CS 598: Communication Cost Analysis of Algorithms Lecture 26: Hierarchically semi-separable (HSS) matrices

Edgar Solomonik

University of Illinois at Urbana-Champaign

November 28, 2016

HSS matrix, two levels



Hierarchically semi-separable (HSS) matrix, space padded around each matrix block, which are uniquely identified by dimensions and color

HSS matrix, three levels



HSS matrix formal definition

Consider matrix $\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$

• the I-level HSS factorization is

$$\mathcal{H}_{l}(\mathbf{A}) = \begin{cases} \{\mathbf{U}, \mathbf{V}, \mathbf{T}_{12}, \mathbf{T}_{21}, \mathbf{A}_{11}, \mathbf{A}_{22}\} & : l = 1\\ \{\mathbf{U}, \mathbf{V}, \mathbf{T}_{12}, \mathbf{T}_{21}, \mathcal{H}_{l-1}(\mathbf{A}_{11}), \mathcal{H}_{l-1}(\mathbf{A}_{22})\} & : l > 1 \end{cases}$$

• the low-rank representation of the diagonal blocks is given by $\mathbf{A}_{21} = \bar{\mathbf{U}}_2 \mathbf{T}_{21} \bar{\mathbf{V}}_1^{\mathsf{T}}$, $\mathbf{A}_{12} = \bar{\mathbf{U}}_1 \mathbf{T}_{12} \bar{\mathbf{V}}_2^{\mathsf{T}}$ where for $a \in \{1, 2\}$,

$$\bar{\mathbf{U}}_{a} = \mathcal{U}_{a}(\mathcal{H}_{l}(\mathbf{A})) = \begin{cases} \mathbf{U}_{a} & : l = 1\\ \left[\mathcal{U}_{1}(\mathcal{H}_{l-1}(\mathbf{A}_{aa})) & \mathbf{0}\\ \mathbf{0} & \mathcal{U}_{2}(\mathcal{H}_{l-1}(\mathbf{A}_{aa})) \right] \mathbf{U}_{a} & : l > 1 \end{cases}$$
$$\bar{\mathbf{V}}_{a} = \mathcal{V}_{a}(\mathcal{H}_{l}(\mathbf{A})) = \begin{cases} \mathbf{V}_{a} & : l = 1\\ \left[\mathcal{V}_{1}(\mathcal{H}_{l-1}(\mathbf{A}_{aa})) & \mathbf{0}\\ \mathbf{0} & \mathcal{V}_{2}(\mathcal{H}_{l-1}(\mathbf{A}_{aa})) \right] \mathbf{V}_{a} & : l > 1 \end{cases}$$

HSS matrix-vector multiplication

We now consider computing $\mathbf{y} = \mathbf{A}\mathbf{x}$

- with $\mathcal{H}_1(\mathbf{A})$ we would just compute $\mathbf{y}_1 = \mathbf{A}_{11}\mathbf{x}_1 + \mathbf{U}_1(\mathbf{T}_{12}(\mathbf{V}_2^\mathsf{T}\mathbf{x}_2))$ and $\mathbf{y}_2 = \mathbf{A}_{22}\mathbf{x}_2 + \mathbf{U}_2(\mathbf{T}_{21}(\mathbf{V}_1^\mathsf{T}\mathbf{x}_1))$
- \bullet for general $\mathcal{H}_{\textit{I}}(\textbf{A})$ we will perform an up-sweep and a down-sweep
 - up-sweep computes $\mathbf{w} = \begin{bmatrix} \mathbf{\bar{V}}_1^\mathsf{T} \mathbf{x}_1 \\ \mathbf{\bar{V}}_2^\mathsf{T} \mathbf{x}_2 \end{bmatrix}$ at every tree node

• down-sweep computes a tree sum of $\begin{bmatrix} \mathbf{\bar{U}}_1 \mathbf{T}_{12} \mathbf{w}_2 \\ \mathbf{\bar{U}}_2 \mathbf{T}_{21} \mathbf{w}_1 \end{bmatrix}$

ullet the up-sweep is performed by using the nested structure of $ar{f V}$

$$\mathbf{w} = \mathcal{W}(\mathcal{H}_{l}(\mathbf{A}), \mathbf{x}) = \begin{cases} \begin{bmatrix} \mathbf{V}_{1}^{\mathsf{T}} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_{2}^{\mathsf{T}} \end{bmatrix} \mathbf{x} & : l = 1 \\ \begin{bmatrix} \mathbf{V}_{1}^{\mathsf{T}} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_{2}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \mathcal{W}(\mathcal{H}_{l-1}(\mathbf{A}_{11}), \mathbf{x}_{1}) \\ \mathcal{W}(\mathcal{H}_{l-1}(\mathbf{A}_{22}), \mathbf{x}_{2}) \end{bmatrix} & : l > 1 \end{cases}$$

HSS matrix-vector multiplication, down-sweep

We now employ each $w=\mathcal{W}(\mathcal{H}_{\textit{I}}(A),x)$ from the root to the leaves to get

$$\mathbf{y} = \mathbf{A}\mathbf{x} = \begin{bmatrix} \mathbf{U}_1 \mathbf{T}_{12} \mathbf{w}_2 \\ \mathbf{U}_2 \mathbf{T}_{21} \mathbf{w}_1 \end{bmatrix} + \begin{bmatrix} \mathbf{A}_{11} \mathbf{x}_1 \\ \mathbf{A}_{22} \mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} \bar{\mathbf{U}}_1 & \mathbf{0} \\ \mathbf{0} & \bar{\mathbf{U}}_2 \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{0} \end{bmatrix} \mathbf{w} + \begin{bmatrix} \mathbf{A}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{22} \end{bmatrix} \mathbf{x}$$

• using the nested structure of
$$\overline{\mathbf{U}}_a$$
 and $\mathbf{v} = \begin{bmatrix} \mathbf{U}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{U}_2 \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{0} \end{bmatrix} \mathbf{w}$,
$$\mathbf{y}_a = \begin{bmatrix} \mathcal{U}_1(\mathcal{H}_{l-1}(\mathbf{A}_{aa})) & \mathbf{0} \\ \mathbf{0} & \mathcal{U}_2(\mathcal{H}_{l-1}(\mathbf{A}_{aa})) \end{bmatrix} \mathbf{v}_a + \mathbf{A}_{aa}\mathbf{x}_a \text{ for } a \in \{1, 2\}$$

• which gives the down-sweep recurrence

$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{z} = \mathcal{Y}(\mathcal{H}_{l}(\mathbf{A}), \mathbf{x}, \mathbf{z}) = \begin{cases} \begin{bmatrix} \mathbf{U}_{1}\mathbf{q}_{1} \\ \mathbf{U}_{2}\mathbf{q}_{2} \end{bmatrix} + \begin{bmatrix} \mathbf{A}_{11}\mathbf{x}_{1} \\ \mathbf{A}_{22}\mathbf{x}_{2} \end{bmatrix} : l = 1 \\ \mathcal{Y}(\mathcal{H}_{l-1}(\mathbf{A}_{11}), \mathbf{x}_{1}, \mathbf{U}_{1}\mathbf{q}_{1}) \\ \mathcal{Y}(\mathcal{H}_{l-1}(\mathbf{A}_{22}), \mathbf{x}_{2}, \mathbf{U}_{2}\mathbf{q}_{2}) \end{bmatrix} : l > 1 \end{cases}$$

where $\mathbf{q} = \begin{bmatrix} \mathbf{0} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{0} \end{bmatrix} \mathcal{W}(\mathcal{H}_{l}(\mathbf{A}), \mathbf{x}) + \mathbf{z}$

Prefix sum as HSS matrix-vector multiplication

We can express the *n*-element prefix sum $y(i) = \sum_{j=1}^{i-1} x(j)$ as

$$\mathbf{y} = \mathbf{L}\mathbf{x} \quad \text{where} \quad \mathbf{L} = \begin{bmatrix} \mathbf{L}_{11} & \mathbf{0} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{bmatrix} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 1 & \cdots & 1 & 0 \end{bmatrix}$$

• L is an
$$\mathcal{H}$$
-matrix since $\mathbf{L}_{21} = \mathbf{1}_{n} \mathbf{1}_{n}^{\mathsf{T}} = \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}$

• L also has rank-1 HSS structure, in particular

$$\mathcal{H}_{l}(\mathsf{L}) = \begin{cases} \left\{ \mathbf{1}_{2}, \mathbf{1}_{2}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \mathcal{H}_{l-1}(\mathsf{L}_{11}), \mathcal{H}_{l-1}(\mathsf{L}_{22}) \right\} & : l = 1 \end{cases}$$

so each $\bm{U},\bm{V},\bar{\bm{U}},\bar{\bm{V}}$ is a vector of 1s, $\bm{T}_{12}=\begin{bmatrix}0\end{bmatrix}$ and $\bm{T}_{21}=\begin{bmatrix}1\end{bmatrix}$

Prefix sum HSS up-sweep

We can use the HSS structure of $\boldsymbol{\mathsf{L}}$ to compute the prefix sum of $\boldsymbol{\mathsf{x}}$

• recall that the up-sweep recurrence has the general form

$$\mathbf{w} = \mathcal{W}(\mathcal{H}_{l}(\mathbf{A}), \mathbf{x}) = \begin{cases} \begin{bmatrix} \mathbf{V}_{1}^{\mathsf{T}} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_{2}^{\mathsf{T}} \\ \mathbf{V}_{1}^{\mathsf{T}} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_{2}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \mathcal{W}(\mathcal{H}_{l-1}(\mathbf{A}_{11}), \mathbf{x}_{1}) \\ \mathcal{W}(\mathcal{H}_{l-1}(\mathbf{A}_{22}), \mathbf{x}_{2}) \end{bmatrix} & : l > 1 \end{cases}$$

for the prefix sum this becomes

$$\mathbf{w} = \mathcal{W}(\mathcal{H}_{l}(\mathbf{L}), \mathbf{x}) = \begin{cases} \mathbf{x} & : l = 1\\ \begin{bmatrix} 1 & 1 & 0 & 0\\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} \mathcal{W}(\mathcal{H}_{l-1}(\mathbf{L}_{11}), \mathbf{x}_{1})\\ \mathcal{W}(\mathcal{H}_{l-1}(\mathbf{L}_{22}), \mathbf{x}_{2}) \end{bmatrix} & : l > 1 \end{cases}$$

• so the up-sweep computes $\mathbf{w} = \begin{bmatrix} \mathcal{S}(\mathbf{x}_{1})\\ \mathcal{S}(\mathbf{x}_{2}) \end{bmatrix}$ where $\mathcal{S}(\mathbf{a}) = \sum_{i} a(i)$

Prefix sum HSS down-sweep

The down-sweep has the general structure

$$\mathbf{y} = \mathcal{Y}(\mathcal{H}_{l}(\mathbf{A}), \mathbf{x}, \mathbf{z}) = \begin{cases} \begin{bmatrix} \mathbf{U}_{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{U}_{2} \end{bmatrix} \mathbf{q} + \begin{bmatrix} \mathbf{A}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{22} \end{bmatrix} \mathbf{x} & : l = 1 \\ \mathcal{Y}(\mathcal{H}_{l-1}(\mathbf{A}_{11}), \mathbf{x}_{1}, \mathbf{U}_{1}\mathbf{q}_{1}) \\ \mathcal{Y}(\mathcal{H}_{l-1}(\mathbf{A}_{22}), \mathbf{x}_{2}, \mathbf{U}_{2}\mathbf{q}_{2}) \end{bmatrix} & : l > 1 \end{cases}$$

where
$$\mathbf{q} = \begin{bmatrix} \mathbf{0} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{0} \end{bmatrix} \mathcal{W}(\mathcal{H}_{l}(\mathbf{A}), \mathbf{x}) + \mathbf{z}$$
, for the prefix sum:
• $\begin{bmatrix} \mathbf{0} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{0} \end{bmatrix} \mathcal{W}(\mathcal{H}_{l}(\mathbf{L}), \mathbf{x}) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \mathcal{S}(\mathbf{x}_{1}) \\ \mathcal{S}(\mathbf{x}_{2}) \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{S}(\mathbf{x}_{1}) \end{bmatrix} = \mathbf{q} - \mathbf{z}$
 $\mathbf{y} = \mathcal{Y}(\mathcal{H}_{l}(\mathbf{L}), \mathbf{x}, \mathbf{z}) = \begin{cases} \begin{bmatrix} z(1) \\ x(1) + z(2) \end{bmatrix} & : l = 1 \\ \mathcal{Y}(\mathcal{H}_{l-1}(\mathbf{L}_{11}), \mathbf{x}_{1}, \mathbf{1}_{2}z(1)) \\ \mathcal{Y}(\mathcal{H}_{l-1}(\mathbf{L}_{22}), \mathbf{x}_{2}, \mathbf{1}_{2}(\mathcal{S}(\mathbf{x}_{1}) + z(2)) \end{bmatrix} & : l > 1 \end{cases}$

• initially the prefix $\mathbf{z} = \mathbf{0}$ and it will always be the case that z(1) = z(2)

Short pause

Cost of HSS matrix-vector multiplication

The down-sweep and the up-sweep perform small dense matrix-vector multiplications at each recursive step

- lets assume k is the dimension of the leaf blocks and the rank at each level (number of columns in each U_a, V_a)
- the computation cost for both the down-sweep and up-sweep is

$$T(n,k) = 2T(n/2,k) + O(k^2 \cdot \gamma), \quad T(k,k) = O(k^2 \cdot \gamma)$$

$$T(n,k) = O(nk \cdot \gamma)$$

- Q: what parallelization approach would be sensible for small k?
- if we assign each tree node to a single processor for the first log₂(P) levels, and execute a different leaf subtree with a different processor

$$T(n, k, P) = 2T(n, k, P/2) + O(k^2 \cdot \gamma + k \cdot \beta + \alpha)$$

= $O((nk/P + k^2 \log(P)) \cdot \gamma + k \log(P) \cdot \beta + \log(P) \cdot \alpha)$

Synchronization-efficient HSS multiplication

Our first algorithm would require $O(\log(P))$ BSP supersteps

- Q: what would we need to do to reduce this to O(1)?
- we can observe that the leaf subtrees can be computed independently

$$T_{\text{leaf-subtrees}}(n, k, P) = O(nk/P \cdot \gamma + k \cdot \beta + \alpha)$$

- thus we can focus on doing the up-sweep and down-sweep on a binary tree with log₂(P) levels
 - executing the root subtree sequentially would yield a cost of

$$T_{\text{root-subtree}}(n,k,P) = O(Pk^2 \cdot \gamma + Pk \cdot \beta + \alpha)$$

- this could be prohibitive on a large number of processors
- instead have P^r (r < 1) processors compute subtrees with P^{1-r} leaves, then recurse on the P^r roots

$$T_{\text{rec-tree}}(k, P) = T_{\text{rec-tree}}(k, P^r) + O(P^{1-r}k^2 \cdot \gamma + P^{1-r}k \cdot \beta + \alpha)$$

• the algorithm has BSP complexity

$$T_{\mathsf{rec-tree}}(k, P) = O(P^{1-r}k^2 \cdot \gamma + P^{1-r}k \cdot \beta + \log_{1/r}(\log(P)) \cdot \alpha)$$

Synchronization-efficient HSS multiplication

We can do better by exploiting what the HSS tree nodes are doing

- again lets focus on the top tree with P leaves (leaf subtrees)
- lets try to assign each processor a unique path from a leaf to the root
- given $\mathbf{w} = \mathcal{W}(\mathcal{H}_{l}(\mathbf{A}), \mathbf{x})$ at every node its clear each processor can compute a down-sweep path in the subtree independently
- for the up-sweep, we can realize that the tree applies a linear transformation, so we can sum the results computed in each path
- for each tree node, there is a contribution from every processor assigned a leaf of the subtree of the node
- therefore, there are P 1 sums of a total of O(P log(P)) contributions, for a total of O(kP log(P)) elements
- we can do these with min(P, k log₂(P)) processors, each obtaining max(P, k log₂(P)) contributions, so

 $T_{\text{root-paths}}(k, P) = O(k^2 \log(P) \cdot \gamma + (k \log(P) + P) \cdot \beta + \alpha)$

• we have not improved the asymptotic number of messages, but only the number of synchronizations, and can leverage efficient reductions

HSS multiplication by multiple vectors

Consider multiplication $\mathbf{C} = \mathbf{A}\mathbf{B}$ where $\mathbf{A} \in \mathbb{R}^{n \times n}$ is HSS and $\mathbf{B} \in \mathbb{R}^{n \times b}$

- lets consider the case that $P \leq b \ll n$
- if we assign each processor all of **A**, each can compute a column of **C** simultaneously
- this requires a prohibitive amount of memory usage
- Q: could you propose a good BSP algorithm for this problem?
- A: use transpose like in the b scans problem
 - perform leaf-level multiplications, processing n/P rows of B with each processor (call intermediate C
 - transpose C
 and apply log₂(P) root levels of HSS tree to columns of C
 independently
- this algorithm requires replication only of the root O(log(P)) levels of the HSS tree, O(Pb) data
- for large k or larger P different algorithms may be desirable