Discovering Hierarchical Matrix Structure Through Recursive Tensor Decomposition

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Fractional PDEs are useful in Scientific applications

- Fractional Partial Differential Equations (fPDEs) are used in modeling turbulence, financial markets, anomalous diffusion.

Definition (Fractional PDE)

For a fractional index $\alpha \in (1, 2)$ and function $f \in L^2[b, c]$, the initial value problem we are trying to solve is:

$$\mathcal{D}_x^\alpha u(x) = f(x), \quad x \in (b, c)$$
$$u(b), u(c) = 0$$

where the Riesz fractional derivative is:

$$\mathcal{D}_x^\alpha f(x) = \frac{-1}{2\cos(\alpha\pi/2)\Gamma(2-\alpha)} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \int_b^c |x - \xi|^{1-\alpha} f(\xi) \mathrm{d}\xi$$

Discretizing the fPDE

- We use the weak formulation of the fPDE and the Galerkin method to get a finite element discretization.
- We can take the discrete solution to get a vector $\vec{u}$, which is the PDE solution at discrete locations.
- This means we get a linear system: $\mathbf{A}\vec{u} = \vec{f}$

X. Zhao *et.al.* "Adaptive finite element method for fractional differential equations using hierarchical matrices," Comput. Methods Appl. Mech. Engrg.325, pp. 56-76, (2017)

Problems with Adaptive Grid on discretized fPDEs

- The stiffness matrices require $\mathcal{O}(n^2)$ storage and $\mathcal{O}(n^3)$ flops to solve exactly.
  - This motivates a need for a storage efficient approximation.
- On a uniform mesh, this matrix has Toeplitz structure, which has known algorithms for efficient storage and fast mat-vecs.
  - Uniform meshes can still have issues with singularities around the boundary even with smooth inputs.
- If we use an adaptive mesh, we could minimize the singularities and get hierarchical structure, leading to low rank off-diagonal blocks. But this is still an appoximation.
- To form a better approximation, we propose a novel tensor based method to construct a matrix that uses less memory to give a better approximation.

Matrix Properties

Definition (Kronecker Product)

Let $\mathbf{A} \in \mathbb{R}^{m \times p}$, $\mathbf{B} \in \mathbb{R}^{n \times l}$. Then the Kronecker Product $\mathbf{A} \otimes \mathbf{B} \in \mathbb{R}^{(mn)\times(pl)}$ is denoted as

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & a_{1p}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots & a_{2p}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & a_{m2}\mathbf{B} & \cdots & a_{mp}\mathbf{B} \end{pmatrix} \tag{1}$$

Definition (Relative Error)

Let $\hat{\mathcal{A}}$ be an approximation to $\mathcal{A}$. The relative error is the norm of the difference between $\mathcal{A} - \hat{\mathcal{A}}$ divided by the norm of the original, namely $\frac{\|\mathcal{A}-\hat{\mathcal{A}}\|}{\|\mathcal{A}\|}$. We use the Frobenius norm for this project.

What is a Tensor?

Definition (Tensor)

A tensor is a multidimensional array of numbers.

Example

- A scalar, $c \in \mathbb{R}$ is a zeroth order tensor.
- A vector, $\vec{v} \in \mathbb{R}^n$ is a first order tensor.
- A matrix, $\mathbf{A} \in \mathbb{R}^{m \times n}$ is a second order tensor.
- A tensor, $\mathcal{T} \in \mathbb{R}^{m \times p \times n}$ is a third order tensor.

Definition (Tensor Order)

The tensor $\mathcal{T} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ is a d^{th}-order tensor, sometimes also read as d-way tensor. The order corresponds to the dimension of tensor.

Tensor Properties

Definition (k^{th}-mode Tensor Unfolding)

Let $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ be a d-way tensor. Then the k^{th}-mode unfolding is defined as

$$\mathbf{A}_{(k)} \in \mathbb{R}^{n_k \times n_1 n_2 \cdots n_{k-1} n_{k+1} \cdots n_d} \tag{2}$$

Definition (mode-k product)

The mode-k product is a way of denoting a tensor-matrix product, where the tensor is unfolded in the k^{th} mode and left multiplied by a matrix, assuming matrix dimensions match. Mathematically,

$$\mathcal{A} \times_k \mathbf{U} := \mathbf{U}\mathbf{A}_{(k)} \tag{3}$$

Tensor Examples

Let $\mathcal{A} \in \mathbb{R}^{2\times2\times2}$, where the frontal slices of the tensor are:

$$\mathcal{A}_{::1} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \quad \mathcal{A}_{::2} = \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix} \tag{4}$$

Then the following are the k^{th}-mode unfoldings ("matricizations")

$$\mathbf{A}_{(1)} = \begin{pmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{pmatrix} \tag{5}$$

$$\mathbf{A}_{(2)} = \begin{pmatrix} 1 & 3 & 5 & 7 \\ 2 & 4 & 6 & 8 \end{pmatrix} \tag{6}$$

$$\mathbf{A}_{(3)} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{pmatrix} \tag{7}$$

Tensor Decompositions

Definition (Higher Order Singular Value Decomposition (HOSVD))

We perform an SVD on each unfolding, keeping the left singular vectors, denoted $\mathbf{U}, \mathbf{V}, \mathbf{W}$ respectively. Then the core tensor $\mathcal{G}$ is computed by

$$\mathcal{G} := \mathcal{A} \times_1 \mathbf{U}^T \times_2 \mathbf{V}^T \times_3 \mathbf{W}^T \tag{8}$$

Once we have the core tensor, we can truncated it in any mode possible to get a tensor approximation, namely

$$\hat{\mathcal{A}} \approx \mathcal{G} \times_1 \mathbf{U} \times_2 \mathbf{V} \times_3 \mathbf{W} \tag{9}$$

Matrix to Tensor Bijective Mapping

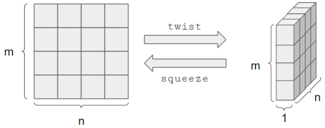


Figure: The bijective mapping between an $m \times n$ matrix and an $m \times 1 \times n$ tensor.

Theorem

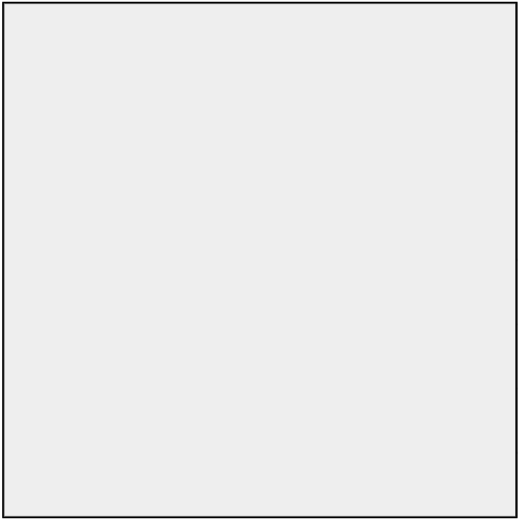
The error between the original matrix $\mathbf{A}$ *and the matrix form of the tensor approximation* $\hat{\mathbf{A}}$ *is the same error as the tensor* $\mathcal{T}$ *and tensor approximation* $\hat{\mathcal{T}}$ *in the Frobenious norm.*[a]

[a] M. Kilmer and A. Saibaba, "Structured Matrix Approximations via Tensor Decompositions," arXiv:2105.01170 [math.NA], May 2021

Algorithmic approach to our Proposed Method

1. Divide the Matrix
2. Form Tensors at different levels
3. Compress with Higher Order SVD
4. Map back to a Matrix

Divide the Matrix (Diagonal + Low Rank)



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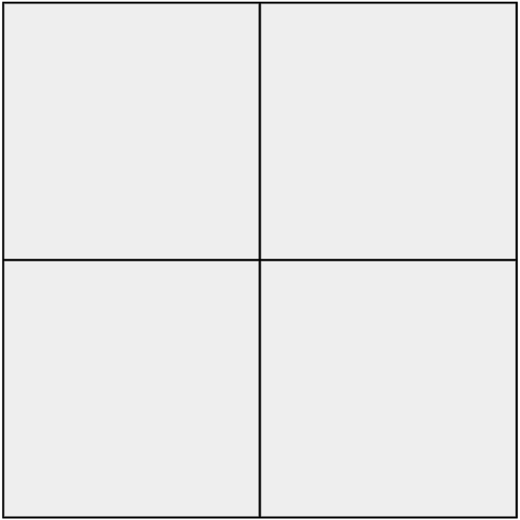

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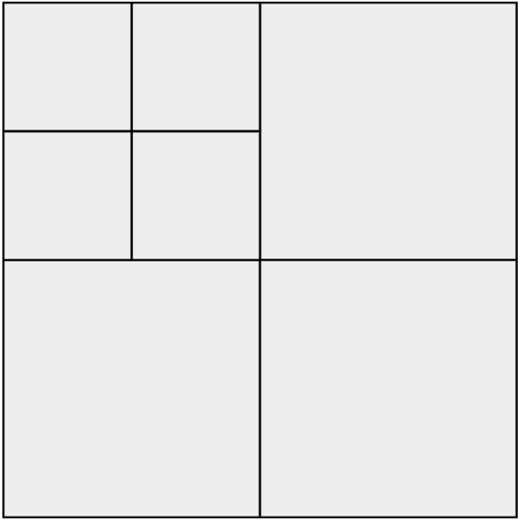

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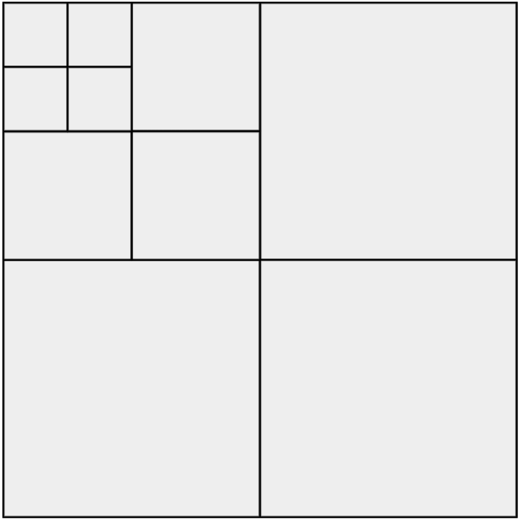

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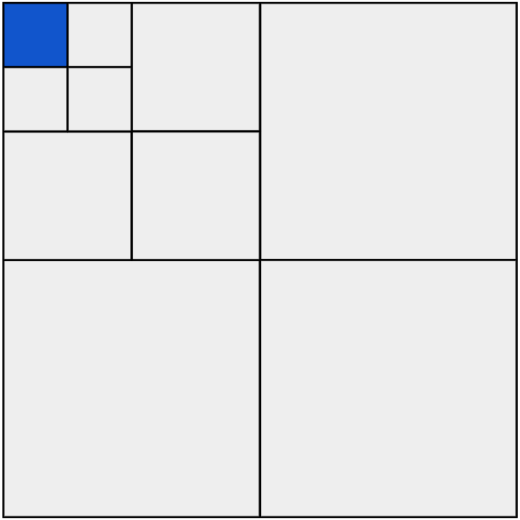

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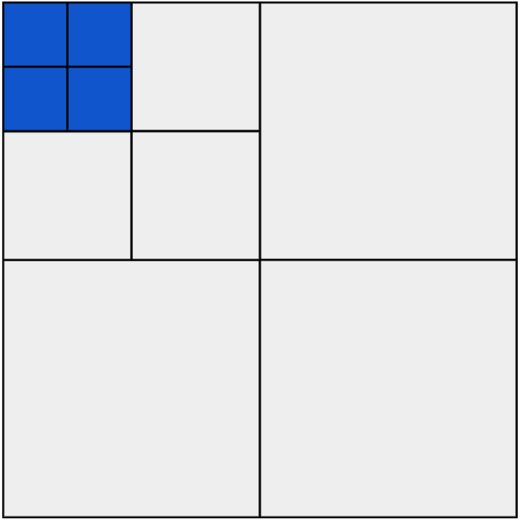

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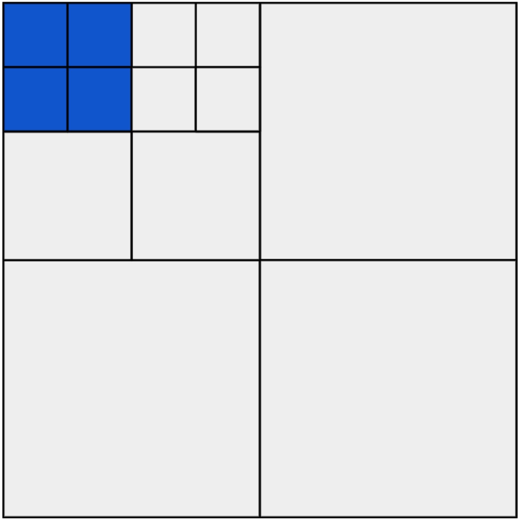

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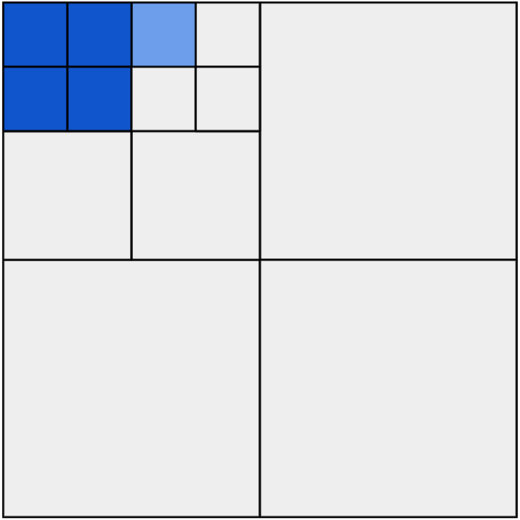

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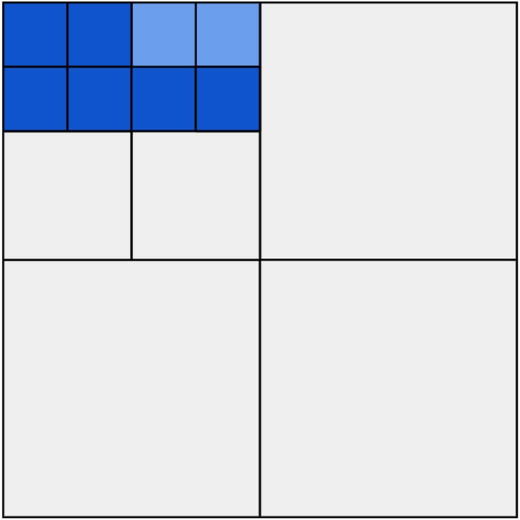

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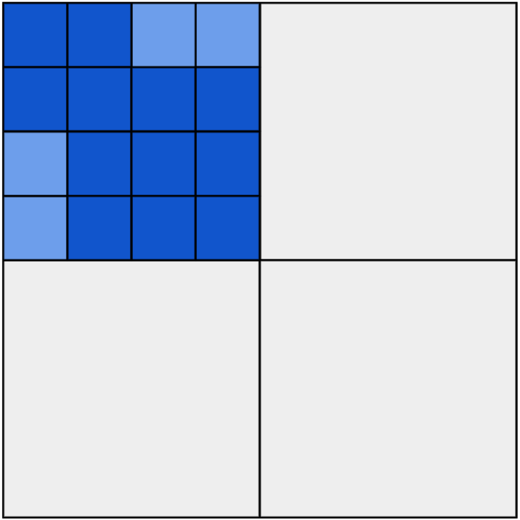

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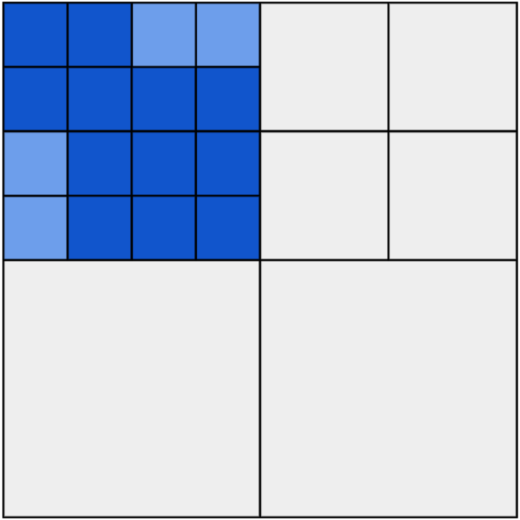

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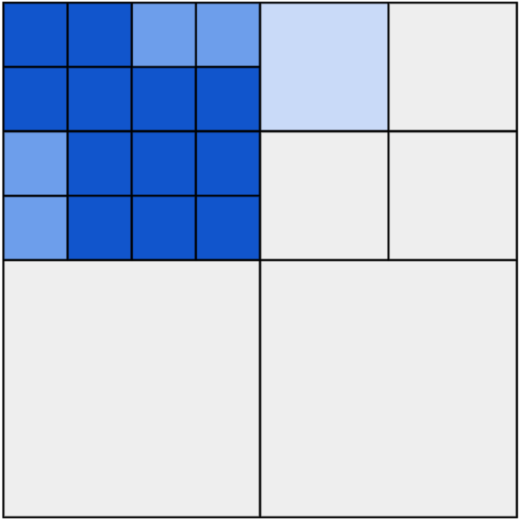

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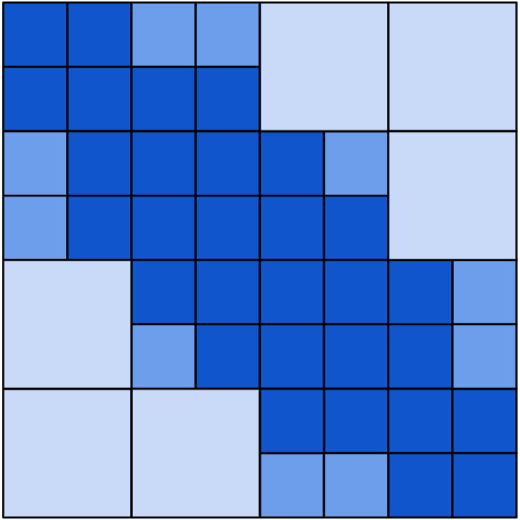
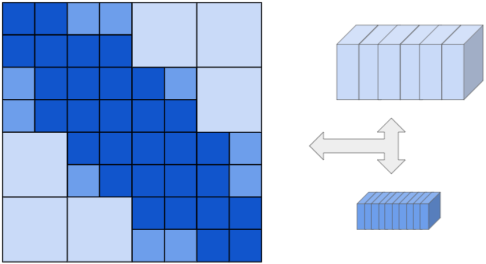


Algorithmic approach to our Proposed Method

1. Divide the Matrix
2. Form Tensors at different levels
3. Compress with Higher Order SVD
4. Map back to a Matrix

Form Tensors at different levels

- This hierarchical structured approximation of the true stiffness matrix allows us to identify candidate submatrices to twist into a tensor.
- These submatrices share more properties than just rank and size, and we plan to use these higher dimensional properties to make our lives easier.



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Compress with Higher Order SVD

- Using either storage or approximation thresholds, we change the structure of the tensor approximations of these ill-conditioned adaptive meshes.

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Map back to a Matrix

- This leads to a structured factorization.
- We can treat it as a sum of kronecker products.
  - Using kronecker properties, we can make this a cheaper representation.

Comparing our preliminary results with current literature

- Using a similar relative error/ compression benchmark, our method has better preconditioning, lower error, and better storage properties.

Method	**Literature**	**Proposed**
Rel Error	1.5905e-5	1.2217e-5
Compression	10.16%	52.67%

Method	**Literature**	**Proposed**
Compression	10.16%	11.13%
Rel Error	1.5905e-5	1.8462e-12

- This is due to exploiting the multidimensional structure of the data, considering it all at once, and not at individual blocks.

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Summary and Future Work

- Right now, our toy problem is small and easy to compute, so we are looking at kronecker based SMW methods to never form the inverse.
  - This leads us to use this method to produce $\hat{\mathbf{A}}$ as a preconditioner for the original $\mathbf{A}$.
- We are looking at using integer programming to determine the optimal truncation rank and weights across the matrix unfoldings and the two levels of tensors.
- We are also looking for techniques in constructing the tensor to ensure even if the adaptive mesh matrix is more general, our tensor-based approach still works.

Questions?

- Thank you organizers for this opportunity.
- Thank *you* for coming to my talk.
- Are there any questions?
- If you have any questions after this talk, you can reach me at
  - mitchell.scott@tufts.edu