Real time evolution with neural network quantum states

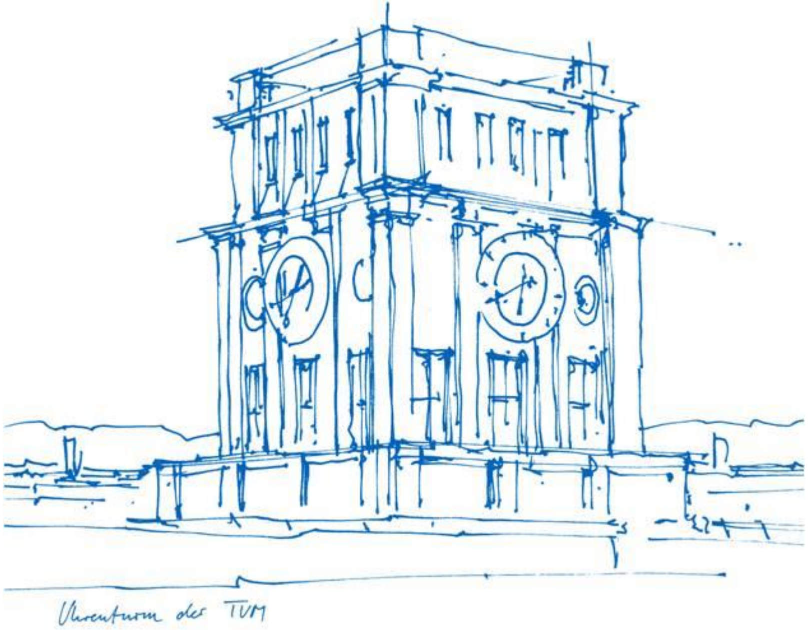
Irene López Gutiérrez and Christian Mendl

Technical University Munich

Faculty of Informatics

Chair of Scientific Computing

Denver, 5th March 2020



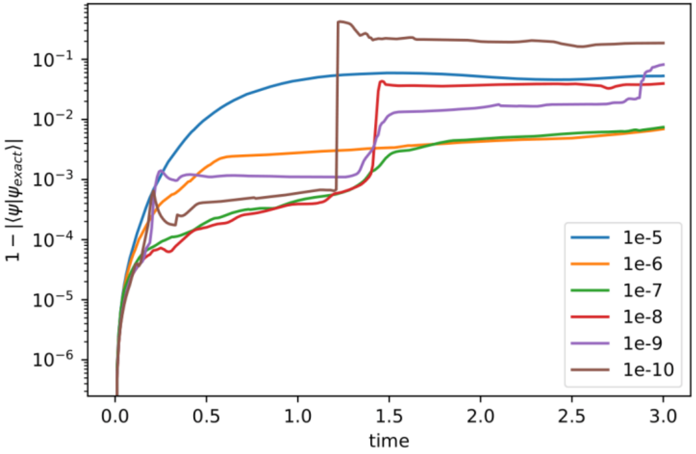
How to optimise the network

In stochastic reconfiguration, one must solve

$$S\dot{\theta} = -iF$$

Many times *S* is singular.

- Solution with pseudo-inverse is very sensitive to chosen cut-off for singular values.
- Krylov subspace methods are not guaranteed to converge to optimal solution.



How to optimise the network

Instead, we can minimise:

$$\left\| \psi[\theta_{n+1}] - \Phi^{\Delta t}(\psi[\theta_n]) \right\|$$

Numerical ODE method

For example, using the implicit midpoint rule

$$\psi[\theta_{n+1}] = \psi[\theta_n] - i\Delta t H \left(\frac{\psi[\theta_{n+1}] + \psi[\theta_n]}{2} \right)$$

$$C(\theta_{n+1}) = \sum_{j=1}^{N} \left| \left((I + \frac{i\Delta t}{2} H)\psi[\theta_{n+1}] - (I - \frac{i\Delta t}{2} H)\psi[\theta_n] \right) (\sigma^{(j)}) \right|^2$$

Backpropagation with complex parameters

To perform an optimization, cost function must be real.

In our case: $$C(\theta) = \|A\psi[\theta] - b\|^2$$

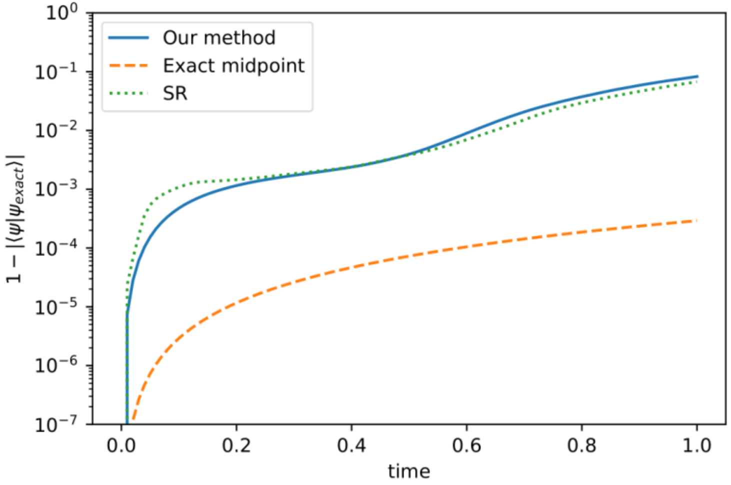
This function is not holomorphic!

To find gradients with respect to parameters, we employ the *Wirtinger formalism.*

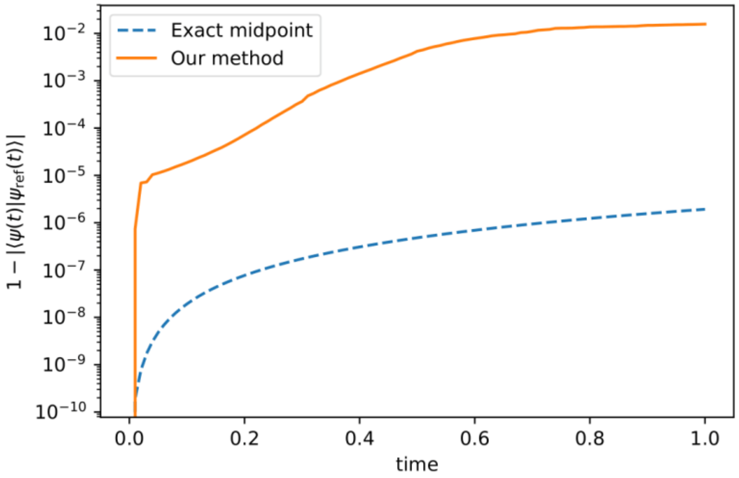
In our case, this leads to: $$\frac{\partial C(\theta)}{\partial \theta_l} = \left\langle A\psi[\theta] - b \middle| A \underbrace{\frac{\partial \psi[\theta]}{\partial \theta_l}}_{\text{Computed as usual}} \right\rangle$$

Test case: Ising model

20 sites, 1D lattice



9 sites, 2D lattice



Questions?