Approximation and Hardness of Quantum Max Cut

Presented by
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Quantum Algorithms and Applications Collaboratory

with Kevin Thompson (Sandia)

including work with: Sevag Gharibian (U Paderborn), Yeongwoo Hwang (Harvard), John Kallaugher (Sandia), Joe Neeman (UT Austin), John Wright (UC Berkeley)
INFORMS Challenge Paper:
Survey article and suggestions to engage QIS for operations researchers

Synergies Between Operations Research and Quantum Information Science
P., 2023
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Special Issue of INFORMS Journal on Computing—Quantum computing and operations research
Broadly targeting research at intersection of OR and QIS

Call will appear soon; papers due January 15, 2024

Guest Editors: Carleton Coffrin, Elisabeth Lobe, Giacomo Nannicini, Ojas Parekh
Quantum Computing
State of Quantum “Speedups”

- **Unproven exponential speedup:**
  Shor’s quantum factorization algorithm
  [Shor, *Polynomial-Time Algorithms for Prime Factorization...*, 1995]

- **Provable modest speedup:**
  Grover’s quantum search algorithm

- **Provable exponential advantage in specialized settings:**
  Query and communication complexity
  [Childs et al., *Exponential Algorithmic Speedup by a Quantum Walk*, 2003]
  [Bar-Yossef et al., *Exponential Separation of Quantum and Classical...*, 2008]
  ...

- **Optimization offers potential for new kinds of quantum advantages:**
  Better quality solutions but not necessarily faster solution times
Quantum Bits Live in a Sphere

Classical bit: (bit)
1 = Head
0 = Tail

Prob. bit: (p-bit)
0 with probability $1 - p$
1 with probability $p$

Quantum bit: (qubit)
$|0\rangle + \beta|1\rangle$
0 with probability $|\alpha|^2$
1 with probability $|\beta|^2$

State space
$\{0, 1\}$

Representation
2-d complex unit vector
3-d real unit vector

3-d real unit vector
Quantum Algorithms Output Distributions

Physically

Sequence of physical manipulations of the $N$ qubits

Conceptually

Sequence of quantum gates

Probability distribution over $2^N$ binary classical states

Seek to maximize probability of good solutions
Quantum Optimization
What is Quantum Optimization?

Classical approaches for quantum Hamiltonians (e.g. DMRG, mean-field methods)

Quantum approaches for classical Hamiltonians (e.g. AQC, QAOA for quantum Hamiltonians)

Quantum approaches for continuous optimization

Classical optimization
Max Cut

Model NP-hard discrete optimization problem and 2-CSP

Has driven developments in approximation algorithms

0.878…-approximation
[Goemans and Williamson, 1995]

0.878…+ \( \varepsilon \) is unique games hard
[Khot, Kindler, Mossel, O'Donnell, 2007]

Cut and related polytopes have advanced discrete optimization
e.g., [Fiorini, Massar, Pokutta, Tiwary, de Wolf, 2012]

Partition vertices of a graph two parts
to maximize (weight of) crossing edges

Constraint Satisfaction Problem (CSP) version:
Boolean assignment satisfying max # XOR clauses

\((x_1 \oplus x_2), (x_1 \oplus x_4), (x_1 \oplus x_6), (x_2 \oplus x_3), ...\)
How far can we go?

0.87856 + ε approximations are **NP-Hard!** (under Unique Games Conjecture)

\[
\frac{1}{2} + \frac{1}{2n} \\
\text{[Haglin, Venkatesan 1991]}
\]

\[
\frac{1}{2} + \frac{1}{2m} \\
\text{[Vitányi 1981]}
\]

\[
\frac{1}{2} + \frac{1}{2\Delta} \\
\text{[Hofmeister, Lefmann 1995]}
\]

\[
0.87856 \\
\text{[Goemans, Williamson 1995]}
\]

\[
\frac{1}{2} \\
\text{Random}
\]

\[
\frac{1}{2} + \frac{1}{2n} \\
\text{[Haglin, Venkatesan 1991]}
\]

\[
1 \\
\text{[Khot, Kindler Mossel, O’Donnell 2007]}
\]

Slide courtesy of Yeongwoo Hwang
It’s Natural to Optimize

Hamiltonian eigenstate problems naturally link quantum mechanics and optimization

$$\min_{\psi} \langle \psi | \sum_S H_S | \psi \rangle$$

Hamiltonian, $\sum_S H_S$, represents energy levels of a physical system composed of “local” parts, $S$

Discrete optimization problem becomes an eigenproblem on a large matrix

Optimal discrete optimization solution $\leftrightarrow$ Min-energy eigenvector

Nature tends towards stable states...
So let nature solve your problems for you?

Image from https://en.wikipedia.org/wiki/Metastability
Hacking Nature to Solve Your Problems

1. Map solution values to energy levels of a physical system
2. Realize said physical system
3. Let Nature relax to a stable low-energy state

Minimum eigenstate is of form: $|\psi\rangle = \alpha |010\rangle + \beta |101\rangle$, with energy -2
Computational Complexity Considerations

Hamiltonian is exponentially large, $2^N \times 2^N$, for an $N$-node graph, but it is a sum of $O(N^2)$ local $4 \times 4$ Hamiltonians, one for each edge.

Local Hamiltonians are efficient and require manipulating only a constant number of qubits.
**The Power of Quantum Computing?**

**Extended Quantum Church-Turing Thesis**

Any “reasonable” model of computing can be *efficiently* simulated by a *quantum* Turing machine.

It would be very surprising if quantum computers could solve NP-complete problems in quantum polynomial time (BQP).

Yet, there are problems in BQP that are very unlikely to be in classical polynomial time (P) or even NP!*

Using nature to solve optimization problems is an old idea.

*In the quantum setting, it is a surprisingly powerful idea that captures universal quantum computing.*

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*Quantum supremacy: [Preskill; arXiv 1801.00862], [Harrow & Montanaro; arXiv 1809.07442], [Aaronson & Chen; arXiv 1612.05903]*
Quantum Approximation Algorithms
A $\alpha$-approximation algorithm runs in polynomial time, and for any instance $I$, delivers an approximate solution such that:

$$\frac{\text{Value(Approximate}_I)}{\text{Value(Optimal}_I)} \geq \alpha$$

$\alpha$ is the largest “gap” between optimal and approximate solutions over all instances.
A $\alpha$-approximation algorithm runs in polynomial time, and for any instance $I$, delivers an approximate solution such that:

$$\frac{\text{Value(Approximate}_I)}{\text{Value(Optimal}_I)} \geq \alpha$$

**Heuristics**
- Guided by intuitive ideas
- Perform well on practical instances
- May perform very poorly in worst case
- Difficult to prove anything about performance

**Approximation Algorithms**
- Guided by worst-case performance
- May perform poorly compared to heuristics
- Rigorous bound on worst-case performance
- Designed with performance proof in mind
Let’s consider diagonal PSD matrices with trace = 1:

\[
\begin{bmatrix}
\frac{1 + a}{2} & 0 \\
0 & \frac{1 - a}{2}
\end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} + \frac{a}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}
\]

Bias $a$ must satisfy $|a| \leq 1$

\[
\begin{bmatrix}
\frac{1 + a_1}{2} & 0 \\
0 & \frac{1 - a_1}{2}
\end{bmatrix} \otimes \begin{bmatrix}
\frac{1 + a_2}{2} & 0 \\
0 & \frac{1 - a_2}{2}
\end{bmatrix} = \frac{I + a_1 Z}{2} \otimes \frac{I + a_2 Z}{2} = \frac{Z_1}{4}
\]

\[
\frac{Z_1}{4} = \frac{Z_2}{4} = \frac{Z_1 Z_2}{4}
\]
Probability Distributions and Polynomials

\[
\begin{bmatrix}
\frac{1 + a_1}{2} & 0 \\
0 & \frac{1 - a_1}{2}
\end{bmatrix} \otimes \begin{bmatrix}
\frac{1 + a_2}{2} \\
\frac{1 - a_2}{2}
\end{bmatrix} = \frac{I + a_1 Z}{2} \otimes \frac{I + a_2 Z}{2} = \frac{Z_1}{4} + Z_2 + a_1 a_2 Z \otimes Z
\]

\[a_1 = -\frac{1}{2} \quad a_2 = \frac{1}{2}\]

\[
\begin{bmatrix}
\frac{1}{4} & 0 \\
0 & \frac{3}{4}
\end{bmatrix} \otimes \begin{bmatrix}
\frac{3}{16} \\
\frac{1}{16}
\end{bmatrix} = \begin{bmatrix}
\frac{3}{16} \\
\frac{9}{16} \\
\frac{3}{16}
\end{bmatrix}
\]

\[= \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} - \frac{1}{8} \begin{bmatrix} 1 & 1 & -1 \\ -1 & 1 & -1 \end{bmatrix} + \frac{1}{8} \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} + \frac{1}{16} \begin{bmatrix} 1 & -1 & -1 \\ -1 & -1 & -1 \end{bmatrix} \]

\[
\begin{align*}
I & \quad Z_1 & \quad Z_2 & \quad Z_1 Z_2
\end{align*}
\]
Quantum “Distributions” and Polynomials

Let’s consider diagonal PSD matrices with trace = 1:

$$\begin{bmatrix}
\frac{1 + a}{2} & 0 \\
0 & \frac{1 - a}{2}
\end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{a}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Bias $a$ must satisfy $|a| \leq 1$

$$\begin{bmatrix}
\frac{1 + a}{2} & \frac{b - ci}{2} \\
\frac{b + ci}{2} & \frac{1 - a}{2}
\end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{a}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} + \frac{b}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{c}{2} \begin{bmatrix} i \\ -i \end{bmatrix}$$

Biases must satisfy $\| (a, b, c) \| \leq 1$
Max Cut and Quantum Max Cut

### Classical Max Cut
2-variable constraint: $x_i \oplus x_j$

<table>
<thead>
<tr>
<th>$x_i, x_j$</th>
<th>0.0</th>
<th>0.1</th>
<th>1.0</th>
<th>1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0, 0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.0, 0.1</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.0, 1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.0, 1.1</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

**Diagonal** matrix
diagonal encodes Boolean function:

$$f(z_i, z_j) = \frac{1}{2}(1 - z_i z_j)$$

$$z_i \in \{-1, 1\}$$

Maximum eigenvectors:

- $(0, 1, 0, 0) = |01\rangle$
- $(0, 0, 1, 0) = |10\rangle$

with (eigen)value 1

### Quantum Max Cut
quantum 2-variable constraint

$$\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 1/2 & -1/2 & 0 \\
0 & -1/2 & 1/2 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}$$

**General** non-diagonal matrix

$$(I - X_i X_j - Y_i Y_j - Z_i Z_j)/4$$

Maximum eigenvector:

$$\left(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right) = \frac{1}{\sqrt{2}} |01\rangle - \frac{1}{\sqrt{2}} |10\rangle,$$

with (eigen)value 1

**Maximum product state:** e.g., $|01\rangle$ with energy 1/2
Polynomials and Quantum Solutions

**Classical**

Real-coeff polynomial $P(I, Z_1, ..., Z_n)$ over **commutative** variables

Problem: $\max_{z_i} \lambda_{\max}(P(I, Z_1, ..., Z_n))$

\[
Z_i^2 = I \\
Z_iZ_j = Z_jZ_i
\]

$P$ represents a **diagonal** $M \in \mathbb{R}^{2^n \times 2^n}$

\[
P = \frac{1}{2}(I - Z_1Z_2)
\]

**Quantum**

Real-coeff polynomial $Q(I, X_1, Y_1, Z_1, ..., X_n, Y_n, Z_n)$ over **non-commutative** variables

$\max_{x_i,y_i,z_i} \lambda_{\max}(Q(I, X_1, Y_1, Z_1, ..., X_n, Y_n, Z_n))$

\[
X_i^2 = Y_i^2 = Z_i^2 = I \\
X_iY_i = -Y_iX_i, X_iZ_i = -Z_iX_i, Y_iZ_i = -Z_iY_i
\]

Variables commute on different indices:

- e.g. $X_iZ_j = Z_jX_i$

$Q$ represents a **Hermitian** $M \in \mathbb{C}^{2^n \times 2^n}$

\[
Q = \frac{1}{4}(I - X_1X_2 - Y_1Y_2 - Z_1Z_2)
\]

\[
\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 1/2 & -1/2 & 0 \\
0 & -1/2 & 1/2 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]
Polynomials and Quantum Solutions

**Classical**

Problem: $\text{Max}_{\{Z_i\}} \lambda_{\max} (P(I, Z_1, \ldots, Z_n))$

$Z_i^2 = I$

$Z_i Z_j = Z_j Z_i$

WLOG can take: $Z_i \in \{-1, 1\}$

\[
\begin{bmatrix}
0,0 & 0 & 0 & 0 & 0 \\
0,1 & 0 & 1 & 0 & 0 \\
1,0 & 0 & 0 & 1 & 0 \\
1,1 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

$P = \frac{1}{2}(I - Z_1 Z_2)$

**Quantum**

$\text{Max}_{\{X_i, Y_i, Z_i\}} \lambda_{\max} (Q(I, X_1, Y_1, Z_1, \ldots, X_n, Y_n, Z_n))$

$X_i^2 = Y_i^2 = Z_i^2 = I$

$X_i Y_i = -Y_i X_i, X_i Z_i = -Z_i X_i, Y_i Z_i = -Z_i Y_i$

Variables commute on different indices:

e.g. $X_i Z_j = Z_j X_i$

WLOG: $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$

e.g. $Z_2 = I \otimes Z \otimes I \ldots$

$Z_1 Z_3 = Z \otimes I \otimes Z \otimes I \ldots$

$X_1 Y_4 = X \otimes I \otimes I \otimes Y \ldots$

\[
\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 1/2 & -1/2 & 0 \\
0 & -1/2 & 1/2 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

$Q = \frac{1}{4}(I - X_1 X_2 - Y_1 Y_2 - Z_1 Z_2)$
Quantum Max Cut: Physical Motivation

Max Cut Hamiltonian: \[ \sum(I - Z_iZ_j)/2 \]

Quantum Max Cut generalization: \[ \sum(I - X_iX_j - Y_iY_j - Z_iZ_j)/4 \]

**Physical motivation**
Heisenberg model is fundamental for describing quantum magnetism, superconductivity, and charge density waves. Beyond 1 dimension, properties of the anti-ferromagnetic Heisenberg model are notoriously difficult to analyze.

**Problem**
Find max-energy value/state of Quantum Max Cut: \[ \sum(I - X_iX_j - Y_iY_j - Z_iZ_j)/4 \]

(\[\equiv\] Find min-energy state of quantum Heisenberg model: \[ \sum(X_iX_j + Y_iY_j + Z_iZ_j)/4 \], but different from approximation point of view)

[Image: Sachdev, arXiv:1203.4565]

[Image: Ground state of the Heisenberg antiferromagnet on the triangular lattice with long-range antiferromagnetic order. This state is not an example of gapped quantum matter.]

[Image: A snapshot of the RVB state on the triangular lattice. Each ellipse represents a singlet valence bond, \(|#i#i|/#p2\). The RVB state is a superposition of all different singlet pairings, of which only one is shown above.]

Spin-charge separation: there are spinon excitations which carry spin \(S = 1/2\) but do not transfer any charge, as shown in Fig. 4.

Our understanding of the physics of RVB states advanced rapidly after the discovery of cuprate high temperature superconductivity in 1986. Baskaran and Anderson pointed out that a natural language for the description of RVB-like states is fundamental for describing quantum magnetism, superconductivity, and charge density waves. Beyond 1 dimension, properties of the anti-ferromagnetic Heisenberg model are notoriously difficult to analyze.

Physical motivation
Heisenberg model is fundamental for describing quantum magnetism, superconductivity, and charge density waves. Beyond 1 dimension, properties of the anti-ferromagnetic Heisenberg model are notoriously difficult to analyze.

Problem
Find max-energy value/state of Quantum Max Cut: \[ \sum(I - X_iX_j - Y_iY_j - Z_iZ_j)/4 \]

(\[\equiv\] Find min-energy state of quantum Heisenberg model: \[ \sum(X_iX_j + Y_iY_j + Z_iZ_j)/4 \], but different from approximation point of view)

[Image:-large, arXiv:1909.08846]

[Physical motivation
Heisenberg model is fundamental for describing quantum magnetism, superconductivity, and charge density waves. Beyond 1 dimension, properties of the anti-ferromagnetic Heisenberg model are notoriously difficult to analyze.

Problem
Find max-energy value/state of Quantum Max Cut: \[ \sum(I - X_iX_j - Y_iY_j - Z_iZ_j)/4 \]

(\[\equiv\] Find min-energy state of quantum Heisenberg model: \[ \sum(X_iX_j + Y_iY_j + Z_iZ_j)/4 \], but different from approximation point of view)
Quantum Max Cut

Has driven advances in quantum approximation algorithms, based on generalizations of classical approaches

QMA-hard and each term is maximally entangled
[Cubitt, Montanaro 2013]

Recent approximation algorithms
[Gharibian and P. 2019], [Anshu, Gosset, Morentz 2020],
[P. and Thompson 2021, 2021, 2022]

Evidence of unique games hardness
[Hwang, Neeman, P., Thompson, Wright 2021]

Likely that approximation/hardness results transfer to 2-LH with positive terms
[P., Thompson 2021, 2022]
Approximation Algorithms for Quantum Max Cut

How far can we go?

Classical Intuition: Best possible?

Beyond product states: 0.53
[Anshu, Gossett, Morenz 2020]

0.498
[Gharibian, P 2019]

0.5
[P, Thompson 2022]

0.53
[P, Thompson 2021]

0.562
[Lee 2022]

0.582 (Δ-free)
[King 2022]

0.956
[Hwang, Neeman, P, Thompson, Wright 2022]

NP-hardness Barrier

Slide courtesy of Yeongwoo Hwang
Max-Cut
in Quantum Language
Max-Cut
in Quantum Language

Treat $|\psi\rangle$ as a classical string!

Measure in $+1/-1$ basis (or $Z$ basis)

Then $s_u \equiv Z_u |\psi\rangle$

Observable: $h_{\text{MAX-CUT}} = \frac{1}{2} (\mathbb{I} - Z_u \otimes Z_v)$
Quantum Max-Cut

Measure in $Z$ basis and the $X$ and $Y$ bases

Observable: $m_{\text{MAX-CUT}} \neq m_z'$ and $\frac{1}{4}(u \neq m_z' \; \text{and} \; m_y \neq m_y' \; \text{and} \; Z_u \otimes Z_v)$

Slide courtesy of Yeongwoo Hwang
Quantum Max-Cut

Slide courtesy of Yeongwoo Hwang
Associate Hamiltonian $h_{(u,v)}$ to each edge.

**Energy:** $\langle \psi | h_{(u,v)} | \psi \rangle$

Overall value given by,

$$\sum_{(u,v) \in E} \langle \psi | h_{(u,v)} | \psi \rangle = \langle \psi | \left( \sum_{(u,v) \in E} h_{(u,v)} \right) | \psi \rangle$$

i.e., this a **maximum eigenvalue** problem for matrix

$$H = \sum_{(u,v) \in E} h_{(u,v)}$$

$\Psi = |\psi\rangle$ maximizes overlap with singlet on each edge

$$h_{(u,v)} = |\Psi^-\rangle \langle \Psi^-| = \left( I - X_i X_j - Y_i Y_j - Z_i Z_j \right)/4$$

Slide courtesy of Yeongwoo Hwang
Quantum Generalization of Constraint Satisfaction (CSP)

Classical 2-CSP clause: \((\neg x_i \land x_j)\)

<table>
<thead>
<tr>
<th></th>
<th>0,0</th>
<th>0,1</th>
<th>1,0</th>
<th>1,1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x_i, x_j = 0,0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(x_i, x_j = 0,1)</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(x_i, x_j = 1,0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(x_i, x_j = 1,1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Quantum 2-CSP clause

\[
\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 1/2 & -1/2 & 0 \\
0 & -1/2 & 1/2 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

Diagonal rank-1 projector

Random assignment “earns” 1/4 of diagonal = \(k/4\) for rank-\(k\) projectors

Research challenge: find classical applications for quantum CSPs, thinking of solutions as probability distributions over classical solutions
First approximations for Max k-Local Hamiltonian

Classical approximation scheme for planar graphs:

First nontrivial general approximations:
Classical approximation scheme for dense instances

Near-optimal product-state approx for special cases:
Uses semidefinite programming (SDP) for bounds

Approximation w.r.t. number of terms and degree:

[Bansal, Bravyi, Terhal 2007: arXiv 0705.1115]

[Gharibian, Kempe 2011: arXiv 1101.3884]

[Brandao, Harrow 2013: arXiv 1310.0017]

[Harrow, Montanaro 2015: arXiv 1507.00739]

All of these results use product states
Recent approximations for Max 2-Local Hamiltonian

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>Max traceless 2-LH:</td>
<td>Max Ising:</td>
<td>$\Omega(1/\log n)$</td>
<td>$\Omega(1/\log n)$ [Bravyi, Gosset, Koenig, Temme ‘18] 0.184 (bipartite, no 1-local terms) [P, Thompson ‘20]</td>
</tr>
<tr>
<td>$\sum_{ij} H_{ij}$, $H_{ij}$ traceless</td>
<td>$\max -\sum_{ij} z_i z_j$, $z_i \in {-1,1}$</td>
<td>[Charikar, Wirth ‘04]</td>
<td></td>
</tr>
<tr>
<td>Max positive 2-LH:</td>
<td>Max 2-CSP</td>
<td>0.874</td>
<td>0.25 [Random assignment] 0.282 [Hallgren, Lee ‘19] 0.328 [Hallgren, Lee, P ‘20] 0.387 / 0.498 (numerical) [P, Thompson ‘20] 0.5 (best possible via product states) [P, Thompson ‘21]</td>
</tr>
<tr>
<td>$\sum_{ij} H_{ij}$, $H_{ij} \geq 0$</td>
<td></td>
<td>[Lewin, Livnat, Zwick ‘02]</td>
<td></td>
</tr>
<tr>
<td>Quantum Max Cut:</td>
<td>Max Cut:</td>
<td>0.878</td>
<td>0.498 [Gharibian, P ‘19] 0.5 [P, Thompson ‘22] 0.53* [Anshu, Gosset, Morenz ‘20] 0.533* [P, Thompson ‘21] 0.562* [Lee ‘22] (also [King ‘22])</td>
</tr>
<tr>
<td>$\sum_{ij} I_i X_i X_j - Y_i Y_j - Z_i Z_j$ (special case of above)</td>
<td>$\max \sum_{ij} I_i - z_i z_j$, $z_i \in {-1,1}$</td>
<td>[Goemans, Williamson ‘95]</td>
<td></td>
</tr>
<tr>
<td>Max 2-Quantum SAT:</td>
<td>Max 2-SAT</td>
<td>0.940</td>
<td>0.75 [Random Assignment] 0.764 / 0.821 (numerical) [P, Thompson ‘20] 0.833... best possible via product states</td>
</tr>
<tr>
<td>$\sum_{ij} H_{ij}$, $H_{ij} \geq 0$, rank 3</td>
<td></td>
<td>[Lewin, Livnat, Zwick ‘02]</td>
<td></td>
</tr>
</tbody>
</table>


* These results are not product-state based
Quantum Relaxations
Max Cut Semidefinite Programming Relaxation

Max $\sum_{i,j \in E} (1 - m_{ij})/2$

\[
\begin{bmatrix}
1 & m_{12} & m_{13} & \cdots \\
m_{12} & 1 & m_{23} & \cdots \\
m_{13} & m_{23} & 1 & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{bmatrix} \succeq 0
\]

Max $\sum_{i,j \in E} (1 - v_i \cdot v_j)/2$

$\|v_i\| = 1$, for all $i \in V$

($v_i \in \mathbb{R}^n$)

Equivalent perspective: unit vectors $v_i$, with $m_{ij} = v_i \cdot v_j$

Max Cut

Exact solution when $v_i \in \mathbb{R}^1$: -1 $\rightarrow$ +1
Quantum Moment Matrices are Positive

State on $n$ qubits

$\langle \psi \rangle \in \mathbb{C}^2^n$

$V = \begin{bmatrix}
\langle x_1 \rangle = \langle \psi | X_1 \\
\langle y_1 \rangle = \langle \psi | Y_1 \\
\langle z_1 \rangle = \langle \psi | Z_1 \\
\vdots \\
\langle x_n \rangle = \langle \psi | X_n \\
\langle y_n \rangle = \langle \psi | Y_n \\
\langle z_n \rangle = \langle \psi | Z_n 
\end{bmatrix}$,

$M_{ij} = \begin{bmatrix}
\langle \psi | X_i X_j | \psi \rangle & \langle x_i | y_j \rangle & \langle x_i | z_j \rangle \\
\langle y_i | x_j \rangle & \langle y_i | y_j \rangle & \langle y_i | z_j \rangle \\
\langle z_i | x_j \rangle & \langle z_i | y_j \rangle & \langle z_i | z_j \rangle 
\end{bmatrix}$

Entries of this $3n \times 3n$ moment matrix are expectation values of all 2-local Pauli terms

$= V V^\dagger \succeq 0 \implies Re(V V^\dagger) \succeq 0$
Quantum Max Cut SDP Relaxation

\[
\begin{bmatrix}
X_1 & Y_1 & Z_1 & X_2 & Y_2 & Z_2 & X_3 & Y_3 & Z_3 \\
1 & 0 & 0 & & & & & & \\
0 & 1 & 0 & M_{12} & M_{13} & & & & \\
0 & 0 & 1 & & & & & & \\
\end{bmatrix}
\]

\[
\vdots
\]

\[
\begin{bmatrix}
X_1 & Y_1 & Z_1 & X_2 & Y_2 & Z_2 & X_3 & Y_3 & Z_3 \\
1 & 0 & 0 & & & & & & \\
0 & 1 & 0 & M_{12} & M_{13} & & & & \\
0 & 0 & 1 & & & & & & \\
\end{bmatrix}
\]

\[
\vdots
\]

Real part of moment matrix

Quantum Max Cut vector relaxation
\[
\text{Max } \sum_{i \in E} (1 - x_i \cdot x_j - y_i \cdot y_j - z_i \cdot z_j)/4
\]

\[
\|x_i\|, \|y_i\|, \|z_i\| = 1, \text{ for all } i \in V
\]

\[
\newx_i \cdot \newy_i = x_i \cdot z_i = y_i \cdot z_i = 0, \text{ for all } i \in V
\]

\[
(v_i \in \mathbb{R}^{3n})
\]

\[\newv_i = (x_i \oplus y_i \oplus z_i)/\sqrt{3}\]

Max Cut vector relaxation
\[
\text{Max } \sum_{i \in E} (1 - 3v_i \cdot v_j)/4
\]

\[
\|\newv_i\| = 1, \text{ for all } i \in V
\]

\[
(v_i \in \mathbb{R}^n)
\]
Quantum Lasserre Hierarchy

Max $\text{Tr}[H\hat{\rho}]$
$\text{Tr}[\hat{\rho}] = 1$
$\text{Tr}[\hat{\rho} S^+ S] \geq 0, \forall \text{deg}-k S$

$\hat{\rho}$ is called degree-$k$ pseudo density

Classical
[Lasserre 2001]
[Parillo 2003]

Non-commutative/Quantum
Rounding Infeasible Solutions

**α-Approximation Algorithm**

Round optimal non-positive pseudo-density $\tilde{\rho}$ to sub-optimal positive density $\rho$ so that:

$$Tr[H\rho] \geq \alpha Tr[H\tilde{\rho}] \geq \alpha \lambda_{\text{max}}(H)$$

- $\forall \text{deg-1} S$
- $\forall \text{deg-2} S$
- $\forall \text{deg-n} S$

$\tilde{\rho}$ is called degree-$k$ pseudo density
Approximating Quantum Max Cut
0.498-approximation for Quantum Max Cut

Use hyperplane rounding generalization inspired by [Briët, de Oliveira Filho, Vallentin 2010] to round the vectors $x_i, y_i, z_i$ to scalars $\alpha_i, \beta_i, \gamma_i$ to obtain:

$$\rho = \frac{1}{2^n} \prod_i (1 + \alpha_i X_i + \beta_i Y_i + \gamma_i Z_i), \quad \alpha_i^2 + \beta_i^2 + \gamma_i^2 = 1$$

Classical rounding ($\mathbb{R}^n \rightarrow \mathbb{R}^1$)

$$v_i \in \mathbb{R}^n \rightarrow \alpha_i = \frac{r^T v_i}{|r^T v_i|}$$

$$r \sim N(0,1)^n$$

Product-state rounding ($\mathbb{R}^{3n} \rightarrow \mathbb{R}^3$)

$$v_i \in \mathbb{R}^{3n} \rightarrow (\alpha_i, \beta_i, \gamma_i) = \left(\frac{r_x^T v_i}{\|r_x^T v_i\|}, \frac{r_y^T v_i}{\|r_y^T v_i\|}, \frac{r_z^T v_i}{\|r_z^T v_i\|}\right)$$

$$r_x, r_y, r_z \sim N(0,1)^{3n}$$

[Garibian, P. 2019]
# Max Cut vs Quantum Max Cut

## Relaxation

\[
\text{Max} \sum_{ij \in E} \frac{(1 - v_i \cdot v_j)}{2}
\]

\[\|v_i\| = 1, \text{ for all } i \in V \quad (v_i \in \mathbb{R}^n)\]

\[\|v_i\| = 1, \text{ for all } i \in V \quad (v_i \in \mathbb{R}^n)\]

## Rounding

\[v_i \in \mathbb{R}^n \rightarrow \alpha_i = \frac{r^Tv_i}{\|r^Tv_i\|}\]

\[v_i \in \mathbb{R}^{3n} \rightarrow (\alpha_i, \beta_i, \gamma_i) = \left(\frac{r^Tv_i}{\|r^Tv_i\|}, \frac{r^Tv_i}{\|r^Tv_i\|}, \frac{r^Tv_i}{\|r^Tv_i\|}\right)\]

## Approximability

<table>
<thead>
<tr>
<th>Method</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lasserre 1 (optimal under unique games conjecture)</td>
<td>0.878</td>
</tr>
<tr>
<td>Lasserre 1</td>
<td>0.5</td>
</tr>
<tr>
<td>Lasserre 2 (optimal using product states)</td>
<td>0.498</td>
</tr>
<tr>
<td>(0.533 using 1- &amp; 2-qubit ansatz)</td>
<td></td>
</tr>
</tbody>
</table>
Monogamy of Entanglement

Star Bound

\[ \sum_{j=1}^{m} \text{Tr}(\rho h_{0j}) \leq \frac{q + 1}{2} \]

- Lasserre\(_1\) gets \(q\)
- Lasserre\(_2\) gets \((q + 1)/2\)

We generalize monogamy of entanglement bounds to edge energies \(\mu_{ij}\) coming from Lasserre hierarchy.

New nonlinear triangle bound:

**Triangle Bound** Lasserre\(_2\) satisfies:

\[
\begin{align*}
\mu_{01} &= \text{Tr}(\rho h_{01}) \\
\mu_{02} &= \text{Tr}(\rho h_{02}) \\
\mu_{12} &= \text{Tr}(\rho h_{12})
\end{align*}
\]

\[
0 \leq \mu_{01} + \mu_{02} + \mu_{12} \leq \frac{3}{2}
\]

\[
4(\mu_{01}^2 + \mu_{02}^2 + \mu_{12}^2) - 8(\mu_{01}\mu_{02} + \mu_{01}\mu_{12} + \mu_{02}\mu_{12}) \leq 0
\]

\[
\mu_{01} = 1 \Rightarrow \mu_{02} = \frac{1}{4}
\]

- These constraints fully capture the allowed values on a triangle!
Rounding Ansatze

Product State Ansatz

\[ \rho = \prod_i \rho_i \] 

Singlets+Product States

\[ \rho = \prod_i \rho_i \cdot \prod_{jk} \rho_{jk} \]

\[ \rho_{jk} = \frac{1 - X_i X_k - Y_j Y_k - Z_j Z_k}{4} \]

\[ \rho_i = \frac{1 + \alpha_i X_i + \beta_i Y_i + \gamma_i Z_i}{2} \]
Better Rounding Algorithm

- PS rounding algorithm and singlet+PS rounding algorithm follow similar meta-algorithm, with different “building blocks”

\[ \mu_{ij} = \text{Tr}(\tilde{\rho}h_{ij}) \]

- 0 ≤ \( \mu_{ij} \) ≤ 1, if \( \mu_{ij} \approx 1 \) then Lasserre_2 “thinks” that edge should be a singlet.

**Overall idea** - Find the edges Lasserre_2 “thinks” should be a singlet, take care to get good objective value on these edges

**Meta-Algorithm**
1. Solve Lasserre_2 to get submatrix of \( M \)
2. Initialize \( L = \{ \} \)
3. For all \( ij \) calculate \( \mu_{ij} \). If \( \mu_{ij} > \gamma \) add \( ij \) to \( L \).
4. Find Maximum matching \( M \) on \( L \).
5. Consider two states
   1. Take optimal state on \( M \), something standard on the rest
   2. PS rounding from [GP ‘19]
6. Take whichever has better objective.
Rounding Algorithm (cont.)

Block 1
- Star/Triangle bounds say that large edges must be adjacent to small edges ⇒
  set L forms a subgraph of small degree
- Threshold controls degree of subgraph

Why set them differently? Technical reasons
Tradeoff in d:
- d is too small ⇒ product state rounding bad
- d is too large ⇒ matching is bad

Block 2/Block 3

\[ d=1 \text{ for PS rounding} \]
\[ d=2 \text{ for Entangled} \]
To learn more about Quantum Max Cut...

**Optimal product-state approximations:**

- [P., Thompson 2022: arXiv 2206.08342]

**Best-known Quantum Max Cut (QMC) approximations:**

- [P., Thompson 2021: arXiv 2105.05698]
- [Lee 2022: arXiv 2209.00789]
- [King 2022: arXiv 2209.02589]
- [P., Thompson 2021, 2022 above]
- [Hwang, Neeman, P., Thompson, Wright 2021: arXiv 2111.01254]
- [Anshu, Gosset, Morenz-Korol, Soleimanifar: arXiv 2105.01193]
- [Kallaugher, P. 2022: arXiv 2206.00213]

**Lasserre hierarchy in 2-LH approximations:**

- [P., Thompson 2021, 2022 above]

**Prospects for unique-games hardness:**

- [Anshu, Gosset, Morenz-Korol, Soleimanifar: arXiv 2105.01193]

**Connections in approximating QMC and 2-LH:**

- [Anshu, Gosset, Morenz-Korol, Soleimanifar: arXiv 2105.01193]

**Optimal space-bounded QMC approximations:**

- (no quantum advantage possible!)
Thanks for reading this!
Goal: New quantum algorithms and rigorous advantages from the interplay of quantum simulation, optimization, and machine learning

- Quantum simulation
- Machine learning
- Optimization

Quantum approaches for differential equations
Quantum circuit optimization
(Convex and gradient-based) optimization
(Convex/semidefinite relaxations)
Quantum query complexity
(Approximate) extremal energy states of physically-inspired Hamiltonians
ML approaches for understanding and mitigating noise
Quantum approaches for linear algebra

We're looking for interns and postdocs!
Quantum Algorithms for *Ideal Abstract* Quantum Computers

**Models:** based on abstract complexity classes (e.g. BQP)
**Goal:** identification of rigorous asymptotic quantum advantages
**Challenge:** potentially difficult or impossible to physically realize advantages

Quantum Algorithms for *Physically-inspired Abstract* Quantum Computers

**Models:** abstract imbued with physically-inspired features
(e.g. DQC1, using few ancilla, restricted gate sets or topologies)
**Goal:** rigorous quantum advantages under resource restrictions
**Challenge:** models and results should help bridge ideal-physical gap

Quantum Algorithms for *Physical* Quantum Computers

**Models:** implementation on current and future quantum computers
(e.g. “quantum software engineering” on IBM, Google systems)
**Goal:** empirical demonstration of quantum “wins”
**Challenge:** wins may be platform-specific, not sustainable asymptotically, or have no immediate practical applications