Sandia National Laboratories

Approximating quantum constraint satisfaction problems

Presented by

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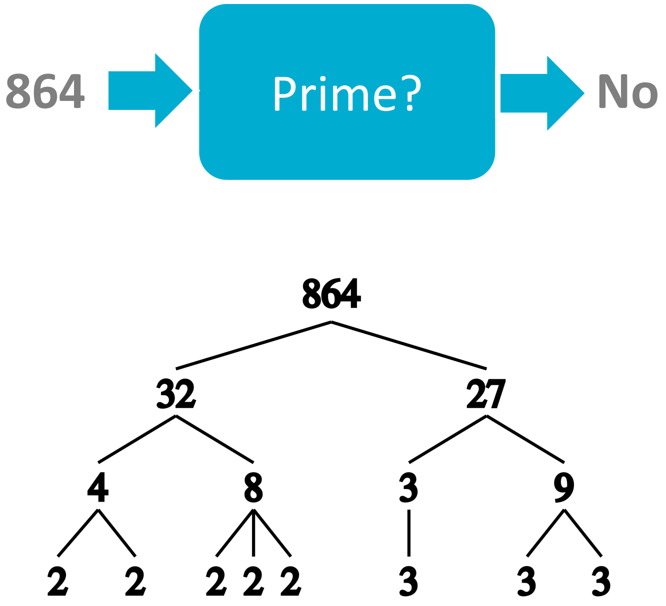
Quantum Advantages

Known quantum speedups are limited for practical applications

	Against *best-known* classical algorithm	Against *best-possible* classical algorithm
Polynomial speedup	e.g. checking if an integer is prime	e.g. Grover's algorithm for unstructured search
Exponential speedup	e.g. Shor's algorithm for integer factorization	?



See https://quantumalgorithmzoo.org for state of quantum speedups

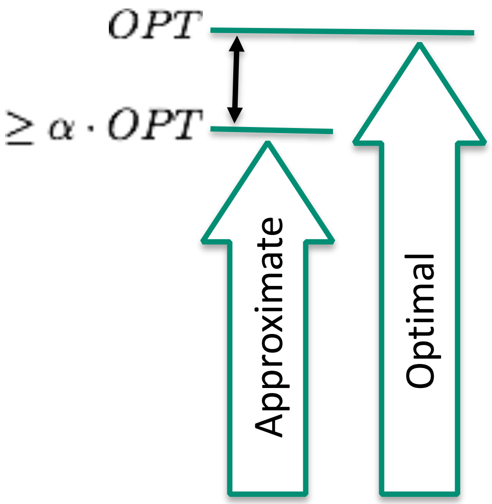
State of Quantum “Speedups”

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

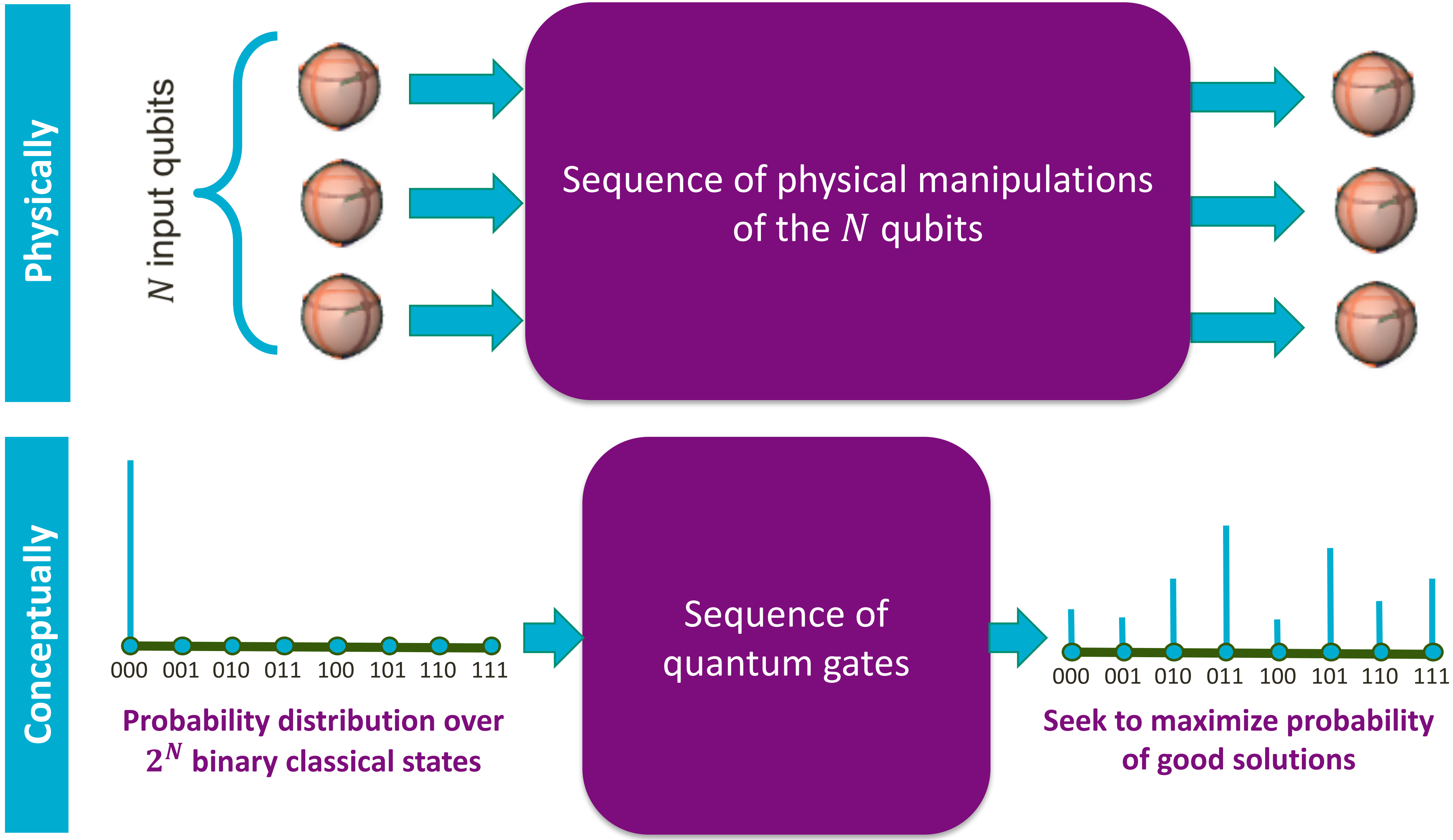
- Provable modest speedup:
  Grover’s quantum search algorithm
  [Grover, *A fast quantum mechanical algorithm for database search*, 1996]

- 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 Algorithms Output Distributions



Quantum Optimization

What is Quantum Optimization?

Algorithm \ Problem	Classical	Quantum
Classical	Classical optimization	Classical approaches for quantum Hamiltonians (e.g. DMRG, mean-field methods)
Quantum	Quantum approaches for classical Hamiltonians (e.g. AQC, QAOA for quantum Hamiltonians) Quantum approaches for continuous optimization	Quantum approaches for quantum Hamiltonians (e.g. AQC, QAOA for quantum Hamiltonians)

It’s Natural to Optimize

Hamiltonian eigenstate problems naturally link quantum mechanics and optimization

$$Min_{\Psi} \left\langle \psi \middle| \sum_{S} H_S \middle| \psi \right\rangle$$

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 ⟷ Min-energy eigenvector

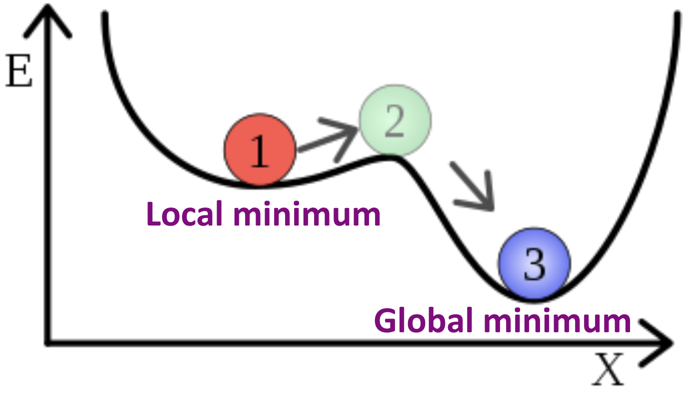


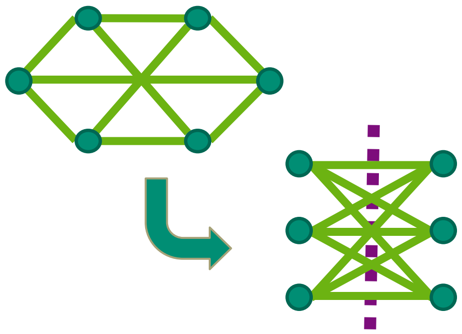
Image from https://en.wikipedia.org/wiki/Metastability

Nature tends towards stable states…

So let nature solve your problems for you?

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



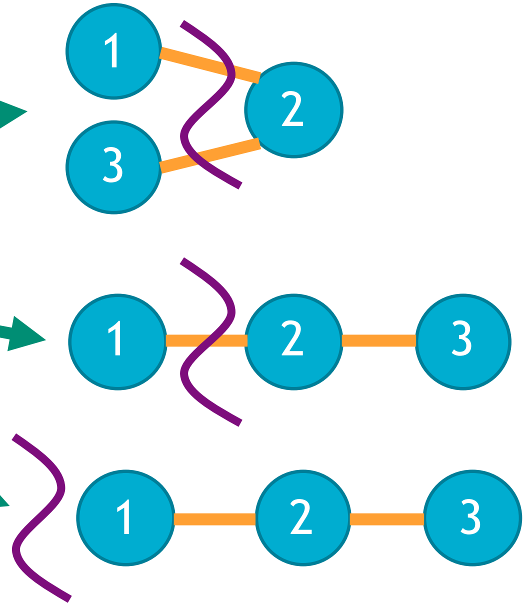
Max Cut

Vertices 1	2	3	State
L,	L,	L	$\equiv \lvert 000\rangle$
L,	L,	R	$\equiv \lvert 001\rangle$
L,	R,	L	$\equiv \lvert 010\rangle$
L,	R,	R	$\equiv \lvert 011\rangle$
R,	L,	L	$\equiv \lvert 100\rangle$
R,	L,	R	$\equiv \lvert 101\rangle$
R,	R,	L	$\equiv \lvert 110\rangle$
R,	R,	R	$\equiv \lvert 111\rangle$

Left or Right side of cut

$$
\begin{array}{c}
|000\rangle \; |001\rangle \; |010\rangle \; |011\rangle \; |100\rangle \; |101\rangle \; |110\rangle \; |111\rangle \\
\begin{bmatrix}
0 & & & & & & & \\
& -1 & & & & & & \\
& & -2 & & & & & \\
& & & -1 & & & & \\
& & & & -1 & & & \\
& & & & & -2 & & \\
& & & & & & -1 & \\
& & & & & & & 0
\end{bmatrix}
\end{array}
$$

Hamiltonian for Max Cut on a path with 3 vertices



Some cuts on a path with 3 vertices

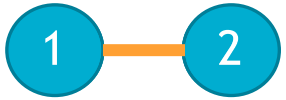
Minimum eigenstate is of form: $|\psi\rangle = \alpha|010\rangle + \beta|101\rangle$, with energy -2

Local Hamiltonians

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

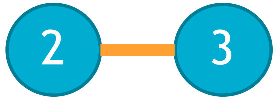
Hamiltonian is exponentially large, $2^N \times 2^N$, for an N-node graph, but it is a sum of $O(N^2)$ local 4×4 Hamiltonians, one for each edge

$$H_{12} = \begin{array}{c} \begin{bmatrix} 0 &&& \\ & -1 && \\ && -1 & \\ &&& 0 \end{bmatrix} \\ |00\rangle \;\; |01\rangle \;\; |10\rangle \;\; |11\rangle \end{array} \otimes I = \begin{array}{cc} \begin{bmatrix} 0 &&&&&&& \\ & 0 &&&&&& \\ && -1 &&&&& \\ &&& -1 &&&& \\ &&&& -1 &&& \\ &&&&& -1 && \\ &&&&&& 0 & \\ &&&&&&& 0 \end{bmatrix} & \begin{array}{c} |000\rangle \\ |001\rangle \\ |010\rangle \\ |011\rangle \\ |100\rangle \\ |101\rangle \\ |110\rangle \\ |111\rangle \end{array} \end{array}$$



$$+$$

$$H_{23} = I \otimes \begin{array}{c} \begin{bmatrix} 0 &&& \\ & -1 && \\ && -1 & \\ &&& 0 \end{bmatrix} \\ |00\rangle \;\; |01\rangle \;\; |10\rangle \;\; |11\rangle \end{array} = \begin{array}{cc} \begin{bmatrix} 0 &&&&&&& \\ & -1 &&&&&& \\ && -1 &&&&& \\ &&& 0 &&&& \\ &&&& 0 &&& \\ &&&&& -1 && \\ &&&&&& -1 & \\ &&&&&&& 0 \end{bmatrix} & \begin{array}{c} |000\rangle \\ |001\rangle \\ |010\rangle \\ |011\rangle \\ |100\rangle \\ |101\rangle \\ |110\rangle \\ |111\rangle \end{array} \end{array}$$



Local Hamiltonians are efficient and require manipulating only a constant number of qubits

The Power of Quantum Computing?

Extended Church-Turing Thesis

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

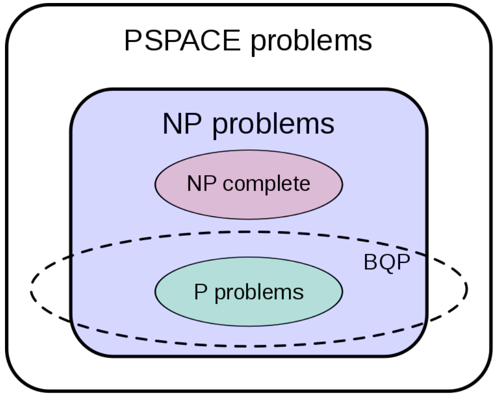


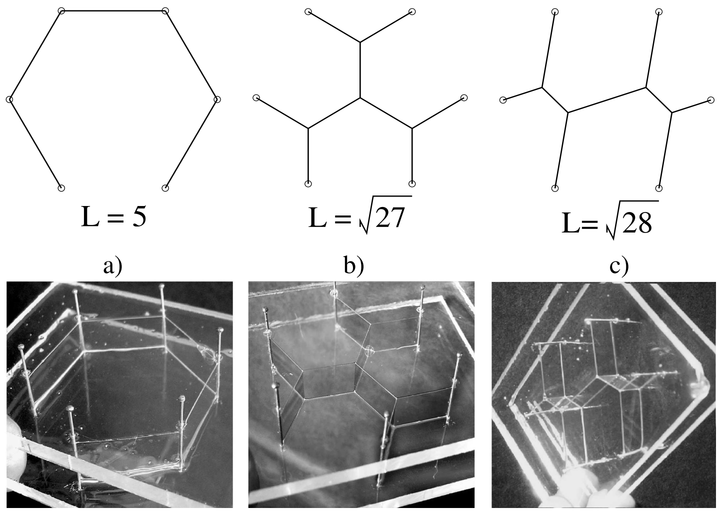
Image from https://en.wikipedia.org/wiki/BQP

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.



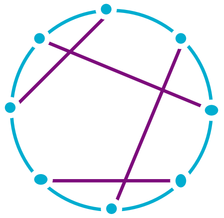
Using soap film to find Steiner Trees

[Datta, Khastgir, & Roy; arXiv 0806.1340]

*Quantum supremacy: [Preskill; arXiv 1801.00862], [Harrow & Montanaro; arXiv 1809.07442], [Aaronson & Chen; arXiv 1612.05903]

Quantum Approximation Algorithms

(Quantum) Approximation Algorithms

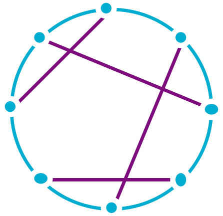


$H = \sum H_{ij}$ → Approximation Algorithm → (description of) state ρ

A α-approximation algorithm runs in polynomial time, and for any instance *I*, delivers an approximate solution such that:

$$\frac{Value(Approximate_I)}{Value(Optimal_I)} \geq \alpha$$

(Quantum) Approximation Algorithms



$H = \sum H_{ij}$ → Approximation Algorithm → (description of) state ρ

A α-approximation algorithm runs in polynomial time, and for any instance *I*, delivers an approximate solution such that:

$$\frac{Value(Approximate_I)}{Value(Optimal_I)} \geq \alpha$$

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

Polynomials and Quantum Solutions

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

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

$Z_1 Z_3 = Z \otimes I \otimes Z \otimes I \ldots$ (constraint only on variables/qubits 1 and 3)

Classical

Polynomial $\mathrm{P}(I, Z_1, \ldots, Z_n)$:
(Multilinear since $Z_i^2 = I$)
Represents a **diagonal** $M \in \mathbb{R}^{2^n \times 2^n}$

Classical solution: M is **PSD** & trace=1
Convex combination of solutions

$$\begin{array}{r} x_1, x_2 = 0,0 \\ x_1, x_2 = 0,1 \\ x_1, x_2 = 1,0 \\ x_1, x_2 = 1,1 \end{array} \begin{bmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 \end{bmatrix}$$

$$P = \frac{1}{4}(I - \frac{1}{2} Z_2 + \frac{1}{2} Z_1 Z_2)$$

Quantum

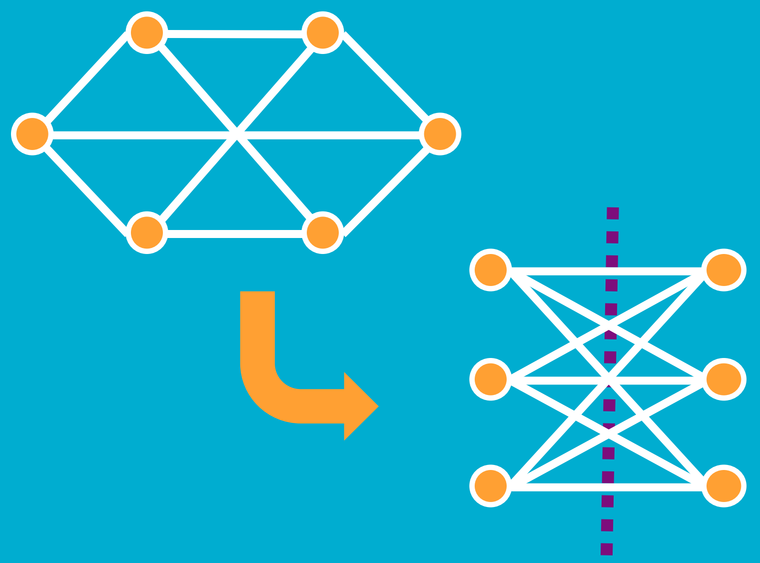
Polynomial $\mathrm{Q}(I, X_1, Y_1, Z_1, \ldots, X_n, Y_n, Z_n)$:
(Multilinear since $X_i^2 = Y_i^2 = Z_i^2 = I$)
Represents a **Hermitian** $M \in \mathbb{C}^{2^n \times 2^n}$

Quantum solution: M is **PSD** & trace=1
Convex combination of pure states

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

$$Q = \frac{1}{4}(I - X_1 X_2 - Y_1 Y_2 - Z_1 Z_2)$$

Max Cut



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

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

$$(x_1 \oplus x_2), (x_1 \oplus x_4), (x_1 \oplus x_6), (x_2 \oplus x_3), \ldots$$

Model NP-hard discrete optimization problem and 2-CSP

Has driven developments in approximation algorithms

0.878…-approximation
[Goemans and Williamson, 1995]

0.878…+ε 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]

Quantum Max Cut: Motivation

Max Cut Hamiltonian:
$\sum(I - Z_i Z_j)/2$

Quantum Max Cut generalization:
$\sum(I - X_i X_j - Y_i Y_j - Z_i Z_j)/4$

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.

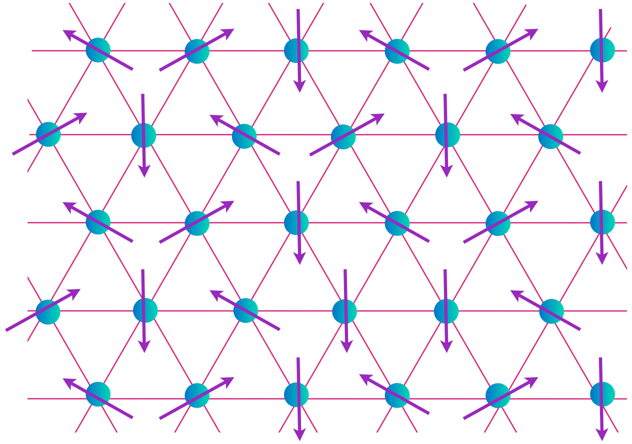
Problem

Find max-energy value/state of Quantum Max Cut: $\sum(I - X_i X_j - Y_i Y_j - Z_i Z_j)/4$

(≡ Find min-energy state of quantum Heisenberg model:

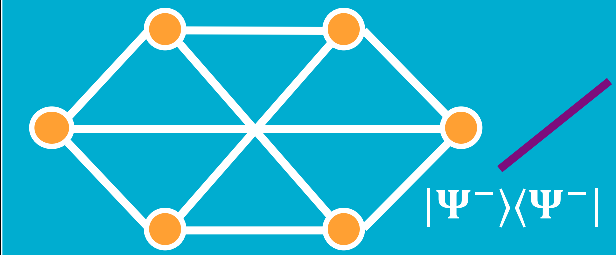
$$\sum(X_i X_j + Y_i Y_j + Z_i Z_j)/4,$$

but different from approximation point of view)



Anti-ferromagnetic Heisenberg model: roughly neighboring quantum particles aim to align in opposite directions. This kind of Hamiltonian appears, for example, as an effective Hamiltonian for so-called Mott insulators.
[Image: Sachdev, arXiv:1203.4565]

Quantum Max Cut



maximize overlap with singlet on each edge

Instance of 2-Local Hamiltonian

Find max eigenvalue of $H = \sum H_{ij}$,

$$H_{ij} = \left(I - X_i X_j - Y_i Y_j - Z_i Z_j\right)/4$$

Each term is singlet projector:

$H_{ij} = |\Psi^-\rangle\langle\Psi^-|$

$|\Psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$

Model 2-Local Hamiltonian?

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, P. 2019], [Anshu, Gosset, Morenz-Korol 2020], [P., Thompson 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 2020, 2022]

Max Cut and Quantum Max Cut

Classical Max Cut

2-variable constraint: $x_i \oplus x_j$

$$\begin{array}{c} \\ x_i, x_j = 0,0 \\ x_i, x_j = 0,1 \\ x_i, x_j = 1,0 \\ x_i, x_j = 1,1 \end{array} \begin{array}{c} \begin{array}{cccc} 0,0 & 0,1 & 1,0 & 1,1 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

Diagonal matrix

diagonal encodes Boolean function:

$$f(z_i, z_j) = 1/2(1 - z_i z_j)$$

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

Maximum eigenvectors:

$(\mathbf{0}, \mathbf{1}, \mathbf{0}, \mathbf{0}) = |\mathbf{01}\rangle$,

$(\mathbf{0}, \mathbf{0}, \mathbf{1}, \mathbf{0}) = |\mathbf{10}\rangle$

with (eigen)value 1

quantum generalization $\Rightarrow$

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:

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

with (eigen)value 1

"anti-aligned" superposition of optimal Max Cut bases

Maximum product state: e.g., $|01\rangle$

with energy 1/2

Quantum Generalization of Constraint Satisfaction (CSP)

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

$$\begin{array}{c} \\ x_i, x_j = 0,0 \\ x_i, x_j = 0,1 \\ x_i, x_j = 1,0 \\ x_i, x_j = 1,1 \end{array} \begin{array}{c} \begin{array}{cccc} 0,0 & 0,1 & 1,0 & 1,1 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

Diagonal rank-1 projector

quantum generalization

Quantum 2-CSP clause

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

General rank-1 projector

Random assignment "earns" 1/4 of diagonal = *k*/4 for rank-*k* projectors

(Product-State) Approximations for Max 2-Local Hamiltonian

QMA-hard 2-LH problem class	NP-hard specialization	P approximation for NP-hard specialization	Product-state approximation for QMA-hard 2-LH problem
Max traceless 2-LH: $\sum_{ij} H_{ij}$, H_{ij} traceless	**Max Ising:** Max $-\sum_{ij} z_i z_j$, $z_i \in \{-1,1\}$	$\Omega(1/\log n)$ [Charikar, Wirth '04]	$\Omega(1/\log n)$ [Bravyi, Gosset, Koenig, Temme '18] 0.184 (bipartite, no 1-local terms) [P, Thompson '20]
Max positive 2-LH: $\sum_{ij} H_{ij}$, $H_{ij} \succcurlyeq 0$	**Max 2-CSP**	0.874 [Lewin, Livnat, Zwick '02]	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 '22]**
Quantum Max Cut: $\sum_{ij} I - X_iX_j - Y_iY_j - Z_iZ_j$ (special case of above)	**Max Cut:** Max $\sum_{ij} I - z_i z_j$, $z_i \in \{-1,1\}$	0.878 [Goemans, Williamson '95]	0.498 [Gharibian, P '19] **0.5 [P, Thompson '22]** 0.53 [Anshu, Gosset, Morenz '20] 0.533 [P, Thompson '21]
Max 2-Quantum SAT: $\sum_{ij} H_{ij}$, $H_{ij} \succcurlyeq 0$, rank 3	**Max 2-SAT**	0.940 [Lewin, Livnat, Zwick '02]	0.75 [Random Assignment] 0.764 / 0.821 (numerical) [P, Thompson '20] **0.833… best possible via product states**

Quantum Relaxations

Max Cut Semidefinite Programming Relaxation

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

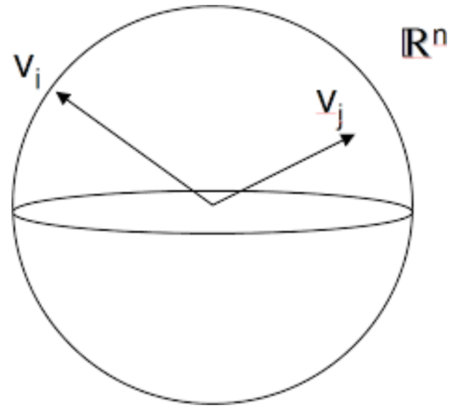
$$\begin{bmatrix} 1 & m_{12} & m_{13} & \cdots \\ m_{12} & 1 & m_{23} & \\ m_{13} & m_{23} & 1 & \\ \vdots & & & \ddots \end{bmatrix} \succcurlyeq 0$$

$\equiv$

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

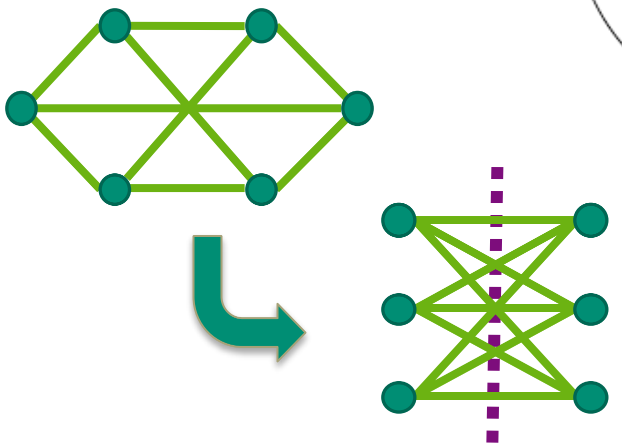
$\|v_i\| = 1$, for all $i \in V$

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



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 ⟵ • ⟶ +1

Quantum Moment Matrices are Positive

State on n qubits

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

$$V = \begin{bmatrix} \langle x_1| = \langle\psi|X_1 \\ \langle y_1| = \langle\psi|Y_1 \\ \langle z_1| = \langle\psi|Z_1 \\ \vdots \\ \langle x_n| = \langle\psi|X_n \\ \langle y_n| = \langle\psi|Y_n \\ \langle z_n| = \langle\psi|Z_n \end{bmatrix}, \quad M_{ij} = \begin{bmatrix} \langle\psi|X_iX_j|\psi\rangle & \langle x_i|y_j\rangle & \langle x_i|z_j\rangle \\ \langle y_i|x_j\rangle & \langle y_i|y_j\rangle & \langle y_i|z_j\rangle \\ \langle z_i|x_j\rangle & \langle z_i|y_j\rangle & \langle z_i|z_j\rangle \end{bmatrix}$$

$$\begin{array}{cc} & \begin{matrix} X_1 & Y_1 & Z_1 & X_2 & Y_2 & Z_2 & X_3 & Y_3 & Z_3 \end{matrix} \\ \begin{matrix} X_1 \\ Y_1 \\ Z_1 \\ X_2 \\ Y_2 \\ Z_2 \\ X_3 \\ Y_3 \\ Z_3 \end{matrix} & \begin{bmatrix} M_{11} & M_{12} & M_{13} & \cdots \\ M_{12}^\dagger & M_{22} & M_{23} & \\ M_{13}^\dagger & M_{23}^\dagger & M_{33} & \\ \vdots & & & \ddots \end{bmatrix} \end{array} = VV^\dagger \succcurlyeq 0 \Longrightarrow Re\left(VV^\dagger\right) \succcurlyeq 0$$

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

Quantum Max Cut SDP Relaxation

$$\begin{array}{cc} & \begin{array}{ccccccccc} X_1 & Y_1 & Z_1 & X_2 & Y_2 & Z_2 & X_3 & Y_3 & Z_3 \end{array} \\ \begin{array}{c} X_1 \\ Y_1 \\ Z_1 \\ X_2 \\ Y_2 \\ Z_2 \\ X_3 \\ Y_3 \\ Z_3 \\ \end{array} & \begin{bmatrix} 1 & 0 & 0 & & & & & & & \cdots \\ 0 & 1 & 0 & & M_{12} & & & M_{13} & & \\ 0 & 0 & 1 & & & & & & & \\ & & & 1 & 0 & 0 & & & & \\ & M_{12}^T & & 0 & 1 & 0 & & M_{23} & & \\ & & & 0 & 0 & 1 & & & & \\ & & & & & & 1 & 0 & 0 & \\ & M_{13}^T & & & M_{23}^T & & 0 & 1 & 0 & \\ & & & & & & 0 & 0 & 1 & \\ \vdots & & & & & & & & & \ddots \end{bmatrix} \end{array} \succcurlyeq 0$$

$$M_{ij} = \begin{bmatrix} x_i \cdot x_j & x_i \cdot y_j & x_i \cdot z_j \\ y_i \cdot x_j & y_i \cdot y_j & y_i \cdot z_j \\ z_i \cdot x_j & z_i \cdot y_j & z_i \cdot z_j \end{bmatrix}$$

Real part of moment matrix

Quantum Max Cut vector relaxation

Max $\sum_{ij \in E}(1 - x_i \cdot x_j - y_i \cdot y_j - z_i \cdot z_j)/4$

$\|x_i\|, \|y_i\|, \|z_i\| = 1$, for all $i \in V$
$x_i \cdot y_i = x_i \cdot z_i = y_i \cdot z_i = 0$, for all $i \in V$
$(v_i \in \mathbb{R}^{3n})$

$v_i = (x_i \oplus y_i \oplus z_i)/\sqrt{3}$

$x_i = v_i \oplus 0 \oplus 0$
$y_i = 0 \oplus v_i \oplus 0$
$z_i = 0 \oplus 0 \oplus v_i$

$$\text{Max} \sum_{ij \in E} (1 - 3 v_i \cdot v_j)/4$$

$\|v_i\| = 1$, for all $i \in V$
$(v_i \in \mathbb{R}^n)$

Max Cut vector relaxation

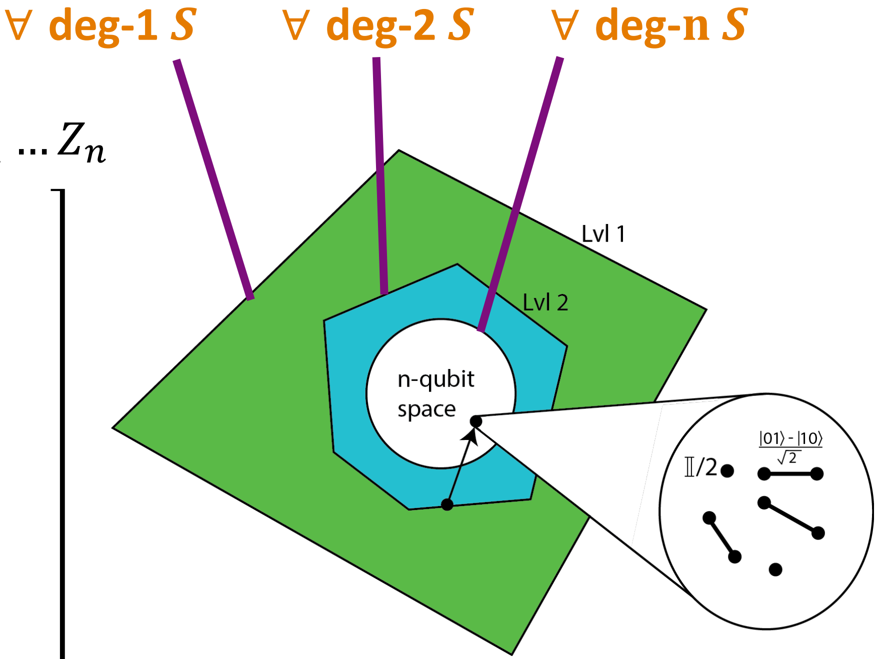
Max $\sum_{ij \in E}(1 - v_i \cdot v_j)$

$\|v_i\| = 1$, for all $i \in V$
$(v_i \in \mathbb{R}^n)$

Quantum Lasserre Hierachy

$Lasserre_1$ $\quad$ $Lasserre_2$

$$
\begin{array}{c|cccccccccccc}
 & I & X_1 & Y_1 & Z_1 & X_2 & \dots & Z_n & X_1X_2 & \dots & Z_{n-1}Z_n & X_1X_2X_3 & \dots & Z_1\dots Z_n \\
\hline
I & 1 & & & & & & & & & & & & \\
X_1 & & 1 & & & & & & & & & & & \\
Y_1 & & & 1 & & & & & & & & & & \\
Z_1 & & & & 1 & & & & & & & & & \\
X_2 & & & & & 1 & & & & & & & & \\
\vdots & & & & & & \ddots & & & & & & & \\
Z_n & & & & & & & 1 & & & & & & \\
X_1X_2 & & & & & & & & 1 & & & & & \\
\vdots & & & & & & & & & \ddots & & & & \\
Z_{n-1}Z_n & & & & & & & & & & 1 & & & \\
X_1X_2X_3 & & & & & & & & & & & 1 & & \\
\vdots & & & & & & & & & & & & \ddots & \\
Z_1Z_2\dots Z_n & & & & & & & & & & & & & 1
\end{array}
$$



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

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

Classical
[Lasserre 2001]
[Parillo 2003]

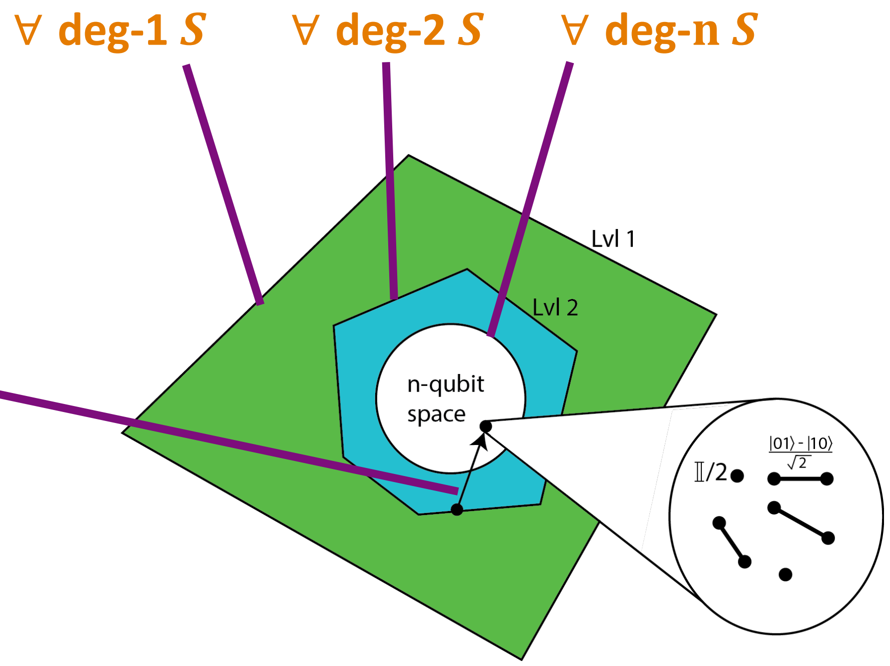
Non-commutative/Quantum
[Navascués, Pironio, Acìn 2009 (2010 SIAM J Opt)]

Rounding Infeasible Solutions

α-Approximation Algorithm

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

$$Tr[H\rho] \geq \alpha\, Tr[H\widetilde{\rho}] \geq \alpha\, \lambda_{max}(H)$$



$$Max\ Tr[H\widetilde{\rho}]$$
$$Tr[\widetilde{\rho}] = 1$$
$$Tr\left[\widetilde{\rho}\, S^{\dagger}S\right] \geq 0, \forall \text{ deg-}k\ S$$

$\widetilde{\rho}$ 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:

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

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

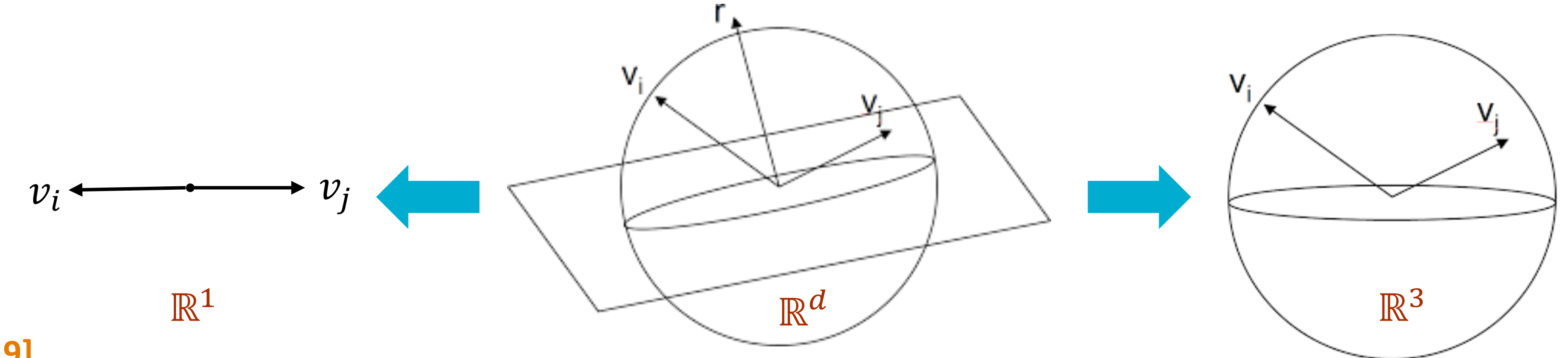
$$v_i \in \mathbb{R}^n \longrightarrow \alpha_i = \frac{r^T v_i}{|r^T v_i|}$$

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

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

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

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



[Garibian, P. 2019]

Max Cut vs Quantum Max Cut

Relaxation (upper bound)

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

$\|v_i\| = 1$, for all $i \in V$
($v_i \in \mathbb{R}^n$)

Max $\sum_{ij\in E}(1 - 3v_i \cdot v_j)/4$

$\|v_i\| = 1$, for all $i \in V$
($v_i \in \mathbb{R}^n$)

Rounding

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

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

Approximability

0.878 Lasserre 1
(optimal under unique games conjecture)

0.498 Lasserre 1
0.5 Lasserre 2 (optimal using product states)
(0.533 using 1- & 2-qubit ansatz)

Approximating General 2-Local Hamiltonian

Objective: $\sum_{ij} c_{ij}\, Tr\Big(\underbrace{\begin{bmatrix} 1 & b_{ij,j}^T \\ b_{ij,i} & A_{ij} \end{bmatrix}}_{A} \begin{bmatrix} 1 & v_0 \cdot x_j & v_0 \cdot y_j & v_0 \cdot z_j \\ v_0 \cdot x_i & x_i \cdot x_j & x_i \cdot y_j & x_i \cdot z_j \\ v_0 \cdot y_i & y_i \cdot x_j & y_i \cdot y_j & y_i \cdot z_j \\ v_0 \cdot z_i & z_i \cdot x_j & z_i \cdot y_j & z_i \cdot z_j \end{bmatrix}\Big),$

where v_0 and x_i, y_i, z_i are unit vectors from relaxation
(involves 15 + 15 parameters!)

Rounding goal:

$v_0 \longrightarrow 1$
$x_i \longrightarrow \alpha_i \in \mathbb{R}$
$y_i \longrightarrow \beta_i \in \mathbb{R}$
$z_i \longrightarrow \gamma_i \in \mathbb{R}$
with $\alpha_i^2 + \beta_i^2 + \gamma_i^2 = 1$

Monogamy of Entanglement

Star Bound

[Lieb, Mattis, '62]
[Anshu, Gosset, Morenz, '20]

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

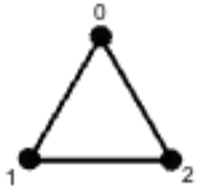
Monogamy of Entanglement

- $Lasserre_1$ gets q
- $Lasserre_2$ gets $(q+1)/2$

We generalize monogamy of entanglement bounds to edge energies μ_{ij} coming from Lasserre hierarchy

New nonlinear triangle bound:

Triangle Bound $\mathrm{Lasserre}_2$ satisfies:



$$\mu_{01} = \mathrm{Tr}(\tilde{\rho} h_{01})$$
$$\mu_{02} = \mathrm{Tr}(\tilde{\rho} h_{02})$$
$$\mu_{12} = \mathrm{Tr}(\tilde{\rho} h_{12})$$

$$\boxed{\begin{aligned} 0 \leq \mu_{01} + \mu_{02} + \mu_{12} \leq 3/2 \\ 4(\mu_{01}^2 + \mu_{02}^2 + \mu_{12}^2) - 8(\mu_{01}\mu_{02} + \mu_{01}\mu_{12} \\ + \mu_{02}\mu_{12}) \leq 0 \end{aligned}}$$

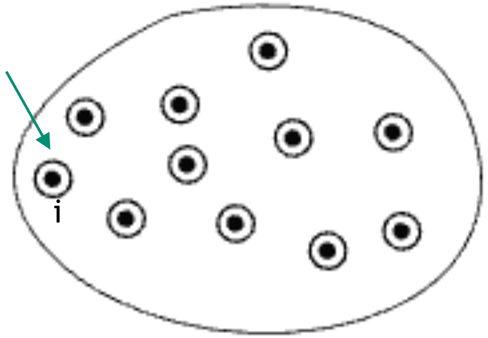
$$\mu_{01} = 1 \Rightarrow \mu_{02} = 1/4$$

- We think these constraints are fully capturing the allowed values on a triangle!

Rounding Ansatze

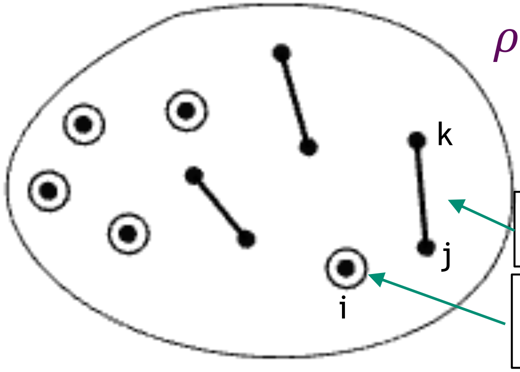
Product State Ansatz

$$\rho = \prod_i \rho_i$$



Singlets+Product States

$$\rho = \prod_i \rho_i \cdot \prod_{jk} \rho_{jk}$$



$$\rho_{jk} = \frac{I - X_j X_k - Y_j Y_k - Z_j Z_k}{4}$$

$$\rho_i = \frac{I + \alpha_i X_i + \beta_i Y_i + \gamma_i Z_i}{2}$$

Why Product States?

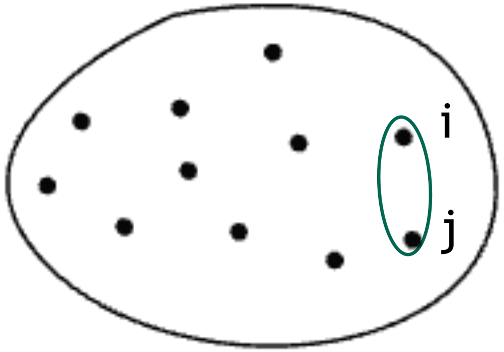
All present approximations for Quantum Max Cut involved product states in an essential way. Why?

As degree or density of graph grows, product states are optimal [Brandão, Harrow 2013]

We show on 3-regular unweighted graphs, product-state approximation is > 0.547 > 0.533, best-known entangled approx

Better Rounding Algorithm

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



$$\mu_{ij} = \mathrm{Tr}(\tilde{\rho} h_{ij})$$

$0 \leq \mu_{ij} \leq 1$, 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 μ_{ij}. If $\mu_{ij} > \boxed{\gamma}$ 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.

Block 1

Threshold

Block 2

Handling large edges

Block 3

Handling qubits outside M

Rounding Algorithm (cont.)

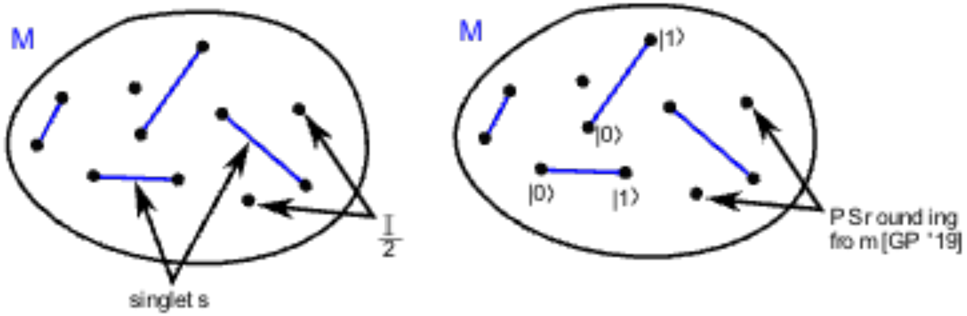
Block 1

- 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

d=1 for PS rounding
d=2 for Entangled

  - 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



To learn more about…

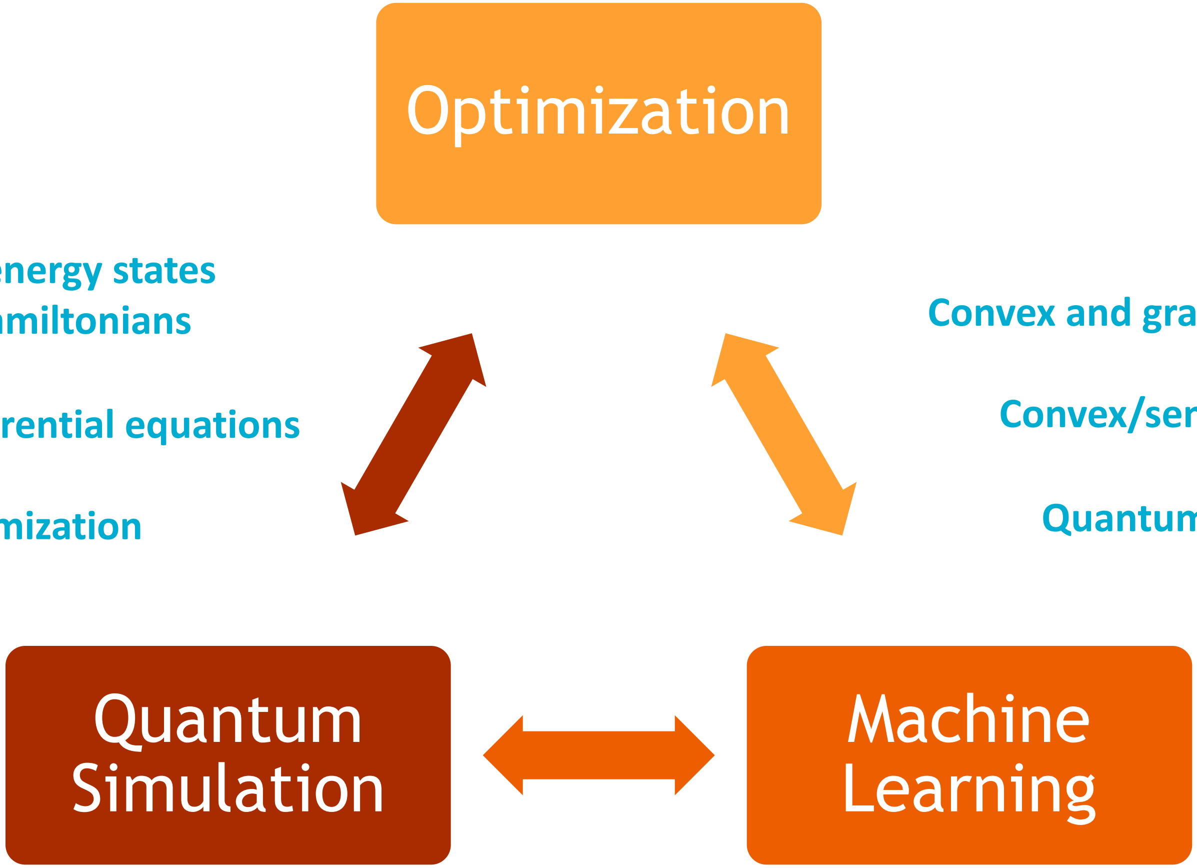
Optimal product-state approximations:	[P., Thompson 2022: arXiv 2206.08342]
Best-known Quantum Max Cut (QMC) approximations:	[Anshu, Gosset, Morenz-Korol 2020: arXiv 2003.14394] [P., Thompson 2021: arXiv 2105.05698]
Lasserre hierarchy in 2-LH approximations:	[P., Thompson 2021, 2022 above]
Prospects for unique-games hardness:	[Hwang, Neeman, P., Thompson, Wright 2021: arXiv 2111.01254]
Connections in approximating QMC and 2-LH:	[P., Thompson 2022 above, 2020: arXiv 2012.12347] [Anshu, Gosset, Morenz-Korol, Soleimanifar: arXiv 2105.01193]
Optimal space-bounded QMC approximations: (no quantum advantage possible!)	[Kallaugher, P. 2022: arXiv 2206.00213]

Thanks for showing up, staying awake, not throwing stuff, etc.!

FAR-QC

Fundamental Algorithmic Research for Quantum Computing

Goal: New quantum algorithms and rigorous advantages from the interplay of quantum simulation, optimization, and machine learning



(Approximate) extremal energy states of physically-inspired Hamiltonians

Quantum approaches for differential equations

Quantum circuit optimization

Convex and gradient-based optimization

Convex/semidefinite relaxations

Quantum query complexity

Quantum sampling complexity

ML approaches for understanding and mitigating noise

Quantum approaches for linear algebra