Error Analysis for Gauss Elimination

We now work on estimating errors in our LU decomposition algorithms. To get a sense of the central issues, we start by considering

$$A = \begin{bmatrix} 0.0001 & 1 \\ 1 & 1 \end{bmatrix} \quad \text{in 3 digit floating point.}$$

Now we can compute (I used Mathematica) the eigenvalues of A.

$$1.61806 \quad \text{and} \quad -0.617962$$

So the condition number of A is

$$\chi(A) \approx \frac{1.61806}{-0.617962} = 2.61839$$

This means that A is well-conditioned and we should be able to solve $Ax=b$ accurately.

Let us perform LU factorization <u>without</u> pivoting.

Step 1.

$$l_{21} = a_{21}/a_{11} = fl\left(1/10^{-4}\right) = 10^4$$

$$u_{12} = a_{12} = 1.$$

$$\tilde{a}_{22} = a_{22} - l_{21}u_{12} = fl\left(1 - 10^4\right) = -10^4$$

in 3 digit floating pt.

so

$$L = \begin{bmatrix} 1 & 0 \\ 10^4 & 1 \end{bmatrix} \quad U = \begin{bmatrix} 10^{-4} & 1 \\ 0 & -10^4 \end{bmatrix}$$

and

$$LU = \begin{bmatrix} 10^{-4} & 1 \\ 1 & 0 \end{bmatrix} \text{ but } A = \begin{bmatrix} 10^{-4} & 1 \\ 1 & 1 \end{bmatrix}.$$

This means that anything in the A_{22} spot which rounds to 10^4 when added to 10^4 gives the same LU decomposition! But

$$A = \begin{bmatrix} 10^{-4} & 1 \\ 1 & 1 \end{bmatrix} \quad \text{and (for example)} \quad A' = \begin{bmatrix} 10^{-4} & 1 \\ 1 & -1 \end{bmatrix}$$

yield totally different answers to

$$Ax = b \quad \text{and} \quad A'x = b.$$

We conclude that our solver (which must give the same answer in both cases) has failed.

Example. $Ax = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$. We see

$$\begin{bmatrix} 10^{-4} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

has solution $\begin{bmatrix} 1.0001 \\ 0.9999 \end{bmatrix}$. But applying our LU decomposition, we solve

$$\begin{bmatrix} 1 & 0 \\ 10^{4} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

to get

$$y_1 = fl(1/1) = 1$$

$$y_2 = fl(2 - 10^{4} \cdot 1) = -10^{4}$$

Then we solve

$$\begin{bmatrix} 10^{-4} & 1 \\ 0 & -10^{4} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^{4} \end{bmatrix}$$

to get

$$x_2 = fl\left(\frac{-10^{4}}{-10^{4}}\right) = 1, \quad x_1 = fl\left(\frac{1-1}{10^{-4}}\right) = 0.$$

This answer, $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, is of course <u>completely</u> <u>wrong</u>.

Example 2. We compute the condition numbers of L and U. For L, the eigenvalues are 1 and 1. But for U they are 10^4 and 10^{-4}, so the condition numbers are

$$\chi(L) = 1 \qquad \chi(U) = 10^8$$

This, too, is a <u>bad</u> <u>sign</u>.

By comparison, if we compute this same example with partial pivoting, we get

Step 1. Permute to get

$$\begin{bmatrix} 1 & 1 \\ 10^{-4} & 1 \end{bmatrix} = PA$$

Now

$$l_{21} = a_{21}/a_{11} = fl\left(\frac{10^{-4}}{1}\right) = 10^{-4}.$$

$$u_{12} = a_{12} = 1.$$

$$\tilde{a}_{22} = a_{22} - l_{21}u_{12} = fl\left(1 - 10^{-4}\cdot 1\right) = 1$$

So we get

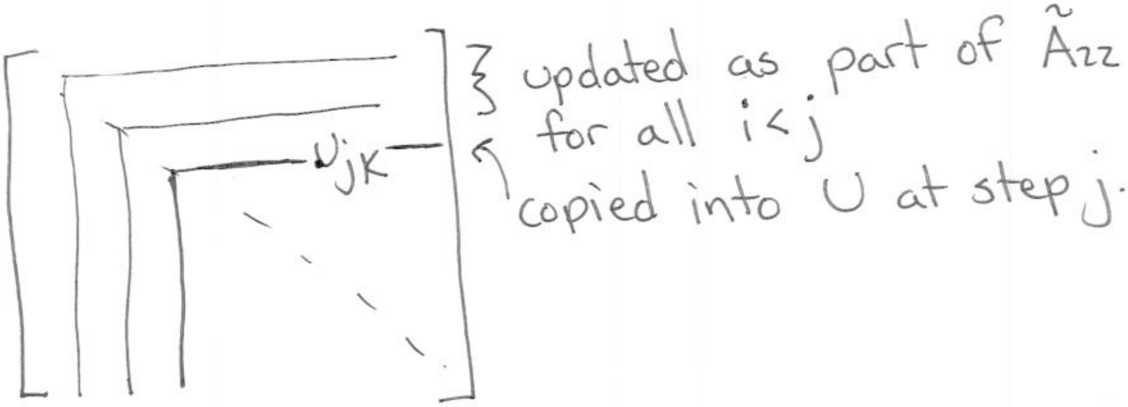
$$L = \begin{bmatrix} 1 & 0 \\ 10^{-4} & 1 \end{bmatrix} \qquad U = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

and

$$LU = \begin{bmatrix} 1 & 1 \\ 10^{-4} & 1+10^{-4} \end{bmatrix} \approx \begin{bmatrix} 1 & 1 \\ 10^{-4} & 1 \end{bmatrix} = PA.$$

Rigorous Error Bounds.

Suppose we have reordered A so that all pivoting is done. We observe that each element in the upper triangular factor is given by

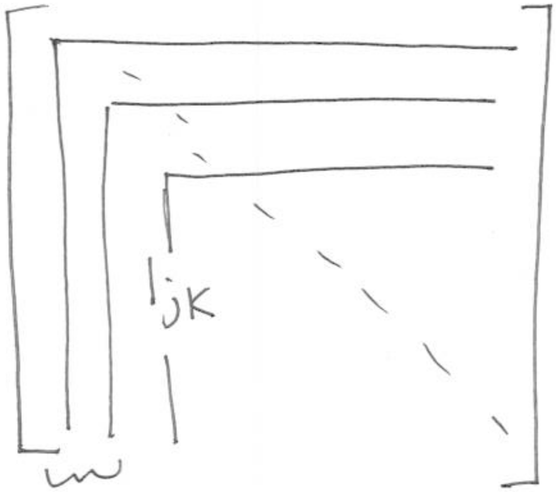


so

$$u_{jk} = a_{jk} - \sum_{i=1}^{j-1} l_{ji} u_{ik}$$

(because the update at step i was
$a_{jk} = a_{jk} - l_{ji} u_{ik}$)

On the other hand, below the diagonal we get



scaled and copied into L at step $i=k$

updated as part of $\tilde{A}_{22}$ for $i<k$

So

$$l_{jk} = \frac{a_{jk} - \sum_{i=1}^{k-1} l_{ji} u_{ik}}{u_{kk}}$$

So

$$u_{jk} = \left(a_{jk} - \sum_{i=1}^{j-1} l_{ji} u_{ik} (1+\delta_i) \right)(1+\delta')$$

where $|\delta_i| \le (j-1)\epsilon$ and $|\delta'| \le \epsilon$. So

$$a_{jk} = \frac{1}{1+\delta'} u_{jk} + \sum_{i=1}^{j-1} l_{ji} u_{ik} (1+\delta_i)$$

If we let $\frac{1}{1+\delta'} = 1+\delta_j$ and use $l_{jj}=1$

we get

$$a_{jk} = (1+\delta_j)\, l_{jj}\, u_{jk} + \sum_{i=1}^{j-1} (1+\delta_i)\, l_{ji}\, u_{ik}$$

$$= \sum_{i=1}^{j} l_{ji}\, u_{ik} + \sum_{i=1}^{j} l_{ji}\, u_{ik}\, \delta_i$$

$$= \sum_{i=1}^{j} l_{ji}\, u_{ik} + E_{jk}.$$

Now we can bound E_{jk}:

$$|E_{jk}| = \left| \sum_{i=1}^{j} l_{ji} \cdot u_{ik} \cdot \delta_i \right|$$

$$\leq \sum_{i=1}^{j} |l_{ji}|\, |u_{ik}| \cdot n\epsilon$$

since each $\delta_i \leq (j-1)\epsilon \leq n\epsilon$. Now recall that $l_{ji} = 0$ for $i > j$ since L is lower triangular. So this is really entry jk of the matrix product $|L|\,|U|$ where $|A|$ = the matrix of entries $|a_{ij}|$.

so

$$|E_{jk}| \le n\epsilon(|L||U|)_{jk}$$

Now we need to do a similar analysis of the error in l_{jk}. to write a formula for a_{jk} where ~~j≤k~~ $j \ge k$. The details are in the book, but we get (in total)

$$A = LU + E$$

where $|E_{ij}| \le n\epsilon |L| \cdot |U|_{ij}$ for all i,j. Taking norms, we get $\| E \| \le n\epsilon \| |L| \| \| |U| \|$. (using homework problem 7).

It turns out to be the case that if we solve $Ly = b$ by back substitution, the solution $\hat{y}$ obeys the equation

$$(L + \delta L)\hat{y} = b$$

where $|\delta L_{ij}| < n\epsilon |L_{ij}|$ and similarly solving $Ux = \hat{y}$ gives a solution satisfying

$$(U + \delta U)\hat{x} = \hat{y}$$

where $|\delta U_{ij}| < n\epsilon |U_{ij}|$. So

$$\begin{aligned} b &= (L+\delta L)\hat{y} \\ &= (L + \delta L)(U + \delta U)\hat{x} \\ &= \left(LU + (\delta L)U + L(\delta U) + (\delta L)(\delta U)\right)\hat{x} \\ &= \left(A - E + (\delta L)U + L(\delta U) + (\delta L)(\delta U)\right)\hat{x} \\ &= (A + \delta A)\hat{x} \end{aligned}$$

Now (componentwise) we have

$$|\delta A_{ij}| \leq |E_{ij}| + |((\delta L)U)_{ij}| + |(L(\delta U))_{ij}| + |(\delta L\,\delta U)_{ij}|$$

$$\leq |E_{ij}| + (|\delta L|\cdot|U|)_{ij} + (|L|\cdot|\delta U|)_{ij} + (|\delta L|\cdot|\delta U|)_{ij}$$

$$\leq n\epsilon\, |L|\cdot|U|_{ij} + (n\epsilon\, |L|\cdot|U|)_{ij} + (|L|\cdot n\epsilon\,|U|)_{ij} + (n\epsilon\,|L|\cdot n\epsilon\,|U|)_{ij}$$

$$\approx 3n\epsilon\,(|L|\cdot|U|)_{ij}$$

Thus to get backward stability for a solution by LU decomposition, we want

$$\frac{\|\delta A\|}{\|A\|} \approx O(\epsilon) \quad \text{or} \quad 3n\epsilon\, \|\,|L|\,\|\cdot\|\,|U|\,\| \lesssim O(\epsilon)\,\|A\|$$

This boils down to a desire that

$$\| |L| \| \, \| |U| \| \approx \|A\|.$$

Remark. This is exactly what <u>didn't</u> happen before, as $\|U\| \approx 10^4$ while $\|A\| \approx 2$. (At least in the ∞-norm), unless we pivoted.

Remark. In practice, GEPP almost always does this. In fact

$$\frac{\max_{ij} |U_{ij}|}{\max_{ij} |A_{ij}|} \approx O(n^{2/3}) \text{ or } O(n^{1/2})$$

for random matrices with partial pivoting.

Unfortunately, matrices exist for which

$$\frac{\max |U_{ij}|}{\max |A_{ij}|} = 2^{n-1},$$

and for these matrices, the GEPP algorithm fails. (It never gets worse, see Prop. 2.1 in Demmel.)