Lecture 8 – Autoencoder and Principal component analysis (PCA)

(Tutorial part 1)

Autoencoder

In our previous two lectures, we have studied ANNs and used them to recognize MNIST images.

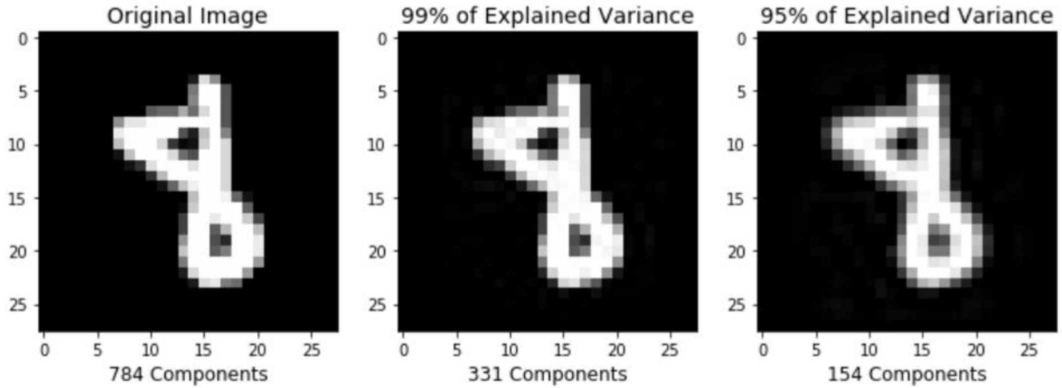
In the next two lectures, we are going to look at another form of an ANN i.e., called Autoendcoder (AE)

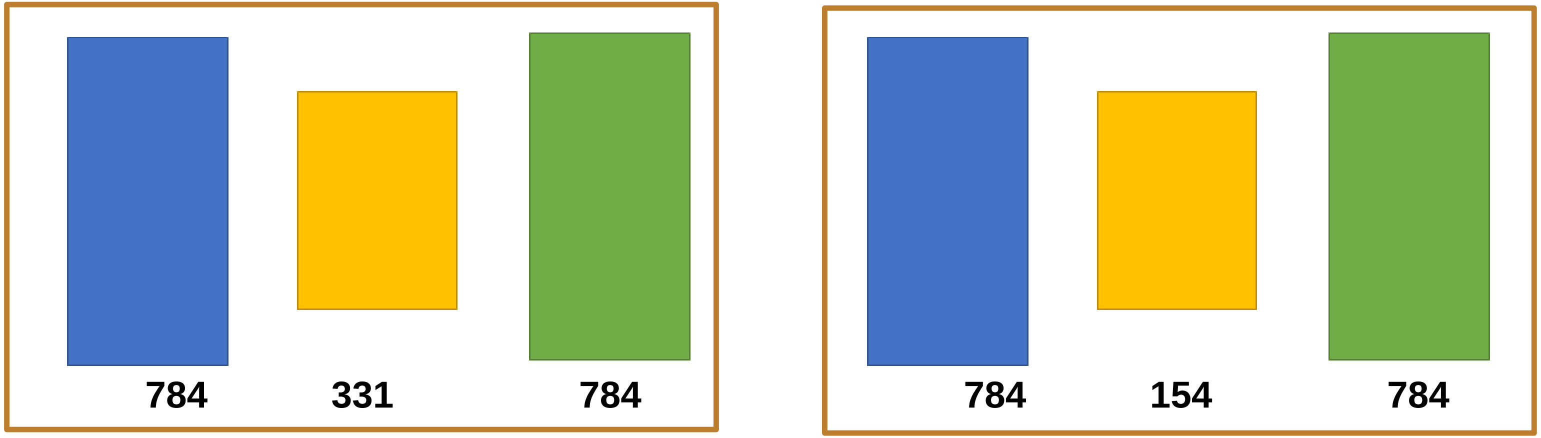
An AE is a type of ANN that is used to learn efficient data codings in an unsupervised manner.

The AE helps to learn a representation (encoding) for a set of data, typically for dimensionality reduction, compression etc.

For example, we can limit the number of features to represent the same image (by limiting the number of hidden units)

Autoencoder example





WS8 - Task 1

The code provided in WS6 –Task 1 could be used to obtain an Autoencoder like functioning. **We will see a proper AE algorithm in Lecture 10. The example here is just to give you an idea.**

Download the “WS8_codes” folder

The provided AE_MNIST code will extract and pre-process the dataset

The provided code also does the post-processing,

For your ease, a few lines are left empty for you to fill.

WS8 - Task 1

1.1. Complete and execute the code for 10, 20, and 30 hidden neurons (HNs)

1.2. Compare and explain these three models.

1.3. Compare and explain the results, in terms of computational complexity and speed e.g. 10-HNs vs. 20-HNs vs. 30-HNs

1.4. Explain the difference between WS6-Task 1 and WS8-Task1

Principal component analysis (PCA)

To better understand AE or in general get the insight into an ANN and its non-linear transformation, we can study Principal component analysis (PCA).

PCA is a statistical procedure that uses an orthogonal linear transformation compared to ANN’s non-linear transformation.

Similar to AE, PCA has application in fields such as face recognition and image compression, and is a common technique for finding patterns in data of high dimension.

Principal component analysis (PCA) - background knowledge

Before implementing PCA, this Lecture/tutorial first introduces the mathematical concepts which will be used in PCA.

We will cover:

- Mean
- Standard deviation
- Variance
- Covariance/covariance matrix
- Eigenvectors and eigenvalues.

This background knowledge will help in understanding the PCA in the next lecture.

Principal component analysis (PCA) - background knowledge

Let’s take a simple example, set X = [1 2 4 6 12 15 25 68 67 65 98]

There are several things we can find about this set. For example,
we can calculate the mean of the sample, given as: $\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n}$

Please note that the mean doesn’t tell us much about the data, except a middle point.

For example, the following two sets have the same mean, but they are different.
DS1 = [0 8 12 20], DS2 = [8 9 11 12]

It is the spread of the data that is different.

Principal component analysis (PCA) - background knowledge

The **Standard Deviation (SD)** of a dataset is a measure of how spread out the data is

SD is defined as, “the average distance from the mean of the data set to a point”.

The way to calculate it is to compute the squares of the distance from each data point to the mean of the set, add them all up, divide by n-1, and take the positive square root.

$$s = \sqrt{\frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}}$$

Where ‘*s*’ is the symbol for standard deviation

Principal component analysis (PCA) - background knowledge

Variance is another measure of the spread of data in a data set, almost identical to the standard deviation, and given as:

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}$$

Principal component analysis (PCA) - background knowledge

Covariance:

Both SD and Variance are purely 1-dimensional i.e. data sets like, heights of all the people in the room, marks for the last exam etc.

However many data sets have more than one dimension, and the aim of the statistical data analysis is to find any relationships between different dimensions.

For example, assume our dataset has both the height of all the students in a class, and the marks they received for that paper – A 2D dataset

In this case, we could perform a statistical analysis to find out if there exist any relationship between the height of a student and obtained marks.

Principal component analysis (PCA) - background knowledge

Covariance is always measured between 2 dimensions.

If we calculate the covariance between one dimension and itself, its the variance.

If we have a 3-dimensional dataset (x,y,z), then covariance could be measured between the x and y dimensions, the x and z dimensions, and the y and z dimensions.

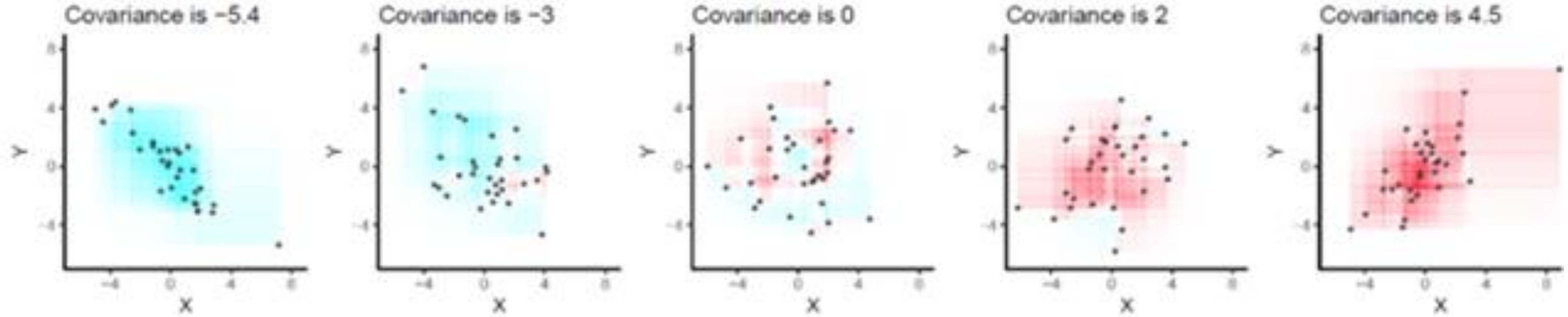
Covariance is similar to the variance, given as.

$$cov(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

Principal component analysis (PCA) - background knowledge

Covariance Matrix:

Here are a few examples with 32 binormal points drawn from distributions with the given covariances, ordered from most negative (bluest) to most positive (reddest).



The exact value is not as important as it’s sign (positive/negative). If the value is positive, it means both dimensions (X and Y) increase together. If the value is negative, it means when one dimension increases the other decreases. If the covariance is zero, it indicates that the two dimensions are independent of each other.

Principal component analysis (PCA) - background knowledge

If our dataset has more than 2 dimensions, there is more than one covariance measurement.

For example, a covariance matrix (C) for an imaginary 3 dimensional data set is given as:

$$C = \begin{pmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{pmatrix}$$

Principal component analysis (PCA) - background knowledge

$$C = \begin{pmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{pmatrix}$$

Note that the main diagonal has covariance between one of the dimensions and itself. These are the variances for that dimension. The matrix is symmetrical about the main diagonal.

WS8 - Task 2

2.1. Work out the covariance between the x and y dimensions and explain the results.

X	10	40	18	Student number (last 2 digits e.g. 54)
Y	41	15	29	24

2.2. Calculate for a 3 dimensional data set

X	1	-1	4
Y	2	1	3
Z	1	3	-1

Principal component analysis (PCA) - background knowledge

Eigenvalues and Eigenvectors

Eigenvectors: Consider a multiplications between a matrix and a vector:

(First Example): $\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \times \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \begin{pmatrix} 11 \\ 5 \end{pmatrix}$

(Second Example): $\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \times \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4 \times \begin{pmatrix} 3 \\ 2 \end{pmatrix}$

Fig. 1. Example of one non-eigenvector and one eigenvector

$$2 \times \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 6 \\ 4 \end{pmatrix}$$

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \times \begin{pmatrix} 6 \\ 4 \end{pmatrix} = \begin{pmatrix} 24 \\ 16 \end{pmatrix} = 4 \times \begin{pmatrix} 6 \\ 4 \end{pmatrix}$$

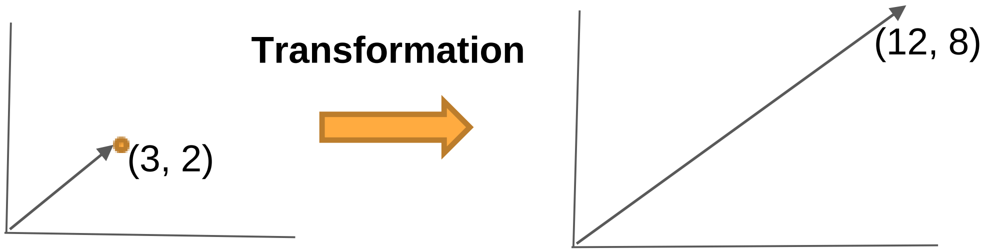
Fig. 2. Example of how a scaled eigenvector is still an eigenvector

Principal component analysis (PCA) - background knowledge

Eigenvalues and Eigenvectors

In the **first example**, the resulting vector is not an integer multiple of the original vector, whereas the **second example** is exactly 4 times the vector we began with.

The vector (3,2) from the **second example** represents an arrow pointing from the origin



The square matrix is a transformation matrix. If you multiply this matrix on the left of a vector, the answer is another vector that is transformed from it’s original position

Principal component analysis (PCA) - background knowledge

Eigenvalues and Eigenvectors

Eigenvectors properties:

- Eigenvectors can only be found for square matrices. And, not every square matrix has eigenvectors. Given a 3x3 matrix, there are 3 eigenvectors.

- If we scale the eigenvector by some amount before multiplication, we get the same multiple of it as a result, as shown in Fig. 2. This is because if we scale a vector by some amount, all we are doing is making it longer, without changing it's direction.

- All eigenvectors of a matrix are perpendicular, i.e. at right angles to each other (orthogonal). This is important because it means that you can express the data in terms of these perpendicular eigenvectors, instead of expressing them in terms of the X and Y axes.

Principal component analysis (PCA) - background knowledge

Eigenvalues and Eigenvectors

Eigenvalues:

- Eigenvalues are closely related to eigenvectors, ‘4’ is an eigenvalue associated with the eigenvector in Figure 1.
- Eigenvectors and eigenvalues always come in pairs.

Principal component analysis (PCA) - background knowledge

Eigenvalues and Eigenvectors

How to find these mystical eigenvectors? **By Solving Homogeneous Systems of Linear Equations**

Homogeneous Systems of Linear Equations is out of scope of this tutorial. **However, I strongly recommend to learn more (its fun!)**, please see a good link below: https://www.khanacademy.org/math/linear-algebra/alternate-bases/eigen-everything/v/linear-algebra-introduction-to-eigenvalues-and-eigenvectors

In the next lecture, we will be using Python/Numpy eigenvalues and eigenvectors functions.

Lecture 9 – Principal component analysis (PCA)

(Tutorial part 2)