NLA Short Notes

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

Norms

→ Properties of a valid norm :

→ Should be real & non-negative

→ $\|\underset{\sim}{x}\| = 0 \iff \underset{\sim}{x} = \underset{\sim}{0}$

→ $\|\alpha \underset{\sim}{x}\| = \alpha \|\underset{\sim}{x}\|$

→ $\|\underset{\sim}{x} + \underset{\sim}{y}\| \leq \|\underset{\sim}{x}\| + \|\underset{\sim}{y}\|$

→ $|\underset{\sim}{x}^T \underset{\sim}{y}| \leq \|\underset{\sim}{x}\|_2 \, \|\underset{\sim}{y}\|_2$ (Cauchy-Shwarz Inequality)

→ $\|\underset{\sim}{A}\|_1 = \max\limits_{1 \leq i \leq m} (\|\underset{\sim}{a_j}\|_1)$

→ $\|\underset{\sim}{A}\|_\infty$ = max. row absolute sum

→ If $\underset{\sim}{A} = \underset{\sim}{u}\underset{\sim}{v}^T$, $\|A\|_2 = \|u\|_2 \|v\|_2$ (when $\underset{\sim}{x} = \dfrac{\underset{\sim}{v}}{\|\underset{\sim}{v}\|}$)

→ $\|\underset{\sim}{A}\underset{\sim}{B}\|_p \leq \|\underset{\sim}{A}\|_p \|\underset{\sim}{B}\|_p$

→ $\|\underset{\sim}{A}\|_F = \sqrt{\sum_{i=0}^{m} \sum_{j=0}^{n} |a_{ij}|^2} = \sqrt{tr(\underset{\sim}{A}\underset{\sim}{A}^T)} = \sqrt{tr(\underset{\sim}{A}^T\underset{\sim}{A})} = \sqrt{\sum_{i=0}^{m} \|\underset{\sim}{a_i}\|^2}$

Conditioning & Stability

→ Absolute cond. no, $\hat{\kappa} = \dfrac{\|\delta f\|}{\|\delta x\|} = \dfrac{\|J(x)\, \delta x\|}{\|\delta x\|} = \|J(x)\|$

→ Relative cond. no. $= \dfrac{\|\delta f\|}{\|f\|} \div \dfrac{\|\delta x\|}{\|x\|} = \dfrac{\|J(x)\| \, \|x\|}{\|f\|}$

→ $\kappa(\underset{\sim}{A}) = \dfrac{\sigma_1}{\sigma_m} = \sqrt{\dfrac{\lambda_{max}(\underset{\sim}{A}^T\underset{\sim}{A})}{\lambda_{min}(A^TA)}}$

→ $\hat{\kappa}^R(\underset{\sim}{A}) = \|\underset{\sim}{A}\| \, \|\underset{\sim}{A}^+\|$, where $\|\underset{\sim}{A}^+\| = (\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T$

→ Backwards stable $\Rightarrow$ Stable $\Rightarrow$ Forward stable
$\cancel{\Leftarrow}$ $\cancel{\Leftarrow}$

→ For a backward stable algo. $f(\tilde{x}) = \tilde{f}(x)$

Backward stability:
$\tilde{f}(x) = f(x + \delta x)$
Forward stability:
$\|\tilde{f}(x) - f(x)\| = O(\varepsilon_m)$

SVD

$$\underset{\sim}{A} = \underset{\sim}{U}\,\underset{\sim}{\Sigma}\,\underset{\sim}{V}^T, \quad \begin{array}{ll} \underset{\sim}{U} \in \mathbb{R}^{m\times m}, & \text{orthogonal} \\ \underset{\sim}{\Sigma} \in \mathbb{R}^{m\times n}, & \text{diagonal} \\ \underset{\sim}{V}^T \in \mathbb{R}^{n\times n}, & \text{orthogonal} \end{array}$$

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

Principal Component Analysis

→ Orthogonal transformation of the feature space.

→ Consider a data matrix $\underset{\sim}{A} \in \mathbb{R}^{m\times n}$

no. of experiments (m)
particular measurement (n)

1) Move the matrix 0-centred by subtracting the mean of the coln. from each element in the coln.

2) Variance of the coln. $= \dfrac{E(X^2) - \cancel{(E(X))^2}}{m} = \dfrac{\|\underset{\sim}{a_i}\|_2^2}{m}$ (crossed-out term $= 0$)

3) Hence, total variance, $T = \|a_1\|_2^2 + \cdots + \|a_n\|^2$
$= \|A\|_F^2$
$= \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_n^2$

Biggest contributor to the variance

→ To get the direction with highest variance, we need to find a vector $\underset{\sim}{\hat{w}_1}$ s.t.: $\underset{\sim}{t_1} = \underset{\sim}{A}\,\underset{\sim}{\hat{w}_1}$, $\|t_1\|_2$ is maximised. The solution is $\underset{\sim}{\hat{w}_1} = \underset{\sim}{v_1}$.

$$\underset{\sim}{t_1} = \underset{\sim}{A}\,\underset{\sim}{v_1} = \sum_{i=1}^{n} \underset{\sim}{u_i}\,\sigma_i\,\underset{\sim}{v_i}^T\underset{\sim}{v_1} \qquad \left[v_i^T v_1 = \begin{cases} 0, & i \neq 1 \\ 1, & i = 1 \end{cases} \right]$$

$$= u_1 \sigma_1 \underbrace{\cancel{v_1^T v_1}}_{1}$$
$$= \sigma_1 \underset{\sim}{u_1}$$

→ Similarly, $\underset{\sim}{t_2} = \sigma_2 \underset{\sim}{u_2}$, where $\underset{\sim}{t_2}$ is the direction along second highest variance.

Projection

→ Projector matrix $\underset{\sim}{P}$, must be:

→ $\underset{\sim}{P}^2 = \underset{\sim}{P}$ (idempotent) → $\underset{\sim}{P}\underset{\sim}{v} - \underset{\sim}{v} \in \text{Null}(\underset{\sim}{P})$

→ Square matrix → Rank-deficient

→ $\underset{\sim}{P}\underset{\sim}{x} = \underset{\sim}{x}\ \forall\ \underset{\sim}{x} \in \text{Range}(\underset{\sim}{P})$ → symmetrical

→ Orthogonal projector also fulfils $P = P^T$ (symmetric)

→ If $\underset{\sim}{P}$ is a projector, so is $(\underset{\sim}{I} - \underset{\sim}{P})$. This the complementary projector of $\underset{\sim}{P}$.

→ Let us have $\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ has no soln., we can solve $\underset{\sim}{A}\underset{\sim}{\hat{x}} = \underset{\sim}{P}\underset{\sim}{b}$ instead. $\underset{\sim}{P}$ projects $\underset{\sim}{b}$ onto the coln. space of $\underset{\sim}{A}$, which makes this eqn. solvable.

Hence, $\underset{\sim}{P} = A(A^T A)^{-1} A^T$

→ If $\underset{\sim}{P}$ is an orthogonal projector, so is $(\underset{\sim}{I} - \underset{\sim}{P})$

→ If $\underset{\sim}{A}$ is orthogonal, $\underset{\sim}{P} = \underset{\sim}{A}\cancel{(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}}^{\,I}\underset{\sim}{A}^T = \underset{\sim}{A}\underset{\sim}{A}^T$

→ Projection & SVD: If $\underset{\sim}{A} = \underset{\sim}{V}\underset{\sim}{\Sigma}\underset{\sim}{V}^T$, $\underset{\sim}{V}$ forms a orthonormal basis of $\underset{\sim}{A}$.
Hence, the projection matrix corresponding to $\underset{\sim}{A}$, $\underset{\sim}{P} = Q\cancel{(Q^T Q)^{-1}}^{\,I} Q^T = QQ^T$

QR Factorisation

→ $\underset{\sim}{Q}$: matrix w/ orthonormal colns. → $\underset{\sim}{R}$: UTM

→ Gram-Schmidt orthogonalisation:

$$\underset{\sim}{v_j} = \underset{\sim}{a_j} - (\underset{\sim}{q_1}^T \underset{\sim}{a_j})\underset{\sim}{q_1} - \cdots - (\underset{\sim}{q_{j-1}}^T \underset{\sim}{a_j})\underset{\sim}{q_{j-1}}$$

$$\underset{\sim}{q_j} = \frac{\underset{\sim}{v_j}}{\|\underset{\sim}{v_j}\|_2}$$

Hence $\underset{\sim}{q_n} = \dfrac{\underset{\sim}{a_n} - \sum_{i=0}^{n-1} r_{in}\underset{\sim}{q_i}}{r_{nn}}$, where $r_{ij} = \begin{cases} q_i^T a_j, & i \neq j \\ \|a_j - \sum_{i=1}^{j-1} r_{ij} q_i\|_2, & i = j \end{cases}$

→ Gram Schmidt with projector : $q_n = \dfrac{P_n a_n}{\|P_n a_n\|}$, where

$$P_n = I - \sum_{i=0}^{n-1} q_i q_i^T = I - \hat{Q}_{j-1} \hat{Q}_{j-1}^T$$

→ Modified Gram-Schmidt :

$$P_n a_n = \left(I - \sum_{i=0}^{n-1} q_i q_i^T\right) a_n = \left[\prod_{i=0}^{n-1} \left(I - q_i q_i^T\right)\right] a_n$$

Algo : for $j = 1 \to n$:

$$v_j^{(1)} = a_j$$

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

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

$$\vdots$$

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

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

→ Householder Triangularisation

→ Perform transformations to convert A to R :

$$Q_n \cdots Q_1 A = R$$

ensure that prev colns. are not changed.

must be an orthogonal matrix

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

→ Let $\hat{x} = \begin{bmatrix} - \\ - \\ - \\ \vdots \\ - \end{bmatrix}$, $\hat{F}$ should be s.t. $Fx = \begin{bmatrix} - \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|x\| \cdot e_1$

Hence, $y = Fx = (I - 2uu^T)x$, where $u = -\dfrac{v}{\|v\|}$, where $\underset{\sim}{v} = \|\underset{\sim}{x}\|_2 \underset{\sim}{e}_1 - \underset{\sim}{x}$

Algo: for $k = 1 \rightarrow n$:

$\underset{\sim}{x} = \underset{\sim}{A}(k:m, k)$ // row k to row m in the k^{th} coln.

$\underset{\sim}{v}_k = sgn(x_1) \cdot \|\underset{\sim}{x}\|_2 \underset{\sim}{e}_1 + \underset{\sim}{x}$

$\underset{\sim}{v}_k = \dfrac{\underset{\sim}{v}_k}{\|\underset{\sim}{v}_k\|}$

$\underset{\sim}{A}(k:m, k:n) -= 2\underset{\sim}{v}_k \underset{\sim}{v}_k^T \underset{\sim}{A}(k:m, k:n)$

Algo	FLOPs	Stability	Error
CGS	$2mn^2$	Unstable	$O(\hat{\kappa}(\underset{\sim}{A})^2 \cdot \varepsilon_m)$
MGS	"	Backward stable	$O(\hat{\kappa}(\underset{\sim}{A}) \cdot \varepsilon_m)$
Householder	$2mn^2 - 2/_3 n^3$	"	$O(\varepsilon_m)$

Symmetric +ve Definite Matrix (SPD)

→ Properties

→ $\underset{\sim}{A} = \underset{\sim}{A}^T$

→ $(\underset{\sim}{x}, \underset{\sim}{A}\underset{\sim}{y}) = (\underset{\sim}{y}, \underset{\sim}{A}\underset{\sim}{x}) \quad \forall\, x, y \in \mathbb{R}^m$

→ $\underset{\sim}{x}^T \underset{\sim}{A} \underset{\sim}{x} > 0, \quad \forall\, \underset{\sim}{x} \in \mathbb{R}^m$

→ If $\underset{\sim}{A}$ is S.P.D. & $\underset{\sim}{X} \in \mathbb{R}^{m \times n}$ is full rank, then $\underset{\sim}{X}^T \underset{\sim}{A} \underset{\sim}{X}$ is also S.P.D.

→ All eigenvalues are +ve for any S.P.D.

Cholesky Decomposition

UTM

→ If $\underset{\sim}{A}$ is S.P.D, $\underset{\sim}{A}$ can be decomposed s.t. $\underset{\sim}{A} = \underset{\sim}{R}^T \underset{\sim}{R}$

→ $n^3/3$ FLOPs

Linear Least Squares

normal eqn.

→ If $\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ is overdetermined, we can solve for $\boxed{\underset{\sim}{A}^T \underset{\sim}{A} \hat{\underset{\sim}{x}} = \underset{\sim}{A}^T \underset{\sim}{b}}$ instead. This shall minimize the residual, i.e $\|\underset{\sim}{r}\|_2$, where $\underset{\sim}{r} = \underset{\sim}{A}\hat{\underset{\sim}{x}} - \underset{\sim}{b}$

→ $\underset{\sim}{A}\hat{\underset{\sim}{x}} = \underset{\sim}{P}\underset{\sim}{b}$ // get b to coln. space of $\underset{\sim}{A}$

$\underset{\sim}{A}\hat{\underset{\sim}{x}} = \underset{\sim}{A}(\underset{\sim}{A}^T \underset{\sim}{A})^{-1} \underset{\sim}{A}^T \underset{\sim}{b} \Rightarrow \hat{\underset{\sim}{x}} = (\underset{\sim}{A}^T \underset{\sim}{A})^{-1} \underset{\sim}{A}^T \underset{\sim}{b}$

→ Soln. by Cholesky decomposition:

$$A^T A \hat{x} = A^T b$$

$$R^T R \hat{x} = A^T b$$

$$R^T w = A^T b \qquad // \text{Let } w = R\hat{x}$$

↓ solve for w

$$R\hat{x} = w$$

↓ solve for x

$$\hat{x}$$

→ Soln. by QR factorisation

$$Ax = Pb$$

$$QRx = QQ^T b$$

$$Rx = Q^T b$$

↓ solve for x

$$x$$

→ Soln with SVD

$$Ax = Pb$$

$$U\Sigma V^T x = UU^T b$$

$$\Sigma V^T x = U^T b$$

$$\Sigma y = U^T b \qquad // \text{Let } V^T x = y$$

↓ solve for y

$$V^T x = y$$

↓ solve for x

$$x$$

Algo	Work
Cholesky	$mn^2 + n^3/3$
QR (Householder)	$2mn^2 - \frac{2n^3}{3}$
SVD	$2mn^2 + 11n^3$

→ If A is close to rank-deficient,

$\boxed{\text{Either } m \geq n \text{ \& } \operatorname{rank}(A) < n, \text{ or } m < n}$

$$Ax = b$$

$$U\Sigma V^T x = b$$

$\boxed{U^T U = I \text{, whereas } UU^T \text{ will be a projector matrix}}$

$$\underbrace{\cancel{U^T U}}_{I} \Sigma V^T x = U^T b$$

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

range (A)

null (A)

Let $x = V_1 y + V_2 z$, where $V = [V_1 \;\; V_2]$

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

Therefore $x = V_1 \Sigma^{-1} U^T b + V_2 z$

inner product

$$\|x\|_2 = \|V_1 \Sigma^{-1} U^T b\|_2 + \|V_2 z\|_2 - \cancel{\|(V_1\Sigma^{-1}U^T b, V_2 z)\|_2} \quad 0$$

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

→ If $b \notin$ Range (A), then we solve $Ax = Pb$.

In this case, $x = V_1 \Sigma^{-1} U^T P b + V_2 z$ $\boxed{P = UU^T}$

$$= V_1 \Sigma^{-1} U^T b + V_2 z$$

Eigen Decomposition

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

→ Characteristic polynomial (P_A) : $P_A(z) = \det(A - zI)$

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

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

→ If λ corresponds to two eigenvectors v_1 & v_2, any vector $x = \alpha_1 v_1 + \alpha_2 v_2$ will be an eigenvector of A:

Pf: $A(\alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 A v_1 + \alpha_2 A v_2 = \alpha_1 \lambda v_1 + \alpha_2 \lambda v_2$

$= \lambda(\alpha_1 v_1 + \alpha_2 v_2)$

$= \lambda x$ (shown)

Similarity Transformation

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

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

→ $\underset{\sim}{A}$ & $\underset{\sim}{B}$ will have same eigenvalues & respective multiplicities

$$P_B(z) = \det(z\underset{\sim}{I} - \underset{\sim}{X}\underset{\sim}{A}\underset{\sim}{X}^{-1})$$
$$= \det(z\underset{\sim}{X}\underset{\sim}{X}^{-1} - \underset{\sim}{X}\underset{\sim}{A}\underset{\sim}{X}^{-1})$$
$$= \det(\underset{\sim}{X}(z\underset{\sim}{I} - \underset{\sim}{A})\underset{\sim}{X}^{-1})$$
$$= \cancel{\det(\underset{\sim}{X})}\det(z\underset{\sim}{I} - \underset{\sim}{A})\cancel{\det(\underset{\sim}{X}^{-1})} \quad \text{(shown)}$$

$\boxed{\text{* Eigen vectors may not be the same for } \underset{\sim}{A} \,\&\, \underset{\sim}{B}}$

Defective Eigenvalues & Matrices

→ An eigenvalue, for which algebraic multiplicity > geometric multiplicity is a defective eigenvalue.

→ Any matrix that has a defective eigenvalue is a defective matrix

→ It does not posses a full set of L.I. eigenvectors.

→ Diagonal matrices are not defective

→ Diagonalisability: If $\underset{\sim}{A} \in \mathbb{R}^{m\times n}$ is not defective iff it has eigenvalue decomposition.

Or orthogonal diagonalisability

not all non-defective matrices are unitary diagonalisable

→ Unitary diagonalisability: If a non-defective matrix $\underset{\sim}{A}$ has eigenvalue decomposition $\underset{\sim}{A} = \underset{\sim}{Q}\underset{\sim}{\Lambda}\underset{\sim}{Q}^{-1} = \underset{\sim}{Q}\underset{\sim}{\Lambda}\underset{\sim}{Q}^{\top}$, where $\underset{\sim}{Q}$ is a $\underbrace{\text{unitary matrix}}$.

Transjugate

$\underset{\sim}{Q} \in \mathbb{C}^{m\times m}$ $\quad \underset{\sim}{Q}^{\top}\underset{\sim}{Q} = \underset{\sim}{Q}\underset{\sim}{Q}^{\top} = \underset{\sim}{I}$

→ Symmetric matrices have all real eigenvalues & eigen vectors.

→ Skew symmetric matrices have all imaginary eigen values. Skew symmetric matrices are also unitary diagonalisable.

Defective Matrices

→ Defective eigenvalue: An eigen value with geometric multiplicity < algebraic multiplicity. If a matrix has ≥ 1 defective eigenvalue, it is defective.

Unitary / Orthogonal Diagonalisability

$\leftarrow$ transjugate

→ $Q \in \mathbb{C}^{m\times m}$ is a unitary matrix if $Q^\perp Q = QQ^\perp = I$

→ A is unitary diagonalisable iff $\exists\, Q$ s.t. $A = Q^\perp \Lambda Q$, Q is unitary

Symmetric Matrices

→ A real symmetric matrix is non-defective & unitary diagonalisable, with real eigenvalues.

→ A real skew-symmetric matrix is also non-defective & unitary diagonalisable, with purely complex eigenvalues.

→ Any normal matrix $A \in \mathbb{C}^{m\times m}$, s.t. $A^\perp A = AA^\perp$, will be unitary diagonalisable.

Schur Factorisation

→ $A = QTQ^\perp$, where Q is unitary, and T is U.T.M.

→ SVD of T = SVD of A.

→ Every sq. matrix has a Schur factorisation.

* If A is real, A can be decomposed to UTU^T, where U & T are real, and T is quasi U.T.M.

→ Schur factorisation need not be unique.

Eigen solvers

→ Phase 1: Reduce A to upper Hessenberg matrix H. (UTM but with additional line of non-zero elements parallel to diagonal). $O(m^3)$ flops

→ Phase 2: Reduce H to U.T.M. $O(m)$ iterations, $O(m^2)$ flops per iteration $\Rightarrow O(m^3)$ flops.

* Without phase 1, we would need $O(m^4)$ flops.

→ Phase 1: Reduce A to H as follows: $A = QHQ^\perp$, where

$$Q = Q_1 \cdots Q_{m-2}.$$

→ Rayleigh quotient: $\alpha = \dfrac{x^T A x}{x^T x}$

→ α will be the eigenvalue of $\underset{\sim}{A}$ closest to $\underset{\sim}{x}$. This is the least sq. soln. that minimises $\| \underset{\sim}{A}\underset{\sim}{x} - \alpha \underset{\sim}{x} \|_2$.

Power Iterations

→ Finds the eigenvector corresponding to largest eigenvector (by magnitude).

Algo: Initialise $\underset{\sim}{v}^{(0)}$ to a random unit vector

for $k = 1 \to \infty$,

$$\underset{\sim}{w} = \underset{\sim}{A}\, \underset{\sim}{v}^{(k-1)}$$

$$\underset{\sim}{v}^{(k)} = \frac{\underset{\sim}{w}}{\|\underset{\sim}{w}\|}$$

$$\lambda^{(k)} = (\underset{\sim}{v}^{(k)})^T A (\underset{\sim}{v}^{(k)})$$

* Convergence is slow if $\lambda_2 \simeq \lambda_1$

Results:

$$\| \underset{\sim}{v}^{(k)} - (\pm \underset{\sim}{q}_1) \|_2 = O\left(\left| \frac{\lambda_2}{\lambda_1} \right|^k \right)$$

$$| \lambda^{(k)} - \lambda_1 | = O\left(\left| \frac{\lambda_2}{\lambda_1} \right|^{2k} \right)$$

If k is even, $\underset{\sim}{v}^{(k)} \to \underset{\sim}{q}_1$, otherwise, $\underset{\sim}{v}^{(k)} \to -\underset{\sim}{q}_1$

Inverse Power Iterations

Algo: Initialise μ = some value near λ_J,
$v^{(0)}$ = " random unit vector

for $k = 1 \to \infty$:

$$\underset{\sim}{w} = (A - \mu I)^{-1} v^{(k-1)}$$ // Solve by finding soln to system of lin eqns.

$$\underset{\sim}{v}^{(k)} = \frac{\underset{\sim}{w}}{\|\underset{\sim}{w}\|}$$

$$\lambda^{(k)} = (\underset{\sim}{v}^{(k)})^T A (\underset{\sim}{v}^{(k)})$$

Converges to closest eigenvalue of μ. If λ_J is the closest to μ and λ_K is second-most closest to μ,

$$\| v^{(k)} - (\pm q_J) \| = O\left(\left| \frac{\mu - \lambda_J}{\mu - \lambda_K} \right|^k \right)$$

$$| \lambda^{(k)} - \lambda_J | = O\left(\left| \frac{\mu - \lambda_J}{\mu - \lambda_K} \right|^{2k} \right)$$

Rayleigh Quotient Iteration

Algo: Initialise $\underset{\sim}{v}^{(0)}$ to some random unit vector

$$\lambda^{(0)} = (\underset{\sim}{v}^{(0)})^T \underset{\sim}{A} (\underset{\sim}{v}^{(0)})$$

for $k = 1 \to \infty$:

$$\underset{\sim}{w} = (\underset{\sim}{A} - \lambda^{(k-1)} \underset{\sim}{I})^{-1} \underset{\sim}{v}^{(k-1)}$$ // again linear system of eqns.

$$\underset{\sim}{q}^{(k)} = \frac{\underset{\sim}{w}}{\|\underset{\sim}{w}\|}$$

$$\lambda^{(k)} = (\underset{\sim}{q}^{(k)})^T \underset{\sim}{A} (\underset{\sim}{q}^{(k)})$$

→ Very fast convergence:

$$\| \underset{\sim}{v}^{(k+1)} - (\pm \underset{\sim}{q_i}) \| = O\left(\| \underset{\sim}{v}^{(k)} - (\pm \underset{\sim}{q_i}) \|^3 \right)$$

$$| \lambda^{(k+1)} - \lambda_i | = O\left(| \lambda^{(k)} - \lambda_i |^3 \right)$$

Analysis of Algos. (per iteration)

→ Power iteration: $O(m^2)$ due to matrix-vector multiplication.

→ Inverse power iteration: $O(m^3)$ due to soln. of linear system of eqns.

→ Can be reduced to $O(m^2)$ by solving $(\underset{\sim}{A} - \mu \underset{\sim}{I})^{-1}$ once

→ Rayleigh quotient iteration: $O(m^3)$, but lesser iterations are reqd.

→ Can be reduced to $O(m^2)$ by reducing $\underset{\sim}{A}$ to tridiagonal / upper Hessenberg.

Multiple Eigenvalues

→ Subspace / simultaneous iterations

→ Take multiple vectors which are L.I.. Provided we have an ∞ precision computer, these will converge to different eigenvectors.

→ Assumption #1: The first n eigenvalues are distinct & well-separated

→ " #2: If $\underset{\sim}{Q_1} = [\underset{\sim}{q_1} \cdots q_n]$, where $\{q_1 \cdots q_n\}$ are eigenvectors of $\underset{\sim}{A}$, $\underset{\sim}{Q_1}^T \underset{\sim}{v}^{(0)}$ is non-singular, and all principal submatrices of $\underset{\sim}{Q_1}^T \underset{\sim}{v}^{(0)}$ are also singular.

→ Orthogonalise at each step to prevent loss of orthogonality, and hence make the algo stable.

→ Works for large, sparse matrices

Algo: Initialise $\underset{\sim}{\hat{Q}}^{(0)} \in \mathbb{R}^{m \times n}$

for $k = 1 \to \infty$:

$$\underset{\sim}{Z}^{(k)} = \hat{A} \hat{\underset{\sim}{Q}}^{(k-1)}$$

$$\hat{\underset{\sim}{Q}}^{(k)}, \hat{\underset{\sim}{R}}^{(k)} = \underset{\sim}{Z} \quad // \text{ QR factorisation}$$

→ Pure QR algorithm (dense matrices)

Algo: $A^{(0)} = A$

for $k = 1 \to \infty$

$Q^{(k)}, R^{(k)} = A^{(k-1)}$ // orthogonalise

$A^{(k)} = R^{(k)} Q^{(k)}$

→ As $k \to \infty$, $A^{(k)}$ approaches Schur form.

→ Mathematically equivalent to simultaneous iterations

→ Can also be considered a simultaneous inverse iteration applied to a flipped identity matrix.

→ Modified QR (most used for eigenvalues)

Full Algo: Define $A^{(0)}$ s.t $(Q^{(0)})^T A^{(0)} (Q^{(0)}) = A$ // tridiagonalisation of A

for $k = 1 \to \infty$:

Pick a shift $\mu^{(k)}$ // many methods for picking, e.g. $\mu^{(k)} = A^{(k-1)}_{mm}$

$Q^{(k)} R^{(k)} = A^{(k-1)} - \mu^{(k)} I$ // shifted QR factorisation

$A^{(k)} = R^{(k)} Q^{(k)} + \mu^{(k)} I$

If any off-diagonal entries are close to 0, set $A_{j,j+1} = A_{j+1,j} = 0$

Split $A^{(k)}$ into A_1 & A_2 s.t $A^{(k)} = \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix}$

Apply QR algo (from tridiagonalisation) on A_1 & A_2.

→ Krylov subspace method (fully iterative):

→ Krylov subspace is a subspace rich in eigenvectors. This is the set of vectors $\{b, Ab, A^2 b, \dots\}$.

→ This seq. is similar to power iterations

→ For this to be an virtual subspace, $\underset{\sim}{b}, \underset{\sim}{A}\underset{\sim}{b}, \underset{\sim}{A}^2\underset{\sim}{b}$ etc. must be L.I. They are confirmed to be L.I. if $\underset{\sim}{A}$ is full-rank.

→ This method is computationally unstable

→ Arnoldi Iteration (To construct Krylov subspace)

Algo: $\underset{\sim}{b}$ = arbitrary vector

$$\underset{\sim}{q}_1 = \frac{\underset{\sim}{b}}{\|\underset{\sim}{b}\|}$$

for $n = 1 \to \infty$

$\underset{\sim}{v} = \underset{\sim}{A}\underset{\sim}{q}_1$

for $j = 1 \to n$

$h_{jn} = \underset{\sim}{q}_j^T \underset{\sim}{v}$

$\underset{\sim}{V} = \underset{\sim}{v} - h_{jn}\underset{\sim}{q}$

$h_{(n+1)n} = \|\underset{\sim}{v}\|$

$$q_{n+1} = \frac{\underset{\sim}{V}}{h_{(n+1)n}}$$

→ At the end of the iterations, we have:

→ Constructed a subspace rich in eigenvalues of $\underset{\sim}{A}$

→ Projected $\underset{\sim}{A}$ onto the subspace, to obtain $\underset{\sim}{H}_n$

→ Hence, $\underset{\sim}{H}_n$ is a projection of $\underset{\sim}{A}$ onto K_n

→ Eigenvalues of $\underset{\sim}{H}_n$ are Arnoldi eigenvalue estimates, a.k.a. Ritz values

→ Arnoldi iterations can be viewed as polynomial approximation

→ Arnoldi approximation problem: Find $p^n \in P^n$ s.t. $\|p^n(\underset{\sim}{A})\underset{\sim}{b}\|_2$ is minimum. P^n is the set of monic polynomials of deg. n.

→ Soln. to this problem is actually $P_{H_n}(z) = \det(z\underset{\sim}{I} - \underset{\sim}{H}_n)$

→ As $n \to \infty$, the soln. approaches eigen values of $\underset{\sim}{A}$.

GMRes

→ Tries to solve $\underset{\underset{\sim}{z} \in K_n}{\operatorname{argmin}} \|\underset{\sim}{A}\underset{\sim}{z} - \underset{\sim}{b}\|_2$ * Use Krylov subspace to minimise residual

Let $\underset{\sim}{x} = \underset{\sim}{\hat{Q}_n} \underset{\sim}{y}$

$$\underset{\underset{\sim}{z} \in K_n}{\operatorname{argmin}} \|\underset{\sim}{A}\underset{\sim}{z} - \underset{\sim}{b}\|_2 = \underset{\underset{\sim}{y} \in \mathbb{R}^n}{\operatorname{argmin}} \|\underset{\sim}{A}\underset{\sim}{\hat{Q}_n}\underset{\sim}{y} - \underset{\sim}{b}\|_2$$

$$\left[\underset{\sim}{A}\underset{\sim}{\hat{Q}_n} = \underset{\sim}{\hat{Q}_{n+1}}\underset{\sim}{\tilde{H}_n}\right] \qquad = \underset{\underset{\sim}{y} \in \mathbb{R}^n}{\operatorname{argmin}} \|\underset{\sim}{\hat{Q}_{n+1}} \underset{\sim}{\hat{H}_n} \underset{\sim}{y} - \underset{\sim}{b}\|_2$$

$$= \underset{\underset{\sim}{y} \in \mathbb{R}^n}{\operatorname{argmin}} \|\underset{\sim}{\hat{H}_n}\underset{\sim}{y} - \|\underset{\sim}{b}\|\underset{\sim}{e_1}\|_2$$

This results in $(n+1) \times n$ least sq. problem

Algo : Let $\underset{\sim}{q_1} = \dfrac{\underset{\sim}{b}}{\|\underset{\sim}{b}\|}$

for $n = 1 \to \infty$

<step n of Arnoldi iteration>

$$\underset{\sim}{y} := \underset{\underset{\sim}{y} \in \mathbb{R}^n}{\operatorname{argmin}} \|\underset{\sim}{\hat{H}_n}\underset{\sim}{y} - \|\underset{\sim}{b}\|\underset{\sim}{e_1}\|_2$$

$$\underset{\sim}{x_n} = \underset{\sim}{Q_n} \cdot \underset{\sim}{y}$$

→ Polynomial approximations of GMRes :

Let $P_n = \{$polynomials of degree $\leq n$ s.t. $p(0) = 1$

Let $\underset{\sim}{x_n} \in K_n \Rightarrow x_n = c_0 \underset{\sim}{b} + \cdots + c_{n-1} \underset{\sim}{A}^{n-1} \underset{\sim}{b}$

" $q_n(z) = c_0 + c_1 \underset{\sim}{z} + \cdots + c_{n-1} \underset{\sim}{z}^{n-1}$ s.t. $x_n = q_n(\underset{\sim}{A}) \cdot \underset{\sim}{b}$

Hence $\underset{\sim}{r_n} = \underset{\sim}{b} - \underset{\sim}{A}\underset{\sim}{x_n} = \underbrace{(\underset{\sim}{I} - q(\underset{\sim}{A}))}_{P_n(\underset{\sim}{A})} \underset{\sim}{b}$

→ Convergence of GMRes

→ Monotonic convergence : $\|\underset{\sim}{r_{n+1}}\| \leq \|\underset{\sim}{r_n}\|$

$\rightarrow$ $O(m)$ iterations with $O(m^2)$ ops/iteration shall be reqd.

$$\|\underset{\sim}{r_n}\| = \|p(\underset{\sim}{A})\cdot \underset{\sim}{b}\|$$
$$\le \|p(\underset{\sim}{A})\|\,\|\underset{\sim}{b}\|$$
$$\frac{\|\underset{\sim}{r_n}\|}{\|\underset{\sim}{b}\|} \le \|p(\underset{\sim}{A})\|$$
$$\le \min_{p_n \in P^n} \|p_n(\underset{\sim}{A})\|$$

$$p_n(\underset{\sim}{A}) \le \|\underset{\sim}{V}\|\,\|p_n(\underset{\sim}{\Lambda})\|\,\|\underset{\sim}{V}^{-1}\| \qquad \left[\text{Let } \underset{\sim}{A} = \underset{\sim}{V}\,\underset{\sim}{\Lambda}\,\underset{\sim}{V}^{-1}\right]$$
$$\le \kappa(\underset{\sim}{V})\,\|p_n(\underset{\sim}{\Lambda})\| \qquad \left[\kappa(\underset{\sim}{V}) = \|\underset{\sim}{V}\|\,\|\underset{\sim}{V}^{-1}\|\right]$$
$$\le \kappa(\underset{\sim}{V})\cdot \max |p_n(\lambda)| \qquad [\text{Cayley Hamilton}]$$

Hence, $\dfrac{\|\underset{\sim}{r_n}\|}{\|\underset{\sim}{b}\|} \le \kappa(\underset{\sim}{V}) \cdot \min\limits_{p_n \in P^n} \left(\max |p_n(\lambda)|\right)$

If A is S.P.D., $\|\underset{\sim}{r_n}\| \le \left(\dfrac{\kappa(\underset{\sim}{A})^2 - 1}{\kappa(\underset{\sim}{A})}\right)^{n/2} \|r_0\|$

Conjugate Gradient

$\rightarrow$ Let A-norm, $\|\underset{\sim}{x}\|_A = \sqrt{\underset{\sim}{x}^T \underset{\sim}{A}\,\underset{\sim}{x}}$

$\rightarrow$ Conjugate gradient is recurrence formulae that generates a sequence s.t. at step n, $\|\underset{\sim}{e_n}\|_A = \|\underset{\sim}{x}^* - \underset{\sim}{x_n}\|_A$ is minimised.

$\rightarrow$ Algo: Initialise $\underset{\sim}{x_0} = \underset{\sim}{0}$ // initial guess
$\underset{\sim}{r_0} = \underset{\sim}{b}$ // " residual
$\underset{\sim}{p_0} = \underset{\sim}{r_0}$ // " direction

for $n = 1 \rightarrow \infty$

$\alpha_n = \dfrac{r_{n-1}^T\, r_{n-1}}{\underset{\sim}{p}_{n-1}^T \underset{\sim}{A}\, \underset{\sim}{p_{n-1}}}$ // step length

$\underset{\sim}{x_n} = \underset{\sim}{x_{n-1}} + \alpha_n \underset{\sim}{p_{n-1}}$ // update approx. soln

$\underset{\sim}{r_n} = \underset{\sim}{r_{n-1}} - \alpha_n \underset{\sim}{A} \cdot \underset{\sim}{p_{n-1}}$ // update residual

$$\beta_n = \frac{r_n^T r_n}{r_{n-1}^T r_{n-1}}$$ // improvement in search direction

$$\underset{\sim}{p_n} = \underset{\sim}{r_n} + \beta_n \underset{\sim}{p_{n-1}}$$ // update search direction

→ Results : $\langle \underset{\sim}{x_1}, \dots, \underset{\sim}{x_n} \rangle = \langle \underset{\sim}{p_0}, \dots, \underset{\sim}{p_{n-1}} \rangle = \langle \underset{\sim}{r_0}, \dots, r_{n-1} \rangle = \text{Krylov}_{n-1}$

→ $\underset{\sim}{r_n}^T \underset{\sim}{r_j} = 0 \quad \forall j < n$ → $\underset{\sim}{p_n}^T \underset{\sim}{A} \underset{\sim}{p_j} = 0 \quad \forall j < n$

→ $\|\underset{\sim}{e_{n+1}}\|_A < \|\underset{\sim}{e_n}\|_A$

→ CG as optimization problem :

$$\|\underset{\sim}{e_n}\|_A^2 = \underset{\sim}{e_n}^T \underset{\sim}{A} \underset{\sim}{e_n} = \dots = 2\phi(x_n) + \text{constant}, \quad \phi(\underset{\sim}{x}) = \frac{\underset{\sim}{x}^T \underset{\sim}{A} \underset{\sim}{x}}{2} - \underset{\sim}{x}^T \underset{\sim}{b}$$

$$\frac{\|\underset{\sim}{e_n}\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^n$$, where κ = condn. no. of $\underset{\sim}{A}$

$O(\sqrt{\kappa})$ iterations shall be reqd