Numerical Linear Algebra

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Fall 2022

Justification

Many algorithms are based in linear algebra, including some non-obvious ones such as graph algorithms. This session will mostly discuss aspects of solving linear systems, focusing on those that have computational ramifications.

Linear algebra

- Mathematical aspects: mostly linear system solving
- Practical aspects: even simple operations are hard
  - Dense matrix-vector product: scalability aspects
  - Sparse matrix-vector: implementation

Let's start with the math...

Two approaches to linear system solving

Solve $Ax = b$

Direct methods:

- Deterministic
- Exact up to machine precision
- Expensive (in time and space)

Iterative methods:

- Only approximate
- Cheaper in space and (possibly) time
- Convergence not guaranteed

Really bad example of direct method

Cramer's rule

write $|A|$ for determinant, then

$$x_i = \begin{vmatrix} a_{11} & a_{12} & \ldots & a_{1i-1} & b_1 & a_{1i+1} & \ldots & a_{1n} \\ a_{21} & & \ldots & & b_2 & & \ldots & a_{2n} \\ \vdots & & & & \vdots & & & \vdots \\ a_{n1} & & \ldots & & b_n & & \ldots & a_{nn} \end{vmatrix} / |A|$$

Time complexity $O(n!)$

Not a good method either

$$Ax = b$$

- Compute explicitly A^{-1},
- then $x \leftarrow A^{-1}b$.
- Numerical stability issues.
- Amount of work?

A close look linear system solving: direct methods

Gaussian elimination

Example

$$\begin{pmatrix} 6 & -2 & 2 \\ 12 & -8 & 6 \\ 3 & -13 & 3 \end{pmatrix} x = \begin{pmatrix} 16 \\ 26 \\ -19 \end{pmatrix}$$

$$\left[\begin{matrix} 6 & -2 & 2 & | & 16 \\ 12 & -8 & 6 & | & 26 \\ 3 & -13 & 3 & | & -19 \end{matrix}\right] \longrightarrow \left[\begin{matrix} 6 & -2 & 2 & | & 16 \\ 0 & -4 & 2 & | & -6 \\ 0 & -12 & 2 & | & -27 \end{matrix}\right] \longrightarrow \left[\begin{matrix} 6 & -2 & 2 & | & 16 \\ 0 & -4 & 2 & | & -6 \\ 0 & 0 & -4 & | & -9 \end{matrix}\right]$$

Solve x_3, then x_2, then x_1

$6, -4, -4$ are the 'pivots'

Gaussian elimination, step by step

$\langle LU$ factorization$\rangle$:

for $k = 1, n-1$:

$\langle$eliminate values in column $k\rangle$

$\langle$eliminate values in column $k\rangle$:

for $i = k+1$ to n:

$\langle$compute multiplier for row $i\rangle$

$\langle$update row $i\rangle$

$\langle$compute multiplier for row $i\rangle$

$a_{ik} \leftarrow a_{ik}/a_{kk}$

$\langle$update row $i\rangle$:

for $j = k+1$ to n:

$a_{ij} \leftarrow a_{ij} - a_{ik} * a_{kj}$

Gaussian elimination, all together

$\langle LU$ factorization$\rangle$:

for $k = 1, n-1$:
  for $i = k+1$ to n:
    $a_{ik} \leftarrow a_{ik}/a_{kk}$
    for $j = k+1$ to n:
      $a_{ij} \leftarrow a_{ij} - a_{ik} * a_{kj}$

Amount of work:

$$\sum_{k=1}^{n-1} \sum_{i,j>k} 1 = \sum_{k}^{n-1} (n-k)^2 \approx \sum_{k} k^2 \approx n^3/3$$

Pivoting

If a pivot is zero, exchange that row and another.
(there is always a row with a nonzero pivot if the matrix is nonsingular)
best choice is the largest possible pivot
in fact, that's a good choice even if the pivot is not zero:
partial pivoting
(full pivoting would be row *and* column exchanges)

Roundoff control

Consider

$$\begin{pmatrix} \varepsilon & 1 \\ 1 & 1 \end{pmatrix} x = \begin{pmatrix} 1+\varepsilon \\ 2 \end{pmatrix}$$

with solution $x = (1,1)^t$

Ordinary elimination:

$$\begin{pmatrix} \varepsilon & 1 \\ 0 & 1-\frac{1}{\varepsilon} \end{pmatrix} x = \begin{pmatrix} 1+\varepsilon \\ 2-\frac{1+\varepsilon}{\varepsilon} \end{pmatrix} = \begin{pmatrix} 1+\varepsilon \\ 1-\frac{1}{\varepsilon} \end{pmatrix}.$$

We can now solve x_2 and from it x_1:

$$\begin{cases} x_2 & = (1-\varepsilon^{-1})/(1-\varepsilon^{-1}) = 1 \\ x_1 & = \varepsilon^{-1}(1+\varepsilon-x_2) = 1 \end{cases}$$

Roundoff 2

If $\varepsilon < \varepsilon_{\mathrm{mach}}$, then in the rhs $1+\varepsilon \to 1$, so the system is:

$$\begin{pmatrix} \varepsilon & 1 \\ 1 & 1 \end{pmatrix} x = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

The solution $(1,1)$ is still correct!

Eliminating:

$$\begin{pmatrix} \varepsilon & 1 \\ 0 & 1-\varepsilon^{-1} \end{pmatrix} x = \begin{pmatrix} 1 \\ 2-\varepsilon^{-1} \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} \varepsilon & 1 \\ 0 & -\varepsilon^{-1} \end{pmatrix} x = \begin{pmatrix} 1 \\ -\varepsilon^{-1} \end{pmatrix}$$

Solving first x_2, then x_1, we get:

$$\begin{cases} x_2 & = \varepsilon^{-1}/\varepsilon^{-1} = 1 \\ x_1 & = \varepsilon^{-1}(1 - 1\cdot x_2) = \varepsilon^{-1}\cdot 0 = 0, \end{cases}$$

so x_2 is correct, but x_1 is completely wrong.

Roundoff 3

Pivot first:

$$\begin{pmatrix}1 & 1\\ \varepsilon & 1\end{pmatrix} x = \begin{pmatrix}2\\ 1+\varepsilon\end{pmatrix} \Rightarrow \begin{pmatrix}1 & 1\\ 0 & 1-\varepsilon\end{pmatrix} x = \begin{pmatrix}2\\ 1-\varepsilon\end{pmatrix}$$

Now we get, regardless the size of epsilon:

$$x_2 = \frac{1-\varepsilon}{1-\varepsilon} = 1, \qquad x_1 = 2 - x_2 = 1$$

LU factorization

Same example again:

$$A = \begin{pmatrix} 6 & -2 & 2 \\ 12 & -8 & 6 \\ 3 & -13 & 3 \end{pmatrix}$$

2nd row minus $2\times$ first; 3rd row minus $1/2\times$ first; equivalent to

$$L_1Ax = L_1b, \qquad L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix}$$

(elementary reflector)

LU 2

Next step: $L_2 L_1 A x = L_2 L_1 b$ with

$$L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{pmatrix}$$

Define $U = L_2 L_1 A$, then $A = LU$ with $L = L_1^{-1} L_2^{-1}$
'LU factorization'

LU 3

Observe:

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix} \qquad L_1^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1/2 & 0 & 1 \end{pmatrix}$$

Likewise

$$L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{pmatrix} \qquad L_2^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 3 & 1 \end{pmatrix}$$

Even more remarkable:

$$L_1^{-1} L_2^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1/2 & 3 & 1 \end{pmatrix}$$

Can be computed in place! (pivoting?)

Solve LU system

$Ax = b \longrightarrow LUx = b$ solve in two steps:
$Ly = b$, and $Ux = y$

Forward sweep:

$$\begin{pmatrix} 1 & & & \emptyset & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & & \ddots & & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \\ \vdots \\ b_n \end{pmatrix}$$

Solve LU system

$Ax = b \longrightarrow LUx = b$ solve in two steps:
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$$\begin{pmatrix} 1 & & & \emptyset & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & & \ddots & & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \\ \vdots \\ b_n \end{pmatrix}$$

$$y_1 = b_1, \quad y_2 = b_2 - \ell_{21} y_1, \ldots$$

Solve LU 2

Backward sweep:

$$\begin{pmatrix} u_{11} & u_{12} & \ldots & u_{1n} \\ & u_{22} & \ldots & u_{2n} \\ & & \ddots & \vdots \\ \emptyset & & & u_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

Solve LU 2

Backward sweep:

$$\begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ & u_{22} & \dots & u_{2n} \\ & & \ddots & \vdots \\ \emptyset & & & u_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$x_n = u_{nn}^{-1} y_n, \quad x_{n-1} = u_{n-1n-1}^{-1}(y_{n-1} - u_{n-1n}x_n), \dots$$

Computational aspects

Compare:

Matrix-vector product:

$$\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \leftarrow \begin{pmatrix} a_{11} & \ldots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \ldots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

Solving LU system:

$$\begin{pmatrix} a_{11} & & \emptyset \\ \vdots & \ddots & \\ a_{n1} & \ldots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

(and similarly the U matrix)

Compare operation counts. Can you think of other points of comparison? (Think modern computers.)

Short detour: Partial Differential Equations

Second order PDEs; 1D case

$$\begin{cases} -u''(x) = f(x) & x \in [a,b] \\ u(a) = u_a,\, u(b) = u_b \end{cases}$$

Second order PDEs; 1D case

$$\begin{cases} -u''(x) = f(x) & x \in [a,b] \\ u(a) = u_a,\, u(b) = u_b \end{cases}$$

Using Taylor series:

$$u(x+h) + u(x-h) = 2u(x) + u''(x)h^2 + u^{(4)}(x)\frac{h^4}{12} + \cdots$$

so

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + O(h^2)$$

Numerical scheme:

$$-\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = f(x, u(x), u'(x))$$

This leads to linear algebra

$$-u_{xx} = f \to \frac{2u(x) - u(x+h) - u(x-h)}{h^2} = f(x, u(x), u'(x))$$

Equally spaced points on $[0,1]$: $x_k = kh$ where $h = 1/(n+1)$, then

$$-u_{k+1} + 2u_k - u_{k-1} = -h^2 f(x_k, u_k, u_k') \quad \text{for } k = 1, \ldots, n$$

Written as matrix equation:

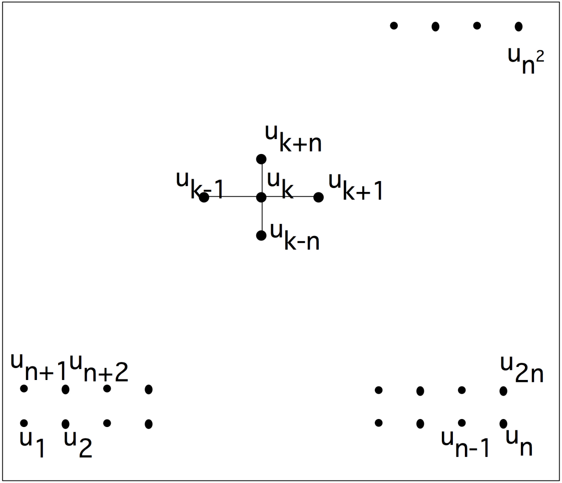
$$\begin{pmatrix} 2 & -1 & & \emptyset \\ -1 & 2 & -1 & \\ \emptyset & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} f_1 + u_0 \\ f_2 \\ \vdots \end{pmatrix}$$

Second order PDEs; 2D case

$$\begin{cases} -u_{xx}(\bar{x}) - u_{yy}(\bar{x}) = f(\bar{x}) & x \in \Omega = [0,1]^2 \\ u(\bar{x}) = u_0 & \bar{x} \in \delta\Omega \end{cases}$$

Now using central differences in both x and y directions.

The stencil view of things



Sparse matrix from 2D equation

$$
\left(\begin{array}{ccccc|ccccc|cc}
4 & -1 & & & \emptyset & -1 & & & & \emptyset & & \\
-1 & 4 & 1 & & & & -1 & & & & & \\
 & \ddots & \ddots & \ddots & & & & \ddots & & & & \\
 & & \ddots & \ddots & -1 & & & & \ddots & & & \\
\emptyset & & & -1 & 4 & \emptyset & & & & -1 & & \\
\hline
-1 & & & & \emptyset & 4 & -1 & & & & -1 & \\
 & -1 & & & & -1 & 4 & -1 & & & & -1 \\
 & \uparrow & \ddots & & & \uparrow & \uparrow & \uparrow & & & & \uparrow \\
 & k-n & & & & k-1 & k & k+1 & & -1 & & k+n \\
 & & & & -1 & & & & -1 & 4 & & \\
\hline
 & & & & & \ddots & & & & & \ddots &
\end{array}\right)
$$

The stencil view is often more insightful.

Matrix properties

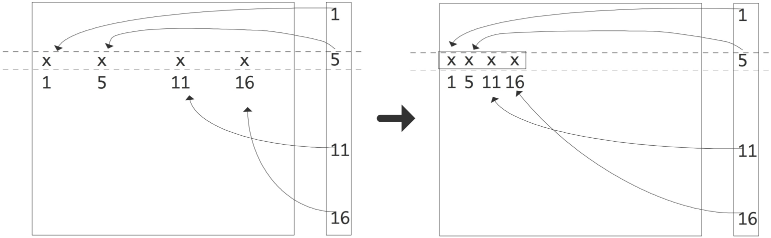
- Very sparse, banded
- Factorization takes less than n^2 space, n^3 work
- Symmetric (only because 2nd order problem)
- Sign pattern: positive diagonal, nonpositive off-diagonal (true for many second order methods)
- Positive definite (just like the continuous problem)
- Constant diagonals: only because of the constant coefficient differential equation
- Factorization: lower complexity than dense, recursion length less than N.

Sparse matrices

Sparse matrix storage

Matrix above has many zeros: n^2 elements but only $O(n)$ nonzeros. Big waste of space to store this as square array.

Matrix is called 'sparse' if there are enough zeros to make specialized storage feasible.



Compressed Row Storage

$$A = \begin{pmatrix} 10 & 0 & 0 & 0 & -2 & 0 \\ 3 & 9 & 0 & 0 & 0 & 3 \\ 0 & 7 & 8 & 7 & 0 & 0 \\ 3 & 0 & 8 & 7 & 5 & 0 \\ 0 & 8 & 0 & 9 & 9 & 13 \\ 0 & 4 & 0 & 0 & 2 & -1 \end{pmatrix} . \tag{1}$$

Compressed Row Storage (CRS): store all nonzeros by row, their column indices, pointers to where the columns start (1-based indexing):

`val`	10	-2	3	9	3	7	8	7	$3 \cdots 9$	13	4	2	-1
`col_ind`	1	5	1	2	6	2	3	4	$1 \cdots 5$	6	2	5	6

`row_ptr`	1	3	6	9	13	17	20

.

Sparse matrix-vector operations

- Simplest, and important in many contexts: matrix-vector product.
- Matrix-matrix product rare in engineering science
  very important in Deep Learning
- Gaussian elimination is a complicated story.
- In general: changes to sparse structure are hard!

Dense matrix-vector product

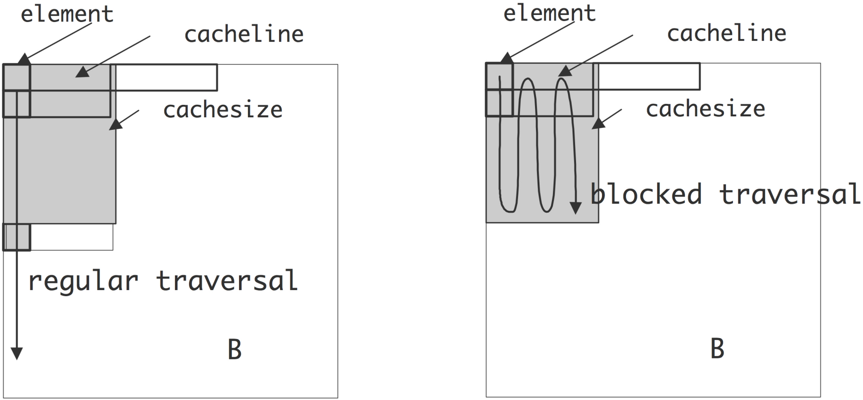
Most common operation in many cases: matrix-vector product

```
aptr = 0;
for (row=0; row<nrows; row++) {
   s = 0;
   for (col=0; col<ncols; col++) {
      s += a[aptr] * x[col];
      aptr++;
   }
   y[row] = s;
}
```

Reuse? Locality? Cachelines?

Better implementation

Three loops: block, columns inside block, row;
permute blocks to outermost



Sparse matrix-vector product

```
aptr = 0;
for (row=0; row<nrows; row++) {
  s = 0;
  for (icol=ptr[row]; icol<ptr[row+1]; icol++) {
    int col = ind[icol];
    s += a[aptr] * x[col];
    aptr++;
  }
  y[row] = s;
}
```

Again: Reuse? Locality? Cachelines?

Indirect addressing of `x` gives low spatial and temporal locality.

Exercise: sparse coding

What if you need access to both rows and columns at the same time? Implement an algorithm that tests whether a matrix stored in CRS format is symmetric. Hint: keep an array of pointers, one for each row, that keeps track of how far you have progressed in that row.

Fill-in

Remember Gaussian elimination algorithm:

for $k = 1, n-1$:
  for $i = k+1$ to n:
    for $j = k+1$ to n:
      $a_{ij} \leftarrow a_{ij} - a_{ik} * a_{kj} / a_{kk}$

Fill-in: index (i,j) where $a_{ij} = 0$ originally, but gets updated to non-zero. (and so $\ell_{ij} \neq 0$ or $u_{ij} \neq 0$.)

Change in the sparsity structure! How do you deal with that?

LU of a sparse matrix

$$\begin{pmatrix} 2 & -1 & 0 & \ldots \\ -1 & 2 & -1 \\ 0 & -1 & 2 & -1 \\ & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \Rightarrow \left(\begin{array}{c|cccc} 2 & -1 & 0 & \ldots \\ \hline 0 & 2-\frac{1}{2} & -1 \\ 0 & -1 & 2 & -1 \\ & \ddots & \ddots & \ddots & \ddots \end{array}\right)$$

How does this continue by induction?

Observations?

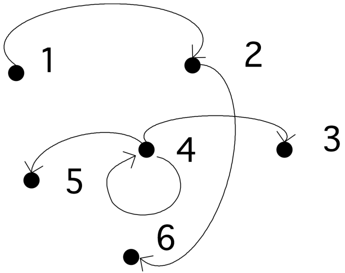
LU of a sparse matrix

$$\left(\begin{array}{ccccc:ccc}
4 & -1 & 0 & \ldots & & -1 & & \\
-1 & 4 & -1 & 0 & \ldots & 0 & -1 & \\
& \ddots & \ddots & \ddots & & & \ddots & \\
\hdashline
-1 & 0 & \ldots & & & 4 & -1 & \\
0 & -1 & 0 & \ldots & & -1 & 4 & -1
\end{array}\right)$$

$$\Rightarrow \quad \left(\begin{array}{c|cccc:ccc}
4 & -1 & 0 & \ldots & & -1 & & \\
\hline
& 4-\frac{1}{4} & -1 & 0 & \ldots & -1/4 & -1 & \\
& \ddots & \ddots & \ddots & & & \ddots & \\
\hdashline
& -1/4 & \ldots & & & 4-\frac{1}{4} & -1 & \\
& -1 & 0 & \ldots & & -1 & 4 & -1
\end{array}\right)$$

A little graph theory

Graph is a tuple $G = \langle V, E \rangle$ where $V = \{v_1, \ldots v_n\}$ for some n, and $E \subset \{(i,j) \colon 1 \leq i,j \leq n,\, i \neq j\}$.

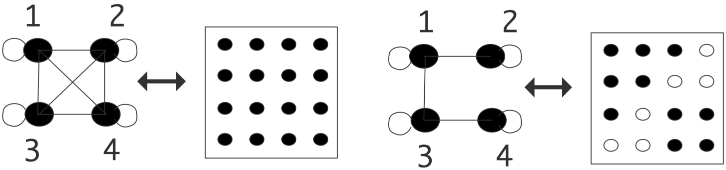


$$\begin{cases} V = \{1,2,3,4,5,6\} \\ E = \{(1,2),(2,6),(4,3),(4,4),(4,5)\} \end{cases}$$

Graphs and matrices

For a graph $G = \langle V, E \rangle$, the adjacency matrix M is defined by

$$M_{ij} = \begin{cases} 1 & (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$

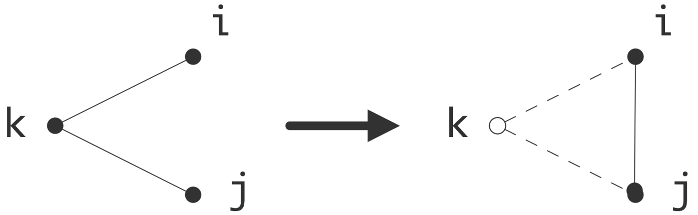


A dense and a sparse matrix, both with their adjacency graph

Fill-in

Fill-in: index (i,j) where $a_{ij} = 0$ originally, but gets updated to non-zero.

$$a_{ij} \leftarrow a_{ij} - a_{ik} * a_{kj} / a_{kk}$$

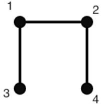


Eliminating a vertex introduces a new edge in the quotient graph

LU of sparse matrix, with graph view: 1

Original matrix.

3

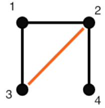


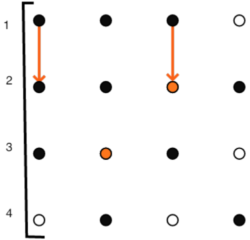
$$
\begin{array}{c}
1 \\ 2 \\ 3 \\ 4
\end{array}
\begin{bmatrix}
\bullet & \bullet & \bullet & \circ \\
\bullet & \bullet & \circ & \bullet \\
\bullet & \circ & \bullet & \circ \\
\circ & \bullet & \circ & \bullet
\end{bmatrix}
$$

LU of sparse matrix, with graph view: 2

Eliminating $(2,1)$ causes fill-in at $(2,3)$.

3

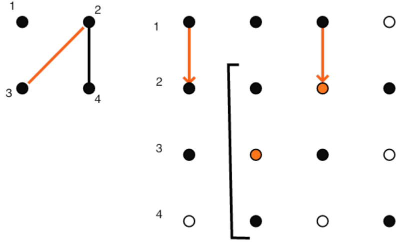




LU of sparse matrix, with graph view: 3

Remaining matrix when step 1 finished.

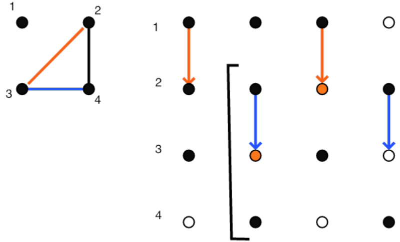
3



LU of sparse matrix, with graph view: 4

Eliminating $(3,2)$ fills $(3,4)$

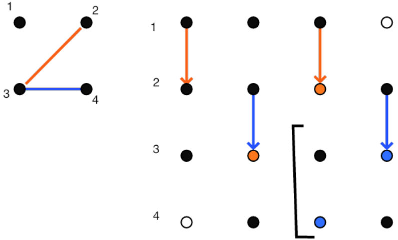
3



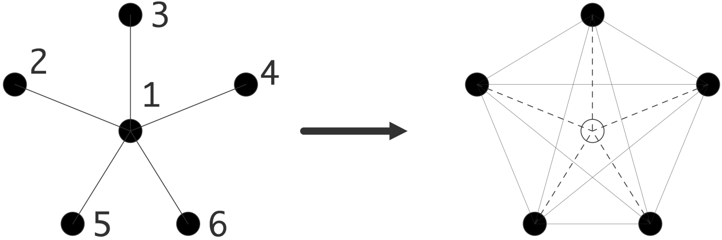
LU of sparse matrix, with graph view: 5

After step 2

3



Fill-in is a function of ordering



$$\begin{pmatrix} * & * & \cdots & * \\ * & * & & \emptyset \\ \vdots & & \ddots & \\ * & \emptyset & & * \end{pmatrix}$$

After factorization the matrix is dense.

Can this be permuted?

Exercise: LU of a penta-diagonal matrix

Consider the matrix

$$\begin{pmatrix} 2 & 0 & -1 \\ 0 & 2 & 0 & -1 \\ -1 & 0 & 2 & 0 & -1 \\ & -1 & 0 & 2 & 0 & -1 \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

Describe the *LU* factorization of this matrix:

- Convince yourself that there will be no fill-in. Give an inductive proof of this.
- What does the graph of this matrix look like? (Find a tutorial on graph theory. What is a name for such a graph?)
- Can you relate this graph to the answer on the question of the fill-in?

Exercise: LU of a band matrix

Suppose a matrix A is banded with *halfbandwidth* p:

$$a_{ij} = 0 \quad \text{if } |i-j| > p$$

Derive how much space an LU factorization of A will take if no pivoting is used. (For bonus points: consider partial pivoting.)

Can you also derive how much space the inverse will take? (Hint: if $A = LU$, does that give you an easy formula for the inverse?)