

Supplementary Information for “Time integration of quantized tensor trains using the interpolative dynamical low-rank approximation”

1 QTT in Fourier space

In Section 2.3, the PDE is solved in the Fourier representation instead of the standard real-space basis. This is still efficient in the low-rank representation. In Fourier space, the quantization procedure is the same, except the basis functions are now of the form $\phi_n(x) = \exp(i2\pi nx)$, and a binary mapping between n and hyperindices $(\sigma_1, \dots, \sigma_L)$ are used:

$$n = \sum_{k=1}^L 2^k \sigma_k = \sigma_L \dots \sigma_3 \sigma_2 \sigma_1.$$

This choice of basis still offers a multiscale representation, with the splitting of the σ at grid level m separating the low frequency modes $(\sigma_1, \dots, \sigma_m)$ from the high frequency modes $(\sigma_{m+1}, \dots, \sigma_L)$

$$n_{\leq m} = \sum_{k=1}^m 2^k \sigma_k, \quad n_{> m} = \sum_{k=m+1}^L 2^k \sigma_k = 2^m \sum_{k=1}^{L-m} 2^k \sigma_k$$

Converting the real-space operations in the PDE to Fourier space is done by taking the Fourier transform. In the case that an analytical form is not readily accessible, one can efficiently compute it numerically in the QTT representation since the Fourier transform is low rank [1, 2]. Constructing the operator explicitly can also be preferable to avoid issues with artificial ringing effects.

For example, consider the convolution operation, which takes two inputs and generates an output. Ref. [3] explains the construction of the QTT representation, determining that it is of rank 2. It can also be expressed explicitly

$$C_{ijk} = \sum_{a,b,c} \mathcal{F}_{kc} \delta_{abc} \mathcal{F}_{ai}^{-1} \mathcal{F}_{bj}^{-1}$$

where $\mathcal{F}$ is the matrix representation of the Fourier transform, such that

$$(x * y)_k = \sum_{ij} C_{ijk} x_i y_j$$

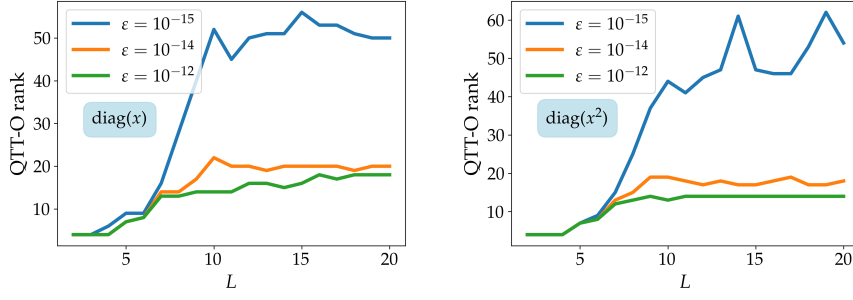


Fig. 1: QTT ranks versus L for Fourier representation of $\text{diag}(x)$ and $\text{diag}(x^2)$.

Since the Fourier transform can be written in QTT form, then this operator can be also be efficiently constructed in a way analogous to the zip-up algorithm¹: starting from $i = 1$, contract all tensors associated with index σ_i . If not at the end of the chain, perform the QR decomposition, setting Q as the i^{th} tensor core and associating R with the $i + 1$ site. Once the new QTTs are constructed, perform the standard canonicalization procedure sweeping from site L to site 1. With an rank-truncation threshold of $\varepsilon = 10^{-14}$, it also returns a QTT of rank 2, regardless of resolution.

To measure the m^{th} spatial moment of some function $\tilde{f}$ that it is in the Fourier basis, one will need to perform the convolution $\mathcal{F}x^m * \tilde{f}$. The linear operator that performs this operation $M\tilde{f} = (\tilde{f} * \mathcal{F}x^m)$ is

$$M_{ij} = \sum_{a,b,c} \mathcal{F}_{kc} \delta_{abc} \mathcal{F}_{ai}^{-1} \sum_j \left(\mathcal{F}_{bj}^{-1} (\mathcal{F}x^m)_j \right) = \sum_j C_{ijk} (\mathcal{F}x^m)_j.$$

For the first and second orders, the ranks are larger than their real-space counterparts, but plateaus at about 20 at high resolutions (large L), as shown in Fig. 1.

Once these operators are constructed offline, one can solve the PDE in the Fourier basis without explicitly converting to a real-space representation.

References

- [1] Chen, J., Stoudenmire, E.M., White, S.R.: Quantum fourier transform has small entanglement. PRX Quantum **4**, 040318 (2023) <https://doi.org/10.1103/PRXQuantum.4.040318>
- [2] Chen, J., Lindsey, M.: Direct interpolative construction of the discrete Fourier transform as a matrix product operator. arXiv. arXiv:2404.03182 [quant-ph] (2024). <https://doi.org/10.48550/arXiv.2404.03182> . <http://arxiv.org/abs/2404.03182> Accessed 2024-07-03

¹see tensornetwork.org

- [3] Kazeev, V.A., Khoromskij, B.N., Tyrtshnikov, E.E.: Multilevel Toeplitz matrices generated by tensor-structured vectors and convolution with logarithmic complexity. *SIAM J. Sci. Comput.* **35**(3), 1511–1536 (2013)