Approximation and Hardness of Quantum Max Cut

Presented by

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including work with: Sevag Gharibian (U Paderborn), Yeongwoo Hwang (Harvard), John Kallaugher (Sandia), Joe Neeman (UT Austin), John Wright (UC Berkeley)

Trends in Computational Discrete Optimization
April, 2023

Synergies between OR and Quantum Information Science (QIS)

INFORMS Challenge Paper:
Survey article and suggestions to engage QIS for operations researchers

Synergies Between Operations Research and Quantum Information Science
P., 2023
https://doi.org/10.1287/ijoc.2023.1268 (open access)

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

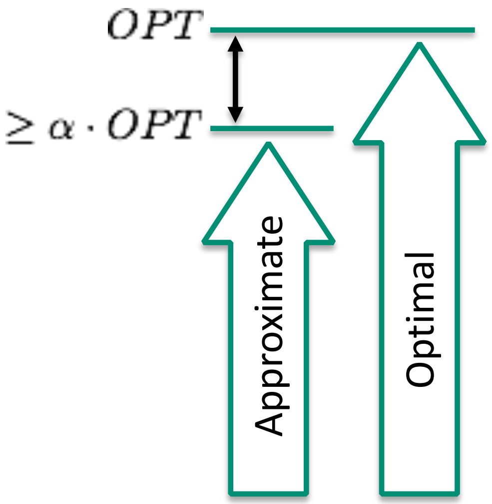
Quantum Computing

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
  [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 Bits Live in a Sphere

Representation

State space

Classical bit:
(bit)

1 = Head

OR

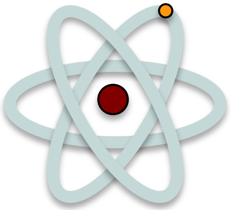
0 = Tail

{0, 1}

Prob. bit:
(p-bit)

0 with probability $1-p$
1 with probability p

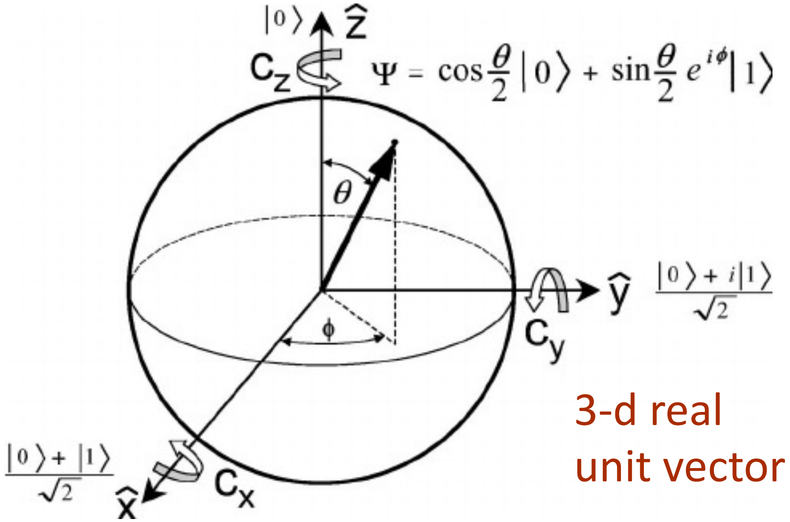
Quantum bit:
(qubit)



$\begin{pmatrix}1\\0\end{pmatrix}$ 2-d complex unit vector $\begin{pmatrix}0\\1\end{pmatrix}$

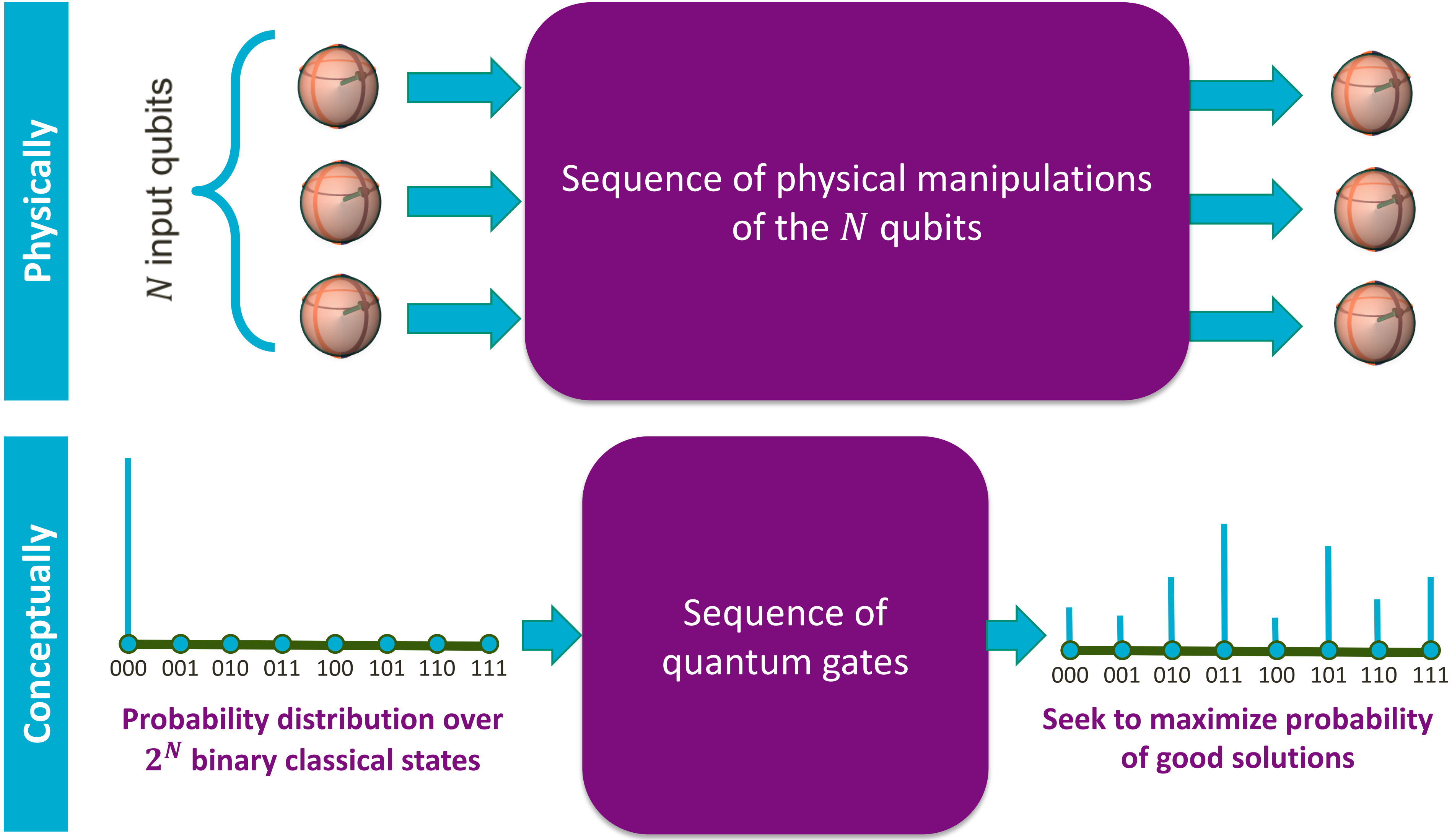
$\alpha|0\rangle + \beta|1\rangle$

0 with probability $|\alpha|^2$
1 with probability $|\beta|^2$



3-d real
unit vector

Quantum Algorithms Output Distributions



Sequence of physical manipulations of the N qubits

Sequence of quantum gates

Probability distribution over 2^N binary classical states

Seek to maximize probability of good solutions

Quantum Optimization

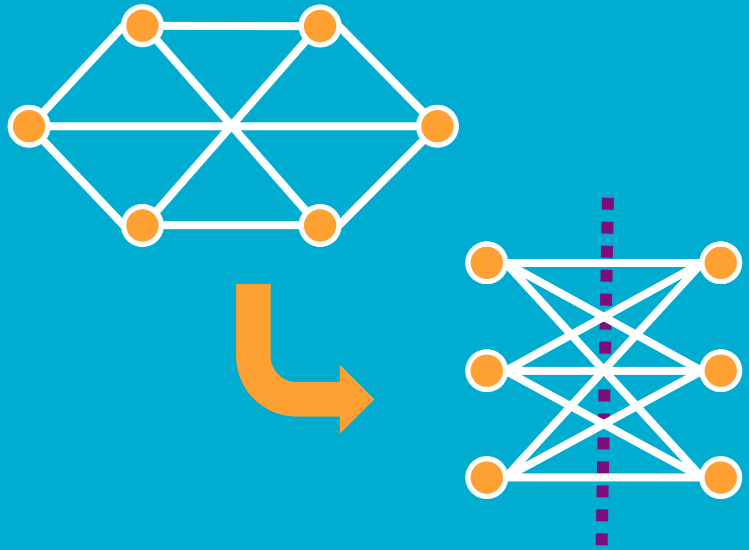
What is Quantum Optimization?

Algorithm

	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)

Problem

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]

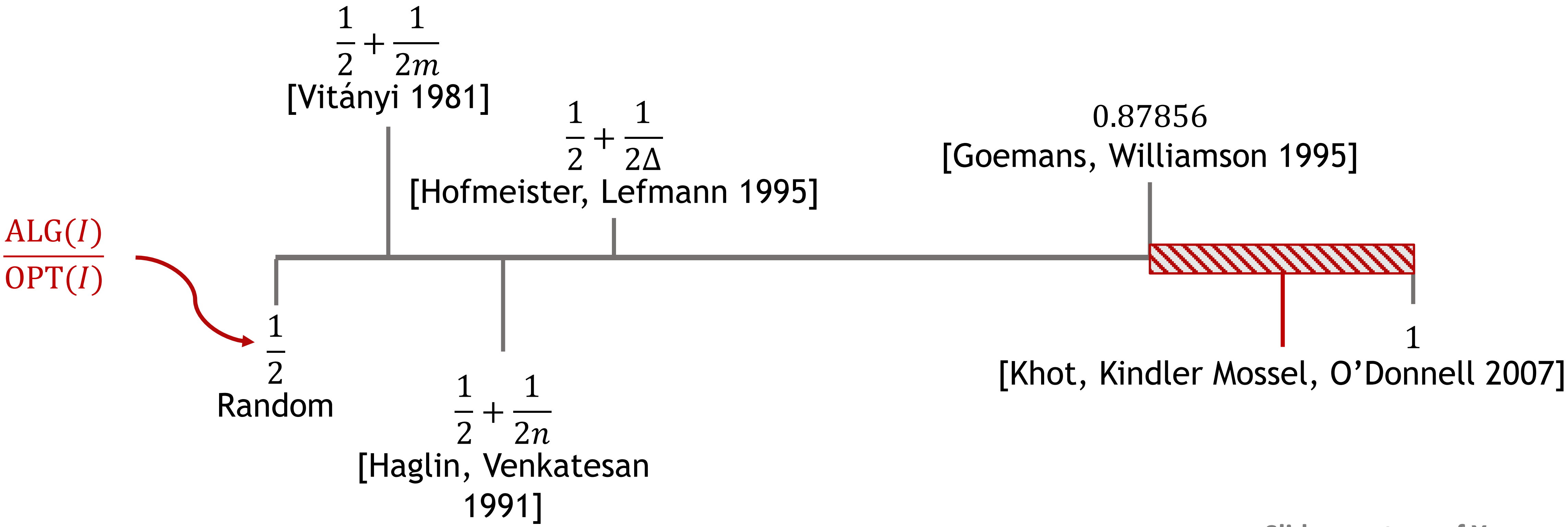
Cut and related polytopes have advanced discrete optimization
e.g., [Fiorini, Massar, Pokutta, Tiwary, de Wolf, 2012]

Algorithms for Max-Cut

Approximation algorithms

How far can we go?

$0.87856 + \epsilon$ approximations are **NP-Hard!** (under Unique Games Conjecture)



$\frac{\mathrm{ALG}(I)}{\mathrm{OPT}(I)}$

$\frac{1}{2}$
Random

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

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

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

0.87856
[Goemans, Williamson 1995]

[Khot, Kindler Mossel, O'Donnell 2007]

1

Slide courtesy of Yeongwoo Hwang

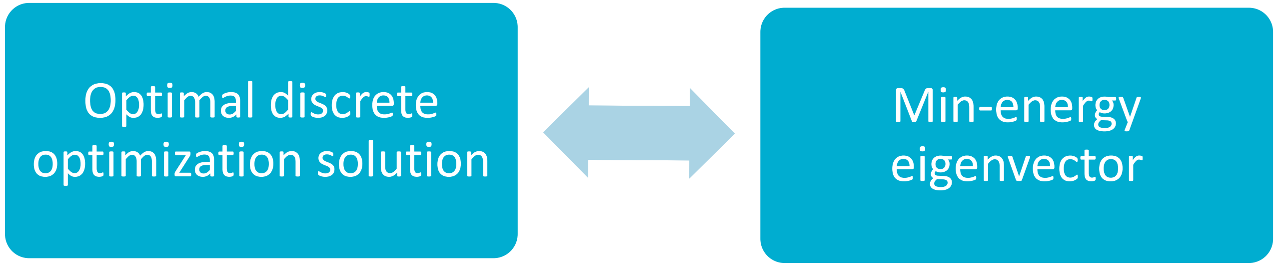
It’s Natural to Optimize

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

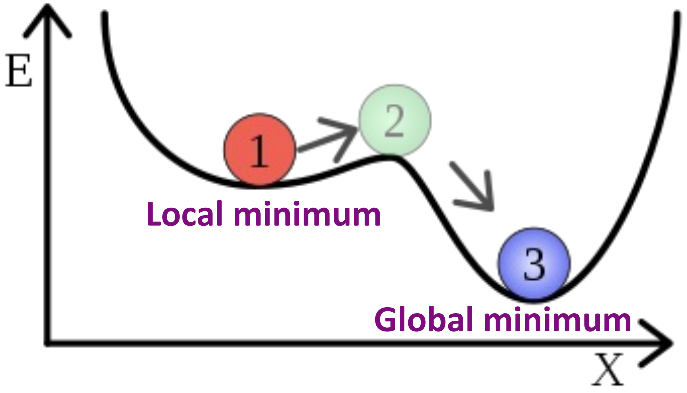


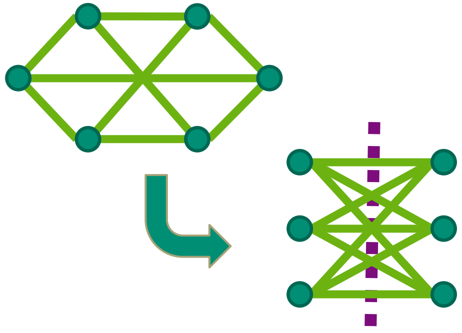
Image from https://en.wikipedia.org/wiki/Metastability

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



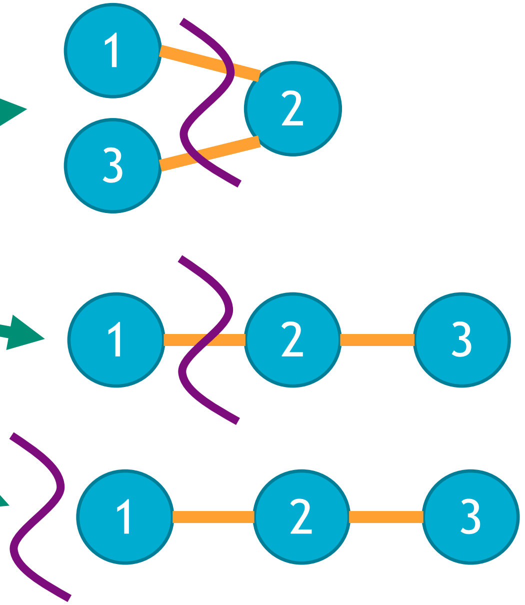
Max Cut

Vertices			
1	**2**	**3**	**State**
L,	L,	L	≡ $|000\rangle$
L,	L,	R	≡ $|001\rangle$
L,	R,	L	≡ $|010\rangle$
L,	R,	R	≡ $|011\rangle$
R,	L,	L	≡ $|100\rangle$
R,	L,	R	≡ $|101\rangle$
R,	R,	L	≡ $|110\rangle$
R,	R,	R	≡ $|111\rangle$

Left or **R**ight side of cut

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

Hamiltonian for Max Cut on a path with 3 vertices



Some cuts on a path with 3 vertices

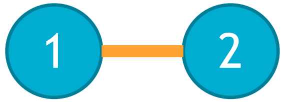
Minimum eigenstate is of form: $|\psi\rangle = \alpha|010\rangle + \beta|101\rangle$, with energy -2

Computational Complexity Considerations

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

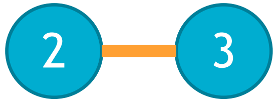
Hamiltonian is exponentially large, $2^N \times 2^N$, for an N-node graph, but it is a sum of $O(N^2)$ local 4×4 Hamiltonians, one for each edge

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



$$+$$

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



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

The Power of Quantum Computing?

Extended Quantum Church-Turing Thesis

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

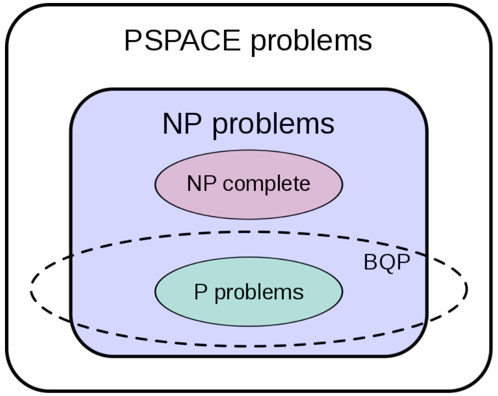


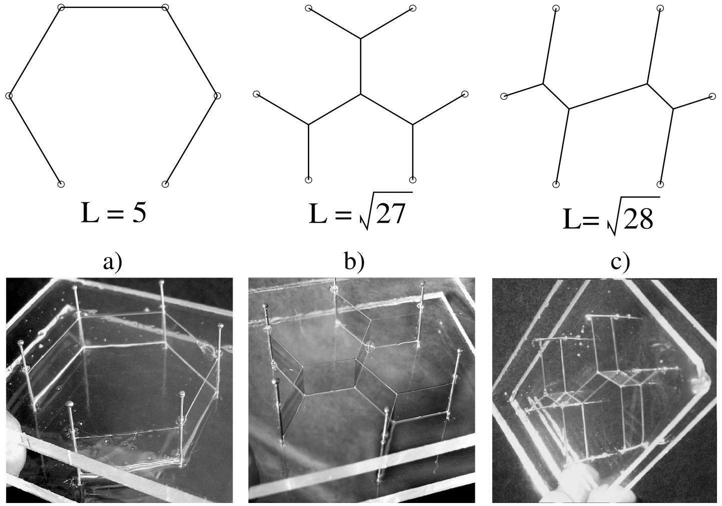
Image from https://en.wikipedia.org/wiki/BQP

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]

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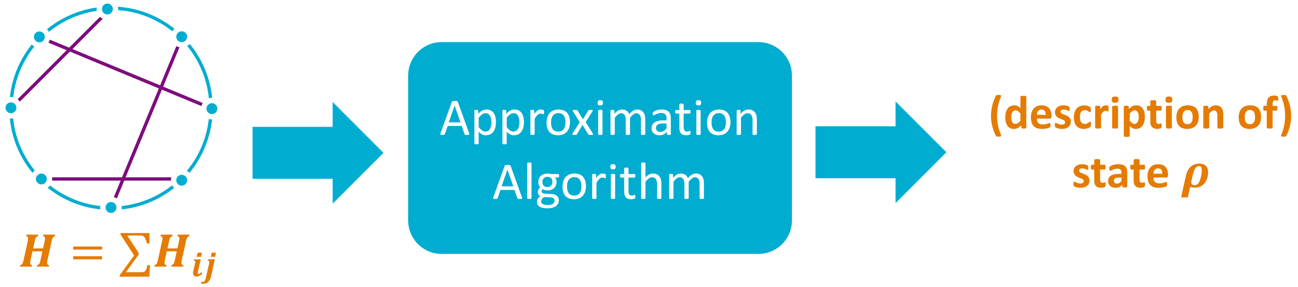
[*] **Quantum supremacy: [Preskill; arXiv 1801.00862], [Harrow & Montanaro; arXiv 1809.07442], [Aaronson & Chen; arXiv 1612.05903]**

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:

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

Optimal value

Approximate solution value

solution quality

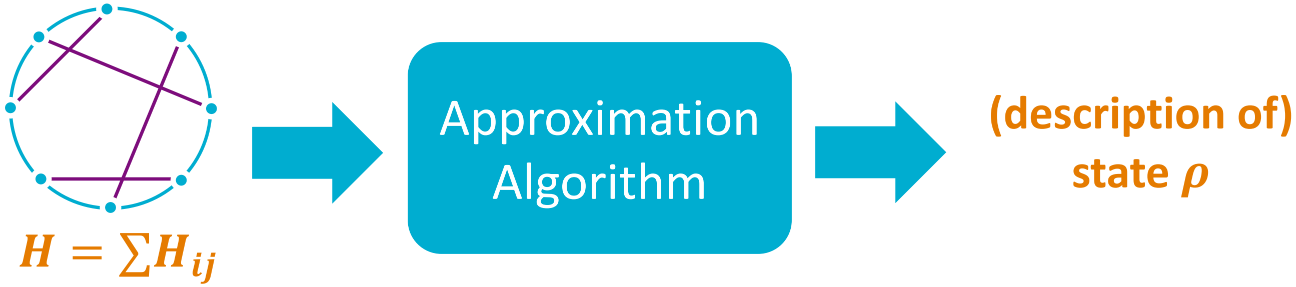
Instance 1

Instance 2

Instance 3 …

α = largest "gap" between optimal and approximate solutions over all instances

(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

Probability Distributions and Polynomials

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

$$\begin{bmatrix} \frac{1+a}{2} & 0 \\ 0 & \frac{1-a}{2} \end{bmatrix} = \frac{1}{2}\underbrace{\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}}_{\boldsymbol{I}} + \frac{a}{2}\underbrace{\begin{bmatrix} 1 & \\ & -1 \end{bmatrix}}_{\boldsymbol{Z}}$$

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

$$\begin{bmatrix} \frac{1+a_1}{2} & 0 \\ 0 & \frac{1-a_1}{2} \end{bmatrix} \otimes \begin{bmatrix} \frac{1+a_2}{2} & \\ & \frac{1-a_2}{2} \end{bmatrix} = \frac{I+a_1 Z}{2} \otimes \frac{I+a_2 Z}{2} = \frac{I + a_1 \overbrace{Z \otimes I}^{\boldsymbol{Z_1}} + a_2 \overbrace{I \otimes Z}^{\boldsymbol{Z_2}} + a_1 a_2 \overbrace{Z \otimes Z}^{\boldsymbol{Z_1 Z_2}}}{4}$$

Probability Distributions and Polynomials

$$\begin{bmatrix} \frac{1+a_1}{2} & 0 \\ 0 & \frac{1-a_1}{2} \end{bmatrix} \otimes \begin{bmatrix} \frac{1+a_2}{2} & \\ & \frac{1-a_2}{2} \end{bmatrix} = \frac{I+a_1 Z}{2} \otimes \frac{I+a_2 Z}{2} = \frac{I + a_1 \overbrace{Z \otimes I}^{\boldsymbol{Z_1}} + a_2 \overbrace{I \otimes Z}^{\boldsymbol{Z_2}} + a_1 a_2 \overbrace{Z \otimes Z}^{\boldsymbol{Z_1 Z_2}}}{4}$$

$$\overbrace{\begin{bmatrix} \frac{1}{4} & 0 \\ 0 & \frac{3}{4} \end{bmatrix}}^{\boldsymbol{a_1 = -\frac{1}{2}}} \otimes \overbrace{\begin{bmatrix} \frac{3}{4} & \\ & \frac{1}{4} \end{bmatrix}}^{\boldsymbol{a_2 = \frac{1}{2}}} = \begin{bmatrix} \frac{3}{16} & & & \\ & \frac{1}{16} & & \\ & & \frac{9}{16} & \\ & & & \frac{3}{16} \end{bmatrix}$$

$$= \frac{1}{4} \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}}_{\boldsymbol{I}} - \frac{1}{8} \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{bmatrix}}_{\boldsymbol{Z_1}} + \frac{1}{8} \underbrace{\begin{bmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{bmatrix}}_{\boldsymbol{Z_2}} - \frac{1}{16} \underbrace{\begin{bmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{bmatrix}}_{\boldsymbol{Z_1 Z_2}}$$

Quantum "Distributions" and Polynomials

Let's consider ~~diagonal~~ PSD matrices with trace = 1:

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

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

$$\begin{bmatrix} \frac{1+a}{2} & \frac{b-ci}{2} \\ \frac{b+ci}{2} & \frac{1-a}{2} \end{bmatrix} = \frac{1}{2}\underbrace{\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}}_{I} + \frac{a}{2}\underbrace{\begin{bmatrix} 1 & \\ & -1 \end{bmatrix}}_{Z} + \frac{b}{2}\underbrace{\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}}_{X} + \frac{c}{2}\underbrace{\begin{bmatrix} & -i \\ i & \end{bmatrix}}_{Y}$$

Biases must satisfy $\| (a, b, c) \| \leq 1$

Max Cut and Quantum Max Cut

Classical Max Cut

2-variable constraint: $x_i \oplus x_j$

$$\begin{array}{r|cccc} & 0{,}0 & 0{,}1 & 1{,}0 & 1{,}1 \\ \hline x_i, x_j = 0{,}0 & 0 & 0 & 0 & 0 \\ x_i, x_j = 0{,}1 & 0 & 1 & 0 & 0 \\ x_i, x_j = 1{,}0 & 0 & 0 & 1 & 0 \\ x_i, x_j = 1{,}1 & 0 & 0 & 0 & 0 \end{array}$$

quantum generalization →

Quantum Max Cut

quantum 2-variable constraint

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

Diagonal matrix

diagonal encodes Boolean function:

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

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

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

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

Polynomials and Quantum Solutions

Classical

Real-coeff polynomial $\mathrm{P}(I, Z_1, \dots, Z_n)$
over **commutative** variables

Problem: $Max_{\{Z_i\}}\, \lambda_{max}(\,\mathrm{P}(I, Z_1, \dots, Z_n)\,)$

$$Z_i^2 = I$$

$$Z_i Z_j = Z_j Z_i$$

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

$$\begin{array}{c}0,0\\0,1\\1,0\\1,1\end{array}\begin{bmatrix}0 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{bmatrix}$$

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

Quantum

Real-coeff polynomial $\mathrm{Q}(I, X_1, Y_1, Z_1, \dots, X_n, Y_n, Z_n)$
over **non-commutative** variables

$Max_{\{X_i, Y_i, Z_i\}}\, \lambda_{max}(\,\mathrm{Q}(I, X_1, Y_1, Z_1, \dots, X_n, Y_n, Z_n)\,)$

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

$$\mathrm{X_i Y_i = -Y_i X_i,\ X_i Z_i = -Z_i X_i,\ Y_i Z_i = -Z_i Y_i}$$

Variables commute on different indices:
e.g. $X_i Z_j = Z_j X_i$

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

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

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

Polynomials and Quantum Solutions

Classical

Problem: $Max_{\{Z_i\}}\,\lambda_{max}(\,\mathrm{P}(I, Z_1, \dots, Z_n)\,)$

$$Z_i^2 = I$$
$$Z_i Z_j = Z_j Z_i$$

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

$$\begin{array}{c} 0,0 \\ 0,1 \\ 1,0 \\ 1,1 \end{array} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

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

Quantum

$Max_{\{X_i, Y_i, Z_i\}}\,\lambda_{max}(\,\mathrm{Q}(I, X_1, Y_1, Z_1, \dots, X_n, Y_n, Z_n)\,)$

$$X_i^2 = Y_i^2 = Z_i^2 = I$$
$$\mathrm{X_i Y_i = -Y_i X_i,\ X_i Z_i = -Z_i X_i,\ Y_i Z_i = -Z_i Y_i}$$

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. $Z_2 = I \otimes Z \otimes I \dots$

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

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

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

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

Quantum Max Cut: Physical Motivation

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

→

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

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

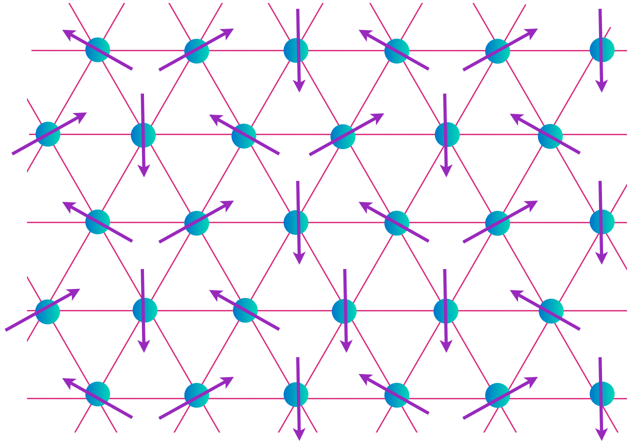
Find max-energy value/state of Quantum Max Cut: $\sum\left(I - X_i X_j - Y_i Y_j - Z_i Z_j\right)/4$

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

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

but different from approximation point of view)

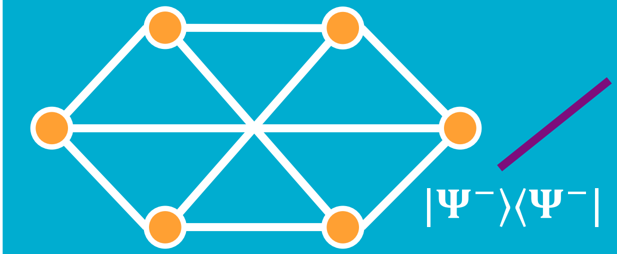
[Gharibian, P; arXiv:1909.08846]



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 $H = \sum H_{ij}$,

$$H_{ij} = \left(I - X_iX_j - Y_iY_j - Z_iZ_j\right)/4$$

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]

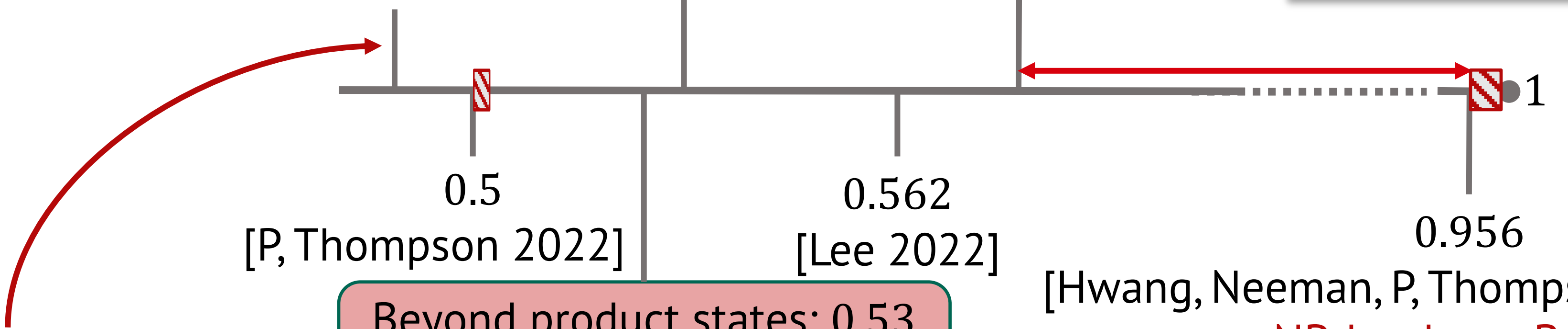
Recent approximation algorithms
[Gharibian and P. 2019], [Anshu, Gosset, Morentz 2020],
[P. and Thompson 2021, 2021, 2022]

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?



0.498
[Gharibian, P 2019]

0.533
[P, Thompson 2021]

0.582 (Δ-free)
[King 2022]

0.5
[P, Thompson 2022]

0.562
[Lee 2022]

1

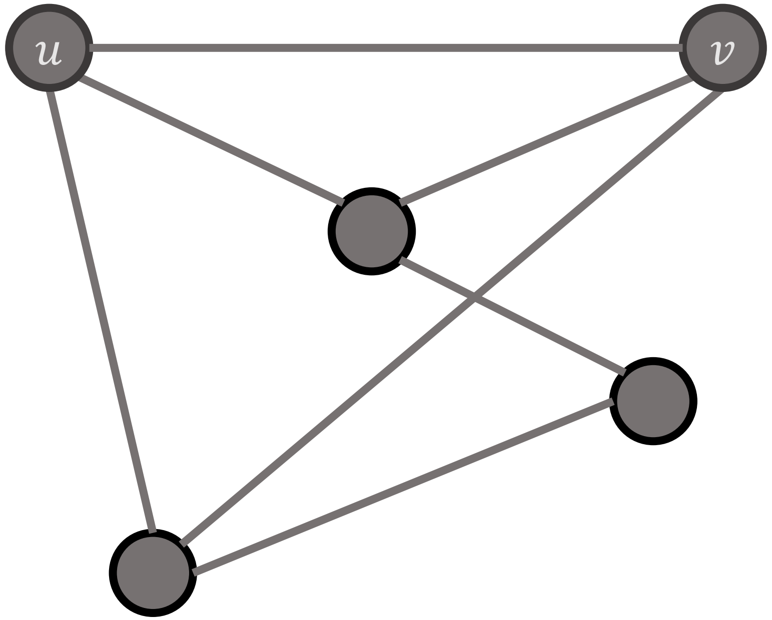
0.956
[Hwang, Neeman, P, Thompson, Wright 2022]
NP-hardness Barrier

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

Classical Intuition:
Best possible?

Slide courtesy of Yeongwoo Hwang

Max-Cut
in Quantum Language



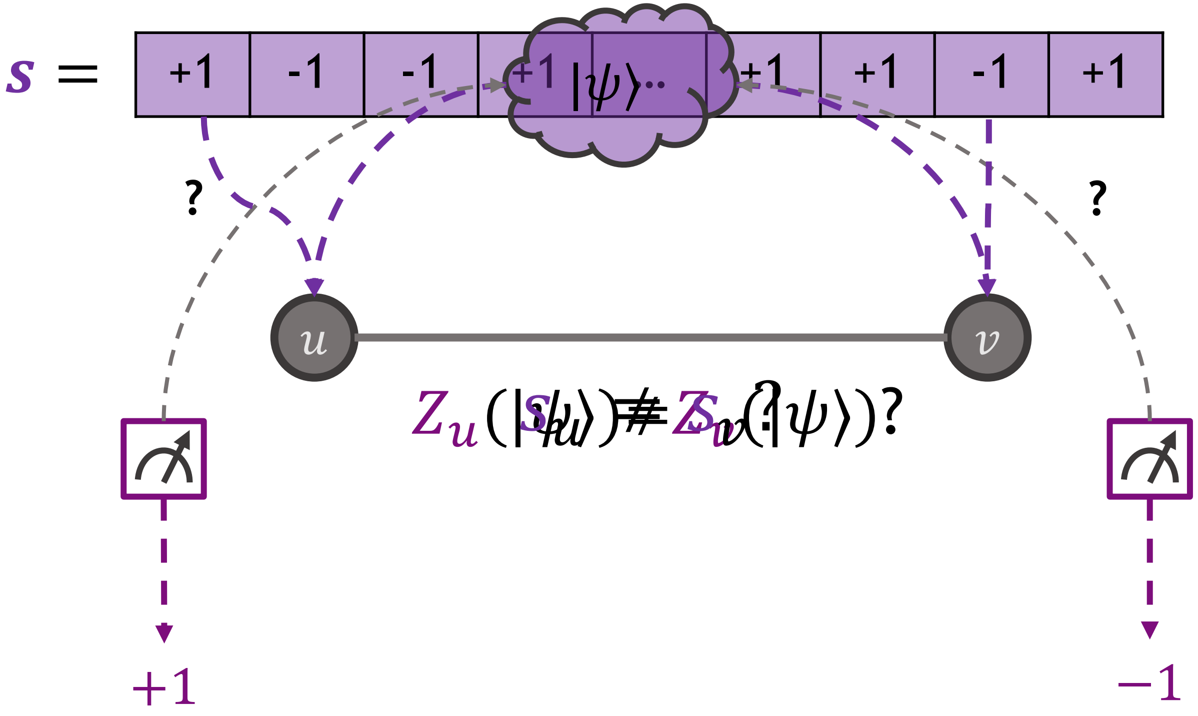
Slide courtesy of Yeongwoo Hwang

Max-Cut
in Quantum Language

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

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

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

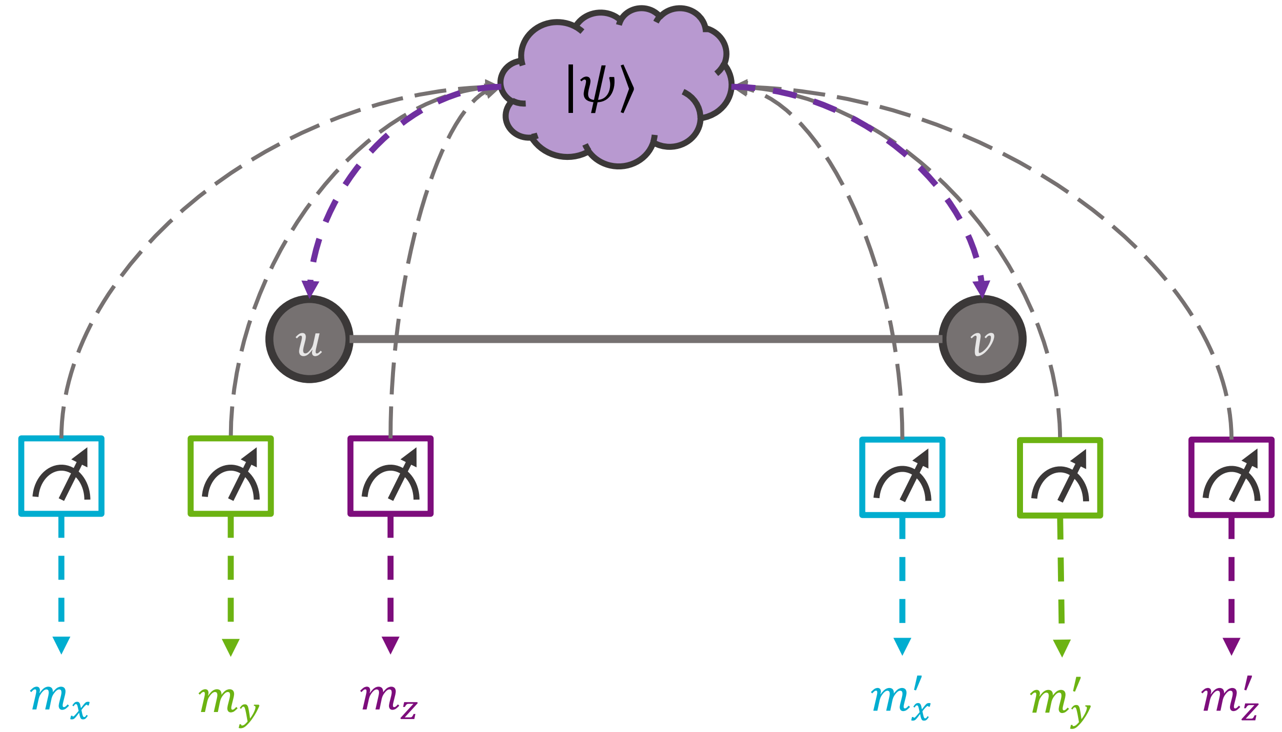


Observable: $h_{MAX-CUT} = \frac{1}{2}(\mathbb{I} - Z_u \otimes Z_v)$

Slide courtesy of Yeongwoo Hwang

Quantum Max-Cut

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



Observable: $m_z \neq m_z'$ and $m_x \neq m_x'$ and $m_y \neq m_y'$?

$h_{QMAX-CUT} = \frac{1}{4}(\mathbb{I} - X_u \otimes X_v - Y_u \otimes Y_v - Z_u \otimes Z_v)$

Slide courtesy of Yeongwoo Hwang

Quantum Max-Cut

Slide courtesy of Yeongwoo Hwang

Quantum Max-Cut
(Local Hamiltonian Problem)

Associate **Hamiltonian** $h_{(u,v)}$ to each edge.

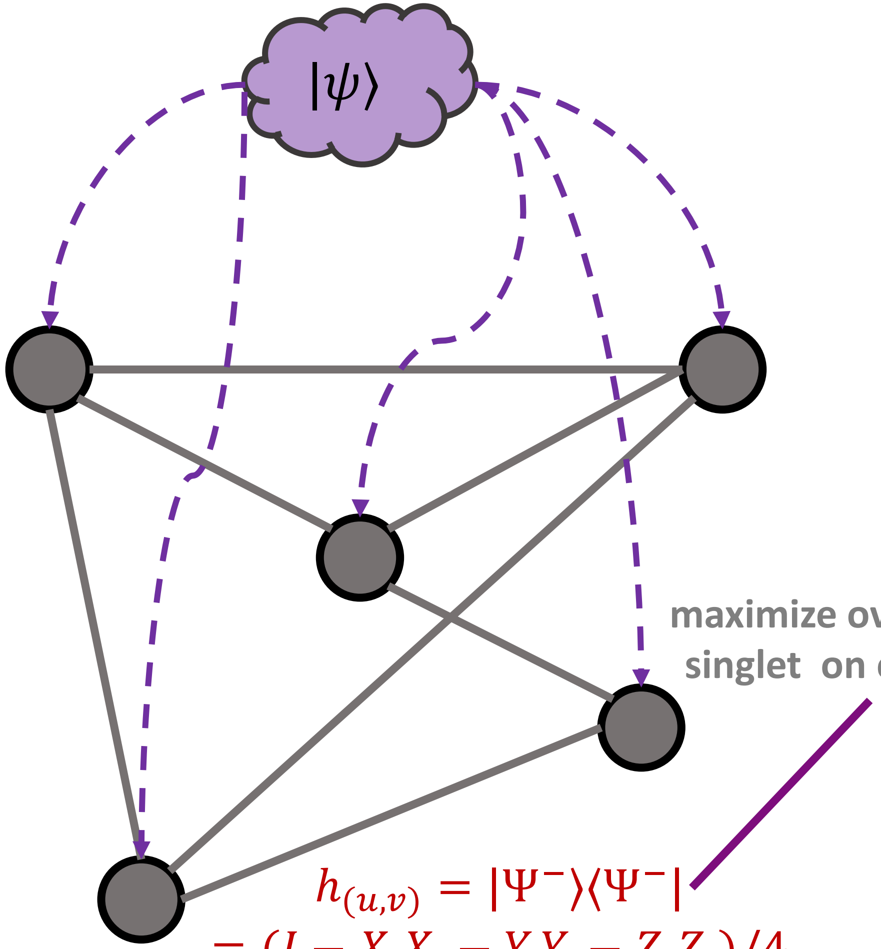
Energy: $\langle\psi|h_{(u,v)}|\psi\rangle$

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

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



maximize overlap with singlet on each edge

$$h_{(u,v)} = |\Psi^-\rangle\langle\Psi^-|$$
$$= (I - X_iX_j - Y_iY_j - Z_iZ_j)/4$$

Slide courtesy of Yeongwoo Hwang

Quantum Generalization of Constraint Satisfaction (CSP)

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

Quantum 2-CSP clause

$$\left.\begin{array}{r|cccc|} & 0,0 & 0,1 & 1,0 & 1,1 \\ \hline x_i, x_j = 0,0 & 0 & 0 & 0 & 0 \\ x_i, x_j = 0,1 & 0 & 1 & 0 & 0 \\ x_i, x_j = 1,0 & 0 & 0 & 0 & 0 \\ x_i, x_j = 1,1 & 0 & 0 & 0 & 0 \end{array}\right. \xrightarrow{\text{quantum generalization}} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & -1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Diagonal rank-1 projector

General 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: [Bansal, Bravyi, Terhal 2007: arXiv 0705.1115]

First nontrivial general approximations: [Gharibian, Kempe 2011: arXiv 1101.3884]
Classical approximation scheme for dense instances

Near-optimal product-state approx for special cases: [Brandao, Harrow 2013: arXiv 1310.0017]
Uses semidefinite programming (SDP) for bounds

Approximation w.r.t. number of terms and degree: [Harrow, Montanaro 2015: arXiv 1507.00739]

All of these results use product states

Recent 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 '21]**
Quantum Max Cut: $\sum_{ij} I - X_i X_j - Y_i Y_j - Z_i Z_j$ (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] 0.562* [Lee '22] (also [King '22])
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**

See [P, Thompson.; arXiv:2012.12347] for table

*** These results are not product-state based**

Quantum Relaxations

Max Cut Semidefinite Programming Relaxation

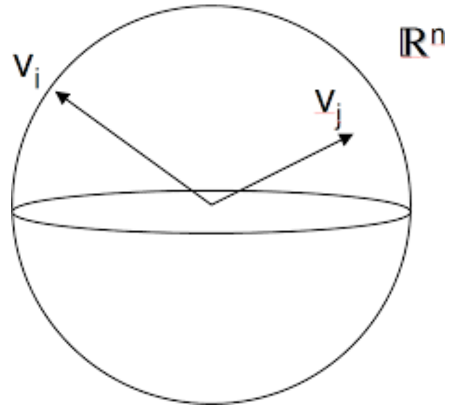
Max $\sum_{ij \in E}(1 - m_{ij})/2$

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

$\equiv$

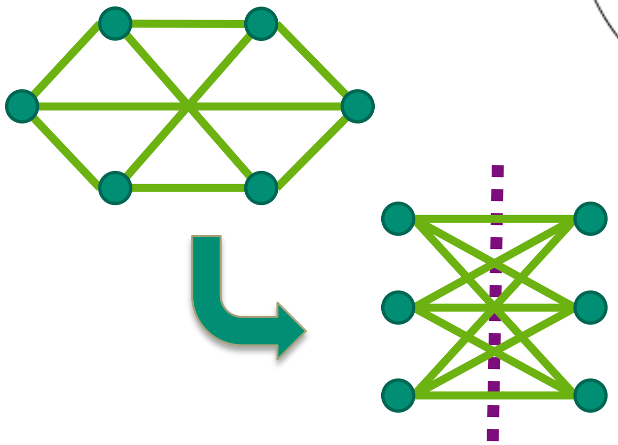
Max $\sum_{ij \in E}(1 - v_i \cdot v_j)/2$

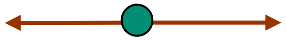
$\|v_i\| = 1$, for all $i \in V$
$(v_i \in \mathbb{R}^n)$



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

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

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

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

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

Quantum Max Cut SDP Relaxation

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

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

Real part of moment matrix

Quantum Max Cut vector relaxation

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

$\|x_i\|, \|y_i\|, \|z_i\| = 1$, for all $i \in V$

$x_i \cdot y_i = x_i \cdot z_i = y_i \cdot z_i = 0$, for all $i \in V$

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

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

$$\longleftrightarrow$$

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

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

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

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

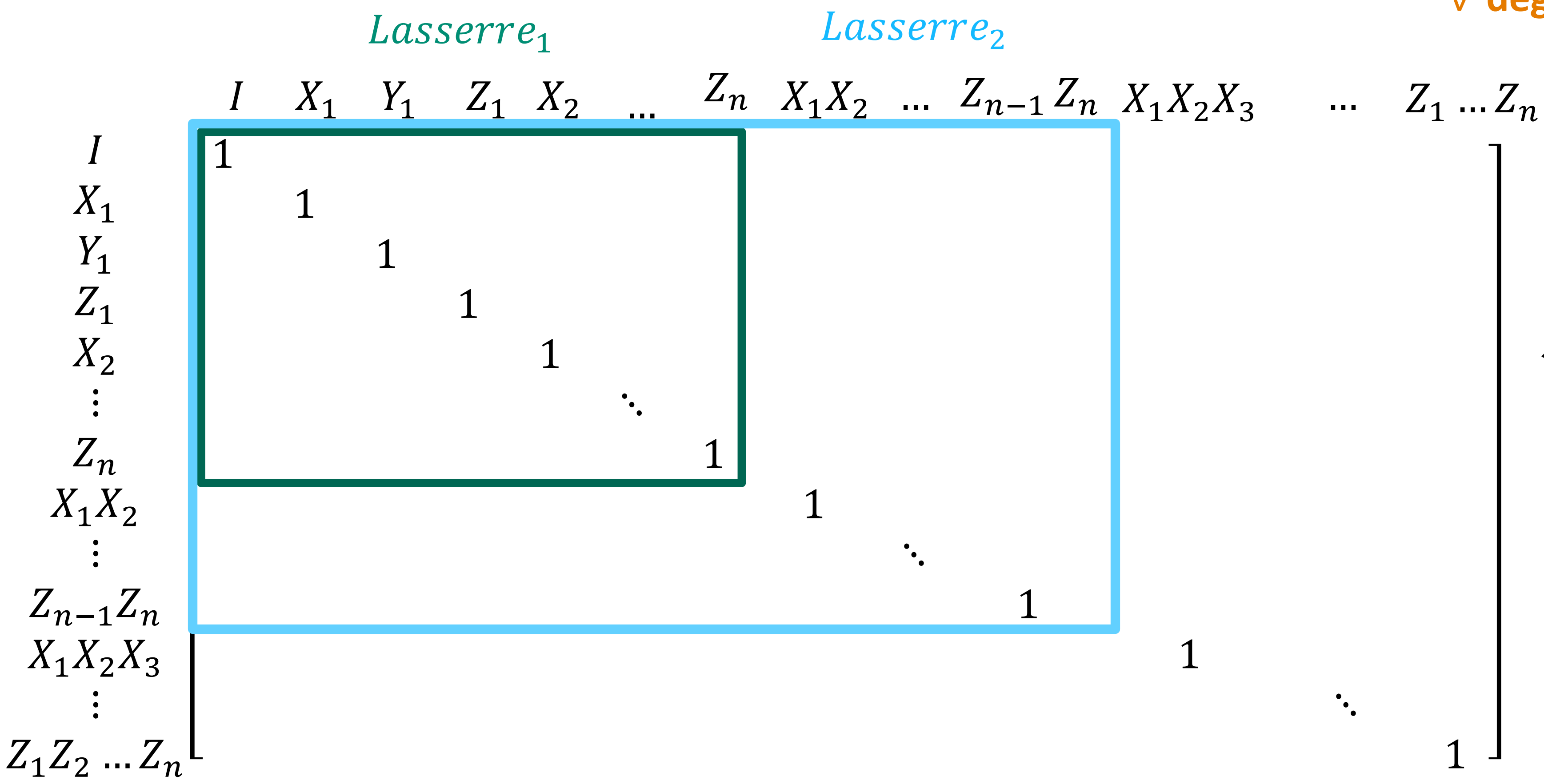
Max Cut vector relaxation

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

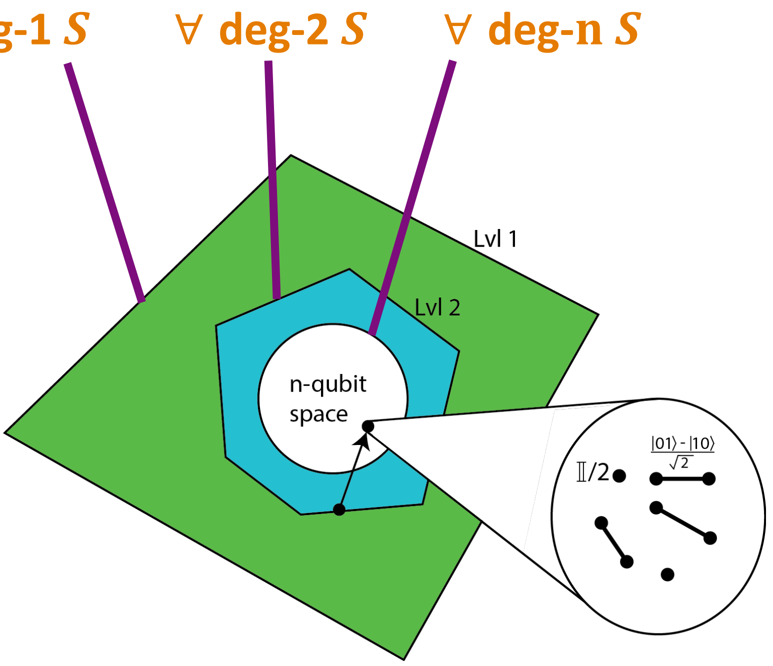
$\|v_i\| = 1$, for all $i \in V$

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

Quantum Lasserre Hierachy



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



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

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

Classical
[Lasserre 2001]
[Parillo 2003]

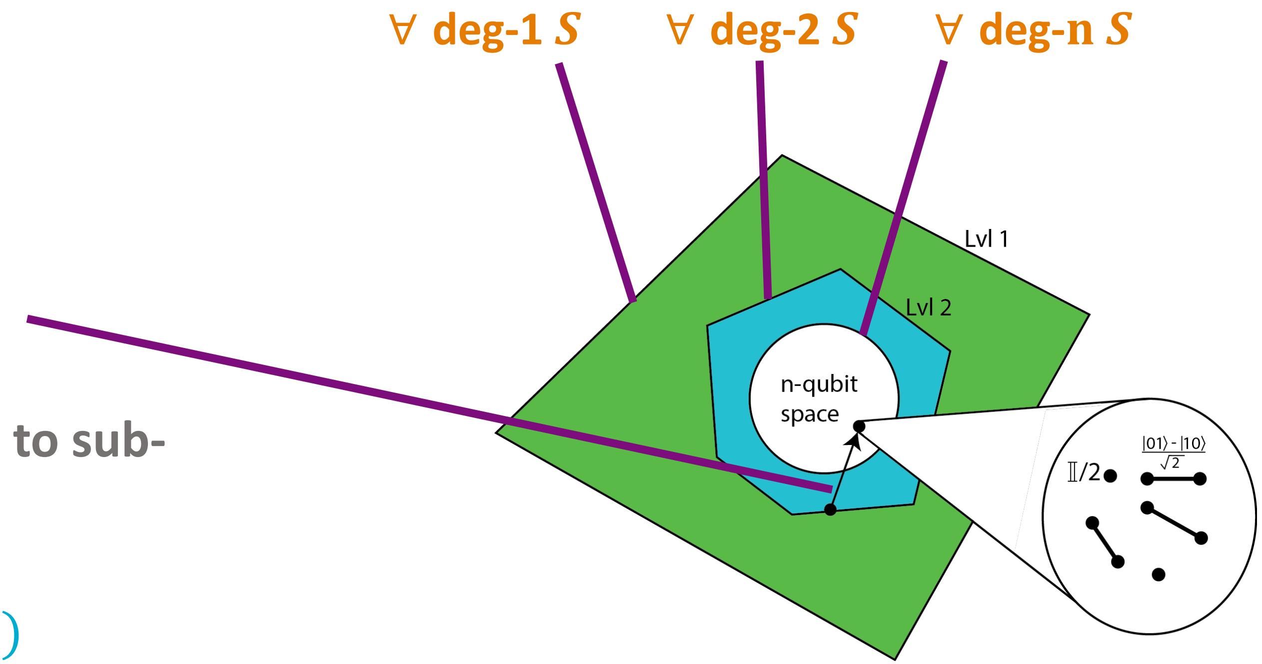
Non-commutative/Quantum
[Navascués, Pironio, Acìn 2009 (2010 SIAM J Opt)]

Rounding Infeasible Solutions

α-Approximation Algorithm

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

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



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

$\tilde{\rho}$ 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:

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

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

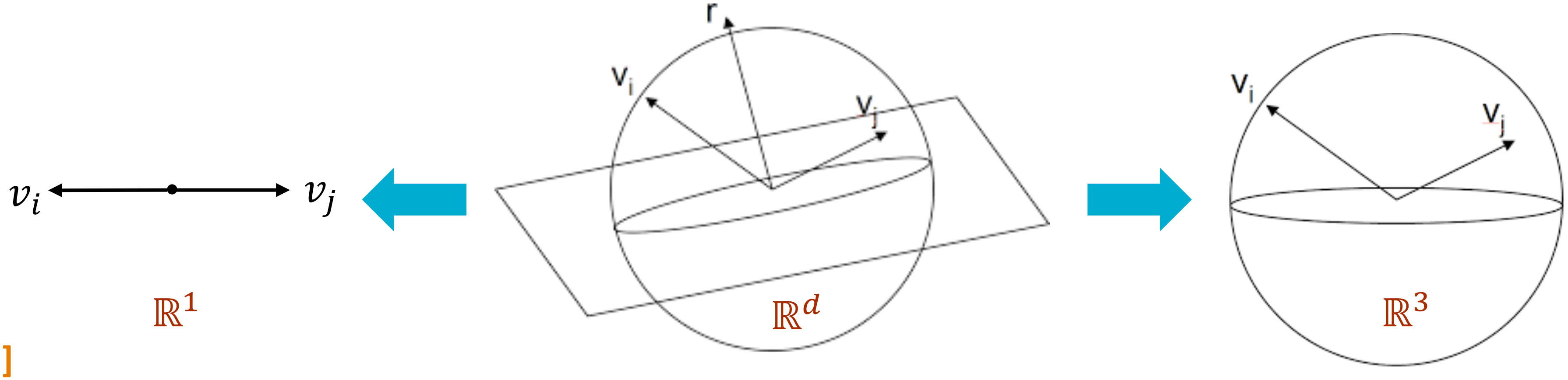
$$v_i \in \mathbb{R}^n \longrightarrow \alpha_i = \frac{r^T v_i}{|r^T v_i|}$$

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

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)

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

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

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

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

Rounding

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

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

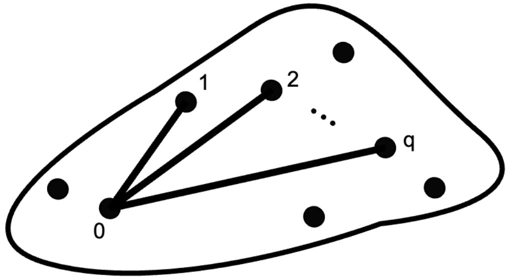
Approximability

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)

Monogamy of Entanglement

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



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

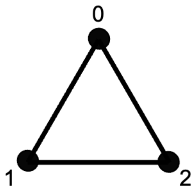
Monogamy of Entanglement

- ➢ $Lasserre_1$ 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:



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

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

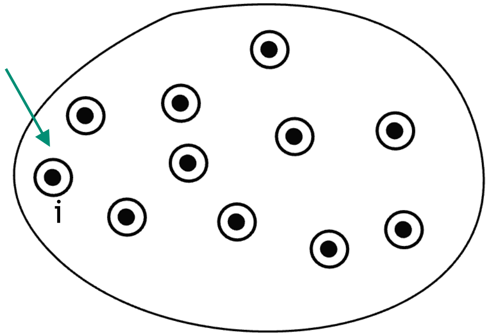
$$\mu_{01} = 1 \Rightarrow \mu_{02} = 1/4$$

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

Rounding Ansatze

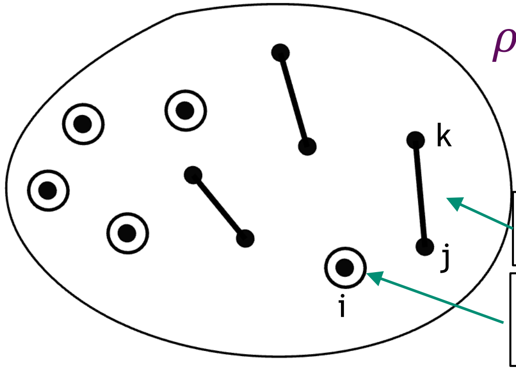
Product State Ansatz

$$\rho = \prod_i \rho_i$$



Singlets+Product States

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

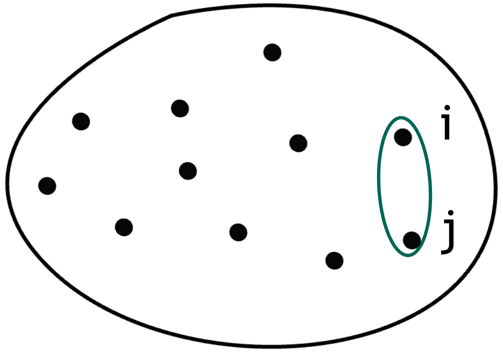


$$\rho_{jk} = \frac{I - X_j X_k - Y_j Y_k - Z_j\, Z_k}{4}$$

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

Better Rounding Algorithm

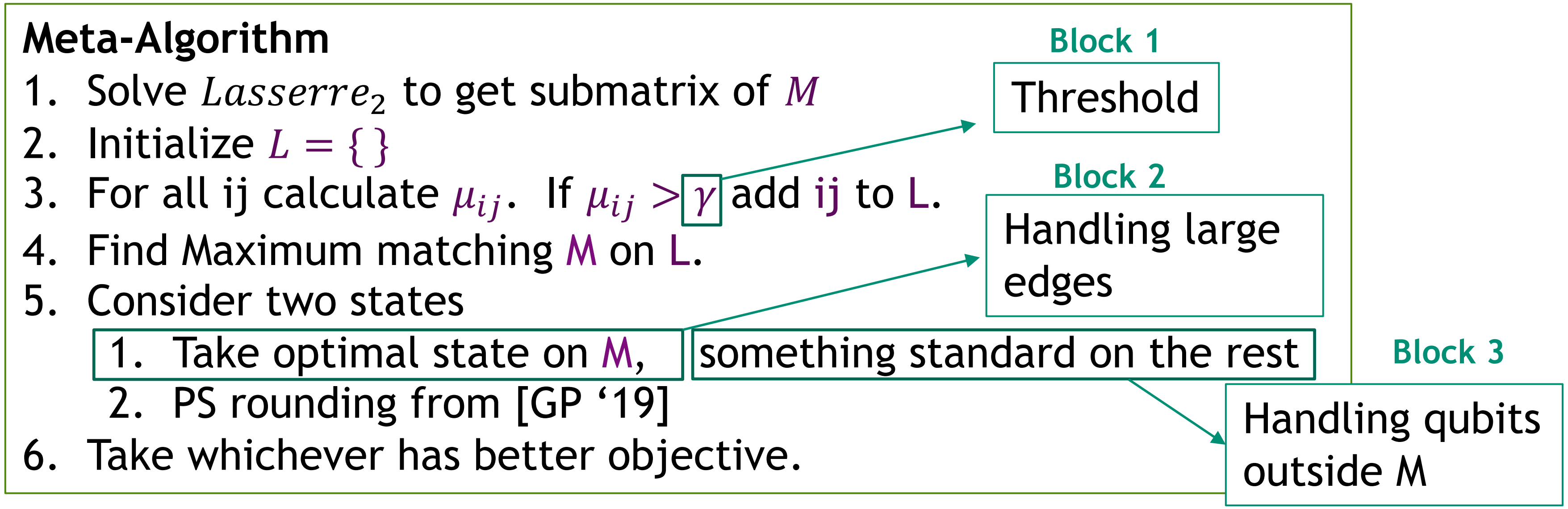
- PS rounding algorithm and singlet+PS rounding algorithm follow similar meta-algorithm, with different “building blocks”



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

$0 \leq \mu_{ij} \leq 1$, 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

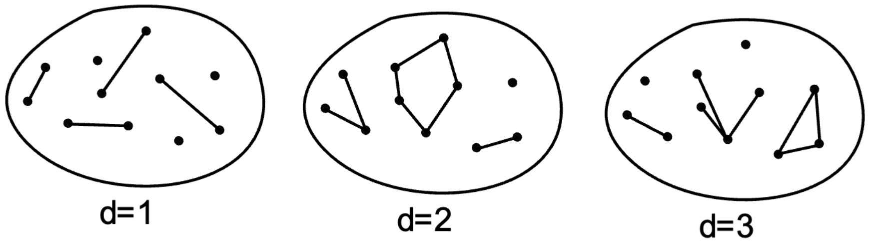
Block 3

Handling qubits outside M

Rounding Algorithm (cont.)

Block 1

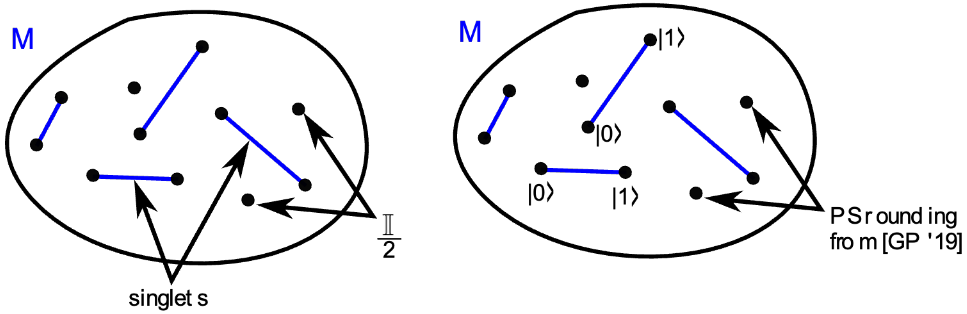
- Star/Triangle bounds say that large edges must be adjacent to small edges ⇒ set L forms a subgraph of small degree
  - Threshold controls degree of subgraph



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 Quantum Max Cut…

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]
[Lee 2022: arXiv 2209.00789]
[King 2022: arXiv 2209.02589]

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]

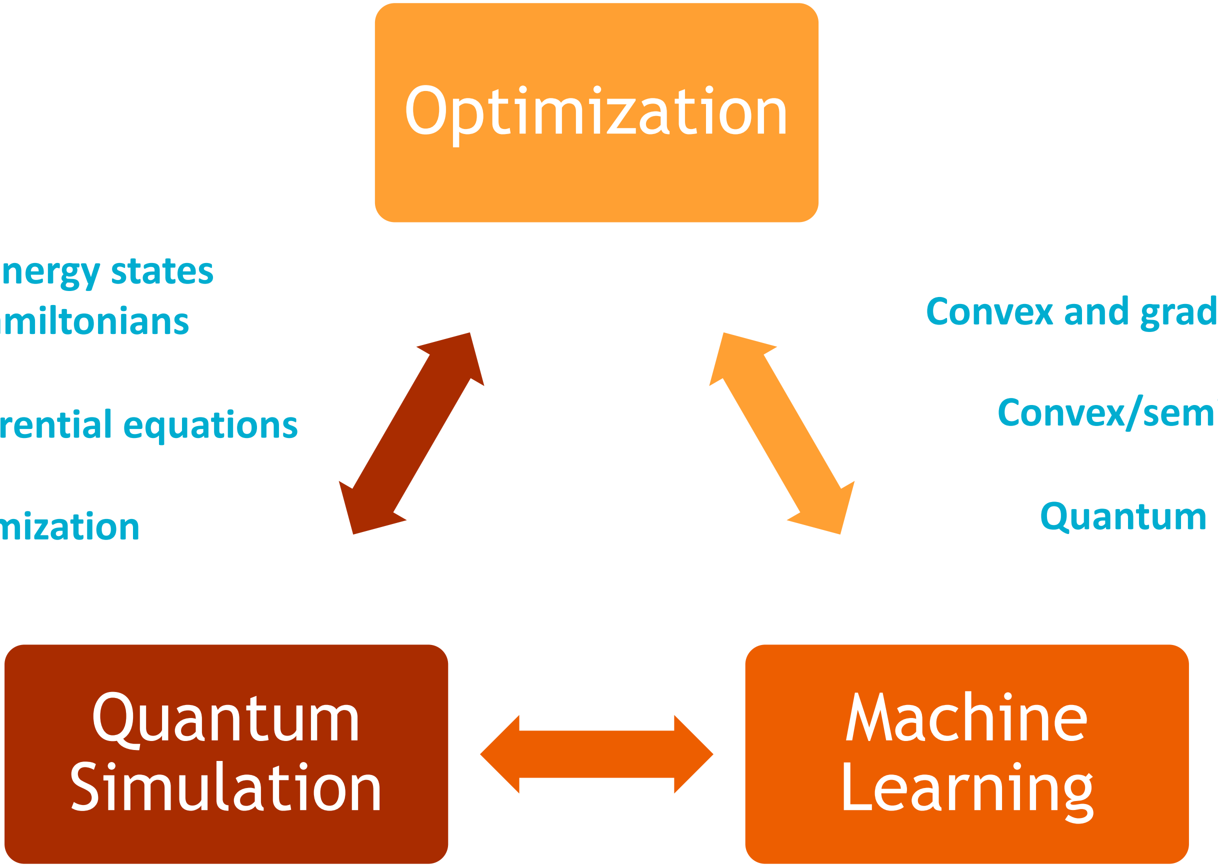
Connections in approximating QMC and 2-LH: [P., Thompson 2022 above, 2020: arXiv 2012.12347]
[Anshu, Gosset, Morenz-Korol, Soleimanifar: arXiv 2105.01193]

Optimal space-bounded QMC approximations:
(no quantum advantage possible!) [Kallaugher, P. 2022: arXiv 2206.00213]

Thanks for reading this!

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

We're looking for interns and postdocs!

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Fundamental Algorithmic Research for Quantum Computing

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

FAR-QC

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