Lecture #5

Stoquastic Hamiltonians

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(based in part on lecture in March 2018 UCSD quantum school by D. Gosset)
Let $H$ be a Hamiltonian specified in the standard basis.

**Definition** $H$ is stoquastic if

$$\langle x | H | y \rangle \leq 0 \quad \text{for all} \quad x \neq y.$$ 

[Bravyi, DiVincenzo, Oliviera, Terhal 2007]

will use a stronger definition:

**vi** hi is stoquastic

$$\langle x | h_i | y \rangle \leq 0 \quad \text{for all} \quad x \neq y.$$
Examples

1. Laplacian matrix of a graph

\[ L = D - A \]

diagonal \( 2\sqrt{\text{deg}(v)} \) adjaceny matrix

2. Hamiltonians from adiabatic computation

When:
- final \( H \) is classical (diagonal)
- initial \( H \) has ground state \( 1 \mapsto \psi_0 \)

\[ H(s) = (1-s) \sum_{i=1}^{n} \frac{E - x_i}{2} + s H_{\text{final}} \]
Many Hamiltonians form physics

- ferromagnetic Heisenberg
- quantum transverse Ising model
- anti-ferromagnetic Heisenberg on cubic lattice

Sometimes with a local change of basis.

- interacting bosons on a lattice
Does the local Hamiltonian become easier if $H$ is stoquastic?

We will show:

\[ 14\rangle = \frac{1}{\sqrt{\beta^*}} \sum_{x \in \mathbb{R}_{\geq 0}} |x\rangle \beta^* \]

Stoquastic local Hamiltonians more like classical (diagonal) Hamiltonians.
Complexity

Given an LH, decide if ground energy $\leq a$ or $\geq b$.

**General $H$**

$a - b \geq \frac{1}{\text{poly}}$

QMA - complete [Kitaev]

$a = 0$ (Frustration - Free)

QMA$_{\pm}$ - complete

Verifier accepts YES instances with prob $= \pm$.

**Stochastic $H$**

$a - b \leq \frac{1}{\text{poly}}$

Stoq FF - complete.

[Bravyi - Bessen - Terhal]

$a = 0$

MA - complete

first MA - complete problem.

[Bravyi - Terhal 2008]
MA (Merlin - Arthur) \[ \text{NP} \leq \text{MA} \leq \text{StoqMA} \leq \text{QMA} \].

\( \text{if } x \in \text{YES } \exists \ y \in \mathbb{Z}_0, \pm 3^m \),

\[ \text{Pr} \left[ V(x,y) \text{ accepts} \right] \geq 2/3 \]

\( \text{if } x \in \text{NO } \forall \ y. \)

\[ \text{Pr} \left[ V(x,y) \text{ accepts} \right] \leq 1/3 \]

\( \text{StoqMA is the same except that verifier can have "quantum-like" circuit with a specific form.} \)

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\[ 1 + \left| x \right| \]

\[ \text{classical reversible circuit.} \]
Numerical Methods

General \( H \)
- brute force diagonalization
  - 20 - 30 qubits.

A diabatic Quantum Computing

- General \( H \)
- capable of efficient universal Quantum Computing.
- [AVKLRL]

Stochastic \( H \)
Quantum Monte Carlo
- "no sign problem"
- works heuristically up to 1000's qubits.

Adiabatic Quantum Computing

- General \( H \)
- capable of efficient universal Quantum Computing.
- [AVKLRL]

Stochastic \( H \)
- frustration-free \( H \)
- a diabatic
- can be simulated classically.
Non-Negative Ground States

Claim: Let $H$ be stochastic. Then $\exists$ ground state $|\psi\rangle$ of $H$ such that $\langle \psi | \psi \rangle \geq 0 \ \forall \ z \in \{0,1\}^n$.

Proof: Let $|\phi\rangle$ be any ground state of $H$

$|\phi\rangle = \sum_x \alpha_x |x\rangle.$

Define $|\psi\rangle = \sum_x \alpha_x |x\rangle$. Then.

$\langle \psi | H | \psi \rangle = \sum_x |\alpha_x|^2 \langle x | H | x \rangle + \sum_{x \neq y} |\alpha_x|^2 \langle x | H | y \rangle$

$\leq \sum_x |\alpha_x|^2 \langle x | H | x \rangle + \sum_{x \neq y} |\alpha_x|^2 |\alpha_y|^2 \langle x | H | y \rangle$

$= \langle \phi | H | \phi \rangle$. 

\[ \leq 0 \]
Ground States of Stochastic Hamiltonians are Non-Negative

Definition: \( H \) is reducible if there exists a permutation matrix \( P \) such that \( P^T H P \) is block diagonal.

Perron-Frobenius Theorem:

1. If \( H \) is irreducible and stoquastic, then ground state \( |\Psi\rangle \) is unique and \( \langle x | \Psi \rangle > 0 \ \forall x \).

2. If \( H \) is reducible and stoquastic, then there exists an orthonormal basis of the ground space \( |\Psi_1\rangle, \ldots, |\Psi_m\rangle \) such that \( \langle x | \Psi_j \rangle \geq 0 \ \forall j, x \).
Markov Chain for stoquastic $H$ \cite{Bravyi-Terhal 2008 arxiv: 0806.1746}

Start with $\sum_{i=1}^{m} h_i$ (assume irreducible for now $\langle x|y \rangle > 0$ for g.s. $|x\rangle$)

Scale + add identity so that:

$0 \leq h_j \leq 1 \Rightarrow 0 \leq \sum h_i \leq m$

$$H = \sum_{i=1}^{m} h_i - E$$ choose $E$ s.t. $H|\psi\rangle = 0$

$\Rightarrow 0 \leq H \leq m$ and ground energy $= 0$. 
Define: \[ G = I - \frac{H}{2m} \Rightarrow \frac{1}{2} \leq G \leq I. \]

and \[ P_{yx} = \frac{\langle y | x \rangle}{\langle x | x \rangle} \langle y | G^{-1} | x \rangle \quad \text{on} \quad \text{Supp} (4) \]

Claim: \[ P_x \rightarrow y \] defines a Markov Chain.

Proof: First show \( P_{xy} \geq 0 \)

Follows from \( \langle y | x \rangle > 0 \) \( \langle x | x \rangle > 0 \)

and \[ \langle y | H | x \rangle = 0 \]

\( x \neq y \) \( \langle y | H | x \rangle \leq 0 \)

\( x = y \) \( \langle y | H | x \rangle \leq m. \)
Next show \( \sum_y P_{x \rightarrow y} = 1 \quad \forall x \)

\[
\sum_y P_{x \rightarrow y} = \sum_y \frac{\langle \psi | y \rangle \langle y | 6 | x \rangle}{\langle \psi | x \rangle} = \frac{\langle 4 | 6 | x \rangle}{\langle \psi | x \rangle}
\]

\( G |\psi \rangle = (I - \frac{4}{2m}) |\psi \rangle = |\psi \rangle \)

(\( H |\psi \rangle = 0 \))
The unique limiting distribution of the Pyx Markov Chain is:

$$\pi_T(x) = \langle x | \chi \rangle^2 \quad x \in \{0, 1\}^n.$$ 

Follows from the fact that $H$ (and hence Pyx M.C.) are irreducible and satisfies detailed balance:

$$\pi_T(x) \cdot P_{x \rightarrow y} = \pi_T(y) \cdot P_{y \rightarrow x}$$

How fast does this M.C. converge?

If not irreducible then take non-negative basis

$14_1 \ldots 14_\ell$

Walk on the support of each $14_1 \ldots 14_\ell$ is irreducible.
Start from arbitrary $\pi \in \mathcal{P}_n$.

$$T_{\text{mix}}(\epsilon, \pi) \triangleq \min \left\{ t \geq 0 : \| P^t \pi - \pi \|_1 \leq \epsilon \right\}$$

Standard mixing time bound

$$T_{\text{mix}}(\epsilon, \pi) \leq \frac{1}{1 - \lambda_2} \log \left[ \frac{1}{2 \epsilon \Pi(\pi)} \right]$$

$\lambda_2$ is the 2nd largest eigenvalue of $P$.

$$\Pi(\pi) = \langle \pi | \pi \rangle^2$$
What is $\lambda_2$ for $P$?

Claim: $1 - \lambda_2 = \frac{\text{gap}(H)}{2m}$

Recall $P_{x \rightarrow y} = \frac{\langle y | \psi \rangle}{\langle x | \psi \rangle} \langle y | \sigma_1 | x \rangle$

$P = D G D^{-1}$ for $D = S x y \langle 41 | x \rangle$

$G$ and $P$ are similar matrices $\Rightarrow$ same eigenvalues

$G = I - \frac{H}{2m}$. //
Upshot:

\[ T_{\text{mix}}(t,z) \leq \frac{1}{1-\chi_2} \log \left[ \frac{1}{2 \epsilon \pi(t,z)} \right] \]

\[ = \frac{2m}{\text{gap}(H)} \log \left[ \frac{1}{2 \epsilon \langle z|H|z \rangle^2} \right] \]

Given a "warm start" \[ \langle z|H|z \rangle^2 \geq \Omega \left( 2^{-\text{poly}(n)} \right) \]

and if \( \text{gap}(H) \geq \Omega \left( \frac{1}{\text{poly}(n)} \right) \)

then chain mixes to \( \Pi \) in poly-time.
Caveat: Running the M.C. requires knowing $P_{x\rightarrow y}$ (which requires knowing $\langle y|\chi\rangle$'s) (which we don't know).

$\Rightarrow$ Bravyi and Terhal show that if $H$ is frustration-free then $\frac{\langle y|\chi\rangle}{\langle x|\chi\rangle}$ can be efficiently computed.
Let \( H|\psi\rangle = 0 \) and \( \langle x|\psi\rangle > 0 \)

If \( P_x \rightarrow y > 0 \) then \( \langle y|H|x\rangle > 0 \)

\[ \Rightarrow \langle y|H|x\rangle < 0 \]

\[ \Rightarrow \langle y|hi|x\rangle < 0 \text{ for some } i \]

Claim: if \( H \) is stoquastic and FF then:

\[ BT \text{ 2008} \]

\[ \frac{\langle y|y\rangle}{\langle x|x\rangle} = \sqrt{\frac{\langle y|Ti|y\rangle}{\langle x|Ti|x\rangle}} \]

\( Ti \) is the projector on to the zero eigenspace of \( hi \)
Intuition: $\Pi$ projector onto groundspace of $H$.

$$\Pi = \sum_a |4_a\rangle \langle 4_a|$$

$|4_a\rangle$ is non-negative

$|4_a\rangle$ ortho-normal (disjoint support)

If:

1. $\Pi |4\rangle$
2. $\langle x | 4 \rangle > 0$
3. $\langle x | \Pi^\dagger y \rangle > 0$

If $FF$ then $\Pi_i |4\rangle = |4\rangle$. Same true for $\Pi_i^\dagger$.

If $\langle x | h_i | y \rangle < 0$ then $\langle x | \Pi_i^\dagger y \rangle > 0$
Implications of Claim (Simulating Adiabatic Computation)

If there is an adiabatic path $H(s) : 0 \to 1$

1. Easy to find $\langle x | y(0) \rangle \approx y(0)$ good state for $H(0)$.

2. $H(s)$ is Stab. TF w/ unique ground state + gap $\geq \frac{1}{\text{poly}(n)}$.

3. Path is smooth $\|d H(s)/ds\| \leq \text{poly}(n)$

Then a classical algorithm can approximately sample from $T(x) \approx \langle 4(x) | x \rangle^2$.
Implications of Claim (Simulating Adiabatic Computation)

If there is an adiabatic path $H(s) : 0 \rightarrow 1$

1. Easy to find $\{ x | \psi(0) \} \rightarrow \text{good state} \text{ of} \ H(1)$.

2. FF without stochastic condition, universal for QC.

3. ($H(s)$ is 2-step FF w/ unique ground state $\pm \text{gap} \geq 1/\text{poly}(n)$.

Then a classical algorithm can approximately sample from $T_T(x) \propto \langle \psi(1) | x \rangle^2$
Adiabatic Evolution with general local $H$ is equivalent to the quantum circuit model.

→ Is there a natural circuit model corresponding to adiabatic evolution of stoquastic (not FF) Hamiltonians?
Given a stoquastic LH determine if:

- \( \exists \mid \psi \rangle \quad H \mid \psi \rangle = 0 \)

or

- \( \forall \mid \psi \rangle \quad \langle \psi | H | \psi \rangle \geq a \quad (a \leq 1/poly) \)

This will be at least NP-hard because Boolean satisfiability is a special case.

Verifier can send as a witness \( x \in \{0,1\}^n \)

\[ \langle x | H | x \rangle \geq \Omega \left( 2^{-\text{poly}(n)} \right) \]
StogFF - LH & MA

- Prover can send a starting point for a random walk:

  \[ x \text{ s.t. } \langle x | x \rangle \geq 2^{-(\text{poly}(n))} \]

- One idea for verification:
  - Implement random walk until convergence, then measure energy.
  - Repeat for accuracy.

Can verify "yes" instances
What about "No" instances?
MA Verification for $\Sigma^*\cdot$MA

Define $S_{\text{good}} = \{ x | \langle x \rangle \cdot \text{TA} | x \rangle > 0 \ \forall a \}$.

$\Rightarrow$ poly-time checkable condition.

$S_{\text{bad}} = S_{\text{good}}^{13^n} - S_{\text{good}}$.

$\Rightarrow$ the random walk is closed on $S_{\text{ground}}$

Show: Starting from $x \in S_{\text{good}} - S_{\text{ground}}$ w.h.p. will reach a string in $S_{\text{bad}}$.

$S_{\text{ground}} = \{ x | \langle x \rangle \cdot \text{TA}_{\text{ground}} | x \rangle > 0 \}$
Verification Procedure:

- Prover sends start string $x$ to Verifier
  (Supposedly $x \in \mathcal{S}_{\text{ground}}$)
  Send $x$ that maximizes $41\langle T(x) \rangle$

- Verifier runs random walk for $T$ steps
  - at each step if current string is in $\mathcal{S}_{\text{bad}}$ \(\Rightarrow\) Reject.

- If $\mathcal{S}_{\text{bad}}$ has not been reached after $T$ steps \(\Rightarrow\) Accept.

+ An additional check always satisfied for yes instances.
How big does $T$ have to be

$\Rightarrow$ No instance $\lambda_0(H) > \epsilon$.

$G = (I - \frac{H}{2m}) \Rightarrow \max \text{ eigenvalue of } G \leq (1 - \frac{\epsilon}{2m})$

\[
\text{Prob Stay Within } S_{\text{good}} = \sum_{x_1, x_2, \ldots, x_T \in S_{\text{good}}} P_{x_0 \rightarrow x_1} \cdot P_{x_1 \rightarrow x_2} \cdots \cdot P_{x_{T-1} \rightarrow x_T}
\]
\[
= \sum_{x_1, x_2, \ldots, x_T \in S_{\text{good}}} \langle x_0 | e | x_1 \rangle \langle x_1 | e | x_2 \rangle \cdots \langle x_{T-1} | e | x_T \rangle
\]

\[
\leq \frac{1}{n} \sum_{x_T} \langle x_0 | G^T | x_T \rangle \leq 2^n \left(1 - \frac{\epsilon}{2m}\right)^T
\]

If $\epsilon > \gamma \text{poly}(n)$, will be exp small with $T \sim \text{poly}(n)$
Hardness of Stog FF LH for MA is shown even when ground state is a uniform superposition. [BT08].

Aharonov and Grilo derandomize this process when $H$ is gapped and has a ground state which is a uniform superposition.

If there is a gap amplification procedure for uniform FF Stog LH then NP = MA.