Lectures on Multivariable Mathematics: Principal Component Analysis and Singular Value Decomposition

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1. Objectives
2. Singular Value Decomposition
3. Means and Variance
4. Principal Component Analysis

Objectives

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5. calculate the covariance matrix for a set of data,
6. use a covariance matrix to determine the principal component of a set of data, and
7. explain why it is called the principal component.

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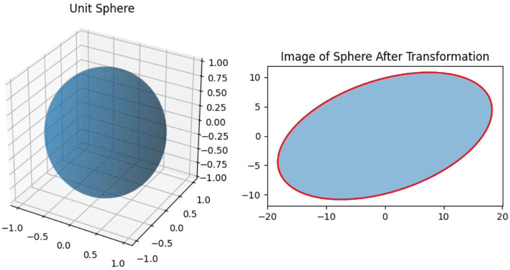
Motivating Example

A 2×3 matrix A is a transformation from $\mathbb{R}^3$ to $\mathbb{R}^2$, for example:

$$\begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix} : \mathbb{R}^3 \longrightarrow \mathbb{R}^2$$



Our goal is to find the major and minor axes of the ellipse.

Minimums and Maximums for Non-Square Transformations

The major and minor axes are the maximum and minimum length non-zero vectors $\vec{x}$ associated with multiplication by A:

$$||A\vec{x}||^2 = (A\vec{x})^T(A\vec{x}) = \left(\vec{x}^T A^T\right) A\vec{x} = \vec{x}^T \left(A^T A\right) \vec{x}$$

From before, the maximum and minimums associated with the symmetric matrix

$$B = A^T A = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix}$$

are given by the eigenvalues and vectors of B.

Minimums and Maximums for Non-Square Transformations

In the case of

$$B = A^T A = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix}$$

the eigenvalues are $\lambda_1 = 360$, $\lambda_2 = 90$, and $\lambda_3 = 0$ with corresponding vectors

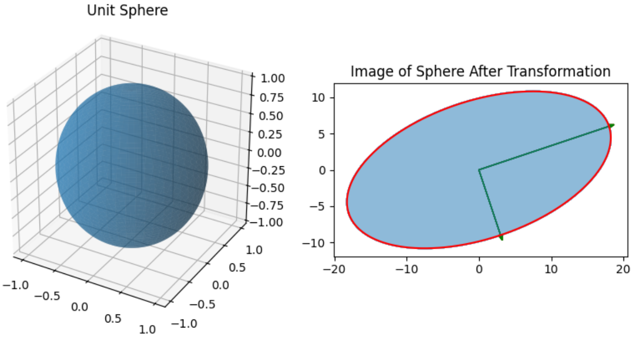
$$\vec{v}_1 = \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix}, \ \vec{v}_2 = \begin{bmatrix} -2/3 \\ -1/3 \\ 2/3 \end{bmatrix}, \text{ and } \vec{v}_3 = \begin{bmatrix} 2/3 \\ -2/3 \\ 1/3 \end{bmatrix}$$

and multiplying by A we get

$$A\vec{v}_1 = \begin{bmatrix} 18 \\ 6 \end{bmatrix}, \ A\vec{v}_2 = \begin{bmatrix} 3 \\ -9 \end{bmatrix}, \text{ and } A\vec{v}_3 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Motivating Example Revisited

The major axis is in the direction of $A\overrightarrow{v}_1 = \langle 18, 6 \rangle$ and the minor is $A\overrightarrow{v}_2 = \langle 3, -9 \rangle$:



Singular Values of a Matrix

Definition (Singular Values of a Matrix)

The singular values of a matrix A are the square roots of the eigenvalues of $A^T A$. We assume that the singular values/eigenvalues are arranged in decreasing order and note that $\sigma_i = \sqrt{\lambda_i} = ||A\overrightarrow{v}_i||$ where $\overrightarrow{v}_i$ is a corresponding eigenvector.

Theorem

Given an $m \times n$ matrix A, $A^T A$ is symmetric and the eigenvectors of $A^T A$, $\{\overrightarrow{v}_1, \overrightarrow{v}_2, \ldots, \overrightarrow{v}_n\}$ form an orthonormal basis for $\mathbb{R}^n$. Assuming the eigenvalues are decreasing order and there are r non-zero values, then $\{A\overrightarrow{v}_1, A\overrightarrow{v}_2, \ldots, A\overrightarrow{v}_r\}$ is an orthogonal basis for the column space (image) of A, a subspace of $\mathbb{R}^M$.

Singular Value Decomposition: Theorem

Theorem

Let A be a $m \times n$ matrix of rank r. Then there exists an $m \times n$ matrix Σ for which the diagonal entries consist of the singular values of A, $\sigma_i = \sqrt{\lambda_i}$, an $m \times m$ orthogonal matrix U, and an $n \times n$ orthogonal matrix V such that

$$A = U \Sigma V^T.$$

Singular Value Decomposition: $A = U\Sigma V^T$

$V = \begin{bmatrix} \vec{v}_1 & \vec{v}_2 & \cdots & \vec{v}_n \end{bmatrix}$ Orthogonal Matrix of Eigenvectors

$D = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_r \end{bmatrix}$ Singular Values $\sigma_i = \sqrt{\lambda_i} = ||A\vec{v}_i||$

$\Sigma = \begin{bmatrix} D & 0_{r,n-r} \\ 0_{m-r,r} & 0_{m-r,n-r} \end{bmatrix}$ $m \times n$ Diagonal Matrix

$U = \begin{bmatrix} \frac{A\vec{v}_1}{||A\vec{v}_1||} & \cdots & \frac{A\vec{v}_r}{||A\vec{v}_r||} & 0 \cdots 0 \end{bmatrix}$ $m \times m$ Matrix of Normed Images

$$\frac{A\vec{v}_i}{||A\vec{v}_i||}\sigma_i = A\vec{v}_i \implies U\Sigma = AV \text{ and } U\Sigma V^T = AVV^T = A$$

Singular Value Decomposition: $m \times n$ with $n > m$

Using our original example

$$A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}$$

we can write $A = U\Sigma V^T = UDV^T$, the Reduced SVD with

$$U = \begin{bmatrix} 3/\sqrt{10} & 1/\sqrt{10} \\ 1/\sqrt{10} & -3/\sqrt{10} \end{bmatrix}$$

$$\Sigma = D = \begin{bmatrix} 6\sqrt{10} & 0 \\ 0 & 3\sqrt{10} \end{bmatrix}$$

$$V^T = \begin{bmatrix} 1/3 & 2/3 & 2/3 \\ -2/3 & -1/3 & 2/3 \end{bmatrix}$$

Singular Value Decomposition: $m \times n$ with $n < m$

If we start with a 3×2 matrix like so:

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 1 \end{bmatrix} \text{ so that } A^T A = \begin{bmatrix} 1 & 1 \\ 1 & 3 \end{bmatrix}$$

and we get eigenvalues of $2 \pm \sqrt{2} \approx 3.414$ and 0.586 and the matrix of eigenvectors is

$$V \approx \begin{bmatrix} 0.383 & 0.924 \\ 0.924 & -0.383 \end{bmatrix}.$$

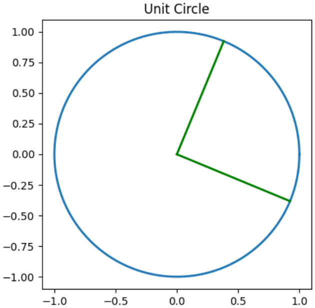
Using these we get

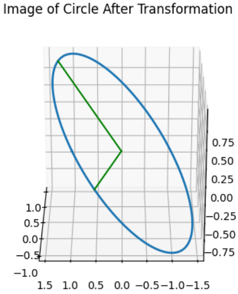
$$U = \begin{bmatrix} 1/2 & -1/2 \\ \sqrt{2}/2 & \sqrt{2}/2 \\ 1/2 & -1/2 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \sqrt{2+\sqrt{2}} & 0 \\ 0 & \sqrt{2-\sqrt{2}} \end{bmatrix} \approx \begin{bmatrix} 1.84 & 0 \\ 0 & 0.765 \end{bmatrix}$$

Singular Value Decomposition: $m \times n$ with $n < m$

The result of transforming the unit circle with

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 1 \end{bmatrix} \approx \begin{bmatrix} 1/2 & -1/2 \\ \sqrt{2}/2 & \sqrt{2}/2 \\ 1/2 & -1/2 \end{bmatrix} \begin{bmatrix} \sqrt{2+\sqrt{2}} & 0 \\ 0 & \sqrt{2-\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0.383 & 0.924 \\ 0.924 & -0.383 \end{bmatrix}$$





Singular Value Decomposition: $m \times n$ with $n = m$

If we start with a 3×2 matrix like so:

$$A = \begin{bmatrix} 2 & 3 \\ 0 & 4 \end{bmatrix} \text{ so that } A^T A = \begin{bmatrix} 4 & 6 \\ 6 & 25 \end{bmatrix}$$

then we get eigenvalues of $\lambda_i \approx 2.41$ and 26.59 and the matrix of eigenvectors is

$$V \approx \begin{bmatrix} -0.966 & -0.257 \\ 0.257 & -0.966 \end{bmatrix}.$$

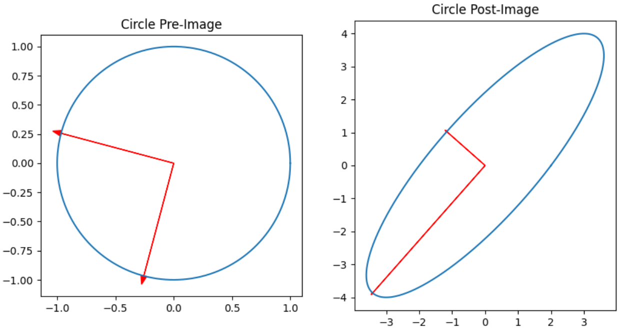
Using these we get

$$U = \begin{bmatrix} -0.750 & -0.662 \\ 0.662 & -0.750 \end{bmatrix} \qquad \Sigma \approx \begin{bmatrix} 1.551 & 0 \\ 0 & 5.157 \end{bmatrix}$$

Singular Value Decomposition: $m \times n$ with $n = m$

The result of transforming the unit circle with

$$A = \begin{bmatrix} 2 & 3 \\ 0 & 4 \end{bmatrix} \approx \begin{bmatrix} -0.750 & -0.662 \\ 0.662 & -0.750 \end{bmatrix} \begin{bmatrix} 1.551 & 0 \\ 0 & 5.157 \end{bmatrix} \begin{bmatrix} -0.966 & 0.257 \\ -0.257 & -0.966 \end{bmatrix}$$



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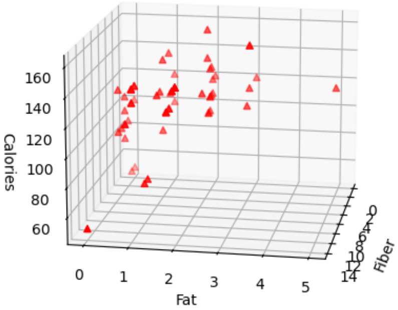
Displaying Some Data

Here we have a matrix of nutritional data for 77 different cereals:

$$Data = \begin{bmatrix} fiber \\ fat \\ calories \end{bmatrix} = \begin{bmatrix} 10.0 & 2.0 & 9.0 & \cdots & 3.0 & 3.0 & 1.0 \\ 1.0 & 5.0 & 1.0 & \cdots & 1.0 & 1.0 & 1.0 \\ 70.0 & 120.0 & 70.0 & \cdots & 100.0 & 100.0 & 110.0 \end{bmatrix}$$

And, here is a scatter plot of that data:



Constructing the Sample Mean Vector

We will begin by finding the mean for each row of data:

$$M = \begin{bmatrix} mean\ fiber \\ mean\ fat \\ mean\ calories \end{bmatrix} = \begin{bmatrix} \overline{fib} \\ \overline{fat} \\ \overline{cal} \end{bmatrix}$$

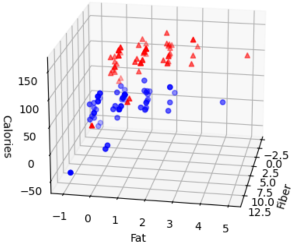
$$= \frac{1}{N} \sum_{cols\ of\ Data} Data_i = \begin{bmatrix} 2.15194805194805 \\ 1.01298701298701 \\ 106.883116883117 \end{bmatrix}$$

Constructing the Mean-Deviation Form

Then we subtract the mean values from each entry to get the signed deviations, $(x - \overline{x})$:

$$B = \begin{bmatrix} fiber - \overline{fib} \\ fat - \overline{fat} \\ calories - \overline{cal} \end{bmatrix} = \begin{bmatrix} 7.85 & -0.152 & \cdots & 0.848 & -1.15 \\ -0.013 & 3.99 & \cdots & -0.013 & -0.013 \\ -36.9 & 13.1 & \cdots & -6.88 & 3.12 \end{bmatrix}$$

If we plot this new data set, it has the same form but is centered on the mean vector:



Construct the Covariance Matrix

Next we construct the covariance matrix

$$S = \frac{1}{N-1} BB^T = \begin{bmatrix} 5.68 & 0.0401 & -13.6 \\ 0.0401 & 1.01 & 9.78 \\ -13.6 & 9.78 & 380.0 \end{bmatrix}$$

in which each entry looks like

$$\sum_i \frac{(x_i - \overline{x})^2}{N-1} \text{ or } \sum_i \frac{(x_i - \overline{x})(y_i - \overline{y})}{N-1}$$

the variance in individual variables or covariance between variables.

Variance, Covariance, and Total Variance

Definition

Given sets of data $X = \{x_1, x_2, \ldots, x_N\}$ and $Y = \{y_1, y_2, \ldots, y_N\}$ with means $\overline{x}$ and $\overline{y}$ the sums

$$\sum_i \frac{(x_i - \overline{x})^2}{N-1} \text{ and } \sum_i \frac{(y_i - \overline{y})^2}{N-1}$$

measure the variance of each individual set data from its mean. While the sum

$$\sum_i \frac{(x_i - \overline{x})(y_i - \overline{y})}{N-1}$$

measures the covariance between the variables (how they change compared to one another), if this is 0 we say they are uncorrelated. Finally the sum of the variances across variables is called the total variance, a measure of how spread out all the data is.

Variance, Covariance, and Total Variance

Returning to the matrix

$$S = \frac{1}{N-1} BB^T = \begin{bmatrix} 5.68 & 0.0401 & -13.6 \\ 0.0401 & 1.01 & 9.78 \\ -13.6 & 9.78 & 380.0 \end{bmatrix}$$

the diagonal entries are the variances, the off diagonal entries are the covariances, and the sum of the diagonal entries, called the trace, is the total variance, $trace(S) \approx 386.32$

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Change of Data Variables: What We Want

Theorem (Principal Axes Theorem)

Let A be an $n \times n$ symmetric matrix, then there is an orthogonal change of variable, $\overrightarrow{x} = P\overrightarrow{y}$, that transforms the quadratic form $\overrightarrow{x}^T A\overrightarrow{x}$ into a quadratic form $\overrightarrow{y}^T D\overrightarrow{y}$ with no cross terms. Note the orthogonal matrix P and diagonal matrix D, with $A = PDP^T$, exist because A is symmetric.

Change of Data Variables: Relation to Covariance

From before we have our covariance matrix

$$S = \frac{1}{N-1} BB^T \approx \begin{bmatrix} 5.68 & 0.0401 & -13.6 \\ 0.0401 & 1.01 & 9.78 \\ -13.6 & 9.78 & 380.0 \end{bmatrix}$$

which by construction is symmetric so that we can find a change of variable with

$$\vec{x}^T S \vec{x} = \vec{y}^T D \vec{y}$$

where D is a diagonal matrix.

Constructing Principal Components: Example

As before, we find D and P so that $S = PDP^{-1} = PDP^T$ using eigenvalues and eigenvectors:

$$D \approx \begin{bmatrix} 380.0 & 0 & 0 \\ 0 & 5.22 & 0 \\ 0 & 0 & 0.726 \end{bmatrix} \text{ and } P \approx \begin{bmatrix} 0.0363 & 0.995 & -0.0874 \\ -0.0257 & 0.0883 & 0.996 \\ -0.999 & 0.0339 & -0.0288 \end{bmatrix}$$

Then we let $\vec{y} = P^T \vec{x}$ to get

$$\vec{y}^{\,T} D \vec{y} = \left(P^T \vec{x}\right)^T DP^T \vec{x} = \vec{x}^{\,T} PDP^T \vec{x} = \vec{x}^{\,T} S \vec{x}.$$

The advantage of working with the $\vec{y}$ is that pairs of variables are uncorrelated, and of course calculations with a diagonal matrix are simpler.

Constructing Principal Components: Example

Since the matrices P and P^T are orthogonal they don't change lengths or angles so

$$Total\ \ Variance = trace(S) = trace(D) \approx 386.32.$$

We can more easily look at variation due to the variables $\vec{y}$ since they are uncorrelated, in particular

- $\vec{y}_1 = \vec{P}_1^T \vec{x}$ accounts for $380/386 \approx 98.45\%$ of variation,
- $\vec{y}_2 = \vec{P}_2^T \vec{x}$ accounts for $5/386 \approx 1.30\%$ of variation, and
- $\vec{y}_3 = \vec{P}_3^T \vec{x}$ accounts for $0.73/386 \approx 0.19\%$ of variation.

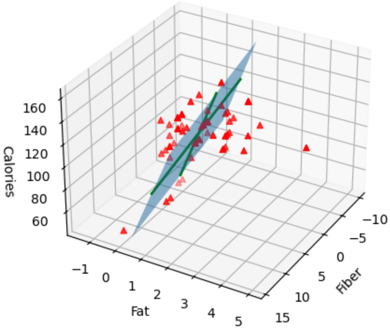
This means if we describe our data using two variables $\vec{y}_1$ and $\vec{y}_2$ instead of three separate variables, we still get approximately 99.75% of the same information.

Constructing Principal Components: Example

With

$$\overrightarrow{v} = \langle 0.036, -0.026, -0.999 \rangle \text{ and } \overrightarrow{w} = \langle 0.996, 0.088, 0.034 \rangle$$

(the eigenvectors corresponding to the two largest eigenvalues) the plane defined by $M + \overrightarrow{v}\,t + \overrightarrow{w}s$ approximates our data in two dimensions:



Constructing Principal Components: A Little Theory

The covariance matrix for the $\overrightarrow{y}$'s as defined above is precisely the diagonal matrix D of eigenvalues for the covariance matrix $S = \frac{1}{N-1}(X - \overline{X})(X - \overline{X})^T$.

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- Define $Y = P^T X$,

$$\begin{aligned} \overline{Y} &= \frac{1}{N}\sum_i Y_i \\ &= \frac{1}{N}\sum P^T X_i \\ &= P^T\left(\frac{1}{N}\sum X_i\right) \\ &= P^T\overline{X} \end{aligned}$$

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$$\begin{aligned} Y - \overline{Y} &= P^T X - P^T \overline{X} \\ &= P^T \left(X - \overline{X}\right) \\ &= P^T B \end{aligned}$$

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- $Y - \overline{Y} = P^T B$

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$$\begin{aligned}
\frac{1}{N-1}\left(Y - \overline{Y}\right)\left(Y - \overline{Y}\right)^T &= \frac{1}{N-1}\left(P^T B\right)\left(P^T B\right)^T \\
&= \frac{1}{N-1}P^T BB^T P \\
&= P^T \frac{1}{N-1}BB^T P \\
&= P^T SP = D
\end{aligned}$$

Constructing Principal Components: A Little Theory

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- $B = X - \overline{X}$, Mean Deviation
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- $S = PDP^T$, Ortho. Diag.
- Define $Y = P^T X$,
- $\overline{Y} = P^T \overline{X}$
- $Y - \overline{Y} = P^T B$
- Covariance of Y is D

$$\begin{aligned} \frac{1}{N-1}\left(Y - \overline{Y}\right)\left(Y - \overline{Y}\right)^T &= \frac{1}{N-1}\left(P^T B\right)\left(P^T B\right)^T \\ &= \frac{1}{N-1}P^T BB^T P \\ &= P^T \frac{1}{N-1}BB^T P \\ &= P^T SP = D \end{aligned}$$

Lectures on Multivariable Mathematics: Principal Component Analysis and Singular Value Decomposition

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