Quantum algorithms (CO 781, Winter 2008)
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LECTURE 20: An example of the success of adiabatic optimization

In this lecture, we describe a simple example of a function that can be minimized by adiabatic optimization in polynomial time.

The ring of agrees Consider n bits $z_1, z_2, \ldots, z_n$ arranged on a ring. For each adjacent pair of bits, we include a clause that is satisfied if and only if the two bits are the same. This instance has exactly two satisfying assignments, namely those for which all the bits agree: $z_1 = z_2 = \cdots = z_n = 0$ and $z_1 = z_2 = \cdots = z_n = 1$. But even though it does not present a computational challenge, it is interesting to ask how well adiabatic optimization does on this simple "problem."

Summing over the n clauses, the cost function is

$$h(z) = \sum_{j=1}^{n} (1 - \delta_{z_j, z_{j+1}}) \tag{1}$$

$$= \sum_{j=1}^{n} \frac{1 - (2z_j - 1)(2z_{j+1} - 1)}{2} \tag{2}$$

where we make the identification $z_{n+1} := z_1$. Thus, the problem Hamiltonian can be written in terms of Pauli operators as

$$H_P := \sum_z h(z) |z\rangle\langle z| \tag{3}$$

$$= \frac{1}{2} \sum_{j=1}^{n} (1 - \sigma_z^{(j)} \sigma_z^{(j+1)}) \tag{4}$$

where we make the similar identification $\sigma_z^{(n+1)} := \sigma_z^{(1)}$. To prepare the ground state of H_P, we will use linear interpolation from a magnetic field in the x direction (i.e., the adjacency matrix of the hypercube), giving

$$H(s) = -(1-s) \sum_{j=1}^{n} \sigma_x^{(j)} + \frac{s}{2} \sum_{j=1}^{n} (1 - \sigma_z^{(j)} \sigma_z^{(j+1)}) \,. \tag{5}$$

To understand how well the resulting adiabatic algorithm performs, we would like to calculate the gap $\Delta(s)$ of this Hamiltonian as a function of s. Strictly speaking, this gap is zero, since the final ground state is degenerate: any state in the two-dimensional subspace $\mathrm{span}\{|0 \ldots 0\rangle, |1 \ldots 1\rangle\}$ has zero energy. However, note that the Hamiltonian commutes with the operator

$$G := \prod_{j=1}^{n} \sigma_x^{(j)} \,, \tag{6}$$

and that the initial state $|S\rangle$ (where $S = \{0,1\}^n$) is an eigenstate of G with eigenvalue $+1$. The evolution takes place entirely within the $+1$ eigenspace of G, so we can restrict our attention to this subspace. So let $\Delta(s)$ denote the gap between the ground state of $H(s)$ and the first excited

state in the $+1$ eigenspace of G. This is the relevant gap for adiabatic evolution starting in $|S\rangle$, with the ultimate goal of producing the unique $G = +1$ ground state of H_P, the GHZ state

$$\frac{|0\ldots0\rangle + |1\ldots1\rangle}{\sqrt{2}}\,. \tag{7}$$

Measurement of this state in the computational basis will yield one of the two satisfying assignments of the n bits, each occurring with probability $1/2$.

The Hamiltonian (5) is well-known in statistical mechanics, where it is referred to as a ferromagnetic Ising model in a transverse magnetic field. It can be diagonalized using the Jordan-Wigner transform, which we describe next.

The Jordan-Wigner transformation: From spins to fermions The Jordan-Wigner transformation is a way of mapping a one-dimensional spin system to a system of free fermions. Since finding the spectrum of the resulting system of noninteracting fermions only requires diagonalizing an $n \times n$ matrix, whereas determining the spectrum of a generic system of n spins requires diagonalizing a $2^n \times 2^n$ matrix, the Jordan-Wigner transformation shows that one-dimensional spin systems are particularly simple, and provides a powerful tool for analyzing them.

We will focus on a one-dimensional Ising spin system in a transverse magnetic field, with nearest-neighbor couplings and magnetic fields that can vary arbitrarily from site to site. In other words,

$$H = \sum_{i=1}^{n} J_i\, \sigma_z^{(i)} \sigma_z^{(i+1)} + \sum_{i=1}^{n} h_i\, \sigma_x^{(i)} \tag{8}$$

for some values of the real numbers J_i and h_i. We may either have periodic boundary conditions (by identifying $\sigma_z^{(n+1)}$ with $\sigma_z^{(1)}$) or open boundary conditions (by setting $J_n = 0$).

The Jordan-Wigner transformation consists of the definition

$$a_j := \sigma_x^{(1)} \sigma_x^{(2)} \cdots \sigma_x^{(j-1)} \tilde{\sigma}_-^{(j)} 1^{(j+1)} \cdots 1^{(n)} \tag{9}$$

(which will turn out to be a fermion annihilation operator), where we have defined spin raising and lowering operators in the x basis,

$$\tilde{\sigma}_\pm := R \frac{\sigma_x \pm \mathrm{i}\sigma_y}{2} R \tag{10}$$

$$= |\mp\rangle\langle\pm| \tag{11}$$

where

$$R := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{12}$$

is the Hadamard transformation, and $|\pm\rangle := (|0\rangle \pm |1\rangle)/\sqrt{2}$ are the eigenvectors of σ_x.

To see that the a_j's correspond to fermion annihilation operators, we observe that a_j and

$$a_j^\dagger = \sigma_x^{(1)} \sigma_x^{(2)} \cdots \sigma_x^{(j-1)} \tilde{\sigma}_+^{(j)} 1^{(j+1)} \cdots 1^{(n)} \tag{13}$$

obey fermion anticommutation relations. In particular, let

$$\{A, B\} := AB + BA \tag{14}$$

denote the anticommutator. For $j < k$, we have

$$\{a_j, a_k\} = \{\tilde{\sigma}_-^{(j)}, \sigma_x^{(j)}\}\sigma_x^{(j+1)} \cdots \sigma_x^{(k-1)}\tilde{\sigma}_-^{(k)} = 0 \tag{15}$$

and

$$\{a_j, a_k^\dagger\} = \{\tilde{\sigma}_-^{(j)}, \sigma_x^{(j)}\}\sigma_x^{(j+1)} \cdots \sigma_x^{(k-1)}\tilde{\sigma}_+^{(k)} = 0. \tag{16}$$

On the other hand, for $j = k$ we have

$$\{a_j, a_j\} = \{\tilde{\sigma}_-^{(j)}, \tilde{\sigma}_-^{(j)}\} = 2(|+\rangle\langle -|+\rangle\langle -|)^{(j)} = 0 \tag{17}$$

$$\{a_j, a_j^\dagger\} = \{\tilde{\sigma}_-^{(j)}, \tilde{\sigma}_+^{(j)}\} = (|+\rangle\langle -|-\rangle\langle +| + |-\rangle\langle +|+\rangle\langle -|)^{(j)} = 1. \tag{18}$$

Thus we find the fermion anticommutation relations

$$\{a_j, a_k\} = 0 \tag{19}$$

$$\{a_j, a_k^\dagger\} = \delta_{j,k}. \tag{20}$$

To fermionize H, we need to express $\sigma_x^{(j)}$ and $\sigma_z^{(j)}\sigma_z^{(j+1)}$ in terms of fermion operators. The important point is that even though the a_j's and $a_j^\dagger$'s are highly nonlocal spin operators, certain local combinations of them correspond to local spin operators, and vice versa. For the magnetic field, we have

$$a_j^\dagger a_j = \tilde{\sigma}_+^{(j)}\tilde{\sigma}_-^{(j)} \tag{21}$$

$$= (|-\rangle\langle -|)^{(j)} \tag{22}$$

$$= \frac{1}{2}(1 - \sigma_x^{(j)}), \tag{23}$$

so

$$\sigma_x^{(j)} = 1 - 2a_j^\dagger a_j \tag{24}$$

$$= a_j a_j^\dagger - a_j^\dagger a_j . \tag{25}$$

For the Ising coupling term, we have (for $j = 1, 2, \ldots, n-1$),

$$(a_j^\dagger - a_j)(a_{j+1}^\dagger + a_{j+1}) = (\tilde{\sigma}_+^{(j)} - \tilde{\sigma}_-^{(j)})\sigma_x^{(j)}(\tilde{\sigma}_+^{(j+1)} + \tilde{\sigma}_-^{(j+1)}) \tag{26}$$

$$= \sigma_z^{(j)}\sigma_z^{(j+1)} . \tag{27}$$

If we want to use periodic boundary conditions, including the operator $\sigma_z^{(n)}\sigma_z^{(1)}$, then we have to treat it separately. We have

$$(a_n^\dagger - a_n)(a_1^\dagger + a_1) = \left(\prod_{j=1}^{n-1}\sigma_x^{(j)}\right)(\tilde{\sigma}_+^{(n)} - \tilde{\sigma}_-^{(n)})(\tilde{\sigma}_+^{(1)} + \tilde{\sigma}_-^{(1)}) \tag{28}$$

$$= -G\sigma_z^{(n)}\sigma_z^{(1)} \tag{29}$$

where G is the spin flip operator defined in (6). Since σ_x anticommutes with σ_z, the operator G commutes with each Ising coupling term, and thus commutes with any H of the form (8). Therefore,

to find the spectrum of H, it suffices to separately determine the spectra in the subspaces with $G = +1$ and $G = -1$.

Note that since $\sigma_x = (-1)^{\frac{1}{2}(1-\sigma_x)}$, we can write

$$G = (-1)^{\sum_{j=1}^n \frac{1}{2}(1-\sigma_x^{(j)})} \tag{30}$$

$$= (-1)^{\sum_{j=1}^n a_j^\dagger a_j}\,. \tag{31}$$

Thus the cases $G = +1$, $G = -1$ correspond to the cases of an even or an odd number of occupied fermion modes, respectively.

Overall, the Jordan-Wigner transformation results in the expression

$$H = \sum_{i=1}^n J_i'(a_i^\dagger - a_i)(a_{i+1}^\dagger + a_{i+1}) - \sum_{i=1}^n h_i(a_i^\dagger a_i - a_i a_i^\dagger) \tag{32}$$

where $a_{n+1} := a_1$, and where

$$J_i' := \begin{cases} J_i & i = 1, 2, \ldots, n-1 \\ -GJ_n & i = n\,. \end{cases} \tag{33}$$

Since this Hamiltonian is quadratic in the fermion operators, it corresponds to a collection of n free fermions. Now it remains to diagonalize such a Hamiltonian.

Diagonalizing a system of free fermions Consider the most general quadratic fermion Hamiltonian,

$$H = \sum_{j,k=1}^n (\mu_{jk}\, a_j^\dagger a_k + \nu_{jk}\, a_j a_k) + \text{h.c.} \tag{34}$$

Using the fermion anticommutation relations (19) and (20), we can rewrite this Hamiltonian as

$$H = \underline{a}^\dagger \begin{pmatrix} \mu & -\nu^* \\ \nu & -\mu^* \end{pmatrix} \underline{a} + \operatorname{tr}\mu \tag{35}$$

where μ and ν denote the matrices whose j, k entries are μ_{jk} and ν_{jk}, respectively, and $\underline{a}$ denotes the column vector whose first block has entries $a_1, \ldots, a_n$ and whose second block has entries $a_1^\dagger, \ldots, a_n^\dagger$. Since H is hermitian, we can always choose μ, ν so that $\mu = \mu^\dagger$ and $\nu = -\nu^T$.

We would like to define a change of basis to a new set of fermion operators $b_j, b_j^\dagger$ in which the Hamiltonian is diagonal. If we let

$$b_j := \sum_{k=1}^n (\kappa_{jk}\, a_k + \lambda_{jk}\, a_k^\dagger) \tag{36}$$

(sometimes referred to as a Bogoliubov transformation), then we have

$$\underline{b} = \begin{pmatrix} \kappa & \lambda \\ \lambda^* & \kappa^* \end{pmatrix} \underline{a}\,. \tag{37}$$

The matrices κ and λ are not arbitrary, since we require that the transformed b_j's and $b_j^\dagger$'s remain fermion operators, i.e., that they satisfy the fermion anticommutation relations

$$\{b_j, b_k\} = 0 \tag{38}$$

$$\{b_j, b_k^\dagger\} = \delta_{j,k}\,. \tag{39}$$

It is a good exercise to check that the condition that these relations are satisfied if an only if the matrix in (37) is unitary.

Although we will not describe the proof here,it turns out that any quadratic fermion Hamiltonian can be diagonalized by such a transformation. In particular, it is always possible to choose κ, λ so that

$$H = \underline{b}^\dagger \begin{pmatrix} \omega & 0 \\ 0 & -\omega \end{pmatrix} \underline{b} + \operatorname{tr} \mu \tag{40}$$

where ω is a diagonal matrix whose diagonal entries are the positive eigenvalues of the 2×2 block matrix (representing a $2n \times 2n$ matrix whose eigenvalues occur in $\pm$ pairs) appearing in (35). Expanding this expression, we have

$$H = \sum_{j=1}^{n} \omega_j (2 b_j^\dagger b_j - 1) + \operatorname{tr} \mu \tag{41}$$

where we have again used the fermion anticommutation relations. Since the $b_j^\dagger b_j$'s are commuting operators with eigenvalues 0 and 1, we see that spectrum of H is given by the 2^n numbers

$$\sum_{j=1}^{n} s_j \omega_j + \operatorname{tr} \mu \tag{42}$$

for each of the 2^n possible assignments of $s_1, s_2, \ldots, s_n = \pm 1$.

Calculating the eigenvalues ω_j is especially simple when μ, ν are real, as they are in the case of (32). In this case, we have (now treating R in (12) as a block matrix)

$$R \begin{pmatrix} \mu & -\nu \\ \nu & -\mu \end{pmatrix} R = \begin{pmatrix} 0 & \mu + \nu \\ \mu - \nu & 0 \end{pmatrix}\,. \tag{43}$$

Since the square of this matrix is

$$\begin{pmatrix} 0 & \mu + \nu \\ \mu - \nu & 0 \end{pmatrix}^2 = \begin{pmatrix} (\mu + \nu)(\mu - \nu) & 0 \\ 0 & (\mu - \nu)(\mu + \nu) \end{pmatrix}\,, \tag{44}$$

we see that the ω_j's are simply the positive square roots of the eigenvalues of the $n \times n$ matrix $(\mu + \nu)(\mu - \nu)$ (or equivalently, of $(\mu - \nu)(\mu + \nu)$).

Finally, we specialize to a Hamiltonian of the Ising form (32). Here we have

$$\mu = \frac{1}{2}\begin{pmatrix} 0 & J_1 & 0 & \cdots & 0 & J'_n \\ J_1 & 0 & J_2 & 0 & \cdots & 0 \\ 0 & J_2 & 0 & J_3 & \ddots & \vdots \\ \vdots & 0 & J_3 & \ddots & \ddots & 0 \\ 0 & \vdots & \ddots & \ddots & 0 & J_{n-1} \\ J'_n & 0 & \cdots & 0 & J_{n-1} & 0 \end{pmatrix} - \begin{pmatrix} h_1 & 0 & \cdots & 0 \\ 0 & h_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & h_n \end{pmatrix} \tag{45}$$

$$\nu = \frac{1}{2}\begin{pmatrix} 0 & J_1 & 0 & \cdots & 0 & -J'_n \\ -J_1 & 0 & J_2 & 0 & \cdots & 0 \\ 0 & -J_2 & 0 & J_3 & \ddots & \vdots \\ \vdots & 0 & -J_3 & \ddots & \ddots & 0 \\ 0 & \vdots & \ddots & \ddots & 0 & J_{n-1} \\ J'_n & 0 & \cdots & 0 & -J_{n-1} & 0 \end{pmatrix}, \tag{46}$$

so the matrix $(\mu+\nu)(\mu-\nu)$ is given by

$$\begin{pmatrix} J_1^2+h_1^2 & -J_1h_2 & 0 & \cdots & 0 & -J'_nh_1 \\ -J_1h_2 & J_2^2+h_2^2 & -J_2h_3 & 0 & \cdots & 0 \\ 0 & -J_2h_3 & J_3^2+h_3^2 & -J_3h_4 & \ddots & \vdots \\ \vdots & 0 & -J_3h_4 & \ddots & \ddots & 0 \\ 0 & \vdots & \ddots & \ddots & J_{n-1}^2+h_{n-1}^2 & -J_{n-1}h_n \\ -J'_nh_1 & 0 & \cdots & 0 & -J_{n-1}h_n & J_n^2+h_n^2 \end{pmatrix}. \tag{47}$$

The eigenvalues corresponding to eigenstates with $G = \pm 1$ can be identified as follows. The transformation (37) is invertible, so any quadratic expression in the a_j's and $a_j^\dagger$'s can be written as a quadratic expression in the b_j's and $b_j^\dagger$'s. Since quadratic fermion operators do not change the parity of the total number of occupied modes, this means that the parity of the a modes is the same as the parity of the b modes. In other words,

$$G = (-1)^{\sum_{j=1}^n b_j^\dagger b_j}. \tag{48}$$

Thus the eigenvalues with $G = +1$ are those with an even number of s_j's equal to $+1$ in (42), whereas the eigenvalues with $G = -1$ are those with an odd number of s_j's equal to $+1$. In particular, we see that the gap between the ground and first excited states in the $G = +1$ subspace is equal to $2(\omega_1+\omega_2)$, where ω_1 and ω_2 are the square roots of the two smallest eigenvalues of (47).

In the case of periodic boundary conditions, note that we have two distinct matrices (47), one for each value of G. However, with a fixed value of G, only half the possible assignments of the s_j's give rise to eigenvalues of the Hamiltonian, so we still find the correct number of eigenvalues. Here again, the gap between the ground and first excited states in the $G = +1$ subspace is equal to $2(\omega_1+\omega_2)$, where now ω_1 and ω_2 are the square roots of the two smallest eigenvalues of (47) with $G = +1$.

Diagonalizing the ring of agrees The Hamiltonian (5) is of the form (8) with $J_i = -s/2$ and $h_i = -(1-s)$ for each $i = 1, 2, \ldots, n$. (Note that we can neglect terms proportional to the identity, since they do not affect the gap.) Then, according to (47), the gap is given by twice the sum of the square roots of the two smallest eigenvalues of the matrix

$$(J_i^2 + h_i^2) - J_i h_i (D + D^{-1}) = \frac{1}{4}\left[s^2 + 4(1-s)^2 - 2s(1-s)(D + D^{-1})\right], \tag{49}$$

where D is the skew-circulant matrix

$$D := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & & & 0 & 1 \\ -1 & 0 & \cdots & 0 & 0 \end{pmatrix} \tag{50}$$

$$= \sum_{x=0}^{n-2} |x+1\rangle\langle x| - |0\rangle\langle n-1|\,. \tag{51}$$

Now just as the circulant matrix

$$C := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & & & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix} \tag{52}$$

$$= \sum_{x=0}^{n-1} |x+1 \bmod n\rangle\langle x| \tag{53}$$

(and hence any circulant matrix) is diagonal in the Fourier basis

$$|\phi_k\rangle := \frac{1}{\sqrt{n}} \sum_{x=0}^{n-1} e^{2\pi \mathrm{i} k x/n} |x\rangle \tag{54}$$

for $k = 0, 1, \ldots, n-1$, one can show that the matrix D (and hence any skew-circulant matrix) is diagonal in the *skew-Fourier basis*

$$|\chi_k\rangle := \frac{1}{\sqrt{n}} \sum_{x=0}^{n-1} e^{\pi \mathrm{i}(2k+1)x/n} |x\rangle\,, \tag{55}$$

also for $k = 0, 1, \ldots, n-1$. In particular,

$$D|\chi_k\rangle = e^{\pi \mathrm{i}(2k+1)/n} |\chi_k\rangle\,. \tag{56}$$

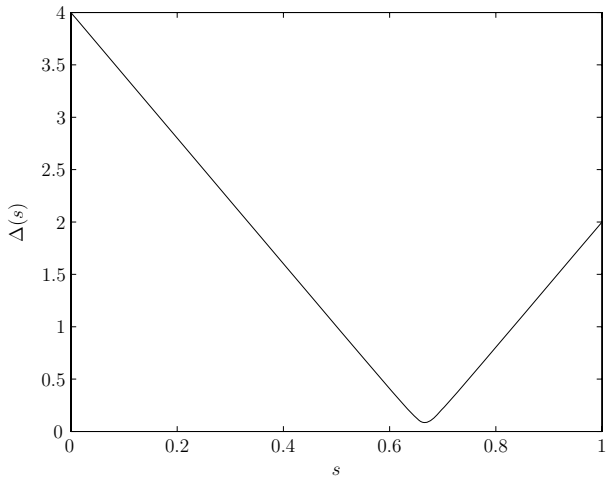
Thus, the eigenvalues of (49) are given by

$$\frac{1}{4}\left[s^2 + 4(1-s)^2 - 4s(1-s)\cos\frac{\pi(2k+1)}{n}\right]. \tag{57}$$

The smallest two eigenvalues (which are equal) occur for $k = 0$ and $k = n - 1$, so the gap as a function of the interpolating parameter is

$$\Delta(s) = 2\sqrt{s^2 + 4(1-s)^2 - 4s(1-s)\cos\frac{\pi}{n}}\,, \tag{58}$$

which looks like this for $n = 50$:



For large n,

$$\cos\frac{\pi}{n} = 1 - \frac{\pi^2}{2n^2} + O(1/n^4)\,, \tag{59}$$

so

$$\Delta(s) = 2\sqrt{(2-3s)^2 + s(1-s)\frac{2\pi^2}{n^2} + O(1/n^4)}\,. \tag{60}$$

Setting $\mathrm{d}\Delta(s)^2/\mathrm{d}s$ equal to zero, we see that the minimum occurs at $s = 2/3 + O(1/n^2)$, at which the minimum gap is

$$\Delta = \frac{4\pi}{3n} + O(1/n^3)\,. \tag{61}$$

Since the minimum gap decreases only as $1/\operatorname{poly}(n)$, we see that adiabatic optimization can efficiently find a satisfying assignment for the ring of agrees. Even though the ring of agrees is not by itself an interesting computational problem, we can take this as preliminary evidence that adiabatic optimization sometimes succeeds.

However, it is also possible for the adiabatic algorithm to fail (at least for certain natural choices of the interpolating Hamiltonian), even for cost functions that are almost as simple as the ring of agrees. For example, suppose we have $4n$ spins arranged on a ring, and we define the cost function

$$h'(z) = \sum_{j=1}^{n}(1-\delta_{z_j,z_{j+1}}) + 2\sum_{j=n+1}^{2n}(1-\delta_{z_j,z_{j+1}}) + \sum_{j=2n+1}^{3n}(1-\delta_{z_j,z_{j+1}}) + 2\sum_{j=3n+1}^{4n}(1-\delta_{z_j,z_{j+1}}). \tag{62}$$

In other words, we again penalize a string when adjacent bits disagree, but the penalty is either 1 or 2 for contiguous blocks of n pairs of spins. In this case one can show that the gap is exponentially small. Unfortunately, we did not have time to discuss the details of this calculation.