Lecture #5

Stoquastic Hamiltonians

Aug 4, 2023

(based in part on lecture in March 2018 UCSD quantum school by D. Gosset)

Let H be a Hamiltonian specified in the standard basis.

[Bravyi, DiVincenzo, Oliviera, Terhal 2007]

Definition H is stoquastic if

$\langle x | H | y \rangle \leq 0$ for all $x \neq y$.

will use a stronger definition:

$\forall i$ h_i is stoquastic

$\langle x | h_i | y \rangle \leq 0$ for all $x \neq y$.

Examples

① Laplacian matrix of a graph

$$L = D - A$$

diagonal $\langle v|D|v\rangle = \text{degree}(v)$

adjacency matrix

H_{prop} from the circuit-to-Hamiltonian construction is stoquastic.

② Hamiltonians from adiabatic computation when:

- final H is classical (diagonal)
- initial H has ground state $|+\rangle^{\otimes n}$

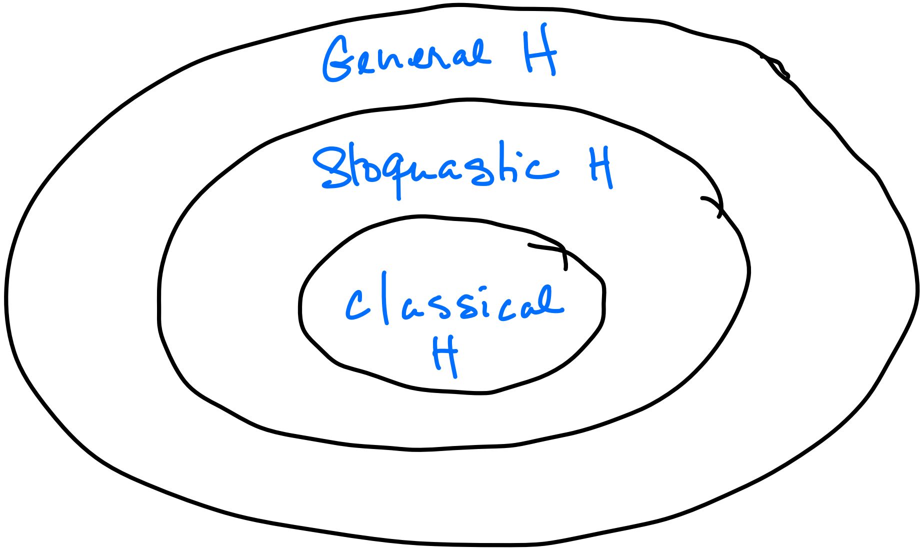
$$H(s) = (1-s)\sum_{i=1}^{n} \frac{I - X_i}{2} + s H_{final}$$

Sometimes with a local change of basis.

(3) Many Hamiltonians from physics

- ferromagnetic Heisenberg
- quantum transverse Ising model
- anti-ferromagnetic Heisenberg on cubic lattice
- interacting bosons on a lattice

Does the local Hamiltonian become easier if H is stoquastic?



Stoquastic local Hamiltonians more like classical (diagonal) Hamiltonians.

We will show:

Ground state of stoquastic H: $|\psi\rangle = \sum_x \alpha_x |x\rangle$

$\alpha_x \in \mathbb{R}^{\geq 0}$

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$_1$ - complete

verifier accepts YES instances with prob $= 1$.

Stoquastic H

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

Stoq FF - complete. [Bravyi-Bessen-Terhal]

$\underline{\underline{a = 0}}$

MA - complete

first MA - complete problem.

[Bravyi - Terhal 2008]

MA (Merlin-Arthur)

$NP \subseteq MA \subseteq StoqMA \subseteq QMA$.

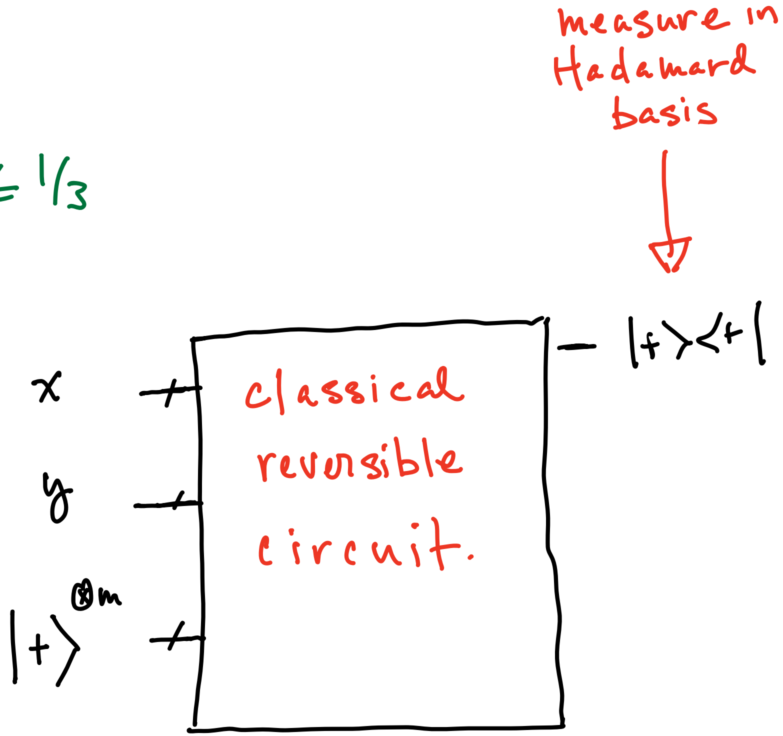
if $x \in YES$ $\exists\, y \in \{0,1\}^m$ classical V

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

if $x \in NO$ $\forall\, y$.

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

StoqMA is the same except that verifier can have "quantum-like" circuit with a specific form.



Numerical Methods

General H

brute force diagonalization

20 - 30 qubits.

Stoquastic 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.

[AvDKLLR]

Stoquastic H

frustration-free stoq H

adiabatic

can be simulated

classically.

Non-Negative Ground States

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

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.

$$\langle\psi|H|\psi\rangle = \sum_x |\alpha_x|^2 \langle x|H|x\rangle + \sum_{x\neq y} |\alpha_x||\alpha_y| \underbrace{\langle x|H|y\rangle}_{\leq 0}$$

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

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

Ground States of Stoquastic Hamiltonians are Non-Negative

Definition: H is **reducible** if $\exists$ 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 $\exists$ orthonormal basis of the ground space $|\psi_1\rangle \dots |\psi_m\rangle$ such that $\langle x|\psi_j\rangle \geq 0$ $\forall j, x$.

Markov Chain from stoquastic H

[Bravyi-Terhal 2008 arXiv: 0806.1746]

Start with $\sum_{i=1}^{m} h_i$

(assume irreducible for now $\langle x|\psi\rangle > 0$ for g.s. $|\psi\rangle$)

Scale + add identity so that:

$$0 \leq h_j \leq I. \Rightarrow 0 \leq \sum h_i \leq m$$

$$H = \sum_{i=1}^{m} h_i - E$$

choose E s.t. $H|\psi\rangle = 0$.

$\Rightarrow$ $0 \leq H \leq m$ and ground energy $= 0$.

Define: $G = I - \frac{H}{2m} \Rightarrow I/2 \leq G \leq I.$

and $P_{yx} = \frac{\langle y|\psi\rangle}{\langle x|\psi\rangle} \langle y|G|x\rangle$

on $\mathrm{Supp}(\psi)$

Claim: $P[x \to y] = P_{x\to y}$ defines a Markov Chain.

Proof: First show $P_{x\to y} \geq 0$

Follows from $\langle y|\psi\rangle > 0$

$\langle x|\psi\rangle > 0$

and

$\langle y|G|x\rangle = \delta_{xy} - \frac{\langle y|H|x\rangle}{2m}.$

$x \neq y \quad \langle y|H|x\rangle \leq 0$

$x = y \quad \langle y|H|x\rangle \leq m.$

Next show $\sum_y P_{x\to y} = 1 \quad \forall x$

$$\sum_y P_{x\to y} = \sum_y \frac{\langle\psi|y\rangle\langle y|G|x\rangle}{\langle\psi|x\rangle} = \frac{\langle\psi|G|x\rangle}{\langle\psi|x\rangle}$$

$$\boxed{\begin{gathered} G|\psi\rangle = \left(I - \frac{H}{2m}\right)|\psi\rangle = |\psi\rangle \\ (H|\psi\rangle = 0) \end{gathered}}$$

$$= \frac{\langle\psi|x\rangle}{\langle\psi|x\rangle}$$

//

The unique limiting distribution of the P_{yx} Markov Chain is:

$$\pi(x) = \langle x | \psi \rangle^2 \qquad x \in \{0,1\}^n.$$

Follows from the fact that H (and hence P_{yx} M.C.) are irreducible and satisfies detailed balance:

$$\pi(x) \cdot P_{x \to y} = \pi(y) P_{y \to x}$$

If not irreducible then take non-negative basis $|\psi_1\rangle \ldots |\psi_r\rangle$

Walk on the support of each $|\psi_i\rangle$ is irreducible.

How fast does this M.C. converge?

Start from arbitrary $z \in \{0,1\}^n$.

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

standard mixing time bound

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

2nd largest eigenvalue of P.

$$\pi(z) = \langle \psi | z \rangle^2$$

What is λ_2 for P?

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

Recall $P_{x\to y} = \dfrac{\langle y|\psi\rangle}{\langle x|\psi\rangle} \langle y|G|x\rangle$

$P = D\,G\,D^{-1}$ for $D = \delta_{xy} \langle\psi|x\rangle$

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

$G = I - H/2m.$

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Upshot:

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

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

Given a "warm start" $\langle z | \psi \rangle^2 \geq \Omega\left(2^{-poly(n)}\right)$

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

then chain mixes to π in poly-time.

Caveat: Running the M.C. requires knowing $P_{x \to y}$ (which requires knowing $\langle \psi | x \rangle$'s) (which we don't know).

L and E.

$\Rightarrow$ Bravyi & Terhal show that if H is frustration-free then

$$\frac{\langle y | \psi \rangle}{\langle x | \psi \rangle}$$

can be efficiently computed.

Let $H|\psi\rangle = 0$ and $\langle x|\psi\rangle > 0$

$G = I - \frac{H}{2m}$

If $P_{x\to y} > 0$ then $\langle y|G|x\rangle > 0$

For a given x, there are poly(n) y s.t. $\langle y|h_i|x\rangle < 0$ for some i.

$\Rightarrow$ $\langle y|H|x\rangle < 0$.

$\Rightarrow$ $\langle y|h_i|x\rangle < 0$ for some i.

Claim: if H is Stoquastic and FF then:

[BT 2008]

$$\frac{\langle\psi|y\rangle}{\langle\psi|x\rangle} = \sqrt{\frac{\langle y|\Pi_i|y\rangle}{\langle x|\Pi_i|x\rangle}}$$

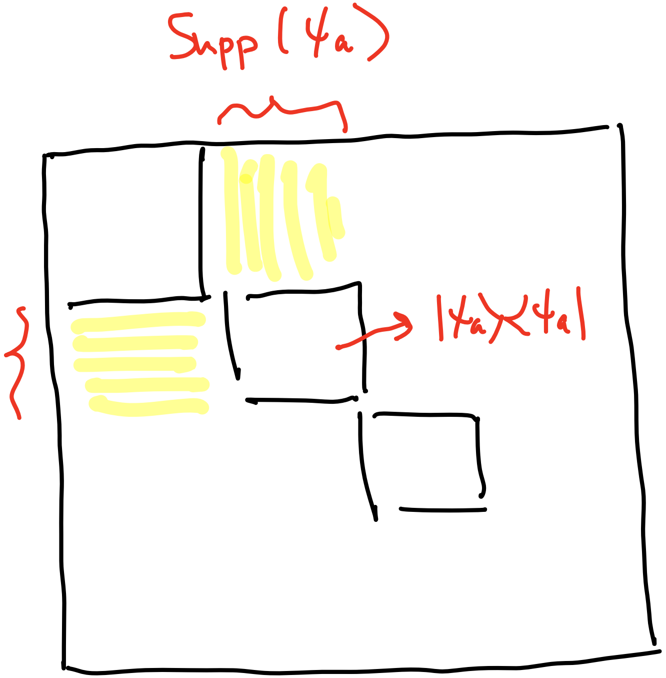
Π_i projector on to zero eigenspace of h_i

Intuition: Π projector onto groundspace of H.

$$\Pi = \sum_a |\psi_a\rangle\langle\psi_a|$$

$|\psi_a\rangle$ is non-negative

$|\psi_a\rangle$ ortho-normal (disjoint support)



If:

① $\Pi|\psi\rangle$

② $\langle x|\psi\rangle > 0$

③ $\langle x|\Pi|y\rangle > 0$

then

$$\frac{\langle x|\psi\rangle}{\langle y|\psi\rangle} = \sqrt{\frac{\langle x|\Pi|x\rangle}{\langle y|\Pi|y\rangle}}$$

If FF then $\Pi_i|\psi\rangle = |\psi\rangle$. same true for Π_i

If $\langle x|h_i|y\rangle < 0$ then $\langle x|\Pi_i|y\rangle > 0$

Implications of Claim (Simulating Adiabatic Computation

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

① Easy to find $\langle x | \psi(0) \rangle$ $|\psi(0)\rangle$ ground state of $H(0)$.

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

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

Then a classical algorithm can approximately sample from $\pi(x) = \langle \psi(1) | x \rangle^2$

Idea: For $J = 0, \ldots, T-1$, use steady state of $H(J/T)$ as a warm start for $H(J+1/T)$.

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~~Without~~ FF ~~stoquastic condition~~, universal for QC.

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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?

Complexity of LH for Stoq-FF Hamiltonians

Given a stoquastic LH determine if:

- $\exists\ |\psi\rangle \quad H|\psi\rangle = 0$

OR

- $\forall\ |\psi\rangle \quad \langle\psi|H|\psi\rangle \geq a$ $\quad (a \geq 1/\text{poly})$

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

- Verifier can send as a witness $x \in \{0,1\}^n$ How to verify??
  $\langle x|\psi\rangle \geq \Omega(2^{-\text{poly}(n)})$

StoqFF-LH $\in$ MA

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

  $$x \text{ s.t. } \langle x|\psi\rangle \geq \Omega\left(2^{-\mathrm{poly}(n)}\right)$$

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

Can verify "yes" instances

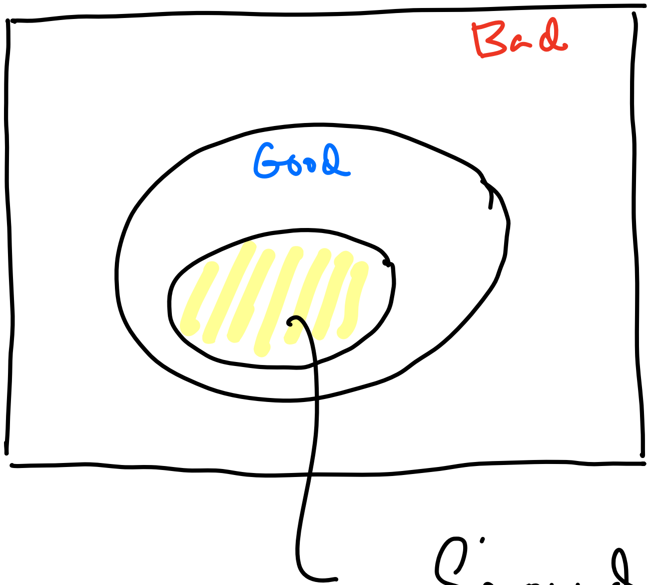
What about "No" instances?

MA Verification for Stoq-MA

Define $S_{good} = \{ x \mid \langle x | \Pi_a | x \rangle > 0 \ \forall a \}$.

↳ poly-time checkable condition.

$S_{bad} = \{0,1\}^n - S_{good}$.



⇒ the random walk is closed on S_{ground}

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

$S_{ground} = \{ x \mid \langle x | \Pi_{ground} | x \rangle > 0 \}$

Verification Procedure:

- Prover sends start string x to Verifier (supposedly $x \in S_{ground}$) send x that maximizes $\langle x|\pi|x\rangle$
- Verifier runs random walk for T steps
  - at each step if current string is in S_{bad} $\Rightarrow$ Reject.
- If S_{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 $\lambda_0(H) > \epsilon$.

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

$P_{x_{i+1} \to x_i} = \frac{\langle x_{i+1} | \psi \rangle}{\langle x_i | \psi \rangle} \langle x_i | G | x_{i+1} \rangle$

Prob Stay Within S_{GOOD} $= \sum_{x_1, x_2 .., x_T \in S_{good}} P_{x_0 \to x_1} \cdot P_{x_1 \to x_2} \cdots \cdot P_{x_{T-1} \to x_T}$

$= \sum_{x_1, x_2 .., x_T \in S_{good}} \langle x_0 | G | x_1 \rangle \langle x_1 | G | x_2 \rangle \cdots \langle x_{T-1} | G | x_T \rangle$

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

If $\epsilon > 1/poly(n)$, will be exp small with $T \sim poly(n)$

Hardness of Stoq FF LH for MA is shown even when ground state is a uniform superposition. [BT 08].

Aharonov & 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 Stoq LH then NP = MA.