Quantized Tensor Trains for Solving Maxwell's Equations with Spectral Methods

Mitchell T. Scott[1], Erika Ye[2]

[1]Emory University, [2]Lawrence Berkeley National Laboratory

ABSTRACT

Numerical simulations of plasmas are critical for designing fusion energy systems and modeling astrophysical bodies. These simulations require solving Maxwell's equations, which describe the behavior of the magnetic and electric fields generated by and applied to the plasma. We aim to reduce computational costs by implementing a spectral solver in the Quantized Tensor Train (QTT) framework.

BACKGROUND

Maxwell's Equations (ME) are given by

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$$

where **E** is the electric field, **B** the magnetic field, and **J** the current density.

Finite Difference Time Domain (FDTD)

The spatial domain is discretized and derivatives are approximated by a first-order finite difference scheme:

$$u'(x) \approx \frac{u(x+h) - u(x)}{h}$$

Spectral Representation

Let $u(x,t)$ be a smooth function. It is approximated by a sum of coefficients $\{a_k\}$ and basis functions $\{\phi_k\}$. With this framework, the derivatives are defined by using a sum of new coefficients $\{a_k^{(p)}\}$ with the same basis functions.

$$u(x,t) \approx u_N(x,t) = \sum_{k=0}^{N} a_k(t)\phi_k(x)$$

$$\frac{\partial^p u(x,t)}{\partial x^p} \approx \frac{\partial^p u_N}{\partial x^p} = \sum_{k=0}^{M} a_k^{(p)}(t)\phi_k(x)$$

Example basis functions:

- *Chebyshev Polynomials*
- *Fourier Series*
- *Spherical Harmonics*
- *Ultraspherical Polynomials*

RESEARCH QUESTION

Can we solve Maxwell's equations in cylindrical coordinates more efficiently by using a spectral representation in the quantized tensor train format?

QUANTIZED TTs

The **quantized tensor train (QTT)** is a low-rank representation for large datasets.Consider a dataset of size N = d^L. In quantization, artificial dimensions are introduced, yielding an L-dimensional tensor of size d along each dimension. Often, the dimensions correspond to different grid resolutions.

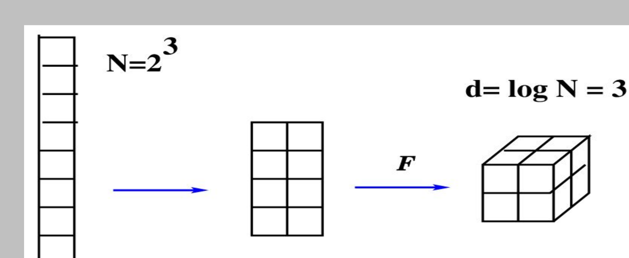

Figure 1: A visual representation of quanticly folding up a vector, N = 2^L, where L = 3. Figure credit: [1]

In a tensor train, the L-dimensional tensor is then approximated as a tensor train of rank R. The storage cost is reduced from N to O(R $\log_d$ N).

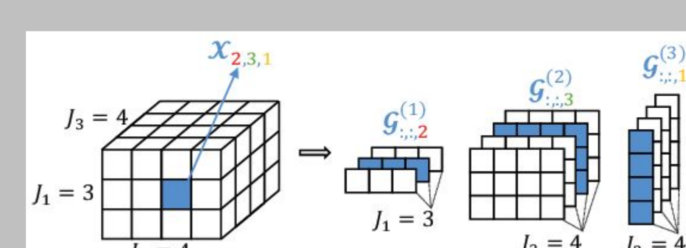

Figure 2: A 3 x 4 x 4 tensor is converted into a tensor train. The blue indicates how **X**(2,3,1) is computed. Figure credit: [2]

Exponential Vector

For example, let an exponential vector be

$$\mathbf{X} = [1, z, z^2, z^3, z^4, z^5, z^6, z^7]^\top \in \mathbb{C}^8$$

where N = 2^3,L = 3. The QTT representation is

$$\mathbf{X} \to \mathbf{A} = \begin{bmatrix} 1 \\ z^4 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z^2 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z \end{bmatrix}$$

Differential Operators

Additionally, differentiation can be efficiently represented in the QTT framework. Let

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{S}^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{S}^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Then on a uniform grid, we approximate the first order derivative (up to scaling) as

$$\frac{\partial}{\partial x} \approx \begin{pmatrix} \mathbf{I} & \mathbf{S}^+ & \mathbf{S}^- \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{S}^+ & \mathbf{S}^- \\ \mathbf{0} & \mathbf{S}^- & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{S}^+ \end{pmatrix} \begin{pmatrix} \mathbf{S}^+ - \mathbf{S}^- \\ \mathbf{S}^- \\ -\mathbf{S}^+ \end{pmatrix}$$

RESULTS

There is a cylindrical domain with periodic conditions in the polar and z-direction, with Chebyshev nodes in the radial direction. This allows for Fourier differentiation in the periodic case and Chebyshev differentiation in the radial component.

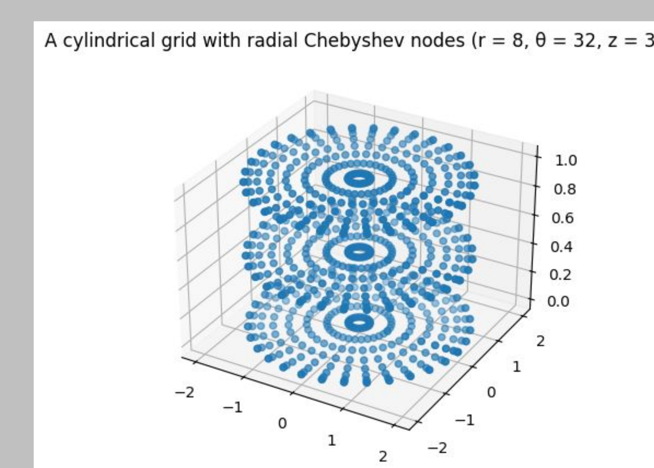

Figure 3: The radial grid points are Chebyshev nodes which allow for no point at the origin and more points around the boundary.

Compared to the finite difference operator, the spectral derivative operator loses sparsity (as the spectral operators are dense), but it maintains circulant structure and improves accuracy.

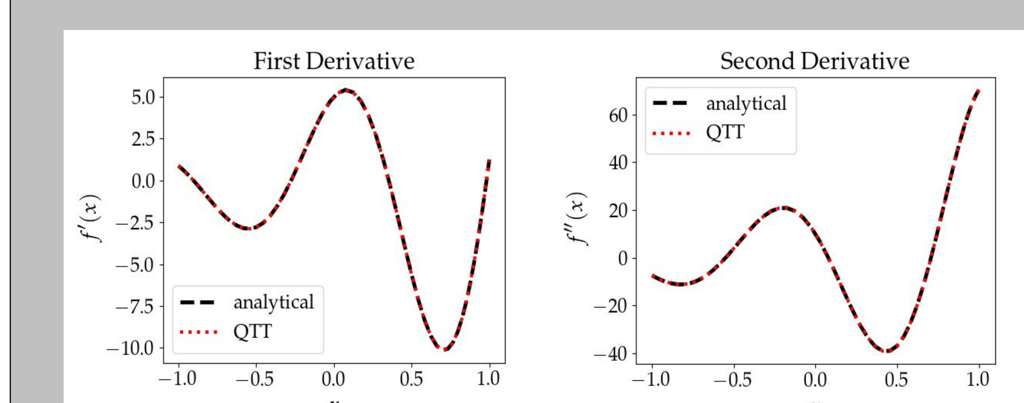

Figure 4: The QTT representation of the first derivative of $e^x \sin(5x)$ (left) and second derivative of the same function (right).

# Tensor Cores	4	5	6	7	8	9
Max Rank	16	32	64	128	256	512
QTT Rank	16	16	56	58	65	66

Table 1: Rank of Chebyshev Derivative Operator versus number of Chebyshev points.

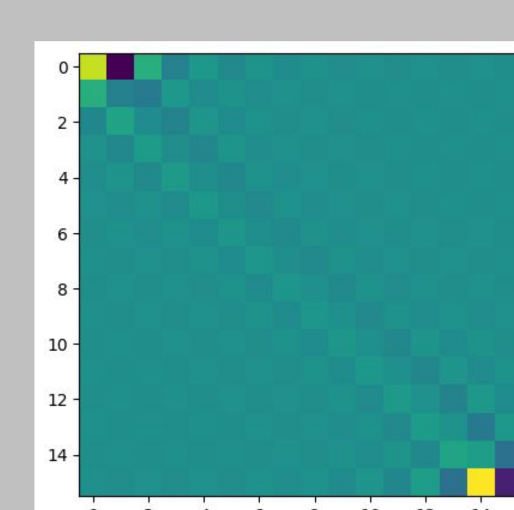

Figure 5: The Chebyshev derivative operator.

FUTURE PLANS

- **Evaluate utility in more practical test problems**
  - Right now, only simple tests problems have been compared, so it would be advantageous to see how spectral methods compare with time varying parameters or boundary conditions.
- **Experiment with rank vs. accuracy**
  - To reduce the rank of the operator, a cutoff threshold on the singular values should be evaluated. Additionally, can an *a priori* rank bound be known?
- **See dependence on physical boundary conditions**
  - There are many boundary conditions used in modeling a plasma reactor, so the problem might change the optimal basis functions and optima rank.
- **Generalize Chebyshev Polynomials**
  - In spectral methods, Chebyshev basis functions are the most versatile. Then using generalizations such as Gegenbauer, Legendre, or Jacobi polynomials might be beneficial.

REFERENCES

[1] Khoromskij, B.N., (2011). "O(Dlog N)-Quantics Approximation of N-d Tensors in High-Dimensional Numerical Modeling."Constr Approx (2011) 34:257–280 DOI 10.1007/s00365-011-9131-1

[2] Xu, Le & Cheng, Lei & Wong, Ngai & Wu, Yik-Chung. (2020). "Learning Tensor Train Representation with Automatic Rank Determination from Incomplete Noisy Data."

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