CS 598 EVS: Tensor Computations

Tensor Networks

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Tensor Networks

- Tensor network methods seek to approximately compute quantities involving high-order tensors, by making use of their decompositions

- Tensor network methods are often employed in problems where the tensor order varies with problem size

Tensor Representation of Quantum States

- An n-qubit state can be represented by an order n *amplitude tensor* $\boldsymbol{\mathcal{T}} \in \mathbb{C}^{2\times\cdots\times 2}$

Hamiltonians

- Quantum states and their evolution are described by *Hamiltonians*

Time-Evolution of Quantum States

- The Schrödinger equation perscribes a time-evolution for a quantum state given a Hamiltonian

- If H is a local Hamiltonian, *Trotterization* provides a method for time-evolution

Time-Evolution of a Matrix Product State (MPS)

- To simulate time-evolution $|\psi(t)\rangle$ from a product state $|\psi(0)\rangle$, we can approximate each $|\psi(j\tau + \tau)\rangle = e^{-iH\tau}|\psi(j\tau)\rangle$ as a matrix product state

Hamiltonians as Matrix Product Operators (MPOs)

- A *matrix product operator (MPO)* is a tensor-train decomposition where every factor tensor is assigned a pair of modes of the original tensor

Hamiltonians as Matrix Product Operators (MPOs)

- Hamiltonians describing quantum systems can typically be represented in an MPO format with low bond dimension

Generation of Efficient MPO Representations of Hamiltonians

- More sophisticated ways of embedding a local Hamiltonian into an MPO yield lower bond dimension

Density Matrix Renormalization Group (DMRG)

- *DMRG* [S. White, 1992] is an alternating optimization scheme to approximate by an MPS the ground state (lowest eigenvector) of a Hamiltonian described by an MPO

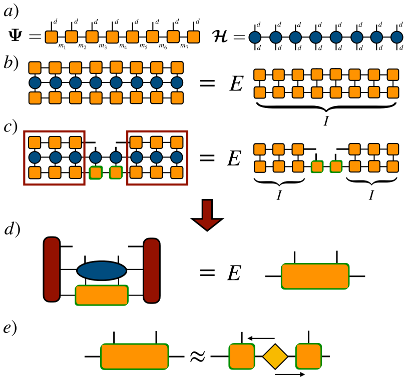


Diagram from [R. Levy, E.S., and B. Clark, 2020]

DMRG Algorithm Description

- A sweep of the DMRG algorithm updates all factor tensors in the MPS

Cost Analysis of DMRG

- Often the maximum bond dimension of the MPS (R) exceeds the MPO bond dimension significantly, and while each subproblem finds an eigenvector of an $O(R^2)$-by-$O(R^2)$ matrix, the optimization of each site in DMRG generally has cost $O(R^3)$

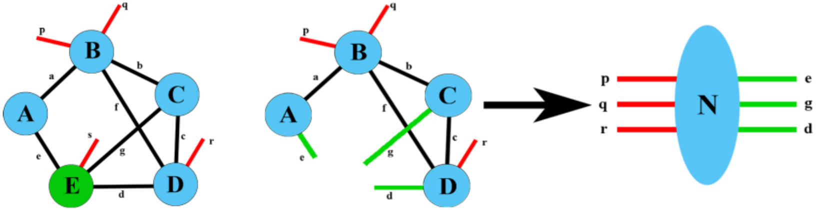
Sources of Error in Tensor Network Calculations

- Tensor network optimization algorithms perform approximations that are local to a few tensor factors

Perturbation Analysis of Tensor Networks

- Suppose we perturb a factor tensor of an tensor network by $\delta\boldsymbol{\mathcal{U}}$, with $\|\delta\boldsymbol{\mathcal{U}}\|_F/\|\boldsymbol{\mathcal{U}}\|_F < \epsilon$, what is the magnitude of the error in the tensor represented by the tensor network $\delta\boldsymbol{\mathcal{T}} = \boldsymbol{\mathcal{T}}(\boldsymbol{\mathcal{U}}) - \boldsymbol{\mathcal{T}}(\boldsymbol{\mathcal{U}} + \delta\boldsymbol{\mathcal{U}})$?

Environment Tensor and Jacobian Matrix



(a) Tensor Network

(b) Environment Matrix

Diagram from [Y. Zhang and E.S., 2020]

Canonical Forms

- A tensor network is in a *canonical form* w.r.t. factor tensor $\boldsymbol{\mathcal{U}}$ if the columns of $\boldsymbol{J}^{(\mathcal{T})}(\boldsymbol{\mathcal{U}})$ are orthonormal, i.e., $\kappa(\boldsymbol{J}^{(\mathcal{T})}(\boldsymbol{\mathcal{U}})) = 1$

Canonical Forms in DMRG

- The DMRG algorithm maintains an appropraite canonical form for all local computations

Tensor Networks beyond 1D

- An MPS is efficiently contractable and easy to put into canonical form, but other tensor networks often provide more desirable representations