Obstacles to State Preparation and Variational Optimization from Symmetry Protection

Robert König

joint work with

Sergey Bravyi, Alexander Kliesch and Eugene Tang

arXiv:1910.08980

robert.koenig@tum.de

Variational methods

How well do these methods perform? (1) What is the best energy attained by a state from S (2) What is the best energy of a state that can be computed efficiently.

many-body Hamiltonian H

optimize over **product states**

mean-field theory

Variational methods

How well do these

methods perform?

(1) What is the best energy attained by a state from S (2) What is the best energy of a state that can be computed efficiently.

Combinatorial optimization

Quantum approximate optimization (QAOA)

Combinatorial optimization

Given: A function $C: \{0,1\}^n \to \mathbb{R}$.

Goal: Find $x^* \in \{0,1\}^n$ such that $C(x^*)$ approximates the maximum

> max $\max_{x \in \{0,1\}^n} C(x)$

Example: MaxCUT for $G = (V, E)$

$$
C_G(x) = \frac{1}{2} \sum_{(u,v) \in E} (1 - (-1)^{x_u} (-1)^{x_v})
$$

Computing maximum exactly Is NP-hard.

Figure of merit for an algorithm \mathcal{A} :

(expected) *approximation ratio*

$$
\alpha(\mathcal{A}) = \frac{\mathbb{E}_{x^* \leftarrow \mathcal{A}}[C(x^*)]}{\max_{x \in \{0,1\}^n} C(x)}
$$

A polynomial-time algorithm achieving α (A) \geq 0.878 for every graph G!

Goemans and Williamson (1995)

Assuming the unique games conjecture and $P \neq NP$ there is no polynomial-time algorithm A satisfying $\alpha(\mathcal{A}) > 0.878$ for every graph G.

S. Khot and N. Vishnoi, FOCS (2005)

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```
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$$

E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028.

$$
H = \sum_{x \in \{0,1\}^n} C(x) |x\rangle\langle x|
$$

 $|x\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$

Level-p QAOA algorithm

1. Prepare state ψ^* such that $\overline{\psi^*} | H | \psi^* \rangle$ approximates

> max $\boldsymbol{\psi}$ $|\psi|H|\psi$

$$
\psi(\beta,\gamma){=}\prod\nolimits_{k=1}^pe^{i\beta_kB}\;e^{i\gamma_kH}\mid{+}\rangle^{\otimes n}
$$

E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028.

$$
\left[H = \sum_{x \in \{0,1\}^n} C(x)|x\rangle\langle x|\right] \left(B = \sum_{j=1}^n
$$

$$
B=\sum_{j=1}^n X_j
$$

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 $e^{i\beta_k B}e^{i\gamma_k H}$ $|+\rangle^{\otimes n}$

 $\psi(\beta, \gamma)$ = $\prod_{k=1}^{P}$

 \overline{p}

E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028.

$$
\left[H = \sum_{x \in \{0,1\}^n} C(x)|x\rangle\langle x|\right] \quad \left(B = \sum_{j=1}^n C(j) |x\rangle\langle x| \right)
$$

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$$

 $|x\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$

QAOA algorithm: Limitations on level p

- descriptive power of variational class of states increases with level p
- energy maximization becomes more challenging with increasing p
- NISQ implementation requires constant (small) p

Main question: Can **constant-level QAOA** outperform the best known classical algorithm (i.e., Goemans-Williamson) for MAXCUT?

Main theme: Lower bounds on *circuit-depth/circuit-range* necessary to prepare low-energy states using symmetric unitary preparation circuits

Symmetric Hamiltonians/unitaries and states

A Hamiltonian H is \mathbb{Z}_2 -symmetric if $[H, X^{\bigotimes n}] = 0.$

Examples:

$$
H_{TF} = -\sum_{k \in \mathbb{Z}_n} X_k
$$

$$
X_k \t\t H_{Ising} = -\sum_{k \in \mathbb{Z}_n} Z_k Z_{k+1}
$$

A state
$$
\psi
$$
 is \mathbb{Z}_2 -symmetric if $X^{\otimes n} \psi = \psi$ or $X^{\otimes n} \psi = -\psi$.

Examples: $|+\rangle^{\otimes n} = |+\rangle \otimes |+\rangle \otimes \cdots \otimes |+\rangle$ 1 2 $(|0\rangle^{\otimes n}+|1\rangle^{\otimes n})$

A unitary U is \mathbb{Z}_2 -symmetric if $\mathit{UX}^{\otimes n}\mathit{U}^\dagger = X^{\otimes n}$.

Examples: $U = X^{\otimes n}$

any circuit U composed of \mathbb{Z}_2 -symmetric gates.

QAOA: a \mathbb{Z}_2 -symmetric circuit

$$
\left[H = \sum_{x \in \{0,1\}^n} C(x) |x\rangle\langle x| \right] \quad \left(B = \sum_{j=1}^n X_j\right)
$$

 $|x\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$

This circuit is Z₂-symmetric if

 $C(x) = C(\bar{x})$ where $\bar{x}_i = 1 - x_i$

symmetric! **Fhis initial state is** \mathbb{Z}_2 -
 E.g., for MAXCUT! |+⟩⊗

level-p QAOA variational state

$$
H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})
$$

Conventions throughout this talk:

- ${H_n}_n$ family of local Hamiltonians with $n =$ number of qubits
- Hamiltonians are sums of local terms of strength $O(1)$
- Ground state energy zero for every Hamiltonian: $min_{\psi} \langle \psi | H_n | \psi \rangle = 0$

$$
H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})
$$

Goal: prepare *a* **ground state** $|\psi\rangle = U|+\rangle^{\otimes n}$ from $|+\rangle^{\otimes n}$

What is the required circuit range for U?

U has

(backward) *range* $R^$ if the backward light-cone of every output qubit *is contained in* $(j - R^{\leftarrow}, j + R^{\leftarrow})$

(forward) *range* R ^{\rightarrow} if the forward light-cone of every input qubit k is contained in $(k - R^{\rightarrow}, k + R^{\rightarrow})$

range $R = \max\{R^{\leftarrow}, R^{\rightarrow}\}.$

$$
H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})
$$

Goal: prepare *a* **ground state** $|\psi\rangle = U|+\rangle^{\otimes n}$ from $|+\rangle^{\otimes n}$

If U is arbitrary (no symmetry):

Choose $|\psi\rangle = |0\rangle^{\otimes n}$ and $U = H^{\otimes n}$ $|\psi\rangle = \alpha |0\rangle^{\otimes n} + \beta |1\rangle^{\otimes n}$, α, β arbitrary ⇒ Easy! (range-1, local)

 $|GHZ_n\rangle =$ 1 2 $(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$ If U is \mathbb{Z}_2 -symmetric: $|\psi\rangle$ has to be Need linear range!

This is a fundamental limitation of ℤ**-symmetric circuits!**

Circuit range lower bound for preparing $|GHZ_n\rangle$

Claim: Suppose a circuit U prepares $|GHZ_n\rangle$ from a product state, i.e., $|GHZ_n\rangle = U|+\rangle^{\otimes n}$. Then the range of U satisfies $R \geq$ \boldsymbol{n} 2 .

Proof:

$$
|GHZ_n^+\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})
$$

$$
|GHZ_n^-\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} - |1\rangle^{\otimes n})
$$

These two states are orthogonal, but *locally indistinguishable*: the reduced density operators on n-1 qubits are identical.

The observable $U O_j U^{-1}$ distinguishes these two states. $|U^{-1}|GHZ_n^+\rangle = |+\rangle^{\otimes n}$

 $|U^{-1}|$ GHZ $^-_n\rangle$

−1

 \overline{U}

These states are *locally distinguishable* because they are orthogonal and the first is a product state

There is a single-qubit observable O_i distinguishing these two states.

S. Bravyi, M. B. Hastings, and F. Verstraete, Phys. Rev. Lett. 97, 050401 (2006).

Saturating the range lower bound: GHZ-preparing circuit

$$
H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})
$$

Goal: prepare *a* **ground state** $|\psi\rangle = U|+\rangle^{\otimes n}$ from $|+\rangle^{\otimes n}$

If U is arbitrary (no symmetry): (range-1 suffices)

If U is \mathbb{Z}_2 -symmetric:

Need linear range!

"Symmetry protection"

Haldane. PRL 50:1153-1156, 1983. Affleck, Kennedy, Lieb, Tasaki. PRL 59:799-802, 1987. Gu, Wen, PRB 80:155131, (2009) Pollmann, Turner, Berg, Oshikawa. PRB 81:054439 (2010) Haegeman, Perez-Garcia, Cirac, Schuch, PRL 102, 050402 (2012) Chiu, Teo, Schnyder, Ryu. Rev. Mod. Phys., 88:035005,2016.

Low-energy states of Ising model: Preparation with symmetry

$$
H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})
$$

Theorem: Suppose $|\psi\rangle = U|+\rangle^{\otimes n}$ where U has range $R < n/4$ and is \mathbb{Z}_2 -symmetric.

Then
$$
\langle \psi | H_n | \psi \rangle \ge \frac{1}{2R+1}n
$$

Preparing any state with an energy density lower than ε *density requires* $R = \Omega(1/\varepsilon)$.

Symmetry obstructs the preparation of low-energy states!

also see G. Mbeng, R. Fazio, G. Santoro, arXiv:190608948 for QAOA

Toric code: no zero-energy trivial states

Geometrically local circuits require $\Omega(\sqrt{n})$ depth.

Bravyi, Hastings, Verstraete, PRL 97, 050401 (2006)

All toric code *zero-energy states* are *non-trivial* (topologically ordered).

Toric code: existence of low-energy trivial states

If $n \geq d^2$ the output state is NOT a ground state of H_n^{toric} PRL 97, 050401 (2006)

Bravyi, Hastings, Verstraete,

All toric code *zero-energy states* are *non-trivial* (topologically ordered).

constant-size patches of local ground states (can be created in parallel)

For every constant $\varepsilon > 0$ there is a **constant-depth** circuit U such that $|\langle + |^{\otimes n} U^{\dagger} H^{toric}_{n} U | + \rangle^{\otimes n} \leq \varepsilon n$

The toric code has *low-energy states that are trivial.*

The NLTS conjecture

Freedman and Hastings, Quant. Inf. Comp. 14 (2014)

No low-energy trivial states (NLTS) property:

There is $\varepsilon > 0$ and a function $f: \mathbb{N} \to \mathbb{N}$ such that for any depth- d (local) circuit U

$$
\langle + |^{\otimes n} U^{\dagger} H_n U | + \rangle^{\otimes n} > \varepsilon n \quad \text{for any} \quad n \ge f(d)
$$

Conjecture: There is a family $\{H_n\ \}_n$ of local Hamiltonians that has the NLTS property.

The following families $\{H_n\}_{n=1}^N$ **do not** satisfy the NLTS property:

The NLTS conjecture

Freedman and Hastings, Quant. Inf. Comp. 14 (2014)

No low-energy trivial states (NLTS) property:

There is $\varepsilon > 0$ and a function $f: \mathbb{N} \to \mathbb{N}$ such that for any depth- d (local) circuit U

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Conjecture: There is a family $\{H_n\ \}_n$ of local Hamiltonians that has the NLTS property.

Evidence for the NLTS conjecture:

- There is a family of toric-code like (CSS-stabilizer) Hamiltonians on simplicial complexes such that an NLTS-like statement holds *when one restricts to a certain subset of excited states*. (Freedman and Hastings)
- There is a family of Hamiltonians satisfying a related "*no lowerror trivial states property*" (Harrow and Eldar, FOCS 2017)

Main result: NLTS with symmetry protection

for a family

 ${H_n}_n$ of local \mathbb{Z}_2 -symmetric Hamiltonians

No low-energy \mathbb{Z}_2 -trivial states property:

There is $\varepsilon > 0$ and a function $f: \mathbb{N} \to \mathbb{N}$ such that for any \mathbb{Z}_2 -symmetric depth- d (local) circuit U

$$
\langle + |^{\otimes n} U^{\dagger} H_n U | + \rangle^{\otimes n} > \varepsilon n \quad \text{for any} \quad n \ge f(d)
$$

Main result: Construction of a family $\{H_n\ \}_n$ of local Hamiltonians that has the NL \mathbb{Z}_2 TS property.

Symmetryprotected NLTS

NL Z₂TS

Let ${G_n}_{n\in I}$ be an infinite family of D-regular graphs such that $h(G_n) \geq h$ for all $n \in I$

Graph
$$
G = (V, E)
$$
 given
\n
$$
\partial(S) = \{e \in E \mid |e \cap S| = 1\}
$$
\nCheeger constant of G :

\n
$$
h(G) = \min_{\substack{S \subseteq V \\ 0 < |S| \le |V|/2}} \frac{|\partial(S)|}{|S|}
$$

We need infinite families of D-regular graphs with $h = \Omega(1)$ **.**

Ramanujan graphs:

- connected
- satisfy $h(G) \geq \frac{1}{2}(D 2\sqrt{D-1})$

There is an infinite family of D -regular Ramanujan graphs for every $D \geq 3$.

Marcus, Spielman, Srivastava, Annals of Mathematics 182, 307 (2015)

Let ${G_n}_{n\in I}$ be an infinite family of D-regular graphs such that $h(G_n) \geq h$ for all $n \in I$

Let
$$
H_n = \frac{1}{2} \sum_{(u,v) \in E_n} (I - Z_u Z_v)
$$

Corollary: Unless $d = \Omega(\log n)$, no low energy (density) state can be prepared.

Let ${G_n}_{n\in I}$ be an infinite family of D-regular graphs such that $h(G_n) \geq h$ for all $n \in I$

Let
$$
H_n = \frac{1}{2} \sum_{(u,v) \in E_n} (I - Z_u Z_v)
$$

Theorem:
$$
(+|\mathcal{D}^n U^\dagger H_n U| + \mathcal{D}^{\otimes n} > (\frac{h}{6})n
$$
 for any $n > 24^2 2^{4d/3}$
and any \mathbb{Z}_2 -symmetric depth- d (local) circuit U
Proof:
 $|+ \rangle$ -symmetric
 $|+ \rangle$ -
circuit U
 $|+ \rangle$ -
of depth d
 $U|+ \mathcal{D}^{\otimes n}$
 $|+ \mathcal{D}^{\otimes n}$
 $|+ \mathcal{D}^{\otimes n}$
 $|+ \mathcal{D}^{\otimes n}$

Let ${G_n}_{n\in I}$ be an infinite family of D-regular graphs such that $h(G_n) \geq h$ for all $n \in I$

Let
$$
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$$

Theorem:		$\langle + ^{\otimes n} U^{\dagger} H_n U + \rangle^{\otimes n} > \left(\frac{h}{6}\right) n$	for any $n > 24^2 2^{4d/3}$		
Proof:		$ + \rangle$ - symmetric	$\sqrt{2}$	x_1	Suppose $\langle + ^{\otimes n} U^{\dagger} H_n U + \rangle^{\otimes n} < \left(\frac{h}{6}\right) n$
Proof:		$ + \rangle$ - circuit U	x_1	Suppose $\langle + ^{\otimes n} U^{\dagger} H_n U + \rangle^{\otimes n} < \left(\frac{h}{6}\right) n$	
1+ \rangle - circuit U		x_2	Consider the distribution		
$ + \rangle$ - of depth d	$\sqrt{2}$	x_n	$p(x) = \langle x U + \rangle^{\otimes n} ^2$ where $x \in \{0,1\}^n$		
By Markov's inequality	$p(S_{low}) \ge 1/2$ where $S_{low} := \{x \in \{0,1\}^n \langle x H x \rangle < \frac{h}{3} n\}$				

"low energy configurations"

Let ${G_n}_{n\in I}$ be an infinite family of D-regular graphs such that $h(G_n) \geq h$ for all $n \in I$

Let
$$
H_n = \frac{1}{2} \sum_{(u,v) \in E_n} (I - Z_u Z_v)
$$

Theorem:		\n $\langle + \frac{\otimes n}{U^{\dagger}}H_nU +\rangle^{\otimes n} > \left(\frac{h}{6}\right)n$ \n	\n for any $n > 24^2 2^{4d/3}$ \n and any \mathbb{Z}_2 -symmetric depth- d (local) circuit U \n	
\n Proof:	\n $ +\rangle = \text{symmetric}$ \n	\n $\sqrt{2}$ \n	\n x_1 \n	\n $\text{Suppose } \langle + \frac{\otimes n}{U^{\dagger}}H_nU +\rangle^{\otimes n} < \left(\frac{h}{6}\right)n$ \n
\n $ +\rangle = \text{circuit } U$ \n	\n $\sqrt{2}$ \n	\n $\text{Consider the distribution}$ \n		
\n $ +\rangle = \text{of depth } d$ \n	\n $\sqrt{2}$ \n	\n $\text{Consider the distribution}$ \n		
\n $p(S_0 \cup S_1) \geq 1/2$ \n	\n $p(S_0) \geq 1/4$ \n	\n $p(S_1) \geq 1/4$ \n	\n $S_0 := \{x \in \{0,1\}^n \mid x < \frac{\pi}{3}\}$ \n	\n $\text{Thus, } \text{the probability of } \mathbb{Q} = \mathbb{Q}(\log n)$ \n
\n $\text{by } \mathbb{Z}_2\text{-symmetry: } \quad p(S_0) \geq 1/4 \quad \text{and } p(S_1) \geq 1/4$ \n	\n $S_0 := \{x \in \{0,1\}^n \mid x < \frac{\pi}{3}\}$ \n	\n $S_1 := \{x \in \{0,1\}^n \mid x > \frac{\pi}{3}\}$ \n	\n $\text{This is only possible if } d =$	

Circuit depth lower bound for sampling from bimodal distributions

Theorem:

(Corollary 43, Eldar & Harrow, 2017) Let $p(x)$ denote the output distribution of a depth-d quantum circuit U. Let $S_0, S_1 \subset \{0,1\}^n$ be such that $p(S_0) > 0$ and $p(S_1) > 0$. Then dist $(S_0, S_1) \leq \frac{4n^{1/2}2^{3d/2}}{\min\{p(S_0), p(S_1)\}}$

A distribution produced by a shallow quantum circuit does not have large support on any two distant subsets of strings at the same time.

level-p QAOA variational state

$$
\psi(\beta,\gamma) = \prod_{k=1}^p e^{i\beta_k B} e^{i\gamma_k H} |+\rangle^{\otimes n}
$$

Sampling from the output distribution of $(p = 1)$ –QAOA cannot be efficiently simulated classically unless the polynomial hierarchy collapses (Farhi & Harrow 2016)

class of "global" classical algorithms. These results suggest that such local classical algorithms are

likely to be at least as promising as the QAOA for approximate optimization.

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$$

Goemans and Williamson, 1995

Main result for MAXCUT-QAOA with $p > 1$

Theorem: For every $D \geq 3$ there is an infinite family of D-regular bipartite graphs $\{G_n\}_{n\in I}$ such that

$$
\alpha(QAOA_p) \leq \frac{5}{6} + \frac{\sqrt{D-1}}{3D}
$$
 if $p \leq D^{-1}(\frac{1}{3}\log_2 n - 4)$

In particular:

 $\alpha(QAOA_n) < 0.87856 = \alpha(Goemans-Williamson)$ if $D \geq 54$

The **best classical polynomial-time algorithm** (Goemans-Williamson) beats QAOA *for any constant* **level p**

Main result for MAXCUT-QAOA with $p > 1$

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$$
\alpha(QAOA_p) \leq \frac{5}{6} + \frac{\sqrt{D-1}}{3D} \qquad \qquad \text{if} \qquad p \leq D^{-1}(\frac{1}{3}\log_2 n - 4)
$$

Proof: Take $\{G_n\}_n$ to be family of D-regular bipartite Ramanujan graphs. (Marcus, Spielman, Srivastava 2015)

$$
\max_{\psi} \quad \langle \psi | H_n | \psi \rangle = |E_n|
$$
\n
$$
\max_{(\beta, \gamma)} \quad \langle \psi(\beta, \gamma) | H_n | \psi(\beta, \gamma) \rangle = \frac{|E_n|}{2} + \max_{(\beta, \gamma)} \quad \langle \widehat{\Psi}(\beta, \gamma) | \widehat{H}_n | \widehat{\Psi}(\beta, \gamma) \rangle \quad \widehat{H}_n = \frac{1}{2} \Sigma_{(u, v) \in E_n} Z_u Z_v
$$
\nbecause G_n is bipartite.

NL \mathbb{Z}_2 TS: $\bra{\widehat{\mathfrak{P}}(\beta,\gamma)}\widehat{H}_n\ket{\widehat{\mathfrak{P}}(\beta,\gamma)}<\frac{|E_n|}{2}$ $\frac{E_n}{2} - \frac{hn}{6}$ $\prod_{k=1}^p e^{i\beta_k B} e^{i\gamma_k H_n}$ is \mathbb{Z}_2 -symmetric depth, depth $d \leq p D$

The **best classical polynomial-time algorithm** (Goemans-Williamson) beats QAOA *for any constant* **level p**

level-p QAOA variational state

$$
\psi(\beta,\gamma) = \prod_{k=1}^p e^{i\beta_k B} e^{i\gamma_k H} |+\rangle^{\otimes n}
$$

The **best classical polynomial-time algorithm** (Goemans-Williamson) beats QAOA *for any constant* **level p**

Conclusions and open problems

- ℤ**-symmetric No Low Energy Trivial States (NLTS) property** for a family of Ising models on expander graphs
	- Other symmetries?
	- General NLTS conjecture still open
- **Limitations to quantum approximate optimization algorithm** (QAOA): Efficient (i.e., constant-level) **QAOA** *underperforms* compared to the **best classical polynomial-time algorithm** (Goemans-Williamson)
	- Comparison for generic instances (instead of worst-case)? Finding independent sets in random graphs:

The Quantum Approximate Optimization Algorithm Needs to See the Whole Graph: A Typical Case

Edward Farhi¹, David Gamarnik², and Sam Gutmann

¹Google Inc., Venice CA 90291 and Center for Theoretical Physics, MIT, Cambridge MA, 02139 ²Operations Research Center and Sloan School of Management MIT, Cambridge MA, 02140

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- **Non-local modifications of QAOA/RQAOA**: some evidence for their suitability:
	- More extensive benchmarks/case studies?