Honors Numerical Analysis

Before discussing pivoted LU, there is one special case where it can be shown that pivoting is not necessary: $\vec{x}^T A \vec{x} > 0$ i.e. A is symmetric positive definite (SPD).

Note The fact that pivoting is not required is one of the earliest results in numerical analysis.

Cholesky Factorization

If A is SPD, then we can write it as

$$A = U^T U \quad \text{since then}$$

$$\begin{aligned} A^T &= (U^T U)^T \\ &= U^T (U^T)^T \\ &= U^T U. \end{aligned}$$

The algorithm is straightforward, set

$$U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ & \bigcirc & \ddots & \\ & & & u_{nn} \end{pmatrix} \qquad u_{jj} \neq 1 \quad \text{(not necessarily.)}$$

Then $$U^T U = \begin{pmatrix} u_{11} & & & 0 \\ u_{12} & u_{22} & & \\ \vdots & & \ddots & \\ u_{1n} & & & u_{nn} \end{pmatrix} \begin{pmatrix} u_{11} & \cdots & & u_{1n} \\ & u_{22} & & \\ & & \ddots & \\ 0 & & & u_{nn} \end{pmatrix}$$

$$= \begin{pmatrix} u_{11}^2 & u_{11}u_{12} & u_{11}u_{13} & \cdots \\ u_{12}u_{11} & u_{12}^2+u_{22}^2 & & \\ u_{13}u_{11} & & \ddots & \\ \vdots & & & \end{pmatrix}$$

$\Rightarrow \quad u_{11}^2 = a_{11} \quad \Rightarrow \quad u_{11} = \sqrt{a_{11}}$

then $\quad u_{12} = a_{12}/u_{11}$

$\vdots$

And so on... The cost is $O(n^3/3)$.

Row Pivoting

When pivoting is necessary when doing an LU decomposition, we effectively write

$$L_m P_{m-1} \cdots L_3 P_2 L_2 P_1 L_1 A = U$$

Each L_j is lower triangular and each P_j is a permutation matrix. Ex:
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \vec{a}_1^T \\ \vec{a}_2^T \\ \vec{a}_3^T \\ \vec{a}_4^T \end{pmatrix} = \begin{pmatrix} \vec{a}_1^T \\ \vec{a}_2^T \\ \vec{a}_4^T \\ \vec{a}_3^T \end{pmatrix}$$ ← interchanged

The question is: How do we obtain an equivalent form of the factorization:

$$\underbrace{PA}_{\substack{\text{a single permutation matrix multiply,}\\ \text{possibly re-ordering all rows.}}} = \overset{\text{lower triangular}}{L}\,\underset{\text{upper triangular}}{U}$$

<u>Note</u> Since P_j involves a <u>single</u> row interchange,

$P_j^{-1} = P_j = P_j^T$.

<u>Example</u> Let $L_2 P_1 L_1 A = U$

then set $L_1' = P_1 L_1 P_1 \implies L_1 = P_1 L_1' P_1$

$L_2' = L_2 \implies L_2 = L_2'$

$$\implies L_2' P_1 (P_1 L_1' P_1) A = U$$

$$L_2' \cancel{P_1 P_1} L_1' P_1 A = U$$

$$L_2' L_1' P_1 A = U$$

$$P_1 A = (L_2' L_1')^{-1} U$$

It can be shown that L_1', L_2' are lower triangular, and therefore in the general case all permutation matrices can be "moved" to the right by the above argument (details omitted).

Conditioning, Backward Stability

relative

Recall from before we computed the <u>condition number</u> of solving $A\vec{x}=\vec{b}$:

$$K(A) = \|A\| \, \|A^{-1}\|$$

$\uparrow$ also called "the condition number of A".

(*) <u>Thm</u> (perturbations of $A, \vec{x}$)

If $A(\vec{x}+\delta\vec{x}) = (\vec{b}+\delta\vec{b})$ then

$$\frac{\|\delta\vec{x}\|}{\|\vec{x}\|} \leq K(A)\frac{\|\delta\vec{b}\|}{\|\vec{b}\|}$$

If $(A+\delta A)(\vec{x}+\delta\vec{x}) = \vec{b}$ then

$$\frac{\|\delta\vec{x}\|}{\|\vec{x}\|} \leq K(A)\frac{\|\delta A\|}{\|A\|} \quad \text{as } \|\delta A\| \to 0.$$

Next, suppose that $\tilde{x}$ is the computed solution to the exact linear system $A\vec{x}=\vec{b}$. $\tilde{x}-\vec{x}$ is unknown since we don't know $\vec{x}$.

Define the residual as:

$$\vec{r} = \vec{b} - A\tilde{x}$$

$\uparrow$ computed solution.

Now note that $\tilde{x}$ solves the linear system

$A\tilde{x} = \vec{b} - \vec{r}$, a perturbed linear system.

<u>Backward error</u> $= \|\vec{r}\|$

= the perturbation from the <u>original</u> problem to the one that is solved exactly.

<u>But</u> small $\|\vec{r}\|$ does <u>not</u> imply small $\|\tilde{x} - \vec{x}\|$:

Let $\vec{h} = \tilde{x} - \vec{x}$, therefore $A\vec{h} = -\vec{r}$ and by Thm $(*)$ we have that

$$\frac{\|\vec{x} - \tilde{x}\|}{\|\vec{x}\|} \le K(A) \frac{\|\vec{r}\|}{\|\vec{b}\|}$$

which may be <u>much</u> larger than the relative error in $\tilde{x}$

The QR Factorization

For the moment, let $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ and $\text{rank}(A) = n$ (i.e. n linearly independent columns).

For a general $\vec{b} \in \mathbb{R}^{m}$, the system $A\vec{x} = \vec{b}$ has no solution if $m > n$. We can, however, ask for the least-squares solution:

$$\vec{x}^* = \underset{\vec{x}}{\operatorname{argmin}} \| A\vec{x} - \vec{b} \|_2 .$$

Furthermore if we can write $A = QR$ with

$Q \in \mathbb{R}^{m \times n}$ orthogonal, i.e. $Q^T Q = I$

$R \in \mathbb{R}^{n \times n}$ upper triangular, &

then clearly $R\vec{x} = Q^T\vec{b}$ has a solution $\vec{x} = R^{-1} Q^T \vec{b}$.

~~and the system~~ Also, note that

$A\vec{x} = QQ^T\vec{b}$ has a solution since QQ^T is the projection onto the column space of A,

and then $QR\vec{x} = QQ^T\vec{b}$

$\Rightarrow \vec{x} = R^{-1} Q^T Q Q^T \vec{b} = R^{-1} Q^T \vec{b}$ is the least squares solution.

(A)

The simple (and naive) way to compute Q is via the Gram-Schmidt process which creates an orthonormal basis for the span of the columns of A, $\vec{a}_1, \ldots, \vec{a}_n \in \mathbb{R}^m$.

$$A = (\vec{a}_1 \ \vec{a}_2 \cdots \vec{a}_n)$$

and let $Q = (\vec{q}_1 \ \vec{q}_2 \cdots q_n)$

If $A = QR$ then

$$\left.\begin{aligned} \vec{a}_1 &= r_{11}\vec{q}_1 \\ \vec{a}_2 &= r_{12}\vec{q}_1 + r_{22}\vec{q}_2 \\ &\vdots \\ \vec{a}_n &= r_{1n}\vec{q}_1 + \ldots + r_{nn}\vec{q}_n \end{aligned}\right\} (*)$$

G-S says: turn $\vec{a}_1, \ldots, \vec{a}_n$ into $\vec{q}_1, \ldots, \vec{q}_n$

The algorithm: On step j, set $\vec{v}_j = \vec{a}_j - \overbrace{(\vec{q}_1, \vec{a}_j)}^{=\text{ inner product } = \vec{q}_1^T\vec{a}_j}\vec{q}_1 - \ldots - (\vec{q}_{j-1}, \vec{a}_j)\vec{q}_{j-1}$

and then $\vec{q}_j = \dfrac{\vec{v}_j}{\|\vec{v}_j\|}$

Comparing with $(*)$ implies that $r_{ij} = (\vec{q}_i, \vec{a}_j)$

and $|r_{jj}| = \left\| \vec{a}_j - \sum_{i=1}^{j-1} r_{ij}\vec{q}_i \right\|_2$

since $r_{jj}\vec{q}_j = \vec{a}_j - r_{1j}\vec{q}_1 - \ldots - r_{j-1,j}\vec{q}_{j-1}$ (and take norms)

Unfortunately this algorithm is num. unstable — a fix next time!