Principal Component Analysis (PCA)

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Introduction to PCA

Principal Component Analysis (PCA) is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components. This transformation is defined in such a way that the first principal component has the largest possible variance (that is, accounts for as much of the variability in the data as possible), and each succeeding component in turn has the highest variance possible under the constraint that it is orthogonal to the preceding components.

Key Concepts: Eigenvectors and Eigenvalues

- **Eigenvectors (Principal Components):** These are the directions (axes) along which the data varies the most. They are orthogonal to each other. The first eigenvector (PC1) points in the direction of the largest variance, the second (PC2) in the direction of the second largest variance, and so on.
- **Eigenvalues:** Each eigenvector has a corresponding eigenvalue, which represents the magnitude of the variance along that eigenvector. A larger eigenvalue indicates that its corresponding eigenvector captures more variance in the data, making it a more "important" principal component.

Real-World Example: Student Performance Data

Let's consider a small dataset of students, where we have two features: "Study Hours per Week" and "Exam Score." We expect these two variables to be positively correlated.

Sample Data

Our dataset X is:

Student	**Study Hours** (x_1)	**Exam Score** (x_2)
1	10	60
2	12	65
3	15	75
4	18	80
5	20	88
6	22	92
7	25	95

Detailed Calculation Steps for Eigenvectors and Eigenvalues

To find the principal components (eigenvectors) and their corresponding variances (eigenvalues), we follow these steps:

Step 1: Center the Data

First, we need to subtract the mean of each feature from its respective values.

- **Mean of Study Hours ($\bar{x}_1$):**

$$\bar{x}_1 = \frac{10 + 12 + 15 + 18 + 20 + 22 + 25}{7} = \frac{122}{7} \approx 17.43$$

- **Mean of Exam Score ($\bar{x}_2$):**

$$\bar{x}_2 = \frac{60 + 65 + 75 + 80 + 88 + 92 + 95}{7} = \frac{555}{7} \approx 79.29$$

Now, we create the centered data matrix X_c by subtracting the means. To ensure the table fits, we'll use slightly abbreviated column headers:

Student	Centered Hours (Δx_1)	Centered Score (Δx_2)
1	-7.43	-19.29
2	-5.43	-14.29
3	-2.43	-4.29
4	0.57	0.71
5	2.57	8.71
6	4.57	12.71
7	7.57	15.71

Step 2: Calculate the Covariance Matrix

The covariance matrix Σ for two variables x_1 and x_2 is given by:

$$\Sigma = \begin{pmatrix} \text{Var}(x_1) & \text{Cov}(x_1, x_2) \\ \text{Cov}(x_2, x_1) & \text{Var}(x_2) \end{pmatrix}$$

Where:

$$\text{Var}(x) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2$$

$$\text{Cov}(x_1, x_2) = \frac{1}{n-1} \sum_{i=1}^{n} (x_{1i} - \bar{x}_1)(x_{2i} - \bar{x}_2)$$

Calculating these values from the centered data:

- Var(Study Hours) ≈ 36.67
- Var(Exam Score) ≈ 141.02
- Cov(Study Hours, Exam Score) ≈ 69.38

So, the approximate covariance matrix Σ is:

$$\Sigma \approx \begin{pmatrix} 36.67 & 69.38 \\ 69.38 & 141.02 \end{pmatrix}$$

Step 3: Perform Eigen-decomposition (Detailed Algebraic Solution)

To find the eigenvalues (λ) and eigenvectors (v) of the covariance matrix Σ, we solve the characteristic equation:

$$\det(\Sigma - \lambda I) = 0$$

where I is the identity matrix.

For our 2×2 covariance matrix:

$$\det \begin{pmatrix} 36.67 - \lambda & 69.38 \\ 69.38 & 141.02 - \lambda \end{pmatrix} = 0$$

Expanding the determinant:

$$(36.67 - \lambda)(141.02 - \lambda) - (69.38)^2 = 0$$
$$(36.67 \times 141.02) - 36.67\lambda - 141.02\lambda + \lambda^2 - 4813.5844 = 0$$
$$5170.4334 - 177.69\lambda + \lambda^2 - 4813.5844 = 0$$

Rearranging into a quadratic equation:

$$\lambda^2 - 177.69\lambda + 356.849 = 0$$

Solving for Eigenvalues (λ)

Using the quadratic formula, $\lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$: Here, $a = 1$, $b = -177.69$, $c = 356.849$.

Calculate the discriminant:

$$\Delta = b^2 - 4ac = (-177.69)^2 - 4(1)(356.849)$$
$$\Delta = 31573.7461 - 1427.396 = 30146.3501$$

Now, find the square root of the discriminant:

$$\sqrt{\Delta} = \sqrt{30146.3501} \approx 173.627$$

The two eigenvalues are:

$$\lambda_1 = \frac{177.69 + 173.627}{2} = \frac{351.317}{2} \approx \mathbf{175.66}$$
$$\lambda_2 = \frac{177.69 - 173.627}{2} = \frac{4.063}{2} \approx \mathbf{2.03}$$

λ_1 is the larger eigenvalue, indicating the direction of most variance.

Solving for Eigenvectors (v)

For each eigenvalue, we substitute it back into the equation $(\Sigma - \lambda I)v = 0$ and solve for $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$.

For $\lambda_1 \approx 175.66$ (First Principal Component, PC1):

$$\begin{pmatrix} 36.67 - 175.66 & 69.38 \\ 69.38 & 141.02 - 175.66 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$\begin{pmatrix} -138.99 & 69.38 \\ 69.38 & -34.64 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

From the first row, we get the equation:

$$-138.99v_1 + 69.38v_2 = 0$$
$$69.38v_2 = 138.99v_1$$
$$v_2 \approx \frac{138.99}{69.38} v_1 \approx 2.003v_1$$

If we choose $v_1 = 1$, then $v_2 \approx 2.003$. So, an unnormalized eigenvector is $\begin{pmatrix} 1 \\ 2.003 \end{pmatrix}$. Normalizing this eigenvector to unit length (so that its magnitude is 1):

$$\|v_1\| = \sqrt{1^2 + (2.003)^2} = \sqrt{1 + 4.012} = \sqrt{5.012} \approx 2.238$$
$$v_1 \approx \begin{pmatrix} 1/2.238 \\ 2.003/2.238 \end{pmatrix} \approx \begin{pmatrix} 0.447 \\ 0.895 \end{pmatrix}$$

This is our first principal component (PC1).

For $\lambda_2 \approx 2.03$ (Second Principal Component, PC2):

$$\begin{pmatrix} 36.67 - 2.03 & 69.38 \\ 69.38 & 141.02 - 2.03 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 34.64 & 69.38 \\ 69.38 & 138.99 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

From the first row, we get the equation:

$$34.64v_1 + 69.38v_2 = 0$$

$$34.64v_1 = -69.38v_2$$

$$v_1 \approx -\frac{69.38}{34.64}v_2 \approx -2.003v_2$$

If we choose $v_2 = 1$, then $v_1 \approx -2.003$. So, an unnormalized eigenvector is $\begin{pmatrix} -2.003 \\ 1 \end{pmatrix}$. Normalizing this eigenvector to unit length:

$$\|v_2\| = \sqrt{(-2.003)^2 + 1^2} = \sqrt{4.012 + 1} = \sqrt{5.012} \approx 2.238$$

$$v_2 \approx \begin{pmatrix} -2.003/2.238 \\ 1/2.238 \end{pmatrix} \approx \begin{pmatrix} -0.895 \\ 0.447 \end{pmatrix}$$

This is our second principal component (PC2). Notice that v_1 and v_2 are orthogonal (their dot product is approximately zero).

Visualization: Data Points with Principal Components

The arrows in the following plot are conceptual representations of these calculated eigenvectors (v_1 and v_2), scaled for better visualization. PC1 aligns with the direction of maximum variance, and PC2 is orthogonal to it, capturing the remaining variance.

Interpretation of the Visualization

- The **red arrow (PC1)** represents the first principal component. Its direction indicates the axis along which the "Study Hours" and "Exam Score" data points show the most spread. Given the positive correlation between study hours and exam scores, PC1 runs diagonally, capturing this primary relationship. The length of this arrow conceptually relates to its large eigenvalue ($\lambda_1 \approx 175.66$), signifying that it accounts for a significant portion of the total variance in the dataset.

- The **green arrow (PC2)** represents the second principal component. It is perpendicular (orthogonal) to PC1. This component captures the remaining variance in the data that is not explained by PC1. Its shorter length conceptually corresponds to a smaller eigenvalue ($\lambda_2 \approx 2.03$), indicating that it explains less variance compared to PC1.

In higher dimensions (more than two features), PCA would find more principal components, but the core idea remains the same: identify orthogonal directions that capture the maximum variance, ordered by their corresponding eigenvalues. This allows us to reduce the dimensionality of the data by keeping only the most important principal components.

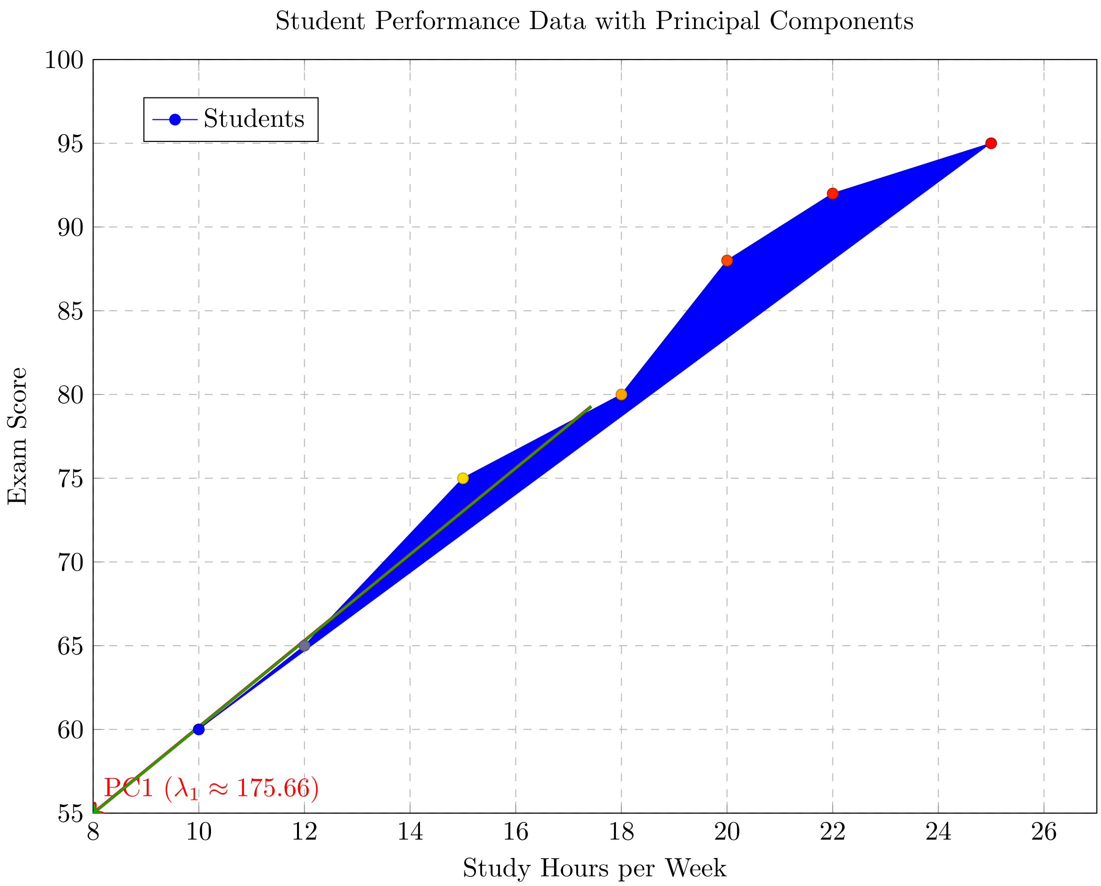

Figure 1: Scatter plot of Study Hours vs. Exam Score with overlaid Principal Components. PC1 (red) shows the primary direction of data spread, and PC2 (green) shows the secondary, orthogonal direction. The lengths of these arrows conceptually represent their corresponding eigenvalues.