Main MPS Algorithms

1. Time marching with direct MPO-MPS product

   Simplest algorithm. See solution to Burgers' equation in Homework 2.

2. Time marching with TDVP

   Define MPO corresponding to PDE, and use TDVP for imaginary time evolution.

$$\frac{\partial}{\partial t} F(t) = H F(t) \longrightarrow F(t) = e^{Ht} F(0)$$

   Do not normalize the MPS, as this will mess up the actual normalization of the function.

   For nonlinear equations, H will be time dependent. Perform time evolution time step after time step, so the time-dependent variables are approximately constant.

$$F(t + \Delta t) = e^{H(F(t))\Delta t} F(t)$$

No known publication!

3. DMRG-like time evolution

Consider a one-dimensional PDE $$\frac{\partial c(x,t)}{\partial t} - Ac(x,t) = 0$$

A can contain nonlinearities and derivatives with respect to *x*.

We want to obtain the MPS $|c\rangle$ that minimizes the cost function $$\left\| \frac{\partial |c\rangle}{\partial t} - A|c\rangle \right\|^2$$

For simplicity, use explicit forward Euler for advancing in time. Other schemes such as Runge-Kutta can also be used. $$\frac{\partial |c(t)\rangle}{\partial t} \approx \frac{|c(t+\Delta t)\rangle - |c(t)\rangle}{\Delta t}$$

Obtaining $|c(t+\Delta t)\rangle$ from $|c(t)\rangle$ can be restated as the minimization problem

$$|c(t+\Delta t)\rangle = \arg\min_{|u\rangle} \Theta(|u\rangle, |c(t)\rangle, \Delta t)$$ with variational function

$$\Theta(|u\rangle, |c(t)\rangle, \tau) = \left\| \frac{|u\rangle - |c(t)\rangle}{\tau} - A|c(t)\rangle \right\|^2$$

We can also write the variational function as $\textcircled{H}(|U\rangle, |c(t)\rangle, \tau) = \frac{1}{\tau^2} \| |U\rangle - H|c(t)\rangle \|^2$

With the MPO Hamiltonian $H = I + A\tau$

$|U\rangle = H|c(t)\rangle$

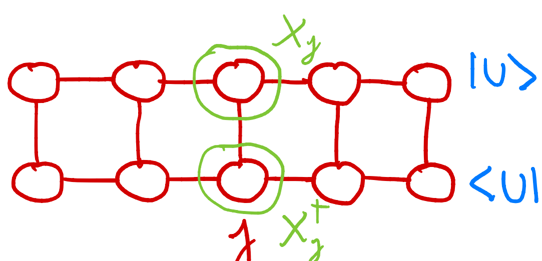
Directly applying H to $|c(t)\rangle$ would correspond to method 1. Instead, we will solve the minimization problem in a way similar to DMRG. Opening the norm

$$\tau^2 \textcircled{H} = \langle U|U\rangle - \langle U|H|c(t)\rangle - \langle c(t)|H^\dagger|U\rangle + \langle c(t)|H^\dagger H|c(t)\rangle$$

We will optimize site by site. When optimizing site *j*, we will derive with respect to tensor $X_j^\dagger$

➡ Terms that do not depend on $\langle U|$ will vanish. This is equivalent to minimizing $\widetilde{\textcircled{H}} = \langle U|U\rangle - \langle U|H|c(t)\rangle$

Diagrammatic representation =



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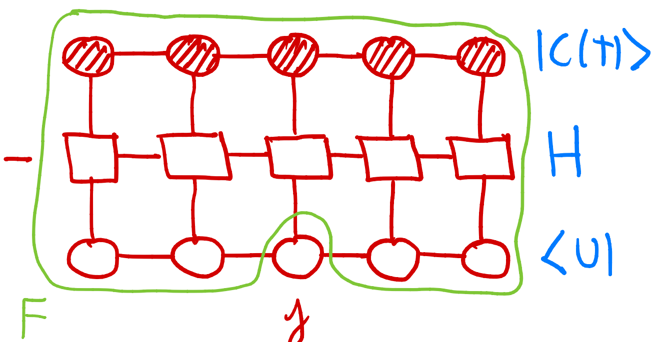


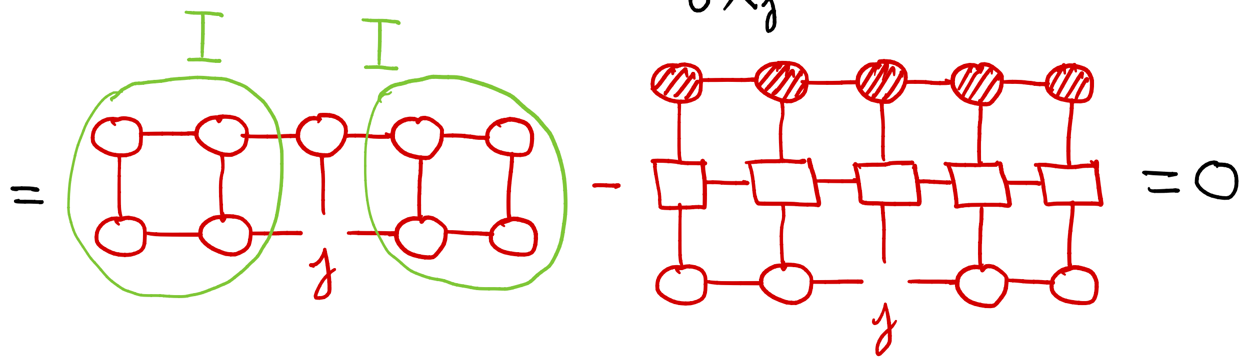
Suppose we want to optimize site *j*. We can rewrite

$$\tilde{H}(X_j) = X_j^\dagger N X_j - X_j^\dagger F$$

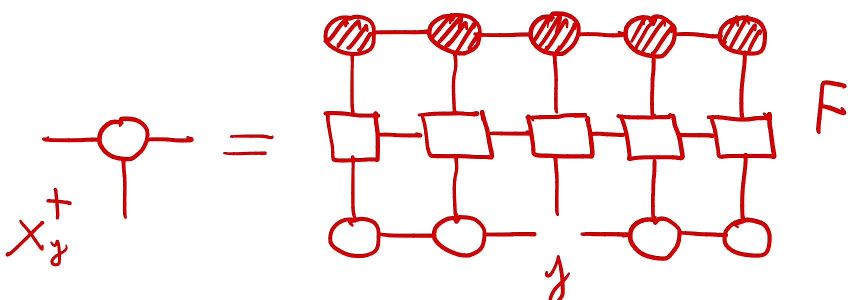
Performing the derivative with respect to X_j $\Rightarrow$

$$\frac{\partial \tilde{H}(X_j)}{\partial X_j^\dagger} = N X_j - F = 0$$

Diagrammatic representation



Assuming site *j* is orthogonalization center, we can use normalization of left and right tensors



Follow the same sequence of sweeps of DMRG, optimizing a site at a time until reaching convergence. This is just variational MPO-MPS product. Use the Fit algorithm from ITensor.

This is the spirit of recent work on tensor networks for simulating Navier-Stokes equations.

- Multidimensional problem
- More complicated local problem (linear system of equations) due to penalty term to ensure incompressibility of the flow

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Nikita Gourianov[1], Michael Lubasch[2], Sergey Dolgov[3], Quincy Y. van den Berg[1], Hessam Babaee[4], Peyman Givi[4], Martin Kiffner[1,5] and Dieter Jaksch[1,5,6]