Solving System of Linear Equations Ax = b1

1.1 p-Norm and Condition Number

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

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

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

- $||x||_1 \ge ||x||_2 \ge ||x||_{\infty}$
- $||x||_1 \le \sqrt{n} ||x||_2 \le \sqrt{n} ||x||_{\infty}$

 $\underline{\text{Matrix } p\text{-Norm}}:$

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

 ∞ -Norm : $||A||_{\infty} = \max_{i} \sum_{j} |a_{ij}|$

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

Function/Vector Condition Number:

$$\operatorname{cond}(f(x)) = \left| \frac{[f(\hat{x}) - f(x)]/f(x)}{[\hat{x} - x]/x} \right|$$
$$= \left| \frac{\Delta y/y}{\Delta x/x} \right| = \left| \frac{y' \cdot \Delta x/y}{\Delta x/x} \right|$$
$$= \left| \frac{xf'(x)}{f(x)} \right|$$

Matrix Condition Number:

$$\frac{\operatorname{cond}_{p}(A) = \|A\|_{p} \cdot \|A^{-1}\|_{p}}{\operatorname{max}_{x \neq 0} \|Ax\|_{p} / \|x\|_{p}} = \operatorname{cond}_{p}(\gamma A) \geq 1$$

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

1.2 Error Bounds and Residuals

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

$$\bullet \quad \|b\| \quad \leq \quad \|A\| \cdot \|x\|$$

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

$$\to \boxed{\frac{\|\Delta x\|}{\|x\|} \le \operatorname{cond}(A) \frac{\|\Delta b\|}{\|b\|}}$$

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

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

 $\leq \|A^{-1}\| \cdot \|r\|$

$$\rightarrow \left| \frac{\|\Delta x\|}{\|\hat{x}\|} \le \operatorname{cond}(A) \frac{\|r\|}{\|A\| \cdot \|\hat{x}\|} \right|$$

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

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

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

$$\to \boxed{\frac{\|\Delta x\|}{\|x\|} \le \operatorname{cond}(A) \frac{\|\Delta A\|}{\|A\|}}$$

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

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

$$\leq \|\Delta A\| \cdot \|\hat{x}\|$$

$$\to \boxed{\frac{\|r\|}{\|A\|\cdot\|\hat{x}\|} \le \frac{\|\Delta A\|}{\|A\|}}, \quad \frac{\|\Delta x\|}{\|x\|} \le \frac{\|A^{-1}\|\cdot\|r\|}{\|\hat{x}\|} \le \operatorname{cond}(A) \quad \frac{\|\Delta A\|}{\|A\|}$$

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

•
$$x'(t) = \frac{b'(t) - A'(t)x(t)}{A(t)} = A^{-1}(t) \left[\Delta b - \Delta A \cdot x(t) \right]$$

•
$$x(t) = x_0 + x'(0)t + \mathcal{O}(t^2)$$

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

Gaussian Elimination with LU/PLU/PLDUQ Decomposition 1.3

Elementary Elimination Matrices, L_k

$$\bullet \ \forall i \neq j \ (L_k^{-1})_{ij} = -(L_k)_{i,j}$$

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

LU/PLU Factorization (w/ partial pivoting)

$$A = LU$$
 (L is gen. triang.)
(U is upp. triang.)
 $L = (\dots L_2 P_2 L_1 P_1)^{-1}$

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

$$b = Ly , \quad y = Ux$$
(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. $(a_{jj} > \sum_{i,i \neq j} a_{ij})$
- A can be singular

$$A = PLU$$
 (P is rowswap permu.)
(L is unit low. triang.)
(U is upp. triang.)
 $P = (\dots P_2 P_1)^{-1}$

$$\{\dots\}b = (\dots P_2 P_1) A x$$
$$P^T b = (P_1^T P_2^T \dots)^{-1} A x$$
$$= P^T (PLU) x = L y$$

$$P^T b = L y \ , \ \ y = U x$$

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

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

$$P^TAQ^T = LDU \qquad \begin{tabular}{l} \mbox{(P is permu. for rows)} \\ \mbox{(Q is permu. for cols.)} \end{tabular}$$

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

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

(growth factor, ρ , 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

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

$$\bullet a_k \text{ is the "pivot"}$$

$$\bullet \forall i \neq j \quad (M_k^{-1})_{ij} = -(M_k)_{ij}$$

MD Factorization (w/ partial pivoting)

$$A = MD$$
 (M is elem. elim.)
 $(D \text{ is diag.})$
 $M = (\dots M_2 P_2 M_1 P_1)^{-1}$

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

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

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

$$M^{-1}b = y , \quad y = Dx$$
 (division)

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

Finding A^{-1} $D^{-1}M^{-1}(A|I) = (I|A^{-1})$ $=D^{-1}M^{-1}\begin{bmatrix}a_{11}&\cdots&1&0\\\vdots&a_{nn}&0&1\end{bmatrix}$ $= \begin{bmatrix} 1 & 0 & a'_{11} & \dots \\ 0 & 1 & \vdots & a'_{nn} \end{bmatrix}$

Symmetric Matrices 1.5

Positive Definite: $|x^T Ax| > 0$

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

- Only lower triangle needed for storage
- Well defined (always works)
- $A = LDL^T$ 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. (Assen) 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

$$\tilde{A}\tilde{x} = b = (A - uv^{T})\tilde{x}$$

$$\rightarrow \tilde{x} = \tilde{A}^{-1}b$$

$$\tilde{A}^{-1} = (A - uv^{T})^{-1} = A^{-1} + \frac{A^{-1}u}{1 - v^{T}(A^{-1}u)} v^{T}A^{-1}$$

$$\tilde{x} = (A^{-1}b) + \frac{A^{-1}u}{1 - v^{T}(A^{-1}u)} v^{T}(A^{-1}b)$$

$$x + \frac{y}{1 - v^{T}y} v^{T}x$$

General Woodbury Formula:

$$(A - UV^{T})^{-1} = A^{-1} + (A^{-1}U)(I - V^{T}A^{-1}U)^{-1} v^{T}A^{-1}$$

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

1.8 Complexity

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

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

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

Symmetric:
$$A = LL^T$$

 $PAP^T = LDL^T$ $\rightarrow \mathcal{O}(n^3/6)$, $LL^Tx = b \rightarrow \mathcal{O}(n^2)$

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

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

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

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

Least ||r|| Linear Regression/Fit for Ax + r = b2

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

Example - Vandermonde Matrix, A:

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

Decompose b: Projector of A, P

$$b = Ax + r$$

$$= y + r$$

$$= Pb + P_{\perp}b$$

Minimize residual, r:

$$\nabla ||r||_2^2 = 0 \qquad \left(\frac{\partial r^2}{\partial x_i} = 0\right)$$

$$= \nabla \left[(b - Ax)^T (b - Ax) \right]$$

$$= \nabla \left(b^T b - 2x^T A^T b + x^T A^T Ax \right)$$

$$0 = 2A^T Ax - 2A^T b$$

$$\downarrow$$

$$= ||Pr||^2 + ||P_{\perp}r||^2$$

$$= ||Pb - Ax||_2^2 + ||P_{\perp}b||_2^2$$

$$\downarrow$$

$$Ax = Pb$$

$$A^T Ax = A^T Pb = (P^T A)^T b$$

 $||r||_2^2 = ||Pr + P_{\perp}r||_2^2 = ||b - Ax||^2$

 $A^T A x = A^T b$ (Solvable with Cholesky)

 $A^T A x = A^T b$ (System of Normal Equations)

Cross-Product Matrix of A: A^TA

Symmetric: $(A^T A)^T = A^T A$

Pos. Def.:
$$\operatorname{rank}(A) = n$$

 $\rightarrow \langle x | A^T A x \rangle = x^T A^T A x$
 $= (Ax)^T (Ax)$
 $= \|Ax\|^2 \ge 0$

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

Pseudoinverse, A^+

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

Nonsingular: $A^T A x = 0$ $\rightarrow \|Ax\|^2 = 0 = Ax$ $\rightarrow (x=0)$

Ortho. Proj., P

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

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: $cond(A^TA) = [cond(A)]^2$

2.1 Error Bounds and Residuals

Norm and Conditioning:

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

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

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

 $\bullet \quad \|\Delta x\| \leq \|A^+\| \cdot \|\Delta b\|$

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

• Cond. number is a func. of cond(A) and b

• $Pb \approx 0$ or $\theta \approx 90^{\circ}$ is highly sensitive

$$\bullet \quad \mathcal{A}^{T} \overrightarrow{Ax} + A^{T} \Delta Ax + (\Delta A)^{T} Ax + (\overline{\Delta A})^{T} \Delta Ax = A^{T} b + (\Delta A)^{T} b$$

$$+ A^{T} A \Delta x + \overline{A}^{T} \Delta A \Delta x + (\overline{\Delta A})^{T} A \Delta x + (\overline{\Delta A})^{T} \Delta A \Delta x$$

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

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

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

2.2 Solving $A^TAx = A^Tb$ with an Augmented Matrix

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

ullet Solvable with LU Decomp or Symm. Pos. Def. Methods

• α "controls the relative weights of the two subsystems in chooing pivots from either"

• $\alpha = \max a_{ij}/1000$ (rule of thumb)

• MATLAB uses it for large, sparse systems

2.3 QR Decomposition

Orthogonal Matrix,
$$Q$$

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

QR Factorization

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

Reduced QR Factorization

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

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

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

- $\bullet \quad ||Qv||^2 = \langle v|Q^TQv\rangle = ||v||^2$ $||Q^T v||^2 = \langle v|QQ^T v\rangle = ||v||^2$
- $\bullet Q^T = H_n \dots H_1$ $\bullet H_i^T H_i = H_i H_i^T = I$
- $\bullet \ A = [a_1 \ \dots \ a_n] \qquad \bullet \ I_n = [e_1 \ \dots \ e_n]$

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

$$H_i \dots H_1 a_i = \sum_{j=1}^{i} c_j e_j = H_n \dots H_1 a_i$$

 $(\|a_i\|^2 = |\alpha_1|^2 = \sum_{j=1}^{i} c_j^2)$

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

$$\langle H_i \dots H_1 r | e_i \rangle = 0$$
 $(1 \le j \le i)$

Q^TA rotates A until the column vectors are aligned with certain axes described above

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

$$\left\{ Q_{\parallel} = Q_{m \times n} \mid \operatorname{span}(Q_{\parallel}) = \operatorname{span}(A) \right\}$$

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

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

$$\rightarrow Q_{\parallel}^{T}Ax = Q_{\parallel}^{T}Pb = Q_{\parallel}^{T}Q_{\parallel}Q_{\parallel}^{T}b$$

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

$$A = Q_{\parallel} R = \begin{pmatrix} | & | & | \\ \vec{q_1} \dots \vec{q_n} \\ | & | & | \end{pmatrix} \begin{pmatrix} r_{11} \dots r_{1n} \\ 0 & \ddots & \vdots \\ 0 & 0 & r_{nn} \end{pmatrix} = \begin{pmatrix} | & | & | \\ \vec{a_1} \dots \vec{a_n} \\ | & | & | \end{pmatrix}$$

$$\bullet \ \vec{a_j} = \sum_{i}^{j} r_{ij} \cdot \vec{q_i}$$

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

Householder Transformation/Elementary Reflector, H

$$H\vec{a_1} = \alpha_1 \vec{e_1} \qquad \|a_1\| = |\alpha_1|$$

$$(\text{rotation})$$

$$= [\vec{a_1} - 2\hat{v}(\hat{v} \cdot \vec{a_1})] \qquad \rightarrow \qquad [H = I - 2vv^T = I - \frac{2vv^T}{v^Tv}] \qquad \bullet \qquad H = H^T = H^{-1}$$

$$(\text{symmetric and orthogonal})$$

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

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

$$\qquad \qquad \alpha_1 = \pm \|a_1\| \quad \rightarrow \quad \boxed{\alpha_i = -\text{sign}(a_i) \|a_i\|} \quad \text{(avoid "cancellation" in finite-calc. of v above)}$$

$$H_j \dots H_1 a_i = a_i^j \quad \rightarrow \quad \begin{bmatrix} v_{j+1} = \begin{pmatrix} 0 \\ \vdots \\ (a_i^j)_i \\ \vdots \\ (a_i^j)_m \end{pmatrix} - \alpha_i e_i \end{bmatrix} \quad \bullet \quad \text{Store v_i and R into A and an extra n-vector.}$$

$$\bullet \quad Q \text{ and H can be computed if needed.}$$

$$\bullet \quad \text{When column i is completed, row i is too.}$$

2.3.2 Givens Rotation, G

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

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

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

•
$$\tau = \frac{a_1}{a_2} < 1 \rightarrow s = \frac{1}{\sqrt{1+\tau^2}}, c = s \cdot \tau$$

2.3.3 Gram-Schmidt Orthogonalization

$$Q_{\parallel}^{T} = \begin{pmatrix} \widehat{q}_{1} : q_{1} = a_{1} \\ \widehat{q}_{2} : q_{2} = a_{2} - \widehat{q}_{1}(\widehat{q}_{1} \cdot a_{2}) \\ \widehat{q}_{3} : q_{3} = a_{3} - \widehat{q}_{1}(\widehat{q}_{1} \cdot a_{3}) - \widehat{q}_{2}(\widehat{q}_{2} \cdot a_{3}) \\ \vdots \\ \widehat{q}_{n} : q_{n} = a_{n} - \sum_{i}^{n} \widehat{q}_{i}(\widehat{q}_{i} \cdot a_{n}) \end{pmatrix}, \quad R = \begin{pmatrix} \|a_{1}\| & \widehat{q}_{1} \cdot a_{2} & \widehat{q}_{1} \cdot a_{3} & \dots & \widehat{q}_{1} \cdot a_{n} \\ 0 & \|a_{2}\| & \widehat{q}_{2} \cdot a_{3} & \dots & \widehat{q}_{2} \cdot a_{n} \\ 0 & 0 & \|a_{3}\| & \dots & \widehat{q}_{3} \cdot a_{n} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & \|a_{n}\| \end{pmatrix}$$

Classical, Column Oriented: Find \widehat{q}_i , then solve for \widehat{q}_{i+1} , and continue up to \widehat{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 $q_i^{[k]} = a_i - \sum_j^k \widehat{q}_j(\widehat{q}_j \cdot a_i)$. 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

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

$$\begin{pmatrix} \mid & \mid & \mid & \mid \\ a_1 \dots a_n & b \\ \mid & \mid & \mid & \mid \end{pmatrix} = \begin{pmatrix} \mid & \mid & \mid & \mid \\ \widehat{q_1} \dots \widehat{q_n} & q_{n+1} \\ \mid & \mid & \mid & \mid \end{pmatrix} \begin{pmatrix} r_{11} \dots r_{1n} \mid \\ 0 & \ddots & \vdots & b'_1 \\ \vdots & \ddots & r_{nn} \mid \\ 0 & \dots & 0 & \rho \end{pmatrix}$$

$$\begin{pmatrix} \text{Use Gram-Schmidt QR on this, then solve } Rx = b \\ \text{This method is preferred numerically to reduce cancelling effects}$$

$$\text{Text didn't recommend what } q_{+1} \text{ or } \rho \text{ should be.}$$

$$\rho \text{ or } (q_{n+1})_i \text{ looks like it should be 0.}$$

$$\text{Idk, not much explained.}$$

- Use Gram-Schmidt QR on this, then solve $Rx = b'_1$
- This method is prefered numerically to reduce cancelling effects

Factorization with Column-Pivoting 2.3.4

- 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.

2.3.5Rank Deficiency (or Other) Case

$$\underline{\operatorname{If} \ \operatorname{rank}(A) = k < n} : \begin{bmatrix} (Q^T A P)(P^T x) & = & Q^T b \\ \binom{R \ S}{0 \ 0'} & \binom{z}{0} & = & \binom{b'_1}{b'_2} \end{bmatrix}$$

- \bullet 0' is approx. 0 since the remaining norms are too small.
- $$\begin{split} \bullet & \ R = R_{k \times k} \\ \bullet & \ S \text{ is the remaining columns after } R \text{ is completed.} \\ \bullet & \boxed{\text{There }} \text{ are multiple solutions for } x. \end{split}$$
- ullet For a quick solution, $Rz = b_1'$, $x = Pinom{z}{0}$
- For the minimized-norm solution with the smallest ||x||, S must be annihilated.
- For another method or if underdetermined (m < n), something like SVD Decomp. can be used.

2.4 Singular Value Decomposition (SVD)

2.5 Complexity

3 Matrix Types

 ${\bf Hermitian:}$

$$m{H}=m{H}^\dagger$$

Unitary:

$$UU^\dagger=I$$

$$H = UDU^{-1}$$

• D is real

$$U=e^{iH}$$

•
$$U = e^{iH} = U_H e^{iD} (U_H)^{-1}$$