Sparse Direct Method.

$Ax=b$, A sparse

Sparse direct method = Gauss elimination for sparse matrices.

$A = LU$. Then

$Ax = b \Rightarrow LUx = b$

$\underbrace{y = L^{-1} b}_{\text{forward substitution}}$. $\underbrace{x = U^{-1} y}_{\text{backward substitution.}}$

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \in \mathbb{R}^{n\times n}. \qquad A_{11} \in \mathbb{R}. \quad A_{11} \neq 0$$

$$\begin{pmatrix} 1 & 0 \\ -A_{21}A_{11}^{-1} & I \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} A_{11}^{-1} & -A_{11}^{-1}A_{12} \\ 0 & I \end{pmatrix}$$

$$= \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix} \begin{pmatrix} A_{11}^{-1} & -A_{11}^{-1}A_{12} \\ 0 & I \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & \underline{A_{22} - A_{21}A_{11}^{-1}A_{12}} \end{pmatrix} \longrightarrow \text{block-diagonal.}$$

Schur complement $= S_{22}$

equivalently.

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ +A_{21}A_{11}^{-1} & I \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & S_{22} \end{pmatrix} \begin{pmatrix} A_{11} & +A_{12} \\ 0 & I \end{pmatrix}$$

$$A = L_1 \begin{pmatrix} 1 & 0 \\ 0 & S_{22} \end{pmatrix} U_1$$

S_{22} is denser than A_{22}, due to fill-in $(-A_{21}A_{11}^{-1}A_{12})$

But in general still sparse.

$$S_{22} = \tilde{L}_2 \begin{pmatrix} 1 & 0 \\ 0 & S_{33} \end{pmatrix} \tilde{U}_2$$

$$L_2 = \begin{pmatrix} 1 & 0 \\ 0 & \tilde{L}_2 \end{pmatrix} \qquad U_2 = \begin{pmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{pmatrix}$$

$$A = L_1 L_2 \begin{pmatrix} \begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix} & 0 \\ 0 & S_{33} \end{pmatrix} U_2 U_1$$

recursively

$$= \underbrace{L_1 L_2 \cdots L_n}_{L} \underbrace{U_n \cdots U_1}_{U}$$

Alg. (LU factorization. column-wise)

for $k = 1, n$.

$L_{kk} = 1$, $U_{kk} = A_{kk}$.

$L_{ik} = A_{ik} A_{kk}^{-1}$, $i > k$

$U_{kj} = A_{kj}$, $j > k$

$A_{ij} \leftarrow A_{ij} - L_{ik} U_{kj}$, $i, j > k$.

only need to work with $A_{ik} \neq 0$, $A_{kj} \neq 0$.

end.

A sym. pos. def. $\in \mathbb{R}^{n\times n}$

$A = LL^T$ Cholesky factorization.

L lower triangular. non-unitary diagonal.

$$\begin{pmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} A_{11}^{\frac{1}{2}} & 0 \\ A_{21}A_{11}^{-\frac{1}{2}} & I \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & A_{22}-A_{21}A_{11}^{-1}A_{12} \end{pmatrix} \cdot \begin{pmatrix} A_{11}^{\frac{1}{2}} & A_{11}^{-\frac{1}{2}}A_{21}^T \\ 0 & I \end{pmatrix}$$

Note: A_{11} is matrix. $A_{11} = L_1 L_1^T$

$$\downarrow$$

"$A_{11}^{\frac{1}{2}}$"

Alg. Cholesky. column-wise.

for $k = 1, n$.

$$L_{kk} = A_{kk}^{\frac{1}{2}}$$

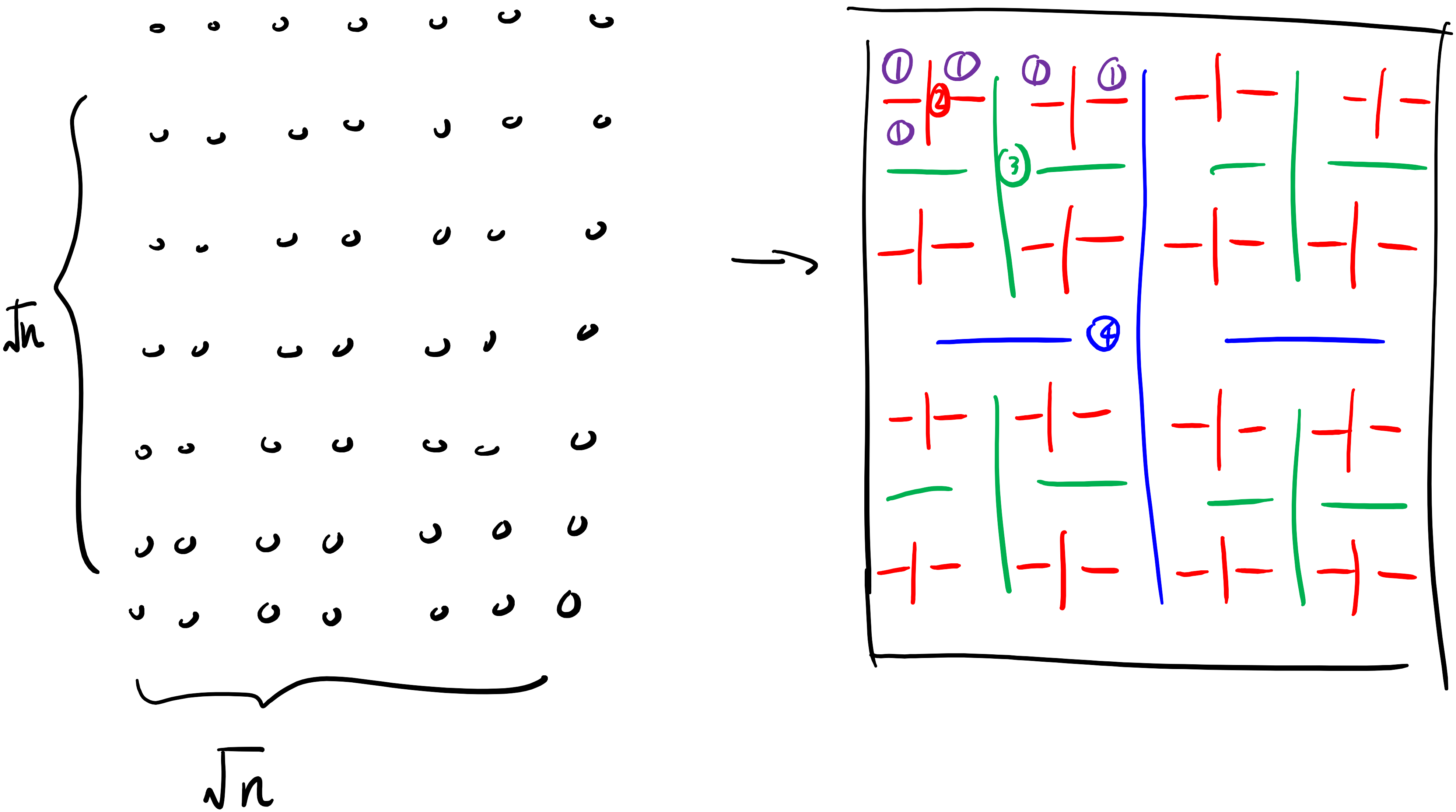
$$L_{ik} = A_{ik} A_{kk}^{\frac{1}{2}} \quad , i > k$$

$$A_{ij} \leftarrow A_{ij} - L_{ik} L_{jk} \quad , i, j > k$$

allows sparsity.

end.

Nested dissection reordering



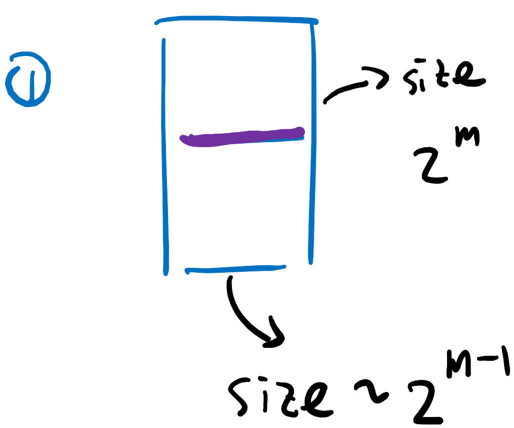
total # levels. $\log_2 \sqrt{n}$

level 1: size of block ~$O(1)$

n blocks.

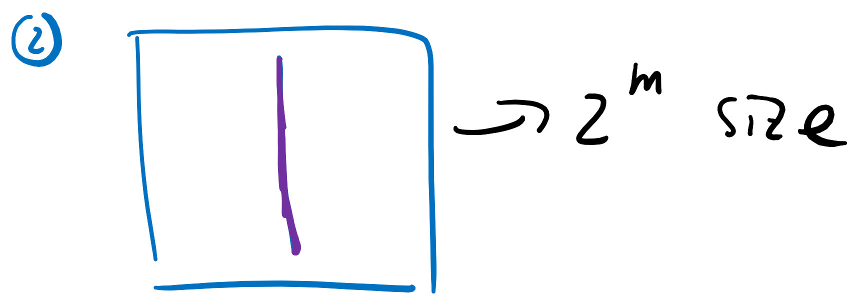
tot nonzeros in L : $O(n)$

level m.



dense matrix

$$2^{m-1}\times(3\cdot 2^{m-1}+2\cdot 2^m)=\frac{7}{4}\cdot 2^{2m}$$



dense matrix

$$2^m\times(5\cdot 2^m)=5\cdot 2^{2m}$$

tot nz in each block.

$$2 \times \frac{7}{4} \times 2^{2m} + 5 \cdot 2^{2m} = \frac{17}{2} \cdot 2^{2m} \sim O(2^{2m})$$

blocks at level m. $O\left(\frac{n}{2^{2m}}\right)$

tot # nz of L at level m.

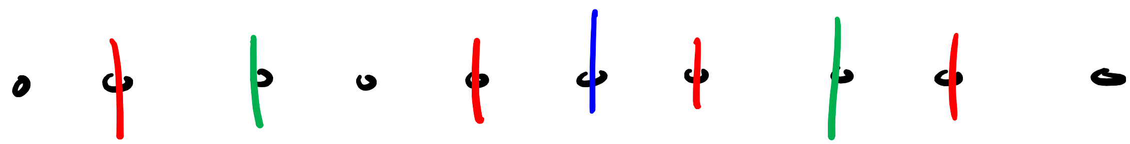
$$O\left(2^{2m} \cdot \frac{n}{2^{2m}}\right) = O(n)$$

tot # nz in L in nested dissection is

$$O(n \log_2 n)$$

1D / 2D / 3D.

1D.



size of separator is $O(1)$.

$\Rightarrow$ each level m, # nz in L for each block $O(1)$

$\frac{n}{2^m}$ blocks.

$\Rightarrow$ tot # nz in L $\sum_{l=1}^{\log_2 n} \frac{n}{2^m} \sim O(n)$

computational complexity $O(n)$.

2D.

each level m. # nz in each block $O(2^{2m})$.

comp. complexity each block $O(2^{3m})$

tot # nz in $L \sim \sum_{l=1}^{\log_2 \sqrt{n}} 2^{2m} \cdot \frac{n}{2^{2m}} \sim n \log_2 n$

blocks

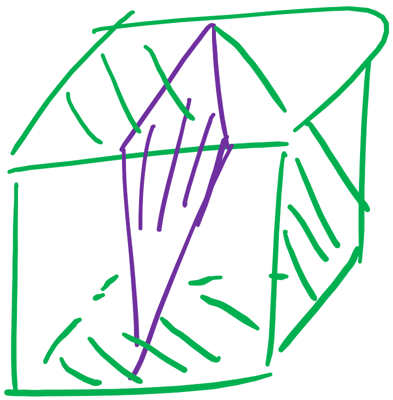
tot comp. complexity $\sim \sum_{l=1}^{\log_2 \sqrt{n}} 2^{3m} \cdot \frac{n}{2^{2m}} \sim \sum_{l=1}^{\log_2 \sqrt{n}} 2^{m} \cdot n$

$\sim O(n^{1.5})$

exer: check # nz. & complexity in natural ordering.

3D

at level m. # nz in each block of L $(2^{2m})^2 \sim 2^{4m}$



comp. complexity each block $(2^{2m})^3 \sim 2^{6m}$

tot # level. $\log_2 n^{\frac{1}{3}}$

2^m

in plane $\cdot\, 2^{2m}$

in plane $\sim 2^{2m} \cdot 6$

tot # nz in L.

$$\sum_{l=1}^{\log_2 n^{\frac{1}{3}}} 2^{4m} \cdot \frac{n}{2^{3m}} \sim n^{\frac{4}{3}}$$

tot complexity

$$\sum_{l=1}^{\log_2 n^{\frac{1}{3}}} 2^{6m} \frac{n}{2^{3m}} \sim n^2 .$$

Lap, nearest neighbor like stencil.

	1D	2D	3D
nz in L	n	$n \log_2 n$	$n^{\frac{4}{3}}$
comp. complexity	n	$n^{\frac{3}{2}}$	n^2

sparse direct method most successful.

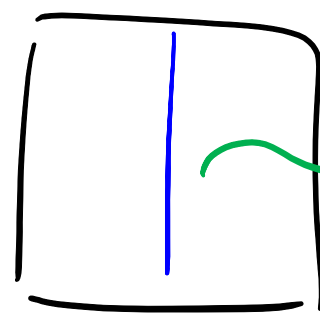
less competitive. consider iterative methods first

Qualitative understanding.

1D root ~ size 1.

blocks n. tot cost ~ n.

2D in the end skeleton

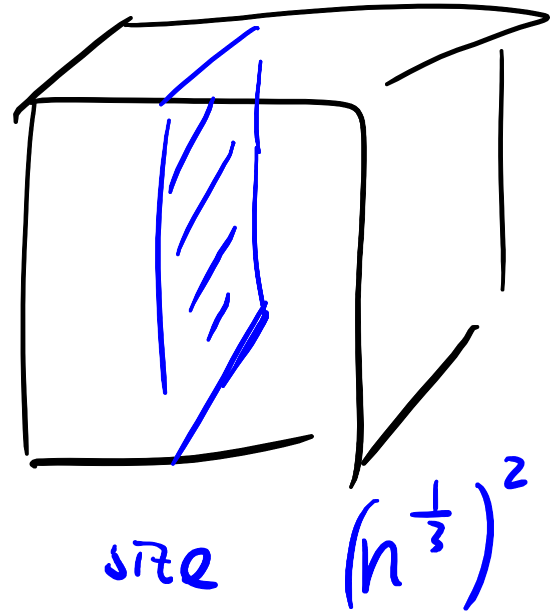


size $\sqrt{n}$ dense mat.

complexity. $(\sqrt{n})^3 = n^{1.5}$

root (last separator) dominates.

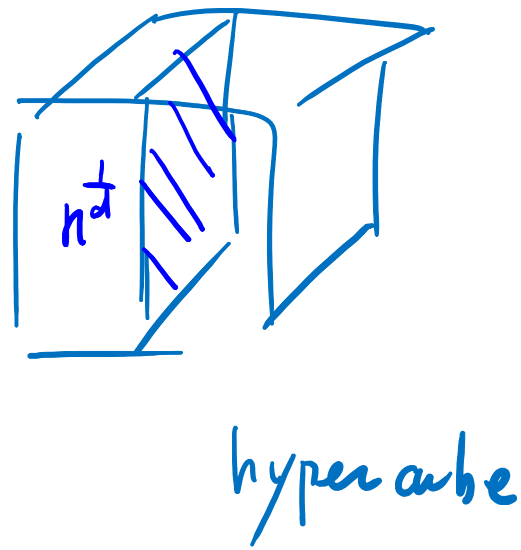
3D. last skeleton



comp. complexity.

$$\left(n^{\frac{2}{3}}\right)^3 \sim O(n^2)$$

root dominates.



d- dimensional Laplacian.

size of separator. $n^{\frac{d-1}{d}}$

cost $\quad n^{3\left(\frac{d-1}{d}\right)} \xrightarrow{d \to \infty} n^3$

infinite dimensional space. sparse direct solve NO BENEFIT.