Simulation of Quantum Systems with Time-Evolving Block Decimation

https://github.com/jchryssanthacopoulos/quantum_information/tree/main/final_project

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Università degli Studi di Padova

Outline

Theory

Simulating Quantum Systems

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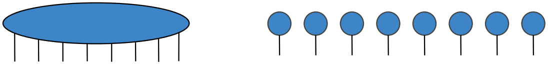
- To study a quantum system, one has to solve Schrodinger equation

$$\hat{H} |\Psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle$$

- One method involves direct numerical integration, where initial state is updated using time evolution operator

$$|\Psi(t + \Delta t)\rangle = e^{-i\hat{H}\Delta t} |\Psi(t)\rangle$$

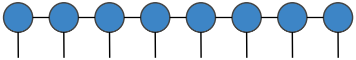
- This requires solving system of equations at every time that scales with system size, but in many-body problems, system size is **exponential** in number of sites, N
- In tensor network notation, general N-body system is shown on left. Mean-field ansatz on right greatly simplifies computation, but it ignores entanglement



How does one **preserve entanglement** while remaining **computationally tractable**?

Matrix Product States

- Matrix product states generalize mean-field ansatz to allow for entanglement between sites. Graphically,



where bond between sites has fixed **bond dimension** χ. When $\chi = 1$, mean-field approximation recovered

- Wavefunction is given by

$$|\Psi\rangle = A_1^{\mu_1} A_{\mu_1,2}^{\mu_2} \cdots A_{\mu_{N-2},N-1}^{\mu_{N-1}} A_{\mu_{N-1},N} |1\,2 \cdots N\rangle$$

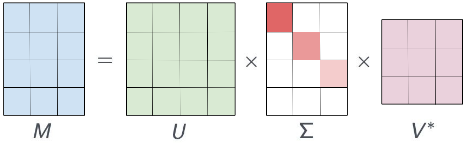
where $A_{\mu_{i-1},i}^{\mu_i}$ tensors have physical dimension $i \in \{1, \dots, d\}$ and **auxiliary dimension** $\mu_i \in \{1, \dots, \chi\}$

- Number of states scales like $Nd\chi^2$, which is **polynomial** in N

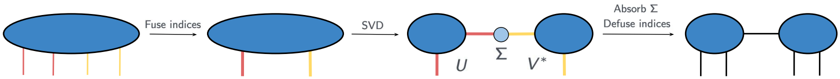
How does one evolve MPS in time without **breaking structure**?

Factoring Quantum State into MPS

- An arbitrary quantum state can be factored as an MPS using matrix factorization technique called **singular value decomposition**
- SVD generalizes eigendecomposition, finding two orthonormal bases u_i, w_i and singular values σ_i such that matrix is factorized into $M = U\Sigma V^*$, with U, V unitary



- SVD can be used to successively factor an MPS using following process:

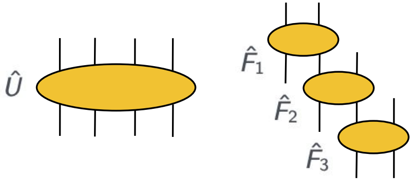


- SVD is driver behind simulating MPS quantum systems, allowing MPS structure to be preserved at each iteration. To keep bond dimension constant, singular values must be **truncated**

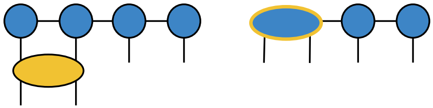
Time-Evolving Block Decimation

- Method for evolving quantum system while efficiently truncating large Hilbert space
- Also called **t-DMRG**, it evolves state using local gate operators and uses SVD to factorize back into MPS structure. The steps are:

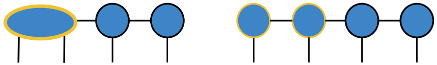
① Factor time evolution operator $\hat{U} : d^N \to d^N$ into two-site gates $\hat{F}_i : d^2 \to d^2$



② Apply first gate to first two sites, contracting indices to produce new state



③ Use SVD to factor state back into MPS form, truncating to bond dimension χ



④ Repeat for each pair of neighbors and time step

Suzuki-Trotter Decomposition

- Approximate decomposition of Hamiltonian based on Baker-Campbell-Hausdorff formula that reduces time and storage complexity of applying time evolution operator
- Hamiltonian $\hat{H}$ can be decomposed into odd and even operators:

$$\hat{H} = \sum_{i} \hat{h}_{i,i+1} = \sum_{i \text{ odd}} \hat{h}_{i,i+1} + \sum_{i \text{ even}} \hat{h}_{i,i+1} \equiv \hat{H}_{\text{odd}} + \hat{H}_{\text{even}}$$

- In **first-order Suzuki-Trotter**, commutator is ignored, leading to error $\mathcal{O}(\Delta t^2)$:

$$\hat{U} = e^{-i\hat{H}\Delta t} = e^{-i\hat{H}_{\text{even}}\Delta t} e^{-i\hat{H}_{\text{odd}}\Delta t} e^{-i\left[\hat{H}_{\text{even}},\hat{H}_{\text{odd}}\right]\Delta t^2} \approx e^{-i\hat{H}_{\text{even}}\Delta t} e^{-i\hat{H}_{\text{odd}}\Delta t} + \mathcal{O}(\Delta t^2)$$

- Higher orders can be built by continuing to factor Hamiltonian into finer time steps. For example, **second-order Suzuki-Trotter** comes with $\mathcal{O}(\Delta t^3)$ error:

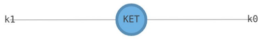
$$\hat{U} \approx e^{-i\hat{H}_{\text{even}}\Delta t/2} e^{-i\hat{H}_{\text{odd}}\Delta t} e^{-i\hat{H}_{\text{even}}\Delta t/2} + \mathcal{O}(\Delta t^3)$$

- When applied to time steps $T/\Delta t$, errors of ST1 and ST2 are $\mathcal{O}(\Delta t)$ and $\mathcal{O}(\Delta t^2)$, respectively. ST2 has lower error but requires more operations

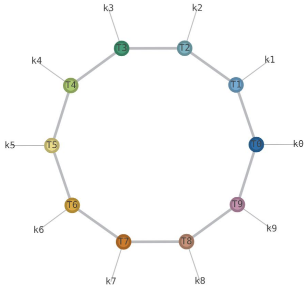
Code Development

QUIMB: Quantum Computing in Python

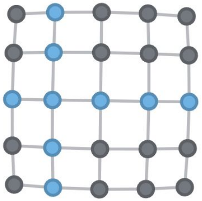
- Contains tools for working with tensors and tensor networks, including contracting, optimizing, and drawing them



`Tensor`



`TensorNetwork`



`TensorNetwork2D`

- Although it supports more complicated geometries and algorithms, only the basic `Tensor` and `TensorNetwork` classes were used

Implementing Matrix Product States

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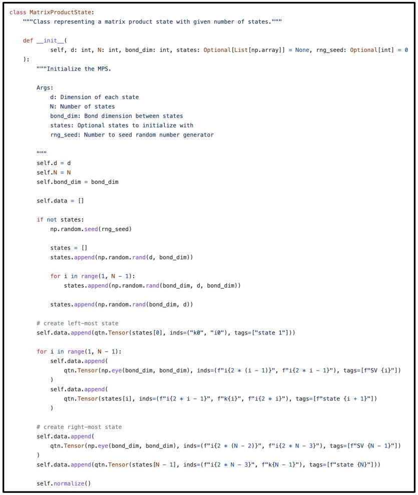
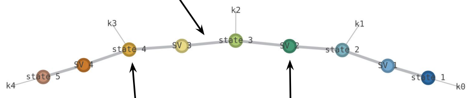
Class used in TEBD algorithm to model basic MPS structure, initializing, contracting, and computing observables from it



```python
class MatrixProductState:
    """Class representing a matrix product state with given number of states."""

    def __init__(
            self, d: int, N: int, bond_dim: int, states: Optional[List[np.array]] = None, rng_seed: Optional[int] = 0
    ):
        """Initialize the MPS.

        Args:
            d: Dimension of each state
            N: Number of states
            bond_dim: Bond dimension between states
            states: Optional states to initialize with
            rng_seed: Number to seed random number generator

        """
        self.d = d
        self.N = N
        self.bond_dim = bond_dim

        self.data = []

        if not states:
            np.random.seed(rng_seed)

            states = []
            states.append(np.random.rand(d, bond_dim))

            for i in range(1, N - 1):
                states.append(np.random.rand(bond_dim, d, bond_dim))

            states.append(np.random.rand(bond_dim, d))

        # create left-most state
        self.data.append(qtn.Tensor(states[0], inds=("k0", "i0"), tags=["state 1"]))

        for i in range(1, N - 1):
            self.data.append(
                qtn.Tensor(np.eye(bond_dim, bond_dim), inds=(f"i{2 * (i - 1)}", f"i{2 * i - 1}"), tags=[f"SV {i}"])
            )
            self.data.append(
                qtn.Tensor(states[i], inds=(f"i{2 * i - 1}", f"k{i}", f"i{2 * i}"), tags=[f"state {i + 1}"])
            )

        # create right-most state
        self.data.append(
            qtn.Tensor(np.eye(bond_dim, bond_dim), inds=(f"i{2 * (N - 2)}", f"i{2 * N - 3}"), tags=[f"SV {N - 1}"])
        )
        self.data.append(qtn.Tensor(states[N - 1], inds=(f"i{2 * N - 3}", f"k{N - 1}"), tags=[f"state {N}"]))

        self.normalize()
```

Edge width indicates bond dimension



Sites

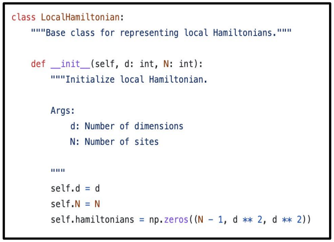
Singular Values

Contains methods for

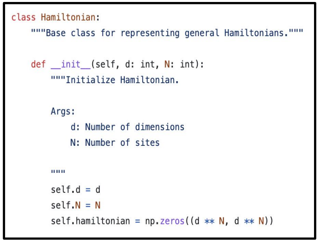
- Generating density matrix tensor
- Computing magnetization
- Calculating entropy
- Extracting wavefunction

Implementing Hamiltonians

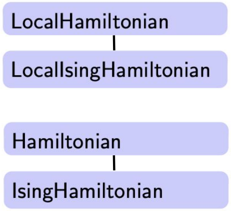
Local and global Hamiltonians implemented to evolve state and compute energy



```python
class LocalHamiltonian:
    """Base class for representing local Hamiltonians."""

    def __init__(self, d: int, N: int):
        """Initialize local Hamiltonian.

        Args:
            d: Number of dimensions
            N: Number of sites

        """
        self.d = d
        self.N = N
        self.hamiltonians = np.zeros((N - 1, d ** 2, d ** 2))
```

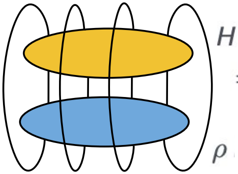


```python
class Hamiltonian:
    """Base class for representing general Hamiltonians."""

    def __init__(self, d: int, N: int):
        """Initialize Hamiltonian.

        Args:
            d: Number of dimensions
            N: Number of sites

        """
        self.d = d
        self.N = N
        self.hamiltonian = np.zeros((d ** N, d ** N))
```



Global Hamiltonian is contracted with density matrix to compute energy

$E = \mathrm{Tr}(\rho H) =$



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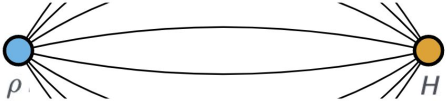

Implementing TEBD Algorithm

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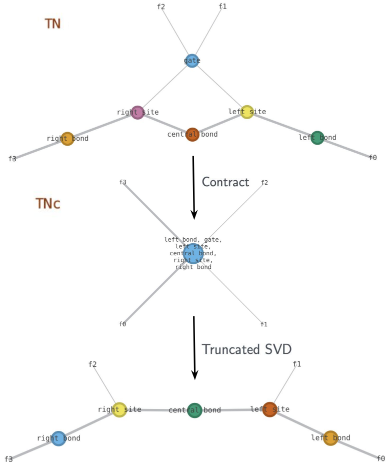
TEBD class accepts `MatrixProductState` and `Hamiltonian` objects and implements `step` method that applies gate on every pair of states from left to right

Apply Gate

Inputs:
`gate`, `left_site`, `right_site`, `left_bond`, `central_bond`, `right_bond`

```
left_bond_T = qtn.Tensor(left_bond_data, inds=('f0', 'k1'), tags=['left bond'])
left_site_T = qtn.Tensor(left_site.data, inds=('k1', 'k2', 'k3'), tags=['left site'])
central_bond_T = qtn.Tensor(central_bond.data, inds=('k3', 'k4'), tags=['central bond'])
right_site_T = qtn.Tensor(right_site.data, inds=('k4', 'k5', 'k6'), tags=['right site'])
right_bond_T = qtn.Tensor(right_bond_data, inds=('k6', 'f3'), tags=['right bond'])
gate_T = qtn.Tensor(gate, inds=('f1', 'f2', 'k2', 'k5'), tags=['gate'])

# contract with gate
TN = left_bond_T & gate_T & left_site_T & central_bond_T & right_site_T & right_bond_T
TNc = TN ^ ...

# perform SVD
nshape = [self.d * left_site.data.shape[0], self.d * right_site.data.shape[2]]
utemp, stemp, vhtemp = LA.svd(TNc.data.reshape(nshape), full_matrices=False)

# truncate to reduced dimension
chitemp = min(self.bond_dim, len(stemp))
utemp = utemp[:, range(chitemp)].reshape(left_site.data.shape[0], self.d * chitemp)
vhtemp = vhtemp[range(chitemp), :].reshape(chitemp * self.d, right_site.data.shape[2])

# remove environment weights to form new MPS tensors
left_site.modify(data=(LA.inv(left_bond_data) @ utemp).reshape(left_site.data.shape[0], self.d, chitemp))
right_site.modify(data=(vhtemp @ LA.inv(right_bond_data)).reshape(chitemp, self.d, right_site.data.shape[2]))
central_bond.modify(data=np.diag(stemp[range(chitemp)] / LA.norm(stemp[range(chitemp)])))
```



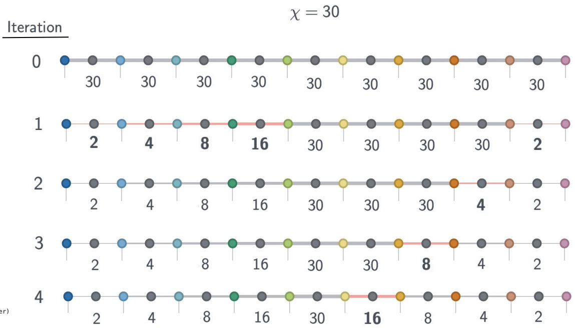
Running TEBD

- Main execution function accepts model, model parameters, and other run parameters
- Bond dimension across chain evolves over first few iterations due to SVD
- Time complexity scales like $\mathcal{O}(\chi^3 d^3 N N_{\text{iter}})$

Run TEBD

Inputs:
`model`, `model_params`, N, χ, Δt, N_{iter}, `mid_steps`, `observables`, `print_to_stdout`, `evol_type`, `st_order`, `initial_state`, `rng_seed`

```
d = 2

if initial_state == "random":
    MPS = MatrixProductState(d=d, N=N, bond_dim=bond_dim, rng_seed=rng_seed)
else:
    MPS = MatrixProductState.init_from_state(initial_state)

# create Hamiltonians
if model == "ising":
    loc_ham = LocalIsingHamiltonian(N=N, **model_params)
    glob_ham = IsingHamiltonian(N=N, **model_params)
elif model == "heisenberg":
    loc_ham = LocalHeisenbergHamiltonian(N=N, **model_params)
    glob_ham = HeisenbergHamiltonian(N=N, **model_params)
else:
    raise Exception(f"Model {model} not supported")

# create TEBD object
tebd_obj = TEBD(MPS, loc_ham, glob_ham, bond_dim=bond_dim, evol_type=evol_type, st_order=st_order)

# run algorithm
observables_at_midsteps = tebd_obj.sweep(tau, num_iter, mid_steps, observables, print_to_stdout)

return observables_at_midsteps
```



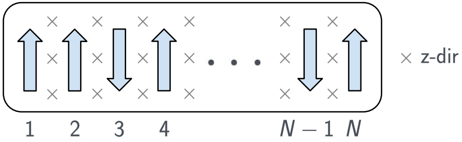
Results

TEBD on Quantum Ising Model

- TEBD can be applied to **quantum Ising model**, a quantum system composed of N spin-1/2 particles on one-dimensional lattice in presence of external magnetic field:

$$\hat{H} = J \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1} \sigma_i^z$$

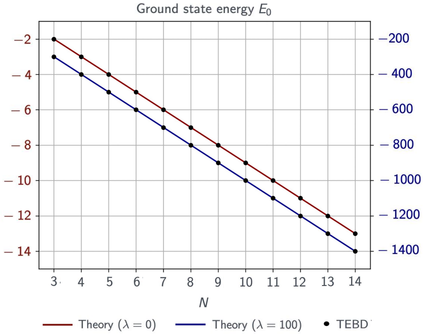
where J is coupling between neighboring spins and λ is coupling to magnetic field

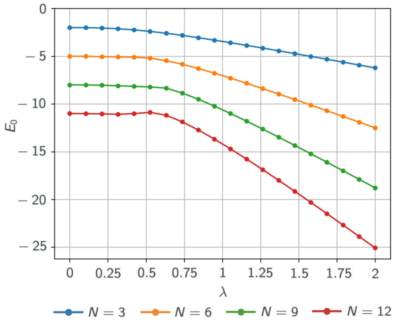


- When $\lambda = 0$, all spins align when $J < 0$ (**ferromagnetic**) and anti-align when $J > 0$ (**antiferromagnetic**). The ground state is two-fold degenerate with energy $-N+1$
- When $\lambda \to \infty$, spins align to magnetic field and ground-state energy is $-\lambda N$

Ground State Energy

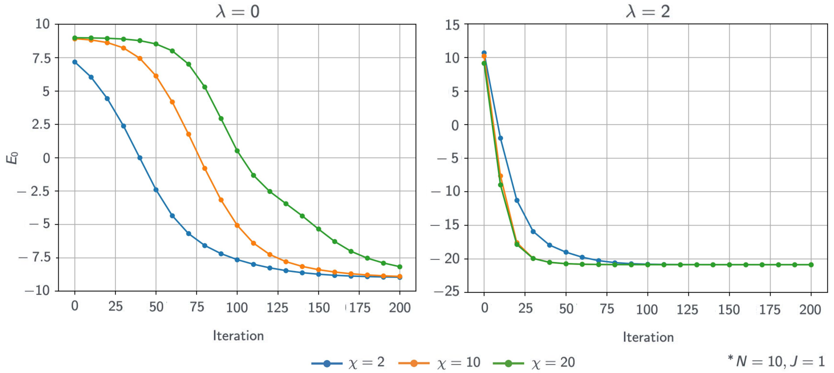
- Ground state energy E_0 can be determined by simulating system using TEBD
- In following experiments, TEBD was run for 500 iterations with a timestep of $\Delta t = 0.01$ and $\chi = 2$. The initial state was random, but was the same across all values of N. Results are robust to choice of χ
- TEBD reproduces E_0 reported in Assignment 7. Results match theoretical expectation very well: $E_0 = -N + 1$ for $\lambda = 0$ and $E_0 = -\lambda N$ for large λ





Effect of Bond Dimension

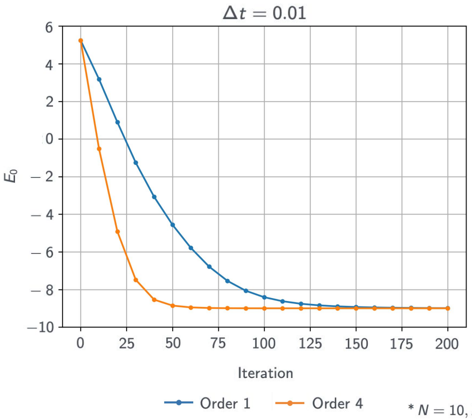
- Increasing bond dimension χ allows model to capture more entanglement, but it takes longer to converge when λ is small since long-range order is low
- When λ is beyond critical point, larger χ leads to faster convergence since degree of long-range order is higher



$^*N = 10, J = 1$

Effect of Suzuki-Trotter Order

- Increasing the order of Suzuki-Trotter decomposition improves convergence rate
- Error of first order is $\mathcal{O}(\Delta t)$ while error of fourth error is $\mathcal{O}(\Delta t^4)$



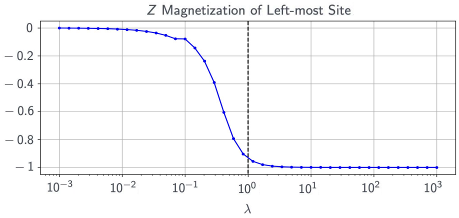
* $N = 10, \lambda = 0, J = 1$

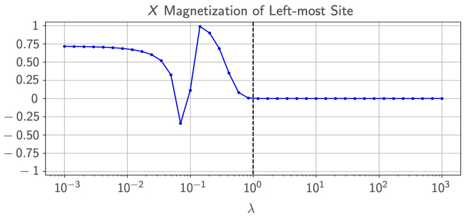
Magnetization

- Magnetization computed for site i along direction j using the magnetic operator:

$$M_{ij} = \mathbb{1}_1 \otimes \cdots \otimes \mathbb{1}_{i-1} \otimes \sigma_i^j \otimes \mathbb{1}_{i+1} \otimes \cdots \otimes \mathbb{1}_N$$

- Average magnetization is given by $\langle M_{ij} \rangle = \mathrm{Tr}(\rho M_{ij}) = \langle \Psi | M_{ij} | \Psi \rangle$
- When λ is low, magnetization along Z is zero as spins have equal probability of being $\uparrow$ or $\downarrow$. When λ increases, approaching phase transition at $\lambda = 1$, spins align to magnetic field and $\langle M_{1Z} \rangle = 0$
- When Z magnetization is -1, average X magnetization is zero as Z-polarized qubit has equal probability of being $\leftarrow$ or $\rightarrow$

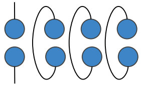




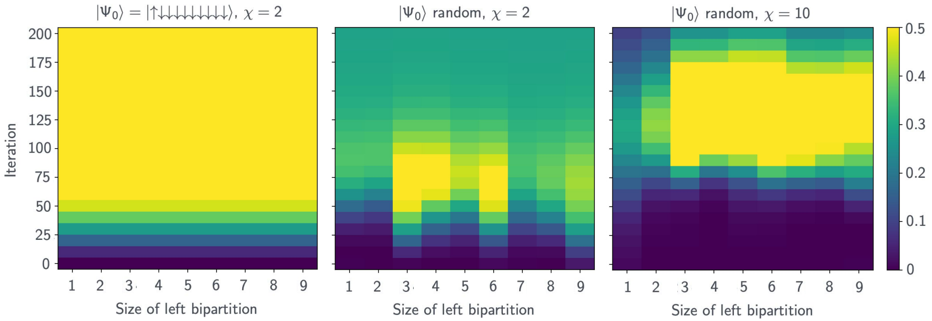
Entanglement Entropy

- Entropy of left bipartition computed by contracting density matrix tensor:

$$S = -\mathrm{Tr}(\rho_L \log \rho_L) \text{ where } \rho_L = \mathrm{Tr}_R\, \rho =$$



- For specific initial state $|\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$, entropy starts uniform and grows uniformly
- For random state, entropy grows and spreads unevenly before becoming uniform. With bigger bond dimension χ, entropy across the chain persists for longer



Entanglement Entropy at Criticality

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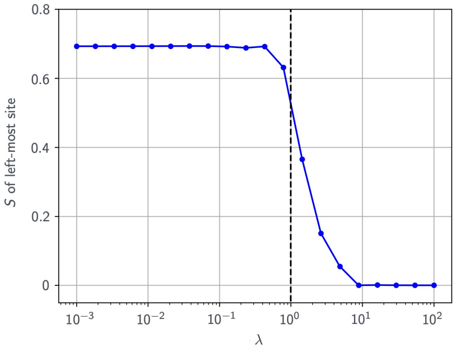
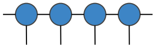
- When λ is low, entanglement entropy of left-most site is high because ground state is degenerate
- When λ exceeds critical value, entropy decreases as all spins align to magnetic field, eliminating degeneracy and creating pure reduced state

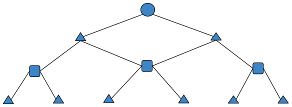


Conclusion

Conclusion



- Time-evolving block decimation is a powerful method of simulating many-body quantum systems using matrix product states
- Through efficient truncation of Hilbert space, algorithm remains computationally tractable while capturing some degree of entanglement
- TEBD can be applied to weakly-coupled one-dimensional quantum systems like Ising or Heisenberg models
- Similar techniques can be used applied using different tensor network structures, like tree tensor networks (e.g., t-MERA)



Appendix

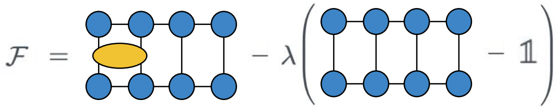
Fidelity Maximization

- TEBD is based on concept of maximizing **fidelity** of reconstruction between MPS structure and evolved state at each time t:

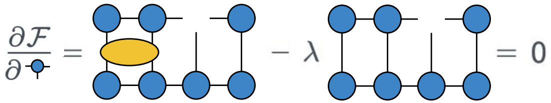
$$\mathcal{F}^* = \max_{\Psi \in M} \langle \Psi | U_t | \Psi \rangle - \lambda(\langle \Psi | \Psi \rangle - 1)$$

  where M is space of MPS tensors, and second term helps to normalize the state

- Graphically, fidelity is represented by

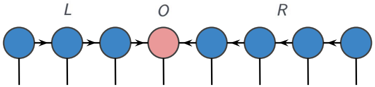


- This can be solved using **gradient descent** by differentiating $\mathcal{F}$ with respect to every tensor. For example, differentiating with respect to the third tensor leads to

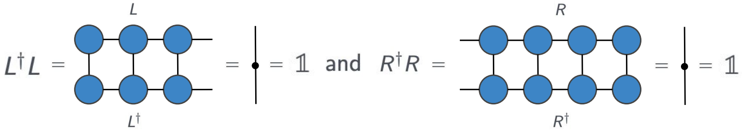


Centers of Orthogonality

- Tensor O is **center of orthogonality** if every branch connected to O is isometry between its legs and index connected to O. For example, O in the tensor network



is center of orthogonality if



- This can be done by finding the principal square roots of $L^\dagger L$ and $R^\dagger R$ and reabsorbing them into O and left and right branches, respectively
- Orthogonality centers are important in TEBD because decomposing tensor O with SVD minimizes **global** error of decomposition if O is center of orthogonality

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