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NLA I: Linear equation solving

Reference:

[D] J. Demmel, Applied NLA, 1997.

Here we discuss the linear equation

$$Ax = b$$

In particular, algorithms for solving it, and their complexity and numerical stability. We focus on direct methods: methods that are exact in the absence of round off. Later in the course we will study iterative methods, that do not produce exact answers in a finite number of steps, but rather decrease the error of some approximation at each step.

1. Gaussian elimination

Let $F = \mathbb{R}$ or $\mathbb{C}$ and

real numbers   complex numbers

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \\ \vdots & & \\ a_{m,1} & \cdots & a_{m,n} \end{pmatrix} \in F^{m \times n}$$

The matrix A defines a linear map

$$A: F^n \to F^m$$

through linear combinations of its columns:

for $x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in F^n$ an n-column vector

$$A \cdot x = x_1 \, col_1(A) + \cdots + x_n \, col_n(A)$$

Ex: $\begin{pmatrix} 2 & 3 \\ 2 & 4 \\ 3 & 7 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = x_1 \begin{pmatrix} 2 \\ 2 \\ 3 \end{pmatrix} + x_2 \begin{pmatrix} 3 \\ 4 \\ 7 \end{pmatrix}$

The image of this map is the column space, that is, the span of the columns of A:

$$Im(A) = Span(col_1(A), \ldots, col_n(A)) .$$

It is a linear subspace of F^m.

The kernel of this linear map is the set of vectors that vanish through this map:

$$Ker(A) = \{ x \in F^n \mid Ax = \underline{0} \}$$

It is a linear subspace of F^n

A fundamental theorem of linear algebra states

$$\dim(\mathrm{Im}(A)) + \dim(\mathrm{Ker}(A)) = n \qquad (*)$$

In other terms

$$\#\text{independent colums} + \dim(\mathrm{Ker}(A)) = \#\text{columns}$$

The first and most fundamental problem of LA is to solve

$$A \cdot x = b \qquad (**)$$

We are given an $n \times n$-matrix A and an n-vector b, and we want to find a solution x, also an n-vector.

The equation $(**)$ being solvable is equivalent to the fact that b belongs to the image of A:

$$b \in \mathrm{Im}(A)$$

If it exists, such a solution is unique if and only if the kernel of A is trivial

$$\mathrm{Ker}(A) = \{0\}$$

By $(*)$, both conditions are equivalent.

$A \in F^{n \times n}$ is <u>non-singular</u> if $Ker(A) = \{0\}$ or equivalently, if $Im(A) = F^n$.

If this is the case, A admits an inverse matrix A^{-1}:

$$A \cdot A^{-1} = A^{-1} \cdot A = \mathbb{1}_n = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}$$

identity matrix

We will study the pb: given $A \in F^{n \times n}$ nonsingular and $b \in F^n$, find $x \in F^n$ such that (s.t.):

$$A \cdot x = b$$

Gaussian elimination (GE) is the basic algorithm for this task.

<u>Ex:</u>

$$\begin{cases} 1 \cdot x_1 + 2 \cdot x_2 = b_1 \\ 3 \cdot x_1 + 4 x_2 = b_2 \end{cases}$$

Substract $3 \times$ first equation from the second equation to eliminate x_1:

$$\begin{cases} 1 \cdot x_1 + 2 x_2 = b_1 \\ \quad - 2 x_2 = b_2 - 3 b_1 \end{cases}$$

then solve by "backward substitution" (compute x_2 and then x_1)

In matrix notation:

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \iff \underbrace{\overset{L^{-1}}{\begin{pmatrix} 1 & 0 \\ -3 & 1 \end{pmatrix}}\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}}_{\begin{pmatrix} 1 & 2 \\ 0 & -2 \end{pmatrix} \; U}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -3 & 1 \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

pivot

Equivalently

$$\underset{A}{\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \underset{L}{\begin{pmatrix} 1 & 0 \\ 3 & 1 \end{pmatrix}} \cdot \underset{U}{\begin{pmatrix} 1 & 2 \\ 0 & -2 \end{pmatrix}}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

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

This decomposition is <u>not always</u> possible, since some <u>pivot</u> may vanish:

$$\begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix} \neq L \cdot U \qquad \forall L, U \text{ nonsingular lower \& upper triangular}$$

<u>Solution</u>: swap rows 1 & 2, which corresponds to multiplication by a <u>permutation matrix</u> P (an identity matrix with permuted rows)

$P \cdot A =$ A with rows permuted following P

$A \cdot P =$ ——— columns ———

Other properties:

- $P^{-1} = P^T$ (transposed)
- $\det(P) = \pm 1$
- P_1, P_2 permutation matrices $\Rightarrow P_1 \cdot P_2$ permutation matrix

<u>Gauss elimination</u> can be interpreted as the factorization

$$A = \underbrace{P}_{\text{permutation}} \cdot \underbrace{L}_{\text{unit lower triangular (1's in the diagonal)}} \cdot \underbrace{U}_{\text{upper triangular}}$$

With this factorization, can solve $Ax = b$ by

1) $LUx = P^{-1}b$ permute the entries of b
2) $Ux = L^{-1}(P^{-1}b)$ forward substitution
3) $x = U^{-1}(L^{-1}P^{-1}b)$ backward substitution

In the example, $P = \mathbb{1}_2$ and so the step (1) is trivial (the entries of $b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$ are not modified).

Recall that

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

Step 2: Set $y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = Ux = \begin{pmatrix} 1 & 2 \\ 0 & -2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

Then $Ly = b \iff \begin{cases} y_1 = b_1 \\ 3y_1 + y_2 = b_2 \end{cases}$

$\iff y_1 = b_1$ and $y_2 = b_2 - 3y_1 = -3b_1 + b_2$

Step 3: $Ux = y \iff \begin{cases} x_1 + 2x_2 = y_1 \\ -2x_2 = y_2 \end{cases}$

$\iff x_2 = -\frac{1}{2} y_2 = \frac{3}{2} b_1 - \frac{1}{2} b_2$

$x_1 = y_1 - 2x_2 = -2b_1 + b_2$

Hence
$$\boxed{x = \begin{pmatrix} -2b_1 + b_2 \\ \frac{3}{2} b_1 - \frac{1}{2} b_2 \end{pmatrix}}$$

To construct the LU factorization, we proceed by induction on n.

Set

$$A = (a_{ij})_{1 \le i,j \le n}$$

For $n=1$ we set

$$P = L = (1) \qquad U = A = (a_{11})$$

Suppose $n \geq 2$. Choose k s.t. $a_{k1} \neq 0$

<u>Remark</u>: In Gaussian elimination with partial pivoting (GEPP) we choose k st $|a_{k1}|$ is <u>maximal</u> for $1 \le k \le n$

Swap rows 1 and k premultiplying A by the permutation matrix

$$P_1 = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & & & 0 & & & \\ \vdots & & \ddots & & \vdots & & & \\ 0 & & & & 1 & 0 & & \\ 1 & 0 & \cdots & & 0 & 0 & & \\ 0 & & & & & & 1 & \\ \vdots & & & & & & & \ddots \\ 0 & & & & & & & & 1 \end{pmatrix}$$

Consider the 2×2 blocks

$$P_1^T \cdot A = \begin{pmatrix} \overset{\text{old } a_{k1}}{a_{11}} & \underbrace{A_{12}}_{1 \times (n-1)} \\ \underbrace{A_{21}}_{(n-1) \times 1} & \underbrace{A_{22}}_{(n-1) \times (n-1)} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \underline{0} \\ L_{21} & \mathbb{1}_{n-1} \end{pmatrix} \cdot \begin{pmatrix} \mu_{11} & U_{12} \\ \underline{0} & \tilde{A}_{22} \end{pmatrix}$$

with $\mu_{11} = a_{11} \quad (\neq 0)$

$L_{21} = A_{21}/a_{11}$

$U_{12} = A_{12}$

$\tilde{A}_{22} = A_{22} - L_{21} U_{12} \quad (n-1)\times(n-1)$ nonsingular

"Schur complement"

<u>Remark</u>: in GEPP, the choice of k implies that all entries in L_{21} have <u>absolute value ≤ 1</u>.

Applying the case $n-1$:

$$\tilde{P}^T \cdot \tilde{A}_{22} = \tilde{L} \cdot \tilde{U}$$

$(n-1)\times(n-1)$ permutation $\qquad$ $(n-1)\times(n-1)$ unit lower & upper triangular

Then

$$P_1^T \cdot A = \begin{pmatrix} 1 & \underline{0} \\ L_{21} & \mathbb{1}_{n-1} \end{pmatrix} \cdot \begin{pmatrix} \mu_{11} & U_{12} \\ \underline{0} & \tilde{P}\tilde{L}\tilde{U} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \underline{0} \\ \underline{0} & \tilde{P} \end{pmatrix} \cdot \begin{pmatrix} 1 & \underline{0} \\ \tilde{P}L_{21} & \tilde{L} \end{pmatrix} \cdot \begin{pmatrix} \mu_{11} & U_{12} \\ 0 & \tilde{U} \end{pmatrix}$$

Hence

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

with

$$P = P_1 \cdot \begin{pmatrix} 1 & \underline{0} \\ \underline{0} & \tilde{P} \end{pmatrix} \quad L = \begin{pmatrix} 1 & \underline{0} \\ \tilde{P} L_2 & \tilde{L} \end{pmatrix} \quad U = \begin{pmatrix} u_{11} & U_{12} \\ \underline{0} & \tilde{U} \end{pmatrix}$$

In GEPP

$$L = (l_{ij})_{ij}$$

with $|l_{ij}| \leq 1 \quad \forall i, j$

Gaussian elimination with complete pivoting (GECP) reorders all rows ~~and~~ and columns in such a way that $|a_{kk}|$ is maximal in the whole matrix.

It can be more numerically stable than GEPP but it is much more expensive in terms of speed. It gives a factorization

$$A = P_1 \cdot L \cdot U \cdot P_2$$

permutations

$\boxed{\text{GEPP}}$

Pseudocode notation

for $i=1$ to $n-1$

- <u>swap</u> row k and i of A and L for k such that

$$|a_{ki}| = \max_{i \le p \le n} |a_{pi}|$$

- compute column i of L

for $j=i+1$ to n

a_{ji} $\quad l_{ji} \leftarrow a_{ji}/a_{ii}$

end for

- compute row i of U

for $j=1$ to n

a_{ij} $\quad u_{ij} \leftarrow a_{ij}$

end for

- update A_{22}

for $j=i+1$ to n and k $\cancel{f}$ $i+1$ to n

$u_{jk} \leftarrow a_{jk} - l_{ji} u_{ik}$

$\quad a_{jk} \qquad\qquad a_{ji}\, a_{ik}$

end for

end for

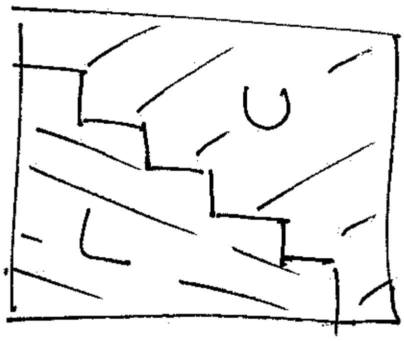
<u>Remark</u>: • the column i of A is used only to compute

________________ L

• the row i of A is used only to compute

________________ U

Need no extra space to store L and U:



~~Ex~~ Using the pseudocode, we can compute the <u>complexity</u> (= # flops) of this algorithm

Recall from <u>calculus</u>: for $k \geq 1$

$$\sum_{i=1}^{n} i^k = \frac{n^{k+1}}{k+1} + \mathcal{O}(n^k)$$

big "Oh" notation

$$C_{GEPP}(n) = \sum_{i=1}^{n-1}\left(\sum_{j=i+1}^{n} 1 + \sum_{j=i+1}^{n}\sum_{k=i+1}^{n} 2\right)$$

complexity of GEPP on $n \times n$ matrices

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

Forward and backward substitution have each a complexity $n^2 + \mathcal{O}(n)$

Hence GEPP solves $Ax = b$ with

$\frac{2}{3}n^3 + \mathcal{O}(n^2)$ flops