Detour to Covariance Matrix and Principal Component Analysis: A simple case of two variables and a simple problem of two coupled simple harmonic oscillators

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1 What is a Covariance Matrix?

Let's illustrate the concept of the covariance matrix for the following data table for two language scores for five team members as given below:

Table 0. Score of Two Languages for 5 Project Team Members

QIV Project Team Member	English Score	Urdu Score
Arafat	10	0
Muneeb	20	10
Aswer	30	0
Suhail	40	70
Javaid	50	70

Let's break down the steps to calculate the covariance matrix in detail.

1. Calculate the Mean of Each Language's Scores:

- Mean of English Scores:

$$\bar{X} = \frac{10 + 20 + 30 + 40 + 50}{5} = \frac{150}{5} = 30$$

- Mean of Urdu Scores:

$$\bar{Y} = \frac{0 + 10 + 0 + 70 + 70}{5} = \frac{150}{5} = 30$$

2. Calculate the Differences from the Mean for Each Score:

- Differences for English Scores:

$$X_i - \bar{X} = [10 - 30, 20 - 30, 30 - 30, 40 - 30, 50 - 30] = [-20, -10, 0, 10, 20]$$

- Differences for Urdu Scores:

$$Y_i - \bar{Y} = [0 - 30, 10 - 30, 0 - 30, 70 - 30, 70 - 30] = [-30, -20, -30, 40, 40]$$

3. Calculate the Covariance for Each Pair of Variables:
The covariance between two variables X and Y is given by:

$$\text{Cov}(X, Y) = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y})$$

where n is the number of observations.
- Covariance between English and English (Variance of English):

$$\text{Cov}(X, X) = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X})^2 = \frac{1}{4} \left[(-20)^2 + (-10)^2 + 0^2 + 10^2 + 20^2\right]$$

$$= \frac{1}{4} [400 + 100 + 0 + 100 + 400] = \frac{1000}{4} = 250$$

- Covariance between Urdu and Urdu (Variance of Urdu):

$$\text{Cov}(Y, Y) = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i - \bar{Y})^2 = \frac{1}{4} \left[(-30)^2 + (-20)^2 + (-30)^2 + 40^2 + 40^2\right]$$

$$= \frac{1}{4} [900 + 400 + 900 + 1600 + 1600] = \frac{5400}{4} = 1350$$

- Covariance between English and Urdu:

$$\text{Cov}(X, Y) = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y}) = \frac{1}{4} [(-20)(-30) + (-10)(-20) + 0(-30) + 10(40) + 20(40)]$$

$$= \frac{1}{4} [600 + 200 + 0 + 400 + 800] = \frac{2000}{4} = 500$$

4. Form the Covariance Matrix:
The covariance matrix is a symmetric matrix where the diagonal elements represent the variances of each variable, and the off-diagonal elements represent the covariances between variables.

$$\text{Covariance Matrix} = \begin{pmatrix} \text{Cov}(X, X) & \text{Cov}(X, Y) \\ \text{Cov}(X, Y) & \text{Cov}(Y, Y) \end{pmatrix} = \begin{pmatrix} 250 & 500 \\ 500 & 1350 \end{pmatrix}$$

Covariance Matrix:

$$\begin{pmatrix} 250 & 500 \\ 500 & 1350 \end{pmatrix}$$

This matrix encapsulates the variances and covariances of the scores for English and Urdu. The diagonal elements (250 and 1350) represent the variances of English and Urdu scores, respectively. The off-diagonal elements (both 500) represent the covariance between the English and Urdu scores.

2 PCA: Finding Eigen Values and Eigen Vectors of a Covriance Matrix

Let's find the eigenvalues and eigenvectors of the covariance matrix:

$$\text{Cov} = \begin{pmatrix} 250 & 500 \\ 500 & 1350 \end{pmatrix}$$

Step 1: Find the Eigenvalues The eigenvalues λ are found by solving the characteristic equation:

$$\det(\text{Cov} - \lambda I) = 0$$

where I is the identity matrix.

First, subtract λ from the diagonal elements of Cov:

$$\begin{pmatrix} 250 - \lambda & 500 \\ 500 & 1350 - \lambda \end{pmatrix}$$

Then, find the determinant of this matrix:

$$\det(\begin{pmatrix} 250 - \lambda & 500 \\ 500 & 1350 - \lambda \end{pmatrix}) = (250 - \lambda)(1350 - \lambda) - (500)(500)$$

Expand and simplify:

$$(250 - \lambda)(1350 - \lambda) - 250000 = 0$$

$$250 \cdot 1350 - 250\lambda - 1350\lambda + \lambda^2 - 250000 = 0$$

$$337500 - 1600\lambda + \lambda^2 - 250000 = 0$$

$$\lambda^2 - 1600\lambda + 87500 = 0$$

Step 2: Solve the Quadratic Equation Solve the quadratic equation $\lambda^2 - 1600\lambda + 87500 = 0$:

$$\lambda = \frac{1600 \pm \sqrt{1600^2 - 4 \cdot 87500}}{2}$$

$$\lambda = \frac{1600 \pm \sqrt{2560000 - 350000}}{2}$$

$$\lambda = \frac{1600 \pm \sqrt{2210000}}{2}$$

$$\lambda = \frac{1600 \pm 1486.61}{2}$$

Thus, the two eigenvalues are:

$$\lambda_1 = \frac{1600 + 1486.61}{2} = 1543.31$$

$$\lambda_2 = \frac{1600 - 1486.61}{2} = 56.69$$

Step 3: Find the Eigenvectors Next, we need to find the eigenvectors corresponding to each eigenvalue.

For $\lambda_1 = 1543.31$: Solve $(\text{Cov} - \lambda_1 I)\vec{v} = 0$:

$$\begin{pmatrix} 250 - 1543.31 & 500 \\ 500 & 1350 - 1543.31 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

$$\begin{pmatrix} -1293.31 & 500 \\ 500 & -193.31 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

This simplifies to:

$$-1293.31x + 500y = 0$$

$$500x - 193.31y = 0$$

Both equations are multiples of each other. Let's use the first equation:

$$-1293.31x + 500y = 0$$

$$y = \frac{1293.31}{500}x = 2.58662x$$

So, one eigenvector is:

$$\vec{v_1} = \begin{pmatrix} 1 \\ 2.58662 \end{pmatrix}$$

For $\lambda_2 = 56.69$: Solve $(\text{Cov} - \lambda_2 I)\vec{v} = 0$:

$$\begin{pmatrix} 250 - 56.69 & 500 \\ 500 & 1350 - 56.69 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

$$\begin{pmatrix} 193.31 & 500 \\ 500 & 1293.31 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

This simplifies to:

$$193.31x + 500y = 0$$

$$500x + 1293.31y = 0$$

Both equations are multiples of each other. Let's use the first equation:

$$193.31x + 500y = 0$$

$$y = -\frac{193.31}{500}x = -0.38662x$$

So, the other eigenvector is:

$$\vec{v_2} = \begin{pmatrix} 1 \\ -0.38662 \end{pmatrix}$$

Step 4: Diagonalization To diagonalize the covariance matrix, we use the eigenvalues and eigenvectors to form the matrices P and D:

$$P = \begin{pmatrix} 1 & 1 \\ 2.58662 & -0.38662 \end{pmatrix}$$

$$D = \begin{pmatrix} 1543.31 & 0 \\ 0 & 56.69 \end{pmatrix}$$

The covariance matrix can be diagonalized as:

$$\text{Cov} = PDP^{-1}$$

This shows the covariance matrix in its diagonal form, where the eigenvalues are on the diagonal, and P contains the eigenvectors as its columns.

3 Interpreting the Results Graphically and Geometrically

4 Pedagogic Example from 11th Class Physics: Linking Problem of Two Coupled Simple Harmonic Oscillators with Principal Component Analysis

The problem of small oscillations, when expressed using matrices, results in an eigenvalue problem that requires simultaneously diagonalizing two real symmetric matrices. Although there is a geometric way to understand this process, it is usually difficult to visualize because of the complex, multi-dimensional coordinate transformations involved. In this part of the tutorial, we use a simple model with just three springs and two masses attached in a way to make one dimentional chain and make the coordinate transformations two-dimensional and easy to visualize. A series of plane diagrams will illustrate how the diagonalization is achieved for this model problem. This in turn illustrates in an elegant way some of the foundational concepts behind one of the most power ML techniques called as Principal Component Analysis (PCA).

The theory of small oscillations is discussed in many mechanics textbooks and has been featured in several articles. The theory is most clearly explained using matrices, where finding the normal modes means diagonalizing two real symmetric matrices that represent kinetic and potential energies. The steps for this diagonalization are straightforward, and students typically solve these problems without difficulty. However, students often miss the interesting geometric interpretation of the diagonalization process and its connection with PCA. This tutorial aims to help students understand this geometric view, enhancing their overall grasp of the subject as well as comprehend some core concepts behind PCA. The geometric explanation mentioned earlier is accurately described in at least two textbooks [1,2], but the complex transformations and lack of diagrams make it difficult to understand. In this tutorial, we use a simple model with just two spring-mass systems which are coupled to make the geometric interpretation clearer. Moreover, the connection to PCA is made smoothly for the first time to the best of our knowledge. We provide a series of diagrams [Figs.

1(a)-(d) below] to help visualize the process. With this clear example, students should find it easier to understand how the PCA procedure works for systems with two or more masses and springs. Unlike the current problem, the geometric interpretation of diagonalizing a single real symmetric matrix is well-known. Students may have seen this when finding the principal axes and moments of inertia of an irregular body: they understand that the diagonalization process involves rotating the coordinate axes to match the symmetry axes of the inertia ellipsoid. However, this straightforward interpretation doesn't apply to the small oscillation problem. Here, diagonalization is done that allows the kinetic energy matrix (represented by a circle) which remains unchanged and the potential energy ellipse is rotated to align with the coordinate axes. The main idea of this tutorial is shown in Fig. 1, which is the key part of the explanation. Just looking at this figure for a few minutes might help you understand the concept without needing too many words. However, we also provide a detailed explanation below. We have organized it so you can read and understand this tutorial on its own, without needing to refer to another text or article or for that matter any other resource.

5 Illustrating Diagonalisation Process: Geometrical Interpretati

The total energy for small oscillations due to two coupled simple harmonic oscillators (Fig.2), can be written as follows

$$Total \quad Energy : E = K.E. + P.E.$$

$$E = \frac{1}{2m_1}p_1^2 + \frac{1}{2m_2}p_2^2 + \frac{1}{2}k_1x_1^2 + \frac{1}{2}k_2x_2^2 + k_{12}x_1x_2$$

Where x_1, x_2 are the position coordinates and p_1, p_2 are corresponding momenta of m_1, m_2 respectively. k, k_{12} are spring constants. Now use $m_1 = m_2 = M = 1$, $k_1 = \omega_1^2$, $k_2 = \omega_2^2$ and $k_{12} = \omega_{12}^2$, in above equation we get the following energy equation for two coupled harmonic oscillators.

$$E = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \frac{1}{2}\omega_1^2x_1^2 + \frac{1}{2}\omega_2^2x_2^2 + \omega_{12}^2x_1x_2$$

$$E = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \frac{1}{2}\omega_1^2x_1^2 + \frac{1}{2}\omega_2^2x_2^2 + \frac{1}{2}\omega_{12}^2x_1x_2 + \frac{1}{2}\omega_{21}^2x_2x_1 \tag{1}$$

Eq.(1) can be written more compactly in matrix form as

$$E = \frac{1}{2}\begin{pmatrix} p_1 & p_2 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} x_1 & x_2 \end{pmatrix}\begin{pmatrix} \omega_1^2 & \omega_{12}^2 \\ \omega_{21}^2 & \omega_2^2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{2}$$

Where P.E. and K.E. matrices are

$$K = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad V = \begin{pmatrix} \omega_1^2 & \omega_{12}^2 \\ \omega_{21}^2 & \omega_2^2 \end{pmatrix}. \tag{3}$$

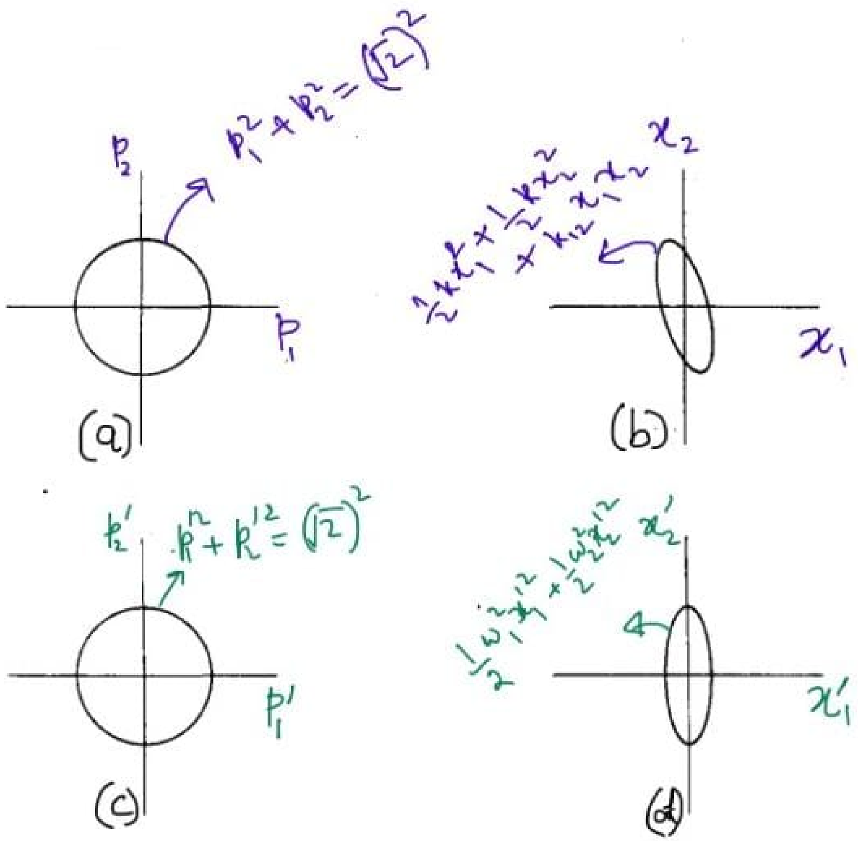

Figure 1: Geometrical representation of kinetic and potential energy quadratic forms for a system with coupled harmonic oscillators: (a) kinetic energy circle given in Eq.(1); (b) potential energy ellipse given in Eq.(1); (c) kinetic energy circle at end of rotation; and (d) potential energy ellipse at end of the procedure/method/diagonalisation. See text for a detailed explanation.

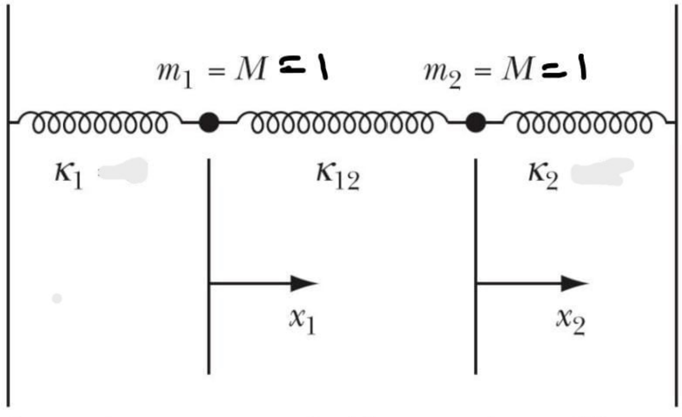

Figure 2: Two coupled harmonic oscillators.

Now any positive definite quadratic form $F(x,y) \equiv p_1x^2 + p_2x_2^2$ gives rise to the equation $F(x,y) = 0$, which can be plotted in the space of p_1, p_2 as a circle [represented by Fig.1(a) in momentum space and mathematically by first two terms of Eq.(1)]. The quadratic form corresponding to V [represented by Fig.1(b) in coordinate space and mathematically by last three terms of Eq.(1)]. Since K matrix is diagonal and is lined up symmetrically with momentum axes p_1, p_2 whereas V matrix is non-diagonal and hence is not lined up with coordinate axes x_1, x_2.

We wish to find a matrix A that diagonalises V and leave K unchanged as it's already diagonal

$$A^TKA = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad A^TVA = \begin{pmatrix} \lambda_1 & 0 \\ 0^2 & \lambda_2 \end{pmatrix}. \tag{4}$$

We shall now show below how to construct such a matrix and establish λ_1 and λ_2 that are the squares of the normal mode frequencies; the connection between the original and normal mode coordinates will also be clear in the process and last but not the least which is indeed the upshot as well of this tutorial, viz., connection to PCA will be made crystal clear.

5.1 Magic by Diagonalisation Procedure

We proceed to the construction of A through following procedure.

Perform a rotation to new coordinates x_1', x_2'in which K remains unchanged and V diagonal. This coordinate transformation is described by the following equations

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \end{pmatrix} \tag{5}$$

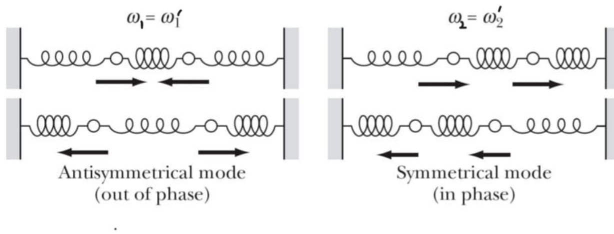

Figure 3: Normal modes of oscillation.

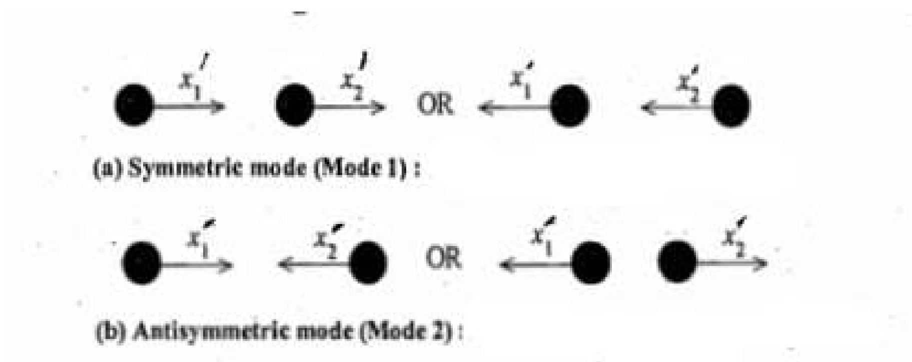

Figure 4: Normal modes of oscillation.

The new kinetic and potential energy matrices after this transformation are

$$K = A^T K A, \qquad V^N = A^T V A \tag{6}$$

The angle θ in Eq.(5) is chosen such that $V_{12}^N = 0$(the $V_{21}^N = 0$) also.Denoting the diagonal elements of V^N by $V_{11}^N = \lambda_1 = {\omega_1'}^2$ and $V_{22}^N = \lambda_2 = {\omega_2'}^2$, the total energy in the new coordinates becomes

$$E = \frac{1}{2}{p_1'}^2 + \frac{1}{2}{p_2'}^2 + \frac{1}{2}{\omega_1'}^2{x_1'}^2 + \frac{1}{2}{\omega_2'}^2{x_2'}^2 \tag{7}$$

The effect of the transformation Eq.(5) is to rotate the potential energy ellipse so that its major and minor axes line up with the new coordinate axes [see Fig. 1(d)]. The kinetic energy being a circle, remains unaffected in the rotation process [see Fig. 1(c)]. This completes the task of diagonalising potential energy matrix.

It is clear that x_1', x_2' are normal coordinates because the total energy Eq.(7) is uncoupled in them. These normal modes of vibration are in Fig.3 below

In other words, we can imagine that the coupled system of oscillators now behaves as two independent oscillators as shown in Fig.4 below

6 Connection of Physics of Two Coupled Harmonic Oscillators (TCHO) with Principal Component Analysis (PCA)

Mapping of Physics Problem (2 CQHO) and Data Science Problem (PCA)		
Steps to Solve Problem from Physics (2 CQHO) and Data Science (PCA)	Physics Example: Diagonalising Coupling Model Matrix V of Two Coupled Harmonic Oscillators Eqn.(3).	Data Science Example: Data of Language Scores of 5 Project Team Members
1. Identifying Covariance Matrix in the domain of Physics and Data Science	V is covariance matrix here consisting of Model Couplings like $\omega_1^2(t)$, $k_{12}(t)$, ,$\omega_2^2(t)$ etc.	The covariance matrix Cov captures the concept or idea of variation of a chunk of data like scores of two languages for five persons.
2. Symmetricity of Covariance Matrix	Potential Energy Matrix V is a symmetric matrix as shown in (3).	The covariance matrix Cov is also always a symmetric matrix.
3. Similarity Transformation (ST) for Diagonising Symmetric Covariance Matricies V and Cov	Here we diagonalise Potential Energy Matrix V with ST, viz., Rotation Matrix as given in Eq(5).	Here we diagonalise Coviariance Matrix Cov with ST as shown in Section 2.
4. Eigen Values after diagonalising Symmetric Covariance Matricies V and Cov	Diagonal elements here are called normal frequencies here, viz., $\omega_1^{'}$ and $\omega_2^{'}$.	Diagonal elements here are called principal components ,viz.,PC_1(Language ability) and PC_2 (to be interpreted, first guess is language exposure)
5. Eigen Vectors after diagonalising Symmetric Covariance Matricies V and Cov	Here they are called normal coordinate axes for decoupled 2 harmonic oscillators.	Here we can call these Principal Component axes as Language Ability axis and Language Exposure Axis

7 Conclusion