Fast direct sparse solvers

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Introduction

- ▶ Laplace equation $-\Delta u = 0$ on a unit square domain $[0, 1]^d$
- ▶ LU factorization of the permuted discrete system $P^*AP = LU$
- ► $N = n^d, d = 2, 3$

Table 1: Complexity of LU

d	Simple ordering	Nested dissection ordering
2	$O(N^2)$	$O(N^{3/2})$
3	$O(N^{7/3})$	$O(N^2)$

Only work for moderate size problems!

Goal for Ch.21

- Linear or near-to-linear complexity, i.e. Fast direct sparse solvers (FDSS)
- I High level view of the general ideas
- I Heuristic understanding of when it will work

Main cost in computing LU of the Schur complement (in the root node).

Schur Complement behaves as a Dirichelet-to-Neumann operator, so it's rank-structured.

Consider it as electrostatic problem.

[Au](k) = $(u(k) - u(k_s)) + (u(k) - u(k_e)) + (u(k) - u(k_n)) + (u(k) - u(k_w))$

The Schur complement is rank structured



Figure 1: Top level of nested dissection

$$\begin{array}{l} \mbox{Schur Complement: } S_1 = A_{1,1} - A_{1,2}A_{2,2}^{-1}A_{2,1} - A_{1,3}A_{3,3}^{-1}A_{3,1} \\ \mbox{Linear system: } \begin{bmatrix} A_{3,3} & 0 & A_{3,1} \\ 0 & A_{2,2} & A_{2,1} \\ A_{1,3} & A_{1,2} & A_{1,1} \end{bmatrix} \begin{bmatrix} u_3 \\ u_2 \\ u_1 \end{bmatrix} = \begin{bmatrix} f_3 \\ f_2 \\ f_1 \end{bmatrix} \\ \mbox{Eliminate points in } I_2: \\ \begin{bmatrix} A_{3,3} & A_{3,1} \\ A_{1,3} & A_{1,3} \end{bmatrix} \begin{bmatrix} u_3 \\ u_1 \end{bmatrix} = \begin{bmatrix} f_3 \\ f_1 - A_{1,2}A_{2,2}^{-1}f_2 + A_{1,2}A_{2,2}^{-1}A_{2,1}u_1 \end{bmatrix}$$

Algorithm 0000000000

Hierarchical-off-diagonal-low-ranked

$$\mathsf{S}_{\alpha,\beta} = \mathsf{S}\left(\mathsf{J}_{\alpha},\mathsf{J}_{\beta}\right) = \mathsf{A}\left(\mathsf{I}_{\alpha},\mathsf{I}_{2}\right)\mathsf{A}\left(\mathsf{I}_{2},\mathsf{I}_{2}\right)^{-1}\mathsf{A}\left(\mathsf{I}_{2},\mathsf{I}_{\beta}\right)$$



Figure 2: Illustration for off-diagonal on the top level

 σ_j is the jth singular value of $S_{\alpha,\beta}$ **Dependence on the problem size**

n	32	64	128	256	512	1024
k	8	10	12	14	16	18

Table 2: 5-pt stencil, precision $\epsilon = 1e - 12$, k is the numerical ranks



Figure 3: σ_j/σ_1 versus j

• Convection term
$$[Au](\mathbf{x}) = -\Delta u(\mathbf{x}) + b \left(\frac{\partial u(\mathbf{x})}{\partial x_1} + \frac{\partial u(\mathbf{x})}{\partial x_2} \right)$$



Figure 4: σ_j/σ_1 versus j, 5-pt stencil for the Laplace operator and centered differences for the convection term

► Rough coefficients and large contrast ratios $[Au](k) = \alpha_{k,k_e} (u(k) - u(k_e)) + \alpha_{k,k_n} (u(k) - u(k_n)) + \alpha_{k,k_w} (u(k) - u(k_w)) + \alpha_{k,k_s} (u(k) - u(k_s)),$ where $\alpha_{k,\ell} = 1 + c\theta_{k,\ell}, \ \theta_{k,\ell} \sim U[0,1]$



Figure 5: σ_j/σ_1 versus j, 5-pt stencil, n=400

Higher order stencils: 5,9,13 points stencil Higher accuracy, thicker mesh separator, the ranks slightly increase.



Figure 6: σ_j/σ_1 versus j

► Wave number for oscillatory problems Discretization for the Helmholtz operator $A = L - \kappa^2 I$ $\begin{array}{c|c} 1/\lambda & 0.5 & 5 & 10 & 15 & 20\\ k & 16 & 17 & 22 & 27 & 31 \end{array}$

Table 3: Wavelength $\lambda = 2\pi/\kappa$, n = 512, precision $\epsilon = 1e - 12$, $k \approx 10 + 1/\lambda$



Figure 7: σ_j/σ_1 versus j

Complexity in 2D

Consider cost to compute LU of $m \times m$ Schur complement is m^{α} , $\alpha \in [1, 3]$, $T \sim \sum_{\ell=0}^{L} 2^{\ell} m_{\ell}^{\alpha} \sim \sum_{\ell=0}^{L} 2^{\ell} 2^{-\alpha \ell/2} n^{\alpha} = n^{\alpha} \sum_{\ell=0}^{L} (2^{1-\alpha/2})^{\ell}$ Since $2^{L} \approx n^{2}$,

 $\boxed{\alpha < 2}$ Geometric sum dominated by the *leaves*. Complexity is O(N). $\boxed{\alpha = 2}$ Every term has the same weight. Complexity is $O(n^2L) = O(N \log N)$. $\boxed{\alpha > 2}$ Geometric sum dominated by the *root*. Complexity is $O(n^{\alpha}) = O(N^{\alpha/2})$.

e.g. ranks scale as $log(m_\ell)$ and then LU scales as $m_\ell log(m_\ell)^2$, much better than m_ℓ^2

Complexity in 3D

$$T \sim \sum_{\ell=0}^{L} 2^{\ell} m_{\ell}^{\alpha} \sim \sum_{\ell=0}^{L} 2^{\ell} 2^{-2\alpha\ell/3} n^{2\alpha} = n^{2\alpha} \sum_{\ell=0}^{L} \left(2^{1-2\alpha/3} \right)^{\ell}$$

$$\alpha < 3/2$$
 Geometric sum dominated by the *leaves*. Complexity is $O(N)$.
 $\alpha = 3/2$ Every term has the same weight. Complexity is $O(n^3L) = O(N \log N)$.
 $\alpha > 3/2$ Geometric sum dominated by the *root*. Complexity is $O(n^{2\alpha}) = O(N^{2\alpha/3})$.

- Possible to parallelize but difficult
- Difficult to achieve the nested dissection ordering



Figure 8: Nested dissection ordering