Algorithms for classical optimization and quantum ground states

Dean Lee
Facility for Rare Isotope Beams
and Physics and Astronomy Department
Michigan State University

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Nuclear Computational Low-Energy Initiative
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Outline

Combinatorial optimization

Adiabatic theorem and adiabatic evolution

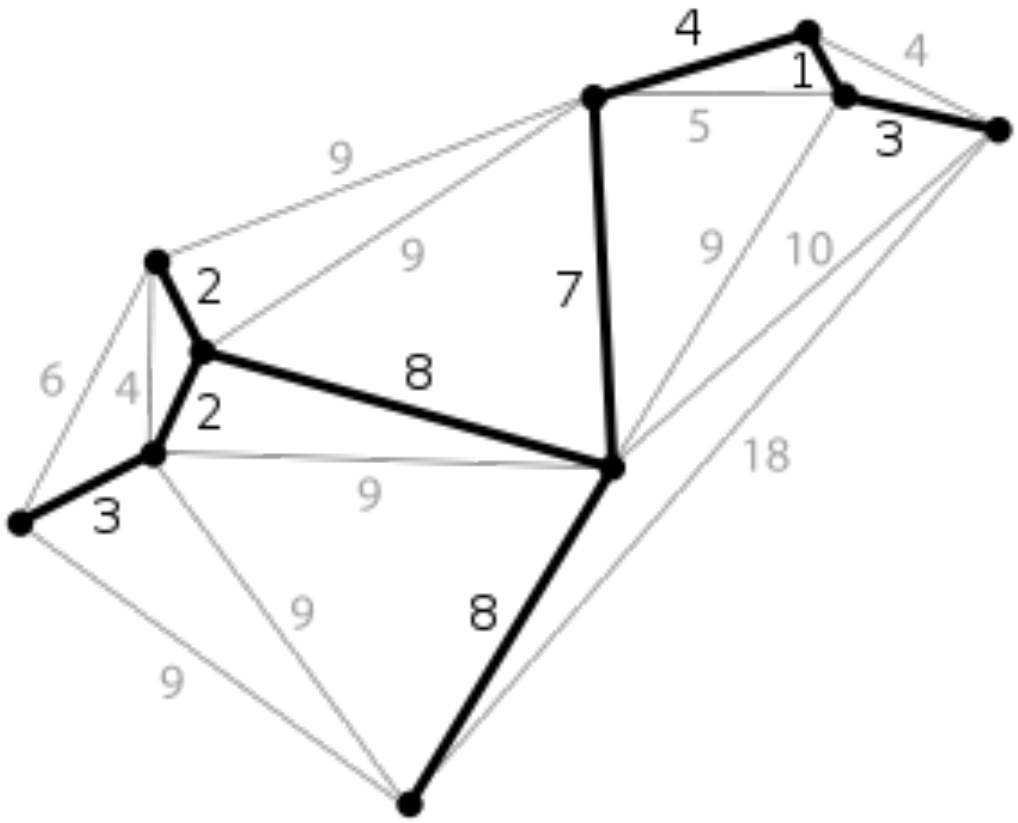
Quantum annealing

Quantum approximate optimization algorithm

Projected cooling algorithm

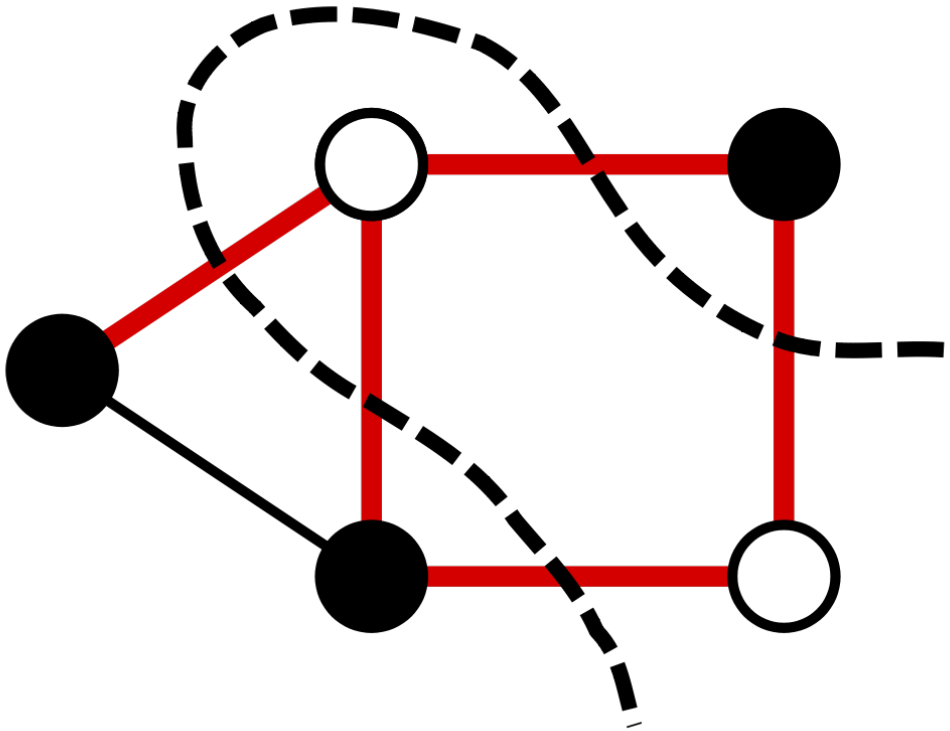
Summary

Minimum spanning tree



wikipedia.org

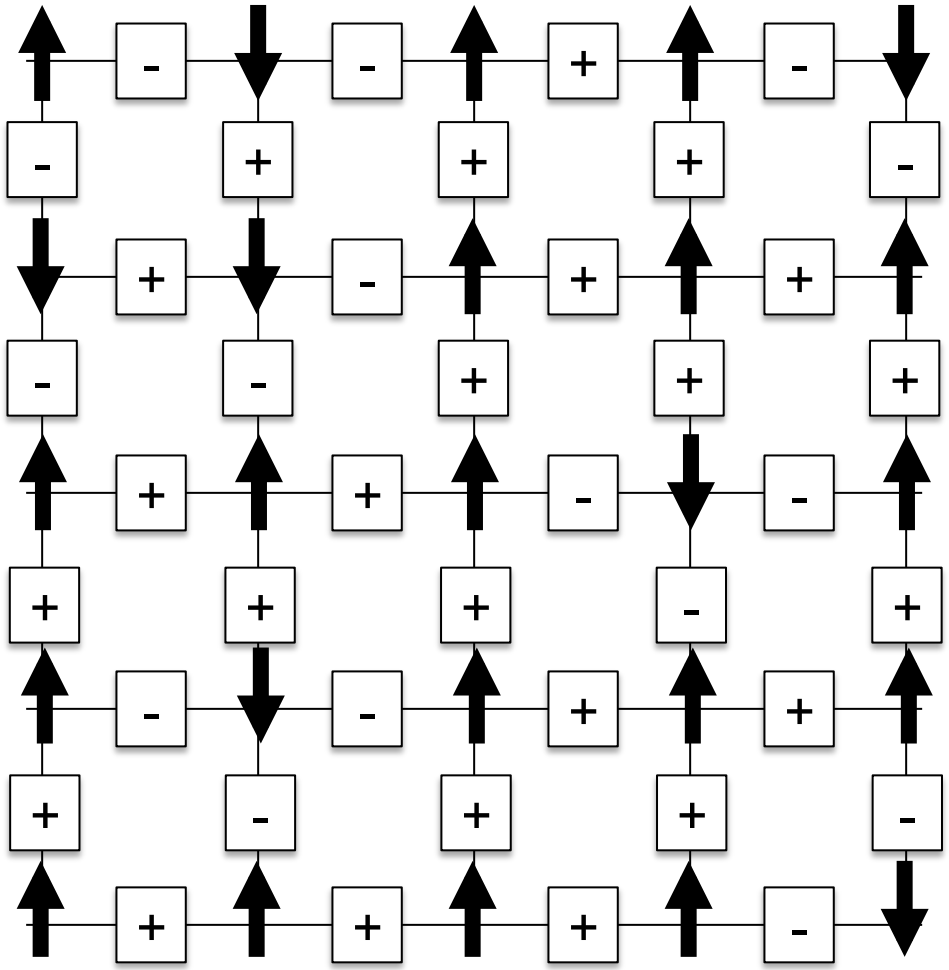
Maximum Cut



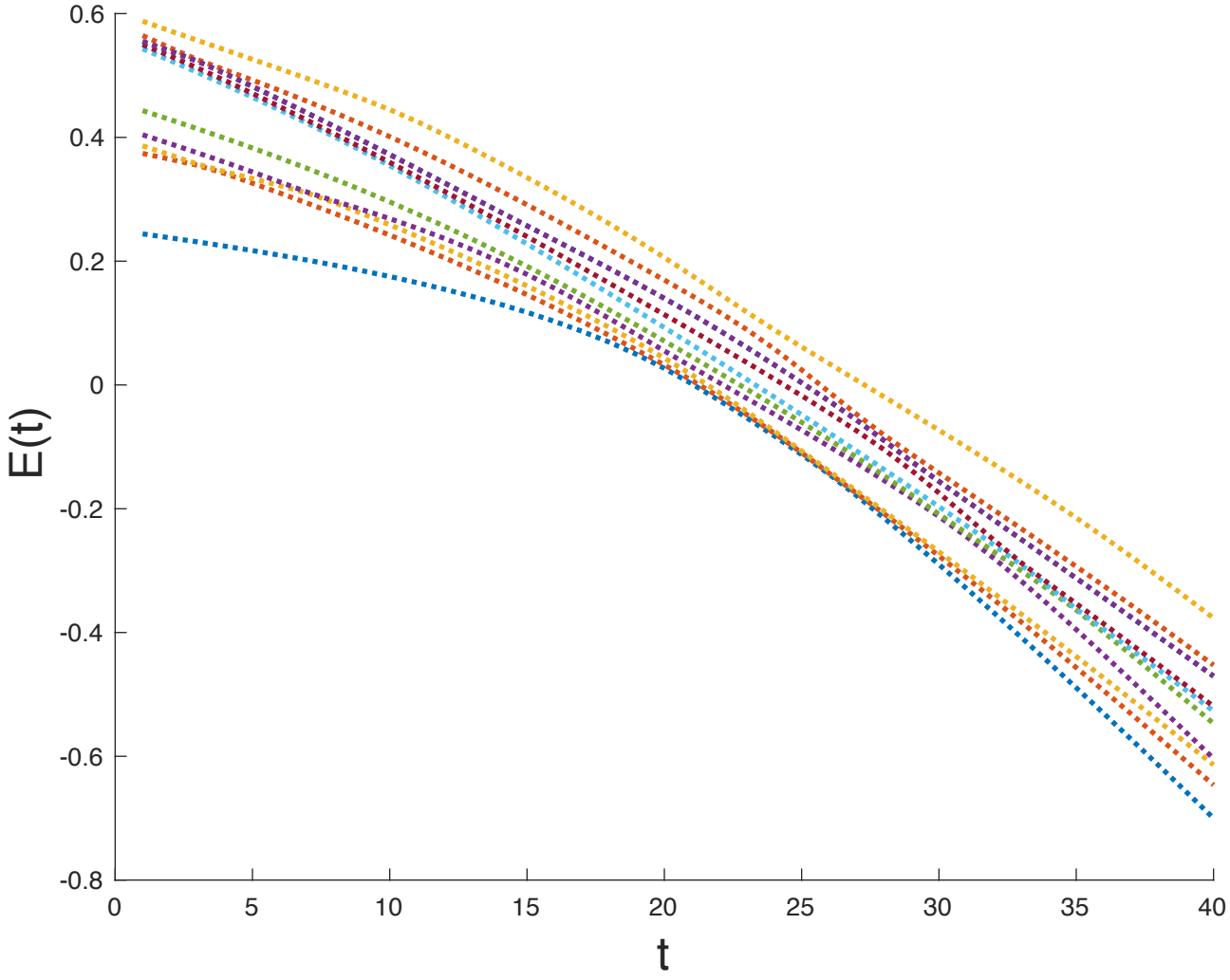
wikipedia.org

Ising spin glass

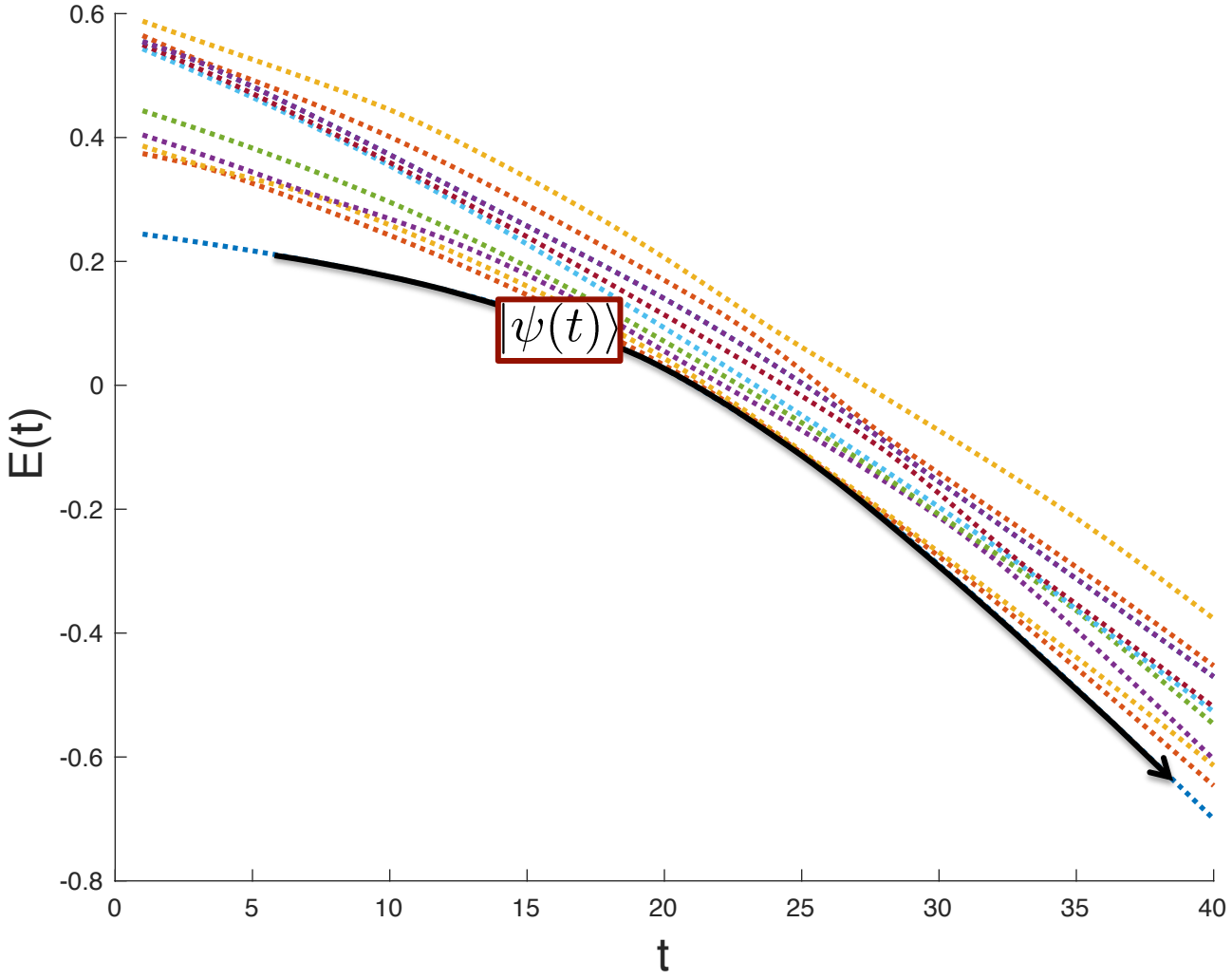
$$H = -\sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z$$



Adiabatic theorem



Adiabatic theorem



Adiabatic evolution

Initial Hamiltonian H_I (simple), final Hamiltonian H_F (target)

$$H(0) = H_I,\ H(t_F) = H_F$$

$$H(t) = \frac{t_F - t}{t_F} H_I + \frac{t}{t_F} H_F$$

The unitary time evolution operator is

$$U(t + dt, t) = e^{-iH(t)dt}$$

$$|\psi(t + dt)\rangle = U(t + dt, t)\,|\psi(t)\rangle$$

$$|\psi(t_2)\rangle = U(t_2, t_1)\,|\psi(t_1)\rangle$$

Start from an eigenstate of the initial Hamiltonian

$$H_I \left|\psi_I\right\rangle = E_I \left|\psi_I\right\rangle$$

In the limit of slow time evolution we remain in an eigenstate of $H(t)$ throughout

$$\left|\psi(t)\right\rangle = U(t,0) \left|\psi_I\right\rangle$$

$$H(t) \left|\psi(t)\right\rangle = E(t) \left|\psi(t)\right\rangle$$

And so at the end of the evolution we have

$$H_F \left|\psi(t_F)\right\rangle = E_F \left|\psi(t_F)\right\rangle$$

Quantum annealing

Quantum annealing is the application of adiabatic evolution to a combinatorial optimization problem. Consider, for example, the Ising spin glass

$$H_F = -\sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z$$

For the initial Hamiltonian we can take the simple operator

$$H_I = -\sum_i \sigma_i^x$$

with ground state

$$|\psi_I\rangle = |\sigma^x = 1\rangle \otimes |\sigma^x = 1\rangle \otimes \cdots$$

We then apply adiabatic evolution

$$H(0) = H_I,\ H(t_F) = H_F$$

$$H(t) = \frac{t_F - t}{t_F} H_I + \frac{t}{t_F} H_F$$

$$|\psi(t)\rangle = U(t,0)\,|\psi_I\rangle$$

At the end of the evolution we have

$$H_F\,|\psi(t_F)\rangle = E_F\,|\psi(t_F)\rangle$$

Trotter approximation

The Hamiltonian usually contains terms that do not commute. For the time evolution we have

$$U(t+dt,t) = e^{-iH(t)dt}$$

for

$$H(t) = \frac{t_F - t}{t_F} H_I + \frac{t}{t_F} H_F$$

We can use the Trotter approximation

$$e^{-iH(t)dt} \approx e^{-i\frac{t_F-t}{t_F}H_I dt} e^{-i\frac{t}{t_F}H_F dt}$$

And so we have

$$U(t_F, 0) \approx \cdots e^{-i\frac{t_F - t_k}{t_F} H_I dt} e^{-i\frac{t_k}{t_F} H_F dt} \cdots e^{-i\frac{t_F - 0}{t_F} H_I dt} e^{-i\frac{0}{t_F} H_F dt}$$

This is very difficult to implement on current quantum devices due to the large number of gates required per qubit.

Quantum approximate optimization algorithm

Farhi, Goldstone, Gutmann, arXiv:1411.4028 (2014) [quant-ph]

The quantum approximate optimization algorithm (QAOA) is a cheap approximation to adiabatic evolution. We make the variational ansatz

$$|\psi(\vec{\beta},\vec{\gamma})\rangle = U(\vec{\beta},\vec{\gamma})\,|\psi_I\rangle$$

$$U(\vec{\beta},\vec{\gamma}) \approx e^{-i\beta_k H_I} e^{-i\gamma_k H_F} \cdots e^{-i\beta_1 H_I} e^{-i\gamma_1 H_F}$$

We then use the variational principle

$$E_F^{\text{ground}} \leq \langle\psi(\vec{\beta},\vec{\gamma})|H_F|\psi(\vec{\beta},\vec{\gamma})\rangle$$

and minimize the value of $E(\vec{\beta},\vec{\gamma}) = \langle\psi(\vec{\beta},\vec{\gamma})|H_F|\psi(\vec{\beta},\vec{\gamma})\rangle$

arXiv:1910.07708

Projected Cooling Algorithm for Quantum Computation

Dean Lee,[1] Joey Bonitati,[1] Gabriel Given,[1] Caleb Hicks,[1] Ning Li,[1]
Bing-Nan Lu,[1] Abudit Rai,[1] Avik Sarkar,[1] and Jacob Watkins[1]

[1]*Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA*

In the current era of noisy quantum devices, there is a need for quantum algorithms that are efficient and robust against noise. Towards this end, we introduce the projected cooling algorithm for quantum computation. The projected cooling algorithm is able to construct the localized ground state of any Hamiltonian with a translationally-invariant kinetic energy. The method can be viewed as the quantum analog of evaporative cooling. We start with an initial state with support over a compact region of a large volume. We then drive the excited quantum states to disperse and measure the remaining portion of the wave function left behind. The method can be used in concert with other techniques such as variational methods and adiabatic evolution to achieve better performance than existing approaches for the same number of quantum gates per qubit. For the nontrivial examples we consider here, the improvement is substantial. The only additional resource required is performing the operations in a volume significantly larger than the size of the localized state.

Projected cooling algorithm

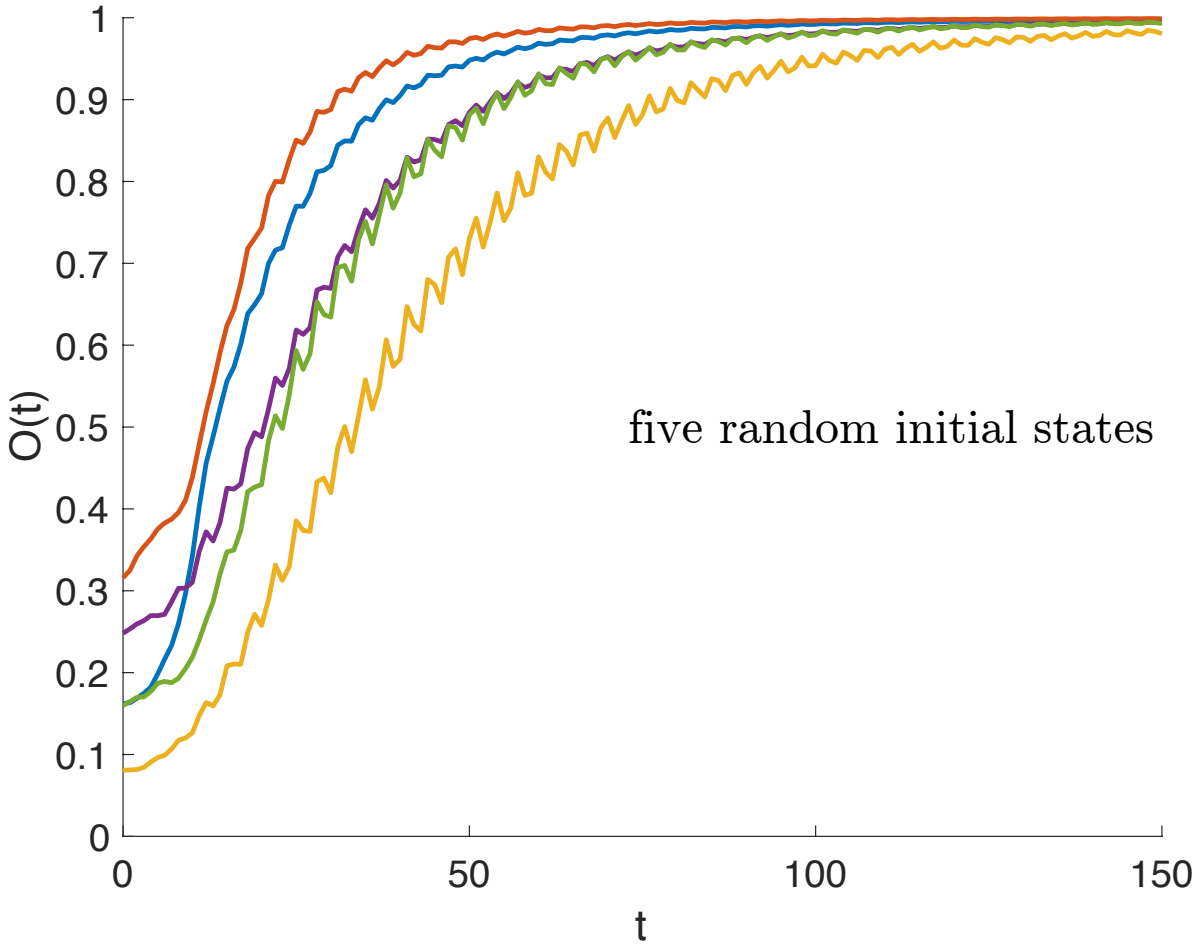
Consider a Hamiltonian H with a translationally-invariant kinetic energy and a localized ground state

$$H\left|\psi_0\right\rangle = E_0\left|\psi_0\right\rangle$$

We first consider the case where there is exactly one bound state. We take the system volume to be infinite (or large enough to avoid rebounding reflections from the boundary). Let P be a projection operator onto a compact region ρ. In the limit of large time t, the projected time evolution has a stable fixed point

$$Pe^{-iHt}P\left|\psi_I\right\rangle \rightarrow e^{-iE_0t}P\left|\psi_0\right\rangle\left\langle\psi_0|P|\psi_I\right\rangle$$

Overlap with $P\,|\psi_0\rangle$

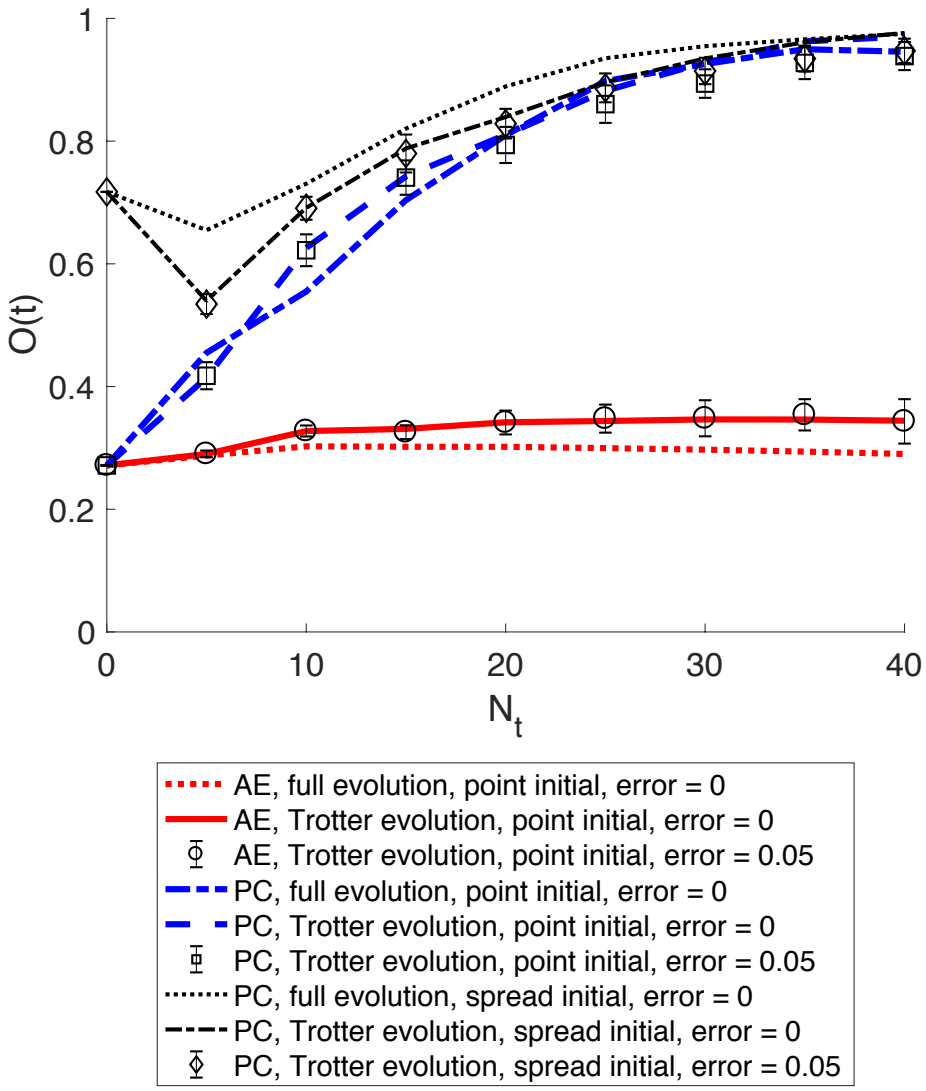


For the case where there are more than one bound state, we need a time-dependent Hamiltonian. We first evolve to the ground state of another Hamiltonian that has only one bound state

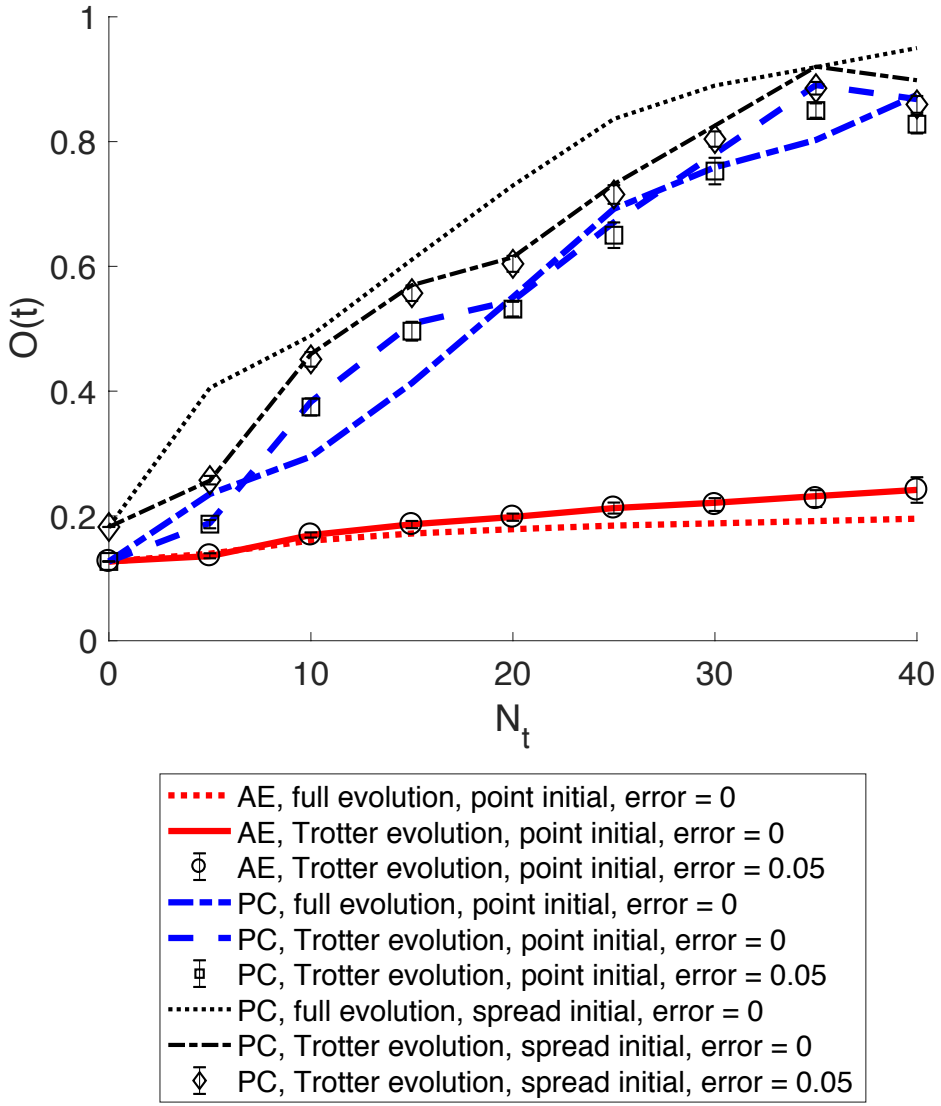
$$H' \left|\psi_0'\right\rangle = E_0' \left|\psi_0'\right\rangle$$

We then use adiabatic evolution to flow to the ground state of the desired Hamiltonian H.

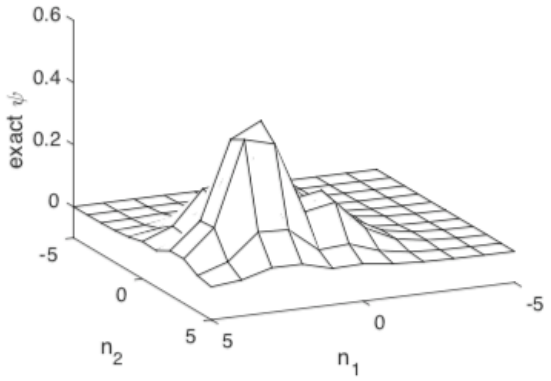
One-particle system on an $L = 51$ chain

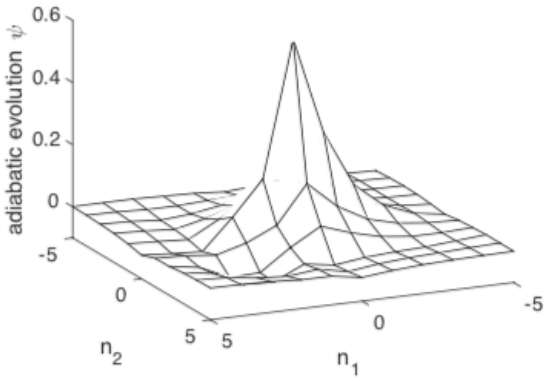


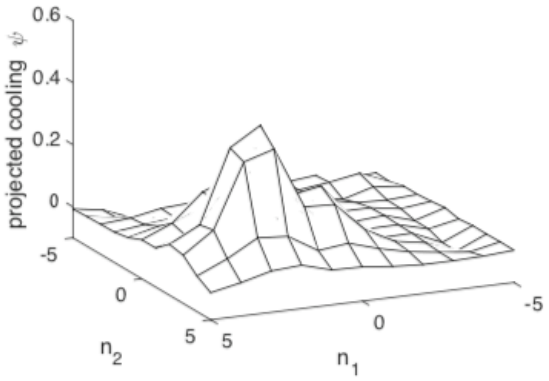
Two-particle system on two linked $L = 51$ chains



Comparison of wave functions







Summary

Quantum annealing is the application of adiabatic evolution to solve combinatorial optimzation problems. Adiabatic evolution relies on the adiabatic theorem, which states that when the time evolution is sufficiently slow, we remain in an eigenstate of the time-dependent Hamiltonian $H(t)$. The quantum approximate optimization algorithm is a variational method which is a cheap approximation to adiabatic evolution. We also discussed a new algorithm called projected cooling that works for localized ground states.