b4 LT dis → wk   After → LT (dist) → Wk

[Source: https://exceednutrition.com/wp-content/uploads/2015/04/Its-never-too-late-for-change..png]

MLAI Session 7: Unsupervised Learning

Learning from unlabelled data

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Based on slides by Neil D. Lawrence, Roger Grosse (Toronto) & Hong-yi Li (NTU, TW)

Overview

What happened last week

- Bayesian you, Bayesian me.
- The model - my belief of teaching is the **prior** MLAI2015 (https://github.com/lawrennd/mlai2015)
- The data - your response and your feedback are data giving the **likelihood**
- The model - I generalised and **marginalised** over model parameters (different ways of teaching), getting the **marginal likelihood**
- The model - I formed the **posterior** (belief after one week's observation / data), made the changes, which is this session

What you will learn this week

- k-means **clustering**
- **Dimensionality reduction** - learning a latent, low-dimensional representation from unlabelled data
- Principal component analysis

- AutoEncoder, i.e., a standard unsupervised **Neural Network**, adapted from [TensorFlow Examples (https://github.com/aymericdamien/TensorFlow-Examples)](https://github.com/aymericdamien/TensorFlow-Examples)

Motivating Example: PCA without Math

[Watch: PCA main ideas in only 5 minutes (https://www.youtube.com/watch?v=HMOI_lkzW08)](https://www.youtube.com/watch?v=HMOI_lkzW08)

Unsupervised Learning

- Supervised learning is learning where each data point has a label (e.g. regression output)
- In unsupervised learning we have no labels for the data.
- Often thought of as structure discovery.
  - Finding features in the data
  - Exploratory data analysis
- In *Nature* 2015,

> We expect unsupervised learning to become far more important in the longer term. Human and animal learning is largely unsupervised: we discover the structure of the world by observing it, not by being told the name of every object!

Clustering - k-means

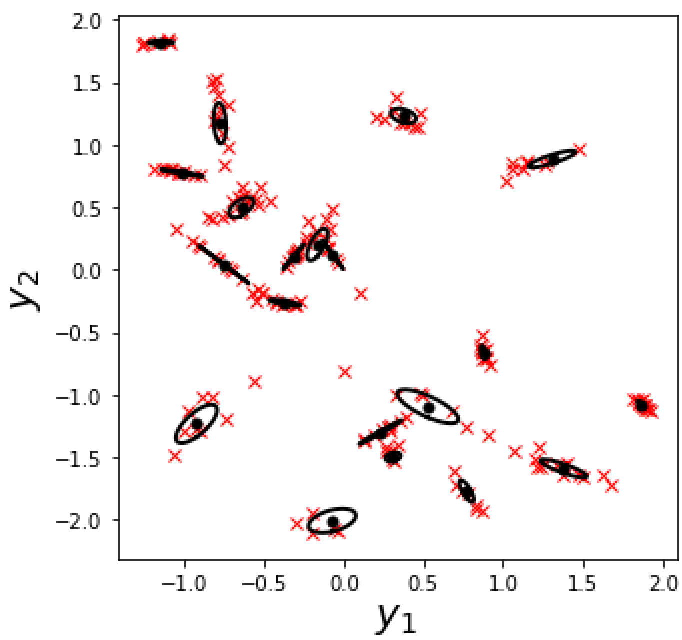
- Associate each data point, $\mathbf{y}_{i,:}$ with one of k different discrete groups.
- For example:
  - Clustering animals into discrete groups. Are animals discrete or continuous?
  - Clustering into different different *political* affiliations.
- **Question**: how to determine k?

In [1]:

```
import pods
import mlai
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

from ipywidgets import *
def display_plots(filebase, directory=None, width=700, height=500, **kwargs):
    """Display a series of plots controlled by sliders. The function relies on Python stri
    def show_figure(filebase, directory, **kwargs):
        """Helper function to load in the relevant plot for display."""
        filename = filebase.format(**kwargs)
        if directory is not None:
            filename = directory + '/' + filename
        display(HTML("<img src='{filename}'>".format(filename=filename)))

    interact(show_figure, filebase=fixed(filebase), directory=fixed(directory), **kwargs)
```

In [2]:

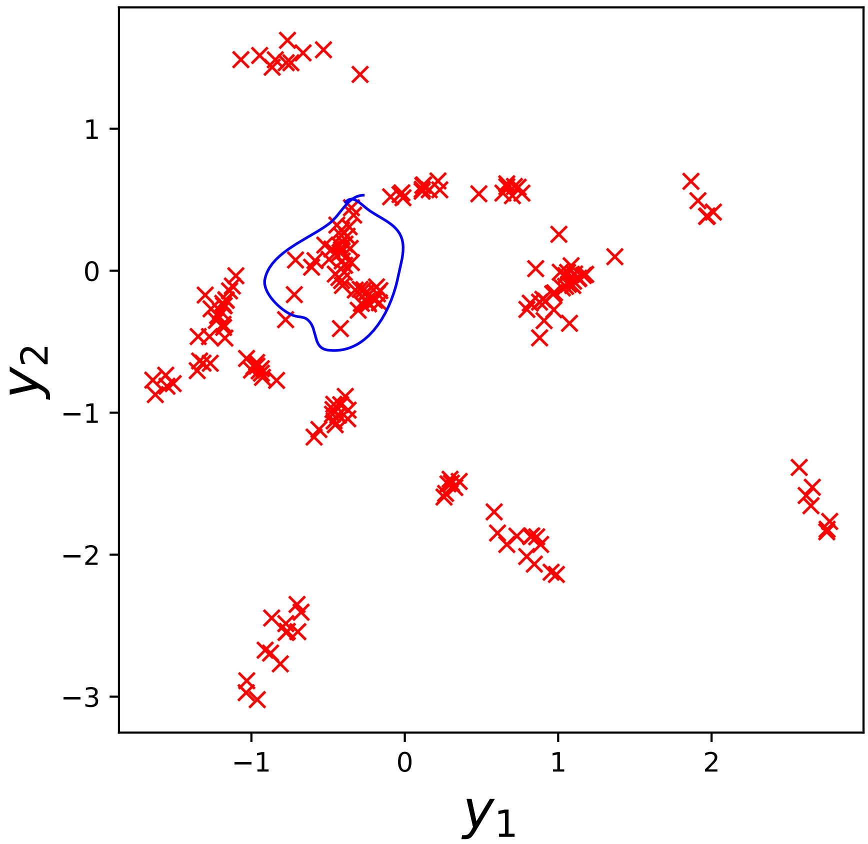
```
fig, ax = plt.subplots(figsize=(5,5))

num_centres = 20
num_data = 200
centres = np.random.normal(size=(num_centres, 2))
w = np.random.normal(size=(num_centres, 2))*0.1
alloc = np.random.randint(0, num_centres, size=(num_data))
sigma = np.random.normal(size=(num_centres, 1))*0.05
epsilon = np.random.normal(size=(num_data,2))*sigma[alloc, :]

Y = w[alloc, :]*np.random.normal(size=(num_data, 1)) + centres[alloc, :] + epsilon

ax.plot(Y[:, 0], Y[:, 1], 'rx')
ax.set_xlabel('$y_1$', fontsize=20)
ax.set_ylabel('$y_2$', fontsize=20)

plt.savefig('./diagrams/cluster_data00.svg')
pi_vals = np.linspace(-np.pi, np.pi, 200)[:, None]
for i in range(num_centres):
    ax.plot(centres[i, 0], centres[i, 1], 'o', markersize=5, color=[0, 0, 0], linewidth=2)
    x = np.hstack([np.sin(pi_vals), np.cos(pi_vals)])
    L = np.linalg.cholesky(np.outer(w[i, :],w[i, :]) + sigma[i]**2*np.eye(2))
    el = np.dot(x, L.T)
    ax.plot(centres[i, 0] + el[:, 0], centres[i, 1] + el[:, 1], linewidth=2, color=[0,0,0]
plt.savefig('./diagrams/cluster_data01.svg')
```



In [3]:

```
display_plots('cluster_data{counter:0>2}.svg', directory='./diagrams', counter=(0, 1))
```

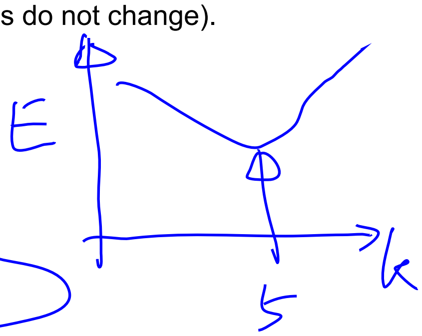
counter 0



k-means Clustering

- Simple algorithm for allocating points to groups.
- *Require*: Set k and a stopping criterion

1. Initialize cluster centres as randomly selected data points.
2. Assign each data point to *nearest* cluster centre (centroid).
3. Update each cluster centre by setting it to the mean of assigned data points.
4. Repeat 2 and 3 until the stopping criterion reached (e.g., cluster allocations do not change).



Objective Function

- This minimizes the objective (compactness)

$$E = \sum_{j=1}^{k} \sum_{i \text{ allocated to } j} \left(\mathbf{y}_{i,:} - \boldsymbol{\mu}_{j,:}\right)^\top \left(\mathbf{y}_{i,:} - \boldsymbol{\mu}_{j,:}\right)$$

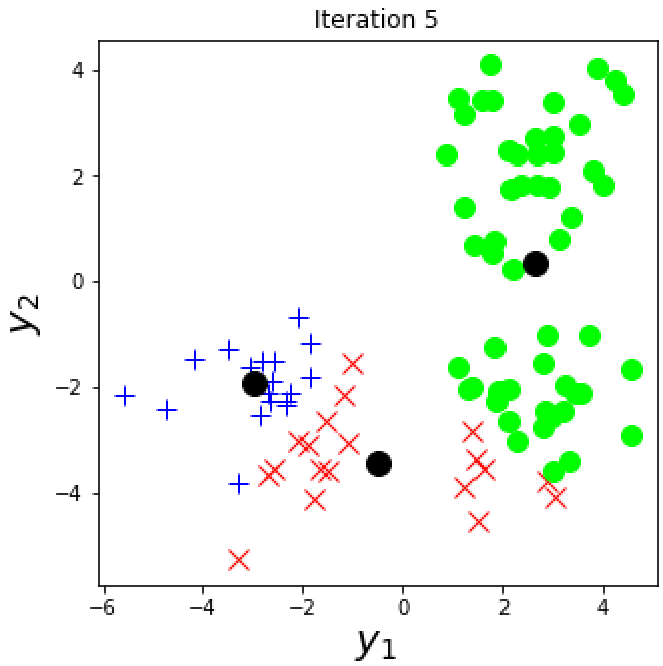
i.e. it minimizes the sum of **Euclidean squared distances** betwen points and their associated centres.

- The minimum is *not* guaranteed to be *global* or *unique*.
- This objective is a non-convex optimization problem.
- **Question**: How to evaluate the clustering results?

k

In [4]:

```
def write_plot(counter, caption):
    filebase = './diagrams/kmeans_clustering_{counter:0>3}'.format(counter=counter)
    plt.savefig(filebase + '.svg')
    f = open(filebase + '.tex', 'w')
    f.write(caption)
    f.close()

fig, ax = plt.subplots(figsize=(5,5))
fontsize = 20

num_clust_points = 30

Y = np.vstack([np.random.normal(size=(num_clust_points, 2)) + 2.5,
       np.random.normal(size=(num_clust_points, 2)) - 2.5,
       np.random.normal(size=(num_clust_points, 2)) + np.array([2.5, -2.5])])

centre_inds = np.random.permutation(Y.shape[0])[:3]
centres = Y[centre_inds, :]

ax.cla()

ax.plot(Y[:, 0], Y[:, 1], '.', color=[0, 0, 0], markersize=10)
ax.set_xlabel('$y_1$')
ax.set_ylabel('$y_2$')
ax.set_title('Data')
counter=0
write_plot(counter, 'Data set to be analyzed. Initialize cluster centres.')
ax.plot(centres[:, 0], centres[:, 1], 'o', color=[0,0,0], linewidth=3, markersize=12)
counter+=1
write_plot(counter, 'Allocate each point to the cluster with the nearest centre')
i = 0

for i in range(6):
    dist_mat = ((Y[:, :, None] - centres.T[None, :, :])**2).sum(1)
    ind = dist_mat.argmin(1)
    ax.cla()
    ax.plot(Y[ind==0, 0], Y[ind==0, 1], 'x', color= [1, 0, 0], markersize=10)
    ax.plot(Y[ind==1, 0], Y[ind==1, 1], 'o', color=[0, 1, 0], markersize=10)
    ax.plot(Y[ind==2, 0], Y[ind==2, 1], '+', color=[0, 0, 1], markersize=10)
    c = ax.plot(centres[:, 0], centres[:, 1], 'o', color=[0,0, 0], markersize=12, linewidt
    ax.set_xlabel('$y_1$',fontsize=fontsize)
    ax.set_ylabel('$y_2$',fontsize=fontsize)
    ax.set_title('Iteration ' + str(i))
    counter+=1
    write_plot(counter, 'Update each centre by setting to the mean of the allocated points
    for j in range(centres.shape[0]):
          centres[j, :] = np.mean(Y[ind==j, :], 0)
    c[0].set_data(centres[:, 0], centres[:, 1])
    counter+=1
    plt.savefig('./diagrams/kmeans_clustering_{counter:0>3}.svg'.format(counter=counter))
    write_plot(counter, 'Allocate each data point to the nearest cluster centre.')
```

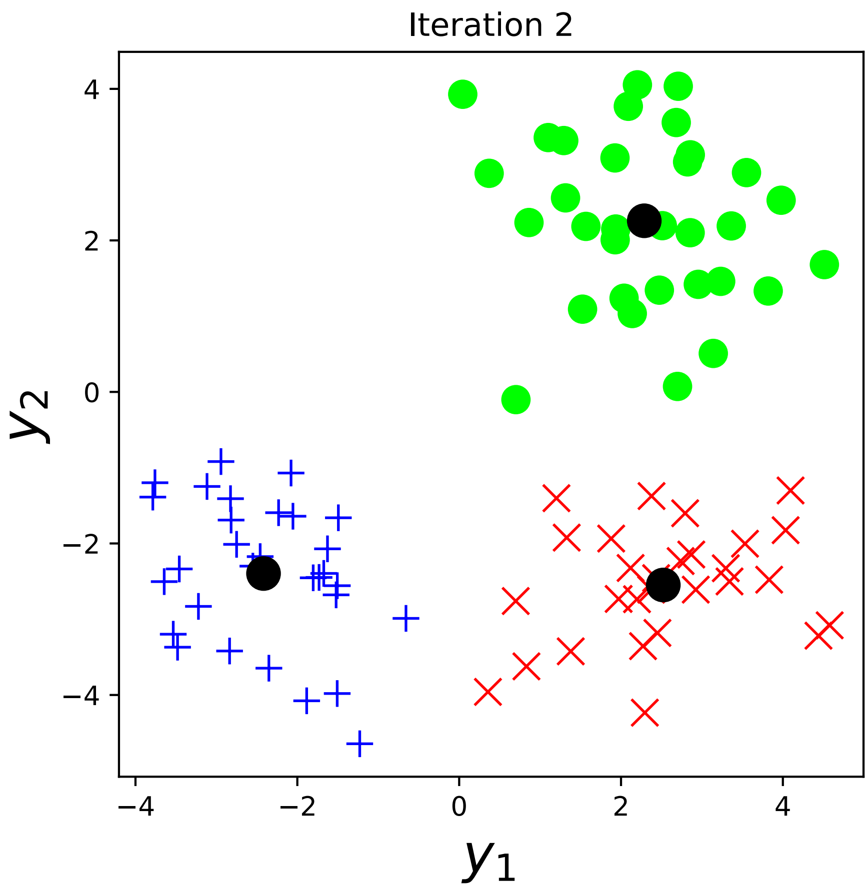

Iteration 5
4
2
0
−2
−4
−6
−4
−2
0
2
4
y_2
y_1

In [5]:

```
display_plots('kmeans_clustering_{counter:0>3}.svg', directory='./diagrams',
                        text_top='kmeans_clustering_{counter:0>3}.tex', counter=(0, 13
```

counter 6

text_top kmeans_clustering_{counter:0>3}



Dimensionality Reduction - PCA

Motivation of Dimensionality Reduction: High Dimensional Data

- USPS Data Set Handwritten Digit
- 3648 dimensions (64 rows, 57 columns)
- Space contains much more than just this digit.
- **Question**: How many possible images of this size and bit depth?

binary

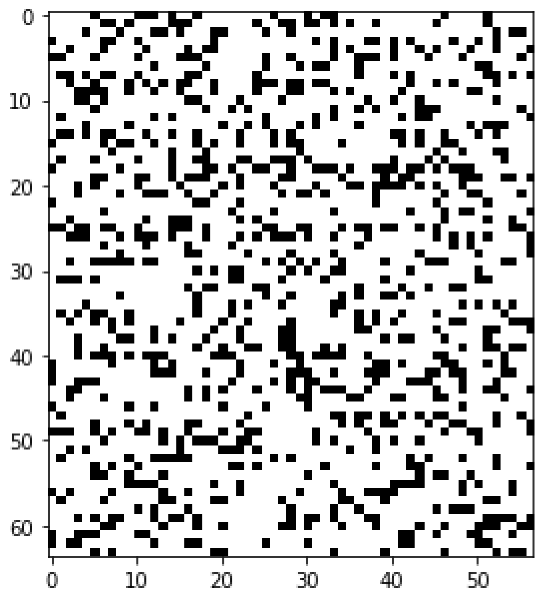
1-bit

$2^{64 \times 57 = 3648}$

= Int

In [6]:

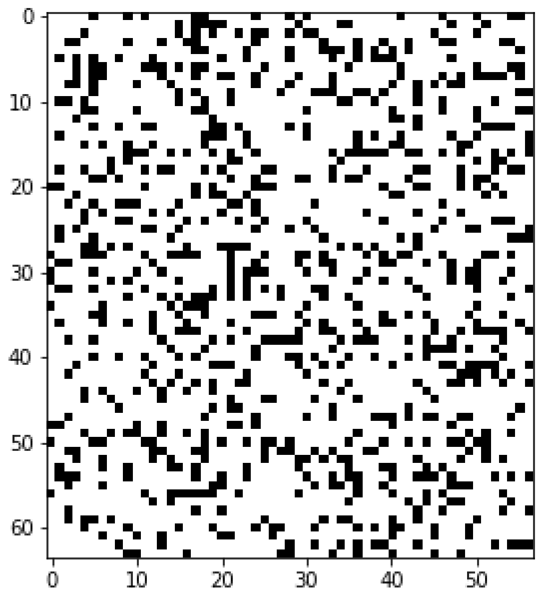
```
fig, ax = plt.subplots(figsize=(5,5))

six_image = mlai.load_pgm('br1561_6.3.pgm', directory ='./diagrams')
rows = six_image.shape[0]
col = six_image.shape[1]

ax.imshow(six_image,interpolation='none').set_cmap('gray')
plt.savefig('./diagrams/dem_six000.png')
for i in range(3):
    rand_image = np.random.rand(rows, col)<((six_image>0).sum()/float(rows*col))
    ax.imshow(rand_image,interpolation='none').set_cmap('gray')
    plt.savefig('./diagrams/dem_six{i:0>3}.png'.format(i=i+1))
```



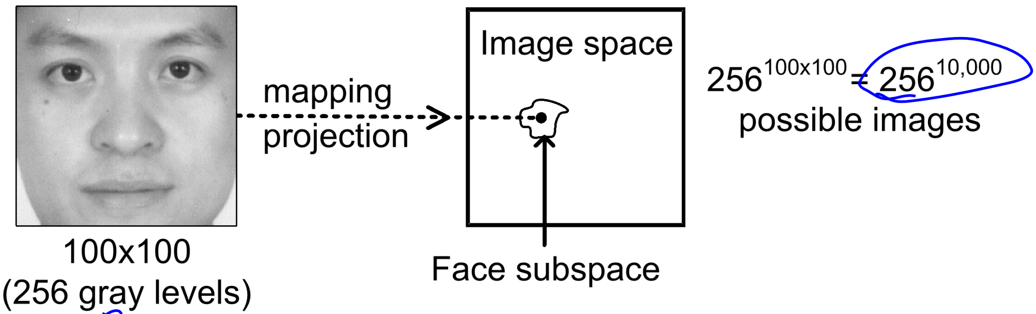
In [7]:

```
display_plots('dem_six{counter:0>3}.png', directory='./diagrams', counter=(0, 3))
```

counter 1



How About a Face?



3x 8-bit

Low Dimensional Subspace/Manifolds

- For high dimensional data with *structure*:
  - We expect fewer variations than dimensions;
  - Therefore we expect the data to live on a lower dimensional manifold.
  - Conclusion: Deal with high dimensional data by looking for a lower dimensional embedding/projection/transformation.

Principal Component Analysis

- PCA (@Hotelling:analysis33) is a linear embedding.
- Today its presented as: =

- Rotate to find 'directions' in data with maximal variance.
- How do we find these directions?

- Algorithmically we do this by diagonalizing the **sample** covariance matrix (a.k.a. scatter matrix, related to correlated Gaussian section in Session 6, rotation matrix)

$$\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{y}_{i,:} - \boldsymbol{\mu}\right)\left(\mathbf{y}_{i,:} - \boldsymbol{\mu}\right)^{\top}$$

- **Interesting observation**: Compare this definition with the k-means objective function

PCA PCA I/P

Principal Component Analysis

- Given data $\{\mathbf{y}\}$, PCA finds *orthogonal* directions defined by a projection $\mathbf{U}$ capturing the **maximum varience** in the data. The projected data (PCA representation) $\mathbf{x} = \mathbf{U}^{\top}\mathbf{y}$. Maximising the variance is equivalent to minimise the reconstruction error.
- **Question**: given the PCA representation $\mathbf{x}$, how to obtain (an approximation/reconstruction) of $\mathbf{y}$?

$S_x =$ λ_1 λ_2

Lagrangian

- Solution for the first direction is found via constrained optimisation (which uses [Lagrange multipliers (https://en.wikipedia.org/wiki/Lagrange_multiplier)](https://en.wikipedia.org/wiki/Lagrange_multiplier)):

$$L\left(\mathbf{u}_1, \lambda_1\right) = \mathbf{u}_1^{\top}\mathbf{S}\mathbf{u}_1 + \lambda_1\left(1 - \mathbf{u}_1^{\top}\mathbf{u}_1\right)$$

unit

- Gradient with respect to $\mathbf{u}_1$

$$\frac{\mathrm{d}L\left(\mathbf{u}_1, \lambda_1\right)}{\mathrm{d}\mathbf{u}_1} = 2\mathbf{S}\mathbf{u}_1 - 2\lambda_1\mathbf{u}_1 = 0$$

rearrange to form

$$\mathbf{S}\mathbf{u}_1 = \lambda_1\mathbf{u}_1.$$

Which is known as an [*eigenvalue problem* (https://en.wikipedia.org/wiki/Eigenvalues_and_eigenvectors)](https://en.wikipedia.org/wiki/Eigenvalues_and_eigenvectors).

- Further directions that are *orthogonal* (uncorrelated) to the first can also be shown to be eigenvectors of the covariance.
- **Eigenvectors**: the *basis functions*, principal components
- **Eigenvalue**: the **variance** captured respectively.
- **Question**: What if further directions are not constrained to be orthogonal (do not have to be orthogonal to the first)?

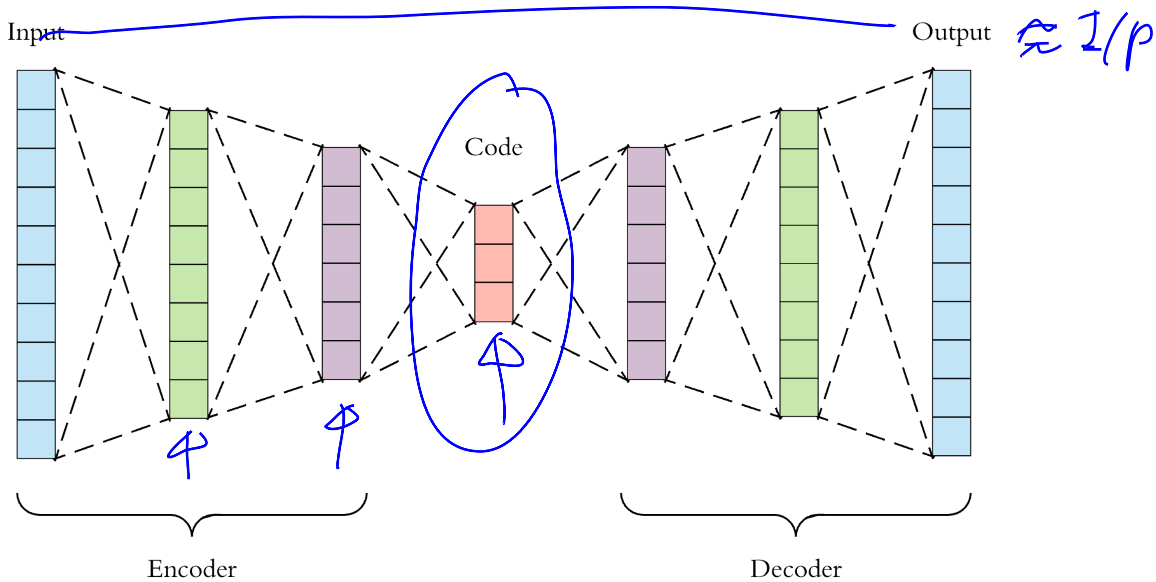
PCA for Visualisation

- A common way to visualise data is to plot PC1 vs PC2 (vs PC3)
- It is a fundamental method for visualisation, see [Google's Embedding projector using TensorFlow (https://projector.tensorflow.org/)](https://projector.tensorflow.org/) with two default visualisation methods 1) PCA, 2) tSNE (have to use PCA as preprocessing for very big data). Go and play with it! You can play with your own data!
- Further reading: [Visualising high-dimensional datasets using PCA and t-SNE in Python (https://medium.com/@luckylwk/visualising-high-dimensional-datasets-using-pca-and-t-sne-in-python-8ef87e7915b)](https://medium.com/@luckylwk/visualising-high-dimensional-datasets-using-pca-and-t-sne-in-python-8ef87e7915b)

Neural Networks for Unsupervised Learning - AutoEncoder (*optional*)

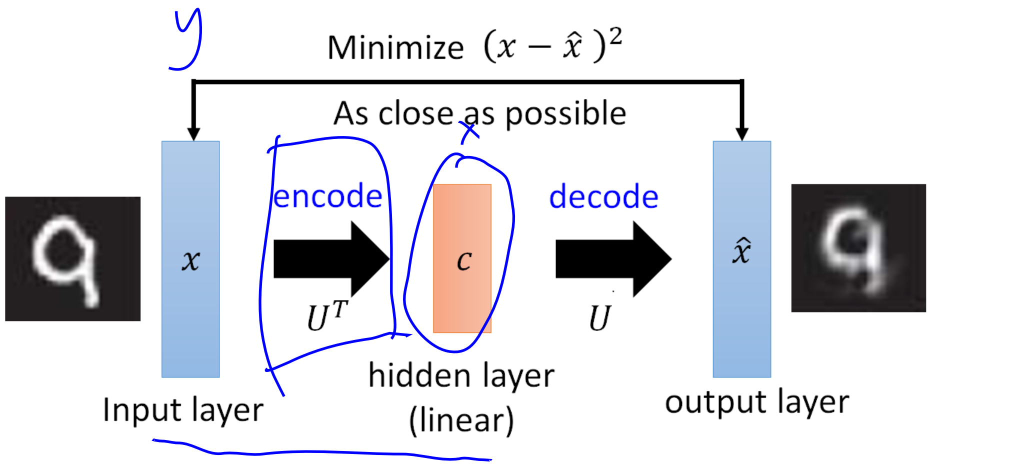
AutoEncoder

- AutoEncoder: a feed-forward neural network taking an input $\mathbf{x}$ and predict $\mathbf{x}$, i.e., reconstructing itself
- To make this non-trivial, we need to add a bottleneck layer whose dimension is much smaller than the input, which is the latent representation of $\mathbf{x}$. Representation Learning (https://en.wikipedia.org/wiki/Feature_learning)



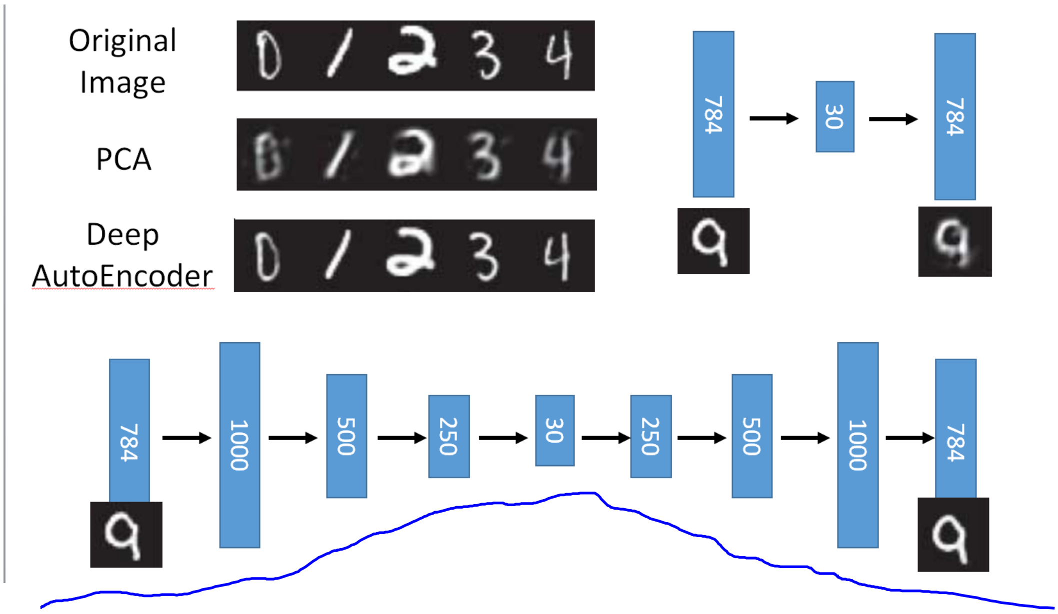
- Encoder: Learn a compact representation, the code, of the input data
- Decoder: Reconstruct the input data from the code

PCA as Linear AutoEncoder



- PCA can be view as a single-layer encoder, single-layer-decoder, AutoEncoder.
- AutoEncoder typically uses nonlinear functions, such as sigmoid function (https://en.wikipedia.org/wiki/Sigmoid_function)
- **Question**: If we stack multiple linear layers as the encoder, do we get a linear or nonlinear encoder?

Deep AutoEncoder



- Issues: architecture, optimisation (no closed-form solution as PCA), initialisation, computational time (many iterations), etc.