Polynomial-time degenerate ground state approximation of gapped 1D Hamiltonians

Christopher T. Chubb Steven T. Flammia

Centre for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia.

arXiv:1502.06967

Introduction

Many algorithms used to compute ground state properties of spin systems, such as the Density Matrix Renormalisation Group, are heuristic methods. As a result while they may be observed to perform well in practice, pathological cases are known to exist which confound them [1], and there do not yet exist theoretical performance guarantees, even in the presence of certain physical restrictions which make the underlying problems computationally tractable.

Summary

We present a ground state approximation algorithm which extends known *provably efficient* techniques [2, 3] to degenerate systems. For a 1D local and gapped spin system of constant degeneracy, our algorithm generates an orthonormal set of approximate ground states. For a spin chain of length n with a spectral gap at least ϵ, this algorithm yields states with ground space overlap at least $1-\eta$ in run-time T, where

$$T = \begin{cases} n^{\mathcal{O}(1/\epsilon)} & \text{for } 1/\eta = n^{\mathcal{O}(1)}, \\ n^{O(1)} & \text{for } 1/\eta = n^{o(1)}. \end{cases}$$

As such the 1D gapped case of the Local Hamiltonian problem remains within P even in the degenerate case.

Entanglement

The curse of dimensionality prohibits us from efficiently representing an arbitrary quantum state. For the Hamiltonians we are considering however, the ground states exhibit limited levels of entanglement, which allow us to use an efficient state ansatz.

Background: Area Law

For a general state the entanglement entropy of a region can scale with the volume. For gapped and local ground states it is conjectured [4] to, at worst, scale with the area of that region. In 1D this means the entanglement entropy of a contiguous region is bounded by a constant. This result has been proven for non-degenerate systems [5], and recently extended to include degeneracy [6], allowing for efficient state representation [7], placing the problem in NP.

The goal: Ground state approximation

Naïvely, exact ground states $\{|\Gamma_i\rangle\}$ could be calculated by calculating the density matrices $\{\sigma_j\}$ by solving the convex programs:

$$\begin{aligned} \text{min} \quad & \mathrm{Tr}(H\sigma_j) && (1) \\ \text{where} \quad & \langle\Gamma_1|\sigma_j|\Gamma_1\rangle = \cdots = \langle\Gamma_{j-1}|\sigma_j|\Gamma_{j-1}\rangle = 0, && (2) \\ & \sigma_j \geq 0,\ \mathrm{Tr}\,\sigma_j = 1, \end{aligned}$$

and taking $|\Gamma_j\rangle$ to be the leading eigenvector of σ_j. The domain of these optimisations is however exponential, rendering them infeasible to solve exactly. By utilising dynamic programming techniques we can instead construct a polynomial-size domain on which these programs *can* be solved, efficiently yielding approximate ground states. Our algorithm constructs such a space iteratively in the form of *viable sets*.

Definition: Viable Set

A set S of states is i-viable if:

- S is efficiently represented.
- States in S are defined on i spins.
- There exists a set of orthonormal witness states $\{|\psi_j\rangle\}$ with large ground space overlap, such that they are appropriately supported by S:

$$\mathrm{Supp}\left(\mathrm{Tr}_{>i}\,|\psi_j\rangle\langle\psi_j|\right) \subseteq \mathrm{Span}\,(S)\,.$$

Algorithm Sketch

The idea here is to extend an existing $(i-1)$-viable set to a i-viable set, whilst carefully controlling the growth of both the size and error. This procedure is performed in three sub-steps:

1) Extension: Element-wise tensor product the viable set with a basis on the ith spin, raising the size but preserving the error.
2) Trimming: Perform convex optimisations that throw out unnecessary high energy states, lowering the size at the expense of a growth in the error.
3) Error Reduction: Apply approximate ground state projectors, raising the size whilst lowering the error.

These steps can be performed such that neither the size nor error grow over the overall procedure. By iterating, this algorithm therefore allows for the efficient construction of an n-viable set, on which we can then perform the desired ground state approximation programs (1).

The two programs

In the case of low LD, a viable set for our first witness also faithfully approximates our second witness. As such we can simply recycle the viable set for the first witness, which is found by solving the *energetic trimming programs*, which take the form:

$$\begin{aligned} \text{min} \quad & \mathrm{Tr}(H_L\sigma_1) && (3) \\ \text{where} \quad & \sigma_1 \geq 0,\ \mathrm{Tr}\,\sigma_1 = 1, \end{aligned}$$

with σ_1 supported on the current viable set, and H_L being the constributions to the Hamiltonian supported on the current left half-chain. This gives us a viable set which is good for the first witness and a low-LD second witness. For the high-LD regime, we restrict to a low-energy subspace and project away from this viable set, giving us *orthogonality trimming programs* of the form:

$$\begin{aligned} \text{min} \quad & \mathrm{Tr}(P\sigma_2) && (4) \\ \text{where} \quad & \mathrm{Tr}(H_L\sigma_2) \leq \mathrm{Tr}(H_L\sigma_1) + \text{small error}\,, \\ & \sigma_2 \geq 0,\ \mathrm{Tr}\,\sigma_2 = 1. \end{aligned}$$

where P is the projector onto the viable set produced by the energetic program (3).

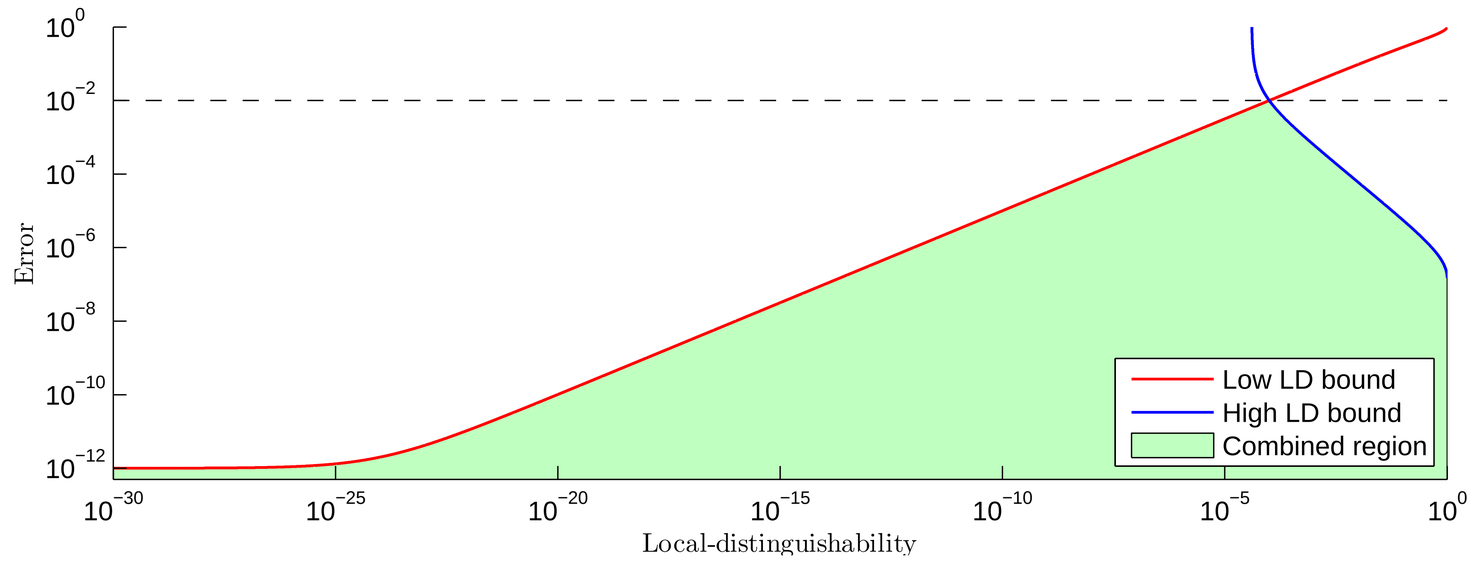

Figure 1: The maximum error levels of a second witness from both the energetic and orthogonality trimming programs, (3) and (4) respectively, in the case of a two-fold degeneracy. By taking our viable set to be the union of these results we can guarantee that our error level lies somewhere in the shaded region, below an overall error threshold (1% in this case).

Degenerate trimming

When trimming we attempt to throw out locally high energy states, whilst maintaining good approximations of our witness states. In the degenerate case care has to be taken that *all* such witnesses have this property. The subtle point is that while two ground states may be orthogonal on the whole system, this does not tell us how much the two states differ locally. As such the trimming procedure will have to vary according to the level of *local-distinguishability* (LD) of the states, which we might not know a priori.

Problem: Local-distinguishability

On the whole system generating a full set of ground states can be ensured by imposing the orthogonality condition (2), but this has no local analogue. Viable sets capture the local contributions to the witness states. If two desired witnesses have high LD, then constructing the viable set for the first witness which is orthogonal to that of the first, analogous to (2), would be appropriate. If however the two witnesses have low LD, then such a constraint would be inappropriate, giving a high error second witness.

Solution: A second trimming program

The problem of LD can be overcome by utilising *two* programs, known as the *Energetic* and *Orthogonality* trimming programs, which are designed to produce low error witnesses in low and high LD regimes respectively. With an appropriate choice of constants, it can be guaranteed that the combination both programs will stay within a given error threshold for any LD (see Figure 1).

References

[1] J. Eisert, "Computational Difficulty of Global Variations in the Density Matrix Renormalization Group," *Physical Review Letters*, **97**, p. 260501, arXiv:quant-ph/0609051, (2006).

[2] Z. Landau, U. Vazirani, and T. Vidick, "A polynomial time algorithm for the ground state of one-dimensional gapped local Hamiltonians," *Nature Physics*, **11**, p. 566-569, arXiv:1307.5143, (2013).

[3] Y. Huang, "A polynomial-time algorithm for approximating the ground state of 1D gapped Hamiltonians," arXiv:1406.6355v1, (2014).

[4] J. Eisert, M. Cramer, and M. B. Plenio, "Colloquium: Area laws for the entanglement entropy," *Reviews of Modern Physics*, **82**, p. 277–306, arXiv:0808.3773, (2010).

[5] M. B. Hastings, "An area law for one-dimensional quantum systems," *Journal of Statistical Mechanics*, arXiv:0705.2024, (2007).

[6] Y. Huang, "Area law in one dimension: Renyi entropy and degenerate ground states," arXiv:1403.0327, (2014).

[7] F. Verstraete and J. Cirac, "Matrix product states represent ground states faithfully," *Physical Review B*, **73**, p. 094423, arXiv:cond-mat/0505140, (2006).