldsymbol{B^{-1}B}\begin{bmatrix}a\\ b\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix} = \begin{bmatrix}a\\ b\end{bmatrix}$$

Therefore

$$\begin{bmatrix}a\\ b\end{bmatrix} = \boldsymbol{B^{-1}}\begin{bmatrix}41\\ 203\end{bmatrix} = \frac{1}{6}\begin{bmatrix}77 & -15\\ -15 & 3\end{bmatrix}\begin{bmatrix}41\\ 203\end{bmatrix} = \frac{1}{6}\begin{bmatrix}(77)(41) + (-15)(203)\\ (-15)(41) + (3)(203)\end{bmatrix} = \begin{bmatrix}18.6\dot{6}\\ -1\end{bmatrix}$$

These steps in matrix algebra therefore lead to the line of best fit defined by $a = 18.6\dot{6}$ and $b = -1$.

Using the non-matrix approach:




$$\bar{x} = \frac{4+5+6}{3} = 5$$

$$\bar{y} = \frac{16+11+14}{3} = 13.66\dot{}$$

$$S_{xx} = (4^2 + 5^2 + 6^2) - 3(5^2) = 2$$

$$S_{xy} = (16 \times 4 + 11 \times 5 + 14 \times 6 +) - 3(5)(13.66\dot{}) = -2$$

$$b = \frac{S_{xy}}{S_{xx}} = \frac{-2}{2} = -1$$

and

$$a = \bar{y} - b\bar{x} = 13.66\dot{} - (-1)(5) = 18.66\dot{}$$

Using three data points to compute the line of best fit is clearly in this case a poor way to determine Young's modulus for the springs. To include all 17 measurements into the calculation the problem is exactly the same but for the use of 17 simultaneous equations rather than three.

$$\begin{matrix} a + bx_1 = y_1 \\ a + bx_2 = y_2 \\ a + bx_3 = y_3 \\ \vdots \\ a + bx_{17} = y_{17} \end{matrix} \quad \Rightarrow \quad \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ & \vdots \\ 1 & x_{17} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{17} \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 4 & 5 & 6 & \cdots & 20 \end{bmatrix} \begin{bmatrix} 1 & 4 \\ 1 & 5 \\ 1 & 6 \\ & \vdots \\ 1 & 20 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 4 & 5 & 6 & \cdots & 20 \end{bmatrix} \begin{bmatrix} 16 \\ 11 \\ 14 \\ \vdots \\ 56 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 17 & 204 \\ 204 & 2856 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 616 \\ 8628 \end{bmatrix}$$

Let $\boldsymbol{B} = \begin{bmatrix} 17 & 204 \\ 204 & 2856 \end{bmatrix}$ then $\det \boldsymbol{B} = 6936$ and

$$\boldsymbol{B^{-1}} = \frac{1}{6939} \begin{bmatrix} 2856 & -204 \\ -204 & 17 \end{bmatrix}$$

Therefore

$$\begin{bmatrix} a \\ b \end{bmatrix} = \boldsymbol{B^{-1}} \begin{bmatrix} 616 \\ 8628 \end{bmatrix} = \frac{1}{6939} \begin{bmatrix} 2856 & -204 \\ -204 & 17 \end{bmatrix} \begin{bmatrix} 616 \\ 8628 \end{bmatrix} = \begin{bmatrix} -0.11765 \\ 3.02941 \end{bmatrix}$$

Thus the gradient for the line of best fit is $b = 3.03$.

### *Linear Transformations*

When considering the problem of linear regression in terms of matrices, a reference to linear transformations was made on more than one occasion. Since the discussion thus far has been concerned with fitting a line to a set of data points plotted on a Cartesian coordinate system, one

might be forgiven for associating the term *linear* in *linear regression* with the use of a line of best fit. In fact the term linear does not relate to the use of a line of best fit. The techniques of linear regression are equally appropriate for finding, should it be required, a quadratic of best fit of the form

$$y(x) = a + bx + cx^2$$

where three parameters are chosen to allow a quadratic polynomial to approximate a set of data in the least squares sense. The use of the term linear indicates the parameters $a$, $b$ and $c$ appear in the fitting function as a power of one, i.e. $a^1$, $b^1$ and $c^1$. By way of contrast, a fitting function of the form

$$y(x) = a(x - b)^2$$

is not linear in the parameter $b$ since $b$ appears in algebraic terms of the form $ab$ and $ab^2$ and therefore does not fall directly into the mathematics of linear regression.

Provided the parameters used to obtain a function of best fit appear only with a power of one in the functional form the problem can be solved using techniques from matrix algebra. In abstract terms, a matrix and the algebra of matrices is an example of a linear transformation from one set of vectors to another satisfying the following relationships, here expressed in terms of vectors in $\mathbb{R}^3$:

$$T\begin{bmatrix} kx \\ ky \\ kz \end{bmatrix} = kT\begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad \cdots \quad (a)$$

$$T\begin{bmatrix} x_1 + x_2 \\ y_1 + y_2 \\ z_1 + z_2 \end{bmatrix} = T\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} + T\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} \quad \cdots \quad (b)$$

$\mathbb{R}^3$ is the symbol used to represent three dimensional space and the linear transformations above defined for vectors in three dimensional space are a mapping from $\mathbb{R}^3$ to $\mathbb{R}^3$, written $T: \mathbb{R}^3 \longrightarrow \mathbb{R}^3$. A linear transformation such as the one used in the above linear regression example based on three simultaneous equations maps $T_r: \mathbb{R}^3 \longrightarrow \mathbb{R}^2$, meaning all 3D vectors after transformation through $T_r$ lie in a 2D plane of 3D space which includes the origin. Since $\mathbb{R}^3$ includes the origin $\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$, a linear transformation obeying the rules (a) and (b) dictate

$$T\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = T\begin{bmatrix} x_1 - x_1 \\ y_1 - y_1 \\ z_1 - z_1 \end{bmatrix} = T\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} + T\begin{bmatrix} (-1)x_1 \\ (-1)y_1 \\ (-1)z_1 \end{bmatrix} = T\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} + (-1)T\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} x'_1 \\ y'_1 \\ z'_1 \end{bmatrix} - \begin{bmatrix} x'_1 \\ y'_1 \\ z'_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Thus the origin is mapped to the origin by a linear transformation. Therefore the transformation $T_r: \mathbb{R}^3 \longrightarrow \mathbb{R}^2$ maps 3D vectors to a 2D plane including the origin.

Given that matrices are a representation for a linear transformation it is clear that the commonly used 2D transformation of rotation, reflection and enlargement are all examples of linear transformation, as in each of these cases the origin is mapped by the corresponding matrix to the origin, whereas a translation is not a linear transformation since the origin is not mapped to the origin by a translation and so cannot be represented by a matrix in the context of matrix algebra.

The mapping $T_r$: $\mathbb{R}^{17} \longrightarrow \mathbb{R}^2$ defined by the matrix formed from the set of 17 data pairs

$$\boldsymbol{A^T} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 4 & 5 & 6 & \cdots & 20 \end{bmatrix}$$

is used to transform the columns of $\boldsymbol{A}$ expressed now in matrix notation as $\boldsymbol{B} = \boldsymbol{A^T A}$ yields the $2 \times 2$ matrix

$$\boldsymbol{B} = \begin{bmatrix} 17 & 204 \\ 204 & 2856 \end{bmatrix}$$

$\boldsymbol{B}$ is an example for a symmetric matrix formed by matrix multiplication which has the special property required to calculate the line of best fit for the set of experimentally determined data points. While the line of best fit can be calculated by the use of an inverse matrix, the properties of symmetric matrices can be used to calculate the inverse using a technique based on characteristic vectors associated with a symmetric matrix. From a practical perspective finding the inverse of $\boldsymbol{B}$ using a computer can be difficult and by considering the eigenvectors for the matrix $\boldsymbol{B}$ some of the practical difficulties are overcome.

An eigenvector of a matrix is a vector which when transformed using the matrix results in a scaling of the original vector. The scale factor is called the eigenvalue corresponding to the eigenvector. Eigenvectors are non-zero although zero is a valid eigenvalue. For a $2 \times 2$ matrix $\boldsymbol{A}$ an eigenvector $\begin{bmatrix} x \\ y \end{bmatrix}$ with eigenvalue $\lambda$ must satisfy the equation

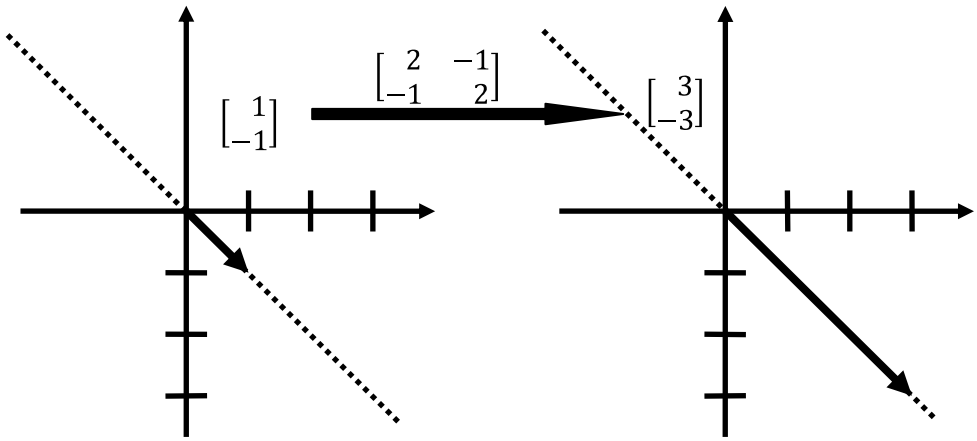
$$\boldsymbol{A}\begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix} \quad \cdots \quad (5)$$

That is, transforming the vector $\begin{bmatrix} x \\ y \end{bmatrix}$ using the matrix $\boldsymbol{A}$ simply changes the magnitude of the vector.

For example

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} (2)(1) + (-1)(-1) \\ (-1)(1) + (2)(-1) \end{bmatrix} = \begin{bmatrix} 3 \\ -3 \end{bmatrix} = 3\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Thus for the matrix $\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$, $\lambda = 3$ is an eigenvalue corresponding to the eigenvector $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$.



An eigenvector represents a direction or a line passing through the origin for which any point on the line is transformed by matrix multiplication to another point on the same line.

To calculate the eigenvalues and eigenvectors for a matrix $\boldsymbol{A}$ Equation (5) is rearranged as follows.

$$\boldsymbol{A}\begin{bmatrix}x\\y\end{bmatrix} = \lambda\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix} = \begin{bmatrix}\lambda & 0\\0 & \lambda\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix}$$

Given $\boldsymbol{A}$ is of the form $\boldsymbol{A} = \begin{bmatrix}a & b\\c & d\end{bmatrix}$

$$\Rightarrow \begin{bmatrix}a & b\\c & d\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix} - \begin{bmatrix}\lambda & 0\\0 & \lambda\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix}$$

$$\Rightarrow \begin{bmatrix}a-\lambda & b\\c & d-\lambda\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix} \quad \cdots \quad (6)$$

Equation (6) has either one solution, namely, $\begin{bmatrix}x\\y\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix}$, which is forbidden from being an eigenvector or the matrix represents the equation of two lines with identical gradients passing through the origin. In matrix terms, this geometric statement is equivalent to the statement the matrix $\begin{bmatrix}a-\lambda & b\\c & d-\lambda\end{bmatrix}$ is singular, which in turn implies $\det\begin{bmatrix}a-\lambda & b\\c & d-\lambda\end{bmatrix} = 0$.

Thus $(a-\lambda)(d-\lambda) - bc = 0$ is a quadratic in $\lambda$ yielding at most two eigenvalues and eigenvectors.

For example, to compute the eigenvalues for the symmetric matrix $\begin{bmatrix}2 & -1\\-1 & 2\end{bmatrix}$ the problem reduces to solving a quadratic equation corresponding to

$$\det\begin{bmatrix}2-\lambda & -1\\-1 & 2-\lambda\end{bmatrix} = 0 \Rightarrow (2-\lambda)(2-\lambda) - 1 = 0 \Rightarrow 3 - 4\lambda + \lambda^2 = 0 \Rightarrow (\lambda-3)(\lambda-1) = 0$$

So there are two distinct eigenvalues $\lambda = 3$ and $\lambda = 1$. The eigenvectors are calculated as a vector with the same direction as the line $(2-\lambda)x + (-1)y = 0$ for each of the two eigenvalues. For $\lambda = 3$ the gradient of the line is $-\frac{(2-3)}{(-1)} = -1$, therefore an eigenvector $\begin{bmatrix}x\\y\end{bmatrix}$ is such that $\frac{y}{x} = -1$. Let $x = 1$ then $\frac{y}{x} = -1 \Rightarrow y = -1$ and an eigenvector corresponding to $\lambda = 3$ is $\begin{bmatrix}1\\-1\end{bmatrix}$. Similarly, for $\lambda = 1$ the gradient of the line is $-\frac{(2-1)}{(-1)} = 1$, therefore an eigenvector $\begin{bmatrix}x\\y\end{bmatrix}$ is such that $\frac{y}{x} = 1$ which is clearly satisfied by the vector $\begin{bmatrix}1\\1\end{bmatrix}$ or the vector . $\begin{bmatrix}2\\2\end{bmatrix}$. There are an infinite number of points on a line through the origin and therefore there are an infinite number of eigenvectors. The matrix $\begin{bmatrix}2 & -1\\-1 & 2\end{bmatrix}$ maps the eigenvector $\begin{bmatrix}1\\-1\end{bmatrix}$ to the eigenvector $\begin{bmatrix}3\\-3\end{bmatrix}$ and $\begin{bmatrix}3\\-3\end{bmatrix}$ is mapped to $\begin{bmatrix}9\\-9\end{bmatrix}$, all of which are eigenvectors. Since it is the direction for the eigenvector that determines this scaling of an eigenvector by the eigenvalue, only the direction for the eigenvectors is important when describing the action of the matrix on this set of vectors. The direction for a vector is defined by the corresponding unit vector and so it is conventional to express eigenvectors in the normalised form of a unit vector.

A unit vector, also referred to as a normalised vector, is obtained by dividing each component of the vector by the magnitude of the vector. The magnitude for a vector is the square root of the sum of

the components squared. For the current example, the unit vector corresponding to the eigenvalue $\lambda = 1$ is calculated from the eigenvector $\begin{bmatrix}1\\1\end{bmatrix}$, which has magnitude $\sqrt{1^2+1^2} = \sqrt{2}$, is $\begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$ and so the normalised eigenvector corresponding to $\lambda = 3$ is $\begin{bmatrix}\frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}}\end{bmatrix}$.

These normalised eigenvectors are of interest to the "line of best fit" problem for the following reasons.

Two matrices can be formed from the eigenvalues and the normalised eigenvectors:

$$\boldsymbol{P} = \begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix} \text{ and } \boldsymbol{D} = \begin{bmatrix}3 & 0\\0 & 1\end{bmatrix}$$

The matrix $\boldsymbol{P}$ formed from the normalised eigenvectors is an example of an orthogonal matrix. A square matrix $\boldsymbol{M}$ with the property $\boldsymbol{MM^T} = \boldsymbol{I}$ is called an orthogonal matrix.

$$\boldsymbol{P^T} = \begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}$$

Therefore

$$\boldsymbol{PP^T} = \begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix} = \begin{bmatrix}\left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right)+\left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right) & \left(\frac{1}{\sqrt{2}}\right)\left(-\frac{1}{\sqrt{2}}\right)+\left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right)\\\left(-\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right)+\left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right) & \left(-\frac{1}{\sqrt{2}}\right)\left(-\frac{1}{\sqrt{2}}\right)+\left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right)\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$$

For a symmetric matrix with positive eigenvalues, the matrix formed from the normalised eigenvectors is orthogonal because the eigenvectors are perpendicular. Clearly for this specific example $\boldsymbol{P^T} = \boldsymbol{P^{-1}}$, a very convenient property when attempting to invert a matrix.

The matrix $\boldsymbol{D}$ formed from the eigenvalues listed along the leading diagonal in the same order as the eigenvectors populate the columns of $\boldsymbol{P}$ is again simply inverted provided the eigenvalues are nonzero as follows.

Given $\boldsymbol{D} = \begin{bmatrix}3 & 0\\0 & 1\end{bmatrix}$ the inverse $\boldsymbol{D^{-1}} = \begin{bmatrix}\frac{1}{3} & 0\\0 & \frac{1}{1}\end{bmatrix}$ is obtained by replacing the diagonal elements of $\boldsymbol{D}$ by the reciprocal of the eigenvalues which can be demonstrated as follows.

$$\begin{bmatrix}3 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}\frac{1}{3} & 0\\0 & \frac{1}{1}\end{bmatrix} = \begin{bmatrix}(3)\left(\frac{1}{3}\right)+(0)(0) & (3)(0)+(0)(1)\\(0)\left(\frac{1}{3}\right)+(1)(0) & (0)(0)+(1)\left(\frac{1}{1}\right)\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$$

The significance of these matrices $\boldsymbol{P}$ and $\boldsymbol{D}$ to the original problem lies in the following observation. Given the eigenvalue equations of the matrix $\boldsymbol{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$

$$\boldsymbol{A}\begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \lambda_1 \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} \text{ and } \boldsymbol{A}\begin{bmatrix} x_2 \\ y_2 \end{bmatrix} = \lambda_2 \begin{bmatrix} x_2 \\ y_2 \end{bmatrix}$$

these two matrix equations can be rewritten as

$$\boldsymbol{AP} = \boldsymbol{A}\begin{bmatrix} x_1 & x_2 \\ y_1 & y_2 \end{bmatrix} = \begin{bmatrix} ax_1 + by_1 & ax_2 + by_2 \\ cx_1 + dy_1 & cx_2 + dy_2 \end{bmatrix} = \begin{bmatrix} \lambda_1 x_1 & \lambda_2 x_2 \\ \lambda_1 y_1 & \lambda_2 y_2 \end{bmatrix} = \begin{bmatrix} \lambda_1 x_1 & \lambda_1 y_1 \\ \lambda_2 x_2 & \lambda_2 y_2 \end{bmatrix}^T$$

Now

$$\begin{bmatrix} \lambda_1 x_1 & \lambda_1 y_1 \\ \lambda_2 x_2 & \lambda_2 y_2 \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \end{bmatrix} = \boldsymbol{DP^T}$$

therefore

$$\boldsymbol{AP} = \left(\boldsymbol{DP^T}\right)^T$$

Since $(\boldsymbol{XY})^T = \boldsymbol{Y^T X^T}$ and $\left(\boldsymbol{X^T}\right)^T = \boldsymbol{X}$

$$\boldsymbol{AP} = \left(\boldsymbol{DP^T}\right)^T \Longrightarrow \boldsymbol{AP} = \left(\boldsymbol{P^T}\right)^T \boldsymbol{D^T}$$

And since a diagonal matrix is symmetric $\boldsymbol{D^T} = \boldsymbol{D}$ therefore

$$\boldsymbol{AP} = \boldsymbol{PD} \Longrightarrow \boldsymbol{APP^T} = \boldsymbol{PDP^T}$$

If $\boldsymbol{P}$ is an orthogonal matrix then $\boldsymbol{PP^T} = \boldsymbol{I}$ hence

$$\boldsymbol{A} = \boldsymbol{PDP^T}$$

and

$$\boldsymbol{A^{-1}} = \left(\boldsymbol{PDP^T}\right)^{-1} = \left(\boldsymbol{P^T}\right)^{-1}(\boldsymbol{PD})^{-1} = \boldsymbol{PD^{-1}P^{-1}} = \boldsymbol{PD^{-1}P^T}$$

For the symmetric matrix

$$\boldsymbol{A} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

with associated matrices

$$\boldsymbol{P} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \text{ and } \boldsymbol{D} = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}$$

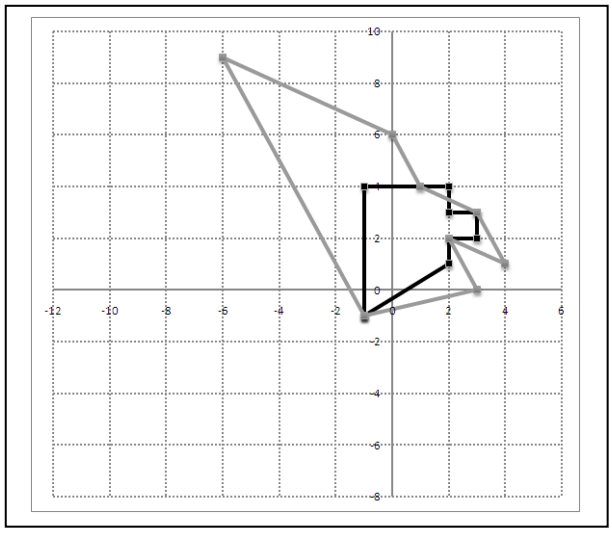
the inverse is given by

$$\boldsymbol{A^{-1}} = \boldsymbol{PD^{-1}P^T} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

Apart from providing a method for finding the inverse matrix, determining the eigenvectors and eigenvalues for the symmetric matrix $\boldsymbol{A} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$ provides a means of understanding the nature of the transformation performed by $\boldsymbol{A}$ in terms of $\boldsymbol{P}$ and $\boldsymbol{D}$. The matrix $\boldsymbol{P}$ is a rotation about the origin by $-\frac{\pi}{4}$ radians while $\boldsymbol{D}$ is an enlargement of 3 in the first coordinate and 1 in the second coordinate. Therefore

$$\boldsymbol{A} = \boldsymbol{PDP^T}$$

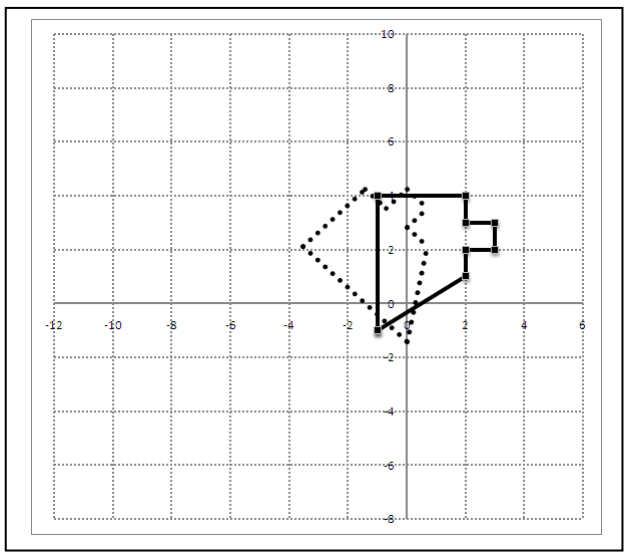
implies the transformation $\boldsymbol{A}$ is a rotation about the origin of $\frac{\pi}{4}$ radians, followed by an enlargement, followed by a rotation by $-\frac{\pi}{4}$ about the origin.



Transformation of 2D shape using direct application of matrix

$$\boldsymbol{A} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

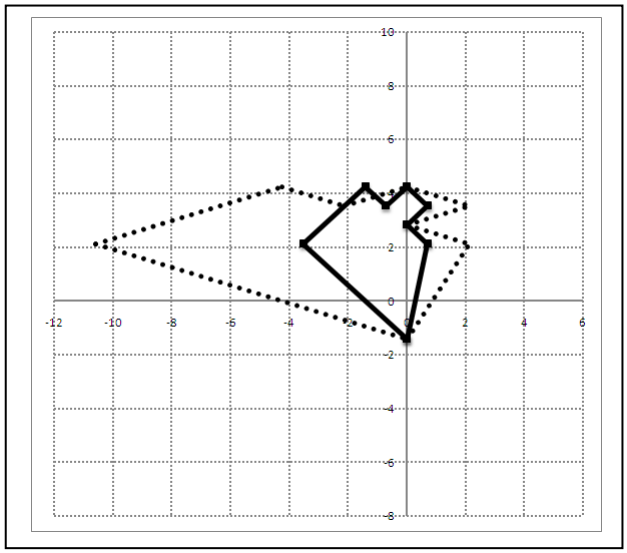
$$\boldsymbol{A} = \boldsymbol{PDP^T}$$



Step 1: Transformation of 2D shape using matrix

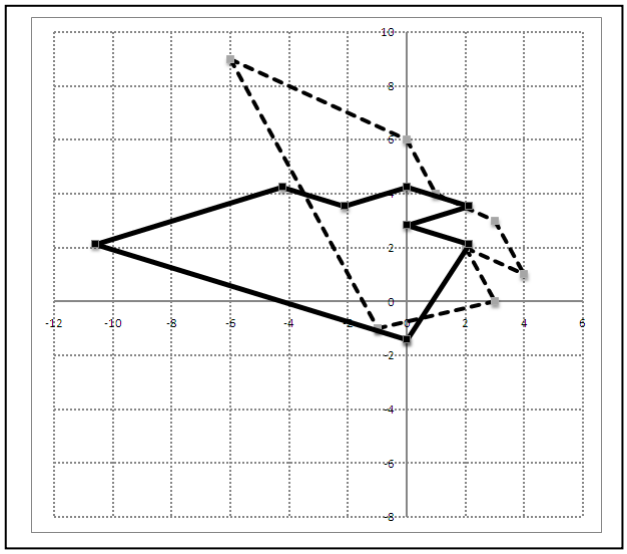
$$\boldsymbol{P^T} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

Rotation about origin by $\frac{\pi}{4}$ radians



Step 2: Transform rotated image using enlargement matrix

$$\boldsymbol{D} = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}$$



Step 3: Transformation of 2D image from step 2 using matrix

$$\boldsymbol{P} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

Rotation about origin by $-\frac{\pi}{4}$ radians

The linear regression problem using 17 experimental measurements reduces to finding the inverse of the matrix $\boldsymbol{B} = \begin{bmatrix} 17 & 204 \\ 204 & 2856 \end{bmatrix}$. The matrix $\boldsymbol{B}$ is also a symmetric matrix $\boldsymbol{B} = \boldsymbol{B^T}$ and a similar eigenanalysis can be performed for $\boldsymbol{B}$ yielding two eigenvalues and eigenvectors.

$$\lambda_1 = 2870.58 \text{ with eigenvector } \hat{\boldsymbol{v}}_1 = \begin{bmatrix} 0.0713 \\ 0.9975 \end{bmatrix}$$

and

$$\lambda_2 = 2.416 \text{ with eigenvector } \hat{\boldsymbol{v}}_2 = \begin{bmatrix} 0.9975 \\ -0.0713 \end{bmatrix}$$

The orthogonal matrix formed from the normalised eigenvectors for $\boldsymbol{B}$ is

$$\boldsymbol{P} = \begin{bmatrix} 0.0713 & 0.9975 \\ 0.9975 & -0.0713 \end{bmatrix}$$

corresponding to the diagonal matrix of eigenvalues

$$\boldsymbol{D} = \begin{bmatrix} 2870.58 & 0 \\ 0 & 2.416 \end{bmatrix}$$

allows the inverse of the symmetric matrix $\boldsymbol{B}$ to be calculated

$$\boldsymbol{B^{-1}} = \boldsymbol{PD^{-1}P^T} = \begin{bmatrix} 0.0713 & 0.9975 \\ 0.9975 & -0.0713 \end{bmatrix} \begin{bmatrix} \frac{1}{2870.58} & 0 \\ 0 & \frac{1}{2.416} \end{bmatrix} \begin{bmatrix} 0.0713 & 0.9975 \\ 0.9975 & -0.0713 \end{bmatrix}$$

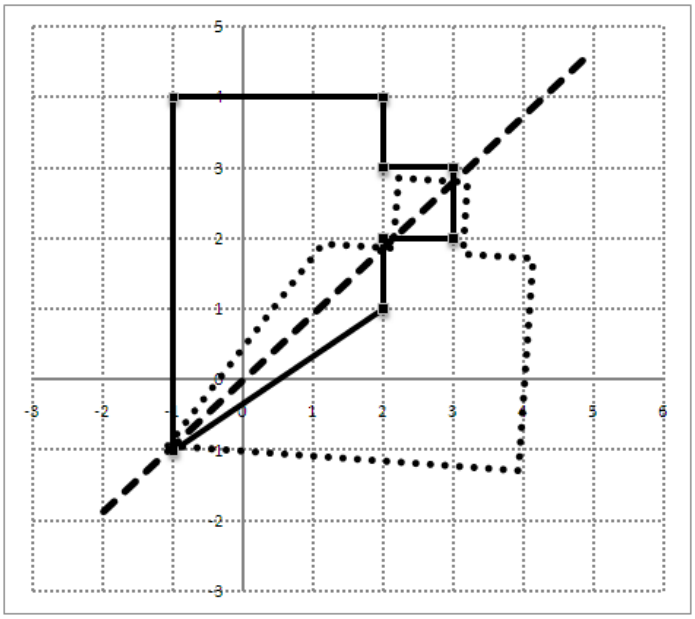
Note, an inverse based on the matrices $\boldsymbol{P}$ and $\boldsymbol{D}$ is only possible because of the special properties of the symmetric matrix $\boldsymbol{B}$ causing $\boldsymbol{P}$ to be orthogonal and eigenvalues all positive.

The line of best fit is again calculated using

$$\begin{bmatrix} a \\ b \end{bmatrix} = \boldsymbol{B^{-1}} \begin{bmatrix} 616 \\ 8628 \end{bmatrix} = \begin{bmatrix} 0.0713 & 0.9975 \\ 0.9975 & -0.0713 \end{bmatrix} \begin{bmatrix} \frac{1}{2870.58} & 0 \\ 0 & \frac{1}{2.416} \end{bmatrix} \begin{bmatrix} 0.0713 & 0.9975 \\ 0.9975 & -0.0713 \end{bmatrix} \begin{bmatrix} 616 \\ 8628 \end{bmatrix} = \begin{bmatrix} -0.11765 \\ 3.02941 \end{bmatrix}$$

yielding the same result, namely the gradient for the line of best fit is $3.03\ Nmm^{-1}$.

The matrix $\boldsymbol{P}$ corresponding to the normalised eigenvectors of $\boldsymbol{B}$ is in this case a reflection rather than a rotation.



Matrix

$$\boldsymbol{P} = \begin{bmatrix} 0.0713 & 0.9975 \\ 0.9975 & -0.0713 \end{bmatrix}$$

represents a reflection in the line through the origin making an angle

$$\theta = \frac{\cos^{-1}(0.0713)}{2} = 42.96°$$

with the x axis.

# Application of Eigenvectors and Eigenvalues to Image Processing

## Images and Vectors

Images are, in essence, a two dimensional array of numerical values mapped to a range of colours so that spatial information can be displayed. At first sight images may seem to have little to do with vectors, let alone 2D vectors, yet interpreting images as vectors is a very useful way to improve an understanding for image data.

One way to make this jump from a pictorial perspective to a 2D vector representation for images is to interpret two images as lists of coordinate values, where the intensities from one image are chosen to be the x-coordinates while the y-coordinates are obtained from the second image. These pairs of coordinate values are precisely the intensities from common pixel locations within these two images. Rather than relying on colour to visualise these images, these image data are represented by a set of points plotted in a 2D plane. Thus from a pair of images numerous coordinate pairs are obtained in a 2D plane and each coordinate pair provides a 2D position vector.

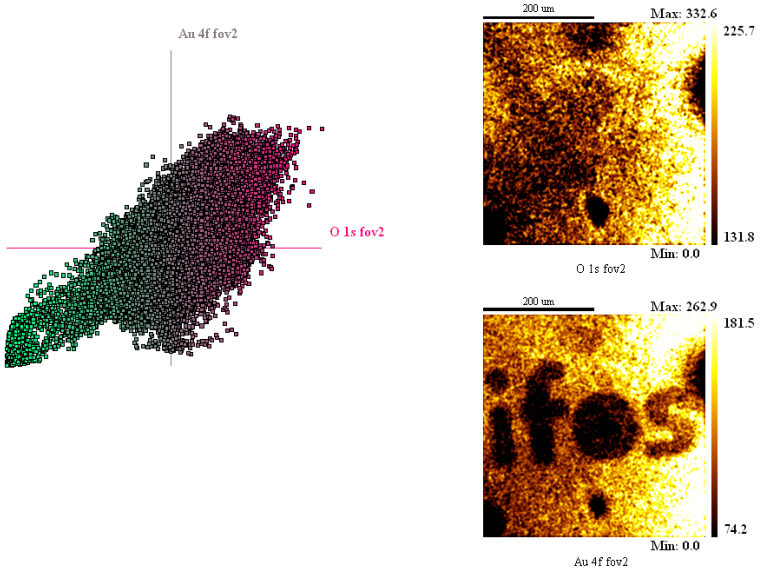



**Figure 1: These two images are plotted in a 2D plane by drawing a point for each pixel. The x-coordinate for the point is taken from the intensity for the same pixel position in the top image as the bottom image, from which the y-coordinate is taken.**

Given a plot of points in a 2D plane the first assessment often made is to calculate a linear regression line. The objective typically is to test for a linear relationship within the scatter plot and attempt to categorise numerically the strength of any linear relationship. If a linear relationship does exist within the data then an obvious transformation which could be applied to the 2D data set is to rotate the scatter plot so that the line of best fit is now the x-axis. Images transformed by such a rotation would then represent, in some sense, an image containing the variation along the line of best fit, while the orthogonal direction is an image of no variation in the direction of the line of best fit.

Whilst linear regression remains an option for a pair of images, the image data can be assessed in terms of linear relationships using a similar approach to linear regression, but where a line of best fit is determined by performing a rotation about some origin selected for a particular distribution of

points. The angle of rotation is chosen to minimise the sum of squares for the $y$-coordinate following the rotation transformation. The origin could be selected to be the minimum point in terms of coordinate values, or alternatively the mean average coordinate could be the origin of choice.

The reason for altering the definition for the line of best fit from the standard regression line to the problem now discussed is linear regression assumes one coordinate is an independent variable, while the second coordinate is a value measured in response to the value set for the first coordinate. That is, for simple regression, the line of best fit can be reasonably assumed to be that obtained from minimising the sum of squares in the original $y$-coordinate alone. For the case of two images the intensities are measured independently of each other, and so the choice for $x$ and $y$ coordinates is not so natural and more importantly the line of best fit should not depend on the choice for assigning images to the $x$ and $y$ coordinates in the scatter plot. Minimising the sum of squares for the transformed $y$-coordinate involves both the original $x$ and $y$ coordinates and therefore removes the bias towards one image over the other introduced by considering the original $y$-coordinate alone.

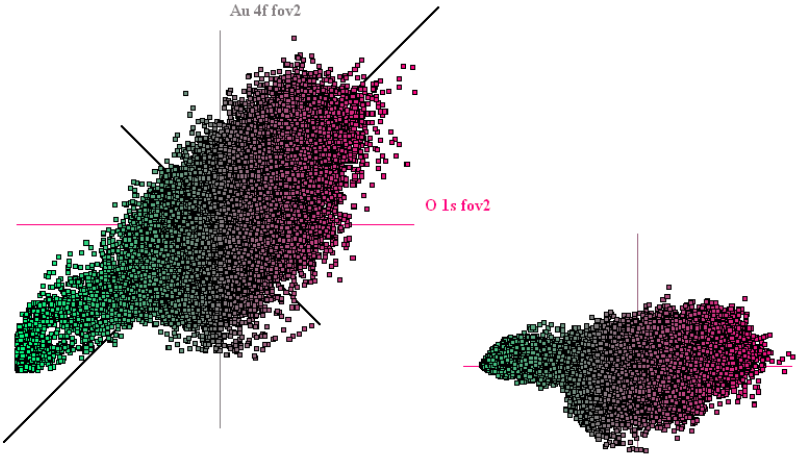



**Figure 2 The image intensities plotted as a scatter plot for the images in Figure 1 showing the line of best fit. A transformation for these data as depicted by a scatter plot representing a rotation about the mean average coordinate pair required to align the line of best fit with the x-axis.**

## Line of Best Fit Revisited

Given two images consisting of intensities at each pixel position these intensities can be expressed as two lists $\boldsymbol{d}_1 = (x_1, x_2, x_3, \cdots, x_n)$ and $\boldsymbol{d}_2 = (y_1, y_2, y_3, \cdots, y_n)$ of numerical values. From these two lists $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ a $2 \times n$ matrix can be defined.

$$\boldsymbol{D} = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ y_1 & y_2 & y_3 & \cdots & y_n \end{bmatrix}$$

The problem is to determine a linear transformation matrix $\boldsymbol{R} = \begin{bmatrix} p & q \\ r & s \end{bmatrix}$ such that

$$\begin{bmatrix} p & q \\ r & s \end{bmatrix} \begin{bmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ y_1 & y_2 & y_3 & \cdots & y_n \end{bmatrix} = \begin{bmatrix} \bar{x}_1 & \bar{x}_2 & \bar{x}_3 & \cdots & \bar{x}_n \\ \bar{y}_1 & \bar{y}_2 & \bar{y}_3 & \cdots & \bar{y}_n \end{bmatrix}$$

where $\Psi = \sum_{i=1}^{n} \bar{y}_i{}^2$ is a minimum with the constraint, to ensure the spatial arrangement of the points in the scatter plot is preserved, $det(\boldsymbol{R}) = 1$.

The constraint $det(\boldsymbol{R}) = 1$ is achieved by defining the transformation in terms of an angle $\phi$ with respect to the positive direction of the $x$ axis about the origin characterising a rotation.

$$\boldsymbol{R} = \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix}$$

Thus $det(\boldsymbol{R}) = \cos^2\phi + \sin^2\phi = 1$.

Since

$$\begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} = \begin{bmatrix} x_i\ \cos\phi - y_i \sin\phi \\ x_i\ \sin\phi + y_i \cos\phi \end{bmatrix} = \begin{bmatrix} \bar{x}_i \\ \bar{y}_i \end{bmatrix}$$

$$\Psi = \sum_{i=1}^{n} (x_i\ \sin\phi + y_i \cos\phi)^2 = \sum_{i=1}^{n} [{x_i}^2 \sin^2\phi + {y_i}^2 \cos^2\phi + 2x_i\, y_i\ \sin\phi \cos\phi]$$

$$\Longrightarrow \Psi = \sin^2\phi \sum_{i=1}^{n} {x_i}^2 + \cos^2\phi \sum_{i=1}^{n} {y_i}^2 + \sin 2\phi \sum_{i=1}^{n} x_i\, y_i$$

Using the notation $S_{xx} = \sum_{i=1}^{n} {x_i}^2$, $S_{xy} = \sum_{i=1}^{n} x_i\, y_i$ and $S_{yy} = \sum_{i=1}^{n} {y_i}^2$

$$\Longrightarrow \Psi = \sin^2\phi\, S_{xx} + \cos^2\phi\, S_{yy} + \sin 2\phi\, S_{xy} \quad \cdots \quad (1)$$

$$\Longrightarrow \Psi = \sin^2\phi\, S_{xx} + \cos^2\phi\, S_{xx} - \cos^2\phi\, S_{xx} + \cos^2\phi\, S_{yy} + \sin 2\phi\, S_{xy}$$

$$\Longrightarrow \Psi(\phi) = S_{xx} + \cos^2\phi \left(S_{yy} - S_{xx}\right) + \sin 2\phi\, S_{xy}$$

To determine the minimum for $\Psi(\phi)$, $\frac{d\Psi}{d\phi} = 0$.

Therefore,

$$\frac{d\Psi}{d\phi} = -2\sin\phi\cos\phi \left(S_{yy} - S_{xx}\right) + 2\cos 2\phi\, S_{xy} = 0$$

$$\Longrightarrow \left(S_{yy} - S_{xx}\right)\sin 2\phi = 2S_{xy}\cos 2\phi$$

$$\Longrightarrow \tan 2\phi = \frac{2S_{xy}}{\left(S_{yy} - S_{xx}\right)} \; for\; S_{yy} - S_{xx} \neq 0 \quad \cdots \quad (2)$$

and for $S_{yy} - S_{xx} = 0, \cos 2\phi = 0$.

Interestingly, if the image data are identical in length ($S_{yy} - S_{xx} = 0$) then the required transformation is a rotation by $\frac{\pi}{4}$,the direction for the rotation only depending on the sign of $S_{xy}$.

The relationship between the required rotation angle and eigenvectors for the covariance matrix can be examined by considering Equation (1) written in terms of sine and cosine, and then expressed as a quadratic form as follows.

$$\Psi = \sin^2\phi\, S_{xx} + \cos^2\phi\, S_{yy} + 2\sin\phi\cos\phi\, S_{xy}$$

Therefore in quadratic form the function of $\phi$ is written in matrix notation as

$$\Psi = [\cos\phi \quad \sin\phi]\begin{bmatrix} S_{yy} & S_{xy} \\ S_{xy} & S_{xx} \end{bmatrix}\begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix}$$

The symmetrical matrix $\boldsymbol{C} = \begin{bmatrix} S_{yy} & S_{xy} \\ S_{xy} & S_{xx} \end{bmatrix}$ is a covariance matrix formed from the image data, the eigenvectors of which provide the same angle of rotation required to optimise $\Psi$. Such an assertion can be supported by the following analysis.

The eigenvalues are calculated by finding the roots of the characteristic quadratic polynomial formed from

$$det(\boldsymbol{C} - \lambda \boldsymbol{I}) = 0$$

$$det\begin{bmatrix} S_{yy} - \lambda & S_{xy} \\ S_{xy} & S_{xx} - \lambda \end{bmatrix} = 0$$

$$\Longrightarrow (S_{yy} - \lambda)(S_{xx} - \lambda) - {S_{xy}}^2 = 0 \Longrightarrow \lambda^2 - (S_{yy} + S_{xx})\lambda + S_{xx}S_{yy} - {S_{xy}}^2 = 0$$

$$\Longrightarrow \lambda = \frac{(S_{yy} + S_{xx}) \pm \sqrt{(S_{yy} + S_{xx})^2 - 4(S_{xx}S_{yy} - {S_{xy}}^2)}}{2}$$

$$\Longrightarrow \lambda = \frac{(S_{yy} + S_{xx}) \pm \sqrt{(S_{yy} - S_{xx})^2 + 4{S_{xy}}^2}}{2}$$

The eigenvector $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$corresponding to the eigenvalue $\lambda$ is calculated from

$$(S_{yy} - \lambda)\alpha + S_{xy}\beta = 0$$

Choosing to calculate the unit eigenvector expressed as $\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix}$ it follows

$$(S_{yy} - \lambda)\cos\phi + S_{xy}\sin\phi = 0$$

$$\Longrightarrow \tan\phi = \frac{(S_{yy} - \lambda)}{S_{xy}}$$

$$\Longrightarrow \tan\phi = \frac{(S_{yy} - S_{xx}) \pm \sqrt{(S_{yy} - S_{xx})^2 + 4{S_{xy}}^2}}{2S_{xy}}$$

Substituting $\tan\phi$ into

$$\tan 2\phi = \frac{2\tan\phi}{1 - \tan^2\phi}$$

and after rearranging

$$\Longrightarrow \tan 2\phi = \frac{2S_{xy}}{(S_{yy} - S_{xx})} \; for \; S_{yy} - S_{xx} \neq 0$$

That is, the same angle is available from the eigenvectors of $\boldsymbol{C}$ as is calculated from the optimisation steps leading to Equation (2). The result is a prescription for rotating the scatter plot to align the maximum variation along the $x$-axis.

Geometrically, the quadratic form

$$\Psi = [\cos\phi \quad \sin\phi] \begin{bmatrix} S_{yy} & S_{xy} \\ S_{xy} & S_{xx} \end{bmatrix} \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix}$$

is the equation for an ellipse $\Psi = constant$ defined with the major axis making an angle $\phi$ with the $x$-axis. The matrix formed from the normalised eigenvectors of $\boldsymbol{C}$ provides the linear transformation required to align the scatter plot as shown in Figure 3.

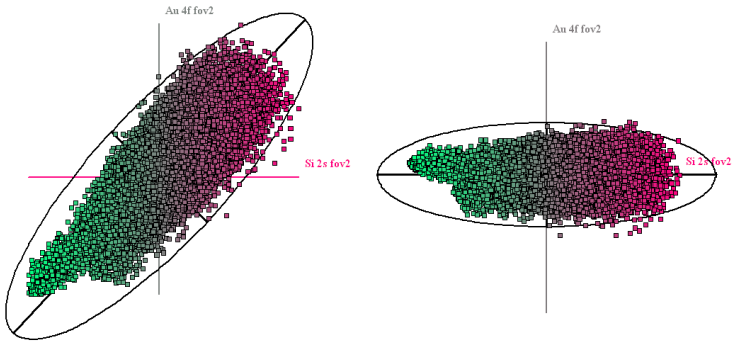



**Figure 3: Shape for a ellipse defined by the quadratic form corresponding to the symmetric matrix $C$ before and after the data are transformed.**

Transforming the scatter plot by a rotation allows the original images to be transformed to provide a new spatial perspective as illustrated in Figure 4. The example illustrates how two essentially similar images are transformed by the 2D transformation to one containing the principal features in these two images while the second image represents the spatial information not in the first.

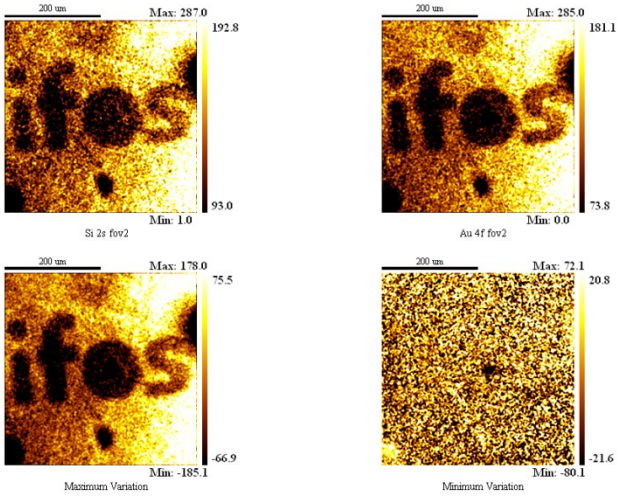



**Figure 4: Top two images are raw data corresponding to the scatter plot in Figure 3 before rotation. The bottom two images represent the transformed data shown in Figure 3 following rotation.**

These concepts of rotating vectors were used by Jacobi to calculate the eigenvectors for a real symmetric matrix. Equation (2), obtained here as a consequence of an optimisation problem, also appears as part of the Jacobi algorithm where the same equation provides the means for eliminating off-diagonal elements in the real symmetric matrix for which eigenvectors are sought.

## Transformation of Data using Rotations

The example now considered is a degradation study for a polymer under the influence of x-ray exposure. These data provide an example of where data evolves gradually with each measurement, and allows the consequences of applying rotations in $n$-dimensional vector space to these $n$-sets of spectra to be investigated.

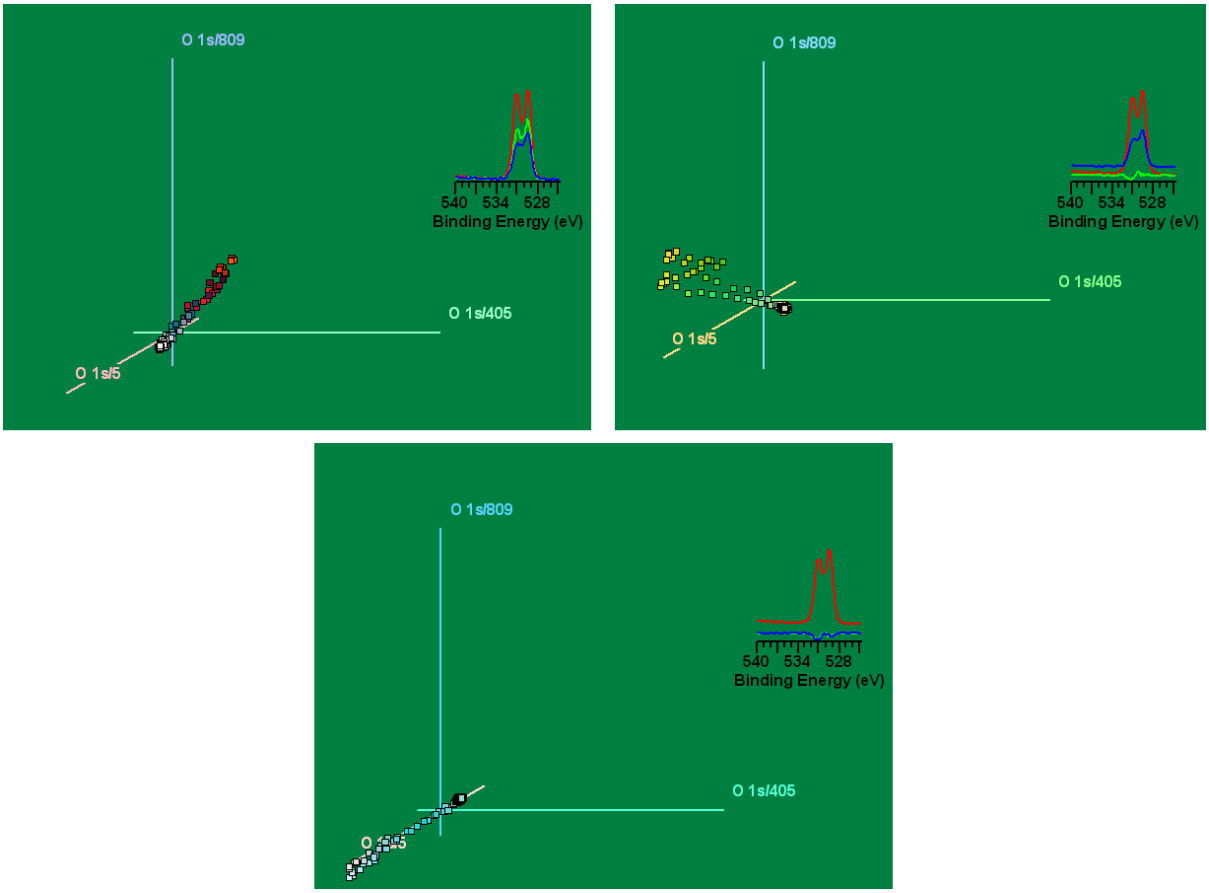



**Figure 5: Three stages involving two rotations leading from a scatter-plot in 3D corresponding to 3 raw spectra to the equivalent (in a spatial sense) scatter-plot calculated to place the scatter-points along the first coordinate axis. First a rotation about the $z$-axis aligns the scatter points around the $xz$ plane, followed by a rotation about the $y$-axis to located the 3D data points about the $x$-axis.**

The method used to transform these spectra rotates a scatter-plot sequentially about each of the other $n-1$ coordinate axes until the variation in the data is aligned with respect to the first coordinate axis. The rotations are calculated to minimize the coordinate values one at a time until the scatter points are located close to the first coordinate axis. To illustrate the rotation transformations Figure 5 represents three states for a set of points derived from three spectra plotted as a scatter diagram. The first scatter diagram (top left) shows the scatter diagram before any transformation. The second plot (top right) illustrates the scatter points after rotation about the $z$-axis achieved by minimizing the sum of squares for the rotated $y$-coordinate following rotation

about the $z$-axis. The result is a scatter of points located close to the $xz$-plane. These points now located around the $xz$-plane are rotated a second time about the $y$-axis resulting in the scatter points being located about the $x$-coordinate axis as seen in the bottom tile in Figure 5. Also, the consequences for the original spectra at each stage can be seen in each tile in Figure 5.

Note how the sequence of rotations gathers the variation in these three data into a dominant vector leaving the minor variations represented in the other two vectors.

Given a set of spectra, a sequence of rotations can be used to examine trends in the data set. For example, a set of C 1s spectra measured from poly (methyl methacrylate) (PMMA) processed using a single pass of rotation transformations equivalent to those illustrated in Figure 5 create an alternative perspective for these spectra. Spectra in Figure 6 appear ordered with respect to time top-left to bottom-right. PMMA is modified by x-ray exposure causing the relative peak intensities for C bonded to O to change relative to C-H chemical state. These changes can be seen in the rotated data shown in Figure 7.

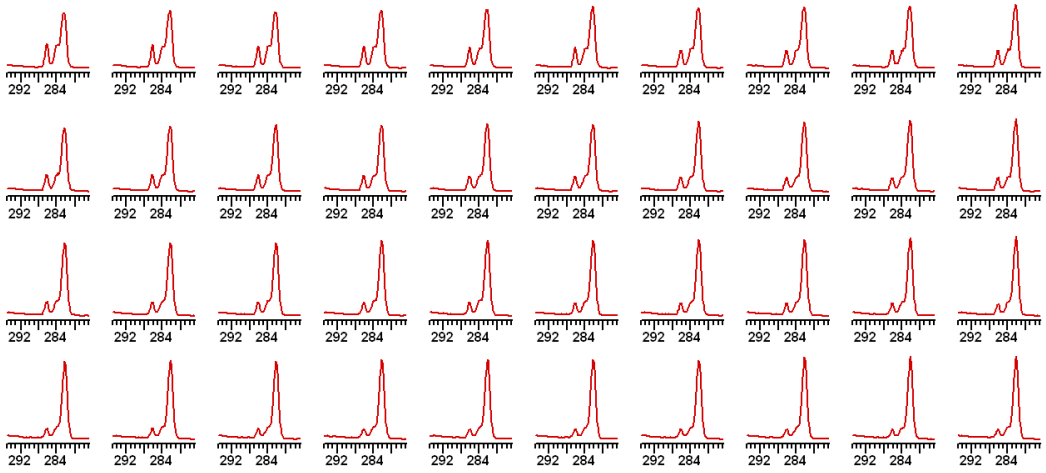



**Figure 6: PMMA spectra measured repeatedly using the same sample. X-ray damage is evident from the changing C=0 C 1s peak to high binding energy of the C 1s transition data envelope.**

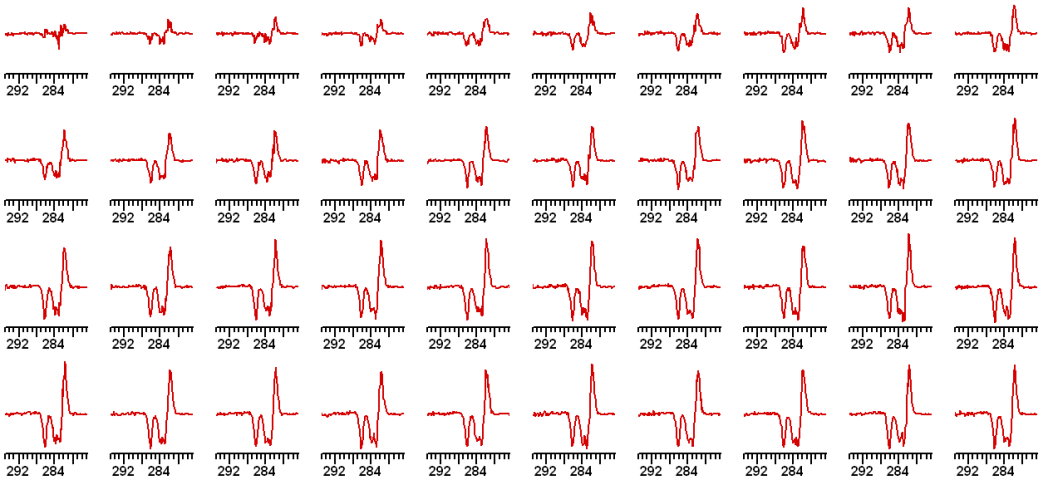



**Figure 7: Spectra after transformation. By applying a sequence of rotations the spectra appear as negative and positive peaks corresponding to the changes in intensity for the C=O, C-O and C-H peaks in PMMA due to x-ray damage. These data are obtained by rotation using the natural chronological order for the spectra.**

# Micro Factor Analysis

The use of Principal Component Analysis to improve signal to noise in XPS spectromicroscopy has been well documented over the last decade. The underlying approach is to perform an eigenanalysis using all data simultaneously and trust the significant information within the data set can be well represented by a limited number of eigenvectors. As an alternative, the approach adopted by micro factor analysis (MFA) is rather than perform an eigenanalysis on the entire data set as a unit, individual vectors from within the data are analysed in three dimensional subspaces of the n-dimensional space spanned by the data vectors. The data vectors are progressively transformed by replacing the data vectors by vectors formed from two-dimensional subspaces corresponding to principal eigenvectors calculated from three vectors sub-sampled from the data set. The success or failure of micro-factor analysis is dependent on the selection of the three vectors used in each step in the procedure.

MFA will be discussed in the context of XPS image data sets and sputter depth profiles, both of which can be chosen to best exemplify MFA in terms of outcome.

## Theory behind the use of Principal Eigenvectors

One reason for considering MFA is the reduced 3D eigenanalysis can be examined in detail and given a physical interpretation.

Given a set of three data vectors $\{\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3\}$, the standard procedure for expressing these three vectors as a corresponding set of abstract vectors $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3\}$ is in terms of a singular valued decomposition

$$\boldsymbol{D} = \boldsymbol{U}\boldsymbol{W}\boldsymbol{V}^T$$

where

$\boldsymbol{d}_i \in \mathbb{R}^n$, $\boldsymbol{u}_i \in \mathbb{R}^n$, $\boldsymbol{D} = [\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3]$ and $\boldsymbol{U} = [\hat{\boldsymbol{u}}_1, \hat{\boldsymbol{u}}_2, \hat{\boldsymbol{u}}_3]$

$\boldsymbol{W}$ is a diagonal matrix with diagonal matrix elements equal to the square root of eigenvalues of the covariance matrix

$$\boldsymbol{Z} = \boldsymbol{D}^T\boldsymbol{D}$$

and $\boldsymbol{V}$ is the matrix formed from the normalised eigenvectors of $\boldsymbol{Z}$ ordered with respect to the eigenvalues. The non-zero values appear ordered in size along the diagonal of $\boldsymbol{W}$. The MFA approximation is simply achieve by replacing the data vector $\boldsymbol{d}_2$ by the linear combination defined by $\overline{\boldsymbol{d}}_2 = c_1\hat{\boldsymbol{u}}_1 + c_2\hat{\boldsymbol{u}}_2$, where $c_1$and $c_2$ are determined in the least squares sense.

The approximation of$\boldsymbol{d}_2$ by $\overline{\boldsymbol{d}}_2$is valid noise reduction step provided the original three vectors $\{\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3\}$ are essentially the same vector but for noise. The use of two terms in the approximation rather than simply one term $c_1\hat{\boldsymbol{u}}_1$ allow for an amount of variation within the data vectors, but if all three vectors are significantly different the approximation fails, hence the need for a slowly varying sequence of data vectors for MFA to be useful. Note, replacing $\boldsymbol{d}_2$by an average of the data vectors is another least squares solution, but one in which there is no possibility of recovering information beyond the value as calculated. MFA could therefore be seen as a more sympathetic mapping

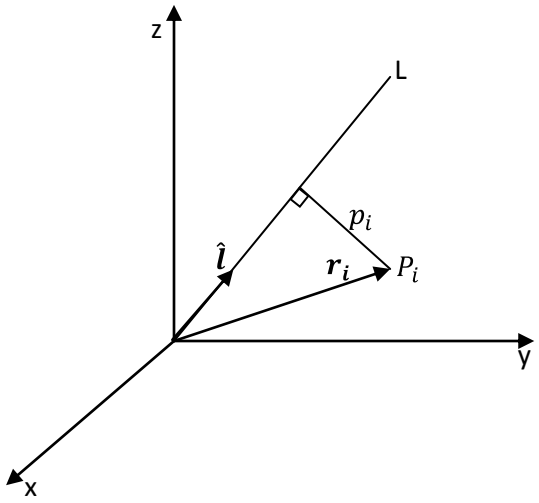
$\mathbb{R}^3 \longrightarrow \mathbb{R}^2$ while an average would enforce a mapping of $\mathbb{R}^3 \longrightarrow \mathbb{R}^1$ with, in the event of slightly varying data vectors, the ensuing loss of information.

The use of the covariance matrix $\boldsymbol{Z}$ to perform the singular valued decomposition of the data matrix $\boldsymbol{D}$ might seem natural in the context of the design matrix used to perform linear least squares fitting of target vectors to a data vector. However to improve an intuitive understanding for the process, the use of the covariance matrix formed from the data can be viewed in terms of physics in the following sense. If each coordinate from the three data vectors are viewed as position coordinates in 3D space of a unit mass particle, then the moments of inertia for a set of unit mass particles when rotated with a fixed angular speed attains a minimum kinetic energy for a specific choice of an axis of rotation in 3D space. This problem from classical mechanics is well known and solved using an eigenanalysis for the matrix

$$\begin{bmatrix} A & -H & -G \\ -H & B & -F \\ -G & -F & C \end{bmatrix}$$

where

$A = \sum_{i=1}^{n}({y_i}^2 + {z_i}^2)$, $B = \sum_{i=1}^{n}({x_i}^2 + {z_i}^2)$, $C = \sum_{i=1}^{n}({y_i}^2 + {x_i}^2)$, $F = \sum_{i=1}^{n}(y_i z_i)$, $H = \sum_{i=1}^{n}(x_i y_i)$ and $G = \sum_{i=1}^{n}(x_i z_i)$




$${p_i}^2 = \left|\hat{\boldsymbol{l}} \times \boldsymbol{r_i}\right|^2$$

$$\Leftrightarrow p^2 = \left(\left|\hat{\boldsymbol{l}}\right|\left|\boldsymbol{r_i}\right| sin\theta_i \hat{\boldsymbol{n}}_i\right).\left(\left|\hat{\boldsymbol{l}}\right|\left|\boldsymbol{r_i}\right| sin\theta_i \hat{\boldsymbol{n}}_i\right)$$

$$\left|\hat{\boldsymbol{l}}\right|^2 = \alpha^2 + \beta^2 + \gamma^2 = 1$$

$$\left|\hat{\boldsymbol{n}}_i\right|^2 = 1$$

The formulation for this matrix is based on minimizing the moments of inertia $I$ about a arbitrary line $L$ passing through the origin for a particle $P_i$ with unit mass and position vector $\boldsymbol{r_i} = (x_i, y_i, z_i)$. If we consider the perpendicular distance $p$ from the point $P$ to the line $L$ with direction cosines $\hat{\boldsymbol{l}} = (\alpha, \beta, \gamma)$, then

$$I = \sum_{i=1}^{n} {p_i}^2$$

and since ${p_i}^2 = \left|\hat{\boldsymbol{l}} \times \boldsymbol{r_i}\right|^2 = (\beta z_i - \gamma y_i)^2 + (\gamma x_i - \alpha z_i)^2 + (\alpha y_i - \beta x_i)^2$

$$I = \sum_{i=1}^{n}[(\beta z_i - \gamma y_i)^2 + (\gamma x_i - \alpha z_i)^2 + (\alpha y_i - \beta x_i)^2]$$

After simplification the moment of inertia for a set of unit mass particles about a line $L$ reduces to

$$I = A\alpha^2 + B\beta^2 + C\gamma^2 - 2F\beta\gamma - 2G\gamma\alpha - 2H\alpha\beta$$

or written as a quadratic form

$$I = [\alpha \quad \beta \quad \gamma]\begin{bmatrix} A & -H & -G \\ -H & B & -F \\ -G & -F & C \end{bmatrix}\begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix}$$

Thus the problem of finding the minimum moment of inertia, i.e. minimizing the sum of the square perpendicular distances by choosing the appropriate direction cosines is that of minimising $I$ subject to the constraint $\alpha^2 + \beta^2 + \gamma^2 = 1$ , that is, the constraint ensures valid direction cosines are involved in the solution.

Applying the method of Lagrange multiplier to minimising $I$ subject to $\alpha^2 + \beta^2 + \gamma^2 = 1$ leads to the requirement to determine eigenvalues and eigenvectors of

$$\mathbf{X} = \begin{bmatrix} A & -H & -G \\ -H & B & -F \\ -G & -F & C \end{bmatrix}$$

So, having observed the requirement to minimise the sum of squares of perpendicular distances to a line yields a minimum moment of inertia for a given distribution of unit mass particles, how does this relate to the covariance matrix $\boldsymbol{Z}$?

The covariance matrix is formed from the data vectors $\{\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3\}$ as follows:

$$\boldsymbol{Z} = \begin{bmatrix} \boldsymbol{d}_1.\boldsymbol{d}_1 & \boldsymbol{d}_1.\boldsymbol{d}_2 & \boldsymbol{d}_1.\boldsymbol{d}_3 \\ \boldsymbol{d}_1.\boldsymbol{d}_2 & \boldsymbol{d}_2.\boldsymbol{d}_2 & \boldsymbol{d}_2.\boldsymbol{d}_3 \\ \boldsymbol{d}_1.\boldsymbol{d}_3 & \boldsymbol{d}_2.\boldsymbol{d}_3 & \boldsymbol{d}_3.\boldsymbol{d}_3 \end{bmatrix}$$

The matrix $\mathbf{X}$ is formed from the data vectors where $\boldsymbol{d}_1 = (x_1, x_2, x_3, \cdots, x_n)$, $\boldsymbol{d}_2 = (y_1, y_2, y_3, \cdots, y_n)$ and $\boldsymbol{d}_3 = (z_1, z_2, z_3, \cdots, z_n)$ as follows

$$\mathbf{X} = \begin{bmatrix} \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3 & -\boldsymbol{d}_1.\boldsymbol{d}_2 & -\boldsymbol{d}_1.\boldsymbol{d}_3 \\ -\boldsymbol{d}_1.\boldsymbol{d}_2 & \boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_3.\boldsymbol{d}_3 & -\boldsymbol{d}_2.\boldsymbol{d}_3 \\ -\boldsymbol{d}_1.\boldsymbol{d}_3 & -\boldsymbol{d}_2.\boldsymbol{d}_3 & \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_1.\boldsymbol{d}_1 \end{bmatrix}$$

Therefore

$$\boldsymbol{Z} + \boldsymbol{X} = \begin{bmatrix} \boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3 & 0 & 0 \\ 0 & \boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3 & 0 \\ 0 & 0 & \boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3 \end{bmatrix}$$

$$\boldsymbol{X} = -\boldsymbol{Z} + (\boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3)\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

If $\boldsymbol{v}$ is an eigenvector of $\boldsymbol{Z}$ with corresponding eigenvalue $\lambda$ then

$$\boldsymbol{Z}\boldsymbol{v} = \lambda \boldsymbol{v}$$

and so

$$\boldsymbol{X}\boldsymbol{v} = -\boldsymbol{Z}\boldsymbol{v} + (\boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3)\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}\boldsymbol{v} = (-\lambda + \boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3)\boldsymbol{v}$$

Therefore $\boldsymbol{v}$ is also an eigenvector of $\boldsymbol{X}$ with eigenvalue $\omega = -\lambda + \boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3$.

Thus, determining the eigenvectors for $\boldsymbol{Z}$ also solves the problem of determining the direction for a line by minimising the sum of the squares of the distances to that line. The least squares problem solved by working with the eigenvectors of the covariance matrix $\boldsymbol{Z}$ is now clear.

The eigenvalues $\omega$ for the matrix $\boldsymbol{X}$ are the moments of inertia about the axes of rotation defined by the eigenvectors for which the system is in a possible maxima or minima. The smallest eigenvalue for $\boldsymbol{X}$ is the minimum moment of inertia for the given system of unit mass particles. The relationship between the eigenvalues of $\boldsymbol{X}$ and the eigenvalues of $\boldsymbol{Z}$ is essentially an adjustment of the absolute values for the eigenvalues for $\boldsymbol{X}$ relative to a new reference value, namely, half the sum of the extreme moments of inertia for three particles positioned on the three coordinate axes at distances from the origin equal to the magnitude for the three data vectors $\{\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3\}$, respectively. Specially

$$\omega + \lambda = \boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3$$

Further, since the eigenvalues of $\boldsymbol{Z}$ are the roots of the characteristic polynomial

$$\boldsymbol{det}\begin{bmatrix}(\boldsymbol{d}_1.\boldsymbol{d}_1 - \lambda) & \boldsymbol{d}_1.\boldsymbol{d}_2 & \boldsymbol{d}_1.\boldsymbol{d}_3\\ \boldsymbol{d}_1.\boldsymbol{d}_2 & (\boldsymbol{d}_2.\boldsymbol{d}_2 - \lambda) & \boldsymbol{d}_2.\boldsymbol{d}_3\\ \boldsymbol{d}_1.\boldsymbol{d}_3 & \boldsymbol{d}_2.\boldsymbol{d}_3 & (\boldsymbol{d}_3.\boldsymbol{d}_3 - \lambda)\end{bmatrix} = 0$$

The sum of the roots for the cubic polynomial is equal to minus the coefficients of $\lambda^2$, namely, $\boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3$, therefore the three eigenvalues of $\boldsymbol{Z}$ ($\lambda_1, \lambda_2$ and $\lambda_3$ ) are such that

$$\boldsymbol{d}_1.\boldsymbol{d}_1 + \boldsymbol{d}_2.\boldsymbol{d}_2 + \boldsymbol{d}_3.\boldsymbol{d}_3 = \lambda_1 + \lambda_2 + \lambda_3$$

Thus the three eigenvalues of $\boldsymbol{X}$ are $\omega_1 = \lambda_2 + \lambda_3$, $\omega_2 = \lambda_1 + \lambda_3$ and $\omega_3 = \lambda_3 + \lambda_1$.

A point worth highlighting is the eigenvalues of $\boldsymbol{X}$ are physically significant and represent the values for the moments of inertia $I$ about the principal axes. The principal axes are in the directions defined by the eigenvectors of $\boldsymbol{X}$, and since if $\boldsymbol{P}$ is a matrix formed from the eigenvectors of $\boldsymbol{X}$ and $\boldsymbol{\Omega}$ is a diagonal matrix with non-zero elements equal to the, assumed distinct, corresponding eigenvalues of $\boldsymbol{X}$, namely

$$\boldsymbol{\Omega} = \begin{bmatrix}\omega_1 & 0 & 0\\ 0 & \omega_2 & 0\\ 0 & 0 & \omega_3\end{bmatrix}$$

then

$$\boldsymbol{X} = \boldsymbol{P}\boldsymbol{\Omega}\boldsymbol{P}^T$$

Thus, the moments of inertia $I$ about an axis with direction cosines $[\alpha \quad \beta \quad \gamma]$ is given by

$$I = [\alpha \quad \beta \quad \gamma]\boldsymbol{X}\begin{bmatrix}\alpha\\ \beta\\ \gamma\end{bmatrix}$$

$$\Longrightarrow I = [\alpha \quad \beta \quad \gamma]\boldsymbol{P\Omega P}^T\begin{bmatrix}\alpha\\ \beta\\ \gamma\end{bmatrix}$$

If $[\alpha_1 \quad \beta_1 \quad \gamma_1]$ is the eigenvector corresponding to eigenvalue $\omega_1$ then since the eigenvectors are constructed to be orthonormal, that is, $\alpha_i\alpha_j+\beta_i\beta_j + \gamma_i\gamma_j = \begin{cases}1 & i = j\\ 0 & i \neq j\end{cases}$

$$\boldsymbol{P}^T\begin{bmatrix}\alpha_1\\ \beta_1\\ \gamma_1\end{bmatrix} = \begin{bmatrix}\alpha_1 & \beta_1 & \gamma_1\\ \alpha_2 & \beta_2 & \gamma_2\\ \alpha_3 & \beta_3 & \gamma_3\end{bmatrix}\begin{bmatrix}\alpha_1\\ \beta_1\\ \gamma_1\end{bmatrix} = \begin{bmatrix}1\\ 0\\ 0\end{bmatrix} \; and \; similarly \; [\alpha_1 \quad \beta_1 \quad \gamma_1]\boldsymbol{P} = [1 \quad 0 \quad 0]$$

Therefore the moments of inertia about the principal axis with direction $[\alpha_1 \quad \beta_1 \quad \gamma_1]$is

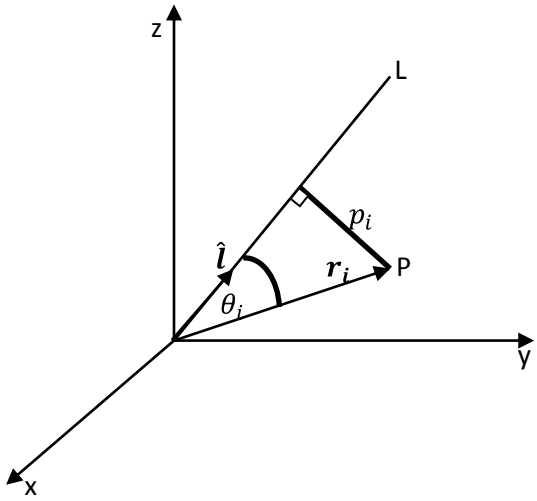
$$I = [\alpha_1 \quad \beta_1 \quad \gamma_1]\boldsymbol{P}\begin{bmatrix}\omega_1 & 0 & 0\\ 0 & \omega_2 & 0\\ 0 & 0 & \omega_3\end{bmatrix}\boldsymbol{P}^T\begin{bmatrix}\alpha_1\\ \beta_1\\ \gamma_1\end{bmatrix} = [1 \quad 0 \quad 0]\begin{bmatrix}\omega_1 & 0 & 0\\ 0 & \omega_2 & 0\\ 0 & 0 & \omega_3\end{bmatrix}\begin{bmatrix}1\\ 0\\ 0\end{bmatrix} = \omega_1$$

## Covariance Matrix and Least Squares Optimisation

While moments of inertia provide a physical interpretation for PCA, the common practice of working with the covariance matrix $\boldsymbol{Z}$ can be understood by following through the logic of minimising the sum of squares of the perpendicular distances from each point in a scatter plot to the principal axis line. If Pythagoras is used to determine the distance from a point in the scatter plot to a line through the origin with direction cosines $\hat{\boldsymbol{l}} = (\alpha, \beta, \gamma)$, the minimisation problem can be expressed as follows.

$$I = \sum_{i=1}^{n} {p_i}^2$$

subject to the constraint $\alpha^2 + \beta^2 + \gamma^2 = 1$




This time, applying Pythagoras theorem to determining the distance $p_i$

$${p_i}^2 = |\boldsymbol{r_i}|^2 - (|\boldsymbol{r_i}|cos\theta_i)^2$$

$$cos\theta_i = \frac{\boldsymbol{r_i}.\hat{\boldsymbol{l}}}{|\boldsymbol{r_i}||\hat{\boldsymbol{l}}|}$$

Since

$$\left|\hat{\boldsymbol{l}}\right|^2 = \alpha^2 + \beta^2 + \gamma^2 = 1$$

$${p_i}^2 = |\boldsymbol{r_i}|^2 - \left(\boldsymbol{r_i}.\hat{\boldsymbol{l}}\right)^2$$

Each point in the scatter plot has coordinates $\boldsymbol{r_i} = (x_i, y_i, z_i)$, therefore

$$p_i{}^2 = x_i{}^2 + y_i{}^2 + z_i{}^2 - (\alpha x_i + \beta y_i + \gamma z_i)^2$$

and

$$I = \sum_{i=1}^{n} (x_i{}^2 + y_i{}^2 + z_i{}^2 - (\alpha x_i + \beta y_i + \gamma z_i)^2)$$

The covariance matrix is derived by applying the method of Lagrange multipliers to include the constraint $\alpha^2 + \beta^2 + \gamma^2 = 1$, namely the optimisation of the parameters $\alpha, \beta \; and \; \gamma$ for the function

$$\Psi = \lambda(\alpha^2 + \beta^2 + \gamma^2 - 1) + I$$

Differentiating with respect to $\alpha$ yields

$$\frac{\partial \Psi}{\partial \alpha} = 2\alpha\lambda + \sum_{i=1}^{n} (-2(\alpha x_i + \beta y_i + \gamma z_i)x_i) = 2\alpha\lambda - 2\alpha \sum_{i=1}^{n} x_i{}^2 - 2\beta \sum_{i=1}^{n} x_i y_i - 2\gamma \sum_{i=1}^{n} x_i \, z_i$$

Equating to zero yields

$$\alpha \sum_{i=1}^{n} x_i{}^2 + \beta \sum_{i=1}^{n} x_i y_i + \gamma \sum_{i=1}^{n} x_i \, z_i = \alpha\lambda$$

Similarly, $\frac{\partial \Psi}{\partial \beta} = 0$ and $\frac{\partial \Psi}{\partial \gamma} = 0$ provides two more equations as follows.

$$\alpha \sum_{i=1}^{n} x_i y_i + \beta \sum_{i=1}^{n} y_i{}^2 + \gamma \sum_{i=1}^{n} y_i \, z_i = \beta\lambda$$

$$\alpha \sum_{i=1}^{n} x_i z_i + \beta \sum_{i=1}^{n} y_i z_i + \gamma \sum_{i=1}^{n} z_i{}^2 = \gamma\lambda$$

Using $\boldsymbol{d}_1.\boldsymbol{d}_1 = \sum_{i=1}^{n} x_i{}^2$, $\boldsymbol{d}_2.\boldsymbol{d}_2 = \sum_{i=1}^{n} y_i{}^2$, $\boldsymbol{d}_3.\boldsymbol{d}_3 = \sum_{i=1}^{n} z_i{}^2$, $\boldsymbol{d}_1.\boldsymbol{d}_2 = \sum_{i=1}^{n} x_i y_i$, $\boldsymbol{d}_1.\boldsymbol{d}_3 = \sum_{i=1}^{n} x_i z_i$ and $\boldsymbol{d}_2.\boldsymbol{d}_3 = \sum_{i=1}^{n} y_i z_i$ and expressing the above simultaneous equations in matrix form the eigenvector problem expressed in terms of the original data vectors reduces as follows.

$$\begin{bmatrix} \boldsymbol{d}_1.\boldsymbol{d}_1 & \boldsymbol{d}_1.\boldsymbol{d}_2 & \boldsymbol{d}_1.\boldsymbol{d}_3 \\ \boldsymbol{d}_1.\boldsymbol{d}_2 & \boldsymbol{d}_2.\boldsymbol{d}_2 & \boldsymbol{d}_2.\boldsymbol{d}_3 \\ \boldsymbol{d}_1.\boldsymbol{d}_3 & \boldsymbol{d}_2.\boldsymbol{d}_3 & \boldsymbol{d}_3.\boldsymbol{d}_3 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = \lambda \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix}$$

Thus, the covariance matrix $\boldsymbol{Z}$ is recovered from the optimisation problem.

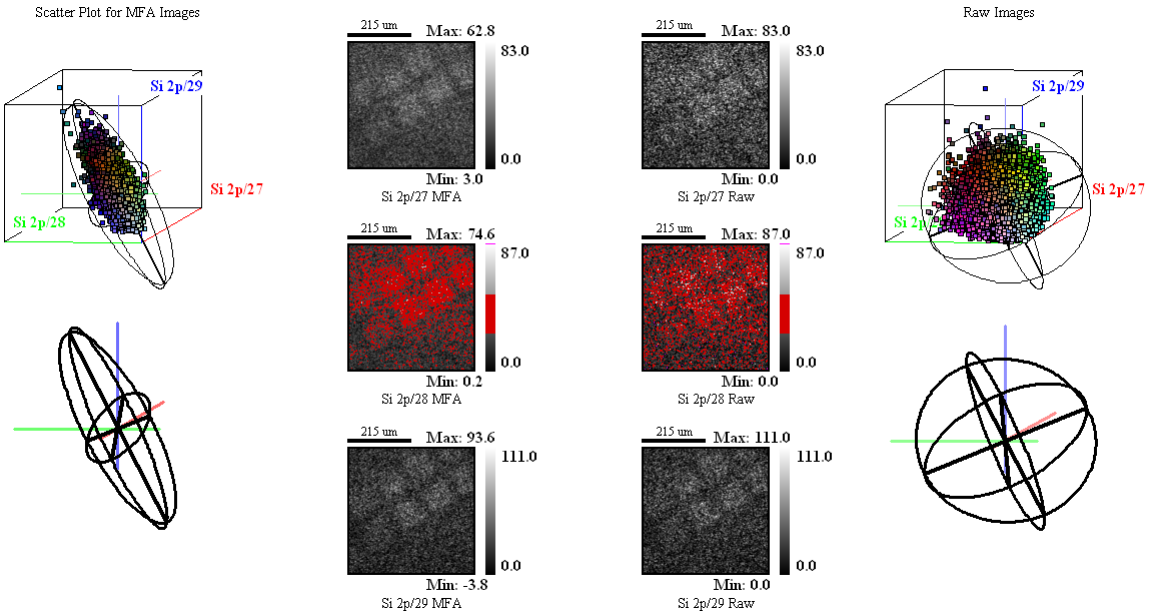
## Visualisation of Principal Axes and Principal Component Vectors

To appreciate the relationship between pixel intensities in an image and the corresponding set of unit mass particles, a set of three images can be displayed as a scatter plot where each point plotted represents the position of a unit mass particle. The following figure depicts three raw images plotted as a scatter plot in a 3D cube. Each pixel from these three raw images provides 3D coordinates for a unit mass particle.

The distribution for the set of unit mass particles defined by the set of image pixels is an indicator for similarity in these images. Three identical non-uniform images when plotted as a scatter plot yield a distribution along the leading diagonal of the coordinate cube. Three images representative of noise resulting from a uniform signal would produce a spherically symmetrical ball of points when viewed as a scatter plot.

The principal axes plotted on a scatter plot show directions about which the moments of inertia takes on extreme values.

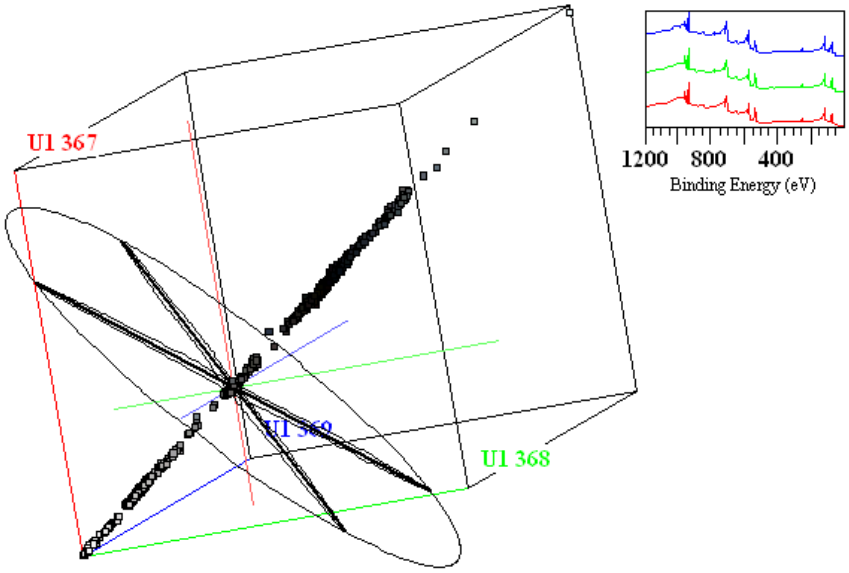
In the following figure, three raw images are displayed together with the MFA enhanced images. To illustrate the transformation performed by the MFA procedure scatter plots based on the raw and MFA are included.




These three raw images are replaced by MFA images formed by projecting onto the two most significant principal directions in the PCA sense of significance. That is, the two directions with largest PCA eigenvalues.

Following processing the entire dataset using the MFA algorithm, the three original images are transformed to a set of images in which the variation is reduced, where the variation eliminated by MFA processing is assumed to be noise. The enhancement for these three images and the change to the pixel distribution is illustrated above. Note how the spherically symmetric scatter plot created from the raw images is transformed to an elliptical shape formed from the corresponding MFA images.

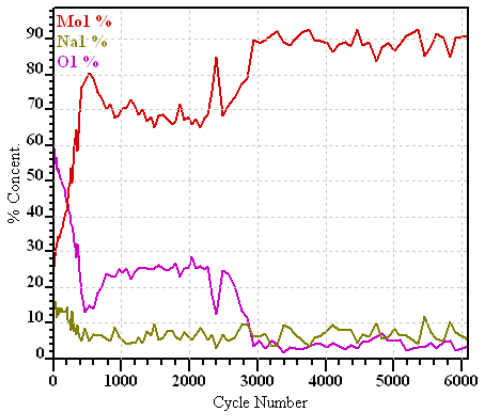
As an alternative to image data, a scatter plot constructed using three spectra taken from a sputter depth profile displaying the principal axes, proportioned using the extreme values for the moments of inertia, show how similar data have a natural direction associated with a system of particles when rotation occurs. The minimum moment of inertia for the set of unit mass particles corresponding to the three spectra points roughly along the cube diagonal.



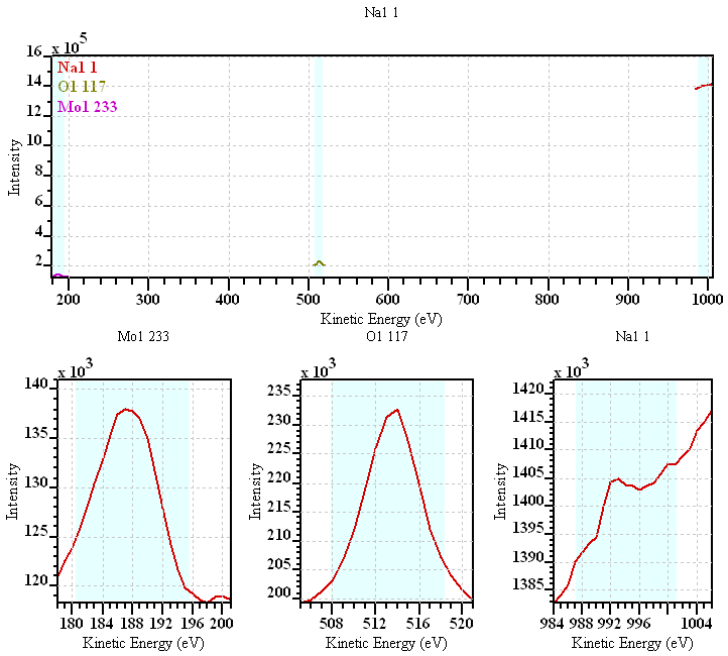

## MFA Applied to Depth Profile Data

A sputter depth profile is potentially appropriate for MFA, particularly if the data is expected to be identical in shape throughout the profile. The example now considered is such a data set, where an Auger depth profile in which sodium is monitored provides a suitable test case for MFA. The sodium signal in this case study is small compared to the other two elements profiled, and what is more the sodium signal is superimposed on large background intensity. Since for pulse counted intensity the noise is expected to increase as the square root of the counts per bin, the sodium Auger peak measured using the same dwell-time as the other peaks is subject to poor signal to noise by comparison. For the sample in question, it was expected the sodium signal would diminish tending to zero. A simple analysis based on the raw data failed to convey the expected result to anyone unfamiliar with Auger data.

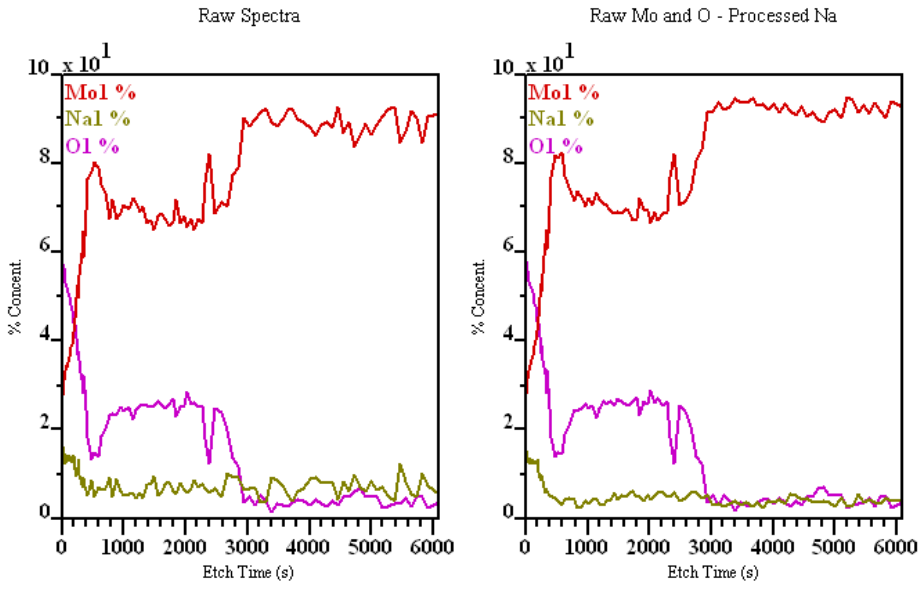
The following profile presents the result of profiling three elements, namely, oxygen, molybdenum and sodium. Apart from apparently including sodium signal greater than the oxygen signal, the scaling of noisy sodium before combining with the other two signals in an atomic concentration calculation injects noise into the molybdenum trace even though the measurement of the molybdenum peak had good signal to noise characteristics. As an attempt to improve the profile from the data set as given, only the sodium spectra will be processed using MFA.



To illustrate the nature of the problem examples of the three spectra in direct mode are displayed below. The sodium peak is clearly poorly defined and small compared to the background signal.



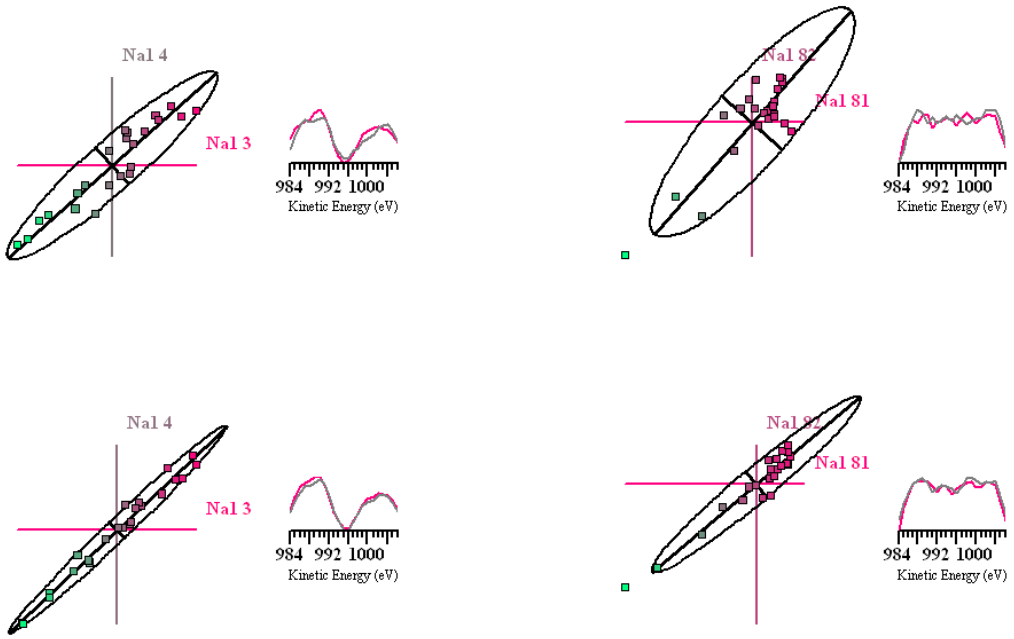

Processing of the Na signal is performed using one eigenvector to perform the MFA step rather than two as described in the introduction section. The reason for using only one eigenvector per MFA step is the Na spectra are very similar throughout the profile. The following two profiles illustrate the improvement in the overall profile even though only the Na spectra are enhanced using MFA.




Note how all profile traces benefit from processing the Na signal only. Scaling a noisy Na signal before combining with the better defined Mo and O intensities to form the atomic concentration causes the uncertainty in the sodium to appear in all three traces.

Processing the Na spectra was performed on the direct spectra. Once noise is reduced by applying the MFA algorithm to the direct spectra, the resulting sodium spectra are differentiated and moved

to the original VAMAS file contain the raw depth profile spectra. Identical regions are used to create the sodium traces for both profiles above so the only change in these profiles is due to the MFA alterations to the direct sodium spectra.




Scatter plots for successive spectra in the profile taken from regions with and without sodium illustrate how the sodium spectra change before (top plots) and after (bottom plots) MFA treatment. The reduction in noise is indicated by the narrowing of the elliptical boundaries about the principal axes.