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NLA IV: Special linear systems

As a principle, we want to take advantage of any special structure to increase speed and reduce storage

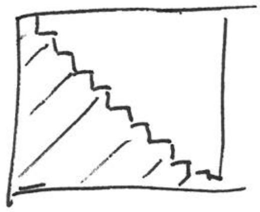
We will consider properties as symmetry, definiteness and bandedness

IV.1 Symmetric matrices [Golub & van Loan, §4.1.2]

An $n \times n$-matrix A is symmetric if

$$A^T = A$$

A symmetric matrix needs half the space to store its coefficients



$\frac{n(n+1)}{2} \approx n^2/2$ entries instead of n^2

Intuition tells we should be able to solve a symmetric

$$Ax = b$$

with half the complexity ($\approx n^3/3$ flops instead of $\frac{2}{3}n^3$?)

Pivoting destroys the symmetry

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} a & b & c \\ b & d & e \\ c & e & f \end{pmatrix} = \begin{pmatrix} c & e & f \\ b & d & e \\ a & b & c \end{pmatrix}$$

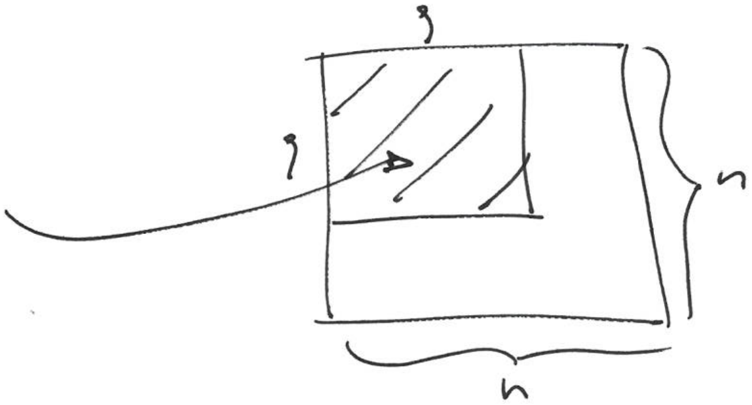
Now let A be an arbitrary (non necessarily symmetric) matrix. When does it admit an LU factorization?

<u>Matlab notation:</u> for $p \leq q$, $r \leq s$

$$A(p:q, r:s) = (a_{ij})_{\substack{p \leq i \leq q \\ r \leq j \leq s}} \in F^{(q-p+1) \times (s-r+1)}$$

The <u>leading</u> $q \times q$-principal submatrix of A is

$A(1:q, 1:q)$



It is equivalent:

(1) $\exists!\ L, U$ s.t. $A = L \cdot U$, with U upper triangular, nonsingular and L unit lower triangular

(2) All leading principal submatrices of A are nonsingular

This result can be found in [D, page 39]

Now suppose A <u>symmetric</u> and has an LU factorization.

These factors have a connection:

$n=2$

$$\begin{pmatrix} a & c \\ c & b \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 \\ c/a & 1 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} a & 0 \\ 0 & d-\frac{c}{a}b \end{pmatrix} \begin{pmatrix} 1 & c/a \\ 0 & 1 \end{pmatrix}}_{U}$$

U is a row scaling of L^T.

This is a general fact: set $d_i = u_{ii}$, then

$$U = \underbrace{D}_{\mathrm{diag}(d_1,\dots,d_n)} \cdot \underbrace{M}_{\text{\underline{unit} upper triangular}}$$

then $\boxed{M = L^T}$

The LU factorization of A can be written as

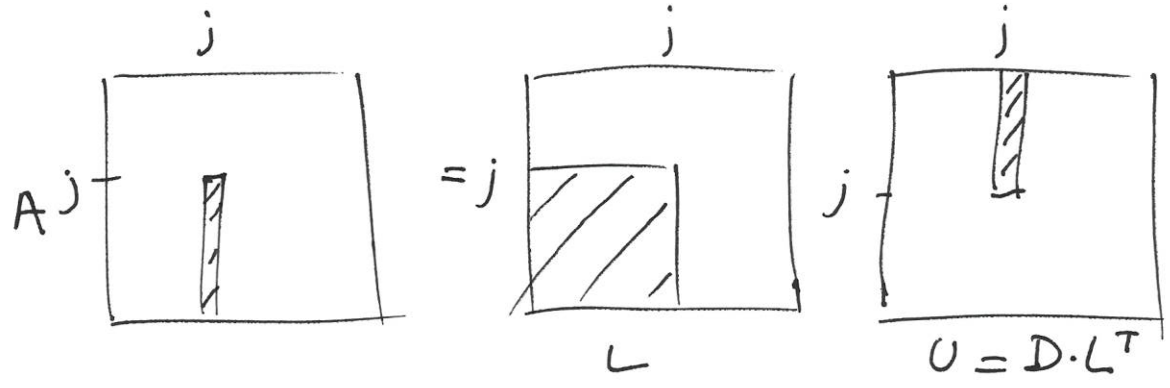
$$A = \underbrace{L}_{\text{unit lower triangular}} \cdot \underbrace{D}_{\text{diagonal}} \cdot L^T$$

How can we compute it?

For $j = 1,\dots,n$

$$A(j:n, j) = L(j:n, 1:j) \cdot w(1:j)$$

$$\cancel{\begin{pmatrix} d_1 l_{j1} \\ \vdots \\ d_{j-1} l_{j,j-1} \\ d_j \end{pmatrix}} \qquad \begin{pmatrix} d_1 l_{j1} \\ \vdots \\ d_{j-1} l_{j,j-1} \\ d_j \end{pmatrix}$$



Hence $$d_j = a_{jj} - \sum_{k=1}^{j-1} d_k \, l_{jk}^2$$

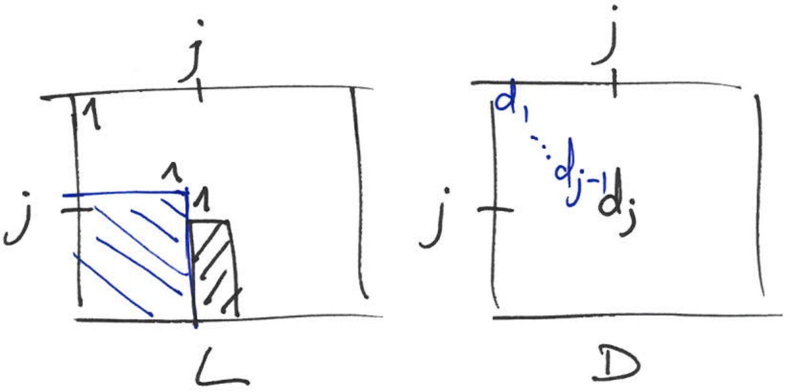
$$A(j+1:n, j) = L(j+1:n, 1:j)\, v(1:j)$$
$$= L(j+1:n, 1:j-1)\, v(1:j-1) + d_j \, L(j+1:n, j)$$

and so

$$L(j+1:n, j) = \frac{1}{d_j}\Big(A(j+1:n, j) - L(j+1:n, 1:j-1)\cdot v(1:j-1)\Big)$$

gives d_j and $L(j+1:n, j)$ in terms of

$d_1, \dots, d_{j-1}$ and $L(j:n, 1:j-1)$ (and A, of course!)



LDL^T algorithm

for $j = 1$ to n

  for $i = 1$ to $j-1$

    $v_i \leftarrow l_{ji} \cdot \cancel{d_i}$ a_{ii}

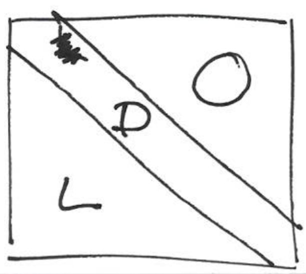
  end

a_j $\cancel{d_j} \leftarrow a_{jj} - \overset{A}{\cancel{L}}(j, 1:j-1)\cdot v(1:j-1)$

A $\cancel{L}(j+1:n, j) \leftarrow \frac{1}{\underset{a_{jj}}{\cancel{d_j}}}\Big(A(j+1:n, j) - \underset{A}{\cancel{L}}(j+1:n, 1:j-1)\, v(1:j-1)\Big)$

end

We might overwrite A



Example

$$A = \begin{pmatrix} 1 & -1 & 2 \\ -1 & 5 & 2 \\ 2 & 2 & 17 \end{pmatrix}$$

$j=1$

$$L = \begin{pmatrix} 1 & & \\ -1 & & \\ 2 & & \end{pmatrix} \qquad D = \begin{pmatrix} 1 & & \\ & & \\ & & \end{pmatrix}$$

$j=2$

$$v_1 = \underset{(-1)\cdot 1}{-1} \qquad L = \begin{pmatrix} & & \\ & & \\ & \underset{\frac{1}{4}(2-2\cdot(-1))}{1} & \end{pmatrix} \qquad D = \begin{pmatrix} & & \\ & \underset{5-(-1)\cdot(-1)}{4} & \\ & & \end{pmatrix}$$

$j=3$

$$v = \begin{pmatrix} \overset{2\cdot 1}{2} \\ \underset{1\cdot 4}{4} \end{pmatrix} \qquad D = \begin{pmatrix} & & \\ & & \\ & & \underset{17-(2\cdot 2+1\cdot 4)}{9} \end{pmatrix}$$

Hence

$$\begin{pmatrix} 1 & -1 & 2 \\ -1 & 5 & 2 \\ 2 & 2 & 17 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 2 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 9 \end{pmatrix} \begin{pmatrix} 1 & -1 & 2 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

In the machine:

$$A \quad \begin{pmatrix} 1 & & \\ 2 & 5 & \\ 2 & 2 & 17 \end{pmatrix} \rightsquigarrow \begin{pmatrix} \boxed{1} & & \\ -1 & \boxed{4} & \\ 2 & 1 & \boxed{9} \end{pmatrix} \qquad L \,\&\, D$$

Beware: the LU factorization of a symmetric matrix can be numerically unstable

Ex:

$$A = \begin{pmatrix} \eta & 1 \\ 1 & 1 \end{pmatrix} \quad \text{with} \quad 0 < \eta < \varepsilon$$

IV.2. Symmetric positive definite systems

[D, §2.7.1], [GvL, §4.2.3 & 4.2.5]

A $n\times n$-matrix A is <u>positive definite</u> if

$$x^T\cdot A\cdot x > 0 \qquad \forall x\neq 0 \qquad (F=\mathbb{R})$$

Symmetric positive definite (spd) constitute one of the most important classes of $Ax=b$ problems

<u>Important fact</u> (from LA)

$$A\in\mathbb{R}^{n\times n} \text{ symmetric} \Rightarrow A = \underbrace{Q^T}_{\text{orthogonal}}\cdot \overbrace{\Lambda}^{\text{diagonal}}\cdot Q$$

A is <u>diagonalizable</u> (over $\mathbb{R}$) with an <u>orthogonal</u> similarity

A is spd $\Leftrightarrow$ $\Lambda = \operatorname{diag}(\lambda_1,\dots,\lambda_n)$ with $\lambda_i>0$.

A spd is nonsingular, and moreover all its leading ppal submatrices are nonsingular (see [D, page 77])

Hence $\exists L$ unit lower triangular and D diagonal s.t.

$$A = L\cdot D\cdot L^T$$

In the spd case we have that $d_i>0$ $\forall i$.
Hence we can write

$$A = G\cdot G^T \qquad \text{Cholesky factorization}$$

with $G = L\cdot\operatorname{diag}(\sqrt{d_1},\dots,\sqrt{d_n})$

To compute, note that

$$a_{ij} = \sum_{k=1}^{j} g_{jk}\, g_{ik}$$

and so

$$g_{jj}\, g_{ij} = a_{ij} - \sum_{k=1}^{j-1} g_{jk}\, g_{ik}$$

If the first $j-1$ columns of G are known, we can compute the j-th one.

<u>Cholesky algorithm</u>

for $j = 1$ to n

$$a_{jj} \quad \cancel{g_{jj}} \leftarrow \Big(a_{jj} - \sum_{k=1}^{j-1} \underset{a_{jk}^2}{\cancel{g_{jk}^2}} \Big)^{1/2}$$

for $i = j+1$ to n

$$a_{ij} \quad \cancel{g_{ij}} \leftarrow \frac{1}{g_{jj}} \Big(a_{ij} - \sum_{k=1}^{j-1} \underset{a_{ik}\, a_{jk}}{\cancel{g_{ik}\, g_{jk}}} \Big)$$

end

We can overwrite A

<u>Example</u>

$$A = \begin{pmatrix} 1 & -1 & 2 \\ -1 & 5 & 2 \\ 2 & 2 & 17 \end{pmatrix}$$

$j = 1$

$$G = \begin{pmatrix} 1 & & \\ -1 & & \\ 2 & & \end{pmatrix}$$

$j=2$

$$G = \begin{pmatrix} & & \\ & 2 & \\ & 2 & \end{pmatrix}$$

$(5-(-1)^2)^{1/2}$

$\frac{1}{2}(2-(-1)\cdot 2)$

$j=3$

$$G = \begin{pmatrix} & & \\ & & \\ & & 3 \end{pmatrix}$$

$(17-(2^2+2^2))^{1/2}$

Hence

$$\begin{pmatrix} 1 & -1 & 2 \\ -1 & 5 & 2 \\ 2 & 2 & 17 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 2 & 0 \\ 2 & 2 & 3 \end{pmatrix} \begin{pmatrix} 1 & -1 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & 3 \end{pmatrix}$$

In the machine

$$A \quad \begin{pmatrix} 1 & & \\ 2 & 5 & \\ 2 & 2 & 17 \end{pmatrix} \rightsquigarrow \begin{pmatrix} 1 & & \\ -1 & 2 & \\ 2 & 2 & 3 \end{pmatrix} \quad G$$

The complexity is

$$\sum_{j=1}^{n} \left((j-1) + (j-2) + 1 + 1 + \sum_{i=j+1}^{n} (2j-1) \right) = \frac{1}{3} n^3 + O(n^2)$$

half the complexity of LU!

Pivoting is not necessary for Cholesky to be
<u>numerically stable</u>

The same analysis of GEPP shows that the computed (by Cholesky) solution of $\hat{x}$ satisfies

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

$\hat{A}$ instead

with

machine epsilon

$$|\delta A| \leq 3n\,\varepsilon\,|G| \cdot |G^T|$$

matrices of absolute values

By Cauchy-Schwartz inequality

$$(|G| \cdot |G^T|)_{ij} = \sum_k |g_{ik}| \cdot |g_{jk}|$$

$$\leq \left(\sum_k g_{ik}^2\right)^{1/2} \left(\sum_k g_{jk}^2\right)^{1/2}$$

$$= a_{ii}^{1/2}\, a_{jj}^{1/2} \leq \max_{ij} |a_{ij}|$$

Hence $\| \, |G| \cdot |G^T| \, \|_\infty \leq n \|A\|_\infty$ and so

$$\boxed{\|\delta A\|_\infty \leq 3n^2 \varepsilon \|A\|_\infty}$$

<u>Remark</u>: Cholesky is also the cheapest way to test if a symmetric matrix is definite positive: this will be the case if and only if the algorithm concludes.

IV.3 Band matrices [D, § 2.7.3]

A is a <u>band matrix</u> with lower band with b_L and upper band with b_U if

$$a_{ij} = 0$$

for $i > j + b_L$ or $i < j - b_U$

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1\,b_U+1} & & 0 \\ & & & \ddots & \\ a_{b_L+1,1} & & & & \ddots\ a_{n-b_U,n} \\ & \ddots & & & \\ 0 & & \ddots\ a_{n,n-b_L} & \cdots & a_{nn} \end{pmatrix}$$

They appear when the equations can be ordered so that each variable x_i appears in few equations in a neighborhood of the i-th equation.

The LU-factorization (Gauss without pivoting) preserves the band structure:

$$A = L \cdot U$$

then L has lower bandwith b_L and U has upper bandwith b_U

It can be computed with $2n\, b_U b_L + \mathcal{O}(n(b_U + b_L))$ flops

Example

$$A = \begin{pmatrix} 2 & -1 & 0 & 0 \\ 4 & -1 & 3 & 0 \\ 0 & -1 & -2 & 1 \\ 0 & 0 & 3 & 4 \end{pmatrix}$$

tridiagonal 4×4

$b_L = b_U = 1$

$$L(1{:}4, 1) = \begin{pmatrix} 1 \\ 2 \\ 0 \\ 0 \end{pmatrix} \qquad U(1, 1{:}4) = \begin{pmatrix} 2 & -1 & 0 & 0 \end{pmatrix}$$

Schur complement: $a_{jk} \leftarrow a_{jk} - l_{j1} u_{1k}$ $\quad j,k = 2,3,4$

$-1 - (2 \cdot (-1))$

$$\rightarrow \; S_1 = \begin{pmatrix} 1 & 3 & 0 \\ -1 & -2 & 1 \\ 0 & 3 & 4 \end{pmatrix}$$

$-2 - ((-1) \cdot 3)$

$$L(2{:}4, 2) = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \qquad U(2, 2{:}4) = \begin{pmatrix} 1 & 3 & 0 \end{pmatrix} \qquad S_2 = \begin{pmatrix} 1 & 1 \\ 3 & 4 \end{pmatrix}$$

$4 - (3 \cdot 1)$

$$L(3{:}4, 3) = \begin{pmatrix} 1 \\ 3 \end{pmatrix} \qquad U(3, 3{:}4) = \begin{pmatrix} 1 & 1 \end{pmatrix} \qquad S_3 = \begin{pmatrix} 1 \end{pmatrix}$$

$$L(4{:}4, 4) = (1) \qquad U(4, 4{:}4) = (1)$$

Hence

$$A = \begin{pmatrix} 2 & -1 & 0 & 0 \\ 4 & -1 & 3 & 0 \\ 0 & -1 & -2 & 1 \\ 0 & 0 & 3 & 4 \end{pmatrix} = L \cdot U = \begin{pmatrix} 1 & & & \\ 2 & 1 & & \\ 0 & -1 & 1 & \\ 0 & 0 & 3 & 1 \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 & 0 \\ & 1 & 3 & 0 \\ & & 1 & 1 \\ & & & 1 \end{pmatrix}$$

<u>Key observation:</u> the Schur complement of a banded matrix is <u>banded</u> (with the same upper & lower bandwiths).

GEPP can exploit band structure, but the band properties of L and U are not so simple.

$$A = P \cdot L \cdot U$$

then U is banded with upper bandwith $b_L + b_U$ and L has at most $b_L + 1$ nonzero entries per column

Indeed, at each step pivoting can only be done within the first b_L rows.
Later permutations can reorder the entries of the earlier columns of L.

Example

$$A = \begin{pmatrix} 2 & -1 & 0 & 0 \\ 4 & -1 & 3 & 0 \\ 0 & -1 & -2 & 1 \\ 0 & 0 & 3 & 4 \end{pmatrix}$$

swap rows 1 & 2:

$$A_1 = \begin{pmatrix} 4 & -1 & 3 & 0 \\ 2 & -1 & 0 & 0 \\ 0 & -1 & -2 & 1 \\ 0 & 0 & 3 & 4 \end{pmatrix} \quad L(1{:}4,1) = \begin{pmatrix} 1 \\ 1/2 \\ 0 \\ 0 \end{pmatrix} \quad U(1,1{:}4) = \begin{pmatrix} 4 & -1 & 3 & 0 \end{pmatrix}$$

$-1 - (\tfrac{1}{2} \cdot (-1))$ $\quad$ $0 - \tfrac{1}{2} \cdot 3$

$$S_1 = \begin{pmatrix} -1/2 & -3/2 & 0 \\ -1 & -2 & 1 \\ 0 & 3 & 4 \end{pmatrix}$$ swap rows 2 & 3

$$L(2{:}4,2) = \begin{pmatrix}1\\ 1/2\\ 0\end{pmatrix} \qquad U(2,2{:}4) = \begin{pmatrix}-1 & -2 & 1\end{pmatrix}$$

$$S_2 = \begin{pmatrix}-1/2 & -1/2\\ 3 & 4\end{pmatrix}$$ swap rows 3 & 4

$$L(3{:}4,3) = \begin{pmatrix}1\\ -1/6\end{pmatrix} \qquad U(3,3{:}4) = \begin{pmatrix}3 & 4\end{pmatrix}$$

$$S_3 = \left(1/6\right) \qquad -\tfrac{1}{2} - \left(\left(-\tfrac{1}{6}\right)\cdot 4\right) \qquad U(4,4{:}4) = \left(1/6\right)$$

upper bandwith 2

$$A = \begin{pmatrix}2 & -1 & 0 & 0\\ 4 & -1 & 3 & 0\\ 0 & -1 & -2 & 1\\ 0 & 0 & 3 & 4\end{pmatrix} = P\,L\,U = \begin{pmatrix}0&0&0&1\\1&0&0&0\\0&1&0&0\\0&0&1&0\end{pmatrix}\cdot\begin{pmatrix}1&&&\\0&1&&\\0&0&1&\\1/2&1/2&-1/6&1\end{pmatrix}\begin{pmatrix}4&-1&3&0\\&-1&-2&1\\&&3&4\\&&&1/6\end{pmatrix}$$

at most 2 nonzeros per column

IV.4 Sparse matrices [D, §2.7.4]

A *sparse matrix* is a matrix with few nonzero entries.

For them, the best choice is usually an *iterative method* (to be explained later in the course)

They are based on *matrix–vector* multiplications, which are cheap when A is sparse.

GE does <u>not</u> preserve the sparse structure:

<u>Example</u>

$$A = \begin{pmatrix} 1 & 0.1 & \cdots & 0.1 \\ 0.1 & 1 & & O \\ \vdots & & \ddots & \\ 0.1 & O & & 1 \end{pmatrix} = \begin{pmatrix} 1 & & & & \\ 0.1 & 1 & & O & \\ \vdots & -0.01 & \ddots & & \\ \vdots & \vdots & & \ddots & \\ 0.1 & -0.01 & & 0.01 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0.1 & 0.1 & \cdots & 0.1 \\ & 0.99 & -0.01 & \cdots & -0.01 \\ & & 0.99 & & \vdots \\ & & & \ddots & -0.01 \\ & & & & 0.99 \end{pmatrix}$$