

Errors

Recall $\begin{bmatrix} \varepsilon & 1 \\ 1 & \lambda \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$. Using $\begin{bmatrix} \varepsilon & 1 \\ 1 & \lambda \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \frac{1}{\varepsilon} & 1 \end{bmatrix} \begin{bmatrix} \varepsilon & 1 \\ 0 & \lambda - \frac{1}{\varepsilon} \end{bmatrix}$

suppose the solution is \hat{x} , while the "true" solution is (say) x^* .

Q. How do we guarantee $\|\hat{x} - x^*\|$ to be small?

Subsidiary questions:

- 1) Why is $\hat{x} \neq x^*$?
- 2) How to calculate $\|\hat{x} - x^*\|$?
- 3) Does $\|\hat{x} - x^*\|$ depend on data (i.e. A, b) or on the algo (LU, LU with pivot, Rank-LU etc) or on both?

[Dorve 3.2]

Floating Point Arithmetic: (we will use Julia commands - same for many other lang.)

E.g.s Int8, Float32, Float64
Integers, Reals

Int8 \rightarrow $\underbrace{d_7 d_6 \dots d_0}_{\text{binary}}$ with $x = \sum_{i=0}^6 d_i 2^i - d_7 2^7$

bitstring(Int8(1)) = "00000001" $\left| \begin{array}{l} x = 1 \cdot 2^0 = 1 \\ x = 2^0 + \dots + 2^6 - 2^7 \\ = 127 - 128 = -1 \end{array} \right.$

" (Int8(-1)) = "11111111"

" (Int8(-128)) = "10000000"

Float32: $\pm \underbrace{\left(1 + \sum_{i=1}^{p-1} d_i 2^{-i}\right)}_{\text{significand / mantissa}} 2^{\underbrace{e}_{\text{exponent}}}$ Base 2

E.g : $3.140625 = \underbrace{(1.5703125)}_{\text{significand}} 2^1 \left| \begin{array}{l} \text{Not stored} \rightarrow \text{always 1 by} \\ \text{our system} \\ e = 1 \\ \text{sign} = + \end{array} \right.$

$$0.5703125 = \frac{1}{2} + \frac{1}{16} + \frac{1}{128} = 2^{-1} + 2^{-4} + 2^{-7}$$

\downarrow \downarrow \downarrow
 0.5 0.0625 0.0078125

bitstring (Float32(3.140625))

$$= \underbrace{0}_{\text{sign}} \quad \underbrace{d_7 \dots d_0}_{e = \sum_{i=0}^7 d_i \cdot 2^i - (2^7 - 1)} \quad \underbrace{100100100 \dots 0}_{23 \text{ bits}}$$

\downarrow \downarrow \downarrow
 0 \rightarrow + Here $e = 2^7 - 2^7 + 1$ $d_{15} d_{14} = d_7 = 1$
 1 \rightarrow - -1

Ex: bitstring (Float32(1.5703125)) $\rightarrow e = 0111111$ (Why?)

Ex: What is bitstring (Float32(0.5703125)) ? Why?

Ex: Show that Float32 can be used to represent nos between 10^{-38} to 10^{38} .

Float64 : Same setup : Sign \rightarrow 1 bit
 $e \rightarrow$ 11 bits

Errors in FPA

Basic Errors :
 1) Overflow } when results go out of range for a particular data type
 2) Underflow }
 3) Roundoff

Roundoff in base 10 (easier than base 2 for explanation)

Let $x = \pm \underbrace{d_0.d_1d_2}_{\text{significant}} \times 10^e$ where $1 \leq d_0 \leq 9$
 $0 \leq d_1 \leq 9$
 $0 \leq d_2 \leq 9$
 $-9 \leq e \leq 9$

Precision is defined by length of significant

e.g. $\pi = 3.14 \times 10^0$ (Error $\approx 10^{-3}$)

Not enough room:

$$(1.23 \times 10^6) + (4.56 \times 10^4) = 1275600$$

$$(1.23 \times 10^6) * (4.56 \times 10^2) = 5608.8$$

Results must be rounded

$$\text{round}(1275600) = 1.28 \times 10^6$$

$$\text{round}(5608.8) = 5.61 \times 10^3$$

There is a lowest & highest m
 (leading to underflow & overflow)

Set of nos is finite (Here $2 \times 9 \times 10 \times 10 \times 19 + 1 = 34201$)

Spacing between consecutive nos. vary
 e.g. diff between 1×10^2 & 1.01×10^2
 is 1.

but diff between 1×10^3 & 1.01×10^3
 is 10.

Defⁿ: Unit Roundoff Error:

$$u = \frac{1}{2} \times \left[\text{gap between } 1 \text{ \& next largest fl. point} \right]_{no}$$

For Float 32 $u \approx 10^{-7}$
 Float 64 $u \approx 10^{-16}$ } Can be checked
 with
 next float (1.0)
 command! \square

FACT: For floating pt. nos. addition is
 not associative

the fl. pt. representation of x
 If $x \in \mathbb{R}$, then, $fl(x) = x(1 + \epsilon)$ $|\epsilon| < u$

Let $x = 1.24 \times 10^0$ (for our example
 3 digit calc. above)
 $y = -1.23 \times 10^0$
 $z = 1.00 \times 10^{-3}$

$$fl(x+y) = 1 \times 10^{-2}$$

$$fl[fl(x+y) + z] = 1.10 \times 10^{-2}$$

But, $fl(y+z) = -1.23 \times 10^0$
 $fl(x + fl(y+z)) = 1 \times 10^{-2}$

error
 $\neq u!$

Q) Why is this happening?

Catastrophic
 Cancellation

$$fl(x) + fl(y) = x(1 + \epsilon_1) + y(1 + \epsilon_2) \quad \left| \begin{array}{l} |\epsilon_1| \approx |u| \ll 1 \\ |\epsilon_2| \approx |u| \ll 1 \end{array} \right.$$

$$= x + y + x\epsilon_1 + y\epsilon_2$$

$$= (x+y) \left[1 + \left(\frac{x}{x+y} \right) \epsilon_1 + \left(\frac{y}{x+y} \right) \epsilon_2 \right]$$

[Watkins 2-5
 pg 144]

If either $x \gg x+y$ or $y \gg x+y$
 then error blows up (larger than u)

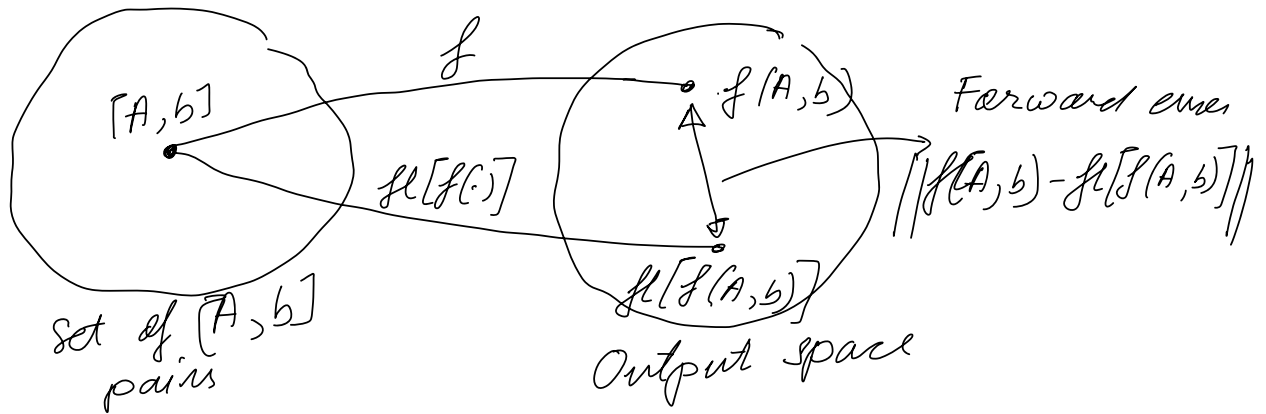
Q. It seems that such errors can accumulate (get magnified) through the steps of any algo. Then how do we guarantee accuracy?

☐ show code for Watkins 2.6.1, 2.6.2, 2.6.9

Some definitions: Let any algo be defined by a map $f: [\text{data}] \rightarrow [\text{result}]$

e.g. in solving $Ax = b$ using LU
 $f(A, b) = A^{-1}b$ Data = $[A, b]$

Since this algo is implemented on a comp. the output is $fl[f(A, b)]$



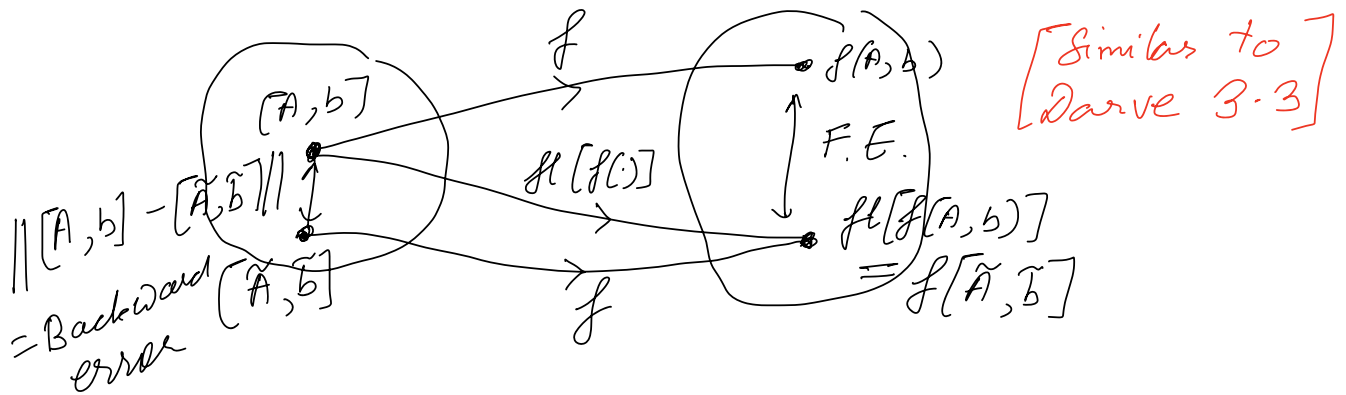
Directly computing "Forward error" is difficult (catastrophic cancellation can occur somewhere in the intermediate steps)

We ask a "strange" new question!

Q) Which $[\tilde{A}, \tilde{b}]$ gives

$$f[\tilde{A}, \tilde{b}] = fl[f(A, b)]$$

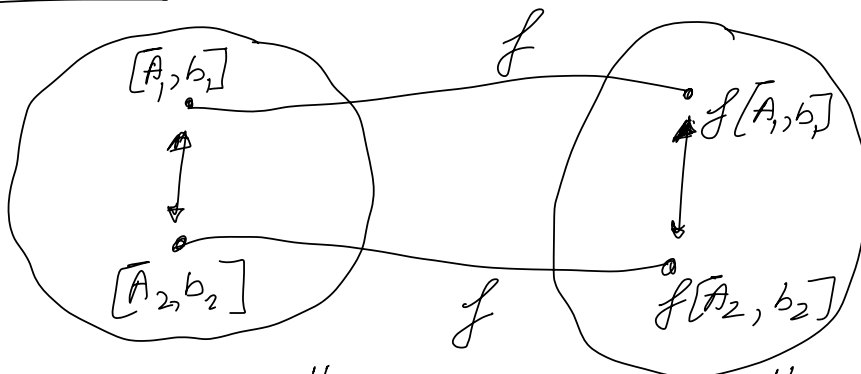
Then define Backward error = $\|[A, b] - [\tilde{A}, \tilde{b}]\|$



It is often easy to bound backward error for a specific algorithm.

Q. How does B.E (even if easy to compute) help in calculating F.E?

Sensitivity



$$\text{Sensitivity} = \frac{\|f[A_1, b_1] - f[A_2, b_2]\|}{\|[A_1, b_1] - [A_2, b_2]\|}$$

Note: 1) Sensitivity has nothing to do with floating point operation.
2) Sensitivity depends on data & f. → hence can be bdd. easily.

$$\begin{aligned}
 \# \quad F.E. &= \|f(\tilde{A}, b) - f(f(A, b))\| = \|f(A, b) - f(\tilde{A}, \tilde{b})\| \\
 &= \frac{\|f(A, b) - f(\tilde{A}, \tilde{b})\|}{\|(A, b) - (\tilde{A}, \tilde{b})\|} \cdot \|(A, b) - (\tilde{A}, \tilde{b})\| \\
 &= \text{Sensitivity} \times B.E
 \end{aligned}$$

If we have bounds on Sensitivity & B.E separately, then we can bound F.E also.

Big-O Notation: A function $f(n)$ is $O(g(n))$ if $\exists n_0 > 0$ & $c > 0$ s.t. for all $n \geq n_0$, $f(n) \leq cg(n)$

1) Sensitivity of Linear Systems ($Ax = b$)

[Golub 2.6.2]

$$\begin{aligned}
 \text{Let } (A + \varepsilon F)x(\varepsilon) &= b + \varepsilon f & x(0) &= x \\
 (A \text{ is non-singular}) & & F \in \mathbb{R}^{n \times n}, f \in \mathbb{R}^n &
 \end{aligned}$$

Clearly, $x(\varepsilon)$ is diff. in the neighborhood of 0.

$$Ax(\varepsilon) + \varepsilon Fx(\varepsilon) = b + \varepsilon f$$

$$\text{Diff. w.r.t } \varepsilon : A\dot{x}(\varepsilon) + Fx(\varepsilon) + \varepsilon F\dot{x}(\varepsilon) = f$$

$$(A + \varepsilon F)\dot{x}(\varepsilon) + Fx(\varepsilon) = f$$

$$\Rightarrow Ax(0) + Fx = f \Rightarrow \dot{x}(0) = A^{-1}[f - Fx]$$

Taylor series of $x(\varepsilon)$ around "0":

$$x(\varepsilon) = x + \varepsilon \dot{x}(0) + O(\varepsilon^2)$$

Then $\|x(\varepsilon) - x\| = \|\varepsilon A^{-1} [f - Fx] + O(\varepsilon^2)\|$

or $\frac{\|x(\varepsilon) - x\|}{\|x\|} \leq |\varepsilon| \|A^{-1}\| \left[\frac{\|f\| + \|F\| \|x\|}{\|x\|} \right] + O(\varepsilon^2)$

$$\leq |\varepsilon| \|A\| \|A^{-1}\| \left[\frac{\|F\|}{\|A\|} + \frac{\|f\|}{\|A\| \|x\|} \right] + O(\varepsilon^2)$$

$$\leq \underbrace{\|A\| \|A^{-1}\|}_{\kappa(A)} \left[\frac{|\varepsilon| \|F\|}{\|A\|} + \frac{|\varepsilon| \|f\|}{\|b\|} \right] + O(\varepsilon^2)$$

$$\leq \kappa(A) \left[\underbrace{\frac{|\varepsilon| \|F\|}{\|A\|}}_{\text{Relative error in } \|A\|} + \underbrace{\frac{|\varepsilon| \|f\|}{\|b\|}}_{\text{Relative error in } b} \right] + O(\varepsilon^2)$$

[since $\|A\| \|x\| \geq \|b\|$]

Defⁿ : Condition No: $\kappa(A) = \|A\| \|A^{-1}\|$
with the convention $\kappa(A) = \infty$ if A singular

Non-parametric bounds on relative errors are also easily derived:

Thm. If A is non-singular, $\frac{\|SA\|}{\|A\|} < \frac{\text{small perturbation}}{\kappa(A)}$, $b \neq 0$
 $Ax = b$ and $(A + SA)(x + \delta x) = b + \delta b$, then

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\kappa(A) \left[\frac{\|SA\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right]}{1 - \kappa(A) \frac{\|SA\|}{\|A\|}}$$

[Watkins 2.3]

Backward Error for Gaussian Elimination

[Watkins 2.7]

FACT: Suppose we compute $\sum_{j=1}^n w_j$ using floating point arithmetic with unit roundoff u .
Then:
$$fl\left(\sum_{j=1}^n w_j\right) = \sum_{j=1}^n w_j (1 + \gamma_j)$$

where $|\gamma_j| \leq (n-1)u + O(u^2)$ — (2)
regardless of the order in which the terms are accumulated.

Proof: By induction, \rightarrow true for $n=1$.

Let (2) be true for all int. $m < n$.

$$\sum_{j=1}^m w_j = \sum_{j=1}^k w_j + \sum_{j=k+1}^m w_j$$

By induction hypothesis, $fl\left(\sum_{j=1}^k w_j\right) = \sum_{j=1}^k w_j (1 + \alpha_j)$
& $fl\left(\sum_{j=k+1}^m w_j\right) = \sum_{j=k+1}^m w_j (1 + \alpha_j)$

where $|\alpha_j| \leq \begin{cases} (k-1)u + O(u^2) & j=1, \dots, k \\ (m-k-1)u + O(u^2) & j=k+1, \dots, m \end{cases}$
(3)

But $k-1 < m-2$ & $(m-k-1) \leq m-2$

Hence for (3) $|\alpha_j| \leq (m-2)u + O(u^2)$ $j=1, \dots, m$

$$\begin{aligned} \text{Now, } fl\left(\sum_{j=1}^m w_j\right) &= fl\left[fl\left(\sum_{j=1}^k w_j\right) + fl\left(\sum_{j=k+1}^m w_j\right)\right] \\ &= \left[\sum_{j=1}^k w_j (1 + \alpha_j) + \sum_{j=k+1}^m w_j (1 + \alpha_j)\right] (1 + \beta) \\ &= \sum_{j=1}^m w_j (1 + \alpha_j) (1 + \beta) \quad [|\beta| < u] \end{aligned}$$

$$\text{Let } \gamma_j^0 = \alpha_j^0 + \beta + \alpha_j \beta$$

$$\Rightarrow \text{fl} \left[\sum_{j=1}^m w_j \right] = \sum_{j=1}^m w_j (1 + \gamma_j)$$

$$\begin{aligned} \text{Then } |\gamma_j| &\leq |\alpha_j| + |\beta| + O(u^2) \\ &\leq (m-2)u + O(u^2) + u + O(u^2) \\ &= (m-1)u + O(u^2) \end{aligned}$$

Notation: $C \in \mathbb{R}^{m \times n}$, then $|C| \in \mathbb{R}^{m \times n}$ with $(|C|)_{ij} = |c_{ij}|$
 $C \leq F \Leftrightarrow c_{ij} \leq f_{ij} \forall i, j$.

B. E. for forward/backward substitution

Thm: Let $G \in \mathbb{R}^{n \times n}$ be non-singular, lower (upper) triangular matrix, and let $b \neq 0$. If $Gy = b$ is solved by any variant of forward (backward) substitution using fl. pt. arithmetic, then the answer \hat{y} satisfies:

$$\begin{aligned} (G + \delta G) \hat{y} &= b \\ \text{where } |\delta G| &\leq 2nu |G| + O(u^2) \quad \left(\begin{array}{l} \text{each entry is} \\ \text{of order } u^2 \end{array} \right) \\ \text{(i.e. } |\delta g_{ij}| &\leq 2nu |g_{ij}| + O(u^2) \quad \forall i, j \end{aligned}$$

Proof: At the i th step: $y_i^0 = \frac{b_i^0 - \sum_{j=1}^{i-1} g_{ij} y_j^0}{g_{ii}^0}$
 ideally.

$$\text{In reality: } \hat{y}_i^0 = \text{fl} \left(\frac{b_i^0 - \sum_{j=1}^{i-1} g_{ij} \hat{y}_j^0}{g_{ii}^0} \right)$$

$$\text{claim: } \text{fl}(g_{ij} \hat{y}_j) = g_{ij} \hat{y}_j (1 + \alpha_{ij}), |\alpha_{ij}| \leq u$$

Proof: Exercise.

From previous FACT:

$$f(b_i - \sum_{j=1}^{i-1} g_{ij} \hat{y}_j (1 + \alpha_{ij}))$$

$$= b_i (1 + \gamma_{ii}) - \sum_{j=1}^{i-1} g_{ij} (1 + \alpha_{ij}) (1 + \gamma_{ij})$$

where $|\gamma_{ij}| \leq (i-1)u + O(u^2) \quad j=1, \dots, i^0$

Next division:

$$\hat{y}_i^0 = \left[\frac{b_i (1 + \gamma_{ii}) - \sum g_{ij} \hat{y}_j^0 (1 + \alpha_{ij}) (1 + \gamma_{ij})}{g_{ii}} \right] (1 + \beta_i^0)$$

where $|\beta_i^0| < u$

$$= \frac{b_i - \sum_{j=1}^{i-1} g_{ij} (1 + \varepsilon_{ij}) \hat{y}_j^0}{g_{ii} (1 + \varepsilon_{ii})} \quad \text{for}$$

$$1 + \varepsilon_{ij} = \begin{cases} \frac{(1 + \alpha_{ij})(1 + \gamma_{ij})}{1 + \gamma_{ii}}, & j < i^0 \\ \frac{1}{(1 + \gamma_{ii})(1 + \beta_i^0)}, & j = i^0 \end{cases}$$

or $\sum g_{ij} (1 + \varepsilon_{ij}) \hat{y}_j^0 = b_i^0$

or $(G_2 + \delta G_2) \hat{y} = b$

L.T with $\delta g_{ij} = \varepsilon_{ij} g_{ij}$ for $i > j^0$

Claim: $|\varepsilon_{ij}| \leq 2au + O(u^2) \quad \forall i, j$

Proof: $\frac{1}{1 + \gamma_{ii}} = 1 - \gamma_{ii} + \gamma_{ii}^2 - \gamma_{ii}^3 + \dots$ { Since $\gamma_{ii} = O(u)$

$$= 1 - \gamma_{ii} + O(u^2)$$

Then for $j < i^0$, $1 + \varepsilon_{ij} = (1 + \alpha_{ij})(1 + \gamma_{ij})(1 - \gamma_{ii} + O(u^2))$

$$= 1 + \alpha_{ij} + \gamma_{ij} - \gamma_{ii} + O(u^2)$$

$$\begin{aligned}
\Rightarrow |\epsilon_{ij}| &\leq |\alpha_{ij}| + |\gamma_{ij}| + |\delta_{ij}| + O(u^2) \\
&\leq u + (i-1)u + (i-1)u + O(u^2) \\
&= (2i-1)u + O(u^2) \\
&\leq 2nu + O(u^2)
\end{aligned}$$

Similarly $|\epsilon_{ii}| \leq iu + O(u^2) \leq 2nu + O(u^2)$

B.E. in LU.

Thm 1: Suppose the LU decomposition of A is computed using fl. pt. arithmetic, & suppose no zero pivots are encountered. Let \hat{L} & \hat{U} are the computed factors. Then:

$$A + E = \hat{L}\hat{U}$$

where $|E| \leq 2nu |\hat{L}| |\hat{U}| + O(u^2)$
& $\|E\|_2 \leq 2nu \|\hat{L}\|_2 \|\hat{U}\|_2 + O(u^2)$

Thm 2: (Same assumptions as above thm), suppose we solve $Ax = b$ numerically using forward & backward substitution using \hat{L}, \hat{U} resp. Then the solution \hat{x} satisfies:

$$(A + \delta A) \hat{x} = b$$

where $|\delta A| \leq 6nu |\hat{L}| |\hat{U}| + O(u^2)$
& $\|\delta A\|_2 \leq 6nu \|\hat{L}\|_2 \|\hat{U}\|_2 + O(u^2)$

Backward stable: (rather loosely used) \rightarrow either
 'B.E. is "small" or $\frac{\text{B.E.}}{\|Data\|}$ (e.g. $\frac{\|SA\|}{\|A\|}$)

From the above then, B.E. is small only when
 $\|L\|$ & $\|U\|$ are small.

\Rightarrow LU without pivoting, LU with partial pivoting
 are both NOT backward stable.

\Rightarrow LU with full pivoting is Backward stable.

Proof: 1) If $A = LU$,
$$l_{ij} = \frac{a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj}}{u_{jj}} \quad i > j$$

&

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj} \quad i < j$$

In actual computation: $\hat{l}_{ij} = fl(\dots \hat{l}_{ik} \hat{u}_{kj})$
 $\hat{u}_{ij} = fl(\dots \dots)$

Then:
$$\hat{l}_{ij} = \frac{a_{ij}(1+\gamma_{ij}) - \sum_{k=1}^{j-1} \hat{l}_{ik} \hat{u}_{kj} (1+\alpha_k)(1+\beta_{ik})(1+\beta)}{\hat{u}_{jj}}$$

$|\gamma_{ij}| \leq (j-1)u + O(u^2) \rightarrow$ from previous thm.

$|\alpha_k| \leq u \leftarrow$ roundoff for mult.

$|\beta| \leq u \leftarrow$ roundoff for div.

Proceeding as in last thm (Exercise),

$$\hat{l}_{ij} = \frac{a_{ij} - \sum_{k=1}^{j-1} \hat{l}_{ik} \hat{u}_{kj} (1+\delta_{ik})}{\hat{u}_{jj} (1+\delta_{ij})}; \quad \text{with } |\delta_{ik}| \leq 2nu + O(u^2)$$

$$k = 1, \dots, j$$

or $a_{ij} + e_{ij} = \sum_{k=1}^j \hat{l}_{ik} \hat{u}_{kj}$ [Consolidating all error term in e_{ij}]

where $e_{ij} = - \sum_{k=1}^j \hat{l}_{ik} \hat{u}_{kj} \delta_{ik}$ [$i > j$]

$\Rightarrow |e_{ij}| \leq |\delta_{ik}| \sum_{k=1}^j |\hat{l}_{ik}| |\hat{u}_{kj}| + O(u^2)$

$= 2nu \sum_{k=1}^j |\hat{l}_{ik}| |\hat{u}_{kj}| + O(u^2)$

For $i < j$, same results can be obtained using the u_{ij} equation.

Hence (2), is true for $\forall i, j$.

In matrix form:

$\rightarrow A + E = \hat{L}\hat{U}$
 $\& |E| \leq 2nu |\hat{L}| |\hat{U}| + O(u^2)$

Proof of 2: $(\hat{L} + \delta\hat{L})\hat{y} = b \Rightarrow |\delta\hat{L}| \leq 2nu |\hat{L}|$
 $(\hat{U} + \delta\hat{U})\hat{x} = \hat{y} \Rightarrow |\delta\hat{U}| \leq 2nu |\hat{U}|$

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

$[\hat{L}\hat{U} + \delta\hat{L}\hat{U} + \hat{L}\delta\hat{U} + \delta\hat{L}\delta\hat{U}]\hat{x} = b$

$[A + E + \dots]\hat{x} = b$

$\delta A = E + \delta\hat{L}\hat{U} + \hat{L}\delta\hat{U} + \delta\hat{L}\delta\hat{U}$
 $|\delta A| \leq (2nu + 2nu + 2nu) |\hat{L}||\hat{U}| + O(u^2)$

$= 6nu |\hat{L}||\hat{U}| + O(u^2)$

Assume
 $A + E = \hat{L}\hat{U}$
 $|E| \leq 2nu |\hat{L}||\hat{U}| + O(u^2)$