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Chapter 1

Introduction

In general, a complex $M \times M$ matrix is a density matrix if it is:

1. Hermitian, $\rho = \rho^\dagger$
2. positive, $\rho \geq 0$
3. normalized, $Tr\rho = 1$

The set of density matrices is convex set and its extremal points are the pure states obeying $\rho^2 = \rho$ We can write a state ρ as

$$\rho = \frac{1}{M}\mathbb{I} + \sum_{i=1}^{M^2-1} \tau_i \sigma_i$$

where σ_i are generators of $SU(M)$ obeying

$$\sigma_i \sigma_j = \frac{2}{M}\delta_{ij} + d_{ijk}\sigma_k + i f_{ijk}\sigma_k.$$

f_{ijk} is totally antisymmetric and equals the Levi-Civita-Symbol for $M = 2$, d_{ijk} is totally symmetric and vanishing for $M = 2$. This is the Bloch representation of quantum states. We can construct the generators as follows:[1]

$$\{\sigma_i\}_{i=1}^{M^2-1} = \{u_{jk}, v_{jk}, w_l\}.$$

where

$$u_{jk} = |k\rangle\langle k| + |k\rangle\langle j|\,,\ v_{jk} = -i(|j\rangle\langle k| - |k\rangle\langle j|),$$

$$w_l = \sqrt{\frac{2}{l(l+1}} \sum_{j=1}^{l} \left(|j\rangle\langle j| - l\,|l+1\rangle\langle l+1|\right),$$

$$1 \leq j \leq k \leq M, 1 \leq l \leq M-1$$

The τ_i are the components of the $M^2 - 1$ dimensional bloch vector and are the expectation values of the σ_i:

$$\tau_i = Tr(\rho\sigma_i)$$

For $M = 2$ the positivity property is equivalent to $Tr\rho^2 \leq Tr\rho$, therefore we have $|\tau| \leq 1$ and characterize the Bloch-vector-space with as a Ball with Radius 1. The generators of $SU(2)$ are the Pauli-matrices

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

For $M \geq 3$ there are bloch vectors which do not correspond to a positive semi-definite matrix. The space spanned by the bloch-vectors is therefore a solid ball with radius 1. The generators of $SU(3)$ are the Gell-Mann-matrices.
In quantum computing, we mostly deal with N 2-level systems, the compositie space of which is $H = H_1 \otimes H_2 \otimes \ldots \otimes H_N$ In this space, there are states ρ which can not be expressed through a tensor product of states in the subsystems $\rho = \rho_1 \otimes \rho_2 \ldots \otimes \rho_N$. We call these states entangled states. States which can be expressed as such are called seperable or product states.

A k-local-Hamiltonian is a hermitian matrix acting on N qudits, which can be written as a sum of Hamiltonians where each acts on at most k qudits. Specifically, here we look at 2-local-Hamiltonians on qubits of the form

$$H = H_1 + H_2.$$

where

$$H_1 = \sum_{j=1}^{3n} D_j P_j, \; H_2 = \sum_{i,j=1}^{3n} C_{i,j} P_i P_j.$$

with the Pauli-operators

$$P_{3a-2} = X_a, \; P_{3a-1} = Y_a, \; P_{3a} = Z_a.$$

Finding the maximal eigenvalue of such a Hamiltonian is relevant to condensed matter and chemistry. This is equivalent to finding the minimal eigenvalue, because $\lambda_{max}(-H) = \lambda_{min}(H)$. [2] We call this the local-Hamiltonian problem, and it is correlated to finding the energy of a system at low temeratures. Since the quantum state achieving this optimal value might be an entangled state which might not be computable in polynomial time, we are interested in finding the product state that achieves the best approximation.
As an elementary example, let us look at a two qubit Hamiltonian:

$$H = X_1 X_2 + Z_1 Z_2.$$

The state achieving the maximal eigenvalue $\lambda_{max} = 2$ is the bell state $|bell\rangle = \frac{\langle 00| + \langle 11|}{\sqrt{2}}$. This is a maximally entangled state. To find out the product state which approximates this the best, look at a general product state and maximize the overlap.

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle = (a_1 |0\rangle + b_1 |1\rangle) \otimes (a_2 |0\rangle + b_2 |1\rangle).$$

with $a_1^2 + b_1^2 = a_2 + b_2^2 = 1$

$$\max_{\psi_1,\psi_2} \left(|\langle bell| \psi \rangle|^2 \right) = \max \left(\left| \frac{1}{\sqrt{2}} (a_1 a_2 + b_1 b_2) \right|^2 \right) = \frac{1}{2}.$$

With either $a_1 = a_2 = 1$ and $b_1 = b_2 = 0$ or $b_1 = b_2 = 1$ and $a_1 = a_2 = 0$. Therefore, the product states with the maximal overlap are $|00\rangle$ and $|11\rangle$ with maximal eigenvalue $\lambda_{sep} = 1$, the approximation ratio being $\frac{\lambda_{sep}}{\lambda_{max}} = 0.5$

The local-Hamiltonian problem is equivalent to constraint satisfaction problems in classical computational theory. It is in the complexity class QMA, which is the quantum analogue to the NP complexity class. It is QMA-complete, meaning that, additionally to being in the class itself, every problem in QMA can be reduced to the local-Hamiltonian problem.[3] Reduction means that for predicates L_1 and L_2 there is a polynomial f, such that $L_1(x) = L_2(f(x))$. We say that f reduces L_1 to L_2 polynomially.[4] It is intructive to think about finding the maximal (or minimal) eigenvalue of such a Hamiltonian as equivalent to the weighted max-cut-problem. Given a Graph $G = (V, E)$, we think about the spin-sites as our vertices, and C as our weighted edges. The task now is to find a maximum cut, which is in NP. This means we cut the graph into two sets of vertices, such that the sum of weights that we cut through is maximized. The most successful classical approximation algorithm for this problem by Goemans and Williamson uses semidefinite programming and randomized rounding. [5] The algorithm discussed here parallelizes this for the quantum case. It is based on relaxation of a semidefinite program.

In semidefinite programing we try to maximize a linear function, such that an affine combination of symmetric matrices is positive semidefinite. [6] An affine combination is a linear combination $\sum_{i=1}^{n} a_i x_i$ where x_i are elements of a vector space, such that $\sum_{i=1}^{n} a_i = 1$ Semidefinite programs are very useful, as they can be solved efficiently both in theory and in practice.

For approximating the optimal solution to the max-cut problem, Goemans and Williamson [5] start with reformulating the problem itself:

$$\text{Maximize } \frac{1}{2} \sum_{i<j} w_{i,j} (1 - y_i y_j)$$

$$\text{subject to: } y_i \in S = \{-1, 1\} \, \forall i \in V$$

given a vertex set $V = \{1, \ldots n\}$ and non-negative weights $w_{i,j} = w_{j,i}$. We call this a quadratic program. As this is in NP, we need to relax the constraints. This is accomplished by extending the objective function to a larger space, namely $S^{n-1} = \{-1, 1\}^{n-1}$. We then have to consider vectors v_i and look at the inner product $v_i \cdot v_j$

The program therefore changes accordingly:

$$\text{Maximize } \frac{1}{2}\sum_{i<j} w_{i,j}\,(1 - v_i v_j)$$
$$\text{subject to: } v_i \in S^n = \{-1, 1\}^n \,\forall i \in V$$

The algorithm that approximates the solution is:

1. Solve the relaxed semidefinite program, obtaining an optimal set of vectors v_i
2. Let r be a vector uniformly distributed on the unit sphere
3. Set the cut to $S = \{i | v_i \cdot r \geq 0\}$

We can build a good geometrical intuition for this. Think of the vector r as the normal of a hyperplane through the origin, and partition the vertices into ones that lie below it and above it. This algorithm has an approximation rate of 0.878.

Chapter 2

Approximation algorithms for the maximal energy of 2-local-Hamiltonians

The algorithm shown in the paper proceeds in the same way as the algorithm for the classical max-cut problem. The aim is to find bounds for the maximum energy of 2-local-Hamiltonians. Before looking at the algorithm itself, there are some prelimaries we have to look at. We Hamiltonians of the kind $H = H_1 + H_2$ where $H_1 = \sum_{j=1}^{3n} D_j P_j,\ H_2 = \sum_{i,j=1}^{3n} C_{i,j} P_i P_j$ have terms, that are linear in Pauli operators. For the theorems presented in this paper, the following lemma will enable us to reduce this Hamiltonian to a purely quadratic one. We form a new $n+1 qubit$ Hamiltonian:

$$H' = H_2 + Z_{n+1} H_1.$$

Lemma1 $\lambda_{max}(H') = \lambda_{max}(H)$. Moreover, given any $(n+1)$-qubit state ω we can efficiently compute an n-qubit state ϕ such that

$$\langle \phi | H | \phi \rangle \geq \langle \omega | H' | \omega \rangle ..$$

If ω is a tensor product of single qubit stabilizer states then so is ϕ. The idea is now, that for any $n - qubit$ Hamiltonian with linear terms, there is a purely quadratic $(n+1)$-qubit Hamiltonian that has the same maximal eigenvalue and has an at best equally good product state approximation. Therefore, the bounds that we proof for quadratic Hamiltonians are valid also for Hamiltonians with linear terms. This enables us to set $H_1 = 0$ The proof idea is that all eigenvalues of H' are either eigenvalues of $H_2 - H_1$ or $H_1 + H_2$, and that $H_2 - H_1$ can be obtained from $H_1 + H_2$ by operations that conserve the spectrum. We can then choose the product state $|\phi\rangle$ according to $|\omega\rangle$, such that its eigenvalues will always be at least equal.
The last statement in the lemma references an elegant concept that is very useful to quantum error correction. We say an operator A stabilizes a state $|\psi\rangle$ if $A|\psi\rangle = |\psi\rangle$. Conversely, a state is called a stabilizer state of an operator, if it is in its $+1$-eigenspace. For practicality, we look at operators from the n-qubit Pauli group. This is favorable because they are unitary and their eigenvalues (± 1) differ

significantly from another, such that we can easily perform phase estimations to find out the eigenvalue. If we are given a set of operators $S = \{A, B, C \ldots\}$, we know that any errors (which are also from the Pauli group) either commute or anticommute with elements in S. One can correct any error E that anticommutes with S, and if the error lies in S it is correctable if they commute with S.[7] We say an operator commutes with a group, or is in the normalizer of the group, if for some $A, B \in S$: $EA = BE$ with possibly $A \neq B$. This criterion is very easy to check and gives us a useful mathematical toolbox.

...In our case, the semidefinite program is:

$$\begin{aligned} max\ tr\left(CM\right) \\ s.t. M_{i,i} = 1 \\ M \geq 0 \end{aligned}$$

where M is a real symmetric matrix. This is without loss of generality, as it does not change the outcome of the objective function. The ideal solution M is connected to our state in the following way:[2]

$$M_{i,j} = tr\left(\rho P_i P_j\right) \ \ i, j = 1 \ldots 3n.$$

From this perspective. the constraints can be understood in the following way:

$$M_{i,i} = tr\left(\rho P_i P_i\right) = tr\left(\rho\right) = 1$$

since $P_i P_i = 1$

$$M \geq 0 \leftrightarrow x^T M x = tr\left(\rho\left(\sum_i^{3n} x_i P_i\right)\left(\sum_j^{3n} x_j P_j\right)\right) = tr\left(\rho X^2\right) \geq 0$$

where $X = \sum_i^{3n} x_i P_i$ and since $X^2, \rho \geq 0$

Appendix A

A

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