

$$\text{NLA solves (approx.)} \quad \left\{ \begin{array}{ll} \text{linear system} & : \mathbf{Ax} = 0, \mathbf{A} \in \mathbb{R}^{n \times n} \\ \text{least square} & : \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{Ax} - \mathbf{b}\|_2, \mathbf{A} \in \mathbb{R}^{m \times n} (m \geq n) \\ \text{eigen-problem} & : \mathbf{Ax} = \lambda \mathbf{x}, \mathbf{A} \in \mathbb{R}^{n \times n}, \mathbf{x} \neq 0, \lambda \in \mathbb{C} \\ \text{singular value} & : \mathbf{A}^T \mathbf{Ax} = \sigma^2 \mathbf{x}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{x} \neq 0, \sigma \geq 0 \end{array} \right.$$

$$\text{Lin. Space} \quad \left\{ \begin{array}{ll} \mathbb{R}^n, \mathbb{C}^n & : \text{vec.} \\ \mathbb{R}^{m \times n}, \mathbb{C}^{m \times n} & : \text{mat.} \end{array} \right. \quad \text{Lin. Trans.} \quad \left\{ \begin{array}{ll} \mathbf{A} \in \mathbb{R}^{m \times n} & : \mathbb{R}^n \rightarrow \mathbb{R}^m \\ \mathbf{A} \in \mathbb{C}^{m \times n} & : \mathbb{C}^n \rightarrow \mathbb{C}^m \end{array} \right.$$

$$\text{Lin. Subspace} \quad \left\{ \begin{array}{ll} N(\mathbf{A}) = \text{Ker}(\mathbf{A}) \triangleq \{\mathbf{x} \in \mathbb{C}^n : \mathbf{Ax} = 0\} & \subseteq \mathbb{C}^n \\ C(\mathbf{A}) = \text{Ran}(\mathbf{A}) \triangleq \{\mathbf{y} \in \mathbb{C}^m : \mathbf{y} = \mathbf{Ax}, \mathbf{x} \in \mathbb{C}^n\} & \subseteq \mathbb{C}^m \end{array} \right.$$

$$\text{span}(\mathbf{A}) \triangleq \{\alpha_1 \mathbf{x}_1 + \alpha_2 \mathbf{x}_2 + \cdots + \alpha_k \mathbf{x}_k\} \quad \left\{ \begin{array}{ll} \mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n & \in \mathbb{C}^n \\ \alpha_1, \alpha_2, \cdots, \alpha_n & \in \mathbb{C} \\ \mathbf{A} = (\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n) & \end{array} \right.$$

$$\text{Vec. Norms} \quad \left\{ \begin{array}{ll} \|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i| & \|\mathbf{x}\|_2 = \left(\sum_{i=1}^n |x_i|^2 \right)^{1/2} \\ \|\mathbf{x}\|_\infty = \max_{1 \leq i \leq n} |x_i| & \|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p} \end{array} \right., \quad \begin{array}{l} \|\gamma \mathbf{x}\| = |\gamma| \cdot \|\mathbf{x}\| \\ \|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\| \end{array}$$

† ℓ^p -norms in \mathbb{R}^n , $p = 1, 2, \infty$

$$\text{Mat. Norms} \quad \left\{ \begin{array}{ll} \|\mathbf{A}\|_1 = \max_{1 \leq j \leq n} \left(\sum_{i=1}^n |a_{ij}| \right) & \|\mathbf{A}\|_2 = \sqrt{\rho(\mathbf{A}^T \mathbf{A})} \\ \|\mathbf{A}\|_\infty = \max_{1 \leq i \leq n} \left(\sum_{j=1}^n |a_{ij}| \right) & \|\mathbf{A}\|_F = \left(\sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^2 \right)^{1/2} \end{array} \right., \quad \begin{array}{l} \|\gamma \mathbf{A}\| \leq |\gamma| \cdot \|\mathbf{A}\| \\ \|\mathbf{A} + \mathbf{B}\| \leq \|\mathbf{A}\| + \|\mathbf{B}\| \\ \|\mathbf{AB}\| \leq \|\mathbf{A}\| \cdot \|\mathbf{B}\| \\ \|\mathbf{Ax}\| \leq \|\mathbf{A}\| \cdot \|\mathbf{x}\| \end{array}$$

† ℓ^p -norms in $\mathbb{R}^{n \times n}$, $p = 1, 2, \infty$ and Frobenius-norm

$$\text{Special Mat.} \quad \left\{ \begin{array}{ll} \text{Hermitian} & : \mathbf{A}^* = \mathbf{A} \\ \text{Normal} & : \mathbf{A}^* \mathbf{A} = \mathbf{A} \mathbf{A}^* \end{array} \right. \quad \begin{array}{ll} \text{Unitary} & : \mathbf{U}^* \mathbf{U} = \mathbf{U} \mathbf{U}^* = \mathbf{I} \\ \text{Orthogonal} & : \mathbf{Q}^T \mathbf{Q} = \mathbf{Q} \mathbf{Q}^T = \mathbf{I} \end{array}$$

$$\text{Eigen-} \quad \left\{ \begin{array}{ll} \text{charct. poly.} & : p(\lambda) = \det(\mathbf{A} - \lambda \mathbf{I}) \quad \text{eigval.} : \{\lambda \in \mathbb{C} : \det(\mathbf{A} - \lambda \mathbf{I}) = 0\} \\ \text{charct. eq.} & : \det(\mathbf{A} - \lambda \mathbf{I}) = 0 \quad \text{eigvec.} : \{\mathbf{x} \in \mathbb{C}^n : \mathbf{Ax} = \lambda \mathbf{x}, \lambda \in \mathbb{C}\} \end{array} \right.$$

† eigval./vec. are only defined for square mat.

† real mat. may have comp. eigval./vec.

† algebraic multiplicity (AM) of λ_i : $\{k \in \mathbb{R} : \det(\mathbf{A} - \lambda \mathbf{I}) = (\lambda - \lambda_i)^k g(\lambda) = 0\}$

† geometric multiplicity (GM) of λ_i : dim. of λ_i 's eigenspace

† similar mat. ($\mathbf{A} = \mathbf{X} \mathbf{B} \mathbf{X}^{-1}$) have same eigval.

† mat. spctm.: $\sigma(\mathbf{A}) \triangleq \{\lambda_1, \cdots, \lambda_n\}$

$$\text{Err. Est.} \begin{cases} \text{abs. err. bound } \varepsilon & : \exists \varepsilon > 0 : |e| \leq \varepsilon \\ \text{rel. err. bound } \varepsilon_r & : \exists \varepsilon_r > 0 : |e_r| \leq \varepsilon_r \end{cases}$$

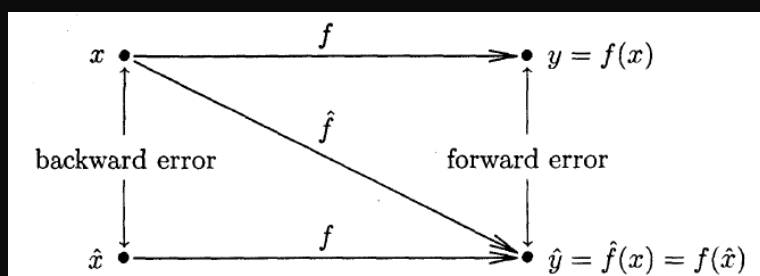
$$\bullet \text{ arithmetic } \begin{cases} \varepsilon(x_1 + x_2) & \leq \varepsilon(x_1) + \varepsilon(x_2) \\ \varepsilon(x_1 x_2) & \leq |x_2| \varepsilon(x_1) + |x_1| \varepsilon(x_2) \end{cases}, \quad \varepsilon\left(\frac{x_1}{x_2}\right) \leq \frac{|x_1| \varepsilon(x_1) + |x_1| \varepsilon(x_2)}{|x_2|^2}$$

$$\bullet \text{ functional } \begin{cases} \varepsilon(f(x)) & \lesssim |f'(x)| \varepsilon(x) \text{ [4,5]} \\ \varepsilon_r(f(x)) & = \text{cond} \cdot \varepsilon_r(x) \end{cases}, \quad \text{cond} \triangleq \left| \frac{\tilde{x} f'(\tilde{x})}{f(\tilde{x})} \right|$$

$$\dagger \varepsilon(f(x)) \approx \sum_{k=1}^n \left| \frac{\partial f(x)}{\partial \tilde{x}_k} \right| \varepsilon(x_k), \quad f(x) = f(x_1, \dots, x_n)$$

\dagger bound the err. rather than compute it (true val. unknown)

$$\text{Err. Anly.} \begin{cases} \text{fore err.} & : \Delta y = \hat{y} - y = \hat{f}(x) - f(x) \\ \text{back err.} & : \Delta x = \hat{x} - x \text{ where } f(\hat{x}) = \hat{y} \end{cases}$$



$\dagger x, f$: exact input and func.

$\dagger \hat{f}$: approx. func.

$\dagger \hat{x}$: exact val. for \hat{f}

$\dagger \hat{f}(x) = f(\hat{x})$ due to the choice of \hat{x} , which defines \hat{x}

\dagger back. err. anly is easier, used to measure algo. stability

\dagger comp. err. $\begin{cases} \text{trunc. err.} & : \text{due to trunc. of inf. series, finite diff., ...} \\ \text{round. err.} & : \text{due to finite-prec., rounding arith., ...} \end{cases}$

$$\dagger \text{ total err.} = \hat{f}(\hat{x}) - f(x) = \underbrace{(\hat{f}(\hat{x}) - f(\hat{x}))}_{\text{comp. err.}} + \underbrace{(f(\hat{x}) - f(x))}_{\text{data err.}}$$

Cond. Num.

$$\text{cond} \triangleq \frac{|\text{rel. change in sol.}|}{|\text{rel. change in input}|} = \frac{(f(\hat{x}) - f(x))/f(x)}{(\hat{x} - x)/x} = \frac{|\Delta y/y|}{|\Delta x/x|}$$

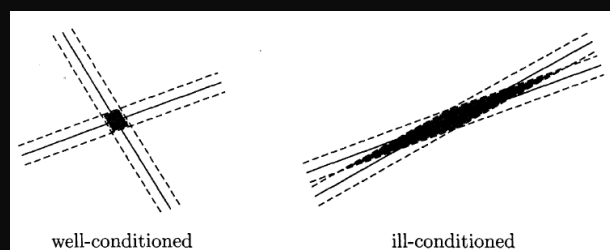
$\dagger \text{ cond} \geq 1 (> 10)$: sensi./ill-cond. prob.

$\dagger |\text{rel. fore. err.}| \lesssim \text{cond} \cdot |\text{rel. back. err.}|$

◦ $\text{cond} \iff$ amplification factor

◦ \lesssim : upper bound for the max. cond.

$$\dagger \text{ cond} \approx \left| \frac{x f'(x)}{f(x)} \right| \text{ [6]}$$



Stability $\left\{ \begin{array}{l} \text{math prob.} \\ \text{(well-posed)} \end{array} \right\} \left\{ \begin{array}{l} \text{sol. exists, unique, depends continuously} \\ \text{small input change } \not\rightarrow \text{ abrupt change in sol.} \\ \text{well-posed} \neq \text{ sol. is insensi. to pertb.} \end{array} \right.$

$\left\{ \begin{array}{l} \text{algo. desp.} \\ \text{(stable)} \end{array} \right\} \left\{ \begin{array}{l} \text{rst. rel. insensi. to pertb. due to approx.} \\ \text{rst. is the exact sol. to a nearby prob.} \\ \text{weaker: } \underline{\text{nearly correct rst. for nearly the correct prob.}} \end{array} \right.$

Accuracy	$\left\{ \begin{array}{l} \text{closeness of comp. sol. to true sol.} \\ \text{depends on algo. cond. and stability} \\ \text{stability} \neq \text{accuracy} \end{array} \right.$		alog.	prob.
		inaccuracy	stable	ill-cond.
			unstable	well-cond.
		accuracy	stable	well-cond.

Mach. Precs. $\left\{ \begin{array}{l} \varepsilon_m = \arg \min_{\varepsilon} \text{fl}(1 + \varepsilon) > 1 \\ \left| \frac{\text{fl}(x) - x}{x} \right| \leq \varepsilon_m \end{array} \right.$

† $\text{fl}(x)$: round to nearest, $\text{fl}(x \oplus y) = (x \oplus y)(1 + \delta)$, $|\delta| \leq \varepsilon_m$

† ε_m determines the max. rel. err. in representing a real num. x

Err. Anly. Sum.

	Total Err.		
	comp. err.		data err.
	trunc. err.	round. err.	
howto est.	theoretical anly.	back. err. anly. hard to quantify	cond.ing, <u>cond</u>
howto rdc.	aglo. selction	stable algo. tips†, dbl-prec.	change prob. form. improve cond.ing

† avoid subtractive cancellation in nums. of nearly equal mag.

† avoid adding large and small nums.

† adjust the order of additions

Mat. Cond.

$\kappa(\mathbf{A}) \triangleq \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\|$

† κ is def. for sqr. non-singlr. mat., $\kappa(\mathbf{A}) = \infty$ if \mathbf{A} singlr.

† $\kappa(\mathbf{A}) \geq 1$, $\kappa(\mathbf{I}) = 1$, $\kappa(\gamma \mathbf{A}) = \kappa(\mathbf{A})$, $\kappa(\mathbf{D}) = (\max |d_i|) / (\min |d_i|)$, $\mathbf{D} = \text{diag}(d_i)$

Perm. Mat.

$$\underline{P^{-1} = P^T} \quad , \quad \|P\| = 1 \quad , \quad \kappa(P) = 1 \quad , \quad \kappa(PA) = \kappa(A)$$

† P is sqr. mat. with only one 1 in each row/col. and is always non-singlr.

† P is orthogonal mat., prod. of P is also perm. mat.

† PA reorders rows, AP reorders cols.

Elem. Elim. Mat.

$$M_k a = \begin{pmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -m_{k+1} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -m_n & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} a_1 \\ \vdots \\ a_k \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad , \quad \begin{matrix} m_i = a_i/a_k \\ i = k+1, \dots, n \end{matrix}$$

† M_k is unit lower tri., non-singlr., annihilates all entries below **pivot** $a_k \neq 0$

† $\left. \begin{matrix} M_k = I - m e_k^T \\ M_k^{-1} = I + m e_k^T \triangleq L_k \end{matrix} \right\}$ reverse signs of multipliers
 $m = (0, \dots, 0, m_{k+1}, \dots, m_n)^T$

† $M_k M_j$ ($j > k$) is their "union", and similar rst. holds for $L_k L_j$ [13]

LU Fact. by Gauss. Elim.

$$\underbrace{M_{n-1} \cdots M_1}_{\text{lower tri. mat. } M} Ax = \overbrace{MAx}^{\text{upper tri. sys.}} = \underbrace{Mb}_y \quad , \quad LUx = b \quad \left\{ \begin{array}{l} Ly = b \quad : \text{ fore. subs.} \\ Ux = y \quad : \text{ back. subs.} \end{array} \right. \quad [12]$$

† LU Fact. is unique $\iff \left\{ \begin{array}{l} L \text{ is unit lower tri., } U \text{ is upper tri.} \\ \text{all leading principle submats. are non-singlr.} \end{array} \right.$

† Gauss. Elim. and LU Fact. are two ways of expressing same process

† zero pivot causes breakdown \rightsquigarrow chooses entry with large mag.

Pivoting

- partial pvt.

† M^{-1} is not necessarily lower tri. due to perm.

† $PA = LU$ where $P = P_{n-1} \cdots P_1$, but can't be determined in advance

† universally used since N.S. is more than adequate

- complete pvt.

† entire remaining unreduced submats. is searched for the max. mag.

† $PAQ = LU$, theoretically superior, but much expensive

LU Fact. Stability

$$\frac{\|\mathbf{r}\|}{\|\mathbf{A}\| \cdot \|\hat{\mathbf{x}}\|} \leq \frac{\|\mathbf{E}\|}{\|\mathbf{A}\|} \leq \rho n \varepsilon_m \quad [11], [Wil61]$$

† \mathbf{E} : back. err. of mat. \mathbf{A}

† growth fac. $\rho \triangleq \frac{\text{max. ele. of } \mathbf{U}}{\text{max. ele. of } \mathbf{A}}$ $\left\{ \begin{array}{ll} \text{without pvt.} & : \text{arbitrarily large} \rightsquigarrow \text{unstable} \\ \text{partial pvt.} & : \rho \leq 2^{n-1} (< 10) \rightsquigarrow \text{stable} \\ \text{complete pvt.} & : \rho \text{ much smaller but not worth} \end{array} \right.$

† $\frac{\|\mathbf{E}\|}{\|\mathbf{A}\|} \lesssim n \varepsilon_m$ in practice $\rightsquigarrow^{\text{always}}$ small res. regardless of cond.ing

† small res. \nleftrightarrow accurate sol. unless \mathbf{A} is well-cond.

LU Fact. Algo.

Algorithm 3: *LU* Fact. with Partial PVT.

```

1  $\mathbf{p} \leftarrow [1:n]$  ; // aux. vec.
2 for  $i \leftarrow 1$  to  $n-1$  do
3    $a_{ki} \leftarrow \max_{i \leq j \leq n} |a_{ji}|$  ; // find pvt.
4   if  $k \neq i$  then
5     for  $j \leftarrow 1$  to  $n$  do
6        $t \leftarrow a_{ij}, a_{ij} \leftarrow a_{kj}, a_{kj} \leftarrow t$  ; // row  $i \rightleftharpoons$  row  $k$ 
7        $\mathbf{p}(k) \leftarrow i, \mathbf{p}(i) \leftarrow k$  ; // upd.  $\mathbf{p}$ 
8   for  $j \leftarrow i+1$  to  $n$  do
9      $a_{ji} \leftarrow a_{ji}/a_{ii}$  ; // calc. col.  $i$ 
10  for  $j \leftarrow i+1$  to  $n$  do
11    for  $k \leftarrow i+1$  to  $n$  do
12       $a_{jk} \leftarrow a_{jk} - a_{ji}a_{ik}$  ; // upd.  $\mathbf{A}[i+1:n, i+1:n]$ 
```

† fact. effectively in-place

† trans. of \mathbf{b} can be included or as a sep. step

- storage only. $\left\{ \begin{array}{l} \mathbf{L}, \mathbf{U} \text{ overwrite init. mat. } \mathbf{A} \left\{ \begin{array}{l} \mathbf{U} \text{ on upper tri.} \\ \mathbf{L} \text{ on } \underline{\text{strict lower tri.}} \end{array} \right. \\ \text{aux. vec. } \mathbf{p} \text{ keeps track of new row order} \end{array} \right.$

- complexity only.: $\frac{2}{3}n^3 + \mathcal{O}(n^2)$ [14]

Special Lin. Sys. $\left\{ \begin{array}{ll} \text{symm./herm.} & : \mathbf{A} = \mathbf{A}^T, \mathbf{A} = \mathbf{A}^H \\ \text{pos. def.} & : \forall \mathbf{x} \neq 0 \quad \mathbf{x}^T \mathbf{A} \mathbf{x} > 0, \mathbf{x}^H \mathbf{A} \mathbf{x} > 0 \\ \text{banded} & : \forall |i-j| > \beta \quad a_{ij} = 0, \text{ where } \beta \triangleq \text{bandwidth} \\ \text{sparse} & : \text{most are zeros} \end{array} \right.$

Symm. Pos. Def. Sys. $\left\{ \begin{array}{l} \text{all eigvals. are pos.} \\ \text{all leading principle mats. are SPD} \\ \text{all elems. on diag. are pos., and } \underline{\max_i \{a_{ii}\} > \max_{i \neq j} \{|a_{ij}|\}} \\ \text{Cholesky Fact.: } \mathbf{A} = \mathbf{L}\mathbf{L}^T \end{array} \right.$

Cholesky Fact.

- $A = LL^T$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{pmatrix} \begin{pmatrix} l_{11} & l_{21} & \cdots & l_{n1} \\ & l_{22} & \cdots & l_{n2} \\ & & \ddots & \vdots \\ & & & l_{nn} \end{pmatrix}$$

$$a_{ij} = \sum_{k=1}^n l_{ik}l_{jk} = l_{jj}l_{ij} + \sum_{k=1}^{j-1} l_{ik}l_{jk} \quad , \quad i, j = 1, 2, \dots, n$$

Algorithm 4: Cholesky LL^T Fact.

```

1 for  $j \leftarrow 1$  to  $n$  do
2    $a_{jj} \leftarrow \left( a_{jj} - \sum_{k=1}^{j-1} a_{jk}^2 \right)^{1/2}$  ;           // diag. elem.
3   for  $i \leftarrow j+1$  to  $n$  do
4      $a_{ij} \leftarrow \left( a_{ij} - \sum_{k=1}^{j-1} a_{ik}a_{jk} \right) / a_{jj}$  ;   // elems. below diag. elem.
```

† $A = LL^T$ is unique when diag. ele. are required to be pos.

† sqr. roots are all of pos. \rightsquigarrow algo is well-def. \rightsquigarrow no pvt. for N.S.: $\rho \leq 1$ [15]

† only access, store, overwrite lower tri. mat. of A

† $\frac{1}{3}n^3 + \mathcal{O}(n^2)$ [16] (half of LU fact.); mcmd.: chol(A)

- $A = LDL^T$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & \ddots & \ddots & \\ l_{n1} & \cdots & l_{n,n-1} & 1 \end{pmatrix} \begin{pmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{pmatrix} \begin{pmatrix} 1 & l_{21} & \cdots & l_{n1} \\ & 1 & \cdots & l_{n2} \\ & & \ddots & \vdots \\ & & & 1 \end{pmatrix}$$

$$a_{ij} = \sum_{k=1}^n l_{ik}d_kl_{jk} = d_jl_{ij} + \sum_{k=1}^{j-1} l_{ik}d_kl_{jk} \quad , \quad i, j = 1, 2, \dots, n$$

Algorithm 5: Cholesky LDL^T Fact.

```

1 for  $j \leftarrow 1$  to  $n$  do
2    $a_{jj} \leftarrow a_{jj} - \sum_{k=1}^{j-1} a_{jk}^2 a_{kk}$  ;           // diag. elem.
3   for  $i \leftarrow j+1$  to  $n$  do
4      $a_{ij} \leftarrow \left( a_{ij} - \sum_{k=1}^{j-1} a_{ik}a_{kk}a_{jk} \right) / a_{jj}$  ;   // elems. below diag. elem.
```

† advantage of not requiring any sqr. roots.

† d_i in LDL^T is the sqr. of l_{ii} in LL^T

Symm. inDef. Lin. Sys.

† $\rho_{chol} \gg 1 \rightsquigarrow$ breakdown using Cholesky fact. \rightsquigarrow unstable algo.

† pvt. \rightsquigarrow asymm. $\xrightarrow[\text{rows \& cols.}]{\text{exchange both}}$ symm.: $PAP^T = LDL^T$

† stable $\left\{ \begin{array}{l} PAP^T = \underline{\underline{L}}TL^T \quad , \quad T \text{ is symm. tri. mat. [Aas71]} \\ PAP^T = \underline{\underline{L}}\tilde{D}L^T \quad , \quad \tilde{D} \text{ is block tridiag. mat. } \left\{ \begin{array}{l} 1 \times 1 \\ 2 \times 2 \end{array} \right. \quad [\text{BK77}] \end{array} \right.$

Tridiag. Lin. Sys.

$$\mathbf{A} = \begin{pmatrix} d_1 & u_1 & & \\ l_2 & \ddots & \ddots & \\ & \ddots & \ddots & u_{n-1} \\ & & l_n & d_n \end{pmatrix}, \quad \begin{array}{l} |d_1| > |u_1| > 0 \\ |d_n| > |l_n| > 0 \\ |d_i| \geq |l_i| + |u_i| > 0 \end{array} \quad \begin{array}{l} \dagger > : \text{irr. strict diag. dom. mat.} \\ \dagger \geq : \text{irr. weak diag. dom. mat.} \end{array}$$

$$\mathbf{A} = \begin{pmatrix} d_1 & u_1 & & \\ l_2 & \ddots & \ddots & \\ & \ddots & \ddots & u_{n-1} \\ & & l_n & d_n \end{pmatrix} = \begin{pmatrix} \alpha_1 & & & \\ l_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & l_n & \alpha_n \end{pmatrix} \begin{pmatrix} 1 & \beta_1 & & \\ & 1 & \ddots & \\ & & \ddots & \beta_{n-1} \\ & & & 1 \end{pmatrix} \triangleq \mathbf{LU}, \quad \begin{array}{l} \alpha_i = d_i - l_i \beta_{i-1} \\ \beta_i = u_i / \alpha_i \ (\beta_0 = 0) \\ i = 1, \dots, n \end{array}$$

$$\mathbf{Ax} = \mathbf{b} \Rightarrow \mathbf{LUx} = \mathbf{b} \left\{ \begin{array}{l} \mathbf{Ly} = \mathbf{b} \Rightarrow y_i = (b_i - l_i y_{i-1}) / \alpha_i, \quad i = 1, \dots, n, \quad y_0 = 0 \\ \mathbf{Ux} = \mathbf{y} \Rightarrow x_i = (y_i - \beta_i x_{i+1}), \quad i = n, \dots, 1, \quad x_{n+1} = 0 \end{array} \right.$$

Algorithm 6: Thomas Algo. for Tridiag. Lin. Sys.

```

1   $\beta_0 = 0, y_0 = 0, x_{n+1} = 0$  ; // init. val.
2  for  $i \leftarrow 1$  to  $n$  do
3     $\alpha_i \leftarrow d_i - l_i \beta_{i-1}$  ; // calc.  $\alpha_i$ 
4     $\beta_i \leftarrow u_i / \alpha_i$  ; // calc.  $\beta_i$ 
5     $y_i \leftarrow (b_i - l_i y_{i-1}) / \alpha_i$  ; // calc.  $y_i$ 
6  for  $i \leftarrow n$  to  $1$  do
7     $x_i \leftarrow (y_i - \beta_i x_{i+1})$  ; // calc.  $x_i$ 

```

$\dagger 0 < |\beta_i| < 1 \rightsquigarrow$ err. in back. subs. is under control

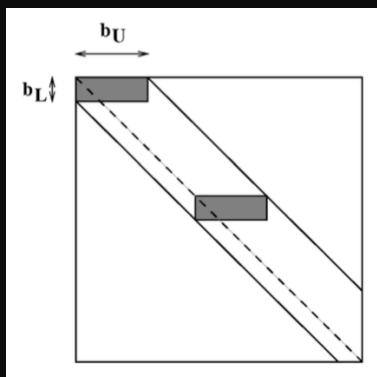
$\dagger 0 < |d_i| - |l_i| < |\alpha_i| < |d_i| + |l_i|, \quad i = 2, 3, \dots, n \rightsquigarrow \alpha_i \neq 0$

\dagger solve $\mathbf{Ly} = \mathbf{b}$ and \mathbf{LU} fact. simultaneously \rightsquigarrow no need to store α_i but β_i

\dagger complexity: $8n$ [17]

Banded Tri. Lin. Sys.

$$a_{ij} = 0 \quad \text{for} \quad \begin{cases} i > j + b_L \\ i < j - b_U \end{cases}$$



- no pvt. $\left\{ \begin{array}{l} \mathbf{L} : \text{lower band} = b_L \\ \mathbf{U} : \text{upper band} = b_U \end{array} \right.$
 (A=LU)

- partial pvt. $\left\{ \begin{array}{l} \mathbf{L} : \text{lower band} = b_L \text{ with at most } b_L + 1 \text{ nz. in each col.} \\ \mathbf{U} : \text{upper band} \leq b_L + b_U \end{array} \right.$
 (PA=LU)

\dagger complexity: $2nb_L b_U + 2n(b_L + b_U)$

Pertb. Anly.

$$\left. \begin{array}{l} Ax = b \\ (A + \delta A)x^* = b + \delta b \\ r = b - Ax^* \end{array} \right\} \xrightarrow{\text{back. anly.}} \begin{array}{l} \delta x = x^* - x \\ = -A^{-1}r \end{array} \quad [18] \quad \left\{ \begin{array}{l} x : \text{exact sol.} \\ x^* : \text{approx. sol.} \\ r : \text{res.} \end{array} \right.$$

- $\delta x \rightsquigarrow x^*$ (A is non-singlr.)

$$\frac{\|\delta x\|}{\|x^*\|} \leq \|A^{-1}\| \cdot \|A\| \cdot \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|A\| \cdot \|x^*\|} \right) \quad [19]$$

$$\frac{\|\delta x\|}{\|x^*\|} \leq \kappa(A) \cdot \frac{\|\delta A\|}{\|A\|} \quad \text{when } \|\delta b\| = 0$$

- $\delta x \rightsquigarrow x$ (A is non-singlr., $\underbrace{\|A^{-1}\| \cdot \|\delta A\|}_{< 1} < 1$)

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\kappa(A)}{1 - \kappa(A) \cdot \frac{\|\delta A\|}{\|A\|}} \cdot \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right) \quad [20]$$

$$\frac{1}{\kappa(A)} \cdot \frac{\|\delta b\|}{\|b\|} \leq \frac{\|\delta x\|}{\|x\|} \leq \kappa(A) \cdot \frac{\|\delta b\|}{\|b\|} \quad \text{when } \|\delta A\| = 0$$

- $\delta x \rightsquigarrow r$ (A is non-singlr.)

$$\|\delta x\| \leq \|A^{-1}\| \cdot \|r\| \quad [18]$$

Accuracy Imprv.

- scaling

† scale by multiplying a diag. mat. D : $DADy = Db$, $x = Dy$;

† scaling affects cond.ing; not practical but worth trying for ill-cond. sys.

† accuracy is usually enhanced if all entries have abt. same order of mag.

- iter. refine. $\left\{ \begin{array}{l} \text{calc. res. } r \text{ for approx. sol. } x: r = b - Ax^* \\ \text{sol. } Az = r \text{ [21] with two tri. lin. sys. [22]: } \mathcal{O}(n^2) \end{array} \right.$

Algorithm 7: Accuracy Enhance. by Iter. Refine.

```

1 let  $PA = LU$ ,  $x^*$  as approx. sol.;
2 repeat
3   | calc.  $r \leftarrow b - Ax^*$ ;
4   | sol.  $Ly = Pr$  ;                               //  $y = L^{-1}Pr$ 
5   | sol.  $Uz = y$  ;                                   //  $z = U^{-1}y$ 
6   |  $x^* \leftarrow x^* + z$  ;                             // new approx. sol.
7 until  $x^*$  converges;
```

† $x^* + z$ is the exact sol., but z^* is found in practice

† $\|r - Az^*\|$ is smaller than $\|r\| \rightsquigarrow x^* + z^*$ is closer to exact sol. than x^*

† A can not be overwritten $\rightsquigarrow A, L, U$ are stored

Lin. LSQ. Prob.

$$\mathbf{Ax} \cong \mathbf{b} \Leftrightarrow \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{b} - \mathbf{Ax}\|_2 = \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{r}\|_2 \quad \begin{cases} m = n & : \mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \text{ if } \mathbf{A} \text{ is non-singlr.} \\ m > n & : \text{overdet. (in most cases)} \\ m < n & : \text{underdet.} \end{cases}$$

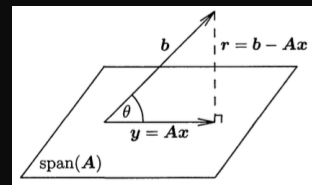
† uniqueness: sol. to $\mathbf{Ax} \cong \mathbf{b}$ is unique **iff.** \mathbf{A} is full col. rank: $\text{rank}(\mathbf{A}) = n$

† existence: sol. always exists but not unique if \mathbf{A} is rank-deficient

Cond.ing of Lin. LSQ. Prob.

• **pseudoinv.** for non-singlr. mat.: $\mathbf{A}^+ \triangleq (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T$

• cond. num. $\begin{cases} \text{full col. rank} & : \kappa(\mathbf{A}) \triangleq \|\mathbf{A}\| \cdot \|\mathbf{A}^+\| \\ \text{defective rank} & : \kappa(\mathbf{A}) = \infty \end{cases}$



Sensitivity of Lin. LSQ. Prob.

$$\text{pertb. in } \mathbf{b} \quad : \quad \frac{\|\Delta \mathbf{x}\|}{\|\mathbf{x}\|} \leq \kappa(\mathbf{A}) \cdot \frac{1}{\cos \theta} \cdot \frac{\|\Delta \mathbf{b}\|}{\|\mathbf{b}\|} \quad [23]$$

$$\text{pertb. in } \mathbf{A} \quad : \quad \frac{\|\Delta \mathbf{x}\|}{\|\mathbf{x}\|} \lesssim \left(\kappa^2(\mathbf{A}) \cdot \tan \theta + \kappa(\mathbf{A}) \right) \cdot \frac{\|\mathbf{E}\|}{\|\mathbf{A}\|} \quad [24]$$

LSQ. Prob. Trans.

$$\mathbf{Ax} \cong \mathbf{b} \underset{\text{overdet.}}{\rightsquigarrow} \text{sqr. lin. sys.} \rightsquigarrow \text{tri. lin. sys.} \quad \begin{cases} 1) \text{ normal eq.} & : \text{fastest} \\ 2) \text{ QR Fact.} & : \text{most important} \\ 3) \text{ SVD Fact.} & : \text{slowest but most reliable} \end{cases}$$

Normal Eq.

$\mathbf{A} \in \mathbb{R}^{m \times n}$ ($m \geq n$), $\mathbf{x}^* \in \mathbb{R}^n$ is lsq. sol. **iff.** $\mathbf{r} = \mathbf{b} - \mathbf{Ax}^* \perp \text{Ran}(\mathbf{A})$

$$\Rightarrow \begin{cases} \mathbf{A}^T \mathbf{Ax} = \mathbf{A}^T \mathbf{b} & : \text{lsq. prob. sol.} \Leftrightarrow \text{normal eq. sol.} \\ \mathbf{A}^T (\mathbf{b} - \mathbf{Ax}) = 0 & : \text{res. } \mathbf{r} = \mathbf{b} - \mathbf{Ax} \text{ is ortho. to } \text{span}(\mathbf{A}) \text{ (geo. view)} \end{cases}$$

† rect. mat. \rightsquigarrow sqr. mat. \rightsquigarrow tri. mat.

$$\dagger \mathbf{A} \text{ is full col. rank} \Rightarrow \begin{cases} \text{rank}(\mathbf{A})=n \\ \mathbf{A}^T \mathbf{A} \text{ is symm. pos. def.} \\ \text{unique lsq. sol.: } \mathbf{x} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b} \\ \text{Cholesky Fact.: } \mathbf{A}^T \mathbf{A} = \mathbf{LL}^T \Rightarrow \begin{cases} \mathbf{Ly} = \mathbf{A}^T \mathbf{b} \\ \mathbf{L}^T \mathbf{x} = \mathbf{y} \end{cases} \end{cases}$$

◦ info. can be lost in forming $\mathbf{A}^T \mathbf{A}$ and $\mathbf{A}^T \mathbf{b}$

◦ cond. num. is **sqr.** of $\kappa(\mathbf{A})$: $\kappa(\mathbf{A}^T \mathbf{A}) = \kappa^2(\mathbf{A}) \rightsquigarrow$ **unstable algo.**

† Chol. Fact. complexity of $\mathbf{A}^T \mathbf{A}$: $mn^2 + \frac{1}{3}n^3 + \mathcal{O}(n^2)$ [26]

$$\mathbf{QR\ Fact.} \quad \left\langle \begin{array}{l} \mathbf{Q} : \text{orthonormal / unitary mat.} \\ \mathbf{R} : \text{upper tri. mat} \end{array} \right. \rightsquigarrow \begin{array}{l} \mathbf{A} = \mathbf{QR} \\ (\mathbf{A} \in \mathbb{C}^{m \times n}, m \geq n) \end{array}$$

† existence: $\exists \mathbf{Q} \in \mathbb{C}^{m \times n} (\mathbf{Q}^* \mathbf{Q} = \mathbf{I})$, $\mathbf{R} \in \mathbb{C}^{n \times n} (r_{ij} = 0, i > j)$

† uniqueness: \mathbf{QR} fact. is unique **iff.** \mathbf{A} is full col. rank, and $r_{ii} > 0$

† app: ¹⁾lin. lsq. prob.; ²⁾eigval. prob.; ³⁾ $\mathbf{Ax} = \mathbf{b}$ when \mathbf{A} is non-singlr. sqr. mat.

QR Fact. \longleftrightarrow Lin. LSQ. Prob.

$$\begin{array}{l} \text{derv. mmz. of lin. lsq. prob.} \\ \text{with } \mathbf{QR} \text{ fact.} \end{array} \rightsquigarrow \begin{array}{l} \text{1) augment } \mathbf{Q} : [\mathbf{1}] \\ \text{2) trans. } \mathbf{b} : [\mathbf{2}] \\ \text{3) normal eq. : } [\mathbf{3}] \end{array} \left. \vphantom{\begin{array}{l} \text{derv. mmz. of lin. lsq. prob.} \\ \text{with } \mathbf{QR} \text{ fact.} \end{array}} \right\} \Rightarrow \mathbf{x}^* = \mathbf{R}^{-1} \mathbf{Q}^T \mathbf{b}$$

$$\begin{aligned} (1) \quad \left. \begin{array}{l} \mathbf{A}_{m \times n} = \mathbf{Q}_{m \times n} \mathbf{R}_{n \times n} \\ (\mathbf{Q}, \hat{\mathbf{Q}}) \in \mathbb{R}^{m \times m} \end{array} \right\} &\Rightarrow \left\| \mathbf{Ax} - \mathbf{b} \right\|_2^2 = \left\| (\mathbf{Q}, \hat{\mathbf{Q}})^T \cdot (\mathbf{Ax} - \mathbf{b}) \right\|_2^2 = \left\| \begin{pmatrix} \mathbf{Q}^T \\ \hat{\mathbf{Q}}^T \end{pmatrix} \cdot (\mathbf{QRx} - \mathbf{b}) \right\|_2^2 \\ &= \left\| \begin{pmatrix} \mathbf{Rx} - \mathbf{Q}^T \mathbf{b} \\ -\hat{\mathbf{Q}}^T \mathbf{b} \end{pmatrix} \right\|_2^2 = \left\| \mathbf{Rx} - \mathbf{Q}^T \mathbf{b} \right\|_2^2 + \left\| \hat{\mathbf{Q}}^T \mathbf{b} \right\|_2^2 \geq \left\| \hat{\mathbf{Q}}^T \mathbf{b} \right\|_2^2 \Rightarrow \mathbf{x}^* = \mathbf{R}^{-1} \mathbf{Q}^T \mathbf{b} \end{aligned}$$

$$\begin{aligned} (2) \quad &\mathbf{A}_{m \times n} = \mathbf{Q}_{m \times n} \mathbf{R}_{n \times n} \text{ , } \mathbf{b} = (\mathbf{Q} \mathbf{Q}^T + \mathbf{I} - \mathbf{Q} \mathbf{Q}^T) \mathbf{b} \\ &\Rightarrow \mathbf{Ax} - \mathbf{b} = \mathbf{Ax} - (\mathbf{Q} \mathbf{Q}^T + \mathbf{I} - \mathbf{Q} \mathbf{Q}^T) \mathbf{b} = (\mathbf{Ax} - \mathbf{Q} \mathbf{Q}^T \mathbf{b}) - (\mathbf{I} - \mathbf{Q} \mathbf{Q}^T) \mathbf{b} \\ &\dagger \Rightarrow \left\| \mathbf{Ax} - \mathbf{b} \right\|_2^2 = \left\| \mathbf{Ax} - \mathbf{Q} \mathbf{Q}^T \mathbf{b} \right\|_2^2 + \left\| (\mathbf{I} - \mathbf{Q} \mathbf{Q}^T) \mathbf{b} \right\|_2^2 = \left\| \mathbf{Q} (\mathbf{Rx} - \mathbf{Q}^T \mathbf{b}) \right\|_2^2 + \left\| (\mathbf{I} - \mathbf{Q} \mathbf{Q}^T) \mathbf{b} \right\|_2^2 \\ &\geq \left\| (\mathbf{I} - \mathbf{Q} \mathbf{Q}^T) \mathbf{b} \right\|_2^2 \Rightarrow \mathbf{x}^* = \mathbf{R}^{-1} \mathbf{Q}^T \mathbf{b} \end{aligned}$$

$$(3) \quad \mathbf{x}^* = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b} = (\mathbf{R}^T \underbrace{\mathbf{Q}^T \mathbf{Q}}_{\mathbf{I}_{n \times n}} \mathbf{R})^{-1} \mathbf{R}^T \mathbf{Q}^T \mathbf{b} = \mathbf{R}^{-1} \mathbf{R}^{-T} \mathbf{R}^T \mathbf{Q}^T \mathbf{b} = \mathbf{R}^{-1} \mathbf{Q}^T \mathbf{b}$$

