GPU-Accelerated Tensor Networks

Harnessing the power of GPUs

arXiv : 2306.00358, in collaboration with Raghav G. Jha

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01 August 2023

- **Goal :** Estimating the Partition Function and Expectation of the subsequent Observables for a system

$$Z = \sum_{\{s_i\}} exp(-\beta H_{s_i}) \tag{1}$$

- Standard Monte Carlo Methods sample states s_i using various techniques but can only compute expectation of the observable
- Tensor Networks can estimate the Partition Function in the Thermodynamic Limit as well as Handle Sign Problems

Tensor Renormalization Group (TRG)

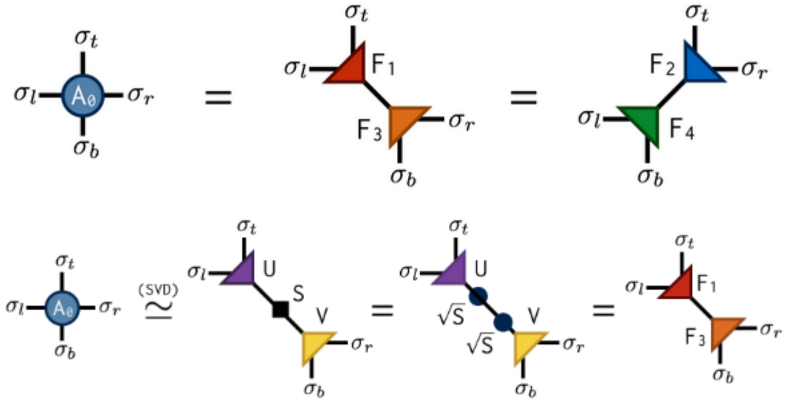
A Tensor Networks Method

- More natural to lattice field theory, based on the Lagrangian of the system.
- First introduced to study discrete spin models and now it has also been used to study spin models with continuous symmetry and gauge theories in two and higher dimensions. **(arxiv : 2202.10051, 2010.06539)**
- Primary reason to use TRG methods is their ability to deal with complex-actions involving terms such as topological-θ, chemical potentials, etc. because no sampling technique is used here.

Tensors Renormalization Group

Algorithm Description, Image source : https://www.tensornetwork.org/trg

- Assuming that the system is represented by a network of 4-rank tensors, A_0. First perform singular value decomposition of each tensor A_0



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Tensors Renormalization Group

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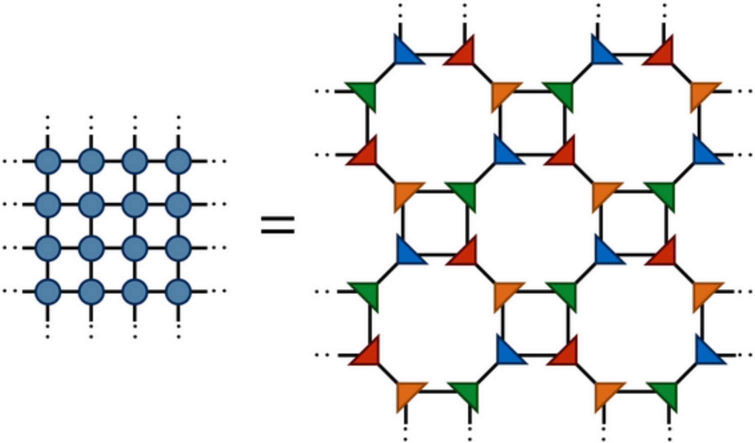
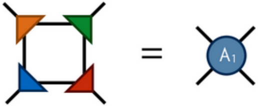
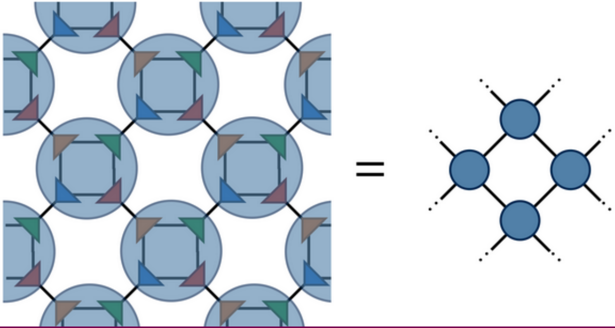
- The original network configuration after SVD looks like,



- Now contract the four F tensors from SVD to get new network configuration with each tensor A_1

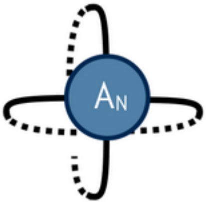




Tensors Renormalization Group

Algorithm Description, Image source : https://www.tensornetwork.org/trg

- Keep repeating this process until only 1 tensor is left in the network configuration and then take the tensor trace which gives the partition function



And that is how we get the Partition Function !

Higher Order Tensors Renormalization Group

TRG + HOSVD = HOTRG

- Higher Order TRG (HOTRG) truncates the diagonal matrix S obtained from SVD at a finite D which reduces the errors in the numerical estimations.
- Truncation means choosing a part of the diagonal matrix consisting of maximum number of non-zero elements with D as an upper bound to this number

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How to use Graphical Processing Units?

Tensor Initialization, Contraction and Linear Algebra Operations on a GPU

- We will use Python Programming Language.
- Define all the tensors using **PyTorch** package. These tensors are all CPU tensors.
- Use **opt_einsum_torch** package which has a compatibility with PyTorch on GPU for tensor contractions.
- This package performs Einstein Summations significantly faster than other python modules such as **ncon, einsteinpy, numpy.einsum**, etc.
- To perform SVD and other Linear Algebra Operations, **torch.linalg** sub-module was used.

Runtime Comparison for HOTRG

Time Complexity Orders on CPU v/s GPU

Device	Scaling	Scaling for $d = 2$
CPU	$\mathcal{O}(D^{4d-1})$	$\mathcal{O}(D^7)$
GPU (This Work)	-	$\mathcal{O}(D^{(5-6)})$

Table: d is the number of Euclidean Dimensions for a system, D is the truncation parameter

- In HOTRG, the dominant contribution in execution time for CPU and GPU both, is from Tensor Contractions.
- HOSVD gets a boost in compute time on a GPU whereas for a CPU the time scaling is given as $\mathcal{O}(D^6)$
- The absolute run-time reduces significantly when GPU is used over a CPU.

GPU v/s CPU

How GPUs are better

- **Number of Cores :** A GPU has large number of cores (in thousands) as compared to a CPU which has only 20-60.
- **Heavy Parallelization :** 32 threads per core for GPU as compared to 2 threads per core for a CPU.
- **Load Management :** Unlike a CPU, a GPU can reduce memory subsystem load by dynamically changing the number of available registers (from 64 to 256 per thread).
- **Shared Memory :** GPUs have shared memory management which is significantly faster than CPU's L1 Cache memory.

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2d Ising Model

Verifying known results

- For 2d Ising Model, we compared the Free Energy with the exact known results to check the accuracy of the HOTRG Algorithm.
- We compute error in free energy as,

$$\left|\frac{\delta f}{f}\right| = \left|\frac{f_{\mathrm{TRG}} - f_{\mathrm{E}}}{f_{\mathrm{E}}}\right| \tag{2}$$

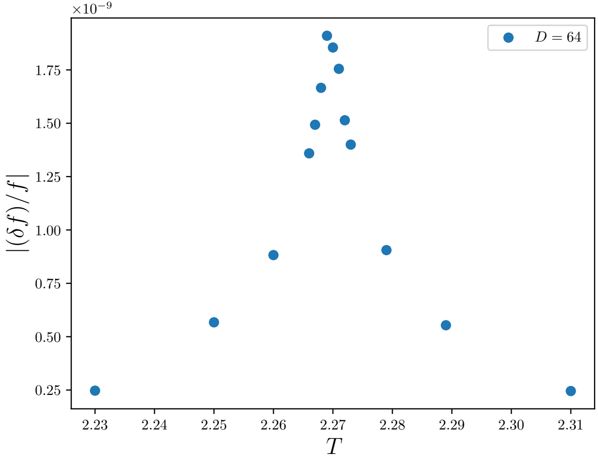
- The starting tensor A_0 for the Ising Model is (By Expanding Boltzmann Weights),

$$A_0 = T_{ijkl} = W_{ia} W_{ja} W_{ka} W_{la}, \tag{3}$$

$$W_{ia} = \begin{bmatrix} \sqrt{\cosh(\beta)} & \sqrt{\sinh(\beta)} \\ \sqrt{\cosh(\beta)} & -\sqrt{\sinh(\beta)} \end{bmatrix} \tag{4}$$

2d Ising Model

Free Energy v/s Temperature



2d Ising Model

Run-time Comparison Table

- Comparison the execution time for a single $T = T_c$ run on CPU and GPU

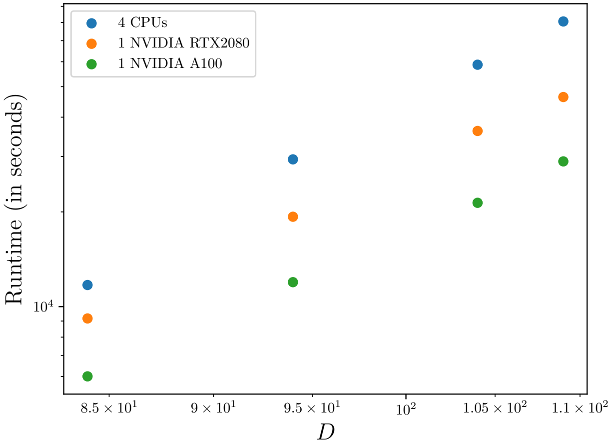
D	$\left\lvert \frac{\delta f}{f} \right\rvert$	A100	RTX 2080	4 CPUs
84	6.6×10^{-10}	6004	9171	11714
94	4.4×10^{-10}	11960	19305	29376
104	2.9×10^{-10}	21376	36159	58715
109	2.4×10^{-10}	28942	46350	80578

Table: Timings (in seconds) for the HOTRG algorithm for Ising model for $2^{20} \times 2^{20}$ lattice at $T = T_c$.

- CPU-time scaling is $\sim D^7$ while the GPU-time is $\sim D^{5.9}$.
- Absolute execution time reduces as the the GPU architecture improves

2d Ising Model

Run-time Comparison Plot



2d Generalized-XY Model

Hamiltonian for 2dGXY

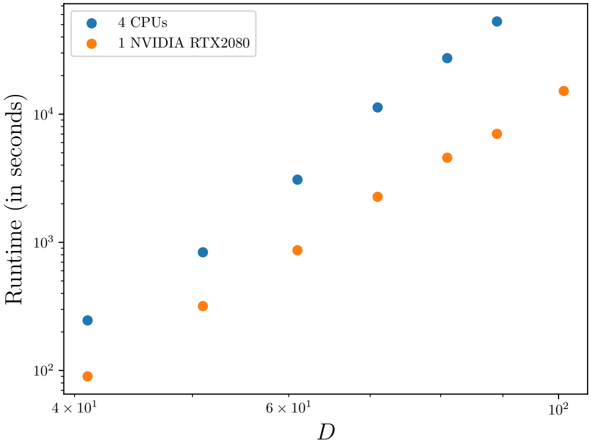
- The generalized XY (GXY) model is a standard XY model with a spin nematic deformation term in the hamiltonian,

$$\mathcal{H} = -\Delta \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - (1-\Delta) \sum_{\langle ij \rangle} \cos(2(\theta_i - \theta_j)) - h \sum_i \cos\theta_i, \quad (5)$$

- where $\langle ij \rangle$ denote the nearest neighbours and $\theta_i \in [0, 2\pi)$
- We performed tensor computations for a fixed value of $\Delta = 0.5$ and for different D, keeping $h = 0$
- GPU run-time scales as $\sim D^{5.4}$ as compared to CPU run-time which scales as $\sim D^7$

2d Generalized-XY Model

System Size : $2^{30} \times 2^{30}$



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4 Summary

Summary

Take-home message

- TRG Methods get a significant boost in compute time if GPUs are used, where absolute execution time reduces as the GPU Architecture improves.
- Run-time for HOTRG Method scales as $\mathcal{O}(D^{(5-6)})$ on a GPU as compared to $\mathcal{O}(D^{7})$ on a CPU for models with 2 Euclidean Dimensions, where the leading contribution comes from tensor contractions.
- Computing Critical Exponents to study system's behaviour around critical point requires higher values of D. Using GPU-Code such exponents can be computed in a reasonable amount of time and memory.
- Large number of cores and large number of threads launched per core enables GPU to perform tensor computations remarkably better than an CPU.

GPU-Accelerated Tensor Networks

Thank you for listening!
Any questions?