An Introduction to Principal Component Analysis

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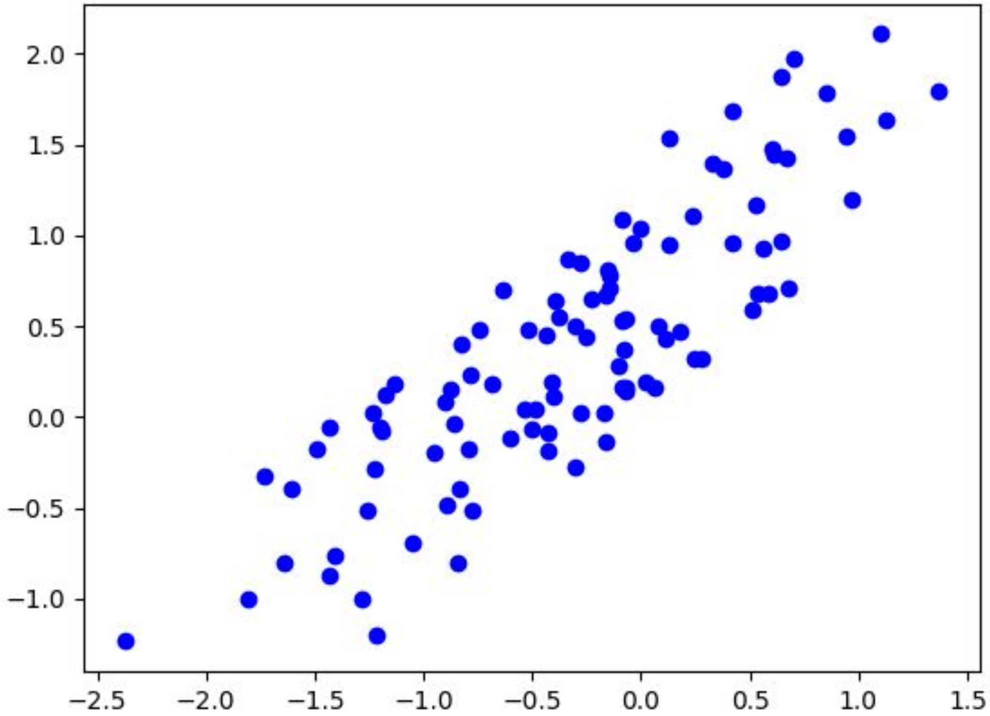
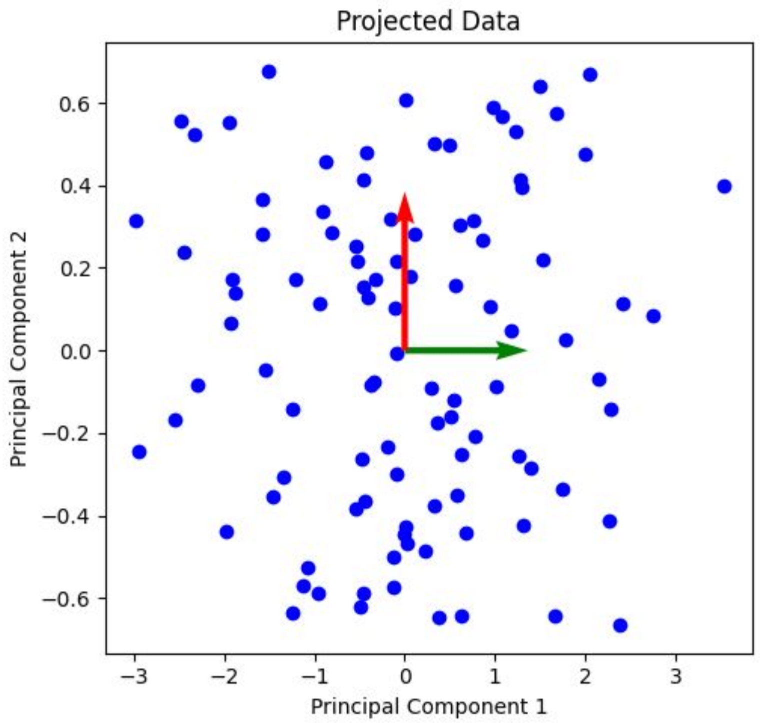
Motivation

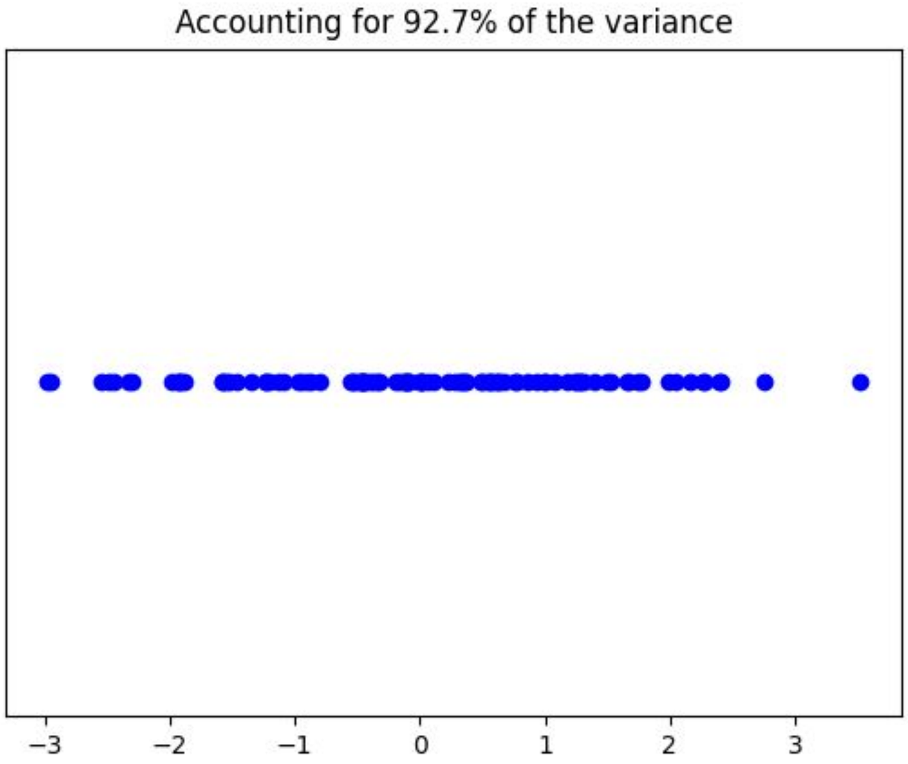


Motivation



Adjusted Data
Principal Component 1
Principal Component 2
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3
Projected Data
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
Principal Component 2
−3
−2
−1
0
1
2
3
Principal Component 1

Motivation



History

- Invented in 1901 by Karl Pearson
- In the 1930s Harold Hotelling independently developed a similar approach
- There are many different names for practically the same method
    - Karhunen Loève Transform (Signal Processing)
    - Hotelling Transform (Multivariate Quality Control)
    - Proper Orthogonal Decomposition (Mechanical Engineering)
    - Singular Value Decomposition (Linear Algebra)
    - Many More

Background Math

Zero-mean and Standardization

Zero-mean

- Shifts the mean to have the values centered at zero

$$X - \bar{X}$$

Standardization (most of the time)

- Shifts all the points to have unit variance

$$\frac{X}{\sigma_X}$$

Z-score equation →

$$z_X = \frac{X - \bar{X}}{\sigma_X}$$

Independent Vectors and Matrix Inverses

Independent Vectors

- Two vectors that can not be made equal by multiplying by a scalar

$$\{1, 1, 2\}$$
$$\{2, -1, 1\}$$

Matrix Inverse

- Equivalent to the reciprocal of a matrix

$$AA^{-1} = I$$

$$A^{-1} = \frac{1}{|A|}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

The Determinant

- Only exists for a square matrix
- Produces a scalar value from a matrix
- Determinant of a product of matrices is the product of their determinants

$$|A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - cb$$

$$|A| = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}$$

Covariance

- The measure of the joint variability of two random variables
- The Covariance Matrix of vectors is a symmetric matrix of the covariance between dimensions of vectors
  - The row and column (i, j) correspond to the i'th and j'th dimension

$$\operatorname{cov}(X, Y) = \mathrm{E}[(X - \mathrm{E}(X))(Y - \mathrm{E}(Y))]$$

Eigenvalues and Eigenvectors

Base Equations

- X: A nonzero vector existing in n-dimensional space known as an eigenvector
- A: A linear transformation applied to X represented as a square matrix
- λ: A scalar value known as an eigenvalue

$$X \in R^n \neq 0$$

$$AX = \lambda X$$

Finding Eigenvalues

- Rework our base equation into a homogeneous system
- Cramer's Rule states that a linear system of equations has nontrivial solutions iff the determinant vanishes
- This is known as the characteristic equation of A

$$AX = \lambda X$$

$$AX - \lambda X = 0$$

$$(A - \lambda I)X = 0$$

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

$$AX = \lambda X$$

Given:

Problem 1:

$$A = \begin{bmatrix} -2 & -2 & 4 \\ -4 & 1 & 2 \\ 2 & 2 & 5 \end{bmatrix}$$

Solve for all non-trivial eigenvalues (λ) of A

Problem 1:

$$A = \begin{bmatrix} -2 & -2 & 4 \\ -4 & 1 & 2 \\ 2 & 2 & 5 \end{bmatrix}$$

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

$$det \begin{bmatrix} -2 & -2 & 4 \\ -4 & 1 & 2 \\ 2 & 2 & 5 \end{bmatrix} - \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} = 0$$

$$det \begin{bmatrix} -2-\lambda & -2 & 4 \\ -4 & 1-\lambda & 2 \\ 2 & 2 & 5-\lambda \end{bmatrix} = 0$$

$$(-2-\lambda)[(1-\lambda)(5-\lambda)-(2)(2)]-(-4)[(-2)(5-\lambda)-(4)(2)]+(2)[(-2)(2)-(4)(1-\lambda)]=0$$

$$-\lambda^3+4\lambda^2+27\lambda-90=0$$

$$\lambda^3-4\lambda^2-27\lambda+90=0$$

$$(\lambda-3)(\lambda^2-\lambda-30)=0$$

$$(\lambda-3)(\lambda+5)(\lambda-6)=0$$

$$AX = \lambda X$$

Problem 2:

Given: $\lambda = 3$

Find the corresponding eigenvector (X)

$$(A-\lambda I)X=0$$

$$A=\begin{bmatrix}-2 & -2 & 4\\ -4 & 1 & 2\\ 2 & 2 & 5\end{bmatrix}$$

$$\begin{bmatrix}-2-\lambda & -2 & 4\\ -4 & 1-\lambda & 2\\ 2 & 2 & 5-\lambda\end{bmatrix}\begin{bmatrix}X\\ Y\\ Z\end{bmatrix}=0$$

$$\lambda=3$$

$$\begin{bmatrix}-5 & -2 & 4\\ -4 & -2 & 2\\ 2 & 2 & 2\end{bmatrix}\begin{bmatrix}X\\ Y\\ Z\end{bmatrix}=0$$

$$\begin{bmatrix}X\\ Y\\ Z\end{bmatrix}=\begin{bmatrix}2\\ -3\\ 1\end{bmatrix}$$

Recap

- If we solve for the nontrivial values of λ we will get up to *n* different eigenvalues (3, -5, 6: in the example)
- When we plug these values into the base equation we will produce n systems of equations to solve
- The results are the eigenvectors corresponding to the eigenvalues