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Chapter 1

Introduction

The aim of this thesis is to introduce the reader to quantum approximation algorithms in general, with special focus on the algorithm by Bravyi et al. [1]. Therefore, I will start with an introduction to the necessary mathematical concepts and to product state approximation. Furthermore, 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:[2]

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

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 $\lambda_{max}(-H) = \lambda_{min}(H)$. [3] 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 EPR-state $|EPR\rangle = \frac{\langle 00|+\langle 11|}{\sqrt{2}}$. 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 $a_1^2 + b_1^2 = a_2 + b_2^2 = 1$

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

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.[4] 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.[5] 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 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. [6] The algorithm discussed here parallelizes this for the quantum case and is based on relaxation of a semidefinite program.

With semidefinite programing we try to maximize a linear function, such that an affine combination of symmetric matrices is positive semidefinite. [7] 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 [6] 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 $V = \{1, \dots n\}$ 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 $S^n = \{-1, 1\}^n$. We then have to consider vectors v_i and look at the inner product $v_i \cdot v_j$ The program therefore changes accordingly:

$$\text{Maximize } \frac{1}{2} \sum_{i<j} w_{i,j} \left(1 - v_i v_j\right)$$

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

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 maximum 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 is a prelimary lemma we have to look at. 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.[8] 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.

We will now look at the algorithm presented, and then understand the ideas as to why it is indeed accurate. It is largely in parallel to the classical max-cut approximation algorithm by Goemans and Williamson. 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. We can understand this better, if we look at the following representation. The ideal solution M is connected to our state in the following way:[3]

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

Setting M as a real symmetric matrix is without loss of generality, because if the Pauli operators act on different matrices they commute, and therefore the matrix entry is real in this case. If they act on the same qubit, the matrix entry is purely imaginary because the operators anticommute. We can eliminate these terms using $M' = \frac{M+M*}{2}$ because they represent linear terms. This does not change the outcome of the objective function and is therefore fully without loss of generality. 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 $X^2, \rho \geq 0$

Since M is real and symmetric, we can express any matrix element as $M_{i,j} = \left\langle v^i \middle| v^j \right\rangle$ for some unit vectors $v^1, v^2, \ldots, v^{3n+1}$. The vectors have unit norm, since $M_{i,i} = 1$. What we have done until now substitutes for the first step in the classical version. In the quantum version, we can interpret the geometry in a different, more instructive way. Since we have to preserve the mathematical structure that states have to fulfill.

Geometrically, this means that our blochvectors are restricted to a sphere of radius one. Since we will still project our optimal vectors obtained from the semidefinite program to a random hyperplane through the origin, we have to make sure trough rounding, that the projections correspond to valid bloch vector components. The way to ensure this is quite elegant. We ask the following question: What is the maximal value that a component of a valid bloch vector can have, if all three components have the same value? In other words, if we pick every value without knowing the others, what is the maximal value that we can assign to it so that it is part of the unit sphere?

$$\|z\| = \sqrt{z_1^2 + z_2^2 + z_3^2} = \sqrt{3z_1^2} = 1.$$

Therefore the maximal value, above which we should round down is $\frac{1}{\sqrt{3}}$. If we round such that no bloch vector component can be above this value, we will always have a valid state. Visually, this is the same as fitting a cube inside the bloch sphere and reducing our state space to inside the cube. The edges of the cube which touch the sphere are the pure states that are possible if all components are ± 1. The projections are $z_i = \frac{\langle r|v^i\rangle}{c\sqrt{\log n}}$ with $c = O(\log n)$. The algorithm looks like this:

1. Solve the relaxed semidefinite program, obtaining an optimal set of vectors v_i
2. Let $|r\rangle$ be a vector of $3n$ indepently and identically distributed $N(0,1)$ random variables
3. If $|z_i| > \frac{1}{\sqrt{3}}$, we round down: $y_i = \frac{sgn(z_i)}{\sqrt{3}}$. Otherwise $y_i = z_i$.

As output we take $\rho = \rho_1 \otimes \ldots \otimes \rho_n$ where:

$$\rho_a = \frac{1}{2}\left(\mathbb{I} + y_{3a-2}P_{3a-2} + y_{3a-1}P_{3a-1} + y_{3a}P_{3a}\right)..$$

The energy of this system is then

$$Tr\left(H\rho\right) = y^T C y.$$

This is the approximation to the maximum eigenvalue. One now has to think about why this works and how good the approximation is. In the introduction, we have found the best product approximation that can be found for the EPR-state. Generally, the optimal product state is not feasible to find, but it important find general bounds, how good or bad this approximation can be. We call the highest eigenvalue achievable by a product state:

$$\lambda_{sep}(H) = \max_{\phi_1,\ldots,\phi_n} \langle \phi_1 \otimes \phi_2 \otimes \ldots \otimes \phi_n | \, H \, | \phi_1 \otimes \phi_2 \otimes \ldots \otimes \phi_n \rangle .$$

We know the following:
Suppose H is traceless 2-local Hamiltonian. then

$$\lambda_{sep}(H) \geq \frac{1}{9}\lambda_{max}(H).$$

We can proof this using entanglement-breaking depolarizing channels. Depolarizing channels are a simple model for noise in quantum information theory. [9] They are implemented by a map Δ_λ, which maps a state ρ into a linear combination of itself and the identity matrix:[10]

$$\Delta_\lambda(\rho) = \lambda\rho + \frac{1-\lambda}{d}\mathbb{I}, .$$

where d is the dimension of state. The parameter λ must satisfy

$$-\frac{1}{d^2-1} \leq \lambda \leq_1 .$$

This channel maps pure states to mixed states and all output states have eigenvalues $\lambda + \frac{1-\lambda}{d}$ (multiplicity 1) and $\frac{1-\lambda}{d}$ (multiplicity $d-1$). For $\lambda = 0$ we get the maximally noisy channel, for $\lambda = 1$ the identity. In our case we look at entanglement breaking channels. These are channels for which the output state is always seperable, i.e. if any entangled density matrix is mapped to a seperable one.[**horodecki08**] Here, the relevant map is defined by its action on the Pauli group.

Appendix A

A

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