LU Factorization with pivoting

$$\underbrace{\begin{bmatrix} c & 1 \\ -1 & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}}_{b}$$

1) We want to solve for x

2) But first we will "construct the problem".

   - start with the true solution

$$x_t = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

   - set $c = 10^{-1}$ (for example)
   - compute matrix-vector multiplication to find $b = Ax_t$

3) Now we can perform the solve $Ax = b$ to find x

4) If "all goes well", $x = x_t$. Is it?

What can go wrong with the previous algorithm for LU factorization?

$$\boldsymbol{M} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & \boxed{\color{red}{\mathbf{4}} & 3 & 3} \\ 1 & 2 & 6 & 2 \\ 1 & 3 & 4 & 2 \end{pmatrix} \qquad \boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \end{pmatrix} \qquad \boldsymbol{U} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 4 & 2 & 0.5 \\ 4 & 2 & 0.5 \\ 4 & 2 & 0.5 \end{pmatrix} \qquad \boldsymbol{M} - \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & \color{red}{\mathbf{0}} & 1 & 2.5 \\ 1 & -2 & 4 & 1.5 \\ 1 & -1 & 2 & 1.5 \end{pmatrix}$$

The next update for the lower triangular matrix will result in a division by zero! LU factorization fails.

What can we do to get something like an LU factorization?

Pivoting

$A = LU$

$A = PLU$

Approach:

1. Swap rows if there is a zero entry in the diagonal
2. Even better idea: Find the largest entry (by absolute value) and swap it to the top row.

The entry we divide by is called the pivot.

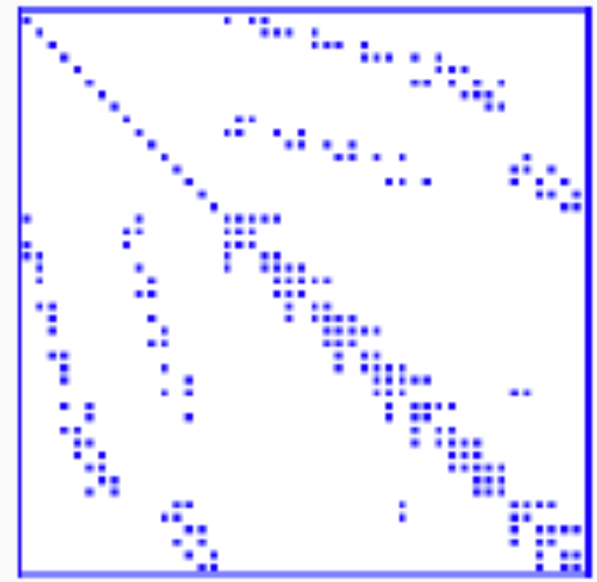
Swapping rows to get a bigger pivot is called (partial) pivoting.

$$\begin{pmatrix} a_{11} & \boldsymbol{a}_{12} \\ \boxed{\boldsymbol{a}_{21}} & \boldsymbol{A}_{22} \end{pmatrix} = \begin{pmatrix} u_{11} & \boldsymbol{u}_{12} \\ u_{11}\,\boldsymbol{l}_{21} & \boldsymbol{l}_{21}\boldsymbol{u}_{12} + \boldsymbol{L}_{22}\boldsymbol{U}_{22} \end{pmatrix}$$

Find the largest entry (in magnitude)

Sparse Systems

Sparse Matrices



Some type of matrices contain many zeros.
Storing all those zero entries is wasteful!

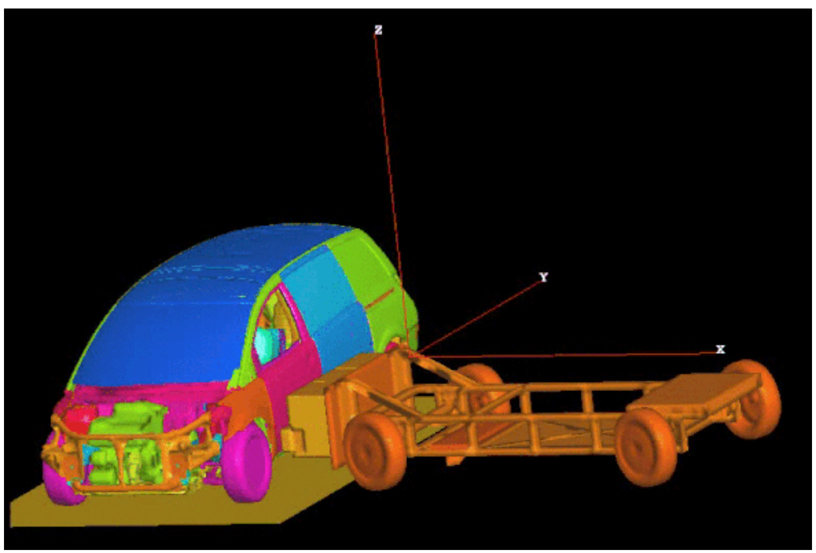
How can we efficiently store large matrices without storing tons of zeros?

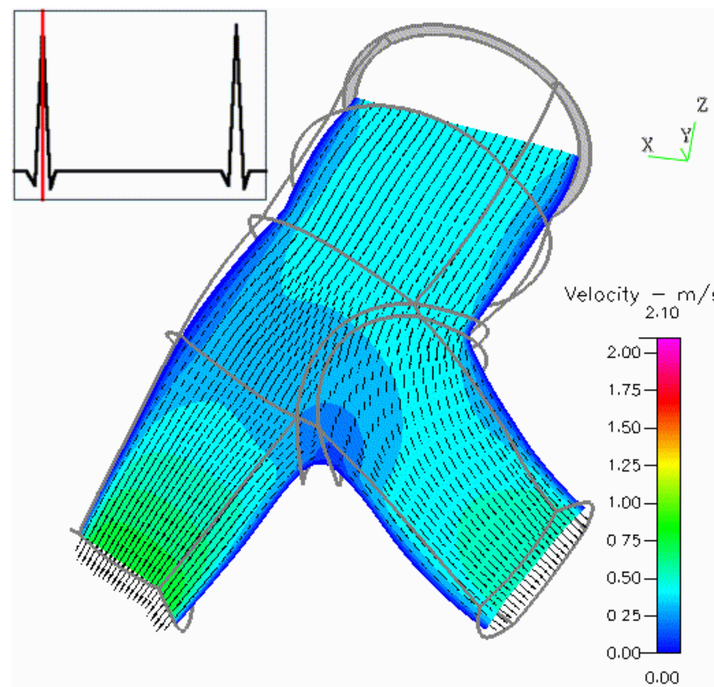
- **Sparse matrices** (vague definition): matrix with few non-zero entries.
- For practical purposes: an $m \times n$ matrix is sparse if it has $O(\min(m, n))$ non-zero entries.
- This means roughly a constant number of non-zero entries per row and column.
- Another definition: "matrices that allow special techniques to take advantage of the large number of zero elements" (J. Wilkinson)

Sparse Matrices: Goals

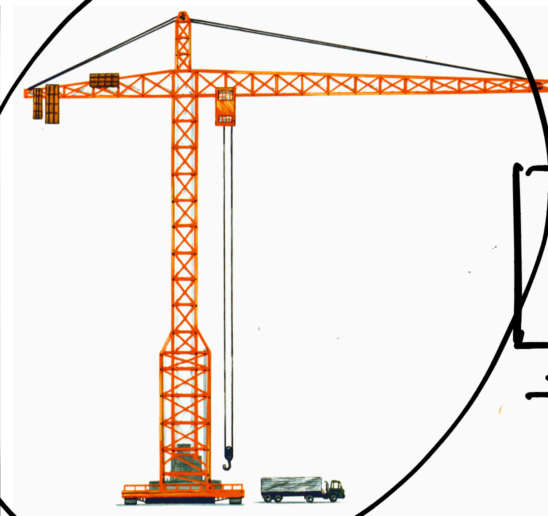
- **Perform standard matrix computations economically, i.e., without storing the zeros of the matrix.**

- For typical Finite Element and Finite Difference matrices, the number of non-zero entries is $O(n)$



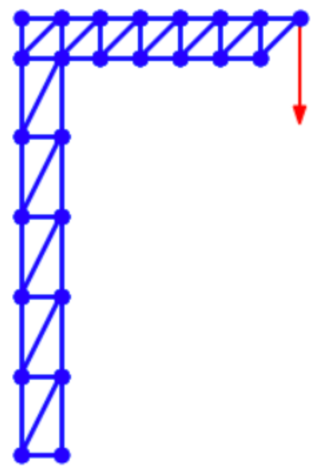


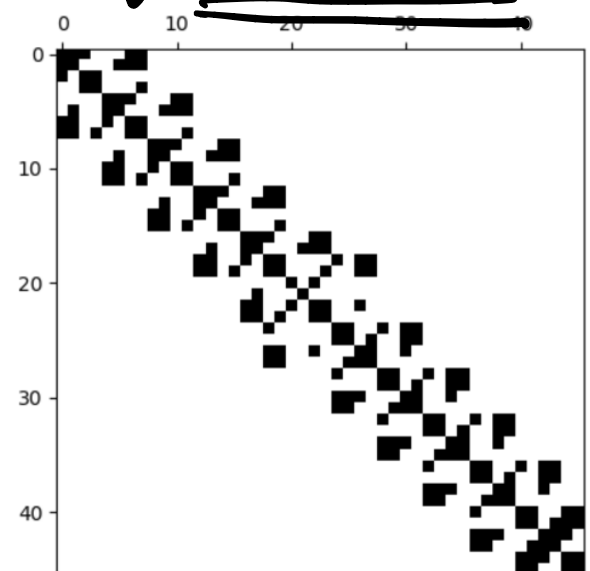
Sparse Matrices: MP example



$$\boxed{KU = F}$$

spy(K)





Sparse Matrices

$$\begin{bmatrix} A \\ n \times n \end{bmatrix} + \begin{bmatrix} B \\ n \times n \end{bmatrix}$$

EXAMPLE:

Number of operations required to add two square dense matrices:

$$O(n^2)$$

Number of operations required to add two sparse matrices **A** and **B**:

$$O(\mathrm{nnz}(\mathbf{A}) + \mathrm{nnz}(\mathbf{B}))$$

where $\mathrm{nnz}(\mathbf{X}) =$ number of non-zero elements of a matrix **X**

Popular Storage Structures

DNS	Dense	**ELL**	Ellpack-Itpack
BND	Linpack Banded	**DIA**	Diagonal
COO	Coordinate	**BSR**	Block Sparse Row
CSR	Compressed Sparse Row	**SSK**	Symmetric Skyline
CSC	Compressed Sparse Column	**BSR**	Nonsymmetric Skyline
MSR	Modified CSR	**JAD**	Jagged Diagonal
LIL	Linked List		

note: CSR = CRS, CCS = CSC, SSK = SKS in some references

We will focus on COO and CSR!

Dense (DNS)

$$A = \begin{bmatrix} 0. & 1.9 & 0. & -5.2 \\ 0.3 & 0. & 9.1 & 0. \\ 4.4 & 5.8 & 3.6 & 0. \\ 0. & 0. & 7.2 & 2.7 \end{bmatrix}$$

$$Ashape = (nrow, ncol)$$

$$A_{dense} = [\underbrace{0. \quad 1.9 \quad 0. \quad -5.2}_{\text{Row } 0} \quad \underbrace{0.3 \quad 0. \quad 9.1 \quad 0.}_{\text{Row } 1} \quad \underbrace{4.4 \quad 5.8 \quad 3.6 \quad 0.}_{\text{Row } 2} \quad \underbrace{0. \quad 0. \quad 7.2 \quad 2.7}_{\text{Row } 3}]$$

- Simple
- Row-wise
- Easy blocked formats
- Stores all the zeros

Coordinate Form (COO)

$$
\begin{array}{cc}
 & \begin{array}{cccc} 0 & 1 & 2 & 3 \end{array} \\
A = & \left[\begin{array}{cccc} 0. & 1.9 & 0. & -5.2 \\ 0.3 & 0. & 9.1 & 0. \\ 4.4 & 5.8 & 3.6 & 0. \\ 0. & 0. & 7.2 & 2.7 \end{array}\right]
\end{array}
\begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \end{array}
$$

floats

data = [1.9 -5.2 0.3 9.1 4.4 5.8 3.6 7.2 2.7]

row = [0 0 1 1 2 2 2 3 3]

col = [1 3 0 2 0 1 2 2 3]

int

data = [-5.2 9.1 3.6 2.7 ...]

row = [0 1 2 3 ....

col = [3 2 2 3 ---

- Simple
- Does not store the zero elements
- Not sorted
- *row* and *col*: array of integers
- *data*: array of doubles

Representing a Sparse Matrix in Coordinate (COO) Form

1 point

Consider the following matrix:

$$
A = \begin{array}{c c}
\begin{array}{ccc} 0 & 1 & 2 \end{array} & \\
\begin{bmatrix}
0 & 0 & 1.3 \\
\boxed{-1.5} & \boxed{0.2} & 0 \\
\boxed{5} & 0 & 0 \\
0 & \boxed{0.3} & \boxed{3} \\
0 & 0 & 0
\end{bmatrix} & \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array}
\end{array}
$$

$nnz(A) = 6$

Suppose we store one row index (a 32-bit integer), one column index (a 32-bit integer), and one data value (a 64-bit float) for each non-zero entry in A. How many bytes in total are stored? Please note that 1 byte is equal to 8 bits.

data = [1.3 0.2 5 -1.5 3 0.3]

col = [2 1 0 0 2 1]

row = [0 1 2 1 3 3]

6 floats + 6 integers

$(6 \times 64 + 12 \times 32)$ bits $= 96$ bytes

Compressed Sparse Row (CSR) format

$$
\begin{array}{c|c}
 & \begin{array}{cccc} 0 & 1 & 2 & 3 \end{array} \\
\begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \end{array} & A = \begin{bmatrix} 0. & 1.9 & 0. & -5.2 \\ 0. & 0. & 0. & 0. \\ 4.4 & 5.8 & 3.6 & 0. \\ 0. & 0. & 7.2 & 2.7 \end{bmatrix}
\end{array}
\quad
\begin{array}{c} 0 \rightarrow 2 \\ 1 \rightarrow 0 \\ 2 \rightarrow 3 \\ 3 \rightarrow 2 \end{array}
\quad 4 + 1 = 5
$$

nnz(A)

float

int

data = [1.9 -5.2 4.4 5.8 3.6 7.2 2.7]

col = [1 3 0 1 2 2 3]

rowptr = [0 2 2 5 7]

+2 +0 +3 +2

(nnz row 0)

nnz row 1

nnz row 2

nnz row 3

nrows + 1

Compressed Sparse Row (CSR)

$$A = \begin{bmatrix} 1 & 0 & 0 & 2 & 0 \\ 3 & 4 & 0 & 5 & 0 \\ 6 & 0 & 7 & 8 & 9 \\ 0 & 0 & 10 & 11 & 0 \\ 0 & 0 & 0 & 0 & 12 \end{bmatrix}$$

$$\begin{aligned} data &= [\ 1.0\ \ 2.0\ \ 3.0\ \ 4.0\ \ 5.0\ \ 6.0\ \ 7.0\ \ 8.0\ \ 9.0\ \ 10.0\ \ 11.0\ \ 12.0\ ] \\ col &= [\ 0\ \ 3\ \ 0\ \ 1\ \ 3\ \ 0\ \ 2\ \ 3\ \ 4\ \ 2\ \ 3\ \ 4\ ] \\ rowptr &= [\ 0\ \ 2\ \ 5\ \ 9\ \ 11\ \ 12\ ] \end{aligned}$$

- Does not store the zero elements
- Fast arithmetic operations between sparse matrices, and fast matrix-vector product
- *col*: contain the column indices (array of nnz integers)
- *data*: contain the non-zero elements (array of nnz doubles)
- *rowptr*: contain the row offset (array of $n+1$ integers)