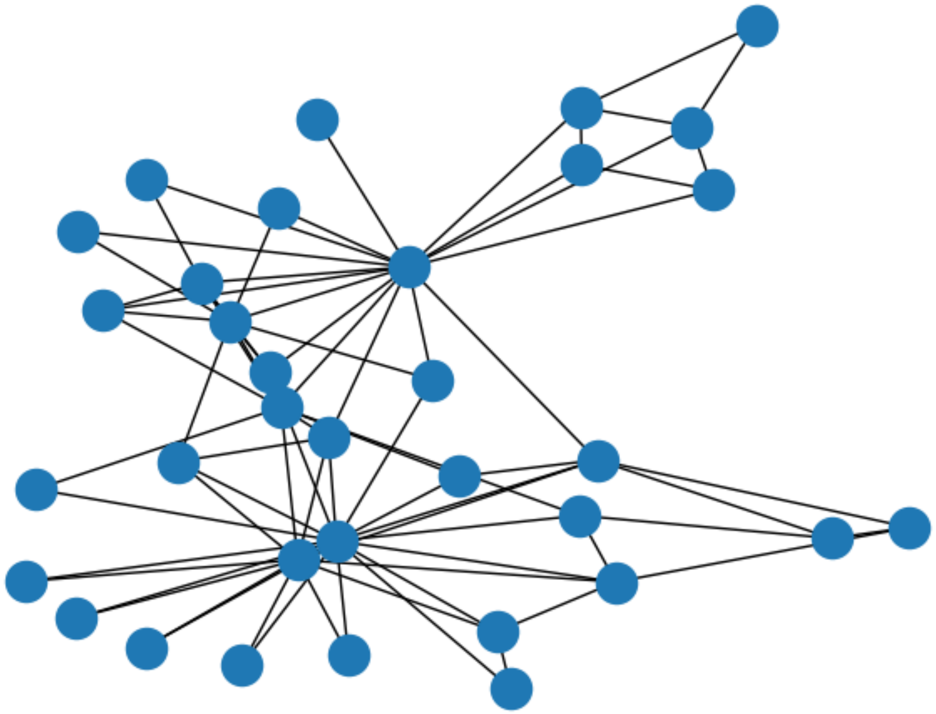
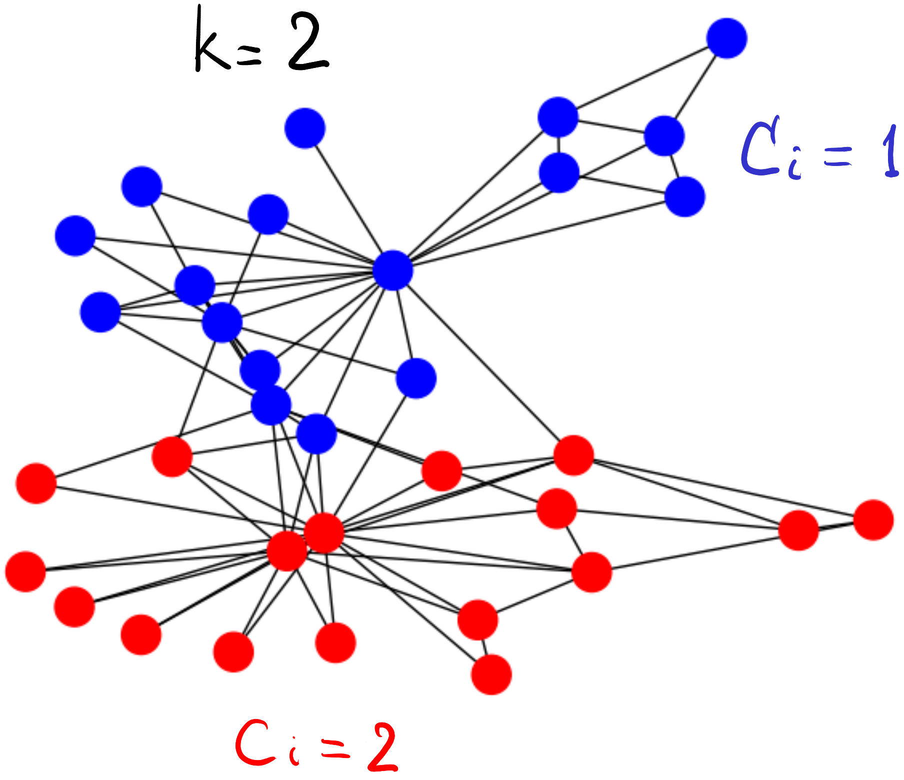
Community detection

on quantum computers

About community detection

$$G : V, E \rightarrow c_1, c_2 \ldots c_{|V|} \in \{1, \ldots, k\}$$





Metrics

Modularity

$$M = \frac{1}{2m} \sum_{ij}' \left(A_{ij} - \frac{g_i g_j}{2m} \right) \delta(c_i, c_j)$$

$g_i = \sum_j' A_{ij}$

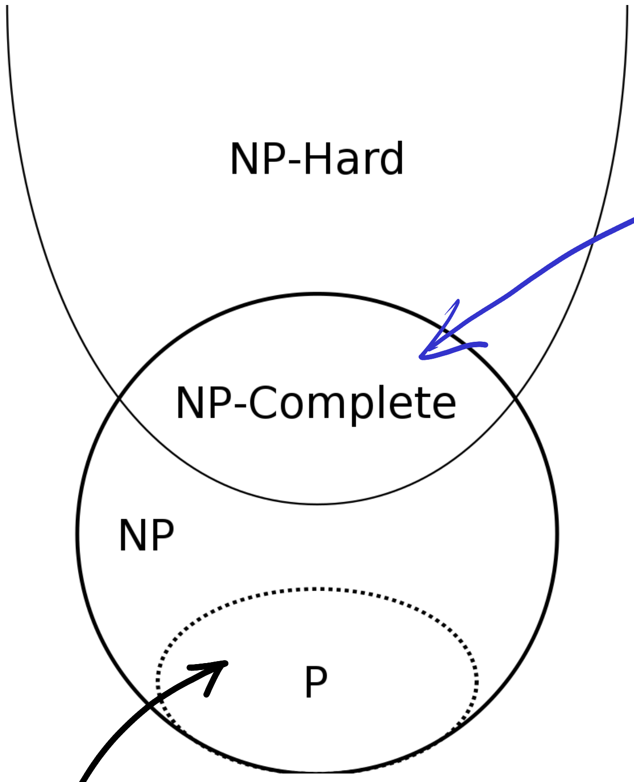
degree

$m = \frac{\sum' g_i}{2}$

adjacency matrix

Kronecker delta

The problem?



We are here :(

Could be solved

For real-world graphs

- Annealing ← $t \to \infty$
- Greedy algorithms ← $M < M_{opt}$

[Submitted on 25 Aug 2006 (v1), last revised 30 Aug 2006 (this version, v2)]

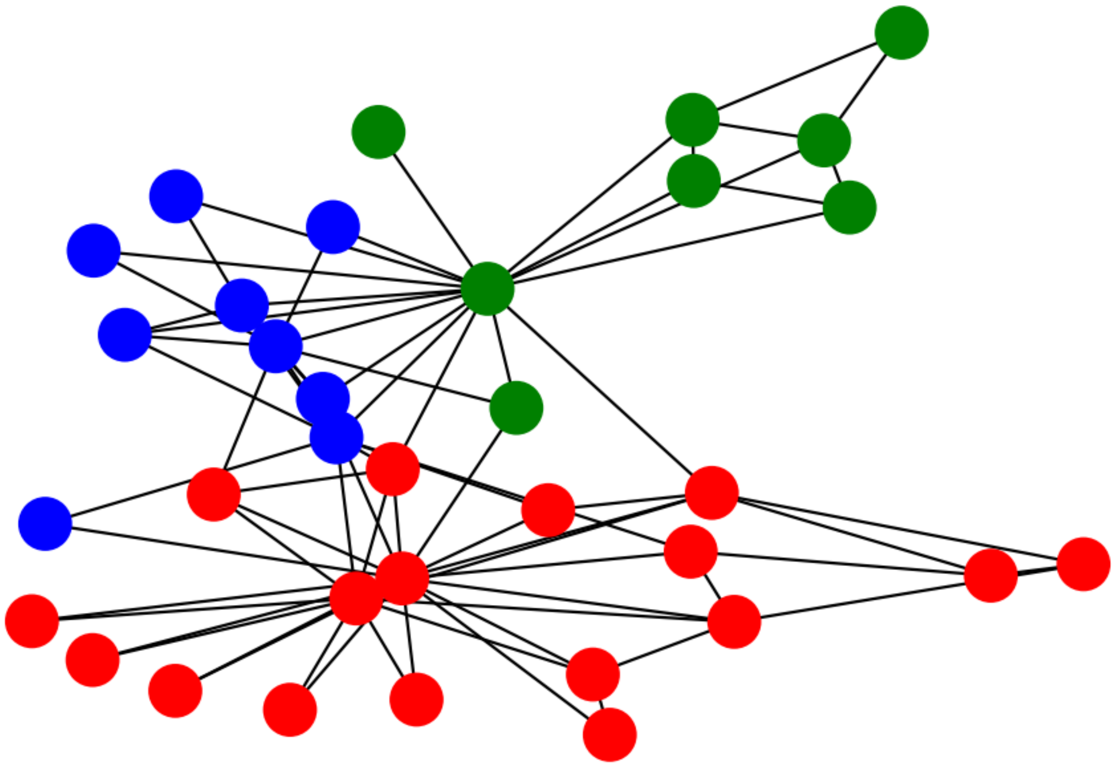
Maximizing Modularity is hard

U. Brandes, D. Delling, M. Gaertler, R. Goerke, M. Hoefer, Z. Nikoloski, D. Wagner

Several algorithms have been proposed to compute partitions of networks into communities that score high on a graph clustering index called modularity. While publications on these algorithms typically contain experimental evaluations to emphasize the plausibility of results, none of these algorithms has been shown to actually compute optimal partitions. We here settle the unknown complexity status of modularity maximization by showing that the corresponding decision version is NP-complete in the strong sense. As a consequence, any efficient, i.e. polynomial-time, algorithm is only heuristic and yields suboptimal partitions on many instances.

Comments: 10 pages, 1 figure
Subjects: **Data Analysis, Statistics and Probability (physics.data-an)**; Statistical Mechanics (cond-mat.stat-mech); Physics and Society (physics.soc-ph)

Greedy solution



$M = 0.380$

Clauset, A., Newman, M. E., & Moore, C. “Finding community structure in very large networks.” Physical Review E 70(6), 2004.

Quantum stuff

Schr. eq.

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

wave function

Hamiltonian (energy operator)

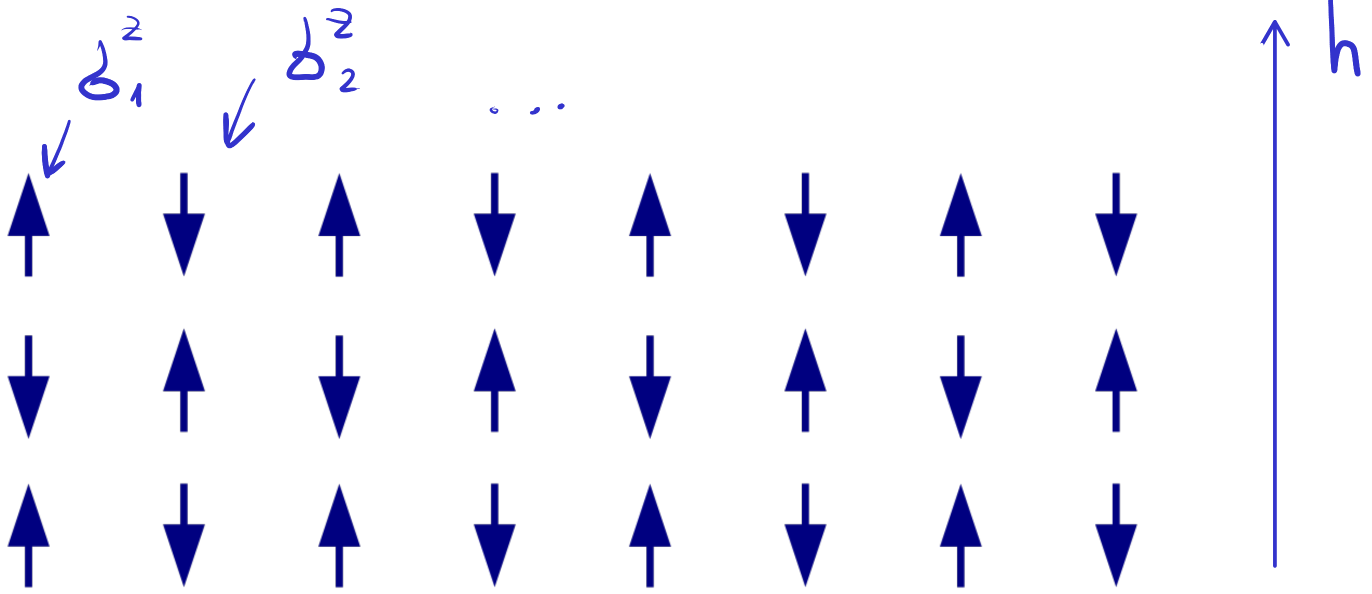
$$\hat{H}|\Psi_i\rangle = E_i|\Psi\rangle$$

Possible states are eigenstates

„Ground state" – – state with min. energy

$$\boxed{E_i \geq E_{g.s.} = \langle\Psi_{g.s.}|\hat{H}|\Psi_{g.s.}\rangle}$$

Ising model



Ernst Ising

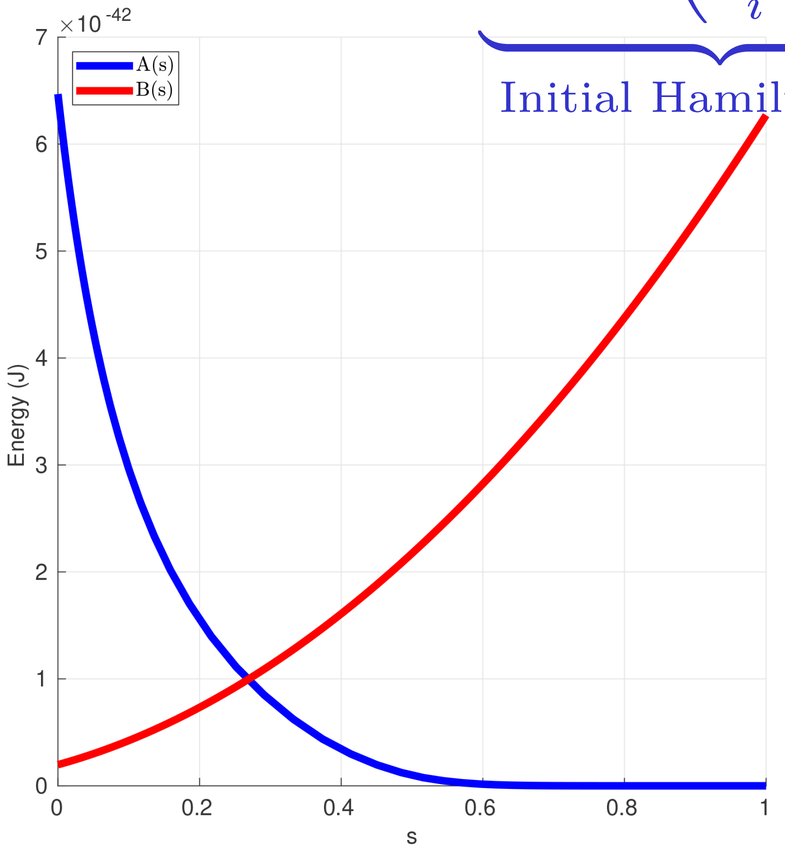
$$\boxed{\hat{H} = -h \sum_i \sigma_i^z - J \sum_{i,j} \sigma_i^z \sigma_j^z}$$

NP-hard

Has an effective approximate q. alg.!

Quantum annealing

$$\hat{H}_{Ising} = \underbrace{-A(t)\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{B(t)\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i,j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}},$$



Adiabatic th.

$\tau \to \infty$

$\hat{H}_0 \to \hat{H}_t$

$|\Psi(0)| \neq |\Psi(t)|$

$\Psi(t)$ – eigenstate of $\hat{H}_t$!

Modularity as Ising

$$x_{i,k} = \begin{cases} 1, \text{if x in } c_k \\ 0, \text{otherwise} \end{cases}$$

Cost part

$$\boxed{\hat{H}_p = P\sum_{i}^{N}(\sum_{c}^{k} x_{i,c} - 1)^2}$$

Constraints

$$B_{i,j} = A_{i,j} - \frac{g_i g_j}{2m}$$

$$\hat{H}_M = -\frac{1}{m}X^T \begin{vmatrix} B & \dots & 0 \\ \dots & \dots & \dots \\ \dots & \dots & B \end{vmatrix} X$$

QUBO matrix

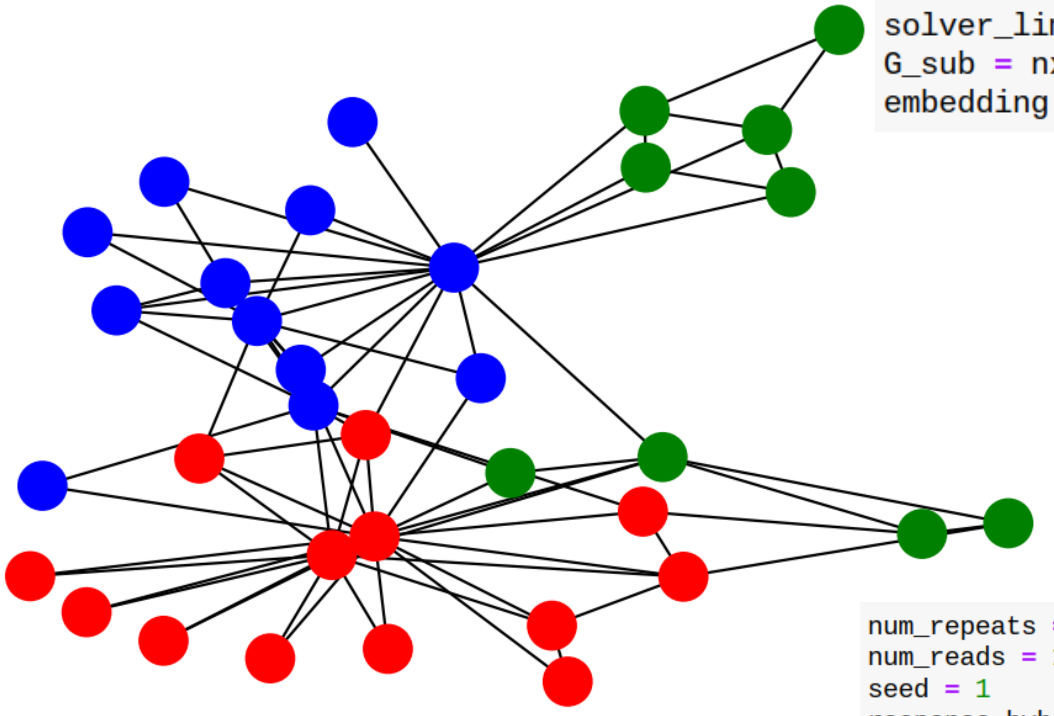
D-wave solution

github.com/aws-samples/amazon-braket-community-detection

```python
from dwave_qbsolv import QBSolv
from dwave.system import DWaveSampler, FixedEmbeddingComposite
```

```python
import minorminer

solver_limit = 50
G_sub = nx.complete_graph(solver_limit)
embedding = minorminer.find_embedding(G_sub.edges, base_sampler.edgelist)
```

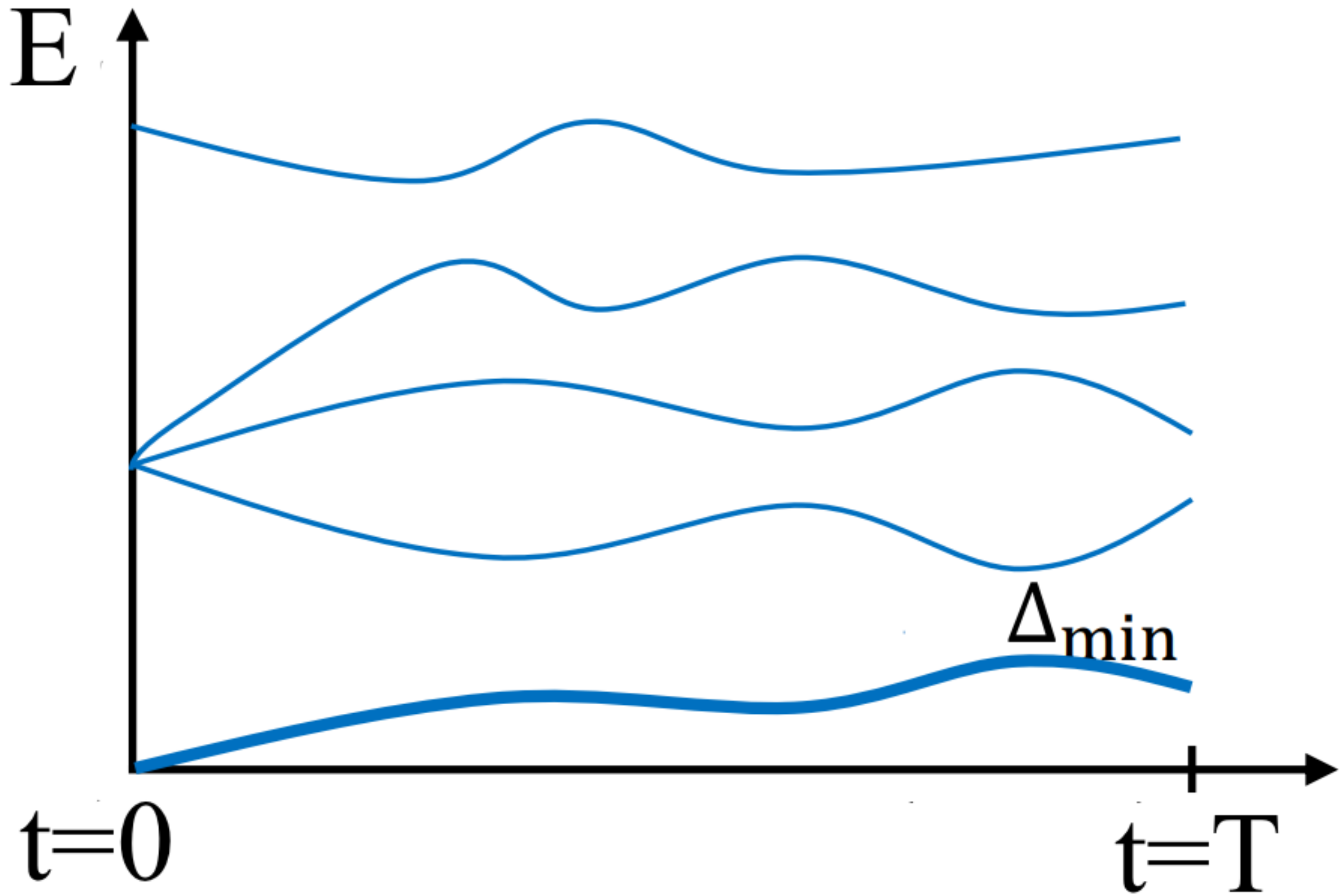


$M = 0.396$

```python
num_repeats = 1
num_reads = 1000
seed = 1
response_hybrid = QBSolv().sample_qubo(qubo, solver=solver,
                                       num_repeats=num_repeats, solver_limit=solver_limit,
                                       num_reads=num_reads, seed=seed)
```

```python
base_sampler = DWaveSampler(token=token)
solver = FixedEmbeddingComposite(base_sampler, embedding)
```

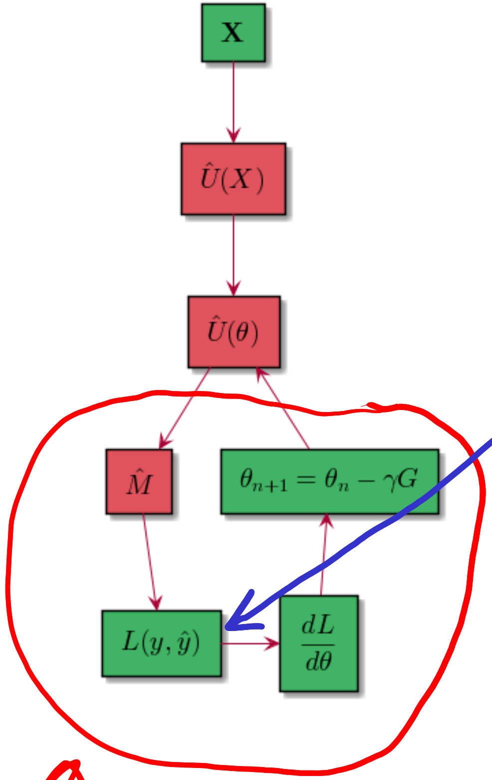
What's the catch?



$\Delta_{min} > 0$?

Another way?

VQE

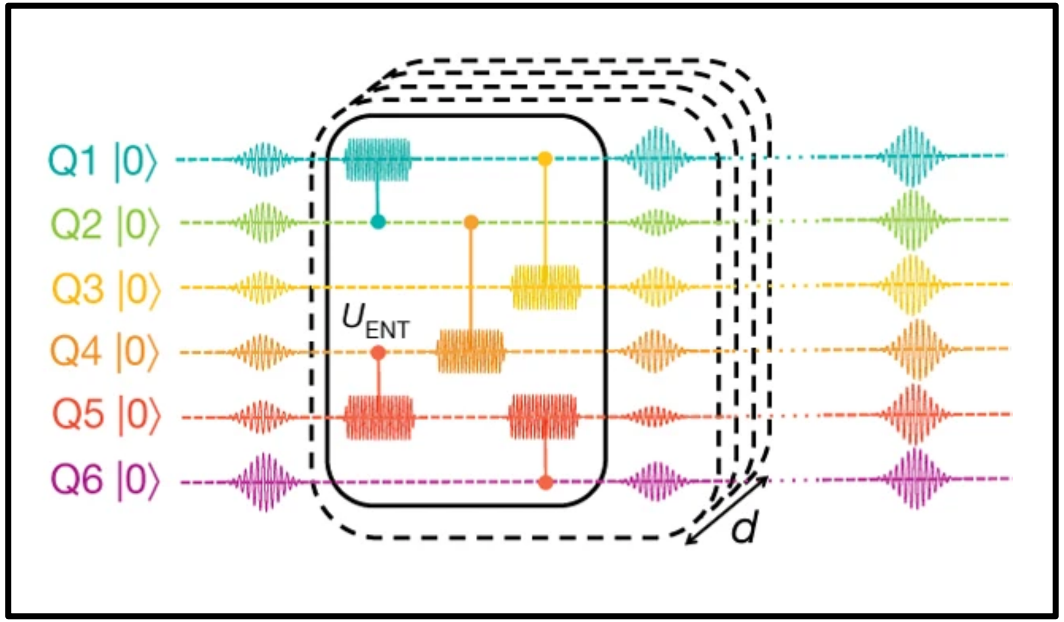


„Gradient descent"

$$L(\theta) = \langle\, 0|\hat{U}^*(\theta)\hat{H}_{Ising}\hat{U}(\theta)|0\rangle$$

$$|\Psi\rangle \simeq \hat{U}(\theta)|0\rangle$$

Approximation



Another way?

„Trotterization"

QAOA

$$|\Psi(t)\rangle = e^{-i\hat{H}_{Ising}(t)t}|\Psi(0)\rangle = e^{-i(A(t)\hat{H}_{initial}+B(t)\hat{H}_{cost})t}|\Psi(0)\rangle$$

Solution from Schr. eq.

$$\begin{array}{l} A(t) \to \gamma_1, \gamma_2, ..., \gamma_N \\ B(t) \to \beta_1, \beta_2, ..., \beta_N \end{array} \rightarrow |\Psi(t)\rangle = e^{-i\gamma_1\hat{H}_{initial}}e^{-i\beta_1\hat{H}_{cost}}...e^{-i\gamma_N\hat{H}_{initial}}e^{-i\beta_N\hat{H}_{cost}}|\Psi(0)\rangle$$

$$\arg \min_{\gamma_1,...,\gamma_N,\beta_1,...,\beta_N} \langle\Psi_{final}|\hat{H}_{cost}|\Psi_{final}\rangle$$

Could be solved by SGD

Want to know more?