MA5233 Computational Mathematics

Lecture 7: Sparse LU Factorisation

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Sparse LU Factorisation

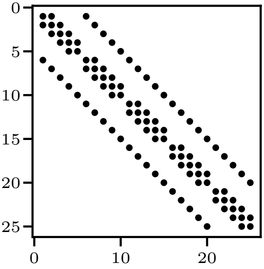
Recap from previous lectures

Poission equation in 1D:

- Tridiagonal system of equations.
- LU factorisation can be performed in $\mathcal{O}(n)$ operations and memory.

Poission equation in 2D:

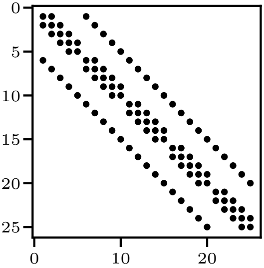
- More complicated sparsity pattern.
- Can LU factorisation still be done efficiently?



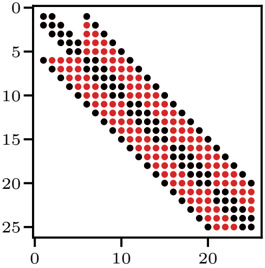
Sparse LU Factorisation

Bad news

- LU factors have more nonzero entries than original matrix.
- These extra entries in L, U are called *fill-in*.
- Fill-in significantly increases the memory consumption and workload of sparse LU factorisation.



Δ_n



$L + U$

Sparse LU Factorisation

Aim for this lecture

- Understand how fill-in arises.
- Find ways to reduce fill-in as much as possible.

Terminology

Let $A = \texttt{sparse(i,j,v)} = LU$ be a sparse matrix with coordinate-list vectors i, j, v. We introduce the following terms.

- *Structure of* `A`*:* the vectors i, j but not v.
- *Structurally nonzero fill-in entries:*
  entries $L[i,j]$, $U[i,j]$ which are nonzero for some v.

In the following, all statements of the form $A[i,j] \neq 0$ are meant in the structural sense.

Sparse LU Factorisation

Example

Consider

$$A_1 := \begin{pmatrix} 1 & & 1 & \\ & 1 & 1 & \\ & & 1 & \\ 1 & 1 & & 1 \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ 1 & 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} 1 & & 1 & \\ & 1 & 1 & \\ & & 1 & \\ & & & 1 \end{pmatrix} =: L_1 U_1,$$

$$A_2 := \begin{pmatrix} 1 & & 1 & \\ & -1 & 1 & \\ & & 1 & \\ 1 & 1 & & 1 \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ 1 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & & 1 & \\ & 1 & 1 & \\ & & 1 & \\ & & & 1 \end{pmatrix} =: L_2 U_2.$$

- A_1 and A_2 have the same *structure*.
- $L_2[4,3] = 0$ is *structurally nonzero* since $L_1[4,3] \neq 0$.

Sparse LU Factorisation

Graph of a sparse matrix $A \in \mathbb{K}^{n \times n}$

Graph $G(A) := \big(V(A), E(A)\big)$ defined by

$$V(A) := \{1, \dots, n\}, \qquad E(A) := \big\{ j \to i \mid A[i,j] \neq 0 \big\}.$$

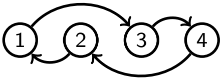
Note transpose in $E(A)$: entry $A[i,j]$ corresponds to edge $j \to i$.

Path in $G = (V, E)$

Ordered sequence $k_0, \dots, k_p \in V$ such that $k_{q-1} \to k_q \in E$ for all q.
Number of edges p is called the length of the path.

Example

$$A = \begin{pmatrix} 1 & \bullet & & \\ & 2 & & \bullet \\ \bullet & & 3 & \\ & & \bullet & 4 \end{pmatrix}$$

$G(A) =$ 

$2 \to 1 \to 3$ is a path of length 2.

Sparse LU Factorisation

Path theorem for matrix powers

$$A^p[i,j] \neq 0 \quad \iff \quad \exists \text{ path } j \to i \text{ of length } p.$$

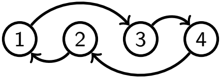
Proof.

$$A^p[i,j] = \sum_{k_{p-1}} \dots \sum_{k_1} A[i, k_{p-1}] \, \dots \, A[k_a, k_{a-1}] \, \dots \, A[k_1, j].$$

Each term is nonzero iff $j \to k_1 \to \dots \to k_{p-1} \to i$ is a path in $G(A)$.

Example (continued)

$$A^2 = \begin{pmatrix} 1 & \bullet & & \bullet \\ & 2 & \bullet & \bullet \\ \bullet & \bullet & 3 & \\ \bullet & & \bullet & 4 \end{pmatrix}$$

$G(A) =$ 

$A^2[4,1] \neq 0$ because $1 \to 3 \to 4$ is a path of length 2 in $G(A)$.
$A^2[2,1] = 0$ because $1 \to 3 \to 4 \to 2$ is a path of length 3 in $G(A)$.

Sparse LU Factorisation

Path theorem for matrix inverses

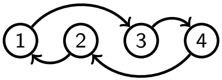
$$A^{-1}[i,j] \neq 0 \quad \iff \quad \exists \text{ path } j \to i.$$

Proof.

- $A^{-1} = p(A)$ for polynomial $p(x)$ interpolating $\frac{1}{x}$ on eigenvalues of A.
- Hence entry (i,j) of $A^{-1} = \sum_{p=0}^{n-1} c_p\, A^p$ is nonzero if there is a path $j \to i$ of arbitrary length.

Example (continued)

$$A^{-1} = \begin{pmatrix} 1 & \bullet & \bullet & \bullet \\ \bullet & 2 & \bullet & \bullet \\ \bullet & \bullet & 3 & \bullet \\ \bullet & \bullet & \bullet & 4 \end{pmatrix}$$

$G(A) =$ 

$A^{-1}[2,1] \neq 0$ because $1 \to 3 \to 4 \to 2$ is a path in $G(A)$.

Sparse LU Factorisation

Corollaries of path theorem

- If $G(A)$ is connected (there exists a path between any pair of vertices), then A^{-1} is dense.
- If $G(A)$ is disconnected, i.e. $A = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}$, then $A^{-1} = \begin{pmatrix} A_{11}^{-1} & 0 \\ 0 & A_{22}^{-1} \end{pmatrix}$.
- Inverse of upper/lower triangular matrix is upper/lower triangular.

Sparse LU Factorisation

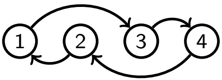
Fill path
Path $i \to k_1 \to \ldots \to k_p \to j$ in $G(A)$ such that $k_1, \ldots, k_p < \min\{i, j\}$.

Fill Path Theorem

$$(L+U)[i,j] \neq 0 \quad \iff \quad \exists \text{ fill path } j \to i.$$

Example (continued)

$$L + U = \begin{pmatrix} 1 & \bullet & & \\ & 2 & & \bullet \\ \bullet & \color{red}{\bullet} & 3 & \\ & & \bullet & 4 \end{pmatrix}$$

$G(A) =$ 

$L[3,2] \neq 0$ because $2 \to 1 \to 3$ is a fill path in $G(A)$.
$L[4,1] = 0$ because $1 \to 3 \to 4$ is not a fill path in $G(A)$.

Sparse LU Factorisation

Lemma

Let $i, j \in \{1, \dots, n\}$ and set $\ell := \big\{1, \dots, \min\{i, j\} - 1\big\}$. Then,

$$\begin{aligned} U[i,j] &= A[i,j] - A[i,\ell]\,A[\ell,\ell]^{-1}\,A[\ell,j] && \text{for } i \le j, \\ U[j,j]\,L[i,j] &= A[i,j] - A[i,\ell]\,A[\ell,\ell]^{-1}\,A[\ell,j] && \text{for } i \ge j. \end{aligned}$$

Proof. Block LU factorisation with $\bar{r} := \big\{\min\{i,j\}, \dots, n\big\}$:

$$\begin{pmatrix} A[\ell,\ell] & A[\ell,\bar{r}] \\ A[\bar{r},\ell] & A[\bar{r},\bar{r}] \end{pmatrix} = \begin{pmatrix} I & \\ A[\bar{r},\ell]\,A[\ell,\ell]^{-1} & I \end{pmatrix} \begin{pmatrix} A[\ell,\ell] & A[\ell,\bar{r}] \\ & A[\bar{r},\bar{r}] - A[\bar{r},\ell]\,A[\ell,\ell]^{-1}\,A[\ell,\bar{r}] \end{pmatrix}.$$

Let $\quad L_1 U_1 = A[\ell,\ell], \quad L_2 U_2 = A[\bar{r},\bar{r}] - A[\bar{r},\ell]\,A[\ell,\ell]^{-1}\,A[\ell,\bar{r}].$

Full factorisation is then given by

$$\begin{pmatrix} A[\ell,\ell] & A[\ell,\bar{r}] \\ A[\bar{r},\ell] & A[\bar{r},\bar{r}] \end{pmatrix} = \begin{pmatrix} L_1 & \\ A[\bar{r},\ell]\,A[\ell,\ell]^{-1} L_1 & L_2 \end{pmatrix} \begin{pmatrix} U_1 & L_1^{-1}\,A[\ell,\bar{r}] \\ & U_2 \end{pmatrix}.$$

Claim follows by noting that $L[i,j] = L_2[i,j]$ and $U[i,j] = U_2[i,j]$ have the given form.

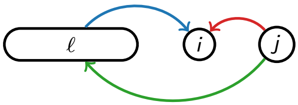
Sparse LU Factorisation

Fill Path Theorem (repeated from previous slide)

$$(L+U)[i,j] \neq 0 \quad \Longleftrightarrow \quad \exists \text{ fill path } j \to i.$$

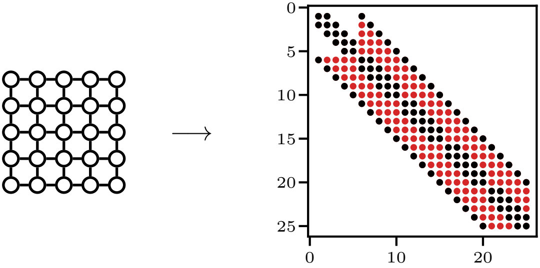
Proof. Follows immediately from

$$\begin{aligned} U[i,j] &= A[i,j] - A[i,\ell]\, A[\ell,\ell]^{-1}\, A[\ell,j] && \text{for } i \le j, \\ U[j,j]\, L[i,j] &= A[i,j] - A[i,\ell]\, A[\ell,\ell]^{-1}\, A[\ell,j] && \text{for } i \ge j. \end{aligned}$$



Sparse LU Factorisation

Corollary for 2d Laplacian ($n \times n$ grid, $N := n^2$ degrees of freedom)



Memory consumption:

- $\mathcal{O}(n)$ fill-in per column.
- Hence, $\mathcal{O}(n^3) = \mathcal{O}(N^{3/2})$ fill-in overall.

Floating-point operations (FLOPs)

- $\mathcal{O}(n)$ subdiagonal entries to eliminate per column.
- Each elimination takes $\mathcal{O}(n)$ FLOPs.
- Hence, $\mathcal{O}(n^4) = \mathcal{O}(N^2)$ FLOPs overall.

Sparse LU Factorisation

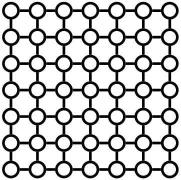
Observations

Amount of fill-in depends on

- physical dimension of problem, and
- ordering of rows and columns.

Can we permute the matrix to reduce fill-in?

1D: 

2D: 

Sparse LU Factorisation

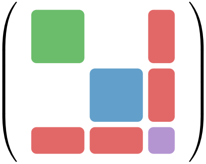
Algorithm 1 Nested dissection ordering

1: Partition the vertices into three sets V_1, V_2, V_{sep} such that every path from V_1 to V_2 visits at least one vertex in V_{sep}.

2: Arrange the vertices in the order V_1, V_2, V_{sep}, where V_1 and V_2 are ordered recursively according to the nested dissection algorithm.

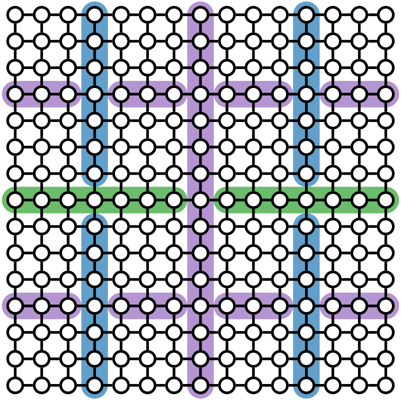
Consequences:

- No fill-in between V_1 and V_2!
- Some fill-in between V_1 / V_2 and V_{sep} (red blocks below).



Sparse LU Factorisation

Separators for 2d mesh



Sparse LU Factorisation

Complexity of LU factorisation with nested dissection ordering

Observations:

- Diagonal block associated with V_{sep} is dense.
- Factorising this block costs $\mathcal{O}\left(|V_{\text{sep}}|^3\right)$.

The following can be shown for 2D and 3D meshes (see references):

- The overall runtime of LU factorisation with nested dissection ordering is dominated by factorisation of largest separator.
- Nested dissection is asymptotically optimal: no other ordering can outperform nested dissection in the big-$\mathcal{O}$ sense.

Sparse LU Factorisation

Complexity of LU factorisation

	Runtime	Memory
$d = 1$	$\mathcal{O}(N)$	$\mathcal{O}(N)$
$d = 2$	$\mathcal{O}(N^{3/2})$	$\mathcal{O}(N \log(N))$
$d = 3$	$\mathcal{O}(N^2)$	$\mathcal{O}(N^{4/3})$

Runtime entries follow immediately from the observation

$$\begin{aligned} d = 1 \quad &\implies \quad |V_{\text{sep}}| = \mathcal{O}(1), \\ d = 2 \quad &\implies \quad |V_{\text{sep}}| = \mathcal{O}(n) = \mathcal{O}(N^{1/2}), \\ d = 3 \quad &\implies \quad |V_{\text{sep}}| = \mathcal{O}(n^2) = \mathcal{O}(N^{2/3}). \end{aligned}$$

Sparse LU Factorisation

Approximate Minimum Degree (AMD) ordering

- Finding good separators can be challenging in practice.
- AMD is another commonly used ordering which is often easier to compute but equally effective.

Sparse algorithms in Julia

Most functions (e.g. `+,*,\,lu()`) are overloaded to automatically exploit sparsity.

Sparse LU Factorisation

Fill-in and pivoting

Recall: LU factorisation of general invertible matrix A requires pivoting to ensure numerical stability.

Bad news: pivoting may undo the effect of fill-in-reducing orderings.

Good news: some classes of matrices provably do not need pivoting.

Matrices which do not require pivoting

- Column-wise diagonally dominant matrices: $A[j,j] \geq \sum_{i \neq j} |A[i,j]|$.
  Column-wise largest pivot will always be on diagonal.
- Symmetric positive semi-definite matrices: $A = A^T$ and $v^T A v \geq 0$.
  Stability of Gaussian elimination is guaranteed.

See Homework Sheet 4.

Sparse LU Factorisation

References and further reading

- T. A. Davis. *Direct Methods for Sparse Linear Systems.* Society for Industrial and Applied Mathematics (2006), `doi:10.1137/1.9780898718881`
- I. S. Duff, A. M. Erisman, and J. K. Reid. *Direct Methods for Sparse Matrices.* Oxford University Press (2017), `doi:10.1093/acprof:oso/9780198508380.001.0001`
- Fill-in on 2D and 3D meshes:

  `https://sites.cs.ucsb.edu/~gilbert/cs219/cs219Spr2013/Notes/fill.pdf`