Data Matrices and Linear Algebra

Eigenvectors and Eigenspaces

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Geometry of Multivariate Data

n observations of p variables can be represented as a $n \times p$ matrix

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ \vdots & \ddots & & \\ x_{n1} & \dots & & x_{np} \end{bmatrix}$$

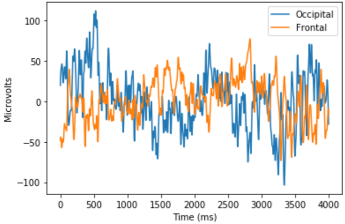
n observations may represent n different participants in an experiment while p are different experimental variables observed in each participant.

In Neuroscience applications, n represents different samples in time, while p represents different locations in the brain.

$\mathbf{X} = \begin{bmatrix} \mathbf{x_1} \\ \vdots \\ \mathbf{x_n} \end{bmatrix}$ The matrix a stack of n row vectors (of size p) of observations. **This is how data is collected.**

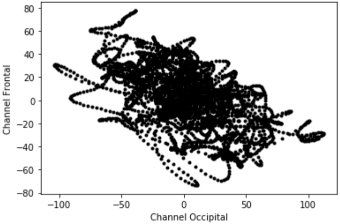
$\mathbf{X} = \begin{bmatrix} \mathbf{x_1} \dots \mathbf{x_p} \end{bmatrix}$ The matrix is a stack of p column vectors (of size n) of variables. **This is the useful way to think about data**

Example



The above example shows EEG traces at two channels, one over the occipital lobe and one over the frontal lobe. The correlation coefficient between the two signals is r = -0.5. This would correspond to an angle of 120 degrees in a 4000 dimensional space, with each dimension corresponding to one of the time points.

Variables as Dimensions



Another useful way to think about our two EEG time series is to plot them in a plane, where the two dimensions correspond to each one of the channels.
The negative correlation between the channels is visible in the geometry of the cloud of points. Each point is a joint observation of the EEG at the two channels. Of course, in reality we observe EEG at many channels, so the dimensionality of our space corresponds to the number of variables we simultaneously observe. The remainder of today's lecture is focused on the geometry of this space

Matrix Properties

1. Matrix A is of dimension m x n if it has m rows and n column. We refer to the elements of A as $a_{ij},\ i = 1, .., m,\ j = 1, .., n$
2. Matrix Addition
$$C = A + B \iff c_{ij} = a_{ij} + bij$$
3. Matrix Multiplication
$$C = A \times B \iff c_{ij} = a_{i1}b_{1j} + a_{i2}b_{2j} + ... + a_{in}b_{nj}$$
In words, matrix multiplication is carried out by the dot product between the rows of matrix A and the columns of matrix B to obtain each element of matrix C. Matrix multiplication can only be applied if the inner dimension of the two matrices are identical.
$$A = (m, n),\ B = (n, p) \implies C = (m, p)$$
4. Matrix/Vector multiplication Matrix and vectors can be multiplied as long as the inner dimensions are matched. For example matrix A of size (m,n) can be multipled to a vector of size (n,1). The result is a vector of size (m,1)
5. The transpose of a matrix is obtained by flipping the matrix so that the rows of the matrix become the columns of the matrix. If A is of size (n,m) then A^T is of size (m,n)

Rotations in the Plane

Lets consider a point (a,b) in the plane.
We would like to rotate the point around the origin by an angle θ, to obtain a new point (c,d).
Since the operation is purely a rotation, its useful to express the location of (a,b) in terms of polar coordinates

$$(a, b) = (rcos(\alpha), rsin(\alpha))$$

Since we want to rotate the point around the origin by an angle θ, the new coordinates can be written as

$$(c, d) = (rcos(\alpha + \theta), rsin(\alpha + \theta))$$

Rotation Matrix

We can use the trig rules for sum of angles to note that

$$c = rcos(\alpha + \theta) = rcos(\alpha)cos(\theta) - rsin(\alpha)sin(\theta)$$
$$d = rsin(\alpha + \theta) = rcos(\alpha)sin(\theta) + rsin(\alpha)cos(\theta)$$

which simplifies to

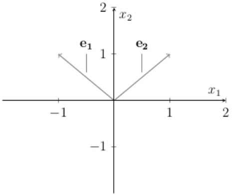
$$c = acos(\theta) - bsin(\theta)$$
$$d = asin(\theta) + bcos(\theta)$$

In matrix form

$$\begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

Basis of a Vector Space

In 2-D, unit vectors along the coordinate axes $\mathbf{u_1} = (1, 0)$ and $\mathbf{u_2} = (0, 1)$ are orthonormal vectors.
Any vector $\mathbf{x}$ in the plane can be written as a linear combination, $\mathbf{x} = x_1\mathbf{u_1} + x_2\mathbf{u_2}$
Thus, together $\{\mathbf{u_1}, \mathbf{u_2}\}$ *span* the vector space of all vectors in a plane, and form a **basis** of the vector space.



In 2-dimensional space, any 2 linearly independent vectors can form an basis.
If n-dimensional space, any n linearly independent vectors can form a basis.
Linearly independent vectors have dot product of zero.

Properties of the Rotation Matrix

$$\begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

The rotation matrix is an example of an orthogonal matrix.

An orthogonal matrix has columns (or rows) that form an orthonormal basis.

Its easy to see that the dot product of the columns of the rotation matrix is zero.

$$cos(\theta)(-sin(\theta)) + sin(\theta)cos(\theta) = 0$$

Its also easy to see that the length of each column of the rotation matrix is 1.

$$cos^2(\theta) + sin^2(\theta) = 1$$

Let $\theta = \frac{\pi}{4}$

$$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$$

The Covariance Matrix

n observations of p variables can be represented as a $n \times p$ matrix

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ \vdots & \ddots & & \\ x_{n1} & \dots & & x_{np} \end{bmatrix}$$

$\mathbf{X} = \begin{bmatrix} \mathbf{x_1} \dots \mathbf{x_p} \end{bmatrix}$ The matrix is a stack of p column vectors (of size n) of variables. **This is the useful way to think about data** When performing data analysis, we should always center the data on the origin of the coordinate system by computing the *deviations*

$$\mathbf{d_k} = \mathbf{x_k} - \bar{x}_k, k = 1, 2, ...p$$

We can define the **covariance** matrix Σ of the multivariate data as the matrix with elements

$$\Sigma_{lk} = \frac{1}{n} \mathbf{d_l} \cdot \mathbf{d_k}$$

Note that the diagonal entries of the matrix are variances, σ_j^2

Covariance Matrix

We can write the covariance matrix as a matrix multiplication

$$\Sigma = \frac{1}{n}\mathbf{X}^T\mathbf{X}$$

where $\mathbf{X}^T$ is the transpose of X. The covariance matrix has a number of important properties.

1. If X is of size (n,p) then Σ is of size (p,p), where p is the number of variables.
2. Σ is a square symmetric matrix, i.e., $\Sigma_{lk} = \Sigma_{kl}$

Similarly, we can define a correlation matrix, **R** with elements that are correlation coefficients, obtained by normalizing the covariance as

$$R_{lk} = \frac{\Sigma_{lk}}{\|\mathbf{d_k}\| \, \|\mathbf{d_l}\|}$$

Eigenvectors

Given a square symmetric matrix A, there exists a set of vectors **x**, known as **eigenvectors** that have the property that

$$\mathbf{Ax} = \lambda \mathbf{x}$$

1. The value λ is the eigenvalues that capture the scale of the eigenvectors.
2. A is of dimension (p,p) then there can be up to p eigenvectors with p distinct eigenvalues.
3. Eigenvectors corresponding to non-zero eigenvalues are linearly independent and have length or norm of 1.
4. If a matrix of dimension (p,p) has p distinct non-zero eigenvalues, the eigenvectors are all linearly independent, and **form a vector basis**.

Eigenvectors form a Rotation Matrix

Let's the define the matrix **M** (known as the modal matrix) whose columns are eigenvectors of the matrix square symmetric (p,p) matrix **A**.

Since eigenvectors are linearly independent vectors of unit length, the matrix M is an orthogonal matrix like a rotation matrix.(In fact it is a rotation matrix!)

$$\mathbf{M}^T\mathbf{A}\mathbf{M} = \Lambda$$

where Λ is a matrix with the eigenvalues λ corresponding to each eigenvector along

the diagonal, and zero at all off-diagonal values.
Thus the matrix **A** can be **diagonalized** by the model matrix **M**. THIS IS THE POINT OF CELL 1 IN THE eigenvalues.py and eigenvalues.m

Eigenvectors of the Covariance Matrix

Consider the covariance matrix Σ of data matrix $\mathbf{X}$

$$\Sigma = \frac{1}{n}\mathbf{X}^T\mathbf{X}$$

of dimensions (p,p) corresponding to the p variables in an experiment.

The covariance matrix has eigenvectors which can be used to form a modal matrix **V**, whose columns are the eigenvectors.

V diagonalizes the covariance matrix Σ such that

$$\mathbf{V}^T\Sigma\mathbf{V} = \Lambda$$

where Λ is a matrix with the eigenvalues along the diagonal.

Interpretation of Eigenvalues and Eigenvectors of a Covariance Matrix

The data covariance matrix Σ has the following structure

1. Along the diagonal, each value $\Sigma_j j$ is the variance of the corresponding variable, σ_j^2.
2. Off the diagonal, each value $\Sigma_j k$ is the covariance of variable j with variable k.

The eigenvectors form a rotation matrix that tell us how to rotate the variables in order to obtain new *Latent* variables, which have a covariance matrix Λ which is diagonal.

1. A diagonal covariance matrix has variances along the diagonal which correspond to each of the eigenvectors. These variances are the eigenvalues, $_j$
2. Off the diagonal, all the values are zero, indicating the Latent variables are uncorrelated, i.e. have covariance of 0.

How do we compute the Latent Variables

We compute the covariance from the data matrix as

$$\Sigma = \frac{1}{n}\mathbf{X}^T\mathbf{X}$$

Given the eigenvectors in a matrix V, we can diagonalize the covariance matrix as

$$\mathbf{V}^T\Sigma\mathbf{V} = \Lambda$$

Substituting the first equation to the second, we get,

$$\frac{1}{n}\mathbf{V}^T\mathbf{X}^T\mathbf{X}\mathbf{V} = \Lambda$$

which can be simplified to

$$\frac{1}{n}(\mathbf{X}\mathbf{V})^T\mathbf{X}\mathbf{V} = \Lambda$$

Thus the covariance matrix Λ is the covariance matrix for the latent variables obtained by multiplying the data matrix by the eigenvector matrix.

$\mathbf{Y} = \mathbf{XV}$ **these new variables are uncorrelated, with covariance equal to zero**.

These *latent* variables are weighted mixtures of the original variables, with the weights given by the eigenvectors.

Inverting the Transformation

Since $\mathbf{V}$ is an orthonormal matrix

$$\mathbf{V}\mathbf{V}^T = \mathbf{I}$$

where I is the identity matrix with 1 along the diagoal and 0 elsewhere.
This implies that we can invert the transformation

$\mathbf{Y} = \mathbf{X}\mathbf{V}$ as

$\mathbf{X} = \mathbf{Y}\mathbf{V}^T$

Principal Components Analysis

The framework just described here is known as Principal Components Analysis (PCA). In this analysis we identify latent variables that capture the variance in our data. In PCA, the critical feature is that the latent variables are **uncorrelated**. The steps in PCA are

1. Compute a covariance matrix from the data.
2. Estimate its eigenvalues and eigenvectors.
3. Use the eigenvectors to project (rotate) the data into the eigenspace.
4. The projected data (sometimes labeled scores) can be used to reduce the number of variables investigated (compress data).
5. They also provide a starting point for the development of data models like classifiers.