NISQ Algorithms for Separable Ground States

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4/5/2022

Thank everyone for being here.

Inner Approximations and NISQ Algorithms for the Separability Problem

with Tobias Haug, Kishor Bharti and Jamie Sikora

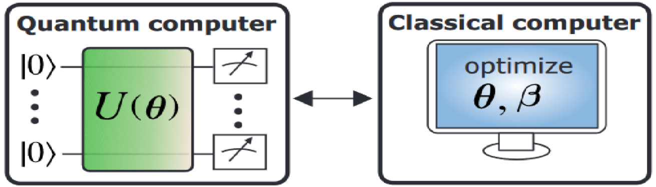
1. Start out by saying that this is still a work in progress in the sense that there are some measurement methods that have not yet been fully looked into.
2. This is part of the work in this paper which is also a work in progress

Outline

1. NSS
2. NSeS
3. Quantification
4. Results

NISQ SDP Solver

Hybrid quantum-classical algorithm to solve SDP.



- Quantum computer encodes an SDP. Only for estimating overlaps.
- Classical optimization routine is also an SDP with dimension given by the size of the ansatz space.
- No classical-quantum feedback loop.

1. Estimating overlaps can be done efficiently on current NISQ devices

Standard form primal SDP

$$
\begin{aligned}
\min \quad & \langle \mathbf{C}, \mathbf{X} \rangle \\
\text{s.t.} \quad & \langle \mathbf{A}_i, \mathbf{X} \rangle = b_i, \; i = \{1, \ldots, m\} \\
& \mathbf{X} \succcurlyeq 0
\end{aligned}
$$

$\mathbf{C}$ and $\mathbf{A}_i, \forall i$ are $n \times n$ Hermitian matrices.

NSS

3 distinct steps:

1. Ansatz selection
2. Overlap measurement
3. Post-processing

Ansatz selection

1. Set of M quantum states $\mathbb{S} = \{|\psi_j\rangle \in \mathcal{H}\}_j$ over a Hilbert space $\mathcal{H}$
2. Hybrid density matrix ansatz

$$\mathbf{X} = \sum_{ij} \beta_{ij} \, |\psi_i\rangle\langle\psi_j|$$

where $\beta_{ij} \in \mathbb{C}$

$\mathbb{S}$ is prepared by a quantum computer.
β is stored on a classical computer.

Lemma

$$\beta \succcurlyeq 0 \implies \mathbf{X} \succcurlyeq 0$$

SDP (Update 1)

$$
\begin{aligned}
\min \quad & \langle \mathbf{C}, \mathbf{X} \rangle \\
\text{s.t.} \quad & \langle \mathbf{A}_i, \mathbf{X} \rangle = b_i, \; i = \{1, \ldots, m\} \\
& \mathbf{X} \succcurlyeq 0
\end{aligned}
$$

$\beta \succcurlyeq 0$

$\mathbf{C}$ and $\mathbf{A}_i, \forall i$ are $n \times n$ Hermitian matrices.

Assumption

Assume $\mathbf{C}$ and $\mathbf{A}_i, \forall i$ can be expressed as the sum of unitaries.

$$\mathbf{C} = \sum_k s_k \mathbf{U}_k$$

$$\mathbf{A}_i = \sum_l f_{il} \mathbf{U}_l^{(i)}$$

Overlap measurement

Measure the following overlap on the quantum system

$$D_{ab} = \sum_k s_k \langle \psi_b | \mathbf{U}_k | \psi_a \rangle$$

SDP (Update 2)

$$
\begin{aligned}
\min \quad & \langle \mathbf{C}, \mathbf{X} \rangle \\
\text{s.t.} \quad & \langle \mathbf{A}_i, \mathbf{X} \rangle = b_i,\ i = \{1, \ldots, m\} \\
& \mathbf{X} \succcurlyeq 0
\end{aligned}
\qquad
\begin{aligned}
\min \quad & \langle \beta, \mathbf{D} \rangle \\
& \\
& \beta \succcurlyeq 0
\end{aligned}
$$

C and $\mathbf{A}_i, \forall i$ are $n \times n$ Hermitian matrices.

Overlap measurement

Measure the following overlap on the quantum system

$$D_{ab} = \sum_k s_k \langle \psi_b | \mathbf{U}_k | \psi_a \rangle$$

$$E_{ab} = \sum_l f_{il} \langle \psi_b | \mathbf{U}_l^{(i)} | \psi_a \rangle$$

Post-processing

$$\begin{aligned} \min \quad & \langle \mathbf{C}, \mathbf{X} \rangle \\ \text{s.t.} \quad & \langle \mathbf{A}_i, \mathbf{X} \rangle = b_i, \; i = \{1, \ldots, m\} \\ & \mathbf{X} \succcurlyeq 0 \end{aligned}$$

$$\begin{aligned} \min \quad & \langle \beta, \mathbf{D} \rangle \\ \text{s.t.} \quad & \langle \beta, \mathbf{E}^{(i)} \rangle = b_i \\ & \beta \succcurlyeq 0 \end{aligned}$$

C and $\mathbf{A}_i, \forall i$ are $n \times n$ Hermitian matrices.

NISQ-friendly overlap measurement method (1)

Assumptions:

1. Unitaries $\mathbf{U}_k$ and $\mathbf{U}_l^{(i)}$ are Pauli strings $\mathbf{P} = \bigotimes_{j=1}^{N} \boldsymbol{\sigma}_j$ with $\boldsymbol{\sigma}_j = \{\mathbb{1}, \boldsymbol{\sigma}^x, \boldsymbol{\sigma}^y, \boldsymbol{\sigma}^z\}$.
   $\because$ Pauli strings form a complete basis, any matrix can be decomposed into a linear combination of Pauli strings.
2. Ansatz space is generated by state $|\psi\rangle$ and a set of M different Pauli strings $\{\mathbf{P}_1, \ldots, \mathbf{P}_M\}$ via $\mathbb{S} = \{\mathbf{P}_j |\psi\rangle\}_{j=1}^{M}$.
   $\implies$ Each overlap element can be expressed as a sum of expectation values of Pauli strings
   $\langle\psi| \mathbf{P}_1\mathbf{P}_2\mathbf{P}_3 |\psi\rangle = a \langle\psi| \mathbf{P}' |\psi\rangle$, where $a \in \{+1, -1, +i, -i\}$.
   Measuring the expectation values of Pauli strings $\implies$ efficient calculation of the overlap elements.

1. How do we actually measure the overlap?

NISQ-friendly overlap measurement method (2)

- On NISQ computers, perform single-qubit rotations into the eigenbasis of the Pauli operator and sample in the computational basis.
- For $\mathbb{S} = \{\mathbf{P}_j \,|\psi\rangle\}_{j=1}^{M}$ we are only required to prepare the reference state $|\psi\rangle$.
- Other states are related to the reference state via single layer Pauli unitaries.
- $\therefore$ we only have to sample $|\psi\rangle$ in a set of Pauli rotated basis elements.

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2. NSeS
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Problem Statement

Given $\rho \in \mathrm{Pos}(\mathcal{A} \otimes \mathcal{B})$, we want to determine whether ρ is *separable* or *entangled*?

Formally, we define

$$\mathrm{Sep}(\mathcal{X} : \mathcal{Y}) = \left\{ \sum_{i=1}^{k} p_i \, |\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i| : \sum_{i=1}^{k} p_i = 1, p_i \geq 0 \; \forall \; i \right\}$$

$$\rho \in \mathrm{Sep}(\mathcal{A} : \mathcal{B})?$$

1. bipartite density matrix ρ – entangled?
2. set of separable states as the convex combination of tensor product of pure states
3. so we ask does ρ belong to this set?
4. This is equivalent to asking the following optimization problem: given a PSD or Herm operator, what is the density matrix that maximizes this HSIP?

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$$\rho \in \mathrm{Sep}(\mathcal{A} : \mathcal{B})?$$

Equivalently: Given $\mathbf{\Pi} \in \{\mathrm{Pos}(\mathcal{A} \otimes \mathcal{B}), \mathrm{Herm}(\mathcal{A} \otimes \mathcal{B})\}$, we want to compute:

$$\alpha = \sup_{\rho \in \mathrm{Sep}} \langle \rho, \mathbf{\Pi} \rangle$$

This is known to be a NP-hard problem [Gurvits, 2003]

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3. so we ask does ρ belong to this set?
4. This is equivalent to asking the following optimization problem: given a PSD or Herm operator, what is the density matrix that maximizes this HSIP?

Ansatz selection

$\mathbb{S}_A = \{|\psi_i\rangle\}_{i=1}^{N} \in \mathcal{A}$
$\mathbb{S}_B = \{|\phi_j\rangle\}_{j=1}^{M} \in \mathcal{B}$
Hybrid density matrix ansatz

$$\mathbf{X} = \sum_{ijkl} \beta_{ijkl} \, |\psi_i\rangle\langle\psi_j| \otimes |\phi_k\rangle\langle\phi_l|$$

where $\beta_{ijkl} \in \mathbb{C}$

Original Problem

$$\begin{aligned} \sup \quad & \langle \mathbf{X}, \mathbf{\Pi} \rangle \\ \text{s.t.} \quad & \mathrm{Tr}(\mathbf{X}) = 1 \\ & \mathbf{X} \in \mathrm{Sep}(\mathcal{A} : \mathcal{B}) \end{aligned}$$

Lemma

$$\beta \in \mathrm{Herm}(\mathcal{A}' \otimes \mathcal{B}')$$

where

$$\mathrm{dim}(\mathcal{A}') << \mathrm{dim}(\mathcal{A}),$$
$$\mathrm{dim}(\mathcal{B}') << \mathrm{dim}(\mathcal{B})$$

Lemma

$$\beta \in \mathrm{Herm}(\mathcal{A}' \otimes \mathcal{B}')$$

where

$$\mathrm{dim}(\mathcal{A}') << \mathrm{dim}(\mathcal{A}),$$
$$\mathrm{dim}(\mathcal{B}') << \mathrm{dim}(\mathcal{B})$$

Lemma

$$\beta \in \mathrm{Sep}(\mathcal{A}' \otimes \mathcal{B}') \implies \mathbf{X} \in \mathrm{Sep}(\mathcal{A} \otimes \mathcal{B})$$

Problem (Update 1)

$$\begin{aligned} \sup \quad & \langle \mathbf{X}, \mathbf{\Pi} \rangle \\ \text{s.t.} \quad & \mathrm{Tr}(\mathbf{X}) = 1 \\ & \mathbf{X} \in \mathrm{Sep}(\mathcal{A} : \mathcal{B}) \end{aligned}$$

$$\beta \in \mathrm{Sep}(\mathcal{A}' : \mathcal{B}')$$

Overlap measurement

Assume $\mathbf{\Pi}$ can be expressed as a sum of unitaries

$$\mathbf{\Pi} = \sum_x c_x \mathbf{U}_x$$

Measure the following overlaps:

$$D_{ijkl} = \sum_x c_x \left|\psi_j\right\rangle \left|\phi_l\right\rangle \mathbf{U}_x \left|\psi_i\right\rangle \left|\psi_k\right\rangle$$

$$E_{ijkl} = \left\langle \psi_j \middle| \psi_i \right\rangle \left\langle \phi_l \middle| \phi_k \right\rangle$$

Post-processing

$$\begin{aligned} \sup \quad & \langle \mathbf{X}, \mathbf{\Pi} \rangle \\ \text{s.t.} \quad & \mathrm{Tr}(\mathbf{X}) = 1 \\ & \mathbf{X} \in \mathrm{Sep}(\mathcal{A} : \mathcal{B}) \end{aligned}$$

$$\begin{aligned} \sup \quad & \langle \beta, \mathbf{D} \rangle \\ \text{s.t.} \quad & \langle \beta, \mathbf{E} \rangle = 1 \\ & \beta \in \mathrm{Sep}(\mathcal{A}' : \mathcal{B}') \end{aligned}$$

Outline

Upper bounds

- β_{PPT}: PPT criterion [Horodecki et al., 1996], [Peres, 1996]
- β_r: Realignment criterion [Chen and Wu, 2003]
- $\{\beta_1, \ldots, \beta_k\}$: Symmetric Extensions [Chen et al., 2014]
- $\{\beta'_1, \ldots, \beta'_k\}$: Bosonic Extensions [Li et al., 2019]

See-saw

Algorithm 1: see-saw

Input: $\boldsymbol{\sigma}_A \in \mathrm{Pos}(\mathcal{A}),\ \boldsymbol{\Pi}$

Output: γ

repeat

$\quad \boldsymbol{\sigma}_B : \sup_{\boldsymbol{\sigma}_B \in \mathrm{Pos}(\mathcal{B})} \langle \boldsymbol{\sigma}_A \otimes \boldsymbol{\sigma}_B, \boldsymbol{\Pi} \rangle$

$\quad \boldsymbol{\sigma}_A : \sup_{\boldsymbol{\sigma}_A \in \mathrm{Pos}(\mathcal{A})} \langle \boldsymbol{\sigma}_A \otimes \boldsymbol{\sigma}_B, \boldsymbol{\Pi} \rangle$

until *convergence or maximum number of iterations*;

$\gamma = \langle \boldsymbol{\sigma}_A \otimes \boldsymbol{\sigma}_B, \boldsymbol{\Pi} \rangle$

Lower-bounds

$$\gamma_{MM} = \text{see-saw}\left(\frac{1}{\dim \mathcal{A}}\,\mathbb{1}, \mathbf{\Pi}\right)$$

$$\gamma_{US} = \text{see-saw}\left(\frac{1}{\dim \mathcal{A}}\sum_i |\mathbf{i}\rangle\langle\mathbf{i}|\,, \mathbf{\Pi}\right)$$

$$\gamma_{rand} = \text{see-saw}\,(\text{random vector}, \mathbf{\Pi}) \;\; \text{for 100 points}$$

Summary

$$\{\gamma_{MM}, \gamma_{US}, \gamma_{rand}\} \leq \alpha \leq \{\beta_{PPT}, \beta_r, \beta_1, \ldots, \beta_k, \beta'_1, \ldots, \beta'_k\}$$

Quantification

How well are we really approximating α?

Define "Tightness of Bound" (TOB) as

$$ToB = \beta - \gamma$$

where

$$\beta = \min\{\beta_{PPT}, \beta_r, \beta_1, \ldots, \beta_k, \beta'_1, \ldots, \beta'_k\}$$

$$\gamma = \max\{\gamma_{MM}, \gamma_{US}, \gamma_{rand}\}$$

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Results

`https://ankith-mohan.shinyapps.io/SEP_app`

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