

Numerical Linear Algebra

Victor Eijkhout and Lars Koesterke

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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

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

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

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

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

Solve x_3 , then x_2 , then x_1

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

Gaussian elimination, step by step

$\langle LU \text{ factorization} \rangle$:

for $k = 1, n - 1$:

$\langle \text{eliminate values in column } k \rangle$

$\langle \text{eliminate values in column } k \rangle$:

for $i = k + 1$ to n :

$\langle \text{compute multiplier for row } i \rangle$

$\langle \text{update row } i \rangle$

$\langle \text{compute multiplier for row } i \rangle$

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

$\langle \text{update row } i \rangle$:

for $j = k + 1$ to n :

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

Gaussian elimination, all together

$\langle LU \text{ factorization} \rangle$:

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 $\epsilon < \epsilon_{\text{mach}}$, then in the rhs $1 + \epsilon \rightarrow 1$, so the system is:

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

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

Eliminating:

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

Solving first x_2 , then x_1 , we get:

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

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:

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

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

$$L_1 A x = L_1 b, \quad L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix}$$

(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:

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

Likewise

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

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:

$$\begin{pmatrix} 1 & & & & 0 \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & & \ddots & & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Solve LU system

$Ax = b \longrightarrow LUX = b$ solve in two steps:

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

Solve LU 2

Backward sweep:

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

Solve LU 2

Backward sweep:

$$\begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ & u_{22} & \dots & u_{2n} \\ & & \ddots & \vdots \\ 0 & & & u_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

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

Computational aspects

Compare:

Matrix-vector product:

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

Solving LU system:

$$\begin{pmatrix} a_{11} & & 0 \\ \vdots & \ddots & \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

(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:

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

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

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

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

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

Written as matrix equation:

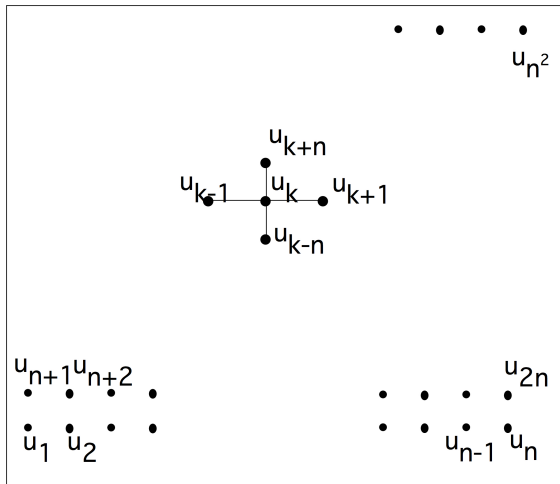
$$\begin{pmatrix} 2 & -1 & 0 & \\ -1 & 2 & -1 & \\ 0 & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} f_1 + u_0 \\ f_2 \\ \vdots \end{pmatrix}$$

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

$$\left(\begin{array}{cccc|cccc|c} 4 & -1 & & & 0 & -1 & & & 0 \\ -1 & 4 & 1 & & & & -1 & & \\ & \ddots & \ddots & \ddots & & & & \ddots & \\ & & \ddots & \ddots & -1 & & & & \\ 0 & & & -1 & 4 & 0 & & -1 & \\ \hline -1 & & & & 0 & 4 & -1 & & -1 \\ & -1 & & & & -1 & 4 & -1 & \\ & \uparrow & \ddots & & & \uparrow & \uparrow & \uparrow & \\ & k-n & & & & k-1 & k & k+1 & -1 \\ & & & & -1 & & & -1 & 4 \\ \hline & & & & & \ddots & & & \ddots \end{array} \right)$$

The stencil view is often more insightful.

Matrix properties

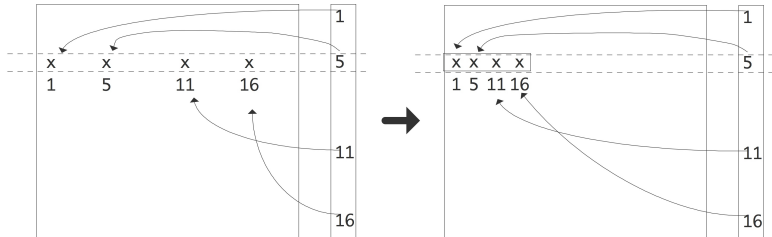
- Very sparse, banded
- Factorization takes less than n^2 space, n^3 work
- Symmetric (only because 2nd order problem)
- Sign pattern: positive diagonal, nonpositive off-diagonal (true for many second order methods)
- Positive definite (just like the continuous problem)
- Constant diagonals: only because 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

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

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 ... 9	13	4	2	-1
col_ind	1	5	1	2	6	2	3	4	1 ... 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

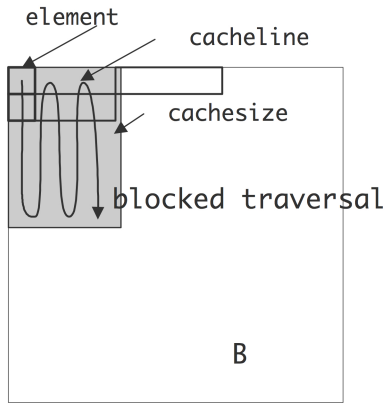
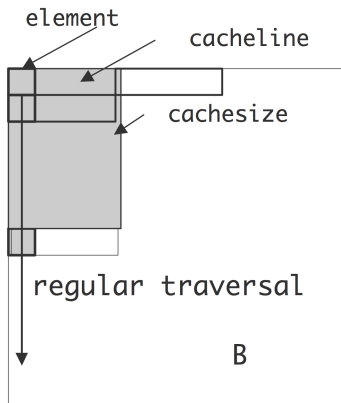
Most common operation in many cases: matrix-vector product

```
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

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

How does this continue by induction?

Observations?

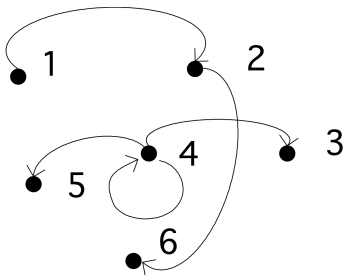
LU of a sparse matrix

$$\Rightarrow \left(\begin{array}{cccc|cc} 4 & -1 & 0 & \dots & -1 \\ -1 & 4 & -1 & 0 & \dots & 0 & -1 \\ & \ddots & \ddots & \ddots & & & \\ -1 & 0 & \dots & & 4 & -1 \\ 0 & -1 & 0 & \dots & -1 & 4 & -1 \end{array} \right)$$

$$\Rightarrow \left(\begin{array}{c|cccc|cc} 4 & -1 & 0 & \dots & -1 \\ \hline & 4 - \frac{1}{4} & -1 & 0 & \dots & -1/4 & -1 \\ & \ddots & \ddots & \ddots & & & \\ -1/4 & \dots & & & 4 - \frac{1}{4} & -1 \\ \hline & -1 & 0 & \dots & -1 & 4 & -1 \end{array} \right)$$

A little graph theory

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

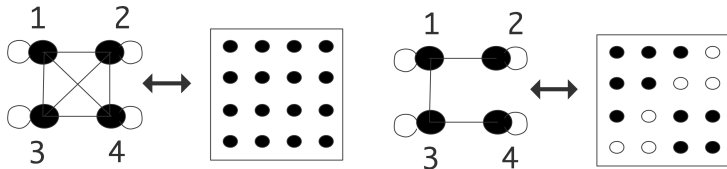


$$\begin{cases} V = \{1, 2, 3, 4, 5, 6\} \\ E = \{(1, 2), (2, 6), (4, 3), (4, 4), (4, 5)\} \end{cases}$$

Graphs and matrices

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

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

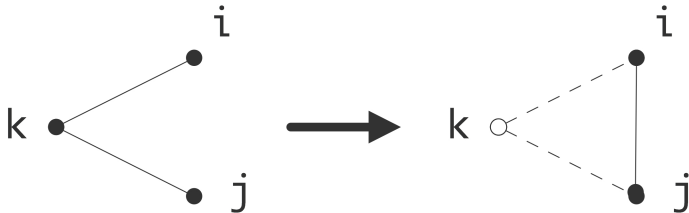


A dense and a sparse matrix, both with their adjacency graph

Fill-in

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

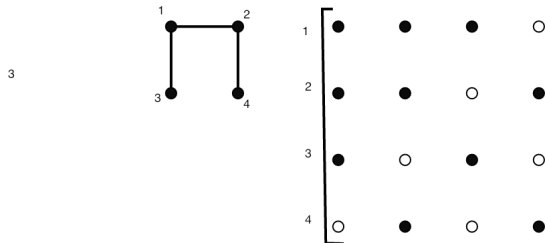
$$a_{ij} \leftarrow a_{ij} - a_{ik} * a_{kj} / a_{kk}$$



Eliminating a vertex introduces a new edge in the quotient graph

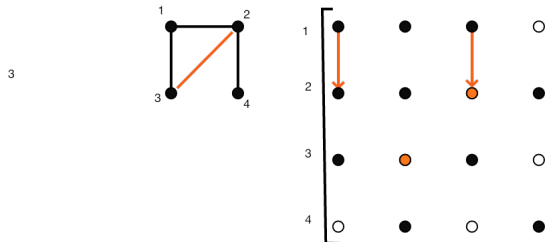
LU of sparse matrix, with graph view: 1

Original matrix.



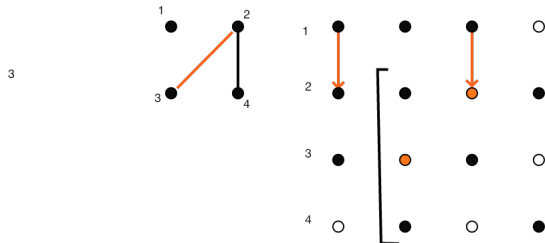
LU of sparse matrix, with graph view: 2

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



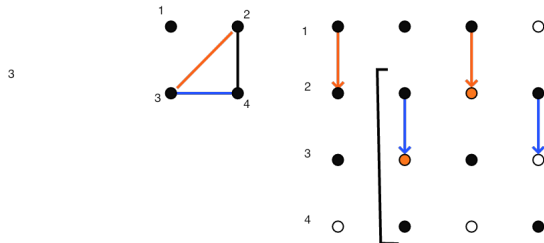
LU of sparse matrix, with graph view: 3

Remaining matrix when step 1 finished.



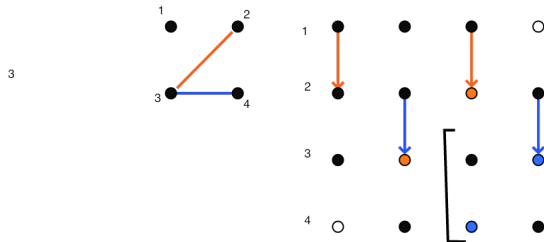
LU of sparse matrix, with graph view: 4

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

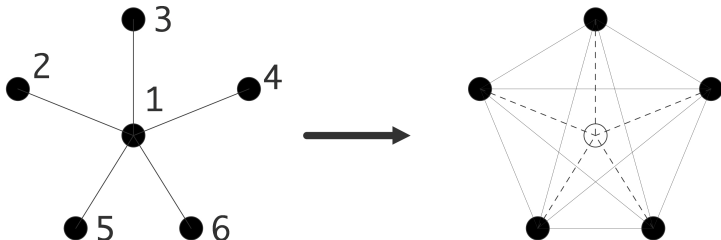


LU of sparse matrix, with graph view: 5

After step 2



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?)