Chapter 1

Ground energy of quantum walk

To get some flavor for QMA-completeness results.

1.1 Encoding computations as states

1.1.1 History states

1.2 Determining ground energy of a sparse adjacency matrix is QMA-complete

1.2.1 Kitaev Hamiltonian

1.2.2 Transformation to Adjacency Matrix

We suppose $\mathcal{C}_x$ implements a unitary

$$U_{\mathcal{C}_x} = U_M \dots U_2 U_1 \tag{1.1}$$

where each U_i is from the universal gate set

$$\mathcal{G} = \{H, HT, (HT)^\dagger, (H \otimes \mathbb{I})\,\text{CNOT}\}$$

with

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix} \quad \text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

The verification circuit $\mathcal{C}_x$ has an n_{input}-qubit input register and $n - n_{\text{input}}$ ancilla qubits initialized to $|0\rangle$ at the beginning of the computation. One of these n qubits serves as an output qubit.

It will be convenient to consider

$$U_{\mathcal{C}_x}^\dagger U_{\mathcal{C}_x} = W_{2M} \dots W_2 W_1$$

where

$$W_t = \begin{cases} U_t & 1 \le t \le M \\ U^\dagger_{2M+1-t} & M+1 \le t \le 2M. \end{cases}$$

As in Section **??** we start with a version of the Feynman-Kitaev Hamiltonian [**?**, **?**]

$$H_x = -\sqrt{2}\sum_{t=1}^{2M}\left(W_t^\dagger \otimes |t\rangle\langle t+1| + W_t \otimes |t+1\rangle\langle t|\right) \tag{1.2}$$

acting on the Hilbert space $\mathcal{H}_{\text{comp}} \otimes \mathcal{H}_{\text{clock}}$ where $\mathcal{H}_{\text{comp}} = (\mathbb{C}^2)^{\otimes n}$ is an n-qubit computational register and $\mathcal{H}_{\text{clock}} = \mathbb{C}^{2M}$ is a $2M$-level register with periodic boundary conditions (i.e., we let $|2M+1\rangle = |1\rangle$). Note that

$$V^\dagger H_x V = -\sqrt{2}\sum_{t=1}^{2M}\left(\mathbb{I} \otimes |t\rangle\langle t+1| + \mathbb{I} \otimes |t+1\rangle\langle t|\right) \tag{1.3}$$

where

$$V = \sum_{t=1}^{2M}\left(\prod_{j=t-1}^{1} W_j\right) \otimes |t\rangle\langle t|$$

and $W_0 = 1$. Since V is unitary, the eigenvalues of H_x are the same as the eigenvalues of (**??**), namely

$$-2\sqrt{2}\cos\left(\frac{\pi\ell}{M}\right)$$

for $\ell = 0, \ldots, 2M-1$. The ground energy of (**??**) is $-2\sqrt{2}$ and its ground space is spanned by

$$|\phi\rangle \frac{1}{\sqrt{2M}}\sum_{j=1}^{2M}|t\rangle, \quad |\phi\rangle \in \Lambda$$

where Λ is any orthonormal basis for $\mathcal{H}_{\text{comp}}$. A basis for the ground space of H_x is therefore

$$V\left(|\phi\rangle\frac{1}{\sqrt{2M}}\sum_{j=1}^{2M}|t\rangle\right) = \frac{1}{\sqrt{2M}}\sum_{t=1}^{2M} W_{t-1}W_{t-2}\ldots W_1|\phi\rangle|t\rangle$$

where $|\phi\rangle \in \Lambda$. The first excited energy of H_x is

$$\eta = -2\sqrt{2}\cos\left(\frac{\pi}{M}\right)$$

and the gap between ground and first excited energies is lower bounded as

$$\eta + 2\sqrt{2} \ge \sqrt{2}\frac{\pi^2}{M^2} \tag{1.4}$$

(using the fact that $1 - \cos(x) \le \frac{x^2}{2}$).

The universal set $\mathcal{G}$ is chosen so that each gate has nonzero entries that are integer powers of $\omega = e^{i\frac{\pi}{4}}$. Correspondingly, the nonzero standard basis matrix elements of H_x are also integer powers of $\omega = e^{i\frac{\pi}{4}}$. We consider the 8×8 shift operator

$$S = \sum_{j=0}^{7} |j+1 \bmod 8\rangle\langle j|$$

and note that ω is an eigenvalue of S with eigenvector

$$|\omega\rangle = \frac{1}{\sqrt{8}} \sum_{j=0}^{7} \omega^{-j}|j\rangle.$$

We modify H_x as follows. For each operator $-\sqrt{2}H$, $-\sqrt{2}HT$, $-\sqrt{2}(HT)^{\dagger}$, or $-\sqrt{2}\,(H \otimes \mathbb{I})\,\mathrm{CNOT}$ appearing in equation (**??**), define another operator that acts on $\mathbb{C}^2 \otimes \mathbb{C}^8$ or $\mathbb{C}^4 \otimes \mathbb{C}^8$ (as appropriate) by replacing nonzero matrix elements with powers of the operator S:

$$\omega^k \mapsto S^k.$$

Matrix elements that are zero are mapped to the 8×8 all-zeroes matrix. Write $B(W)$ for the operators obtained by making this replacement, e.g.,

$$-\sqrt{2}HT = \begin{pmatrix} \omega^4 & \omega^5 \\ \omega^4 & \omega \end{pmatrix} \mapsto B(HT) = \begin{pmatrix} S^4 & S^5 \\ S^4 & S \end{pmatrix}.$$

Adjoining an 8-level ancilla as a third register and making this replacement in equation (**??**) gives

$$H_{\mathrm{prop}} = \sum_{t=1}^{2M} \Big(B(W_t)^{\dagger}_{13} \otimes |t\rangle\langle t+1|_2 + B(W_t)_{13} \otimes |t+1\rangle\langle t|_2 \Big) \tag{1.5}$$

which is a symmetric 0-1 matrix (the subscripts indicate which registers the operators act on). Note that H_{prop} commutes with S (acting on the 8-level ancilla) and therefore is block diagonal with eight sectors. In the sector where S has eigenvalue ω, H_{prop} is identical to the Hamiltonian H_x that we started with (see equation (**??**)). There is also a sector (where S has eigenvalue ω^*) where the Hamiltonian is the complex conjugate of H_x. We will add a term to H_{prop} that introduces an energy penalty for states in any of the other six sectors, ensuring that none of these states lie in the ground space.

To see what kind of energy penalty is needed, we lower bound the eigenvalues of H_{prop}. Note that for each $W \in \mathcal{G}$, $B(W)$ contains at most 2 ones in each row or column. Looking at equation (**??**) and using this fact, we see that each row and each column of H_{prop} contains at most four ones (with the remaining entries all zero). Therefore $\|H_{\mathrm{prop}}\| \leq 4$, so every eigenvalue of H_{prop} is at least -4.

The matrix A_x associated with the circuit $\mathcal{C}_x$ acts on the Hilbert space

$$\mathcal{H}_{\mathrm{comp}} \otimes \mathcal{H}_{\mathrm{clock}} \otimes \mathcal{H}_{\mathrm{anc}}$$

where $\mathcal{H}_{\text{anc}} = \mathbb{C}^8$ holds the 8-level ancilla. We define

$$A_x = H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} + H_{\text{output}} \tag{1.6}$$

where

$$H_{\text{penalty}} = \mathbb{I} \otimes \mathbb{I} \otimes \left(S^3 + S^4 + S^5\right)$$

is the penalty ensuring that the ancilla register holds either $|\omega\rangle$ or $|\omega^*\rangle$ and the terms

$$H_{\text{input}} = \sum_{j=n_{\text{input}}+1}^{n} |1\rangle\langle 1|_j \otimes |1\rangle\langle 1| \otimes \mathbb{I}$$
$$H_{\text{output}} = |0\rangle\langle 0|_{\text{output}} \otimes |M+1\rangle\langle M+1| \otimes \mathbb{I}$$

ensure that the ancilla qubits are initialized in the state $|0\rangle$ when $t = 1$ and that the output qubit is in the state $|1\rangle\langle 1|$ when the circuit $\mathcal{C}_x$ has been applied (i.e., at time $t = M + 1$). Observe that A_x is a symmetric 0-1 matrix.

Now consider the ground space of the first two terms $H_{\text{prop}} + H_{\text{penalty}}$ in (**??**). Note that $[H_{\text{prop}}, H_{\text{penalty}}] = 0$, so these operators can be simultaneously diagonalized. Furthermore, H_{penalty} has smallest eigenvalue $-1-\sqrt{2}$, with eigenspace spanned by $|\omega\rangle$ and $|\omega^*\rangle$. One can also easily confirm that the first excited energy of H_{penalty} is -1.

The ground space of $H_{\text{prop}} + H_{\text{penalty}}$ lives in the sector where H_{penalty} has minimal eigenvalue $-1-\sqrt{2}$. To see this, note that within this sector H_{prop} has the same eigenvalues as H_x, and therefore has lowest eigenvalue $-2\sqrt{2}$. The minimum eigenvalue e_1 of $H_{\text{prop}} + H_{\text{penalty}}$ in this sector is

$$e_1 = -2\sqrt{2} + \left(-1 - \sqrt{2}\right) = -1 - 3\sqrt{2} = -5.24\ldots, \tag{1.7}$$

whereas in any other sector H_{penalty} has eigenvalue at least -1 and (using the fact that $H_{\text{prop}} \geq -4$) the minimum eigenvalue of $H_{\text{prop}} + H_{\text{penalty}}$ is at least -5. Thus, an orthonormal basis for the ground space of $H_{\text{prop}} + H_{\text{penalty}}$ is furnished by the states

$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} W_{t-1}W_{t-2}\ldots W_1 |\phi\rangle|t\rangle|\omega\rangle \tag{1.8}$$
$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} (W_{t-1}W_{t-2}\ldots W_1)^* |\phi^*\rangle|t\rangle|\omega^*\rangle \tag{1.9}$$

where $|\phi\rangle$ ranges over the basis Λ for $\mathcal{H}_{\text{comp}}$ and $*$ denotes (elementwise) complex conjugation.

1.2.3 Upper bound on the smallest eigenvalue for yes instances

Suppose x is a yes instance; then there exists some n_{input}-qubit state $|\psi_{\text{input}}\rangle$ satisfying $\text{AP}\left(\mathcal{C}_x, |\psi_{\text{input}}\rangle\right) \geq 1 - \frac{1}{2^{|x|}}$. Let

$$|\text{wit}\rangle = \frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} W_{t-1}W_{t-2}\ldots W_1 \left(|\psi_{\text{input}}\rangle|0\rangle^{\otimes n - n_{\text{input}}}\right) |t\rangle|\omega\rangle$$

and note that this state is in the e_1-energy ground space of $H_{\text{prop}} + H_{\text{penalty}}$ (since it has the form (**??**)). One can also directly verify that $|\text{wit}\rangle$ has zero energy for H_{input}. Thus

$$\begin{aligned}\langle \text{wit}|A_x|\text{wit}\rangle &= e_1 + \langle \text{wit}|H_{\text{output}}|\text{wit}\rangle \\ &= e_1 + \frac{1}{2M}\langle \psi_{\text{input}}|\langle 0|^{\otimes n-n_{\text{input}}} U^{\dagger}_{\mathcal{C}_x}|0\rangle\langle 0|_{\text{output}} U_{\mathcal{C}_x}|\psi_{\text{input}}\rangle|0\rangle^{\otimes n-n_{\text{input}}} \\ &= e_1 + \frac{1}{2M}\left(1 - \text{AP}(\mathcal{C}_x, |\psi_{\text{input}}\rangle)\right) \\ &\leq e_1 + \frac{1}{2M}\frac{1}{2^{|x|}}.\end{aligned}$$

1.2.4 Lower bound on the smallest eigenvalue for no instances

Now suppose x is a no instance. Then the verification circuit $\mathcal{C}_x$ has acceptance probability $\text{AP}\left(\mathcal{C}_x, |\psi\rangle\right) \leq \frac{1}{3}$ for all n_{input}-qubit input states $|\psi\rangle$.

We backtrack slightly to obtain bounds on the eigenvalue gaps of the Hamiltonians $H_{\text{prop}}+H_{\text{penalty}}$ and $H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}}$. We begin by showing that the energy gap of $H_{\text{prop}} + H_{\text{penalty}}$ is at least an inverse polynomial function of M. Subtracting a constant equal to the ground energy times the identity matrix sets the smallest eigenvalue to zero, and the smallest nonzero eigenvalue satisfies

$$\gamma(H_{\text{prop}} + H_{\text{penalty}} - e_1 \cdot \mathbb{I}) \geq \min\left\{\sqrt{2}\frac{\pi^2}{M^2}, -5 - e_1\right\} \geq \frac{1}{5M^2}. \tag{1.10}$$

since $-5 - e_1 \approx 0.24\ldots > \frac{1}{5}$. The first inequality above follows from the fact that every eigenvalue of H_{prop} in the range $[e_1, -5)$ is also an eigenvalue of H_x (as discussed above) and the bound (**??**) on the energy gap of H_x.

Now use the Nullspace Projection Lemma (Lemma **??**) with

$$H_A = H_{\text{prop}} + H_{\text{penalty}} - e_1 \cdot \mathbb{I} \qquad H_B = H_{\text{input}}.$$

Note that H_A and H_B are positive semidefinite. Let S_A be the ground space of H_A and consider the restriction $H_B|_{S_A}$. Here it is convenient to use the basis for S_A given by (**??**) and (**??**) with $|\phi\rangle$ ranging over the computational basis states of n qubits. In this basis, $H_B|_{S_A}$ is diagonal with all diagonal entries equal to $\frac{1}{2M}$ times an integer, so $\gamma(H_B|_{S_A}) \geq \frac{1}{2M}$. We also have $\gamma(H_A) \geq \frac{1}{5M^2}$ from equation (**??**), and clearly $\|H_B\| \leq n$. Thus Lemma **??** gives

$$\gamma(H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} - e_1 \cdot \mathbb{I}) \geq \frac{\left(\frac{1}{5M^2}\right)\left(\frac{1}{2M}\right)}{\frac{1}{5M^2} + \frac{1}{2M} + n} \geq \frac{1}{10M^3\left(1+n\right)} \geq \frac{1}{20M^3 n}. \tag{1.11}$$

Now consider adding the final term H_{output}. We use Lemma **??** again, now setting

$$H_A = H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} - e_1 \cdot \mathbb{I} \qquad H_B = H_{\text{output}}.$$

Let S_A be the ground space of H_A. Note that it is spanned by states of the form (**??**) and (**??**) where $|\phi\rangle = |\psi\rangle|0\rangle^{\otimes n-n_{\text{input}}}$ and $|\psi\rangle$ ranges over any orthonormal basis of the n_{input}-qubit input register. The restriction $H_B|_{S_A}$ is block diagonal, with one block for states of the form

$$\frac{1}{\sqrt{2M}}\sum_{t=1}^{2M} W_{t-1}W_{t-2}\dots W_1\left(|\psi\rangle|0\rangle^{\otimes n-n_{\text{input}}}\right)|t\rangle|\omega\rangle \tag{1.12}$$

and another block for states of the form

$$\frac{1}{\sqrt{2M}}\sum_{t=1}^{2M} (W_{t-1}W_{t-2}\dots W_1)^*\left(|\psi\rangle^*|0\rangle^{\otimes n-n_{\text{input}}}\right)|t\rangle|\omega^*\rangle. \tag{1.13}$$

We now show that the minimum eigenvalue of $H_B|_{S_A}$ is nonzero, and we lower bound it. We consider the two blocks separately. By linearity, every state in the first block can be written in the form (**??**) for some state $|\psi\rangle$. Thus the minimum eigenvalue within this block is the minimum expectation of H_{output} in a state (**??**), where the minimum is taken over all n_{input}-qubit states $|\psi\rangle$. This is equal to

$$\min_{|\psi\rangle}\frac{1}{2M}\left(1-\text{AP}(\mathcal{C}_x,|\psi\rangle)\right)\geq\frac{1}{3M}$$

where we used the fact that $\text{AP}\left(\mathcal{C}_x,|\psi\rangle\right)\leq\frac{1}{3}$ for all $|\psi\rangle$. Likewise, every state in the second block can be written as (**??**) for some state $|\psi\rangle$, and the minimum eigenvalue within this block is

$$\min_{|\psi\rangle}\frac{1}{2M}\left(1-\text{AP}(\mathcal{C}_x,|\psi\rangle)^*\right)\geq\frac{1}{3M}$$

(since $\text{AP}(\mathcal{C}_x,|\psi\rangle)^*=\text{AP}(\mathcal{C}_x,|\psi\rangle)\leq\frac{1}{3}$). Thus we see that $H_B|_{S_A}$ has an empty nullspace, so its smallest eigenvalue is equal to its smallest nonzero eigenvalue, namely

$$\gamma(H_B|_{S_A})\geq\frac{1}{3M}.$$

Now applying Lemma **??** using this bound, the fact that $\|H_B\|=1$, and the fact that $\gamma(H_A)\geq\frac{1}{20M^3n}$ (from equation (**??**)), we get

$$\gamma(A_x-e_1\cdot\mathbb{I})\geq\frac{\frac{1}{60M^4n}}{\frac{1}{20M^3n}+\frac{1}{3M}+1}\geq\frac{1}{120M^4n}.$$

Since $H_B|_{S_A}$ has an empty nullspace, $A_x-e_1\cdot\mathbb{I}$ has an empty nullspace, and this is a lower bound on its smallest eigenvalue.