

Angle bet. two vectors = $\cos^{-1} \left[\frac{(x, y)}{\|x\|_2 \|y\|_2} \right]$

Norms

- Properties of valid norm:
- Should be real & non-negative $\rightarrow \|x\| = 0 \Leftrightarrow x = 0$
 - $\| \alpha x \| = |\alpha| \|x\|$
 - $\|x + y\| \leq \|x\| + \|y\|$
 - $|x^T y| \leq \|x\|_2 \|y\|_2$ (Cauchy-Schwarz inequality)
 - $\|A\|_1 = \max_{1 \leq i \leq m} (\sum_{j=1}^n |a_{ij}|)$ $\rightarrow \|A\|_\infty = \max_{1 \leq j \leq n} (\sum_{i=1}^m |a_{ij}|)$ (max. row absolute sum)
 - If $A = uv^T$, $\|A\|_2 = \|u\|_2 \|v\|_2$ (when $x = \frac{v}{\|v\|}$)
 - $\|AB\|_p \leq \|A\|_p \|B\|_p$
 - $\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2} = \sqrt{\text{tr}(AA^T)} = \sqrt{\text{tr}(A^T A)} = \sqrt{\sum_{i=1}^m \|a_i\|_2^2}$

Conditioning & Stability

- $\kappa(A) = \frac{\sigma_1}{\sigma_m} = \sqrt{\frac{\lambda_{\max}(A^T A)}{\lambda_{\min}(A^T A)}}$
- $\kappa^R(A) = \|A\| \|A^+\|$, where $\|A^+\| = (A^T A)^{-1} A^T$
- Backwards stable \Rightarrow Stable \Rightarrow Forward stable
- For a backward stable algo, $f(\tilde{x}) = \tilde{f}(x)$
- Backward stability:
 $\tilde{f}(x) = f(x + \delta x)$
 Forward stability:
 $\|f(x) - \tilde{f}(x)\| = O(\epsilon_m)$

SVD

$A = U \Sigma V^T$, $U \in \mathbb{R}^{m \times m}$, orthogonal
 $\Sigma \in \mathbb{R}^{m \times n}$, diagonal
 $V^T \in \mathbb{R}^{n \times n}$, orthogonal

$\|A\|_2 = \sigma_1$, $\|A\|_F = \sqrt{\sigma_1^2 + \dots + \sigma_n^2}$

Principal Component Analysis

- Consider a data matrix $A \in \mathbb{R}^{m \times n}$
- Move the matrix 0-centered by subtracting the mean of the coln. from each element in the coln.
 - Variance of the coln. = $\frac{E(X^2) - (E(X))^2}{m} = \frac{\|a_j\|_2^2}{m}$
 - Hence, total variance, $T = \|a_1\|_2^2 + \dots + \|a_n\|_2^2$

Biggest contributor to the variance = $\|A\|_F^2 = \sigma_1^2 + \sigma_2^2 + \dots + \sigma_n^2$

- To get the direction with highest variance, we need to find a vector \hat{w}_1 s.t. $t_1 = A \hat{w}_1$, $\|t_1\|_2$ is maximised. The solution is $\hat{w}_1 = v_1$.
- $t_1 = A v_1 = \sum_{j=1}^n u_j \sigma_j v_j^T v_1 = \sigma_1 u_1$

- Similarly, $t_2 = \sigma_2 u_2$, where t_2 is the direction along second highest variance.

Projectors

- Projector matrix P , must be:
- $P^2 = P$ (idempotent) $\rightarrow P v - v \in \text{Null}(P)$
 - Square matrix \rightarrow Rank-dependent
 - $P x = x \forall x \in \text{Range}(P)$ \rightarrow Symmetrical
 - If P is an orthogonal projector so is $(I - P)$
 - If A is orthogonal, $P = A(A^T A)^{-1} A^T = A A^T$
 - Projector & SVD: If $A = U \Sigma V^T$, U forms an orthonormal basis of A . Hence, the projection matrix corresponding to A , $P = Q(Q^T Q)^{-1} Q^T = Q Q^T$

QR Factorisation

- Q : matrix w/ orthonormal coln. $\rightarrow R$: UTM
- Gram-Schmidt orthogonalisation:
- $v_j = a_j - (q_1^T a_j) q_1 - \dots - (q_{j-1}^T a_j) q_{j-1}$
- $\hat{q}_j = \frac{v_j}{\|v_j\|_2}$
- Hence $q_n = \frac{a_n - \sum_{i=1}^{n-1} r_{in} q_i}{r_{nn}}$, where $r_{ij} = \begin{cases} v_i^T a_j, & i \neq j \\ \|a_j - \sum_{i=1}^{j-1} r_{ji} q_i\|_2, & i = j \end{cases}$
- Gram-Schmidt with projector: $q_n = \frac{P_n a_n}{\|P_n a_n\|}$, where $P_n = I - \sum_{i=1}^{n-1} q_i q_i^T = I - Q_{j-1} Q_{j-1}^T$

Modified Gram-Schmidt

$P_n a_n = (I - \sum_{i=1}^{n-1} q_i q_i^T) a_n = \left[\prod_{i=1}^{n-1} (I - q_i q_i^T) \right] a_n$

for $j = 1 \rightarrow n$:

$v_j^{(1)} = a_j$

$v_j^{(2)} = P_{\perp q_1} a_j = (I - q_1 q_1^T) a_j = v_j^{(1)} - q_1 q_1^T v_j^{(1)}$

$v_j^{(3)} = P_{\perp q_2} a_j = v_j^{(2)} - q_2 q_2^T v_j^{(2)}$

\vdots

$v_j^{(j)} = v_j^{(j-1)} - q_{j-1} q_{j-1}^T v_j^{(j-1)}$

$q_j = \frac{v_j^{(j)}}{\|v_j^{(j)}\|_2}$

Householder Triangularisation

\rightarrow Perform transformations to convert A to R :

$Q_n \dots Q_1 A = R$

$Q_k = \begin{bmatrix} I_{(k-1) \times (k-1)} & 0 \\ 0 & \hat{F}_{(m-k+1) \times (m-k+1)} \end{bmatrix}$

\rightarrow Let $\hat{x} = \begin{bmatrix} x \\ y \end{bmatrix}$, \hat{F} should be s.t. $\hat{F} \hat{x} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$

$= \|x\|_2 e_1$

Hence, $y = \hat{F} x = (I - 2uu^T)x$, where $u = -\frac{x}{\|x\|_2}$

where $v = \|x\|_2 e_1 - x$

Algo: for $k=1 \rightarrow n$:
 $\tilde{x} = \tilde{A}(k:m, k) \parallel \text{row } k \text{ to column in the } k^{\text{th}} \text{ coln.}$
 $\tilde{v}_k = \text{sgn}(x_1) \cdot \|\tilde{x}\|_2 \tilde{e}_1 + \tilde{x}$
 $\tilde{v}_k = \frac{\tilde{v}_k}{\|\tilde{v}_k\|}$
 $\tilde{A}(k:m, k:n) = 2\tilde{v}_k \tilde{v}_k^T \tilde{A}(k:m, k:n)$

Algo	FLOPs	Stability	Error
CGS	$2mn^2$	Unstable	$O(\kappa(A)^2 \cdot \epsilon_m)$
MGs	"	Boundedly stable	$O(\kappa(A) \cdot \epsilon_m)$
Householder	$2mn^2 - \frac{2}{3}n^3$	"	$O(\epsilon_m)$

Cholesky Decomposition

\rightarrow If \tilde{A} is S.P.D., \tilde{A} can be decomposed s.t. $\tilde{A} = \tilde{R}^T \tilde{R}$
 $\rightarrow n^3/3$ FLOPs

Symmetric Positive Definite Matrix (SPD)

\rightarrow Properties
 $\rightarrow A = A^T$
 $\rightarrow (\tilde{x}, \tilde{A}\tilde{x}) = (\tilde{y}, \tilde{A}\tilde{y}) \quad \forall \tilde{x}, \tilde{y} \in \mathbb{R}^m$
 $\rightarrow \tilde{x}^T \tilde{A} \tilde{x} > 0, \quad \forall \tilde{x} \in \mathbb{R}^m$

\rightarrow If \tilde{A} is S.P.D. & $\tilde{x} \in \mathbb{R}^{m \times n}$ is full rank, then $\tilde{x}^T \tilde{A} \tilde{x}$ is also S.P.D.
 \rightarrow All eigenvalues are +ve for any S.P.D.

Linear Least Squares

$\rightarrow \tilde{A}\tilde{x} = \tilde{P}\tilde{b}$ // get \tilde{x} to calc. space of \tilde{A}
 $\tilde{A}\tilde{x} = \tilde{A}(\tilde{A}^T \tilde{A})^{-1} \tilde{A}^T \tilde{b} \Rightarrow \tilde{x} = (\tilde{A}^T \tilde{A})^{-1} \tilde{A}^T \tilde{b}$

\rightarrow Soln. by Cholesky decomposition: \rightarrow Soln. by QR factorisation

$\tilde{A}^T \tilde{A} \tilde{x} = \tilde{A}^T \tilde{b}$
 $\tilde{R}^T \tilde{R} \tilde{x} = \tilde{A}^T \tilde{b}$
 $\tilde{R}^T \tilde{w} = \tilde{A}^T \tilde{b}$ // Let $\tilde{w} = \tilde{R} \tilde{x}$
 \downarrow solve for \tilde{w}
 $\tilde{R} \tilde{x} = \tilde{w}$
 \downarrow solve for \tilde{x}
 \tilde{x}

$\tilde{A}\tilde{x} = \tilde{P}\tilde{b}$
 $\tilde{Q}\tilde{R}\tilde{x} = \tilde{Q}\tilde{Q}^T \tilde{b}$
 $\tilde{R}\tilde{x} = \tilde{Q}^T \tilde{b}$
 \downarrow solve for \tilde{x}
 \tilde{x}

\rightarrow Soln with SVD

$\tilde{A}\tilde{x} = \tilde{P}\tilde{b}$
 $\tilde{U} \tilde{\Sigma} \tilde{V}^T \tilde{x} = \tilde{U} \tilde{U}^T \tilde{b}$
 $\tilde{\Sigma} \tilde{V}^T \tilde{x} = \tilde{U}^T \tilde{b}$
 $\tilde{\Sigma} \tilde{x} = \tilde{U}^T \tilde{b}$ // Let $\tilde{V}^T \tilde{x} = \tilde{y}$
 \downarrow solve for \tilde{x}
 $\tilde{V} \tilde{y} = \tilde{x}$
 \downarrow solve for \tilde{x}
 \tilde{x}

Algo	Work
Cholesky	$mn^2 + \frac{1}{3}n^3$
QR (Householder)	$2mn^2 - \frac{2}{3}n^3$
SVD	$2mn^2 + \frac{1}{3}n^3$

\rightarrow If \tilde{A} is close to rank-deficient,
 $\tilde{A}\tilde{x} = \tilde{b}$

$\tilde{U} \tilde{\Sigma} \tilde{V}^T \tilde{x} = \tilde{b}$

$\tilde{U} \tilde{U}^T \tilde{\Sigma} \tilde{V}^T \tilde{x} = \tilde{U}^T \tilde{b}$

$\tilde{V}^T \tilde{x} = \tilde{\Sigma}^{-1} \tilde{U}^T \tilde{b}$

Let $\tilde{x} = \tilde{V}_1 \tilde{y} + \tilde{V}_2 \tilde{z}$, where $\tilde{V} = [\tilde{V}_1 \tilde{V}_2]$

Hence $\tilde{x} = \tilde{\Sigma}^{-1} \tilde{U}^T \tilde{b}$

Therefore $\tilde{x} = \tilde{V}_1 \tilde{\Sigma}^{-1} \tilde{U}^T \tilde{b} + \tilde{V}_2 \tilde{z}$

$\|\tilde{x}\|_2 = \|\tilde{V}_1 \tilde{\Sigma}^{-1} \tilde{U}^T \tilde{b}\|_2 + \|\tilde{V}_2 \tilde{z}\|_2 = \|\tilde{U} \tilde{\Sigma}^{-1} \tilde{U}^T \tilde{b}\|_2 + \|\tilde{V}_2 \tilde{z}\|_2$

To minimise $\|\tilde{x}\|_2$, we set $\tilde{z} = 0$

\rightarrow If $\tilde{b} \notin \text{Range}(\tilde{A})$, then we solve $\tilde{A}\tilde{x} = \tilde{P}\tilde{b}$

In this case, $\tilde{x} = \tilde{V}_1 \tilde{\Sigma}^{-1} \tilde{U}^T \tilde{P}\tilde{b} + \tilde{V}_2 \tilde{z}$

$= \tilde{V}_1 \tilde{\Sigma}^{-1} \tilde{U}^T \tilde{b} + \tilde{V}_2 \tilde{z}$

Eigen Decomposition

$\rightarrow \tilde{A} = \tilde{X} \tilde{\Lambda} \tilde{X}^{-1}$, $\tilde{\Lambda}$ is a diagonal matrix containing eigenvalues and \tilde{X} is a matrix comprising of the respective eigenvectors

\rightarrow Characteristic polynomial (P_A): $P_A(z) = \det(\tilde{A} - z\tilde{I})$

\rightarrow Eigenvectors are essentially Nullspace of $(\tilde{A} - \lambda\tilde{I})$. Hence, $(\tilde{A} - \lambda\tilde{I})$ must be a rank-deficient (singular) matrix, with $\det(\tilde{A} - \lambda\tilde{I}) = 0$

\rightarrow Geometric multiplicity of λ : No. of L.I. eigenvectors associated with an eigenvalue λ .

\rightarrow If λ corresponds to two eigenvectors $\tilde{v}_1 \in \tilde{V}_\lambda$, any vector $\tilde{x} = \alpha_1 \tilde{v}_1 + \alpha_2 \tilde{v}_2$ will be an eigenvector of \tilde{A} :

$\text{If } \tilde{A}(\alpha_1 \tilde{v}_1 + \alpha_2 \tilde{v}_2) = \alpha_1 \tilde{A}\tilde{v}_1 + \alpha_2 \tilde{A}\tilde{v}_2 = \alpha_1 \lambda \tilde{v}_1 + \alpha_2 \lambda \tilde{v}_2$
 $= \lambda(\alpha_1 \tilde{v}_1 + \alpha_2 \tilde{v}_2)$
 $= \lambda \tilde{x} \text{ (shown)}$

Similarity Transformation

\rightarrow If $\tilde{X} \in \mathbb{R}^{m \times m}$ is non-singular, $\tilde{X}\tilde{A}\tilde{X}^{-1}$ is known as similarity transformation of \tilde{A} .

\rightarrow Two matrices \tilde{A} & \tilde{B} are said to be similar if there exists a similarity transformation bet. them, i.e. $\tilde{B} = \tilde{X}\tilde{A}\tilde{X}^{-1}$.

$\rightarrow \tilde{A}$ & \tilde{B} will have same eigenvalues & respective multiplicities

$P_B(z) = \det(z\tilde{I} - \tilde{X}\tilde{A}\tilde{X}^{-1})$
 $= \det(z\tilde{X}\tilde{X}^{-1} - \tilde{X}\tilde{A}\tilde{X}^{-1})$
 $= \det(\tilde{X}(z\tilde{I} - \tilde{A})\tilde{X}^{-1})$
 $= \det(\tilde{X}) \det(z\tilde{I} - \tilde{A}) \det(\tilde{X}^{-1}) \text{ (shown)}$

* Eigenvectors may not be the same for \tilde{A} & \tilde{B}