Dense linear algebra : direct methods

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Outline

Linear Algebra Basics

Gaussian Elimination and LU factorization

LU Factorization with partial pivoting

Symmetric matrices

Cholesky Factorization

System of linear equations ?

Example:

$$
\begin{array}{rcrcrcr}
2\ x_1 & - & 1\ x_2 & + & 3\ x_3 & = & 13 \\
-4x_1 & + & 6\ x_2 & - & 5\ x_3 & = & -28 \\
6\ x_1 & + & 13\ x_2 & + & 16\ x_3 & = & 37
\end{array}
$$

can be written under the form:

$$\mathbf{Ax} = \mathbf{b},$$

with $\mathbf{A} = \begin{pmatrix} 2 & -1 & 3 \\ -4 & 6 & -5 \\ 6 & 13 & 16 \end{pmatrix}$, $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$, and $\mathbf{b} = \begin{pmatrix} 13 \\ -28 \\ 37 \end{pmatrix}$

Gaussian Elimination

Example:

$$
\begin{aligned}
2x_1 - x_2 + 3x_3 &= 13 && (1)\\
-4x_1 + 6x_2 - 5x_3 &= -28 && (2)\\
6x_1 + 13x_2 + 16x_3 &= 37 && (3)
\end{aligned}
$$

With 2 * (1) + (2) $\to$ (2) and -3*(1) + (3) $\to$ (3) we obtain:

$$
\begin{aligned}
2x_1 - x_2 + 3x_3 &= 13 && (4)\\
0x_1 + 4x_2 + x_3 &= -2 && (5)\\
0x_1 + 16x_2 + 7x_3 &= -2 && (6)
\end{aligned}
$$

Thus x_1 is eliminated from (5) and (6). With -4*(5) + (6) $\to$ (6):

$$
\begin{aligned}
2x_1 - x_2 + 3x_3 &= 13\\
0x_1 + 4x_2 + x_3 &= -2\\
0x_1 + 0x_2 + 3x_3 &= 6
\end{aligned}
$$

The linear system is then solved by backward ($x_3 \to x_2 \to x_1$) substitution: $x_3 = \frac{6}{3} = 2$, $x_2 = \frac{1}{4}(-2 - x_3) = -1$, and finally $x_1 = \frac{1}{2}(13 - 3x_3 + x_2) = 3$

LU Factorization

- Find $\mathbf{L}$ unit lower triangular and $\mathbf{U}$ upper triangular such that: $\mathbf{A} = \mathbf{L} \times \mathbf{U}$

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 3 \\ -4 & 6 & -5 \\ 6 & 13 & 16 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 3 & 4 & 1 \end{bmatrix} \times \begin{bmatrix} 2 & -1 & 3 \\ 0 & 4 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$

- Procedure to solve $\mathbf{Ax} = \mathbf{b}$
  - $\mathbf{A} = \mathbf{LU}$
  - Solve $\mathbf{Ly} = \mathbf{b}$ (*forward elimination*, down)
  - Solve $\mathbf{Ux} = \mathbf{y}$ (*backward substitution*, up)

$$\mathbf{Ax} = (\mathbf{LU})\mathbf{x} = \mathbf{L}(\mathbf{Ux}) = \mathbf{Ly} = \mathbf{b}$$

From Gaussian Elimination to LU Factorization

$\mathbf{A} = \mathbf{A}^{(1)}$, $\mathbf{b} = \mathbf{b}^{(1)}$, $\mathbf{A}^{(1)}\mathbf{x} = \mathbf{b}^{(1)}$:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \qquad \begin{array}{l} 2 \leftarrow 2 - 1 \times a_{21}/a_{11} \\ 3 \leftarrow 3 - 1 \times a_{31}/a_{11} \end{array}$$

$\mathbf{A}^{(2)}\mathbf{x} = \mathbf{b}^{(2)}$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2^{(2)} \\ b_3^{(2)} \end{pmatrix} \qquad \begin{array}{l} b_2^{(2)} = b_2 - a_{21} b_1 / a_{11} \\ a_{32}^{(2)} = a_{32} - a_{31} a_{12} / a_{11} \end{array}$$

<u>Finally</u> $3 \leftarrow 3 - 2 \times a_{32}/a_{22}$ gives $\mathbf{A}^{(3)}\mathbf{x} = \mathbf{b}^{(3)}$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} \\ 0 & 0 & a_{33}^{(3)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2^{(2)} \\ b_3^{(3)} \end{pmatrix} \qquad a_{33}^{(3)} = a_{33}^{(2)} - a_{32}^{(2)} a_{23}^{(2)} / a_{22}^{(2)}$$

Typical Gaussian elimination at step k:

$$
\begin{pmatrix}
a_{11}^{(1)} & \cdots & \cdots & \cdots & \cdots & \cdots & a_{1n}^{(1)} \\
0 & \ddots & & & & & \vdots \\
\vdots & \ddots & a_{k-1k-1}^{(k-1)} & \cdots & \cdots & \cdots & a_{k-1n}^{(k-1)} \\
\vdots & & 0 & a_{kk}^{(k)} & a_{kk+1}^{(k)} & \cdots & a_{kn}^{(k)} \\
\vdots & & \vdots & a_{k+1k}^{(k)} & a_{k+1k+1}^{(k)} & \cdots & a_{k+1n}^{(k)} \\
\vdots & & \vdots & \vdots & \vdots & & \vdots \\
0 & \cdots & 0 & a_{nk}^{(k)} & a_{nk+1}^{(k)} & \cdots & a_{nn}^{(k)}
\end{pmatrix}
\quad
\begin{pmatrix}
b_1^{(1)} \\ \vdots \\ b_{k-1}^{(k-1)} \\ b_k^{(k)} \\ b_{k+1}^{(k)} \\ \vdots \\ b_n^{(k)}
\end{pmatrix}
$$

$$\boxed{a_{ij}^{(k+1)} = a_{ij}^{(k)} - \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} a_{kj}^{(k)}, \text{ for } i > k}$$

(and $a_{ij}^{(k+1)} = a_{ij}^{(k)}$ for $i \leq k$)

From Gaussian Elimination to **LU** factorization

$$\begin{cases} a_{ij}^{(k+1)} = a_{ij}^{(k)} - \dfrac{a_{ik}^{(k)}}{a_{kk}^{(k)}} a_{kj}^{(k)}, \text{ for } i > k \\ a_{ij}^{(k+1)} = a_{ij}^{(k)}, \text{ for } i \leq k \end{cases}$$

- One step of Gaussian elimination can be written: $\mathbf{A}^{(k+1)} = \mathbf{L}^{(k)}\mathbf{A}^{(k)}$ (and $b^{(k+1)} = \mathbf{L}^{(k)} b^{(k)}$), with

$$\mathbf{L}^k = \begin{pmatrix} \mathbf{1} & & & & & \\ & \cdot & & & & \\ & & \cdot & & & \\ & & & \mathbf{1} & & \\ & & & -\mathbf{l_{k+1,k}} & \cdot & \\ & & & \cdot & & \cdot \\ & & & -\mathbf{l_{n,k}} & & & \mathbf{1} \end{pmatrix} \text{ and } l_{ik} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}.$$

- After $n-1$ steps, $\mathbf{A}^{(n)} = \mathbf{U} = \mathbf{L}^{(n-1)} \ldots \mathbf{L}^{(1)}\mathbf{A}$ gives $\boxed{\mathbf{A} = \mathbf{LU}}$, with $\mathbf{L} = [\mathbf{L}^{(1)}]^{-1} \ldots [\mathbf{L}^{(n-1)}]^{-1} =$

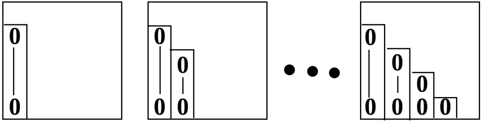
$$\begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & & & \\ & \ddots & & \\ & & 1 & \\ & & l_{n,n-1} & 1 \end{pmatrix} = \begin{pmatrix} \mathbf{1} & & \mathbf{0} & & \\ l_{21} & \mathbf{1} & & & \\ \cdot & & \cdot & & \\ \cdot & & & \cdot & \\ l_{n1} & \ldots & & l_{n,n-1} & \mathbf{1} \end{pmatrix}$$

LU Factorization Algorithm

- Overwrite matrix **A**: we store $a_{ij}^{(k)}, k = 2, \ldots, n$ in `A(i,j)`
- In the end, $\mathbf{A} = \mathbf{A}^{(n)} = \mathbf{U}$

```
do k=1, n-1
   L(k,k) = 1
   do i=k+1, n
      L(i,k) = A(i,k)/A(k,k)
      do j=k, n   ! (better than: do j=1,n)
         A(i,j) = A(i,j) - L(i,k) * A(k,j)
      end do
   enddo
enddo
L(n,n)=1
```

- Matrix **A** at each step:



- Avoid building the zeros under the diagonal
- Before

```
L(n,n)=1
do k=1, n-1
    L(k,k) = 1
    do i=k+1, n
        L(i,k) = A(i,k)/A(k,k)
        do j=k, n
            A(i,j) = A(i,j) - L(i,k) * A(k,j)
```

- After

```
L(n,n)=1
do k=1, n-1
    L(k,k) = 1
    do i=k+1, n
        L(i,k) = A(i,k)/A(k,k)
        do j=k+1, n
            A(i,j) = A(i,j) - L(i,k) * A(k,j)
```

- Use lower triangle of array **A** to store $\mathbf{L}_{i,k}$ multipliers
- Before:

```
L(n,n)=1
do k=1, n-1
   L(k,k) = 1
   do i=k+1, n
      L(i,k) = A(i,k)/A(k,k)
      do j=k+1, n
         A(i,j) = A(i,j) - L(i,k) * A(k,j)
```

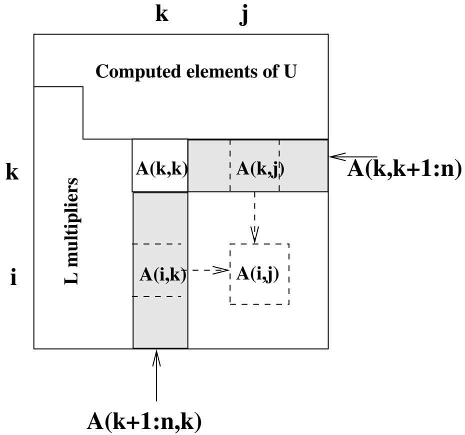
- After (diagonal 1 of L is not stored):

```
do k=1, n-1
   do i=k+1, n
      A(i,k) = A(i,k)/A(k,k)
      do j=k+1, n
         A(i,j) = A(i,j) - A(i,k) * A(k,j)
```

- More compact array syntax (Matlab, scilab):

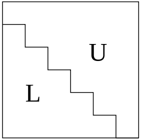
```
do k=1, n-1
  A(k+1:n,k) = A(k+1:n,k) / A(k,k)
  A(k+1:n,k+1:n) = A(k+1:n,k+1:n)
                         - A(k+1:n,k) * A(k,k+1:n)
end do
```

- corresponds to a rank-1 update:



What we have computed

- we have stored the **L** and **U** factors in **A**:
  - $\mathbf{A}_{i,j}$, i $>$ j corresponds to l_{ij}
  - $\mathbf{A}_{i,j}$, i $\leq$ j corresponds to u_{ij}
  - with $l_{ii} = 1, i = 1, n$
- Finally,



after factorization: $\mathbf{A} = \mathbf{L} + \mathbf{U} - I$

LU factorization : summary

- Step by step columns of $\mathbf{A}$ are set to zero and $\mathbf{A}$ is updated
  $\mathbf{L}^{(n-1)} \ldots \mathbf{L}^{(1)} \mathbf{A} = \mathbf{U}$ leading to
  $\mathbf{A} = \mathbf{LU}$ where $\mathbf{L} = [\mathbf{L}^{(1)}]^{-1} \ldots [\mathbf{L}^{(n-1)}]^{-1}$
- At each step $\mathbf{A}(k,k)$ is referred to as the pivot
  - zero entries in column of $\mathbf{A}$ can be replaced by entries in $\mathbf{L}$
  - row entries of $\mathbf{U}$ are stored in corresponding locations of $\mathbf{A}$

Algorithm 1 **LU** factorization

```
for k = 1, n − 1 do
  if |A(k, k)| too small then
    exit (small pivots are not allowed)
  end if
  A(k+1:n,k) = A(k+1:n,k) / A(k,k)
  A(k+1:n,k+1:n) = A(k+1:n,k+1:n) - A(k+1:n,k)*A(k,k+1:n)
end for
```

When $|\mathbf{A}(k,k)|$ is too small, one could consider other pivots: numerical pivoting strategies will be introduced later.

Existence and uniqueness of LU decomposition

Theorem 1

$\mathbf{A} \in R^{n\times n}$ has an LU factorization (where $\mathbf{L}$ is unit lower triangular and $\mathbf{U}$ is upper triangular) if $det(\mathbf{A}(1:k, 1:k)) \neq 0$ for all $k \in \{1 \dots n-1\}$. If the $\mathbf{LU}$ factorization exists, then it is unique and $det(\mathbf{A}) = u_{11} \dots u_{nn}$.

Theorem 2

For each nonsingular matrix $\mathbf{A}$, there exists a permutation matrix $\mathbf{P}$ such that $\mathbf{PA}$ possesses an LU factorization $\mathbf{PA} = \mathbf{LU}$.

Definition 1

$\mathbf{A} \in R^{n\times n}$ is *strictly diagonally dominant* iff $|a_{ii}| > \sum_{j=1, j\neq i}^{n} |a_{ij}|$ for all $i = 1, \dots, n$

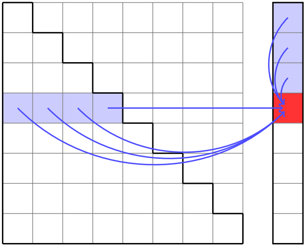
Theorem 3

If $\mathbf{A}^T$ is strictly diagonally dominant then $\mathbf{A}$ is non-singular and $\mathbf{A}$ has an LU factorization and $l_{ij} < 1$

Solution phase : $\mathbf{Lx} = \mathbf{b}$ (Left-Looking and Right-looking)

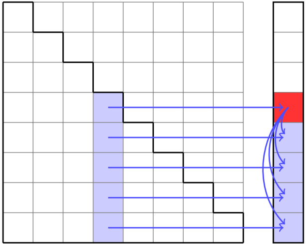
Algorithm 2 LL (sans report)

$x = b$
for $j = 1,\ n$ **do**
  for $i = 1,\ j-1$ **do**
    $x_j = x_j - l_{ji} x_i$
  end for
  $x_j = \dfrac{x_j}{l_{jj}}$
end for



Algorithm 3 RL (avec report)

$x = b$
for $j = 1,\ n$ **do**
  $x_j = \dfrac{x_j}{l_{jj}}$
  for $i = j+1,\ n$ **do**
    $x_i = x_i - l_{ij} x_j$
  end for
end for



Blocked **LU** and Schur decomposition

Exercise 1 (Blocked **LU** and Schur decomposition)

Let $\mathbf{A}$ *be a non singular matrix of order* n *for which* $\exists\mathbf{P}$ *permutation matrix such that* $\mathbf{PA}$ *can be factored without pivoting and consider the block form* $\mathbf{PA} = \begin{pmatrix} \mathbf{A}_{1,1} & \mathbf{A}_{1,2} \\ \mathbf{A}_{2,1} & \mathbf{A}_{2,2} \end{pmatrix}$. *We define the so called Schur matrix* $\mathbf{S}$ *as*

$$\mathbf{S} = \mathbf{A}_{2,2} - \mathbf{A}_{2,1} \left(\mathbf{A}_{1,1}\right)^{-1} \mathbf{A}_{1,2}$$

1. *Explain how to adapt the* **LU** *factorisation algorithm to obtain the following decomposition of* $\mathbf{PA}$. $\mathbf{PA} = \begin{pmatrix} \mathbf{L}_{1,1} & 0 \\ \mathbf{L}_{2,1} & I \end{pmatrix} \begin{pmatrix} \mathbf{U}_{1,1} & \mathbf{U}_{1,2} \\ 0 & \mathbf{S} \end{pmatrix} = \begin{pmatrix} \mathbf{L}_{1,1} & 0 \\ \mathbf{L}_{2,1} & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \mathbf{S} \end{pmatrix} \begin{pmatrix} \mathbf{U}_{1,1} & \mathbf{U}_{1,2} \\ 0 & I \end{pmatrix}$
2. *Prove that* $det(\mathbf{A}) = det(\mathbf{P}) det(\mathbf{A}_{1,1}) det(\mathbf{S})$
3. *We assume that we know how to compute* $\mathbf{Y}$ *such that* $\mathbf{Y} = \mathbf{S}^{-1}\mathbf{Z}$. *Describe how to use previous incomplete blocked factorization to solve* $\mathbf{AX} = \mathbf{B}$.

Blocked factorization and null space

Exercise 2 (Null space)

We suppose that after $n - r$ steps of $\mathbf{LU}$ *factorization we have* $\mathbf{PA} = \begin{pmatrix} \mathbf{L}_{1,1} & 0 \\ \mathbf{L}_{2,1} & I_r \end{pmatrix} \begin{pmatrix} \mathbf{U}_{1,1} & \mathbf{U}_{1,2} \\ 0 & \mathbf{S}_r \end{pmatrix}$ *where* $\mathbf{S}_r$ *is the Schur complement matrix of order* r*. We also suppose that* $\mathbf{S}_r = 0$ *(in practice one could also assume that* $\|\mathbf{S}_r\| \leq \varepsilon \|\mathbf{A}\|$ *for some matrix norm). Finally we assume that* $\det(\mathbf{U}_{11}) \neq 0$*.*
Prove that the dimension of the null-space is r *and compute a basis of the null space.*

Number of floating-point operations (flops)

- In forward elimination ($Ly = b$), computing the k^{th} unknown

$$y_k = b_k - \sum_{j=1}^{k-1} L_{kj} y_j$$

  leads to (k-1) multiplications and (k-1) additions, for $1 \leq k \leq n$

  $n^2 - n$ flops overall
- Idem for $Ux = y$ and at worst n divisions ($U_{kk} \neq 1$).
- Number of flops during factorization:
  - $n - k$ divisions
  - $(n-k)^2$ multiplications, $(n-k)^2$ additions
  - $k = 1, 2, ..., n-1$
  - total: $\approx \frac{2 \times n^3}{3}$
    (Strassen's algorithm can reduce this to $\Theta(n^{log_2 7}) \simeq \Theta(n^{2.8})$)

Computational complexity

Exercise 3 (How to compute $\mathbf{x}$ such that $\mathbf{x} = \left(\mathbf{A}^2\right)^{-1}\mathbf{b}$)

Let $\mathbf{A}$ be a non singular matrix of order n (i.e. it exists $\mathbf{L}$, $\mathbf{U}$ and $\mathbf{P}$ such that $\mathbf{PA} = \mathbf{LU}$ (note that $\mathbf{A}^2$ is also non singular).

1. *Compare the computational complexity of solving $\mathbf{A}^2\mathbf{x} = \mathbf{b}$ with the following two algorithms:*
   1.1 *Compute $\mathbf{B} = \mathbf{A}^2$, factor $\mathbf{B}$ and solve $\mathbf{Bx} = \mathbf{b}$*
   1.2 *Factor $\mathbf{A}$ and use the factored form to solve $\mathbf{A}^2\mathbf{x} = \mathbf{b}$*
2. *Explain why computing directly $\mathbf{C} = \left(\mathbf{A}^2\right)^{-1}$ and performing $\mathbf{x} = \mathbf{Cb}$ is not a method of choice.*

Linear Algebra Basics

Gaussian Elimination and LU factorization

LU Factorization with partial pivoting

Symmetric matrices

Cholesky Factorization

$$\text{Consider } A = \begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \frac{1}{\varepsilon} & 1 \end{bmatrix} \times \begin{bmatrix} \varepsilon & 1 \\ 0 & 1 - \frac{1}{\varepsilon} \end{bmatrix}$$

$$\kappa_2(A) = \frac{\lambda_{max}}{\lambda_{min}} = \frac{1 + \varepsilon + \sqrt{5 + \varepsilon^2 - 2\varepsilon}}{-1 - \varepsilon + \sqrt{5 + \varepsilon^2 - 2\varepsilon}} \simeq 2.6$$

If one solves:

$$\begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 + \varepsilon \\ 2 \end{bmatrix}$$

Exact solution $x^* = (1, 1)$.

$$A = \begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \frac{1}{\varepsilon} & 1 \end{bmatrix} \times \begin{bmatrix} \varepsilon & 1 \\ 0 & 1 - \frac{1}{\varepsilon} \end{bmatrix}$$

ε	$\frac{\|x^* - x\|}{\|x^*\|}$	$\kappa_2(A)$
10^{-3}	6×10^{-16}	2.621
10^{-6}	2×10^{-11}	2.618
10^{-9}	9×10^{-8}	2.618
10^{-12}	9×10^{-5}	2.618
10^{-15}	7×10^{-2}	2.618

Table: Relative error as a function of ε.

- Even if A is well conditioned, Gaussian elimination may introduce errors

$$A = \begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \frac{1}{\varepsilon} & 1 \end{bmatrix} \times \begin{bmatrix} \varepsilon & 1 \\ 0 & 1 - \frac{1}{\varepsilon} \end{bmatrix}$$

ε	$\frac{\|x^* - x\|}{\|x^*\|}$	$\kappa_2(A)$
10^{-3}	6×10^{-16}	2.621
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10^{-9}	9×10^{-8}	2.618
10^{-12}	9×10^{-5}	2.618
10^{-15}	7×10^{-2}	2.618

Table: Relative error as a function of ε.

- Even if A is well conditioned, Gaussian elimination may introduce errors
- Explanation: pivot ε is too small and leads to a large element growth (growth factor) in L and U: $\frac{1}{\varepsilon}$ in L leads to a loss of information/accuracy in $1 - \frac{1}{\varepsilon}$

$$A = \begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \frac{1}{\varepsilon} & 1 \end{bmatrix} \times \begin{bmatrix} \varepsilon & 1 \\ 0 & 1 - \frac{1}{\varepsilon} \end{bmatrix}$$

- Let us try to exchange rows 1 and 2 of A and b:

$$\begin{bmatrix} 1 & 1 \\ \varepsilon & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 + \varepsilon \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ \varepsilon & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \varepsilon & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 - \varepsilon \end{bmatrix}$$

$\rightarrow$ Multipliers are bounded: $\forall i = k+1 : n, \quad \dfrac{|a_{i,k}^{(k)}|}{|a_{k,k}^{(k)}|} \leq 1$

$\rightarrow$ terms of original matrix remain significant in LU factors

$\rightarrow$ perfect accuracy obtained !

Partial Pivoting

- Partial pivoting: choose at each step the largest element of the column as the pivot

$\rightarrow$ avoids large elements in factors matrix (growth factor)

- Then (P: permutation), $PA = LU, \quad Ly = Pb, \quad Ux = y$
- LU with partial pivoting is practically *backward stable*

$$\frac{\|Ax - b\|}{\|A\| \times \|x\| + \|b\|} \approx \varepsilon \qquad (1)$$

$$\frac{\|x - x^*\|}{\|x^*\|} \approx \varepsilon \times \kappa(A) \qquad (2)$$

(1) small backward error (and small residual) independently of the conditioning

(2) accuracy depends on conditioning
if $\varepsilon \approx 10^{-q}$ et $\kappa(A) \approx 10^{p}$ then x has approximately $(q - p)$ correct digits

LU factorization with partial pivoting

Next algorithm computes $\mathbf{L}$ and $\mathbf{U}$ such that $\mathbf{PA} = \mathbf{LU}$, and computes $\mathbf{Pb}$.

Algorithm 4 LU factorization with partial pivoting

for $k = 1, n-1$ **do**
  Pivot search : Find index i of largest entry in $\mathbf{A}(k : n, k)$
  if $|A(i,k)| \leq \varepsilon \|A\|$ **then**
    exit since $\mathbf{A}$ is numerically singular
  end if
  Swap rows i and k of $\mathbf{A}$ and $\mathbf{b}$
  A(k+1:n,k) = A(k+1:n,k) / A(k,k)
  A(k+1:n,k+1:n) = A(k+1:n,k+1:n) - A(k+1:n,k)*A(k,k+1:n)
end for

To solve $\mathbf{Ax} = \mathbf{b}$ one should thus perform $\mathbf{LU} = \mathbf{Pb}$. Permutation $\mathbf{P}$ is either applied on $\mathbf{b}$ during Algorithm 4 or needs be saved to be applied later.

Extensions to **LU** factorization with partial pivoting

Exercise 4 (LU with pivoting)

1. *Explain how to modify algorithm 4 to factor singular matrices in the form proposed at exercice 2 (so that using exercice 2 one could then also compute the null-space of* $\mathbf{A}$*)*
2. *Let us suppose then that in algorithm 4, we want at each step of* **Pivot search** *step to find the largest entry not only in the column (*$\mathbf{A}(k:n,k)$*) both also (*$\mathbf{A}(k:n,k:n)$*), so called* **total pivoting**. *Describe how algorithm 4 should be modified.*
3. *Compare algorithm proposed at questions 1 and 2.*

Linear Algebra Basics

Symmetric matrices

- Assumption: A has a LU factorization
- A symmetric: only store lower or upper triangle
- $A = LU$ and $A^T = A \Rightarrow LU = U^T L^T$,
  thus $LU(L^T)^{-1} = U^T \Rightarrow (U)(L^T)^{-1} = L^{-1}U^T = D$ diagonal
  and $U = DL^T$,
  finally $A = L(DL^T) = LDL^T$, with $D = \text{Diag}(U)$ and
- Example:

$$\begin{bmatrix} 4 & -8 & -4 \\ -8 & 18 & 14 \\ -4 & 14 & 25 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1 & 3 & 1 \end{bmatrix} \times \begin{bmatrix} 4 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \times \begin{bmatrix} 1 & -2 & -1 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{bmatrix}$$

- Solution of $Ax = b$: with $A = LDL^T$:
  1. $Ly = b$ then $Dz = y$ followed by
  2. $L^T x = z$

Properties of LDL^T Algorithm

We have shown that if **A** symmetric and $A = LU$ exists then $\exists L$ and $D (= \text{Diag}(U))$ such that $A = LDL^T$. **LU** Algorithm 1 thus already computes all we need: L and D.

Proposition 1 (LDL^T Algorithm)

Given a symmetric matrix A for which an LU factorisation exists, the LU algorithm 1 can be adapted to compute LDL^T factorization.

Proposition 2 (Complexity of LDL^T factorization)

If only the lower triangular part of the matrix (including diagonal) is used/updated and if only L and D matrices are stored, then the cost of LDL^T factorisation is $\approx \frac{n^3}{3}$

LDL^T Algorithm for symmetric matrices

- let l_k be column k of L and u_k be row k of U then in Algorithm 1, $A(k+1:n, k+1:n) = A(k+1:n, k+1:n) - l_k * u_k^T$
- since $l_k = u_k/u_{kk}$, when U is not stored, one must temporarily save u_k to perform the update.

Algorithm 5 LDT^T factorization

---

for $k = 1, n-1$ **do**
    if $|\mathbf{A}(k,k)|$ too small exit (small pivots
    $\mathbf{v}_k$ = A(k+1:n,k) (corresponds to u_k in **LU** Agorithm)
    A(k+1:n,k) = A(k+1:n,k) / A(k,k)
    for $j = k+1, n$ **do**
        A(j:n,j) = A(j:n,j) - A(j:n,k)*$\mathbf{v}_k(j)$
    end for
end for

Complexity of LDL^T factorization

```
for k = 1, n − 1 do
   if |A(k, k)| too small exit (small pivots
   v_k = A(k+1:n,k) (corresponds to u_k in LU Agorithm)
   A(k+1:n,k) = A(k+1:n,k) / A(k,k)
   for j = k + 1, n do
      A(j:n,j) = A(j:n,j) - A(j:n,k)*v_k(j)
   end for
end for
```

- $$\text{flops}(LDL^T) = 2\sum_{k=1}^{n-1}\left(\sum_{i=1}^{n-k} i\right) = 2\sum_{k=1}^{n-1}\left(\frac{(n-k)(n-k+1)}{2}\right)$$

  $$\text{flops}(LDL^T) \approx \sum_{k=1}^{n-1}(n-k)^2 \qquad \left(\text{thus } \tfrac{1}{2}\text{flops}(\mathbf{LU})\right)$$

  $$LDL^T \approx \frac{n^3}{3}\text{floating point operations}$$

Symmetric matrices and pivoting

- Diagonal pivoting preserves symmetry but is insufficient for stability
- In general one looks for a permutation P such that:

$$PAP^T = LDL^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ x & 1 & 0 & 0 \\ x & 0 & 1 & 0 \\ x & x & x & 1 \end{bmatrix} \times \begin{bmatrix} x & 0 & 0 & 0 \\ 0 & x & x & 0 \\ 0 & x & x & 0 \\ 0 & 0 & 0 & x \end{bmatrix} \times \begin{bmatrix} 1 & x & x & x \\ 0 & 1 & 0 & x \\ 0 & 0 & 1 & x \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- D: matrix of diagonal 1×1 and 2×2 blocks

  Examples of 2x2 pivots: $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \begin{bmatrix} \varepsilon_1 & 1 \\ 1 & \varepsilon_2 \end{bmatrix}$

- Pivot choice more complex: 2 columns at each step Let $PAP^T = \begin{bmatrix} E & C^T \\ C & B \end{bmatrix}$. If E is a 2x2 pivot, form E^{-1} to get:

$$PAP^T = \begin{bmatrix} I & 0 \\ CE^{-1} & I \end{bmatrix} \begin{bmatrix} E & 0 \\ 0 & B - CE^{-1}C^T \end{bmatrix} \begin{bmatrix} I & E^{-1}C^T \\ 0 & I \end{bmatrix}$$

Linear Algebra Basics

Gaussian Elimination and LU factorization

LU Factorization with partial pivoting

Symmetric matrices

Cholesky Factorization

Cholesky Factorization

- $\mathbf{A}$ positive definite if $\mathbf{x}^T\mathbf{A}\mathbf{x} > 0 \quad \forall \mathbf{x} \neq 0$
- $\mathbf{A}$ symmetric positive definite $\Rightarrow$ Cholesky factorization

  $\mathbf{A} = \mathbf{L}\mathbf{L}^T$ with L lower triangular, $\mathbf{L}$ is unique
- By identification :

$$\begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \times \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

- It follows: $\begin{array}{lll} a_{11} = l_{11}^2 & a_{21} = l_{21} \times l_{11} & a_{31} = l_{31} \times l_{11} \\ a_{22} = l_{21}^2 + l_{22}^2 & a_{32} = l_{31} \times l_{21} + l_{32} \times l_{22} & a_{33} = l_{31}^2 + l_{32}^2 + l_{33}^2 \end{array}$

  Thus:

$$\begin{array}{lll} l_{11} = \sqrt{a_{11}} & l_{21} = a_{21}/l_{11} & l_{31} = a_{31}/l_{11} \\ a_{22}^{(1)} = a_{22} - l_{21}^2 & a_{32}^{(1)} = a_{32} - l_{31} \times l_{21} & a_{33}^{(1)} = a_{33} - l_{31}^2 \\ l_{22} = \sqrt{a_{22}^{(1)}} & l_{32} = a_{32}^{(1)}/l_{22} & a_{33}^{(2)} = a_{33}^{(1)} - l_{32}^2 \\ l_{33} = \sqrt{a_{33}^{(2)}} & & \end{array}$$

Cholesky Factorization

Cholesky Factorization

```
do k=1, n
     A(k,k)=sqrt(A(k,k))
     A(k+1:n,k) = A(k+1:n,k)/A(k,k)
     do j=k+1, n
         A(j:n,j) = A(j:n,j) - A(j:n,k) A(j,k)
     end do
end do
```

- Cholesky is backward stable (without pivoting)
- Factorization: $\approx \frac{n^3}{3}$ flops
- Similar to LU, but only on the lower triangle. **LU** factorization:

```
A(k+1:n,k) = A(k+1:n,k)/A(k,k)
A(k+1:n,k+1:n) = A(k+1:n,k+1:n) -  &
                 A(k+1:n,k) * A(k,k+1:n)
```