From COM4509 Lecture 9

PCA: Eigenvalue = Variance

- Focus on first PC: maximise the variance in projected space (i.e. maximise variance of $y = u^T x$)
  - x = original data
  - y = the compressed projection
  - μ = average
  - u = projection vector (the vector of transformations of all of the pcs)
  - $S = (x - \mu)(x - \mu)^T$ = variance of x $$\mathbf{S} = \frac{1}{n} \sum_{i=1}^{n} \left(\mathbf{x}^{(i)} - \boldsymbol{\mu}\right) \left(\mathbf{x}^{(i)} - \boldsymbol{\mu}\right)^\top$$

$$\operatorname{var}(y) = \frac{1}{n} \sum_{i=1}^{n} \left(y^{(i)} - \mu_y\right)^2 = \frac{1}{n} \sum_{i=1}^{n} \mathbf{u}^\top \left(\mathbf{x}^{(i)} - \boldsymbol{\mu}_{\mathbf{x}}\right) \left(\mathbf{x}^{(i)} - \boldsymbol{\mu}_{\mathbf{x}}\right)^\top \mathbf{u} = \mathbf{u}^\top \mathbf{S} \mathbf{u}$$

- The projection **u** is what we want to find
- **Projection vector u**, we use the unit norm constraint then take the derivative of the variance w.r.t u
  - **λ -** the variance(s) captured by **u**

$$L(\mathbf{u}, \lambda) = \mathbf{u}^\top \mathbf{S} \mathbf{u} + \lambda \left(1 - \mathbf{u}^\top \mathbf{u}\right)$$
$$\mathrm{d}L(\mathbf{u}, \lambda)/\mathrm{d}\mathbf{u} \implies \mathbf{S}\mathbf{u} = \lambda \mathbf{u}$$

- **Question**: which solution (eigen-pair) to choose?
  - There are many solutions for eigenvalues so we take the maximum eigenvalue
    - Maximum eigenvalue = maximum variance = most useful

$$\operatorname{var}(y) = \mathbf{u}^\top \mathbf{S} \mathbf{u} = \lambda \mathbf{u}^\top \mathbf{u} = \lambda$$

PCA: Max Variance <-> Min MSE

- **Maximum Variance Direction -** what you maximise
  - For the below, mean = 0 so S simplifies to XX^T
  - $$\frac{1}{n} \sum_{i=1}^{n} (\mathbf{v}^T \mathbf{x}_i)^2 = \mathbf{v}^T \mathbf{X} \mathbf{X}^T \mathbf{v}$$
- **Minimum Reconstruction Error -** what you minimise
  - v = u = projection matrix
  - Mse of original data - reconstruction $Y = U^T X$, $YU = U^T X U = X$^
  - $$\frac{1}{n} \sum_{i=1}^{n} \|\mathbf{x}_i - (\mathbf{v}^T \mathbf{x}_i) \mathbf{v}\|^2$$