

# 1 Solving System of Linear Equations $Ax = b$

## 1.1 $p$ -Norm and Condition Number

Vector  $p$ -Norm:  $\boxed{\|\vec{x}\|_p = \sqrt[p]{\sum_i |x_i|^p}}$

1-Norm :  $\|\vec{x}\|_1 = \sum_i |x_i|$

$\infty$ -Norm :  $\|\vec{x}\|_\infty = \max |x_i|$

- $\|x\|_1 \geq \|x\|_2 \geq \|x\|_\infty$
- $\|x\|_1 \leq \sqrt{n} \|x\|_2 \leq \sqrt{n} \|x\|_\infty$

Matrix  $p$ -Norm:  $\boxed{\|A\|_p = \max_{x \neq 0} \frac{\|Ax\|}{\|x\|}}$

1-Norm :  $\|A\|_1 = \max_j \sum_i |a_{ij}|$

$\infty$ -Norm :  $\|A\|_\infty = \max_i \sum_j |a_{ij}|$

- $\|AB\| \leq \|A\| \cdot \|B\|$
  - $\|Ax\| \leq \|A\| \cdot \|x\|$
- For  $p$ -norms (not necessarily in general)

Function/Vector Condition Number:

$$\begin{aligned} \text{cond}(f(x)) &= \left| \frac{[f(\hat{x}) - f(x)]/f(x)}{[\hat{x} - x]/x} \right| \\ &= \left| \frac{\Delta y/y}{\Delta x/x} \right| = \left| \frac{y' \cdot \Delta x/y}{\Delta x/x} \right| \\ &= \left| \frac{x f'(x)}{f(x)} \right| \end{aligned}$$

Matrix Condition Number:

$\boxed{\text{cond}_p(A) = \|A\|_p \cdot \|A^{-1}\|_p}$  ( $\infty$  if singular)

$$= \frac{\max_{x \neq 0} \|Ax\|_p / \|x\|_p}{\min_{x \neq 0} \|Ax\|_p / \|x\|_p} = \text{cond}_p(\gamma A) \geq 1$$

- Diagonal,  $D$  :  $\text{cond}(D) = \frac{\max |d_i|}{\min |d_i|}$
- $\|z\| = \|A^{-1}y\| \leq \|A^{-1}\| \cdot \|y\|$   
 $\rightarrow \frac{\|z\|}{\|y\|} \leq \max \frac{\|z\|}{\|y\|} \stackrel{?}{=} \|A^{-1}\|$  (optimize)

## 1.2 Error Bounds and Residuals

Error Bound:  $\boxed{\frac{\|\hat{x} - x\|}{\|x\|} \lesssim \text{cond}(A) \epsilon_{\text{mach}}}$   $\rightarrow$  A computed solution is expected to lose about  $\log_{10}(\text{cond}(A))$  digits, so the input data must be more accurate to these digits and the working precision must carry more than these digits.

$$A\hat{x} = b + \Delta b = Ax + A\Delta x$$

- $\|b\| \leq \|A\| \cdot \|x\|$
- $\|\Delta x\| \leq \|A^{-1}\| \cdot \|\Delta b\|$

$$\rightarrow \boxed{\frac{\|\Delta x\|}{\|x\|} \leq \text{cond}(A) \frac{\|\Delta b\|}{\|b\|}}$$

$$A\hat{x} + r = b$$

- $\|\Delta x\| = \|A^{-1}(A\hat{x} - b)\| = \|-A^{-1}r\|$   
 $\leq \|A^{-1}\| \cdot \|r\|$

$$\rightarrow \boxed{\frac{\|\Delta x\|}{\|\hat{x}\|} \leq \text{cond}(A) \frac{\|r\|}{\|A\| \cdot \|\hat{x}\|}}$$

$$(A + \Delta A)\hat{x} = b$$

- $\|\Delta x\| = \|-A^{-1}(\Delta A)\hat{x}\|$   
 $\leq \|A^{-1}\| \cdot \|\Delta A\| \cdot \|\hat{x}\|$

$$\rightarrow \boxed{\frac{\|\Delta x\|}{\|x\|} \leq \text{cond}(A) \frac{\|\Delta A\|}{\|A\|}}$$

$$(A + \Delta A)\hat{x} = b$$

- $\|r\| = \|b - A\hat{x}\| = \|\Delta A \cdot \hat{x}\|$   
 $\leq \|\Delta A\| \cdot \|\hat{x}\|$

$$\rightarrow \boxed{\frac{\|r\|}{\|A\| \cdot \|\hat{x}\|} \leq \frac{\|\Delta A\|}{\|A\|}}, \quad \frac{\|\Delta x\|}{\|x\|} \leq \frac{\|A^{-1}\| \cdot \|r\|}{\|\hat{x}\|} \leq \text{cond}(A) \frac{\|\Delta A\|}{\|A\|}$$

$$\left[ A(t)x(t) = b(t) \right] = \left[ (A_0 + \Delta A \cdot t)x(t) = b_0 + \Delta b \cdot t \right]$$

- $x'(t) = \frac{b'(t) - A'(t)x(t)}{A(t)} = A^{-1}(t) \left[ \Delta b - \Delta A \cdot x(t) \right]$
- $x(t) = x_0 + x'(0)t + \mathcal{O}(t^2)$

$$\rightarrow \boxed{\frac{\|x(t) - x_0\|}{\|x_0\|} \leq \text{cond}(A) \left( \frac{\|\Delta b\|}{\|b\|} + \frac{\|\Delta A\|}{\|A\|} \right) |t| + \mathcal{O}(t^2)}$$

## 1.3 Gaussian Elimination with LU/PLU/PLDUQ Decomposition

Elementary Elimination Matrices,  $L_k$

$$\begin{pmatrix} 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 1 & 0 & \dots & 0 \\ 0 & \dots & \frac{-a_{k+1}}{a_k} & 1 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \frac{-a_n}{a_k} & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} a_1 \\ \vdots \\ a_k \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

- $a_k$  is the “pivot”
- is lower triangular
- $\forall i \neq j \quad (L_k^{-1})_{ij} = -(L_k)_{ij}$

Ex :

$$\begin{pmatrix} 1 & 0 & \dots \\ -a_1/a_2 & 1 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ 0 \\ \vdots \end{pmatrix}$$

LU/PLU Factorization (w/ partial pivoting)

$$\boxed{A = LU \quad \begin{array}{l} (L \text{ is gen. triang.}) \\ (U \text{ is upp. triang.}) \end{array}} \\ \boxed{L = (\dots L_2 P_2 L_1 P_1)^{-1}}$$

$$\{\dots\}b = (\dots L_2 P_2 L_1 P_1)Ax$$

$$L^{-1}b = (P_1^T L_1^{-1} P_2^T L_2^{-1} \dots)^{-1} Ax \\ = L^{-1}(LU)x = y$$

$$\boxed{b = Ly \quad y = Ux} \\ \text{(forw.-sub.) , (back.-sub.)}$$

- Permutation matrix,  $P_i$ , rowswaps s.t.  $a_k \neq 0$
- $P_i$  rowswaps s.t.  $a_k$  is largest s.t.  $a_{k+i}/a_k \leq 1$  for numerical stability/minimize errors
- Pivoting isn't needed if  $A$  is diag. dom. ( $a_{jj} > \sum_{i \neq j} a_{ij}$ )
- $A$  can be singular

$$\boxed{A = PLU \quad \begin{array}{l} (P \text{ is rowswap permu.}) \\ (L \text{ is unit low. triang.}) \\ (U \text{ is upp. triang.}) \end{array}} \\ \boxed{P = (\dots P_2 P_1)^{-1}}$$

$$\{\dots\}b = (\dots P_2 P_1)Ax$$

$$P^T b = (P_1^T P_2^T \dots)^{-1} Ax \\ = P^T (PLU)x = Ly$$

$$\boxed{P^T b = Ly \quad y = Ux}$$

$$\boxed{P^T A = LDU \quad (D \text{ is diag.})}$$

- $LDU$  is unique up to  $D$
- $LDU$  is unique if  $L/U$  are unit low./upp. diag., resp.

$$\boxed{P^T A Q^T = LDU \quad \begin{array}{l} (P \text{ is permu. for rows}) \\ (Q \text{ is permu. for cols.}) \end{array}}$$

- “Complete pivoting” search for largest  $a_k$
- Would be most numerically stable
- Expensive, so not really used

$$\text{Error Bound: } \frac{\|r\|}{\|A\|\|x\|} \leq \frac{\|\Delta A\|}{\|A\|} \leq \rho n^2 \epsilon_{\text{mach}} \sim n \epsilon_{\text{mach}} \\ \text{(Wilkinson) (usually)}$$

(growth factor,  $\rho$ , is the largest entry at any point during factorization - usually at  $U$  - divided by the largest entry of  $A$ )

## 1.4 Gaussian-Jordan with MD Decomposition

Elementary Elimination Matrices,  $M_k$

$$\begin{pmatrix} 1 & \dots & \frac{-a_1}{a_k} & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 1 & 0 & \dots & 0 \\ 0 & \dots & \frac{-a_{k+1}}{a_k} & 1 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \frac{-a_n}{a_k} & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_{k-1} \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_k \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

- $a_k$  is the “pivot”
- $\forall i \neq j \quad (M_k^{-1})_{ij} = -(M_k)_{ij}$

MD Factorization (w/ partial pivoting)

$$\boxed{A = MD \quad \begin{matrix} (M \text{ is elem. elim.}) \\ (D \text{ is diag.}) \end{matrix}}$$

$$M = (\dots M_2 P_2 M_1 P_1)^{-1}$$

$$\{\dots\}b = (\dots M_2 P_2 M_1 P_1)Ax$$

$$M^{-1}b = (P_1^T M_1^{-1} P_2^T M_2^{-1} \dots)^{-1} Ax$$

$$= M^{-1}(MD)x = y$$

$$\boxed{M^{-1}b = y, \quad y = Dx}$$

(division)

- Permutation matrix,  $P_i$ , rowswaps s.t.  $a_k \neq 0$
- $P_i$  rowswaps cannot ensure numerical stability ( $\leq 1$ )
- Division is  $\mathcal{O}(n)$ , so may be useful for parallel comps.
- Can also find  $A^{-1}$

Finding  $A^{-1}$

$$D^{-1}M^{-1}(A|I) = (I|A^{-1})$$

$$= D^{-1}M^{-1} \left[ \begin{array}{ccc|cc} a_{11} & \dots & 1 & 0 \\ \vdots & & a_{nn} & 0 & 1 \end{array} \right]$$

$$= \left[ \begin{array}{cc|ccc} 1 & 0 & a'_{11} & \dots \\ 0 & 1 & \vdots & a'_{nn} \end{array} \right]$$

## 1.5 Symmetric Matrices

Positive Definite:  $x^T Ax \geq 0$

Cholesky Factorization for Sym., Pos. Def.:  $A = LL^T = LDL^T$

$$\begin{pmatrix} a_{11} & a_{21} & a_{31} & \dots \\ a_{21} & a_{22} & a_{32} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 & \dots \\ l_{21} & l_{22} & 0 & \dots \\ l_{31} & l_{32} & l_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} l_{11} & l_{21} & l_{31} & \dots \\ 0 & l_{22} & l_{32} & \dots \\ 0 & 0 & l_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} l_{11}^2 & \dots & \dots & \dots \\ l_{21}l_{11} & l_{21}^2 + l_{22}^2 & \dots & \dots \\ l_{31}l_{11} & l_{31}l_{21} + l_{32}l_{22} & l_{31}^2 + l_{32}^2 + l_{33}^2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- Pivoting not needed
- Well defined (always works)
- Only lower triangle needed for storage
- $A = LDL^T$  is sometimes useful, where  $D$  is diag.

Symmetric Indefinite Matrices

- Pivoting Needed :  $PAP^T = LDL^T$
- Ideally,  $D$  is diag., but if not possible, then  $D$  is tridiag. (Aasen) or 1x1/2x2 block diag. (Bunch, Parlett, Kaufmann, etc.)

## 1.6 Banded Matrices

- Similar to normal Gaussian Elim., but less work since more zeroes
- Pivoting means bandwidth will expand no more than double
- Only  $\mathcal{O}(\beta n)$  storage needed

## 1.7 Rank-1 Update with Sherman-Morrison

$$\tilde{A}\tilde{x} = b = (A - uv^T)\tilde{x} \quad \left| \quad \begin{array}{l} \tilde{A}^{-1} = (A - uv^T)^{-1} = A^{-1} + \frac{A^{-1}u}{1 - v^T(A^{-1}u)} v^T A^{-1} \\ \tilde{A}^{-1}b = \quad \quad \quad \tilde{x} = (A^{-1}b) + \frac{A^{-1}u}{1 - v^T(A^{-1}u)} v^T(A^{-1}b) \\ \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad x + \frac{y}{1 - v^T y} v^T x \end{array} \right.$$

General Woodbury Formula:  $\boxed{(A - UV^T)^{-1} = A^{-1} + (A^{-1}U)(I - V^T A^{-1}U)^{-1} v^T A^{-1}}$

- $U$  and  $V$  are general  $n \times k$  matrices
- No guarantee of numerical stability, so caution is needed

## 1.8 Complexity

Explicit Inversion :  $LU A^{-1} = I \rightarrow \mathcal{O}(n^3) \quad , \quad A^{-1}b = x \rightarrow \mathcal{O}(n^2)$

Gaussian Elimination :  $A = LU \rightarrow \mathcal{O}(n^3/3) \quad , \quad LUx = b \rightarrow \mathcal{O}(n^2)$

Gaussian-Jordan :  $A = MD \rightarrow \mathcal{O}(n^3/2) \quad , \quad MDx = b \rightarrow \mathcal{O}(n)$

Symmetric :  $\begin{matrix} A = LL^T \\ P A P^T = L D L^T \end{matrix} \rightarrow \mathcal{O}(n^3/6) \quad , \quad LL^T x = b \rightarrow \mathcal{O}(n^2)$

Banded :  $A_\beta = LU \rightarrow \mathcal{O}(\beta^2 n) \quad , \quad LUx = b \rightarrow \mathcal{O}(\beta n)$

Sherman-Woodbury :  $\tilde{A} = A - uv^T \rightarrow \mathcal{O}(n^2) \quad , \quad \tilde{x} = \tilde{A}b \rightarrow \mathcal{O}(n^2)$

## 1.9 Diagonal Scaling

Ill-conditioned

$$\begin{pmatrix} 1 & 0 \\ 0 & \epsilon \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ \epsilon \end{pmatrix}$$

Well-conditioned

$$\begin{pmatrix} 1 & 0 \\ 0 & 1/\epsilon \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \epsilon \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1/\epsilon \end{pmatrix} \begin{pmatrix} 1 \\ \epsilon \end{pmatrix}$$

- No general way to correct poor scaling

## 1.10 Iterative Refinement

$$\begin{aligned} r_0 &= b - Ax_0 = A\Delta x_0 \\ r_1 &= b - A(x_0 + \Delta x_0) = b - Ax_1 = A\Delta x_1 \\ r_2 &= b - A(x_1 + \Delta x_1) = b - Ax_2 = A\Delta x_2 \end{aligned}$$

$$\boxed{x = x_0 + \lim_{n=0}^{\infty} \Delta x_n} \quad (\text{terminate when } r_n \text{ is small enough})$$

- Double storage needed to hold original matrix
- $r_n$  usually must be computed with higher precision than  $x_n$
- Useful for badly scaled systems, or making unstable systems stable
- If  $x_n$  is not accurate,  $r_n$  might not need better accuracy

## 2 Least $\|r\|$ Linear Regression/Fit for $Ax + r = b$

- $A = A_{m \times n}$   $(m > n, \text{ underdetermined})$
- $r(y = Ax)$  is cont. & coer.  $\rightarrow \exists \|r(y)\|_{\min}$
- $r(y)$  is strictly convex  $\rightarrow y = Ax$  is unique
- $\text{rank}(A) = n$   
(full column rank)  $\Rightarrow A(x_1 - x_2) = 0$  (unique  $x$ )  
 $(x_1 - x_2) = 0 \rightarrow x_1 = x_2$

Example - Vandermonde Matrix,  $A$ :

$$Ax = \begin{pmatrix} -\vec{f}(t_1) \\ \vdots \\ -\vec{f}(t_m) \end{pmatrix} \begin{pmatrix} | \\ \vec{x} \\ | \end{pmatrix} = \begin{pmatrix} y(t_1) \\ \vdots \\ y(t_m) \end{pmatrix} = \begin{pmatrix} | \\ \vec{y} \\ | \end{pmatrix} = (x^T A^T)^T, \quad y(t) = \sum_{i=1}^n x_i f_i(t) = \vec{x} \cdot \vec{f}$$

Decompose  $b$ :

$$\begin{aligned} b &= Ax + r \\ &= y + r \\ &= Pb + P_{\perp} b \end{aligned}$$

Projector of  $A$ ,  $P$

$$\text{Projector : } P^2 = P \rightarrow PA = A$$

(Idempotent)                      (Projector of  $A$ )

$$\text{Orthogonal Projector : } P^T = P \rightarrow P_{\perp} A = (I - P)A = 0$$

Minimize residual,  $r$ :

$$\begin{aligned} \nabla \|r\|_2^2 &= 0 \quad \left( \frac{\partial x^2}{\partial x_i} = 0 \right) \\ &= \nabla [(b - Ax)^T (b - Ax)] \\ &= \nabla (b^T b - 2x^T A^T b + x^T A^T A x) \\ 0 &= 2A^T A x - 2A^T b \\ &\downarrow \\ A^T A x &= A^T b \quad (\text{Solvable with Cholesky}) \end{aligned}$$

$$\begin{aligned} \|r\|_2^2 &= \|Pr + P_{\perp} r\|_2^2 = \|b - Ax\|_2^2 \\ &= \|Pr\|_2^2 + \|P_{\perp} r\|_2^2 \\ &= \cancel{\|Pb - Ax\|_2^2} + \|P_{\perp} b\|_2^2 \\ &\downarrow \\ Ax &= Pb \\ A^T A x &= A^T Pb = (P^T A)^T b \\ A^T A x &= A^T b \quad (\text{System of Normal Equations}) \end{aligned}$$

Cross-Product Matrix of  $A$ :  $A^T A$

$$\text{Symmetric : } (A^T A)^T = A^T A$$

$$\begin{aligned} \text{Pos. Def. : } \text{rank}(A) &= n \\ &\rightarrow \langle x | A^T A x \rangle = x^T A^T A x \\ &= (Ax)^T (Ax) \\ &= \|Ax\|^2 \geq 0 \end{aligned}$$

$$\begin{aligned} \text{Nonsingular : } A^T A x &= 0 \\ &\rightarrow \|Ax\|^2 = 0 = Ax \\ &\rightarrow (x = 0) \end{aligned}$$

System of Normal Equations:  $A^T A x = A^T b$

Pseudoinverse,  $A^+$

$$\begin{aligned} x &= (A^T A)^{-1} A^T b \\ &\equiv A^+ b \end{aligned} \rightarrow \begin{aligned} A^+ &\equiv (A^T A)^{-1} A^T \\ A^+ A &= I \end{aligned}$$

Ortho. Proj.,  $P$

$$\begin{aligned} Ax &= A(A^T A)^{-1} A^T b \\ &= Pb \end{aligned} \rightarrow \begin{aligned} P &= A(A^T A)^{-1} A^T \\ &= AA^+ \end{aligned}$$

## System of Normal Equations Issues:

- Info can be lost forming  $A^T A$ , e.g,  $A = \begin{pmatrix} 1 & 0 \\ \epsilon & 0 \\ 0 & \epsilon \end{pmatrix} \rightarrow A^T A = \begin{pmatrix} 1+\epsilon^2 & 1 \\ 1 & 1+\epsilon^2 \end{pmatrix} \approx \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$  (singular)

- System of Normal Equations:  $\boxed{\text{cond}(A^T A) = [\text{cond}(A)]^2}$

## 2.1 Error Bounds and Residuals

Error Bound:  $\boxed{\frac{\|\Delta x\|}{\|x\|} \lesssim \text{cond}(A) \epsilon_{\text{mach}}}$   $\rightarrow$  A computed solution is expected to lose about  $\log_{10}(\text{cond}(A))$  digits, so the input data must be more accurate to these digits and the working precision must carry more than these digits.

## Norm and Conditioning:

$$\|A\| = \max_{x \neq 0} \left( \frac{\|Ax\|}{\|x\|} = \frac{\|AA^+b\|}{\|A^+b\|} \right)$$

$$\text{cond}(A) = \begin{cases} \|A\|_2 \cdot \|A^+\|_2 & \text{rank}(A) = n \\ \infty & \text{rank}(A) < n \end{cases}$$

$$A^T A(x + \Delta x) = A^T A(b + \Delta b)$$

$$(A + \Delta A)^T (A + \Delta A)(x + \Delta x) = (A + \Delta A)^T b$$

- $\|\Delta x\| \leq \|A^+\| \cdot \|\Delta b\|$

- $\cancel{A^T Ax} + A^T \Delta Ax + (\Delta A)^T Ax + \cancel{(\Delta A)^T \Delta Ax} = \cancel{A^T b} + (\Delta A)^T b$   
 $+ A^T A \Delta x + \cancel{A^T \Delta A \Delta x} + \cancel{(\Delta A)^T A \Delta x} + \cancel{(\Delta A)^T \Delta A \Delta x}$

$$\rightarrow \boxed{\frac{\|\Delta x\|}{\|\hat{x}\|} \leq \left( \text{cond}(A) \frac{\|b\|}{\|Ax\|} \right) \frac{\|\Delta b\|}{\|b\|}} \\ = \left( \text{cond}(A) \frac{1}{\cos \theta} \right) \frac{\|\Delta b\|}{\|b\|}$$

- $\|\Delta x\| = \|(A^T A)^{-1} (\Delta A)^T r - A^+ \Delta Ax\|$   
 $\leq \|(A^T A)^{-1}\| \cdot \|\Delta A\| \cdot \|r\| + \|A^+\| \cdot \|\Delta A\| \cdot \|x\|$

- Cond. number is a func. of  $\text{cond}(A)$  and  $b$
- $Pb \approx 0$  or  $\theta \approx 90^\circ$  is highly sensitive

$$\rightarrow \boxed{\frac{\|\Delta x\|}{\|\hat{x}\|} \leq \left( [\text{cond}(A)]^2 \frac{\|r\|}{\|Ax\|} + \text{cond}(A) \right) \frac{\|\Delta A\|}{\|A\|}} \\ = \left( [\text{cond}(A)]^2 \tan \theta + \text{cond}(A) \right) \frac{\|\Delta A\|}{\|A\|}$$

## 2.2 Solving $A^T Ax = A^T b$ with an Augmented Matrix

$$\begin{matrix} r + Ax = b \\ A^T r = 0 \end{matrix} \Rightarrow \begin{pmatrix} I & A \\ A^T & 0 \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} \alpha I & A \\ A^T & 0 \end{pmatrix} \begin{pmatrix} r/\alpha \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$$

- Solvable with  $LU$  Decomp or Symm. Pos. Def. Methods
- $\alpha$  "controls the relative weights of the two subsystems in choosing pivots from either"
- $\alpha = \max a_{ij}/1000$  (rule of thumb)
- MATLAB uses it for large, sparse systems

## 2.3 QR Decomposition

Motivation:  $Q^T A = \begin{pmatrix} R \\ 0 \end{pmatrix} \rightarrow Q^T A x + Q^T r = Q^T b \rightarrow \begin{pmatrix} Rx \\ 0 \end{pmatrix} + \begin{pmatrix} r'_1 \\ r'_2 \end{pmatrix} = \begin{pmatrix} b'_1 \\ b'_2 \end{pmatrix} \rightarrow \begin{matrix} \|r'\|^2 = \|b'_1 - Rx\|^2 + \|b'_2\|^2 \\ \downarrow \\ Rx = b'_1, r' = \begin{pmatrix} 0 \\ b'_2 \end{pmatrix} \text{ (solve with back-sub)} \end{matrix}$

Orthogonal Matrix,  $Q$

$$Q^T Q = Q Q^T = I$$

QR Factorization

$$A = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$$

Reduced QR Factorization

$$A = Q \begin{pmatrix} R \\ 0 \end{pmatrix} = \begin{pmatrix} Q_{\parallel} & Q_{\perp} \end{pmatrix} \begin{pmatrix} R \\ 0 \end{pmatrix} = Q_{\parallel} R$$

1.  $Q^T$  is a  $\text{span}(A)$  Plane Rotation through  $\mathbb{R}^m$  to  $\text{span}([R \ 0]^T)$

2-norm Preserved ( $Q$  is a rotation/reflection)

- $\|Qv\|^2 = \langle v | Q^T Q v \rangle = \|v\|^2$
- $\|Q^T v\|^2 = \langle v | Q Q^T v \rangle = \|v\|^2$

- $Q^T = H_n \dots H_1$
- $H_i^T H_i = H_i H_i^T = I$
- $A = [a_1 \dots a_n]$
- $I_n = [e_1 \dots e_n]$

$$H_1 a_1 = \alpha_1 e_1 \quad (\|a_1\| = |\alpha_1|)$$

$$H_i \dots H_1 a_i = \sum_j^i c_j e_j = H_n \dots H_1 a_i$$

$$(\|a_i\|^2 = |\alpha_1|^2 = \sum_j^i c_j^2)$$

$$\langle r | a_i \rangle = 0 \quad (1 \leq i \leq n)$$

$$\langle H_i \dots H_1 r | e_j \rangle = 0 \quad (1 \leq j \leq i)$$

→  $Q^T A$  rotates  $A$  until the column vectors are aligned with certain axes described above

2.  $A$  is a Lin. Sum of  $Q_{\parallel}$ 's Orthogonal Column Vectors Given by  $R$

$$\{Q_{\parallel} = Q_{m \times n} \mid \text{span}(Q_{\parallel}) = \text{span}(A)\}$$

$$\rightarrow Q^+ = (Q^T Q)^{-1} Q^T = Q^T$$

$$\rightarrow P = Q_{\parallel} Q_{\parallel}^T$$

$$\rightarrow Q_{\parallel}^T A x = Q_{\parallel}^T P b = \cancel{Q_{\parallel}^T Q_{\parallel}} Q_{\parallel}^T b$$

$$= Q_{\parallel}^T b \quad (\text{System of Orthogonal Equations?})$$

$$A = Q_{\parallel} R = \begin{pmatrix} | & | & | \\ \vec{q}_1 & \dots & \vec{q}_n \\ | & | & | \end{pmatrix} \begin{pmatrix} r_{11} & \dots & r_{1n} \\ 0 & \ddots & \vdots \\ 0 & 0 & r_{nn} \end{pmatrix} = \begin{pmatrix} | & | & | \\ \vec{a}_1 & \dots & \vec{a}_n \\ | & | & | \end{pmatrix}$$

- $\vec{a}_j = \sum_i^j r_{ij} \cdot \vec{q}_i$

→  $R$  transforms the  $Q_{\parallel}$  column vectors about  $\text{span}(A)$ , an  $\mathbb{R}^n$  plane, until they equal the column vectors of  $A$



### 2.3.1 Householder Transformation/Elementary Reflector, $H$

$$\begin{aligned}
 H\vec{a}_1 &= \alpha_1 \vec{e}_1 \quad \begin{array}{l} \|\vec{a}_1\| = |\alpha_1| \\ \text{(rotation)} \end{array} \\
 &= \boxed{\vec{a}_1 - 2\hat{v}(\hat{v} \cdot \vec{a}_1)} \quad \begin{array}{l} [v_\perp \text{ bisects } \theta(a_1, e_1)] \end{array} \rightarrow \boxed{H = I - 2vv^T = I - \frac{2vv^T}{v^T v}} \quad \bullet \ H = H^T = H^{-1} \\
 &\quad \text{(symmetric and orthogonal)}
 \end{aligned}$$

$$\bullet \ \alpha_1 e_1 = a_1 - (2v_1) \frac{v_1 \cdot a_1}{v_1 \cdot v_1} \Rightarrow v_1 = (a_1 - \alpha e_1) \frac{v_1 \cdot v_1}{2v_1 \cdot a_1} \quad \text{(magnitude doesn't matter)}$$

$$\rightarrow \boxed{v_1 = (a_1 - \alpha e_1)}$$

$$\alpha_1 = \pm \|\vec{a}_1\| \rightarrow \boxed{\alpha_i = -\text{sign}(a_i) \|\vec{a}_i\|} \quad \text{(avoid "cancellation" in finite-calc. of } v \text{ above)}$$

$$H_j \dots H_1 a_i = a_i^j \rightarrow \boxed{v_{j+1} = \begin{pmatrix} 0 \\ \vdots \\ (a_i^j)_i \\ \vdots \\ (a_i^j)_m \end{pmatrix} - \alpha_i e_i} \quad \begin{array}{l} \bullet \text{ Store } v_i \text{ and } R \text{ into } A \text{ and an extra } n\text{-vector.} \\ \bullet \text{ } Q \text{ and } H \text{ can be computed if needed.} \\ \bullet \text{ When column } i \text{ is completed, row } i \text{ is too.} \end{array}$$

### 2.3.2 Givens Rotation, $G$

$$\begin{aligned}
 \boxed{G = \begin{pmatrix} c & s \\ -s & c \end{pmatrix}} &\rightarrow Gx = G \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \pm \begin{pmatrix} \|a\| \\ 0 \end{pmatrix} \quad \begin{array}{l} \bullet \text{ creates 0's one at a time} \\ \bullet \text{ useful for sparse matrices} \\ \bullet \text{ When column } i \text{ is completed, row } i \text{ is too.} \end{array} \\
 &\rightarrow \boxed{c = \frac{a_1}{\sqrt{a_1^2 + a_2^2}}, \quad s = \frac{a_2}{\sqrt{a_1^2 + a_2^2}}}
 \end{aligned}$$

Avoid squaring any number  $\gg 1$  to prevent overflow/underflow

$$\begin{array}{l} \bullet \ t = \frac{a_2}{a_1} < 1 \rightarrow c = \frac{1}{\sqrt{1+t^2}}, \quad s = c \cdot t \\ \bullet \ \tau = \frac{a_1}{a_2} < 1 \rightarrow s = \frac{1}{\sqrt{1+\tau^2}}, \quad c = s \cdot \tau \end{array}$$

### 2.3.3 Gram-Schmidt Orthogonalization

$$Q_{||}^T = \begin{pmatrix} \hat{q}_1 : q_1 = a_1 \\ \hat{q}_2 : q_2 = a_2 - \hat{q}_1(\hat{q}_1 \cdot a_2) \\ \hat{q}_3 : q_3 = a_3 - \hat{q}_1(\hat{q}_1 \cdot a_3) - \hat{q}_2(\hat{q}_2 \cdot a_3) \\ \vdots \\ \hat{q}_n : q_n = a_n - \sum_j^n \hat{q}_j(\hat{q}_j \cdot a_n) \end{pmatrix}, \quad R = \begin{pmatrix} \|a_1\| & \hat{q}_1 \cdot a_2 & \hat{q}_1 \cdot a_3 & \dots & \hat{q}_1 \cdot a_n \\ 0 & \|a_2\| & \hat{q}_2 \cdot a_3 & \dots & \hat{q}_2 \cdot a_n \\ 0 & 0 & \|a_3\| & \dots & \hat{q}_3 \cdot a_n \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & \|a_n\| \end{pmatrix}$$

Classical, Column Oriented: Find  $\hat{q}_i$ , then solve for  $\widehat{q_{i+1}}$ , and continue up to  $\hat{q}_n$ .

- For a program, obviously  $a_k$  can be replaced by  $q_k$ , so less storage is needed.
- Cancellation that causes loss of orthogonality occurs more when ill-conditioned.
- As a result, performing  $Q_{\parallel}^T b = b'_1$  isn't always best.
- Can't column-pivot, since that depends on rows being completed first.

Modified, Row Oriented: Let  $q_i^{[k]} = a_i - \sum_j^k \hat{q}_j (\hat{q}_j \cdot a_i)$ . For all  $1 \leq i \leq n$ , solve for  $q_i^{[k]}$  starting first at  $k = 1$ , then continue until  $k = n$ .

- Allows for column pivoting since rows are completed first.
- Cancellation, though still present, is less severe.

Augmented Matrix:

$$(A | b) = (Q_{\parallel} | q_{n+1}) \begin{pmatrix} R & b'_1 \\ 0 & \rho \end{pmatrix}$$

$$\left( \begin{array}{c|c|c|c|c} | & | & | & | & | \\ a_1 & \dots & a_n & b & \\ | & | & | & | & | \end{array} \right) = \left( \begin{array}{c|c|c|c|c} | & | & | & | & | \\ \hat{q}_1 & \dots & \hat{q}_n & q_{n+1} & \\ | & | & | & | & | \end{array} \right) \left( \begin{array}{c|c|c|c|c} r_{11} & \dots & r_{1n} & | & \\ 0 & \ddots & \vdots & b'_1 & \\ \vdots & \ddots & r_{nn} & | & \\ 0 & \dots & 0 & \rho & \end{array} \right)$$

- Use Gram-Schmidt QR on this, then solve  $Rx = b'_1$
- This method is preferred numerically to reduce cancelling effects
- Text didn't recommend what  $q_{+1}$  or  $\rho$  should be.
- $\rho$  or  $(q_{n+1})_i$  looks like it should be 0.
- Idk, not much explained.

Reorthogonalizing: Repeating procedure to straighten vectors (usually not needed)

### 2.3.4 Factorization with Column-Pivoting

- Column with largest norm is pivoted to the current column  $i$  to be reduced, and current row  $i$  is completed too.
- Choose the next pivoting column based on norms of the smaller columns from remaining uncompleted submatrix.
- Repeat until the end (rank might be  $n$ ) or if the max norm is smaller than some tolerance (rank might be  $k < n$ )
- Pivoting avoids working with 0's on the diag.

### 2.3.5 Rank Deficiency (or Other) Case

If  $\text{rank}(A) = k < n$  :

$$\boxed{(Q^T A P)(P^T x) = Q^T b}$$

$$\boxed{\begin{pmatrix} R & S \\ 0 & 0' \end{pmatrix} \begin{pmatrix} z \\ 0 \end{pmatrix} = \begin{pmatrix} b'_1 \\ b'_2 \end{pmatrix}}$$

- $0'$  is approx. 0 since the remaining norms are too small.
- $R = R_{k \times k}$
- $S$  is the remaining columns after  $R$  is completed.
- There are multiple solutions for  $x$ .

- For a quick solution,  $Rz = b'_1, \quad x = P \begin{pmatrix} z \\ 0 \end{pmatrix}$
- For the minimized-norm solution with the smallest  $\|x\|$ ,  $S$  must be annihilated.
- For another method or if underdetermined ( $m < n$ ), something like SVD Decomposition can be used.

## 2.4 Singular Value Decomposition (SVD)

$$\begin{aligned}
A &= \boxed{U \Sigma V^T} = \left( \begin{array}{c|c|c|c|c} & & & & \\ \hline & & & & \\ \hline u_1 & \dots & u_k & .. & u_m \\ \hline & & & & \\ \hline \end{array} \right) \left( \begin{array}{ccccc} \sigma_1 & 0 & \dots & 0 & \\ \hline 0 & \sigma_2 & \ddots & & \vdots \\ \hline 0 & 0 & \ddots & 0 & \\ \hline \vdots & \vdots & \ddots & \sigma_n & \\ \hline 0 & 0 & \dots & 0 & \\ \hline \vdots & \vdots & & \vdots & \\ \hline 0 & 0 & \dots & 0 & \end{array} \right) \left( \begin{array}{c} \text{---} v_1 \text{---} \\ \vdots \\ \text{---} v_k \text{---} \\ \vdots \\ \text{---} v_n \text{---} \end{array} \right) \\
&= \boxed{U_{\parallel} \Sigma_1 V^T} = (U_{\parallel} \quad U_{\perp}) \begin{pmatrix} \Sigma_1 \\ \mathbf{0} \end{pmatrix} \begin{pmatrix} V_{0\perp}^T \\ V_{0\parallel}^T \end{pmatrix} = \boxed{\sum_i^n \sigma_i \cdot u_i v_i^T}
\end{aligned}$$

- Underdetermined,  $m < n$  is possible too.
- Analogous to Gaussian-Jordan Diagonalization method.
- $U$  and  $V$  are orthogonal;  $u_i$  and  $v_i$  are the respective “left” and “right” singular vectors.
- Usually, the singular values are ordered such that  $\sigma_1 \geq \sigma_2 \geq \dots$
- $\forall (k < i), \sigma_i = 0 \Rightarrow \text{rank}(A) = k < n$
- $U_{\parallel} = U_{m \times k} : \text{span}(U_{\parallel}) = \text{span}(A), \text{span}(U_{\perp}) = \text{span}(A)^{\perp}$
- $V_{0\perp} = V_{n \times k} : \text{span}(V_{0\parallel}) = \text{null}(A), \text{span}(V_{0\perp}) = \text{null}(A)^{\perp} \quad \text{null}(A) = \{x : Ax = 0\}$

Pseudoinverse:

$$\begin{aligned} A^+ &\equiv V \Sigma^+ U^T \\ \Sigma^+ &\equiv \left[ \Sigma^T \quad \text{and} \quad \sigma_i \rightarrow 1/\sigma_i \quad \forall (\sigma_i \neq 0) \right] \end{aligned}$$

- $Ax + r = b \rightarrow$

$$\boxed{x = A^+b = (V\Sigma^+U^T)b}$$

- $$x_{\min} = \sum_{\sigma_i \neq 0} \frac{u_i \cdot b}{\sigma_i} v_i$$
 useful for ill-conditioned or rank deficient since small  $\sigma$  can be dropped.

### 2.4.1 Other uses

Euclidean 2-norm :  $\|A\|_2 = \max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \sigma_{\max}$

Euclid. Cond. Num. :  $\text{cond}_2(A) = \sigma_{\max}/\sigma_{\min}$

Lower Rank Approx. :  $A \approx A_k = \sum_i^k \sigma_i (u_i v_i^T)$

- Closest rank= $k$  matrix to  $A$  in the Frobenius norm.
- Frobenius Norm = Euclid. Norm for a “vector” in  $\mathbb{R}^{mn}$ .

Total Least Squares :  $[A \mid y]_{m \times (n+1)} = U \Sigma V_{(n+1) \times (n+1)}^T$

$$\text{rank}([\hat{A} \mid y]) \leq n \rightarrow \sigma_{n+1} = 0 \rightarrow \hat{A} \cdot v_{n+1} = 0$$

$$\left[\widehat{A} \mid y\right] \cdot \begin{bmatrix} x \\ -1 \end{bmatrix} = 0 \rightarrow \begin{bmatrix} x \\ -1 \end{bmatrix} \propto v_{n+1} = \begin{bmatrix} \vec{\nu}_n \\ \nu_{n+1} \end{bmatrix} \rightarrow \boxed{x = \frac{\vec{\nu}_n}{-\nu_{n+1}}}$$

- $\hat{A}$  is an  $A$  with uncertainty, like how  $y$  normally is.

## 2.5 Complexity

Normal, Cholesky

- $A^T A = A'$  costs  $\frac{mn^2}{2}$
- $A' = LL^T$  costs  $\frac{n^3}{6}$
- Rel. Err.  $\propto [\text{cond}(A)]^2$
- Bad if  $\text{cond}(A) \approx 1/\sqrt{\epsilon_{\text{mach}}}$

Householder

- $Q^T A = R$  costs  $mn^2 - \frac{n^3}{3}$
- Rel. Err.  $\propto [\text{cond}(A)]^2 \|r\|_2 + \text{cond}(A)$
- Bad if  $\text{cond}(A) \approx 1/\epsilon_{\text{mach}}$
- More accurate than Cholesky and broadly applicable
- Usable for rank deficient or nearly rank-deficient

Givens

- The normal implementation needs 50% more work than Householder.
- A more complex implementation makes it comparable to Householder.
- Useful if matrix is sparse or zeros need to be maintained.

SVD

- Most expensive cost at  $\propto mn^2 + n^3$ , perhaps 4-10 times or more.
- Robust and reliable.

### 3 Matrix Information

Symmetric :  $S = S^T$

Hermitian :  $H = H^\dagger$

Orthogonal :  $QQ^T = Q^TQ = I$

Unitary :  $UU^\dagger = U^\dagger U = I$

Normal :  $AA^\dagger = A^\dagger A$

D

•  $H = UDU^{-1}$  ( $D$  is real)

•  $U = e^{iH} = U_H e^{iD} (U_H)^\dagger$

•  $Ax = \lambda x$ ,  $\det(A) \neq 0 \Rightarrow A^{-1}x = (1/\lambda)x$

#### 3.1 Error Bound and Conditioning

$$A + \Delta A = Q(D + \Delta D)Q^{-1}$$

•  $v = (\Delta\lambda I - D)^{-1}(\Delta D)v$

•  $\|(\Delta\lambda I - D)^{-1}\|_2^{-1} \leq \|\Delta D\|_2$

$$|\Delta\lambda - \lambda_i| \leq \|Q(\Delta A)Q^{-1}\|_2$$

$$\rightarrow \boxed{|\Delta\lambda - \lambda_i| \leq \text{cond}(Q) \|\Delta A\|_2}$$

$$(A + \Delta A)(x + \Delta x) = (\lambda + \Delta\lambda)(x + \Delta x)$$

•  $Ax = \lambda x$ ,  $y^H A = \lambda y^H$

•  $\lambda$  is simple  $\Rightarrow y^H x \neq 0$  (?)

$$\begin{aligned} & y^H \cancel{Ax} + y^H \cancel{A\Delta x} + y^H (\Delta A)x + y^H \cancel{(\Delta A)\Delta x} \\ & \approx y^H \lambda x + y^H \lambda \Delta x + y^H (\Delta\lambda)x + y^H \cancel{(\Delta\lambda)\Delta x} \end{aligned}$$

$$\rightarrow \boxed{|\Delta\lambda| \lesssim \frac{\|y\|_2 \cdot \|x\|_2}{|y^H x|} \|\Delta A\|_2 = \frac{1}{\cos \theta} \|\Delta A\|_2}$$

•  $AA^\dagger = A^\dagger A \rightarrow \text{cond}(A) = 1$

• Non-simple (multiple) eigenvalue is complicated:

• allows  $y^H x = 0$ , depends on eigenvalue spacings, vector angles, etc.

• Balancing can improve conditioning - diagonal rescaling