Sparse matrices

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Boundary value problems

Consider in 1D

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

in 2D:

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

Approximation of 2nd order derivatives

Taylor series (write h for δx):

$$u(x+h) = u(x) + u'(x)h + u''(x)\frac{h^2}{2!} + u'''(x)\frac{h^3}{3!} + u^{(4)}(x)\frac{h^4}{4!} + u^{(5)}(x)\frac{h^5}{5!} + \cdots$$

and

$$u(x-h) = u(x) - u'(x)h + u''(x)\frac{h^2}{2!} - u'''(x)\frac{h^3}{3!} + u^{(4)}(x)\frac{h^4}{4!} - u^{(5)}(x)\frac{h^5}{5!} + \cdots$$

Subtract:

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

so

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

Numerical scheme:

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

(2nd order PDEs are very common!)

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

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

Written as matrix equation:

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

Matrix properties

- Very sparse, banded
- 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 (from constant coefficients in the DE)

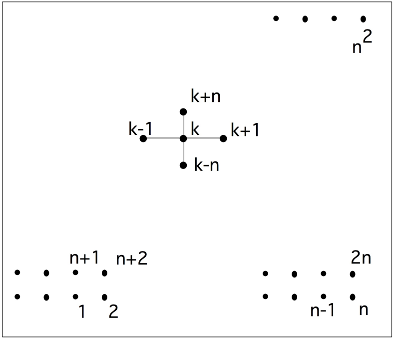
Sparse matrix in 2D case

Sparse matrices so far were tridiagonal: only in 1D case.

Two-dimensional: $-u_{xx} - u_{yy} = f$ on unit square $[0,1]^2$

Difference equation:

$$4u(x,y) - u(x+h,y) - u(x-h,y) - u(x,y+h) - u(x,y-h) = h^2 f(x,y)$$



This is a graph!

The graph view of things

Poisson eq:

$$4u_k - u_{k-1} - u_{k+1} - u_{k-n} - u_{k+n} = f_k$$

Consider a graph where $\{u_k\}_k$ are the edges
and (u_i, u_j) is an edge iff $a_{ij} \neq 0$.

This is the (adjacency) graph of a sparse matrix.

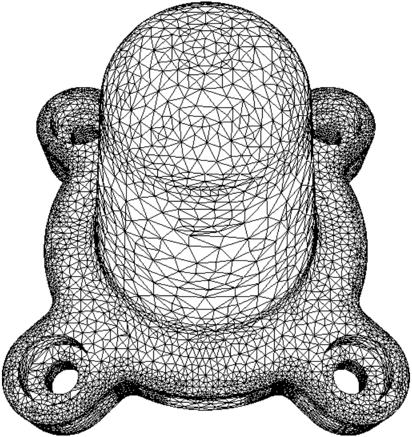
Sparse matrix from 2D equation

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

Matrix properties

- Very sparse, banded
- 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

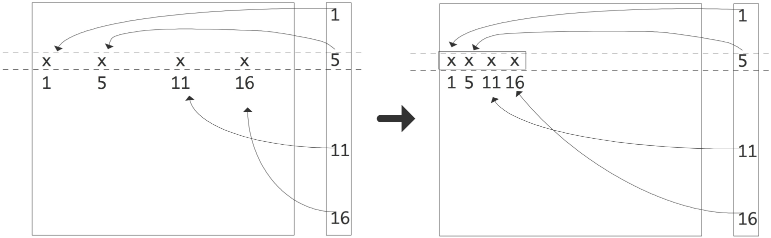
Realistic meshes



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 operations

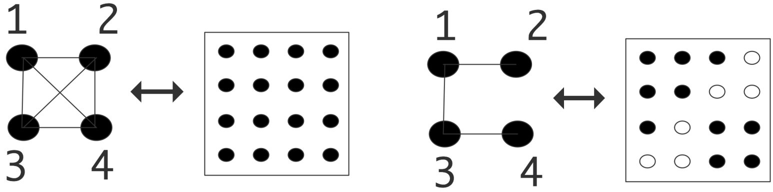
Most common operation: matrix-vector product

```
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;
}
```

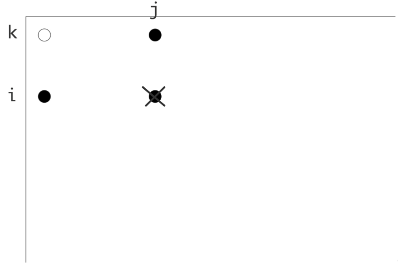
Operations with changes to the nonzero structure are much harder!

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

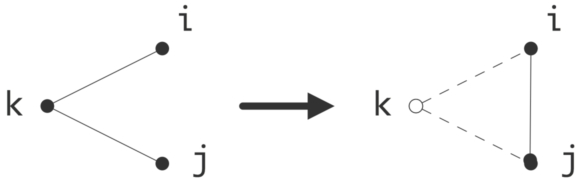
Graph theory of sparse matrices



Graph theory of sparse elimination



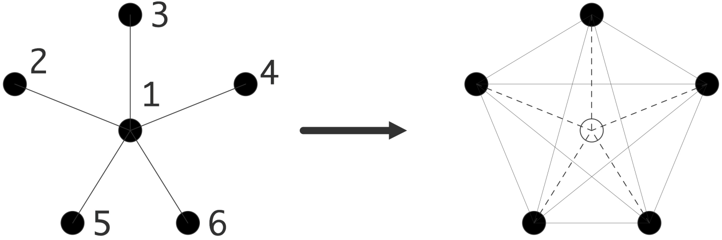
$$a_{ij} \leftarrow a_{ij} - a_{ik} a_{kk}^{-1} a_{kj}$$



Fill-in

Fill-in: index (i,j) where $a_{ij}=0$ but $\ell_{ij}\neq 0$ or $u_{ij}\neq 0$.

Fill-in is a function of ordering



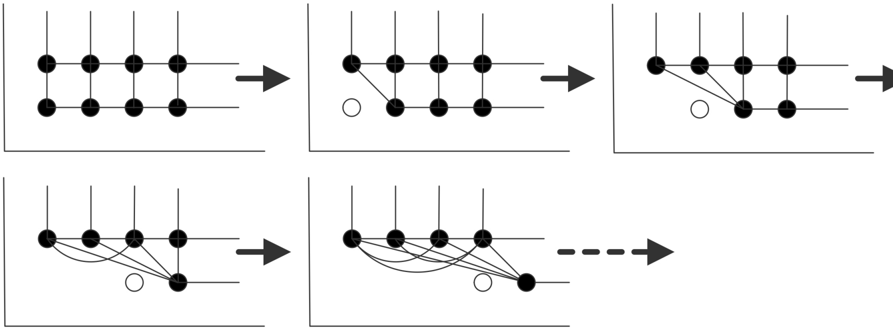
$$\begin{pmatrix} * & * & \cdots & * \\ * & * & & \emptyset \\ \vdots & & \ddots & \\ * & \emptyset & & * \end{pmatrix}$$

After factorization the matrix is dense.
Can this be permuted?

LU of a sparse matrix

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

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



Remaining matrix has a dense leading block

Fill-in during LU

2D BVP: Ω is $n \times n$, gives matrix of size $N = n^2$, with bandwidth n.

Matrix storage $O(N)$

LU storage $O(N^{3/2})$

LU factorization work $O(N^2)$

Cute fact: storage can be computed linear in #nonzeros