

# Principal Component analysis

References:

Applied Machine Learning (Forsyth) <https://link.springer.com/book/10.1007/978-3-030-18114-7>  
sections 4.3.2, 5.1.1 - 5.1.4

## Primer from section 4.3.2 on diagonalizing matrices

- a matrix  $M$  is symmetric if  $M = M^T$
- $S = d \times d$  matrix,  $u = d \times 1$  vector,  $\lambda = \text{Scalar}$

$$Su = \lambda u \quad \text{eigenvalue}$$

↑  
eigenvector

- Symmetric matrices: eigenvalues are real
- $d$  distinct eigenvectors normal to one another
- Stack these into a matrix  $U = [u_1, \dots, u_d]$
- Now:

$$SU = U\Lambda$$

↑                      ↖  
orthogonal matrix      diagonal matrix

- Convention: elements of  $U$  are ordered  
so elements of  $\Lambda$  are sorted along  
diagonal, largest first

to convert any symmetric matrix  $S$  to  
diagonal form:  $U^T S U = \Lambda$  ← result

↑                      ↖  
input                  matrix of  
                         eigenvectors

# PCA

• objective: Encode high dimensional data into a lower dimensional space for analysis and/or visualization

$\{x\}$  = dataset of  $N$ -dimensional vectors

→ Subtract the mean from the dataset to get  $\{m\}$

$$m_i = x_i - \text{mean}(\{x\})$$

→ diagonalize covariance matrix (note that  $\text{cov}(\{m\}) = \text{cov}(\{x\})$ )

$$\underbrace{U^T}_{\text{covariance matrix}} \underbrace{\text{cov}(\{x\})}_{\text{matrix of eigenvectors}} \underbrace{U}_{\text{diagonal matrix of eigenvalues}} = \Lambda$$

Note: the book uses  $\Sigma = \text{cov}(\{x\})$

→ form dataset  $\{r\}$  with:

$$r_i = U^T m_i = U^T (x_i - \text{mean}(\{x\}))$$

→ mean of  $\{r\}$  is 0, covariance is diagonal matrix, or most of the diagonal entries in the covariance matrix are small

Calculating the error:

→ datapoint  $r_i$  has  $d$  components, choose an  $s$  s.t.  $s < d$  to represent  $r_i$  in lower ( $s$ ) dimensions call this  $p_i$

$$\text{error: } \frac{1}{N} \sum_i [(r_i - p_i)^T (r_i - p_i)]$$

$p_i = r_i$  in components  $0 \dots s$

$p_i = 0$  in components  $s+1 \dots d$

So error =

$$\begin{aligned} & \frac{1}{N} \sum_i \left[ \sum_{j=s+1}^d (r_i^{(j)})^2 \right] \\ &= \sum_{j=s+1}^d \left[ \frac{1}{N} \sum_i (r_i^{(j)})^2 \right] = \sum_{j=s+1}^d \text{var}(\{r^{(j)}\}) \\ &= \sum_{j=s+1}^d \lambda_j \end{aligned}$$

• eigenvalues of the covariance matrix give the error when that component is left out

• reprojection error = sum of eigenvalues of components that were left out.

Representing Data on Principal components

$$\hat{x}_i = \bigcup p_i + \text{mean}(\{x\})$$

weighted sum of first  $s$  columns of  $U$

$$\hat{x}_i = \sum_{j=1}^s w_{ij} u_j + \text{mean}(\{x\})$$

$$w_{ij} = r_i^{(j)} = (x_i - \text{mean}(\{x\}))^T u_j$$

$$\hat{x}_i = \text{mean}(\{x\}) + \sum_{j=1}^s [u_j^T (x_i - \text{mean}(\{x\}))] u_j$$