Gauss elemination

$$0.0003x + 1.566y = 1.569$$
$$0.3454x + 2.436y = 1.018 \qquad \text{exact sol: } (10, 1)$$

4 digits: $m = 0.3454/0.0003 = 1151$

$\Rightarrow 0.3454 - 1151 \cdot 0.0003$

etc.

$x = 3.333 \quad y = 1.001$ ill conditioned matrix

$\boxed{\text{Swapping rows}}$ improves results

Fundamental eq. of NLA (FENLA)

A, b given. x is the solution: $Ax = b$

$\hat{x}$ is a guess. $e = x - \hat{x}$ is the error

$r = b - A\hat{x}$ is the residual.

$$\boxed{A \cdot e = r}$$

if we knew e we could get x!

$$A(x - \hat{x}) = b - A\cdot\hat{x} = r$$

Iterative improvement: (an approximate)

1. compute a solution $\hat{x}$
2. $r = b - A\hat{x}$
3. solve for e from $Ae = r$
4. $\hat{x} \to \hat{x} + e$
5. exit if $\|e\|$ is small enough, otherwise goto 2.

(Mixed precision methods: step 3 could use less precision.)

Works if we have at least 1 correct digit in $\hat{x}$, and e

Error analysis, recall induced matrix norm $\|\underline{A}\| = \sup\limits_{x \neq 0} \frac{\|Ax\|}{\|x\|}$,

so $\|Ax\| \le \|A\| \, \|x\|$

Condition number $\text{cond}(A) = \|A^{-1}\| \cdot \|A\|$

for symmetric $\underline{A}$

$\|A\|_2 = \max |\lambda|$ (λ is eigenval of A) $\Rightarrow$ cond. number $\approx \frac{|\text{maximal } \lambda|}{|\text{minimal } \lambda|}$

~~Ax̂~~ $\underline{\underline{A}}\,\underline{x} = \underline{b}$ and we have an approximate solution $-\underline{\underline{A}}\,\underline{\hat{x}} + \underline{b} = \underline{r}$

Then: $$\frac{\|x-\hat{x}\|}{\|x\|} \leq \operatorname{cond}(\underline{\underline{A}}) \cdot \frac{\|r\|}{\|b\|}$$

proof: $\underline{\underline{A}}\,\underline{e} = \underline{r} \qquad \underline{e} = \underline{\underline{A}}^{-1} \cdot \underline{r}$

$$\|e\| \leq \|A^{-1}\|\,\|r\|$$
$$\|b\| \leq \|A\|\,\|x\|$$
$$\|e\|\,\|b\| \leq \|A^{-1}\|\,\|A\|\,\|r\| \cdot \|x\| \implies \frac{\|e\|}{\|x\|} \leq \operatorname{cond}(A)\frac{\|r\|}{\|b\|}$$

QED.

More complicated theorem:

solving $Ax = b$ in finite precision w. rounding errors is equivalent to solving

$$(\underline{\underline{A}} + \underline{\underline{E}})\,\underline{\hat{x}} = \underline{b} + \underline{f} \quad \text{exactly}$$

with $\frac{\|\underline{\underline{E}}\|}{\|\underline{\underline{A}}\|}, \frac{\|f\|}{\|b\|} = O(\text{machine precision})$

one can easily show if either errors are there

$$\frac{\|x-\hat{x}\|}{\|x\|} \leq \operatorname{cond}(A) \cdot \frac{\|E\|}{\|A\|} \quad \text{or} \quad \frac{\|x-\hat{x}\|}{\|x\|} \leq \operatorname{cond}(A)\frac{\|f\|}{\|b\|}$$

Some properties of the condition number

- $\operatorname{cond}(A) \geq 1 \qquad (\|AB\| \leq \|A\| \cdot \|B\|)$
- Scaling does not matter: $\operatorname{cond}(\alpha A) = \operatorname{cond}(A)$ while $\det(\alpha A) = \alpha^n \det(A)$
- depends on the norm used, but usually one gets the same order of magnitude
- $\operatorname{cond}_2(A) = |\lambda|_{max} / |\lambda|_{min}$
- $\operatorname{cond}(A^{-1}) = \operatorname{cond}(A)$
- eigenvalue calculations: error also governed by $\operatorname{cond}(A)$

with some more work for both errors:

$$\frac{\|x-\hat{x}\|}{\|x\|} \leq \frac{\operatorname{cond}(A)}{1 - \|A^{-1}\|\,\|E\|} \cdot \left(\frac{\|E\|}{\|A\|} + \frac{\|f\|}{\|b\|}\right)$$

LU decomposition:

Suppose we can decompose A into LU

$\underline{\underline{A}} = \underline{\underline{L}} \cdot \underline{\underline{U}}$

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 & 0 \\ l_{31} & \cdots & 1 & & \vdots \\ & & & 1 & \\ l_{n1} & & & l_{nn-1} & 1 \end{pmatrix} \qquad U = \begin{pmatrix} u_{11} & u_{12} & \cdots & & \\ 0 & u_{22} & & & \\ 0 & 0 & \ddots & & \\ 0 & 0 & & \ddots & \\ 0 & 0 & & 0 & u_{nn} \end{pmatrix}$$

$\underline{\underline{L}}$ is lower triangular with 1 on the diagonal

$\underline{\underline{U}}$ is upper triangular

Now the solution is easy

$$\underline{\underline{L}}\,\underline{\underline{U}} \cdot \underline{x} = \underline{b} \quad = \underline{\underline{L}}\,\underline{y} \qquad \underline{y} = \underline{\underline{U}}\,\underline{x}$$

first solve $\underline{\underline{L}}\,\underline{y} = \underline{b}$ $\qquad y_1 = b_1$

$$l_{21} y_1 + y_2 = b_2 \qquad y_1 \text{ we know already}$$

$$y_i = b_i - \sum_{j=1}^{i-1} l_{ij}\, y_j \qquad \text{Forward substitution}$$

$\underline{\underline{U}}\,\underline{x} = \underline{y}$ $\qquad$ now start with the last element

$$u_{nn} \cdot x_n = y_n$$

$$u_{n-1,n-1}\, x_{n-1} + u_{n-1,n}\, x_n = y_{n-1} \qquad x_n \text{ is known.}$$

$$x_i = \frac{1}{u_{ii}} \left(y_i - \sum_{j=i+1}^{n} u_{ij}\, x_j \right) \qquad \text{Backward substitution}$$

Doolittle and Crout formulas

1. $u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik}\, u_{kj} \qquad i = 1 \ldots j-1$

2. $\gamma_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik}\, u_{kj} \qquad i = j \ldots n$

3. $u_{jj} = \gamma_{jj}$

4. $l_{ij} = \dfrac{\gamma_{ij}}{\gamma_{jj}} \qquad i = j+1 \ldots n$

Column-wise, left looking
calculate in place
(right-looking version also exists)

Notation $\underline{\underline{A}} = (a^1, a^2, a^3 \sim a^n) = \begin{pmatrix} a(1) \\ \vdots \\ a(n) \end{pmatrix}$ ← rows

↑ columns

$$\left(\underline{\underline{A}} \right) = \begin{pmatrix} 1 & & \\ l_{21} & 1 & \\ l_{31} & & \ddots \end{pmatrix} \begin{pmatrix} u_{11} & \cdots & u_{1n} \\ & \ddots & \vdots \\ & & u_{nn} \end{pmatrix}$$

$a(1) = u(1)$

$a(2) = u(1) + l_{21}\, u(2)$

$\vdots$

$a(n) = l_{nk}\, u(k) + u(n)$

$a^1 = u_{11} \cdot e^1$

$a^2 = u_{12} e^1 + u_{22} e^2$

$\vdots$

$a^n = \sum u_{kn} e^n$

solution: $u(1) = a(1)$

$$\ell^1 = \frac{1}{u_{11}} a^1$$

$$u(2) = a(2) - \ell_{21} \cdot u(1)$$

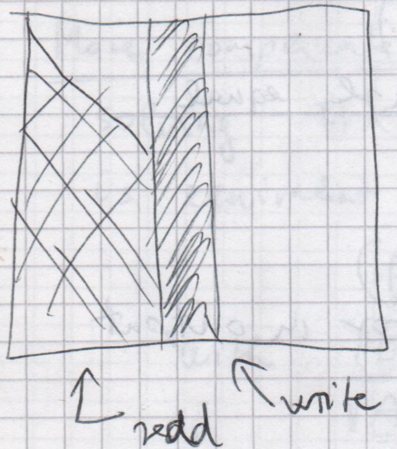
$$\ell^2 = (a^2 - u_{12}\, e^1)\frac{1}{u_{22}}$$

$\vdots$

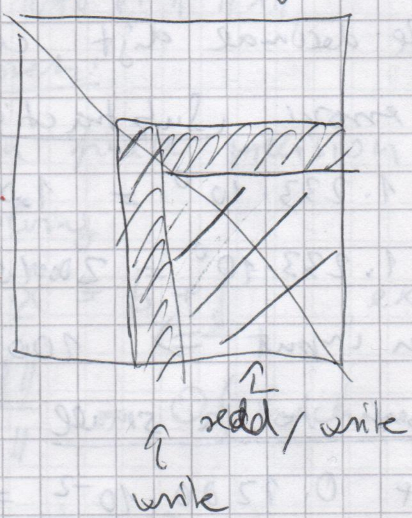
and so on.

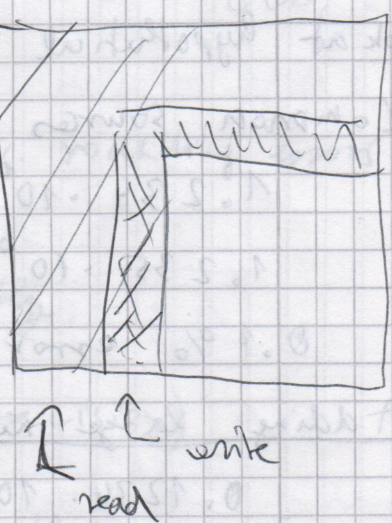
Many versions

left looking

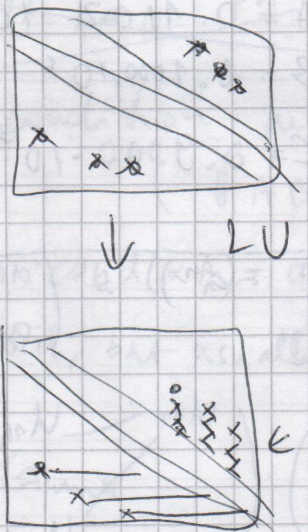


right looking





LU for sparse matrices

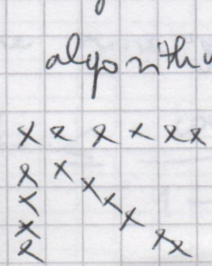
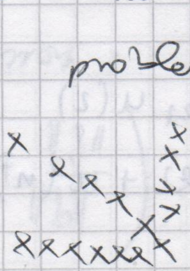
sparse matrix = 

many zeros

fill in no longer zero

swap rows and columns to minimize fill in

– many algorithms, "recipes" no clear best algorithm, depends on problem

e.g.  $\Rightarrow$ reorder  no fill in

Cost $O(N^3)$

$$\det \underline{\underline{A}} = \cancel{\det} = \det \underline{\underline{L}}\,\underline{\underline{U}} = \det \underline{\underline{L}} \cdot \det \underline{\underline{U}} = \det \underline{\underline{U}}$$

$$= \prod_{i=1}^{n} u_{ii}$$ We also get the determinant!

Exercise 1:

$$A = \begin{matrix} 1 & 5348621 & 1608 \\ 5348687 & 43709 & 2000 \\ 6114 & 2 & 910132 \end{matrix}$$

$x = ?$ $\|A \cdot x - b\| = ?$

What happens if you switch some rows?

$$b = \begin{matrix} 1 & 2 & 7 & 4 & 5 \\ 6 & 7 & 8 & 9 & 0 \\ 8 & 7 & 6 & 4 & 2 \end{matrix}$$

Pivoting

suppose $a_{11} = 0$ $a_{11} = \ell_{11} \cdot u_{11} = 0 \Rightarrow \ell_{11} = 0$ or $u_{11} = 0$

$\Rightarrow \det L \cdot \det U = 0 \Rightarrow \det A = 0$?

In this case decomposition fails

we need to be able to swap rows $\Rightarrow A = P \cdot L \cdot U$

permutation matrix

each column and row has exactly one 1 entry, others are 0

$P \cdot M$ rows of M swapped

permutation matrix

$M \cdot P$ columns of M swapped

insert in the LU procedure above

2.5 swap rows $(j \ldots n)$

such that $|\gamma_{jj}|$ is maximal: "partial pivoting"

if all γ_{ij} $i = j \ldots n$ is zero, matrix is singular (i.e. $\det A = 0$)

$A \cdot x = b$ unsolvable

Theorem: if LU decomposition exists, it is unique

it exists if $\det A_{1\dots j,\,1\dots j} \neq 0$ for all j

Complex matrices: LU works with complex arithmetic, for pivoting take abs. value

$$(\underline{\underline{A}} + i\underline{\underline{C}})(\underline{x} + i\underline{y}) = \underline{b} + i\underline{d}$$

$$\begin{pmatrix} \underline{\underline{A}} & -\underline{\underline{C}} \\ \underline{\underline{C}} & \underline{\underline{A}} \end{pmatrix} \begin{pmatrix} \underline{x} \\ \underline{y} \end{pmatrix} = \begin{pmatrix} \underline{b} \\ \underline{d} \end{pmatrix}$$ real matrix of double size

$\underline{\underline{H}} = \underline{\underline{A}} + i\underline{\underline{C}}$ if $\underline{\underline{H}}$ is hermitic, $M = \begin{pmatrix} \underline{\underline{A}} & -C \\ \underline{\underline{C}} & \underline{\underline{A}} \end{pmatrix}$ is symmetric

$$\underline{\underline{A}}^T - i\underline{\underline{C}}^T = \underline{\underline{A}} + i\underline{\underline{C}} \Rightarrow \underline{\underline{A}} = \underline{\underline{A}}^T \quad \underline{\underline{C}}^T = -\underline{\underline{C}}^T$$

Special cases: $\boxed{\text{if } \underline{\underline{A}} = \underline{\underline{A}}^+}$

$LU = U^+L^+$ if all $u_{ii} = 1 \Rightarrow U = L^+$

generally this isn't true

$D = \mathrm{diag}(u_{11}, u_{22}, \dots u_{nn})$

$U = D \cdot \tilde{U}$ $\quad \tilde{u}_{ij} = \dfrac{u_{ij}}{u_{ii}}$ for $j > i$

$\tilde{u}_{ii} = 1$

$A = LD\tilde{U}$

$\tilde{U}^+ D^+ L^+ = A = LU$

~~unicity~~ unicity of $LU \Rightarrow \tilde{U}^+ = L \qquad A = LDL^+$

$$LD^+L^+ = A = A^+ = L^+DL = LD\tilde{U} = LDL^+$$

$\Rightarrow D = D^+ \qquad u_{ii} \in \mathbb{R}$

$\underline{\underline{A}} = \underline{\underline{A}}^+$ and positiv definit

positiv definit $\Longleftrightarrow$ $\underline{v}^+ \underline{\underline{A}}\, \underline{v} > 0$ for all $\underline{v} \neq 0$

$A = L D L^+$ D has real elements u_{ii}

$v^+ A v = v^+ L D L^+ v = w^+ D w > 0$ $\underline{w} = \underline{\underline{L}}^+ \underline{v}$

$\det L^+ = 1 \Rightarrow L^{+^{-1}}$ exists

$\Rightarrow \forall w \quad (\underline{\underline{L}}^+)^{-1} \underline{w} = \underline{v} \neq 0$ exists

$w^+ D w > 0$ for all $w \neq 0$

$\Rightarrow$ D is positive definit : $u_{ii} > 0$ for all i

$D = P \cdot P$ with $P = \mathrm{diag}\left(\sqrt{u_{11}}, \dots, \sqrt{u_{nn}}\right)$

$\underline{\underline{A}} = L P \cdot P \cdot L^+ = L \cdot P \, (L \cdot P)^+ = T \cdot T^+$

with $T = L \cdot P$

This is called the Cholesky decomposition

Tridiagonal matrices LU - no pivot

$$\begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & a_3 & \ddots & \ddots & \\ & & \ddots & \ddots & c_{n-1} \\ & & & a_n & b_n \end{pmatrix} =$$

$u_1 = b_1$

$e_j = a_j / u_{j-1}$ $u_j = b_j - e_j c_{j-1}$

$$\begin{pmatrix} 1 & & & \\ e_2 & 1 & & \\ & \ddots & 1 & \\ & & \ddots & 1 \\ & & & e_n \; 1 \end{pmatrix} \begin{pmatrix} u_1 & c_1 & & \\ & \ddots & \ddots & \\ & & & c_{n-1} \\ & & & u_n \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} r_1 \\ \vdots \\ r_n \end{pmatrix}$$

Forward subs

$y_1 = r_1$

$y_j = r_j - e_j y_{j-1}$

Backward subs

$x_n = y_n / u_n$ $x_j = \left(y_j - c_j x_{j+1}\right) u_j$

Hilbert matrix $a_{ij} = \dfrac{1}{i+j-1}$ cond number $\sim \dfrac{(1+\sqrt{2})^{4n}}{\sqrt{n}}$