Outline

Eigenvalue Decomposition (EVD)

Eigenvalue decomposition places significant role in PCA. PCs are eigenvectors of $X^\top X$ and PCA properties are derived from those of eigenvectors and eigenvalues.

- For any $p \times p$ *symmetric* matrix S (think for example $X^\top X$), there exists p eigenvectors $v_1, \ldots, v_p$ that are pairwise orthogonal and p associated eigenvalues $\lambda_1, \ldots, \lambda_p$ which satisfy the eigenvalue equation $Sv_i = \lambda_i v_i \ \forall i$.
- S can be written as $S = V \Lambda V^\top$ where
  - $V = [v_1, \ldots, v_p]$ is a $p \times p$ orthogonal matrix
  - $\Lambda = diag\{\lambda_1, \ldots, \lambda_p\}$
  - and if $S_{ij} \in \mathbb{R} \ \forall i, j$, $\lambda_i \in \mathbb{R} \ \forall i$
- The relevant R-command is `eigen`. Look at `?eigen` to get help on the command.

Singular Value Decomposition (SVD)

The SVD of a matrix X is an equally useful matrix factorisation that is related to the EVD.

- Though the EVD does not exist for $\mathbb{R}^{n \times p}$ matrices if $p \neq n$, SVDs *always* exists.
- X can be written as $X = UDV^\top$ where
  - U is an $n \times n$ matrix with orthogonal columns.
  - D is a $n \times p$ matrix with decreasing non-negative elements on the diagonal (the singular values) and zero off-diagonal elements.
  - V is a $p \times p$ matrix with orthogonal columns.

  The relevant R-command is `svd`.
- SVD can be computed using very fast and numerically stable algorithms.

Some Properties of the SVD

- Let $X = UDV^\top$ be again the SVD of the $n \times p$ matrix X.
- Note that

$$X^\top X = (UDV^\top)^\top (UDV^\top) = VD^\top U^\top UDV^\top = VD^\top DV^\top,$$

  using orthogonality ($U^\top U = I_n$) of U.
- The eigenvalues of $S = X^\top X$ are thus the squares of the singular values of X and the columns of the orthogonal matrix V are the eigenvectors of S.
- We also have

$$XX^\top = (UDV^\top)(UDV^\top)^\top = UDV^\top VD^\top U^\top = UDD^\top U^\top,$$

  using orthogonality ($V^\top V = I_p$) of V.
- Consider the following optimization problem:

$$\min_{\tilde{X}} \|\tilde{X} - X\|^2 \qquad \text{s.t. } \tilde{X} \text{ has maximum rank } r < n, p.$$

  This problem can be solved by keeping only the r largest singular values of X, zeroing out the smaller singular values in the SVD.