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

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Abstract

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 two spring and two masses attached 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).

1 Introduction

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 [1,2,3], 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 through a general linear transformation that includes deformations (like stretching and compressing) as well as rotations. This extra flexibility allows the kinetic energy matrix (represented by an ellipse) to be transformed into a circle before 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.

2 Illustrating Diagonalisation Process: Geometrical Interpretation and Connection with PCA

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

$$TotalEnergy : E = K.E. + P.E.$$

$$E = \frac{1}{2m_1}p_1^2 + \frac{1}{2m_2}p_2^2 + \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 + k_{12}x_1x_2$$

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 $m_1 = m_2 = M = 1$, $k = \omega^2$, and $k_{12} = \omega_{12}^2$, in above equation we get the following energy equation for two coupled harmonic oscillators.

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

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

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

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

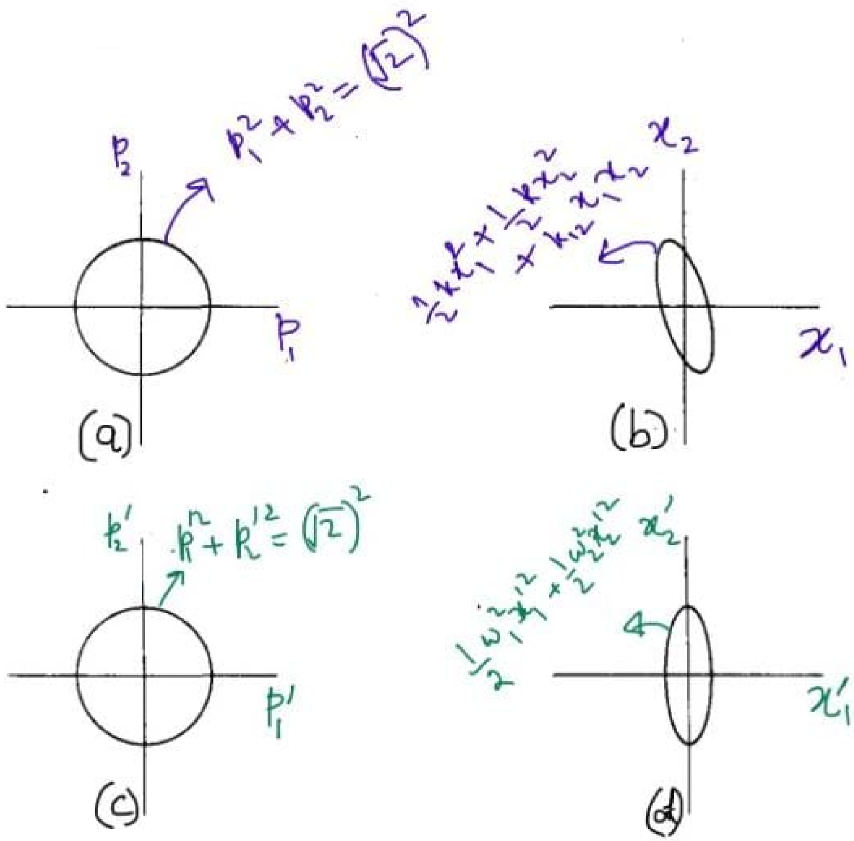

Figure 1: Geometrical representation of kinetic and potential energy quadratic forms for a system with coupled harmonic oscillators: (a) kinetic energy circle given in Eq.(1); (b) potential energy ellipse given in Eq.(1); (c) kinetic energy circle at end of rotation; and (d) potential energy ellipse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

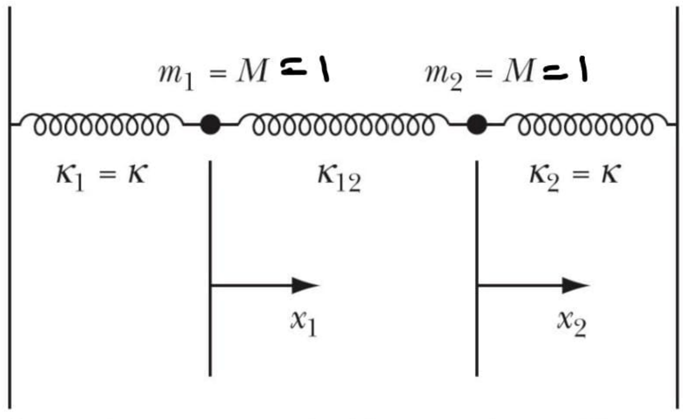

Figure 2: Two coupled harmonic oscillators.

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

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

Now any positive definite quadratic form $F(x, y) \equiv p_1 x^2 + p_2 x_2^2$ 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

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

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.

3 Magic by Diagonalisation Procedure

We proceed to the construction of A through following procedure.

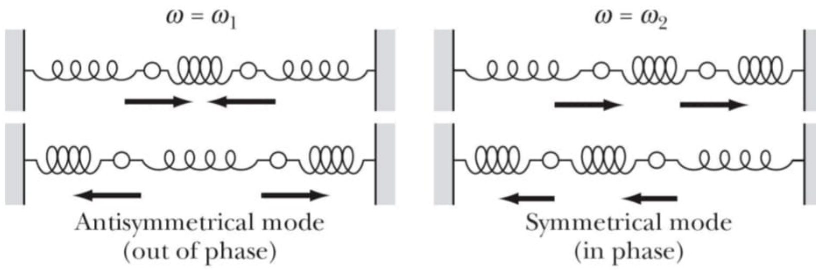

Figure 3: Normal modes of oscillation.

Perform a rotation to new coordinates x'_1, x'_2in which K remains unchanged and V diagonal. This coordinate transformation is described by the following equations

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix} \tag{5}$$

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 $V^N_{12} = 0$(the $V^N_{21} = 0$)$also$.Denoting the diagonal elements of V^N by $V^N_{11} = \lambda_1 = \omega_1^2$ and $V^N_{22} = \lambda_2 = \omega_2^2$, 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

4 Detour to PCA: A simple case of two variables

Let's consider two variables representing scores for two batsmen A and B and having the distribution as shown in Table 1.

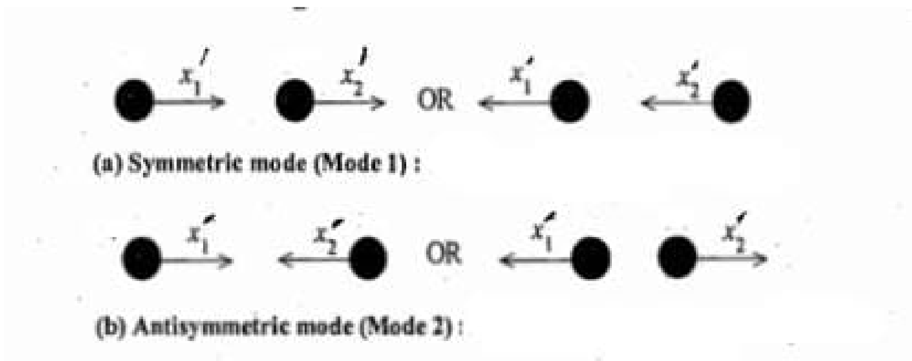

Figure 4: Normal modes of oscillation.

Table 1. Score of Two Batsmen A and B for 5 Cricket Matches		
Match	Batsman A	Batsman B
1	10	0
2	20	10
3	30	0
4	40	70
5	50	70

So which batsmen is performing better. To make sense of it we need to calculate some quantity which can quantify the consistency or dispersion or spread in the distribution. One such quantify is called variance.

Let's calculate the variance through Table 2

Table 2. Finding Variance and Covariance of Batsmen A and B for 5 Cricket Matches							
Match	A	B	$(X_A - \bar{X}_A)$	$(X_A - \bar{X}_A)^2$	$(X_B - \bar{X}_B)$	$(X_B - \bar{X}_B)^2$	$(X_A - \bar{X}_A)(X_B - \bar{X}_B)$
1	10	0	-20	400	-30	900	600
2	20	10	-10	100	-20	400	200
3	30	0	0	0	0	0	0
4	40	70	10	100	-40	1600	-400
5	50	70	20	400	-40	1600	-800
Total				1000		3500	-400

Covariance of a variable with itself is called as variance and that is what is we calculated in the begging for two batsmen A and B.

Once we have covariance, we can go and define covariance matrix as follows for two batsmen

Table 3. Covariance Matrix for Scores of Two Batsmen A and B for 5 Cricket Matches

Covariance	Batsman A	Batsman B
Batsman A	1	-0.21
Batsman B	-0.21	1

5 Connection of P.E. Matrix V of Two Coupled Harmonic Oscillators (TCHO) with Principal Component Analysis (PCA)

Mapping of P.E of TCHO in Mechanics with PCA in Data Science		
Propertry	P.E Matrix V of Two Coupled Harmonic Oscillators.	PCA for Scores of Two Batsmen A and B
1. Covariance	Captures the propoetionality constant of Hook's Law k and k_{12} of two three springs.	Captures the concept or idea of variation of a chunk of data like scores of two batsmen for five matches.
2. Symmetric Matrix	PE Matrix is a symmetric matrix as shown in Eq(3).	The covariance matrix used in PCA is also always a symmetric matrix as shown in Table 3.
3. Similarity Transformation (ST) for Diagonising Symmetric Matrix	Here we diagonalise PE Matrix V with ST, viz., Rotation Matrix as given in Eq(5).	Here we diagonalise Coviariance Matrix with ST as shown in Table 3.
4. Eigen Values of P.E. Matrix V/Covariance Matrix in Table 3	Diagonal elements are called normal frequencies here, viz., ω_1 and ω_2.	Diagonal elements are called principal components here,viz.,PC_1 and PC_2
5. Eigen Vectors of P.E. Matrix V/Covariance Matrix in Table 3	Here they are called normal coordinate axes.	Here we can call them Principal Component axes