# Fast Memory Efficient Construction Algorithm for Hierarchically Semi-separable Representations



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# **Overview**

- Review of Hierarchically Semi-Separable (HSS) Representation
  - Notation
- Previous HSS Algorithm Complexities
- Memory Efficient Algorithm
  - Phase 1
  - Phase 2
- Memory Consumption
- "A Fast Memory Efficient Construction Algorithm for Hierarchically Semi-Separable Representations" submitted for publication

## **Use a Partition Tree to Block Partition a Matrix**

- Partition A according to the integers at the first level of the partition tree

$$A_{0;1,1} = \frac{m_{1;1}}{m_{1;2}} \begin{pmatrix} A_{1;1,1} & A_{1;1,2} \\ A_{1;2,1} & A_{1;2,2} \end{pmatrix}$$

- Recursively partition the block rows and columns of  ${\cal A}$ 

$$A_{0;1,1} = \begin{array}{cccc} m_{2;1} & n_{2;2} & n_{2;3} & n_{2;4} \\ m_{2;1} & A_{2;1,1} & A_{2;1,2} & A_{2;1,3} & A_{2;1,4} \\ A_{2;2,1} & A_{2;2,2} & A_{2;2,3} & A_{2;2,4} \\ A_{2;3,1} & A_{2;3,2} & A_{2;3,3} & A_{2;3,4} \\ A_{2;4,1} & A_{2;4,2} & A_{2;4,3} & A_{2;4,4} \end{array} \right)$$

## **Definition – Complete Partition Tree**



## **HSS Representation**



- Off-Diagonal blocks thus have low rank and can be compressed
- Only store smaller basis matrices ( $U_{k;i}, V_{k;i}$ ) and translation operators ( $R_{k;i}, W_{k;i}$ )

# **Definition - Hankel Blocks**



Block rows/columns of *A*, excluding diagonal blocks

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## Larger Basis Matrices Can Be Stored as Translated Versions of Smaller Basis Matrices



# **Example 2 Level Column and Row Bases**





# Example 2 Level HSS Representation and Corresponding HSS Tree



Note: Notice the larger U's and V's are not stored, and do not appear in the HSS Tree

# **Definition - HSS Tree**

- An HSS tree of a matrix is the corresponding partition tree decorated with  $U_{k;i}, V_{k;i}, D_{k;i}, R_{k;i}, W_{k;i}$  and  $B_{k;i,j}$ .
  - The matrices  $U_{k;i}, V_{k;i}, D_{k;i}$ , are stored at each leaf node (k; i).
  - The matrices  $R_{k;i}$  and  $W_{k;i}$  are stored at each edge which connects parent to child node, (k;i).
  - We add edges to the partition tree from node (k;i) to node (k;j) corresponding to  $B_{k;i,j}$ .

# **Definition of HSS Representation**

- If (k; i) is a leaf node,  $D_{k;i} = A_{k;i,i}$
- If (k; i) is not a leaf node,

$$A_{k;2i-1,2i} = U_{k;2i-1}B_{k;2i-1;2i}V_{k;2i}^{T},$$
  

$$A_{k;2i-1,2i} = U_{k;2i}B_{k;2i;2i-1}V_{k;2i-1}^{T},$$

• Where,

$$U_{k;i} = \begin{pmatrix} U_{k+1;2i-1}R_{k+1;2i-1} \\ U_{k+1;2i}R_{k+1;2i} \end{pmatrix}, \quad V_{k;i} = \begin{pmatrix} V_{k+1;2i-1}W_{k+1;2i-1} \\ V_{k+1;2i}W_{k+1;2i} \end{pmatrix}$$



## An Inefficient Method to Compute the HSS Representation

- One obvious way to form the HSS representation of a matrix would be to take a Singular Value Decomposition (SVD) all Hankel blocks at each level of the HSS representation.
- This is extremely slow,  $O(n^3)$  flops.
- Not memory efficient,  $O(n^2)$  memory





# A More Efficient Way to Compute the HSS Representation

- Previous HSS construction algorithms (Xia, Chandrasekeran, Martinsson) focused on speed, requiring  $O(n^2)$  flops.
- It seems they were unaware they require  $O(n^2)$  memory in the worst case.
- We present an HSS construction algorithm which requires  $O(n^{1.5})$  peak workspace memory in the worst case, while still requiring only  $O(n^2)$  flops.
- We require only  $O(n \log n)$  memory for a complete tree.

## Main Points of this Talk

- Basic building blocks for  $O(n^2)$  flop construction algorithm
- Peak memory consumption

## Phase 1 & Phase 2 of our Construction Algorithm

- Phase 1 Computation of Basis Matrices,  $U_{k;i}$ , and  $V_{k;i}$ , as well as Translation Operators  $R_{k;i}$  and  $W_{k;i}$
- Phase 2 Computation of Expansion Coefficients  $B_{k;i,j}$

## **Phase 1 - Take SVD's Hankel Blocks at Leaf Nodes**

































## **Phase 1 Complete**



























#### **Phase 2 – A Better Way: Divide and Conquer**




























| $egin{array}{c} egin{array}{c} egin{array}$ | $U_1R_1B_{big}W_2^TV_2^T$     | $U_1 B_1 V_1^T$     | $U_1 B_2 V_2^T$   |
|--|-------------------------------|---------------------|-------------------|
| $egin{array}{c} U_2 R_2 B_{big} W_1^T V_1^T \end{array}$   | $U_2 R_2 B_{big} W_2^T V_2^T$ | $U_2 \ B_3 \ V_1^T$ | $U_2 \ B_4 V_2^T$ |



















### Phase 1 & 2 Complete

• We have calculated every  $U_{k;i}$ ,  $V_{k;i}$ ,  $R_{k;i}$ ,  $W_{k;i}$  and  $B_{k;i,j}$  in the HSS Representation



## **Algorithm Memory Consumption**

- Other algorithms can take as much as  $O(n^2)$  memory due to a depth first traversal of the HSS tree
- Our algorithm traverses the tree in a deepest first order instead, and takes  $O(p^{0.5}n^{1.5})$  memory in the worst case, where p is the rank of the off diagonal blocks of the matrix A, while still taking only  $O(n^2p)$  flops

### What is the Worst Case Memory Consumption for Our Algorithm?

- Phase 2 of our algorithm (computation of Expansion Coefficients  $B_{k;i,j}$ ) consumes at most O(pn) memory
  - One  $p \times p$  block is stored in memory for each recursive call.
  - Tree of max depth is O(n/p)
  - This implies O(pn) peak memory consumption for a tree of maximal depth
- We need to focus on Phase 1 (computation of basis matrices,  $U_{k;i}$  and  $V_{k;i}$ , and translation operators  $R_{k;i}$  and  $W_{k;i}$ ) of our algorithm in order to determine peak workspace consumption





































- Each block shown is of dimension  $n \times p$ , where p is the rank of the off-diagonal blocks of the original matrix
- Maximum Depth of this tree is O(n/p)
- This implies a memory consumption of  $O(n^2)$

## How to fix this: Deepest First Traversal

- Traverse in a Deepest first ordering
- Peak workspace memory consumption of  ${\cal O}(np)$  for a tree of maximal depth




























### Method We Use: Deepest First Traversal





### Method We Use: Deepest First Traversal





## **Deepest First Traversal Memory Count**

- For the maximal depth tree, only 2 blocks of size  $n \times p$  are in memory at any given time
- Peak workspace consumption for a tree of maximal depth is O(pn) using deepest first traversal vs  $O(n^2)$  for depth-first traversal
- Further, for a complete tree, the deepest first traversal leads to a peak workspace consumption of  $O(pn \log n)$

### Worst Case Memory Consumption for our Algorithm

- How does worst case memory usage grow with matrix size, *n*?
- This can be formulated as a graph theory problem

### **Memory Block Cardinality for a Root-leaf Path**

• Without loss of generality, any HSS tree can be re-ordered such that the depth of the left subtree is always equal to or greater than the depth of the right subtree.

• Block is stored in memory when we return from a left call.

• Memory Block Cardinality for a root-leaf path is equal to the number of right children in that path plus one.



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### The Search for Maximum Memory Consumption Can Be Formulated as a Graph Theory Problem

- Branch with maximum memory block cardinality will give peak memory consumption.
- Number of leaf nodes,  $N_L$ , is proportional to the size of the matrix n.
- Number of leaf nodes,  $N_L$ , is proportional to the number of nodes, N.
- We are looking for a class of trees that maximizes the ratio of the worst case memory block cardinality to number of nodes.



### We Can Narrow Down Our Search By Excluding Some Classes of Trees

• We can rule out the class of trees that don't have the worst case memory block cardinality along their right-most branch.

• Worst-case memory block cardinality = 3 for both trees shown below.





### Complete Trees Do Not Give Rise to Worst Case Memory Usage

- Complete trees have the property that the worst case memory block cardinality occurs along the right-most branch.
- Worst-case memory block cardinality = 4 for both trees shown below.





### Class of 'Worst Case' Trees\* Has a Surprising Structure



\* K. Lessel, M. Hartman, and S. Chandrasekaran. A Fast Memory Efficient Construction Algorithm for Hierarchically Semi-Separable Representations. *Submitted to SIAM J. Matrix Analysis and Applications* 

### Worst Case Memory Consumption for our Algorithm

- Worst case number of memory blocks we can generate is  $O(N^{0.5})$ , and is generated by the binary tree with a structure as shown



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## Worst Case Number of Memory Blocks is $O(N^{0.5})$



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# Relationship between the number of nodes, $\underline{N}$ and the size of our matrix, n

• Number of non-leaf nodes,  $N_N$ , is one less than the number of leaf nodes,  $N_L$ , i.e,

$$N_N = N_L - 1$$

• 
$$N_L = n/p$$

- $N = N_N + N_L$ =  $\frac{2n}{p} - 1$
- The worst case number of memory blocks is  $O(N^{0.5})$
- Peak memory consumption is  $O(p^{0.5}n^{1.5})$

### **Numerical Results**

• Upper bound for worst case peak memory consumption is  $O(p^{0.5}n^{1.5})$ , and we can show this is a tight bound for 'Worst Case' trees.



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### Conclusion

- Our 2 Phase Algorithm allows for a deepest first traversal of the HSS tree, yielding a reduction in peak memory complexity from  $O(n^2)$  to  $O(p^{0.5}n^{1.5})$  as compared with previous algorithms, while still taking only  $O(n^2)$  flops.
- Open question: Does there exist a 'linear' memory algorithm which does not give up the  $O(n^2)$  flop constraint?

### References

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[2] K. Lessel, M. Hartman, and S. Chandrasekaran. A Fast Memory Efficient Construction Algorithm for Hierarchically Semi-Separable Representations. *Submitted to SIAM J. Matrix Analysis and Applications* 

[3] Per-Gunnar Martinsson. A Fast Randomized Algorithm for Computing a Hierarchically Semiseparable Representation Matrix. *SIAM Journal on Matrix Analysis and Applications*, 32(4):1251-1274, 2011.

[4] Jianlin Xia, Shivkumar Chandrasekaran, Ming Gu, and Xiaoye~S Li. Fast Algorithms for Hierarchically Semiseparable Matrices. *Numerical Linear Algebra with Applications*, 17(6):953—976, 2010.

### Appendix





- Matrix vector multiply:  $O(n^2)$  flops vs HSS vector multiply: O(n) flops
- Solution, x, of Ax = b. Gaussian Elimination:  $O(n^3)$  flops vs Fast HSS solver: O(n) flops

### **Leaf Node Computations**

• For 
$$(k_1, i)$$
,  $(k_2, j)$  leaf nodes define

$$B_{k_1;i,k_2,j} = U_{k_1,i}^T A_{k_1;i,k_2,j} V_{k_2;j}$$

- For  $(k_1, i)$  a leaf node, and  $(k_2, j)$  is not, define  $B_{k_1;i,k_2;j} = B_{k_1;i,k_2+1;2j-1}W_{k_2+1;2j-1}$   $+ B_{k_1;i,k_2+1;2j}W_{k_2+1;2j},$
- For  $(k_1, i)$  not a leaf node, and  $(k_2, j)$  is a leaf node, define

$$B_{k_1;i,k_2;j} = R_{k_1+1;2i-1}^T B_{k_1+1;2i-1,k_2,j} + R_{k_1+1;2i}^T B_{k_1+1;2i,k_2,j}.$$

### **Non-Leaf Node Computations**

• For  $(k_1, i)$ ,  $(k_2, j)$  not leaf nodes, we will have  $k_1 = k_2$  and can then write

$$B_{k;i,j} = B_{k_1;i,k_2;j}$$

where  $k = k_1 = k_2$ 

• Then define

$$B_{k;i,j} = R_{k+1;2i-1}^T B_{k+1;2i-1,2j-1} W_{k+1;2j-1} + R_{k+1;2i-1}^T B_{k+1;2i-1,2j} W_{k+1;2j} + R_{k+1;2i}^T B_{k+1;2i,2j-1} W_{k+1;2j-1} + R_{k+1;2i}^T B_{k+1;2i,2j} W_{k+1;2j},$$

### **Phase 1 - Leaf Node Computations**

$${}_{r}\dot{H}_{k;i} = \left(\begin{array}{cc} U_{k;i} & * \end{array}\right) \left(\begin{array}{cc} \Sigma_{k;i} & 0 \\ 0 & * \end{array}\right) \left(\begin{array}{cc} Q_{k;i}^{T} \\ * \end{array}\right)$$
$${}_{c}\dot{H}_{k;i} = \left(\begin{array}{cc} P_{k;i} & * \end{array}\right) \left(\begin{array}{cc} \Lambda_{k;i} & 0 \\ 0 & * \end{array}\right) \left(\begin{array}{cc} V_{k;i}^{T} \\ * \end{array}\right).$$

# **Phase 1 – Non-leaf Node Computations**

$$_{r}\tilde{H}_{k;2i-1} = \Sigma_{k;2i-1} Q_{k;2i-1}^{T}$$

$$_{c}\tilde{H}_{k;2i-1} = P_{k;2i-1}\Lambda_{k;2i-1}$$

$$_{r}\tilde{H}_{k;2i} = \Sigma_{k;2i} Q_{k;2i}^{T}$$

$$_{c}\tilde{H}_{k;2i} = P_{k;2i}\Lambda_{k;2i}$$

### **Phase 1 – Non-leaf Node Computations**

• Remove block cloumns of  $Q_{k;i,j}^T$  which corresond to the columns that lie in the diagonal block  $D_{k-1;i}$ 

$$Q_{k;i}^{T} = \begin{pmatrix} Q_{k;i,1}^{T} & Q_{k;i,2}^{T} & \dots & Q_{k;i,2^{k}-1}^{T} \end{pmatrix}$$
$$\tilde{Q}_{k;i}^{T} = \begin{pmatrix} Q_{k;i,1}^{T} & \dots & Q_{k;i,i-1}^{T} & Q_{k;i,i+1}^{T} & \dots & Q_{k;i,2^{k}-1}^{T} \end{pmatrix}$$

• Compressed Hankel blocks at node(k-1;i)

$${}_{r}H_{k-1;i} = \begin{pmatrix} \Sigma_{k;2i-1} \tilde{Q}_{k;2i-1}^{T} \\ \Sigma_{k,2i} \tilde{Q}_{k;2i}^{T} \end{pmatrix}$$
$${}_{c}H_{k-1;i} = \begin{pmatrix} \tilde{P}_{k;2i-1} \Lambda_{k;2i-1} & \tilde{P}_{k;2i} \Lambda_{k;2i} \end{pmatrix}$$

### **Algorithm 1 Pass 1U**

Algorithm 1 Pass 1U - Memory Efficient HSS Algorithm 1: function HSS\_BASIS(tree) if *tree* is a leaf node then 2: $(U_{k;i}, \Sigma_{k;i}, Q_{k;i}^T) = \text{TRUNC\_SVD}([A_{k;i,1} \ A_{k;i,2} \ \dots \ A_{k;i,i-1} \ A_{k;i,i+1} \ \dots \ A_{k;i,end}])$ 3: return  $\Sigma_{k;i} \tilde{Q}_{k;i}^T$  $\triangleright \tilde{Q}_{k:i}$  is defined as previously stated in equation (3.8) 4:  $\triangleright$  tree is **not** a leaf node else 5:  $_{-}, treeL, treeR = tree$ 6: if DEPTH(treeL) > DEPTH(treeR) then 7:  $_{r}H_{k+1:2i-1} = \text{HSS}_{BASIS}(treeL)$ 8:  $_{r}H_{k+1;2i}=\mathrm{HSS\_BASIS}(treeR)$ 9: else 10:  $_{r}H_{k+1:2i} = \text{HSS}_{-}\text{BASIS}(treeR)$ 11:  $_{r}H_{k+1;2i-1} = \text{HSS}_{\text{BASIS}}(treeL)$ end if 12:13:  $_{r}H_{k;i} = \left(\begin{array}{c} _{r}H_{k+1;2i-1} \\ _{r}H_{k+1;2i} \end{array}\right)$ 14:  $\begin{array}{c} {}_{r}H_{k+1;2i-1} = (); \\ {}_{r}H_{k+1;2i-1} \\ {}_{R_{k+1;2i}} \end{array} \right), \ \Sigma_{k;i}, \ X_{k;i} = \text{TRUNC\_SVD}(_{r}H_{k;i}) \end{array}$ 15: 16:  $\triangleright \tilde{X}_{k:i}$  is defined as previously stated in equation (3.8) return  $\Sigma_{k;i} X_{k;i}^T$ 17:end if 18: 19: end function

### Algorithm 2 Pass 2BU

Algorithm 2 Pass 2BU - Computation of Expansion Coefficients  $(B_{k;i-1,i})$  Corresponding to Diagonal Blocks

```
Require: tree is not a leaf node
 1: function B_DIAG(tree)
        -, treeL, treeR = tree
                                                   \triangleright \exists (k1; i) s.t. it is the numbering for the root node of treeL.
 2:
                                                  \triangleright \exists (k2; j) s.t. it is the numbering for the root node of treeR.
 3:
        if treeL is a leaf node and treeR is a leaf node then
 4:
            B_{k_1;i,k_2;j} = U_{k_1;i}^T A_{k_1;i,k_2;j} V_{k_2;j}
 5:
        else if treeL is not a leaf node and treeR is not a leaf node then
 6:
            B_{k_1:i,k_2:i} = B_OFFDIAG(treeL, treeR)
 7:
            B_DIAG(treeL)
 8:
            B_DIAG(treeR)
 9:
        else if treeL is a leaf node and treeR is not a leaf node then
10:
            -, treeRL treeRR = treeR
11:
            B_{k_1;i,k_2+1;2j-1} = B_OFFDIAG(treeL, treeRL)
12:
            B_{k_1:i,k_2+1:2i} = B_OFFDIAG(treeL, treeRR)
13:
            B_{k_1;i,k_2;j} = B_{k_1;i,k_2+1;2j-1}W_{k_2+1;2j-1} + B_{k_1;i,k_2+1;2j}W_{k_2+1;2j}
14:
            B_{k_1;i,k_2+1;2i-1} = (); \qquad B_{k_1;i,k_2+1;2i} = ()
15:
            B_DIAG(treeR)
16:
        else if treeL is not a leaf node and treeR is a leaf node then
17:
            -, treeLL, treeLR = treeL
18:
            B_{k_1+1;2i-1,k_2,j} = B_OFFDIAG(treeLL,treeR)
19:
            B_{k_1+1:2i,k_2,j} = B_OFFDIAG(treeLR, treeR)
20:
            B_{k_1;i,k_2;j} = R_{k_1+1;2i-1}^T B_{k_1+1;2i-1,k_2;j} + R_{k_1+1;2i}^T B_{k_1+1;2i,k_2;j}
21:
            B_{k_1+1;2i-1,k_2;j} = (); \qquad B_{k_1+1;2i,k_2;j} = ()
22:
            B_DIAG(treeL)
23:
        end if
24:
25: end function
```

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### **Algorithm 3 Pass 2BU**

**Algorithm 3** Pass 2BU - Computation of Expansion Coefficients  $(B_{k;i-1,i})$  Corresponding to Off-Diagonal Blocks

1: function B\_OFFDIAG(treeL.treeR) -, treeLL, treeLR = treeL 2: 3: -, treeRL, treeRR = treeRif treeL is a leaf node and treeR is a leaf node then 4:  $B_{k_1;i,k_2;j} = U_{k_1:i}^T A_{k_1;i,k_2;j} V_{k_2;j}$ 5: return  $B_{k_1:i,k_2:i}$ 6: else if treeL is not a leaf node and treeR is not a leaf node then 7:  $B_{k_1+1:2i-1,k_2+1:2i-1} = B_OFFDIAG(treeLL,treeRL)$ 8:  $B_{k_1+1:2i-1,k_2+1:2i-} = B_OFFDIAG(treeLL,treeRR)$ 9:  $B_{k_1+1;2i,k_2+1;2j-1} = B_OFFDIAG(treeLR,treeRL)$ 10:  $B_{k_1+1;2i,k_2+1;2j} = B_OFFDIAG(treeLR,treeRR)$ 11:  $B_{k_1;i,k_2;j} = R_{k_1+1;2i-1}^T B_{k_1+1;2i-1,k_2+1;2j-1} W_{k_2+1;2j-1} + R_{k_1+1;2i-1}^T B_{k_1+1;2i-1,k_2+1;2j} W_{k_2+1;2j}$ 12:  $+R_{k_1+1:2i}^TB_{k_1+1;2i,k_2+1;2j-1}W_{k_2+1;2j-1}+R_{k_1+1:2i}^TB_{k_1+1:2i,k_2+1;2j}W_{k_2+1;2j}$  $B_{k_1+1;2i-1,k_2+1;2j-1} = ();$   $B_{k_1+1;2i-1,k_2+1;2j} = ();$ 13:  $B_{k_1+1:2i,k_2+1:2i-1} = (); \qquad B_{k_1+1:2i,k_2+1:2i} = ()$ 14: 15: return  $B_{k_1:i,k_2:i}$ else if treeL is a leaf node and treeR is **not** a leaf node **then** 16:  $B_{k_1:i,k_2+1:2i-1} = B_OFFDIAG(treeL,treeRL)$ 17:  $B_{k_1:i,k_2+1:2i} = B_OFFDIAG(treeL,treeRR)$ 18:  $B_{k_1;i,k_2;j} = B_{k_1;i,k_2+1;2j-1}W_{k_2+1;2j-1} + B_{k_1;i,k_2+1;2j}W_{k_2+1;2j}$ 19:  $B_{k_1;i,k_2+1;2i-1} = ();$  $B_{k_1;i,k_2+1;2j} = ()$ 20: return  $B_{k_1:i,k_2:i}$ 21: else if *treeL* is not a leaf node and *treeR* is a leaf node then 22:  $B_{k_1+1;2i-1,k_2;j} = B_OFFDIAG(treeLL,treeR)$ 23: $B_{k_1+1:2i,k_2:i} = B_OFFDIAG(treeLR,treeR)$ 24: $B_{k_1;i,k_2;j} = R_{k_1+1;2i-1}^T B_{k_1+1;2i-1,k_2;j} + R_{k_1+1;2i}^T B_{k_1+1;2i,k_2;j}$ 25: $B_{k_1+1:2i-1,k_2;j} = (); \qquad B_{k_1+1:2i,k_2;j} = ()$ 26: return  $B_{k_1;i,k_2;j}$ 27:end if 28: 29: end function

### Worst Case Memory Consumption for our Algorithm



### Example Block Partitioning of a Matrix with Corresponding Partition Trees



### **Future Work**

- Fast Multipole Method (FMM) construction Algorithm
- FMM × FMM
- Application to classical HSS algorithms: HSS Multiply & HSS Solver