Lecture 19: Dimensionality Reduction

Dimensionality reduction

- Representing data using **a smaller number of variables** while preserving the "interesting" structure of the data
- Purposes:
  - Visualisation
  - Computational efficiency in a pipeline
  - Data compression or statistical efficiency in a pipeline
- Results in loss of information in general
  - Trick: ensure that most of the "interesting" information (signal) is preserved (while what is lost is mostly noise)

Pricinpal component analysis (PCA)

- Popular method for dimensionality reduction and data analysis
- Aim: find **a new coordinate system** s.t. most of the **variance is concentrated** along the first coordinate, then most of the remaining variance along the second coordinate, etc.
- Dimensionality reduction is based on **discarding coordinates** except the first $l < m$

Formulating the problem

- Projection of u on v: $u_v = u \cdot v / ||v||$
  - If $||v|| = 1$, $u_v = u \cdot v$
- Vector v can be considered as a candicate **coordinate axis**
  - and u_v the coordinate of point u (on the new coordinate axis)
- Data transformation
  - Projecting all data points to a new coordinate axis p_1
    - result: $X' p_i$
    - Where $||p_i|| = 1$
    - X has original data points in columns
- Sample covariance matrix:
  - For centered (mean subtracted) matrix X
  - $\Sigma_X = \frac{1}{n-1} X' X$

PCA

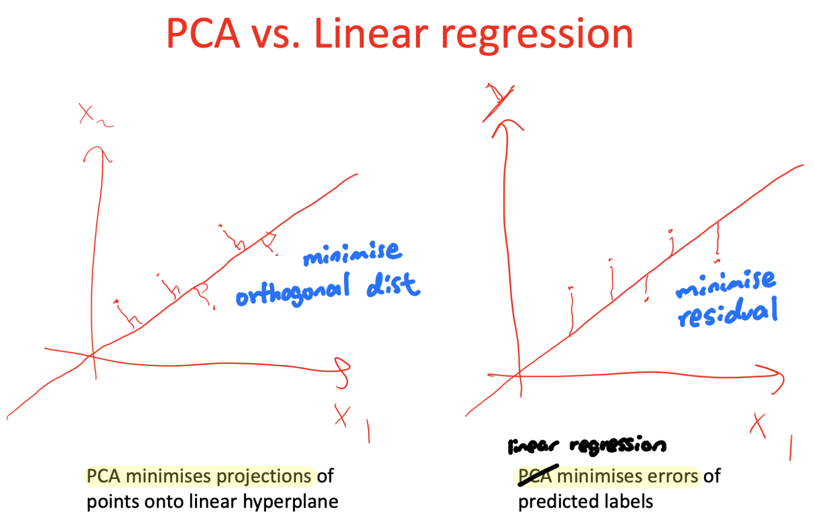
- Objective:
  - assume the data is centered
  - find p_1 to maximise variance along this PC: $p_1' \Sigma_x p_1$ subject to ||p_1|| = 1
- Constrained problem -> Use Lagrange multipliers
- Solution: p_1 is the eigenvector with corresponding λ_1 being the **max** eigenvalue (of covariance matrix Σ_X)
  - Variance captured by PC1: $\lambda_1 = p_1' \Sigma_X p_1$
- (Spectrum of a matrix is a set of its eigenvalues)
- Choose dimensions to keep from "knee" in scree plot

Efficient algorithm for PCA

- Setting p_i as all eigenvectors of the **centered** data covariance matrix Σ_X in decreasing eigenvalue order
- Lemma: a real symmetric m x m matrix has m real eigenvalues and corresponding eigenvectors are orthogonal
- Lemma: a PSD matrix further has non-negative eigenvalues

Linear regression v.s. PCA

- Another view of PCA: $s - dim$ plane minimising residual sum squares to data
- It turns out:
  - PCA chooses the **direction** to be a hyperplane that minimise these errors (RSS)
  - Since variance and squared distance have something in common (both sum of squares)



Additional effect of PCA

- Consider candidate axes i and $(i+1)$, if there is correlation between them
  - This means that axis i can be rotated further to capture more variance
- PCA should end up finding new axes (transformation) s.t. the transformed data is uncorrelated

Non-linear data and kernel PCA

- Low dimensional approximation need not be linear
- Kernel PCA: **map** data to feature space, **then** run **PCA**
  - Express PC in terms of data points
  - Solution uses X'X that can be kernelised:
    - $(X'X)_{ij} = K(x_i, x_j)$
  - Solution strategy differs from regular PCA
  - Modular: Changing kernel leads to a different feature space transformation