# Introduction to Machine Learning

## Lecture 10
## Principle Component Analysis

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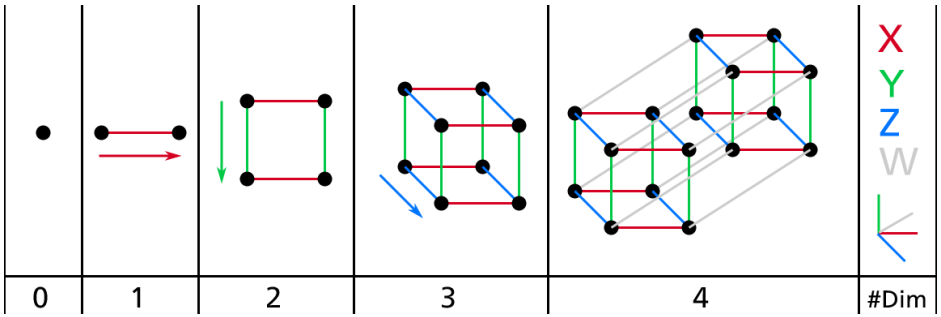
# Introduction

- `https://git.io/ml2019-11`
- Today we will look at a dimensional reduction technique call *Principal Components Analysis*
- This will be good for visualization and to create reduced datasets that can be fit quicker/easier with less resources

# Large Dimensions




- High dimensional behaviour is hard to visualize
- As you increase the number of dimensions, the ratio of the volume of a hypersphere to a hypercube tends to 0
  - This mean there is no "center" to high dimensional objects, all points exist on the border
- This has non-intuitive consequences, e.g., the expected value of the difference between the largest and smallest distance between two randomly picked points tends to zero as the dimensions increase

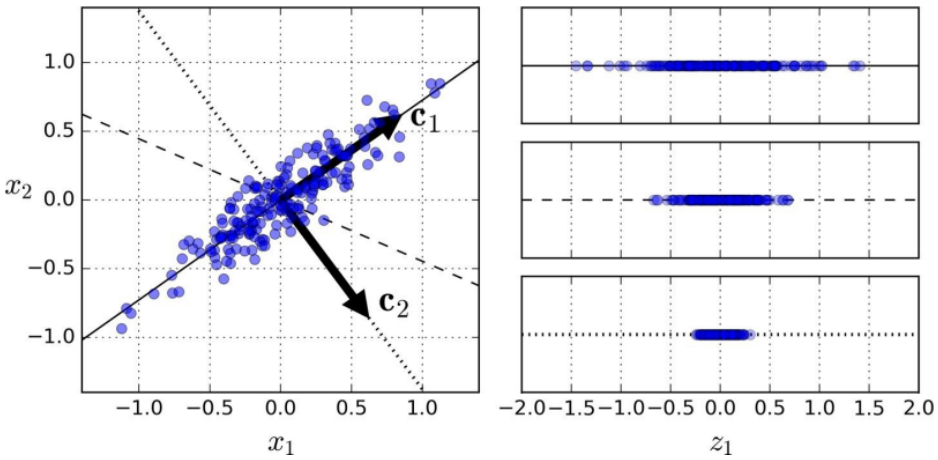
# The Curse of Dimensionality

- In ML, each of our "features" is a dimension
- We think naively collecting more features will result in better discrimination
- But in fact, it can lead to worse results due to the
  - We're usually define some kind of "distance" between datapoints when we are building models
  - But with too many dimensions, the distance between points stops being useful, so our algorithms are unable to be trained
  - In high dimensions, the volume becomes so massive, its impossible to get enough datapoints to fill out space
  - The "curse of dimensionality"

# In Machine Learning

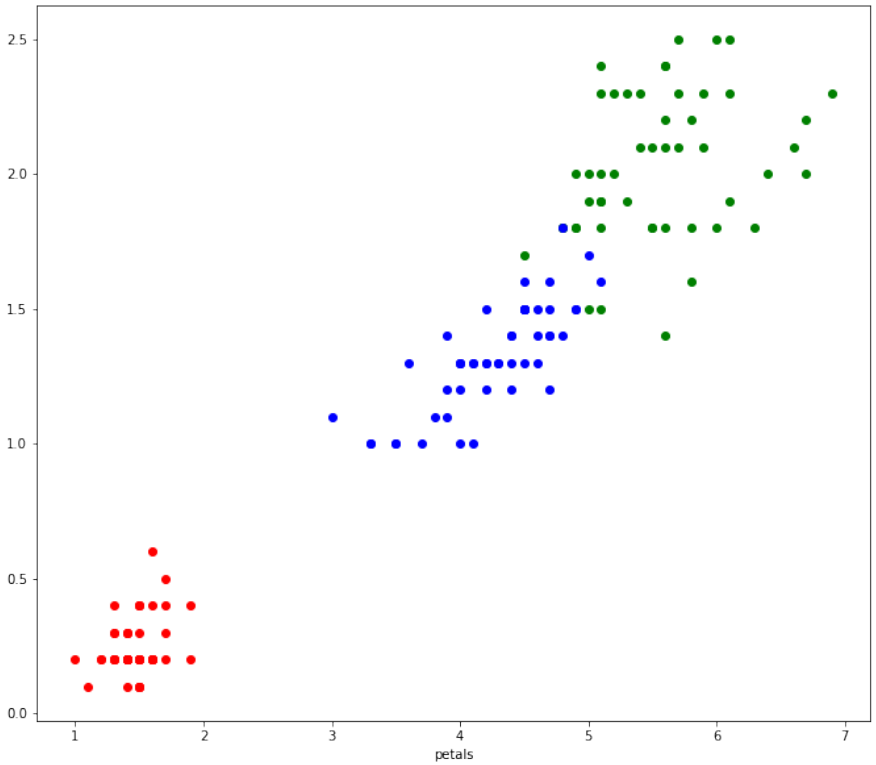
- The assumption was that we're evenly distributed over the unit hypercube
- The whole point of classification in machine learning is that different categories distribute differently
- Quite often, the data tends to clump in lower dimensional subspaces
- We want to reduce the number of dimensions while retaining variance
  - I.e. we will need feature selection
- PCA is one way to automatically reduce the number of data dimensions in a "sensible" manner

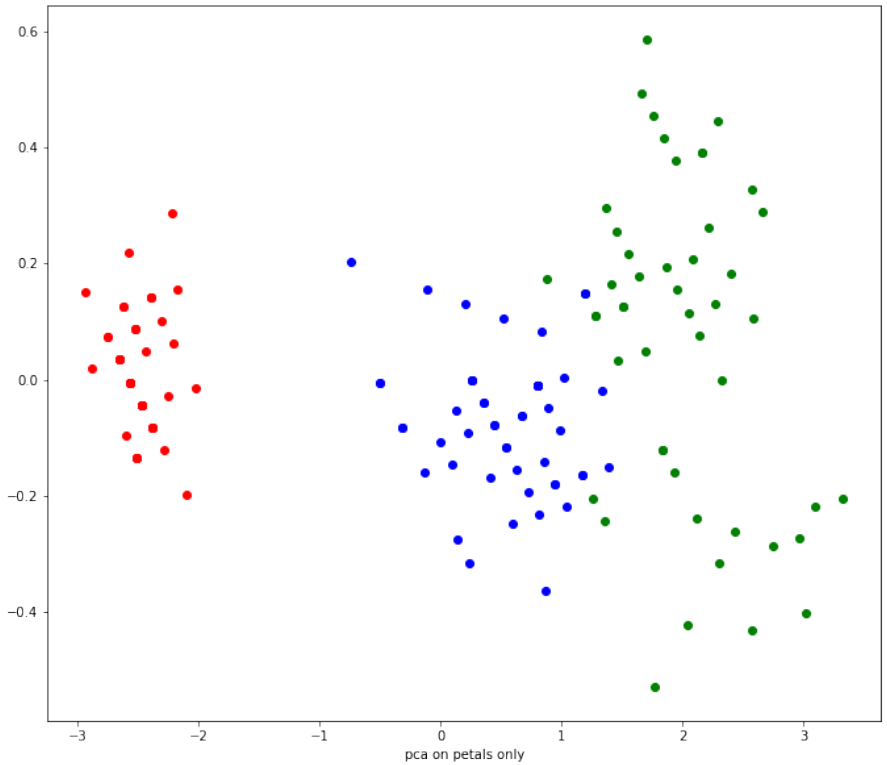
# Principal Component Analysis




- In PCA we search for the axis along which the data has the maximum variance
  - This becomes our first axis
- Then, project out that axis, flatten the data onto a hyperplane where the variance due to the first axis is gone (the plane perp. to the axis)
- Now, find the next axis in the (n-1) space with the highest variance
- Keep going until we have a fully orthogonal set of basis vectors
- We can instead stop this procedure after d dimensions
  - Then we have a reduced dimensional dataset

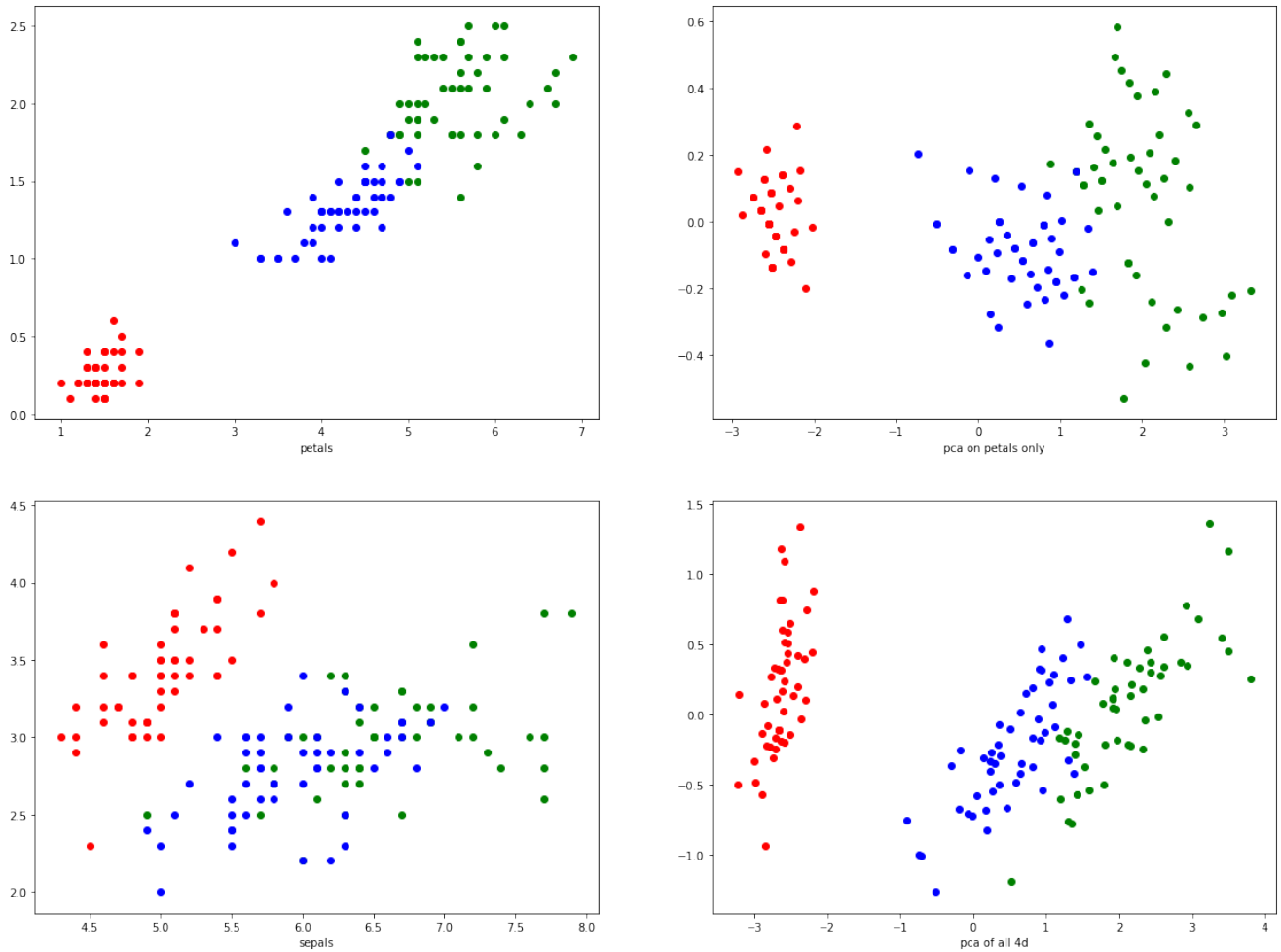
# Example Iris Dataset




- Using only the sepal features (length and width, show left), PCA in 2d transforms the data along the diagonal axis (right)
  - In 2D, once we have first vector, second automatically found, since we end up with an orthogonal basis after PCA

# Example Iris continued




- Using all the features (bot. right), you can see that mostly the same axis is found, but with some additional variation
  - The covariance of the full datasets removed, not necessarily each individual component to be classified

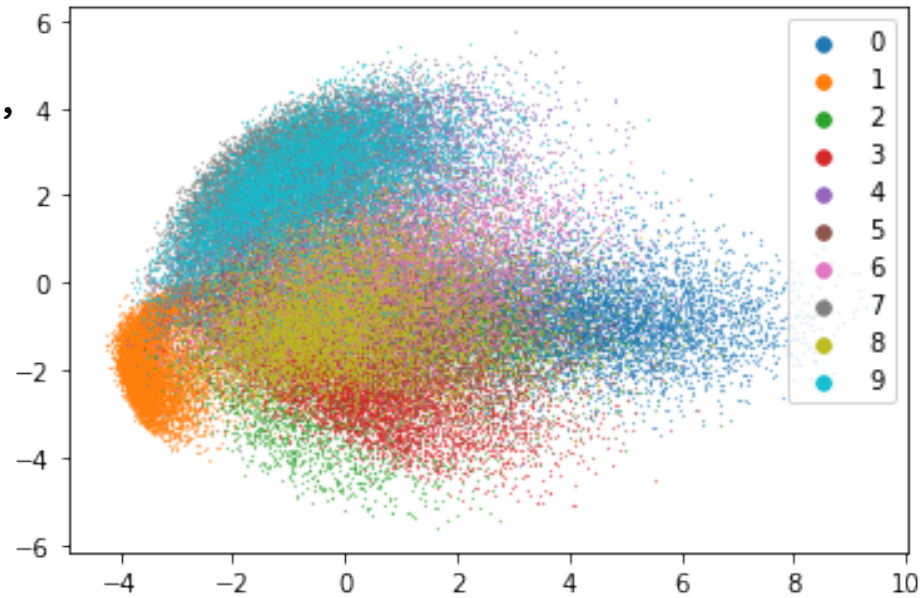
# MNIST after PCA

```
from sklearn.datasets import fetch_openml
from sklearn.decomposition import PCA
import matplotlib.cm as cm
import numpy as np

X, y = fetch_openml('mnist_784', version=1,
                    return_X_y=True)
X = X / 255.

pca = PCA(n_components=2)
pca.fit(X)
x = pca.transform(X)
 # y is stored as a string
y = y.astype(np.int)

for n in range(10):
    xx = x[y==n]
    plt.scatter(xx[:,0], xx[:,1],
                s=0.05, label=str(n))
leg = plt.legend(markerscale=25)
```

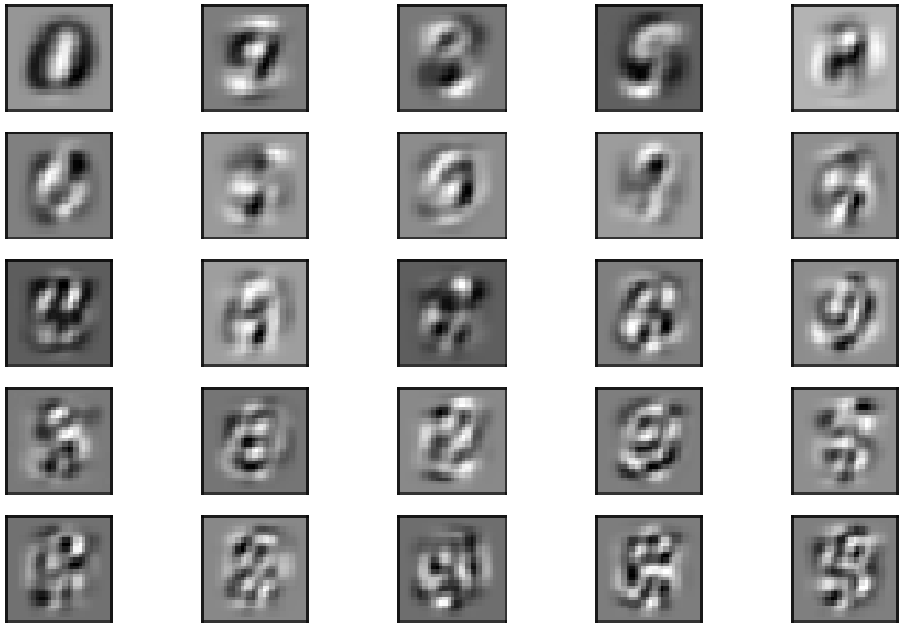



- Two-component PCA on the MNIST digit dataset
  - A 28x28 grayscale image is just a 784-dim. hypercube

# MNIST PCA Components

```
pca=PCA(n_components=25)
pca.fit(X)
for i in range(25):
    plt.subplot(5, 5, (i+1))
    plt.imshow(pca.components_[i].reshape(28,28),
               cmap='gray_r')
    plt.gca().xaxis.set_visible(False)
    plt.gca().yaxis.set_visible(False)
print(np.cumsum(pca.explained_variance_ratio_[:25]))
```

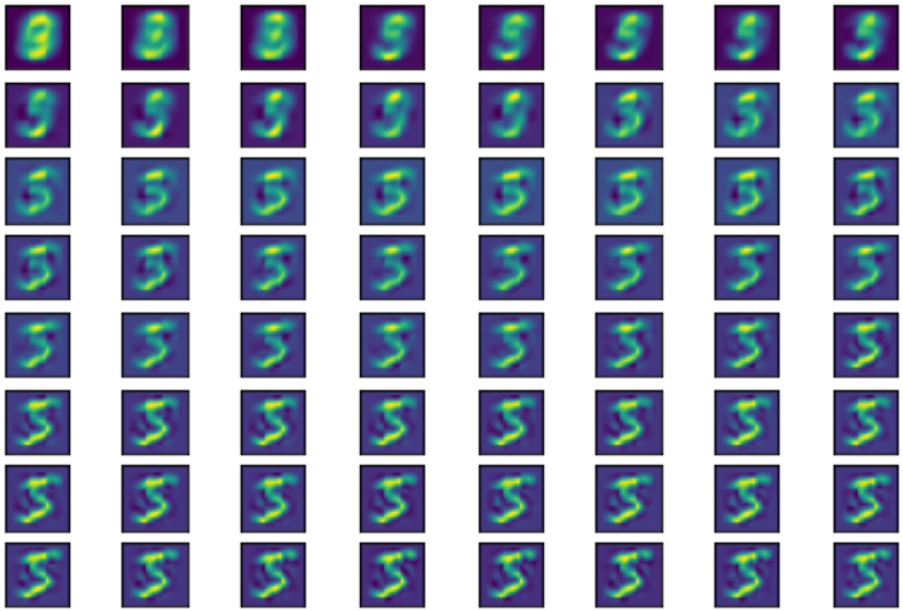
```
[0.09746116 0.16901561 0.23051091 0.28454476 0.3334341
 0.37648637 0.40926898 0.4381654  0.46574904 0.48917044
 0.51023733 0.53061286 0.5476835  0.5646237  0.58045752
 0.59532097 0.60851455 0.62130469 0.6331771  0.64470642
 0.65536679 0.66546472 0.67505596 0.68415214 0.69298103]
```



- A component is just a vector in the 784D space, so we can plot them as 28x28 images (bearing in mind that here they can go negative)
- First two images in the top row are the components of the prev. page
- We can see what fraction of the variance of the dataset is explained by each component, and take the cumulative sum (`np.cumsum`) to see the fraction explained by the first N components

# As a Compression Technique

```
for i in range(64):
    pca=PCA(n_components=i+1)
    pca.fit(X)
    t = pca.transform([X[0]])
    plt.subplot(8, 8, (i+1))
    plt.imshow(pca.inverse_transform(t).\
               reshape(28,28))
    plt.gca().xaxis.set_visible(False)
    plt.gca().yaxis.set_visible(False)
```



- We can use PCA as a rudimentary "compression" technique
- Fit PCA and transform the image, but only keep N components
- Can reconstruct by summing up the components (of course, this also requires you the keep N images, one showing each component)
- Here, we see the first image of MNIST reconstructed with progressively more and more components

# Technical Points

- If we represent our data as rows in a matrix $X$, then PCA is equivalent to finding basis which diagonalizes $X^T X$
- $X^T X$ is essentially the covariance, so we also have:
  - The principal components are the eigenvectors of the covariance matrix
  - The prinicpal components are a decorrelated basis for our measurement
- The principal components can also be obtained by SVD decomposition
  - $X = USV^T$ where S is diagonal, values gives the "strength" of the decomposition, reducing S to the top n gives the n-dim PCA

```
pca=PCA(2)
pca.fit(x)
X_centered = x - x.mean(axis=0)
U, s, Vt = np.linalg.svd(X_centered.astype(np.float))
c1 = Vt.T[:, 0]
c2 = Vt.T[:, 1]
print("Via SVD:", c1, '\n', c2, '\nVia sklearn PCA:', pca.components_)
```

```
Via SVD: [ 0.36158968 -0.08226889  0.85657211  0.35884393]
 [-0.65653988 -0.72971237  0.1757674   0.07470647]
Via sklearn PCA: [[ 0.36158968 -0.08226889  0.85657211  0.35884393]
 [ 0.65653988  0.72971237 -0.1757674  -0.07470647]]
```

# Exercises