Determining coefficients using matrix linear algebra

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The approach outlined requires an understanding of matrix linear algebra in order to calculate the numeric solutions and contributions of input variables to predict outputs. Below, I have provided a brief lesson, with a small example, so that scientists can better understand our approach.

Basic notations

Matrix: a rectangular array of values.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Vector: a matrix having single column.

Matrix multiplication:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & \cdots & \cdots & a_{11}b_{14} + a_{12}b_{24} \\ a_{21}b_{11} + a_{22}b_{21} & \cdots & \cdots & a_{21}b_{14} + a_{22}b_{24} \\ a_{31}b_{11} + a_{32}b_{21} & \cdots & \cdots & a_{31}b_{14} + a_{32}b_{24} \end{bmatrix}$$

An example

Matrix A represents the library of fingerprints with each column representing a single case and each row representing the value of a specific variable:

$a_{11} = 3$ $a_{12} = 5$
$a_{21} = 8$ $a_{22} = 4$
$a_{31} = 17$ $a_{32} = 13$

Matrix B represents the actual output corresponding to a case:

b_1=53.1
b_2=75.8
b_3=193.2

Matrix C represents the weighing factors x and y for each fingerprint, which we will calculate:
c_1=x
c_2=y

The relationship among the matrices can be represented as:

Matrix A   Matrix C   Matrix B

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} * \begin{matrix} x \\ y \end{matrix} = \begin{matrix} b_1 \\ b_2 \\ b_3 \end{matrix}$$

Filling in the values of the Matrix A and B:

$$\begin{bmatrix} 3 & 5 \\ 8 & 4 \\ 17 & 13 \end{bmatrix} * \begin{matrix} x \\ y \end{matrix} = \begin{matrix} 53.1 \\ 75.8 \\ 193.2 \end{matrix}$$

These matrices can be represented as the following equations:

$3x + 5y = 53.1$
$8x + 4y = 75.8$
$17x+13y=193.2$

To calculate approximate values Matrix C, we first need to convert A*C=B to

A^T*A*C=A^T*B, where superscript 'T' in A^T represents the transposed matrix A.

A^T*A:

$$\begin{bmatrix} 3 & 8 & 17 \\ 5 & 4 & 13 \end{bmatrix} * \begin{bmatrix} 3 & 5 \\ 8 & 4 \\ 17 & 13 \end{bmatrix} = \begin{bmatrix} 3*3+8*8+17*17 & 5*3+4*8+13*17 \\ 5*3+4*8+13*17 & 5*5+4*4+13*13 \end{bmatrix} = \begin{matrix} 362 & 268 \\ 268 & 210 \end{matrix}$$

A^T*B:

$$\begin{bmatrix} 3 & 8 & 17 \\ 5 & 4 & 13 \end{bmatrix} * \begin{bmatrix} 53.1 \\ 75.8 \\ 193.2 \end{bmatrix} = \begin{bmatrix} 3*53.1+8*75.8+17*193.2 \\ 5*53.1+4*75.8*13*193.2 \end{bmatrix} = \begin{matrix} 4048 \\ 3078 \end{matrix}$$

Hence, in the form $A*A^T*C=A^T*B$:

$362x + 268y = 4048$
$268x + 210y = 3078$

Second, we need to invert matrix (i.e., A to A^{-1}) to solve for matrix C (i.e., *x* and *y*). The superscript '-1' in A^{-1} represents the inverted matrix A.

Tip: How to inverse a matrix.

$$\text{inv}\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} \text{d/((a * d) - (b * c))} & \text{b/((b * c) - (a * d))} \\ \text{c/((b * c) - (a * d))} & \text{a/((a * d) - (b * c))} \end{bmatrix}$$

Inverting the expression $(A^T * A)^{-1}$:

$$\text{inv}\begin{bmatrix} 362 & 268 \\ 268 & 210 \end{bmatrix} = \text{inv}\begin{bmatrix} 0.05 & -0.064 \\ -0.064 & 0.086 \end{bmatrix}$$

Recall that $A*A^T*C=A^T*B$.

We can solve Matrix C by:

$$(A^T * A)^{-1}*A^T*A*C = (A^T * A)^{-1} * A^T * B$$

and rearranging taking into account that $(A^T * A)^{-1}*A^T*A$ is a unity matrix:

$$C = (A^T * A)^{-1} * A^T * B$$

$$C = \begin{bmatrix} 0.05 & -0.064 \\ -0.064 & 0.086 \end{bmatrix} * \begin{matrix} 4048.4 \\ 3079 \end{matrix} = \begin{matrix} 5.958 \\ 7.064 \end{matrix}$$

Hence, x=5.958 and y=7.064.

To make sure that these solutions make sense, we need to plug them back into the original equations.

$3x + 5y = 53.1$	17.874 +35.32 = 53.194
$8x + 4y = 75.8$	47.664 + 28.256 = 75.92
$17x+13y=193.2$	101.286 + 91.832 = 193.118

Determining the difference between calculated and actual values?

	Calculated	Actual	Difference
Probe 1	53.194	53.1	0.094
Probe 2	75.92	75.8	0.12
Probe 3	193.118	193.2	-0.082

There was little difference between calculated and actual values of probe intensities of the mixtures. Rather than determine the difference, we calculated the R^2 value of the regression line of calculated versus actual values. The value of the R^2 value can be used to account for variability in the solution. If the R^2 value is 0.90, we can say that the numerical solution accounts for ~90% of the variability of the data, with the rest being attributed to noise or other unexplained factors.

Determining the proportion of Fingerprint 1 and 2 was in the solution?
The way to determine relative contribution of each fingerprint is the following:

Fingerprint 1:

$$F1 = \frac{x}{x + y} = \frac{5.958}{5.958 + 7.064} \approx 0.46$$

Fingerprint 2:

$$F1 = \frac{y}{x + y} = \frac{7.064}{5.958 + 7.064} \approx 0.54$$