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Ground state expansion and the spectral gap of local Hamiltonians

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$$\Delta_H \leq 2(\|H\| - E_0)\frac{\Psi^2(\partial S)}{\Psi^2(S)}$$

- **Isoperimetric inequality:** relates the geometry of the ground state probability distribution to the spectral gap

- Constrains the kind of probability distributions that can be efficienctly sampled with adiabatic optimization

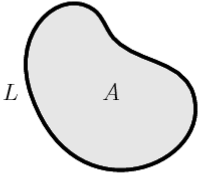
- Applies to **non-stoquastic** as well as stoquastic Hamiltonians

- Corroborates past results about small gaps arising from local minima that are far in Hamming distance

- Suggests speed ups from increased range k-local couplings

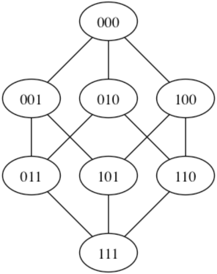
Isoperimetric inequalities

- $\dfrac{\text{Measure on the boundary of a set}}{\text{Measure inside a set}}$



$L^2 \geqslant 4\pi A$

- Can be defined for graphs in terms of **vertex expansion**



$$S = \{000, 100, 010, 001\} \implies \partial S = \{100, 010, 001\} \implies \frac{|\partial S|}{|S|} = \frac{3}{4}$$

Hilbert space graph $G_{\Omega,H}$

- Hamiltonian H and basis set Ω
- Vertices are elements of Ω
- Edges corresponding to non-zero off-diagonal matrix elements
- e.g. computational basis $\Omega = \{0,1\}^n$, transverse Ising Hamiltonian H, $G_{\Omega,H}$ is an n-dimensional boolean hypercube
- The boundary of a set of vertices $S \subseteq \Omega$ are the vertices in S connected to vertices outside of S,

$$\partial S = \{x \in S : \exists y \notin S \text{ with } \langle x|H|y\rangle \neq 0\}$$

Isoperimetric Inequality for Quantum Ground States

- Define $\Psi^2(S) := \langle \Psi | 1_S | \Psi \rangle := \sum_{x \in S} |\Psi(x)|^2$

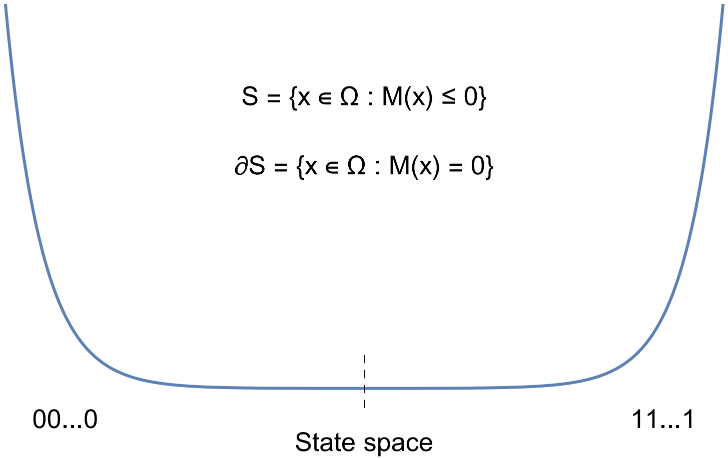
- **Theorem:** If $G_{\Omega,H}$ is a connected graph, then any subset $S \subseteq \Omega$ with $\Psi^2(S) \leq 1/2$ satisfies

$$\Delta_H \leq 2(\|H\| - E_0)\frac{\Psi^2(\partial S)}{\Psi^2(S)},$$

  where $|\Psi\rangle$ is the ground state of H with energy E_0, Δ_H is the spectral gap, and $\|H\|$ is the operator norm.

- Depends on locality of the Hamiltonian and geometry of the ground state, but not the details of the Hamiltonian couplings!

Example: Ferromagnetic Transverse Ising Model



- Probability of $M = 0$ in the ferromagnetic phase is $\sim e^{-\Omega(n)}$
- $\frac{\Psi^2(\partial S)}{\Psi^2(S)} \lesssim e^{-\Omega(n)} \implies \Delta_H \lesssim n\, e^{-\Omega(n)}$

Proof in the stoquastic case: map H to a Markov chain

- Define $\alpha := (\|H\| - E_0)^{-1}$ and $\beta := \|H\|^{-1}$ so that $G := \alpha(I - \beta H)$ non-negative and satisfies $G|\Psi\rangle = |\Psi\rangle$
- $G_{\Omega,H}$ is connected $\implies \Psi(x) > 0 \; \forall \, x \in \{0,1\}^n$
- Define Markov chain transition probabilities by

$$P(x,y) := \frac{\langle\Psi|y\rangle}{\langle\Psi|x\rangle}\langle y|G|x\rangle$$

- Slightly novel mapping, but mostly builds on past results

  [**Bravyi and Terhal 08', Al-Shimary and Pachos 10', Jarret and Jordan 14', Nishimori, Tsuda, and Knysh 14'**].

- P is a **stochastic matrix** because $P(x,y) \geq 0 \; \forall x, y \in \Omega$ and

$$\sum_{y \in \Omega} P(x,y) = \sum_{y \in \Omega} \frac{\langle \Psi | y \rangle}{\langle \Psi | x \rangle} \langle y | G | x \rangle = \frac{\langle \Psi | G | x \rangle}{\Psi | x \rangle} = 1$$

- Define $\pi(x) := |\Psi(x)|^2$, then $|\pi\rangle = \sum_{x \in \Omega} \pi(x) |x\rangle$ satisfies

$$\begin{aligned} \langle \pi | P &= \sum_{x,y \in \Omega} \langle y | \pi(x) P(x,y) = \sum_{x,y \in \Omega} \langle y | \langle \Psi | x \rangle \langle x | G | y \rangle \langle y | \Psi \rangle \\ &= \sum_{y \in \Omega} \langle y | \langle \Psi | G | y \rangle \langle y | \Psi \rangle = \sum_{y \in \Omega} \langle y | |\Psi(y)|^2 = \langle \pi | \end{aligned}$$

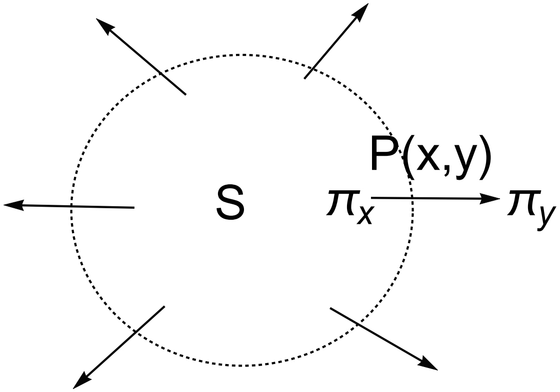
- P satisfies detailed balance, $\pi(x) P(x,y) = \pi(y) P(y,x)$

- P has eigenfunctions $|\phi_k\rangle := \sum_{x \in \Omega} \Psi(x) \Psi_k(x)$ with eigenvalues $\alpha(1 - \beta E_k)$, so the gap is $\Delta_P = \alpha\beta\Delta_H$.

Conductance inequality for Markov chains

- Δ_P satisfies the conductance inequality for Markov chains,

$$\frac{\Phi^2}{2} \leq \Delta_P \leq 2\Phi \quad , \quad \Phi = \min_{S \subset \Omega} \frac{1}{\pi(S)} \sum_{x \in S, y \notin S} \pi(x) P(x,y)$$



From Conductance to Vertex Expansion

- Applying the definitions of P and π,

$$\sum_{x\in S, y\in S^c} \pi(x)P(x,y) = \sum_{x\in S, y\in S^c} \langle\Psi|y\rangle\langle y|G|x\rangle\langle x|\Psi\rangle = \langle\Psi|1_{\partial S}G1_{\partial S^c}|\Psi\rangle$$

- Using the fact that H is stoquastic,

$$\langle\Psi|1_{\partial S}G1_{\partial S^c}|\Psi\rangle \leq \langle\Psi|1_{\partial S}G|\Psi\rangle = \Psi^2(\partial S)$$

which shows that $\Phi(S) \leq \Psi^2(\partial S)/\Psi^2(S)$.

Lower Bound for the Stoquastic Case

- $\forall x \in \Omega$, $\sum_{y\in\Omega} P(x,y) = 1$, and this can be used to show that

$$\frac{H_{\min}}{\|H\|} \leq \frac{\Psi_y}{\Psi_x} \leq 1 \quad \forall\, x,y \in \Omega \;\; s.t. \langle x|H|y\rangle \neq 0$$

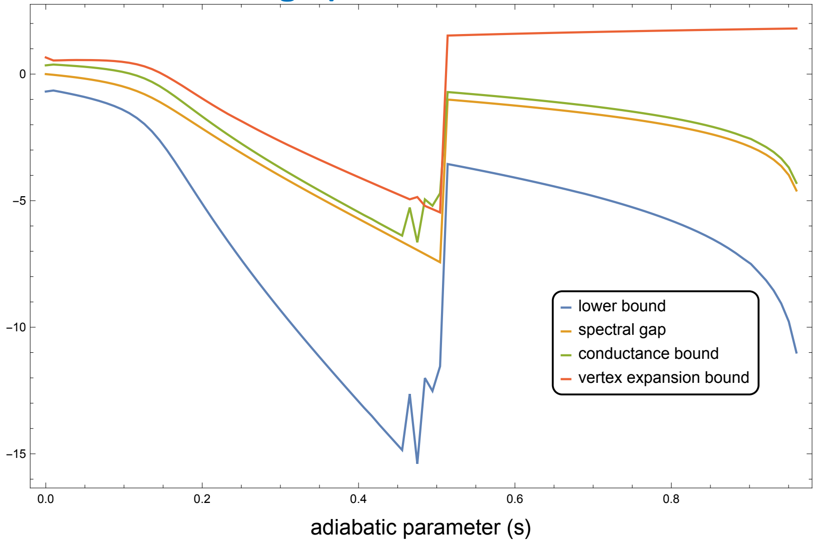
  where $H_{\min} := \min_{x,y:\langle x|H|y\rangle\neq 0} |\langle x|H|y\rangle|$.

- This allows for a lower bound in terms of vertex expansion,

$$\frac{H_{\min}^2}{2\|H\|^2(\|H\| - E_0)}\Phi_V^2 \leq \Delta_H \leq 2(\|H\| - E_0)\Phi_V$$

  where $\Phi_V := \min_{S:\Psi^2(S)\leq 1/2} \frac{\Psi^2(\partial S)}{\Psi^2(S)}$.

Transverse Ising Spin Glass with n = 12 Qubits



- Thanks to John Bowen, from the University of Chicago, who worked on these ideas during a Caltech SURF this Summer!

Proof in the Non-Stoquastic Case

- P retains many properties of a reversible transition matrix despite having complex entries of unbounded magnitude!
- Enables the use of similar techniques as those that are used to show the Markov chain conductance bounds
- **Obstacle:** $\Psi(x) = 0$ is possible even if $G_{\Omega,H}$ is connected.
- **Solution:** consider states close to Ψ with $|\Psi(x)| \geq \epsilon > 0$ for all x, and prove the main theorem by taking the limit $\epsilon \to 0$.
- Counterexamples for non-stoquastic $H \implies \Delta_H$ can be small even if the ground state is highly expanding.

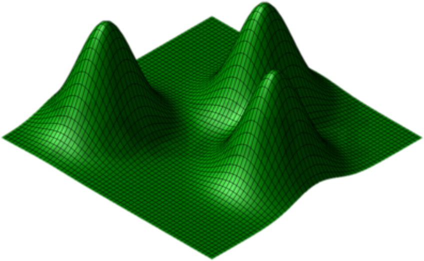
- What if H is non-stoquastic, but $P(x,y) \geq 0$ for all $x, y \in \Omega$?
- e.g. the phases in $\langle y|G|x\rangle$ and $\langle\Psi|y\rangle/\langle\Psi|x\rangle$ could cancel
- **Definition:** if H appears to be non-stoquastic but P is non-negative then H is "secretly stoquastic."
- **Observation:** If $G_{\Omega,H}$ is a connected line graph, then H is secretly stoquastic in the basis Ω.

$$H = \begin{bmatrix} a_1 & b_1 & 0 \\ b_1^\dagger & a_2 & b_2 \\ 0 & b_2^\dagger & \ddots \end{bmatrix}$$

- **Lesson:** genuine non-stoquasticity requires frustration in the off-diagonal couplings!

Implications for Adiabatic Optimization

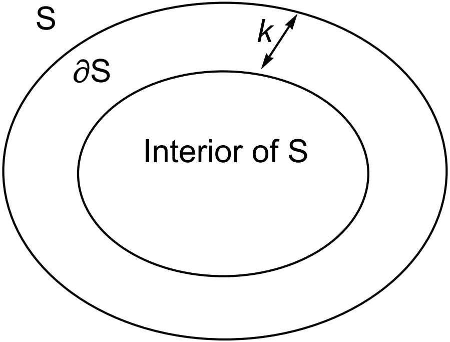
- Ground state distributions with low expansion are difficult to produce using local Hamiltonian adiabatic optimization



- Small gap whenever the ground state is a mixture of modes centered on local minima far apart in Hamming distance

Optimism for k-local Couplings

- Increasing k increases $\Psi^2(\partial S)$ for every S!



Conclusion and Outlook

- Ground state bottlenecks slow down adiabatic optimization
- Limitations on improvement from non-stoquastic couplings for sampling target multimodal distributions
- Larger spectral gaps from path changes require reshaping the ground state throughout the evolution
- Diabatic transitions and thermal effects can escape these limitations on pure ground state adiabatic optimization
- Suggests benefit from k-local couplings for stoquastic systems
- Thank you for your attention! :)