4, Gauss Elimination

Def. (triang. Matrix) $A_{ij} = 0$ for $i > j$ ... „upper" triangular"
for $i < j$ ... „lower triangular"

$A_{ii} = 1 \ \forall i$ ... „normalized"

Goal: solve $A\vec{x} = \vec{b}$

Algorithm (Gauss elim. without pivoting)

Input: A, Output: L, U st. $A = L \cdot U$

for $k = 1, \dots n-1$
  for $i = k+1, \dots n$
    $L_{ik} = \frac{A_{ik}}{A_{kk}}$
    for $j = k+1, \dots n$
      $U[i,j] \mathrel{+}= -L_{ik} \cdot A[k,j]$

Remark (Gauss produces LU-fact.)

$$L^{(k)} := \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & l_{k+1,k} & \ddots & \\ & & \vdots & & \\ & & l_{n,k} & & 1 \end{pmatrix} \Rightarrow \left(L^{(k)}\right)^{-1} = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -l_{k+1,k} & \ddots & \\ & & \vdots & & \\ & & -l_{n,k} & & 1 \end{pmatrix}$$

$l_{i,k} := \frac{A_{ik}}{A_{kk}}$ ... factors produced during Gauss elim.

$\Rightarrow$ Gauss Elim is actually: $L^{-1} \cdot A = U$ (ie. finding L^{-1})
or for $A\vec{x} = \vec{b}$: $\underbrace{L^{-1} \cdot A}_{=U}\vec{x} = L^{-1}\vec{b} = U\vec{x}$

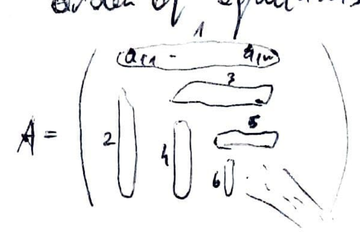
$\Rightarrow$ $A = L \cdot U$

LU-factorization
1. Find L, U st. $LU = A$
2. solve $L\vec{y} = \vec{b}$ (ie finding L^{-1}) by forw. subst.
3. solve $U\vec{x} = \vec{y}$ by backw. subst.

Algorithm (Crout)

$$\begin{pmatrix} 1 & & \\ l_{21} & \ddots & \\ \vdots & & \\ l_{n1} & \dots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & \dots & u_{1n} \\ & \ddots & \vdots \\ 0 & & u_{nn} \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix},$$

order of equations:

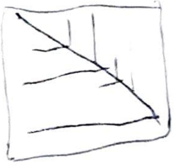


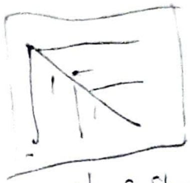
cost: $\mathcal{O}(n^3)$

Remark: different LU-implementations differ in order of access of matrix entries
(they require 3 loops $\Rightarrow$ 3 possible algorithms)

Banded & Skyline matrices

$O(npq)$
$\quad ||$
band width





Proof by induction

Cholesky fact.

if A is spd $\Leftrightarrow$ $\vec{x}^T A \vec{x} > 0 \; \forall \vec{x} \neq 0$, we can
find C s.t. $A = C \cdot C^T$ using an adapted Crouts algor.

Theorem (Existence of LU decomp)

$(a_{11} \overset{!}{\neq} 0)$

$A = \begin{pmatrix} 0 & 1 \\ 3 & 2 \end{pmatrix}$ has no LU decomp.

Proof: $A \overset{!}{=} LU = \begin{pmatrix} 1 & 0 \\ l & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{pmatrix} \Rightarrow u_{11} \overset{!}{=} 0 \Rightarrow \det(U) = 0$
but $\det(A) \neq 0$ ↯

■

Theorem (Permutation)

$\exists P$ s.t. $PA = LU$

e.g.

$$P = \begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 0 & 0 & 1 & & \\ & & 0 & 1 & 0 & & \\ & & 1 & 0 & 0 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} \Rightarrow$$

$P \cdot A$ swaps 3^{rd} and 5^{th} rows ~~column~~
$A \cdot P$ swaps column

Definition (Permutation)

$\pi : X \to Y$ is a permutation if
π .. bijective, associative, invertible, inverse element ..

Matrix $P_\pi := (e_{\pi(1)}, \dots e_{\pi(n)}) \overset{(?)}{\Rightarrow} P_\pi^{-1} = P_\pi^T$ (do proof)

Algorithm (Gauss Elim. with pivoting)

in each elim. step on A, the ~~[illegible]~~ rows are ~~[illegible]~~ interchanged, s.t. the largest entry of ~~[illegible]~~ the column* of A is in the diagonal

* that is manipulated in this very step

this ~~also~~ ~~works~~ helps for $A = \begin{pmatrix} \varepsilon & - & - \\ - & - & \\ & & - \end{pmatrix}$, with $\varepsilon \ll$ all other entries

Def (matrix norm)

$$\|A\| := \max_{\vec{x}} \frac{\|A\vec{x}\|}{\|\vec{x}\|}$$

$$\left(\text{if } \|\cdot\|_2 \Rightarrow \|A\| = \sqrt{\lambda_{max}(A^T A)} \right.$$

Theorem

$\|AB\| \leq \|A\| \cdot \|B\|$ (No proof)

Example (LSE)

$A\vec{x} = \vec{b}$ perturb „input" $\vec{b}$ by $\Delta\vec{b}$

$A \cdot (\vec{x} + \Delta\vec{x}) = \vec{b} + \Delta\vec{b}$ $\Rightarrow$ is $\Delta\vec{x}$ large? (perturb. of „output")

relative error: $$\frac{\|\Delta x\|}{\|x\|} = \frac{\|A^{-1}\Delta b\|}{\|A^{-1}b\|} \leq \underbrace{\|A\| \|A^{-1}\|}_{=: K_{rel}} \frac{\|\Delta b\|}{\|b\|}$$

abs err: $$\|\Delta x\| = \|A^{-1} b\| \leq \underbrace{\|A^{-1}\|}_{=: K_{Abs}} \|b\|$$

Def (Orthogonal mat.)

$Q \in \mathbb{R}^{n \times n}$ is orthog. iff. $Q^T Q = \mathbb{I} \Leftrightarrow Q^T = Q^{-1}$

Denote $Q \in O_n$

Theorem

- Product of orthog. mat. is orthog.
- Inverse — " —
- Q orthog. $\Rightarrow \|Q\vec{x}\|_2 = \|\vec{x}\|_2$
  i.e. $Q \in O_n$

No proof.

Def.

$R \in \mathbb{R}^{m \times n}$ is a generalized upper triangular matr. if $R = \begin{pmatrix} \tilde{R} \\ 0 \end{pmatrix}$, $\tilde{R} \in \mathbb{R}^{n \times n}$ and $\tilde{R}$ upper triangular.

Theorem (Existence)

$A \in \mathbb{R}^{n \times n}$, invertible $\Rightarrow A = QR$, $Q \in O_n$, R gen. upper triangular

square!

(QR unique up to sign)

Remark Multiplication by Q is num. stable

$$\frac{\|Q(x+\Delta x) - Qx\|_2}{\|Qx\|_2} = \frac{\|Q\Delta x\|}{\|Qx\|} = \underbrace{1}_{=K_{rel}} \cdot \frac{\|\Delta x\|}{\|x\|}$$

QR by Gram Schmidt $A \in \mathbb{R}^{n \times n}$, $A = (\vec{a}_1, \vec{a}_2, \dots \vec{a}_n)$

Define $Q := (\vec{q}_1, \dots \vec{q}_n)$ st.

$\vec{q}_1 = \vec{a}_1$

$\vec{q}_2 = \vec{a}_2 + \alpha_2 \cdot \vec{q}_1$ and $\vec{q}_2 \perp \vec{q}_1$

$\vdots$

$\Rightarrow$ $Q = A \cdot \tilde{R}$, where $\tilde{R}$ is dependent on α_i and happens to be upper triangular

for $\tilde{R}$ invertible $\to$ $A = Q\tilde{R}^{-1} =: QR$

Definition (Housholderreflection) $\vec{v} \in \mathbb{R}^n$, $\|\vec{v}\|_2 = 1$, $H \in \mathbb{R}^{n \times n}$ st.

$H = \mathbb{I} - 2\vec{v}\cdot\vec{v}^T$ .. Hh. refl.

Lemma $\circ$ H is sym ($H^T = H$)
$\circ$ $H^2 = \mathbb{I}$
$\Big\} \Rightarrow H^T = H^{-1}$ .. orthogonal $\Leftrightarrow H \in O_n$

$\to$ How to find $\vec{v}$?

Lemma $\vec{x} \in \mathbb{R}^n$, $\vec{e}^1 = (1, \dots)^T$, $\vec{v} = \frac{x + \lambda \vec{e}^1}{\|x + \lambda \vec{e}^1\|_2}$ with $\lambda = \text{sign}(x_1) \cdot \|\vec{x}\|_2$

$\Longrightarrow$ $H\vec{x} = (I - 2\vec{v}\vec{v}^T)\vec{x} = -\lambda \vec{e}^1$ (H not unique)

Proof: $H\vec{x} = (I - 2\vec{v}\vec{v}^T)\vec{x} = \vec{x} - 2 \frac{1}{2\|x\|^2 + 2|x_1|\|x\|} (\vec{x} + \lambda\vec{e}^1) \cdot (\vec{x} + \lambda \vec{e}^1)^T \cdot \vec{x}$

$= - " - (\vec{x} + \lambda\vec{e}^1) \cdot \underbrace{(\vec{x} + \text{sign}(x_1) \cdot \|\vec{x}\| \vec{e}^1)^T \cdot \vec{x}}_{= \|x\|^2 + |x_1|\|x\|} = -\lambda e^1$ ∎

Algorithm (Householder refl.) input A, output $Q \cdot R = A$

select Q_1 as a Hh. refl. st. $(Q_1 \cdot A)_{i1} \parallel \vec{e}^1$ (remove entries from 1^{st} column)

Repeat: $Q = Q_1 \cdot Q_2 \cdots Q_n \Rightarrow A = Q \cdot R$

Cost: $\mathcal{O}(\frac{4}{3} n^3)$ .. QR $\leftarrow$ numerically stable also for ill-cond. matrices

$\mathcal{O}(\frac{2}{3} n^3)$ .. LU

$\mathcal{O}(\frac{1}{3} n^3)$ .. Cholesky !

<u>Solve System</u> $A\vec{x}=\vec{b}$ $\quad A = QR \Rightarrow \quad QR\vec{x}=\vec{b} \Rightarrow \quad R\vec{x} = Q^T\vec{b}$

upper triangl.

<u>Housholder QR with pivoting</u>

in each Housholder step on A, the ~~rows~~ colums of A are interchanged, st. the column with largest L2-norm is where the zeros are being produced (ie. this column is where the Hh. refl. produces a multiple of $\vec{e}^i$)

<u>QR with Givens rot.</u> : more costly than Hh. refl. (still $O(n^3)$) change less entries of A $\Rightarrow$ parallelizable

$c := \cos(\theta)$, $s := \sin(\theta)$

$$G(i,j,\theta) := \begin{array}{cc} \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & c & s & \\ & & -s & c & \\ & & & \ddots & \\ & & & & 1 \end{pmatrix} & \begin{matrix} \\ \\ i \\ j \\ \\ \\ \end{matrix} \\ \begin{matrix} \quad\quad i & j \quad\quad \end{matrix} & \end{array}$$

.. manipulates only i^{th} & j^{th} colum/row

$G \in O_n$

<u>Lemma</u> $\exists\, G(i,i',\theta)$ st. $(G^TA)_{ij} = 0$

<u>Remark</u>: $O(n^2)$ for A - upper Hessenberg, ie. $A_{ij}=0$ for $i>j+1$

$A =$ 

1 subdiagonal non-zero