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Simulated quantum annealing can be exponentially faster than classical simulated annealing

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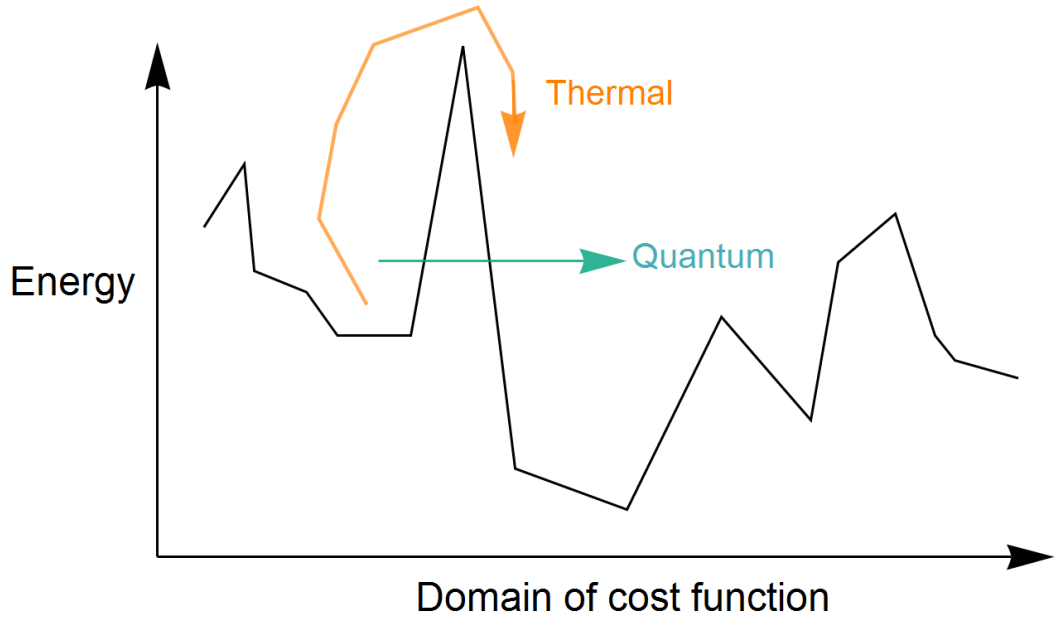
Optimization and Physics

- **Combinatorial Optimization:** minimize $f : \{0,1\}^n \to \mathbb{R}$
- **Physical inspiration:** take advantage of dynamics that drive physical systems to low energy states.

- **Classical simulated annealing (SA):** MCMC algorithm simulates thermal cooling by attempting to sample $\pi(x) = e^{-\beta f(x)}/Z$ for $\beta_0 = 0 \leq \beta_1 \leq \ldots \leq \beta_{final}$.
- Can quantum dynamics inspire faster optimization methods?

Do quantum effects help annealing?

- **Intuition:** quantum dynamics allow for "tunneling" through high barriers in the energy landscape.



- **Theory:** QA can be exponentially faster than classical SA for particular cost functions with tall narrow energy barriers.

  (FGG '02, Reichardt '04, Muthukrishnan et al. '15, Kong and EC '15, Jiang et al. '15, Brady and van Dam '16).

Adiabatic optimization and quantum annealing

- Minimize a cost function $f : \{0,1\}^n \to \mathbb{R}$ by sampling the ground state of an n-qubit Hamiltonian,

$$H_p = \sum_{z \in \{0,1\}^n} f(z)|z\rangle\langle z|$$

- Initialize the qubits in the ground state of a uniform transverse field $H_B = -\sum_{i=1}^{n} \sigma_i^x$ and interpolate from H_B to H_p,

$$H(s) = (1-s)H_B + s\,H_p \quad , \quad 0 \leq s \leq 1$$

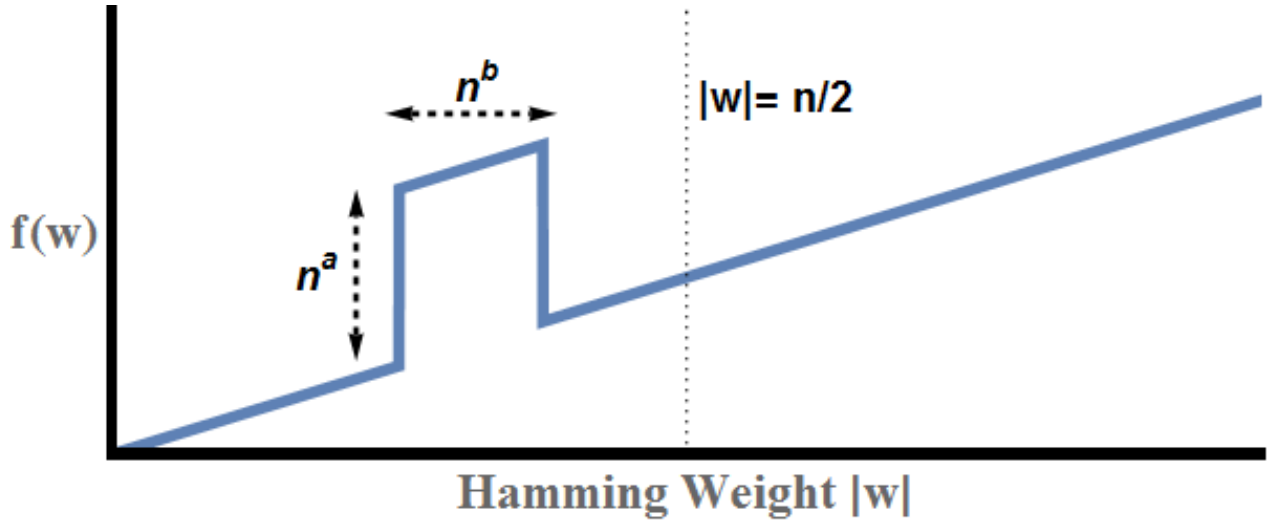
- **Adiabatic optimization:** If $\Delta = \min_s gap(H(s))$ is the minimum spectral gap of $H(s)$, then time $\mathrm{poly}(n, \Delta^{-1})$ suffices to prepare the ground state of H_p.

- **Quantum annealing:** includes more realistic effects e.g. being in a low temperature Gibbs state $\rho(s) = e^{-\beta H(s)}/\mathcal{Z}(s)$.

Exponential separation between QA and SA

- **Spike cost function:** bit-symmetric cost function with a large energy barrier that creates a local minimum.

$$f(w) = \begin{cases} |w| + n^a & n/4 - n^b/2 \leq |w| \leq n/4 + n^b/2 \\ |w| & o.w. \end{cases}$$



- Takes time $2^{\Omega(n^a)}$ to solve with SA, but QA succeeds in $O(n)$ time when $a + b < 1/2$ (Reichardt '04).

However, traditional QA Hamiltonians are "stoquastic"

- **Stoquastic Hamiltonians** have real and non-positive matrix entries and can be scaled to substochastic matrices,

$$H_{z,z'} \leq 0 \quad \text{for all} \quad z, z' \in \{0,1\}^n$$

- Adiabatic computation with *frustration-free* stoquastic H can be classically simulated in poly time (Bravyi and Terhal, 2008)

- Stoquastic LH problem is in AM (Bravyi et al., 2006)

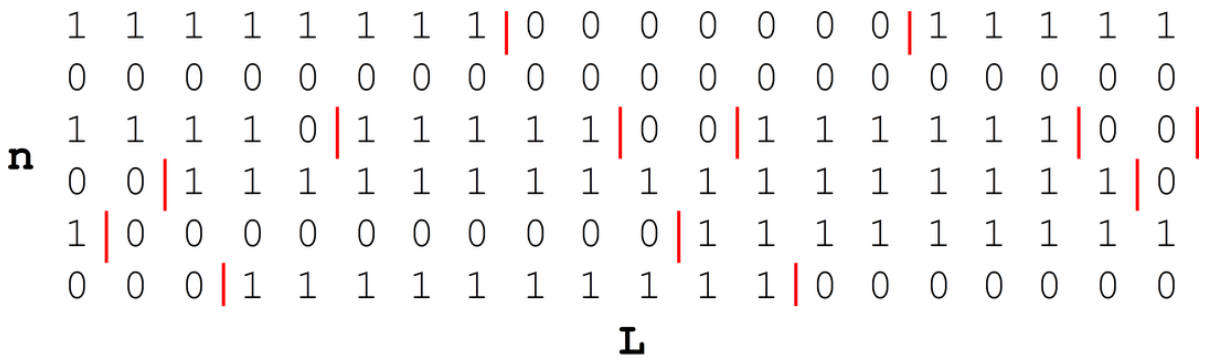
- **Open question:** Can stoquastic QA be classically simulated in time $\mathrm{poly}(n, \Delta^{-1})$?

- Classical simulations motivate implementation of non-stoq QA

Simulated Quantum Annealing

- All amplitudes in stoquastic thermal state path integrals are positive, making some paths more important than others!

$$\pi(z_1, ..., z_L) = \frac{1}{Z} \prod_{i=1}^{L} \langle z_i | e^{-\frac{\beta H}{L}} | z_{i+1} \rangle \quad , \quad z_i \in \{0,1\}^n$$



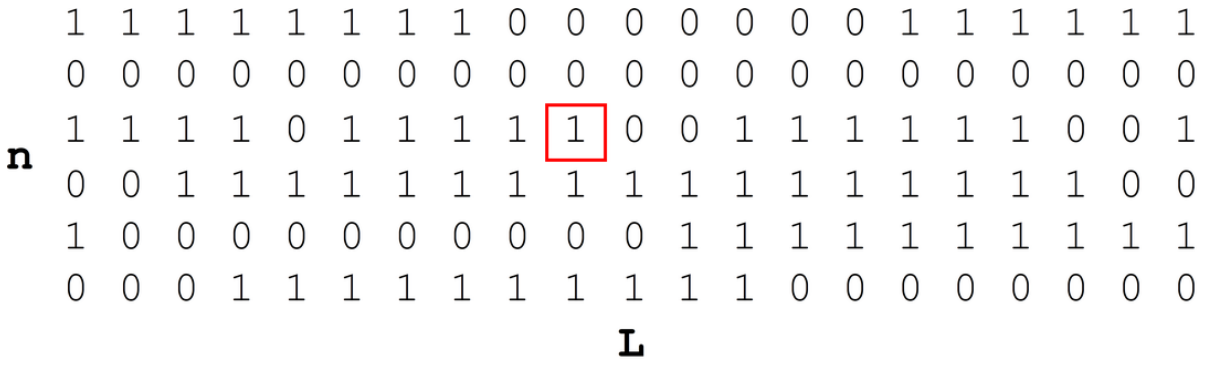
- **SQA** discretizes the adiabatic path and samples π at each point using a Markov chain. The samples can be used for Monte Carlo estimation of physical observables.

- π penalizes configurations for the proportion of "time" they spend on bit strings with high f, and also for the total number of "jumps" along the path.

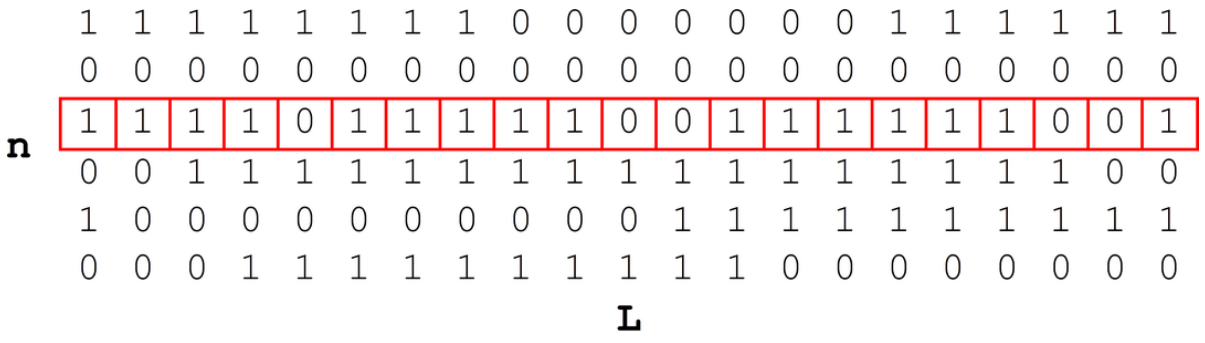
SQA for the spike converges in poly time

- **Our result:** SQA equilibrates in polynomial time and finds the minimum of the spike cost function whenever $a + b < 1/2$.

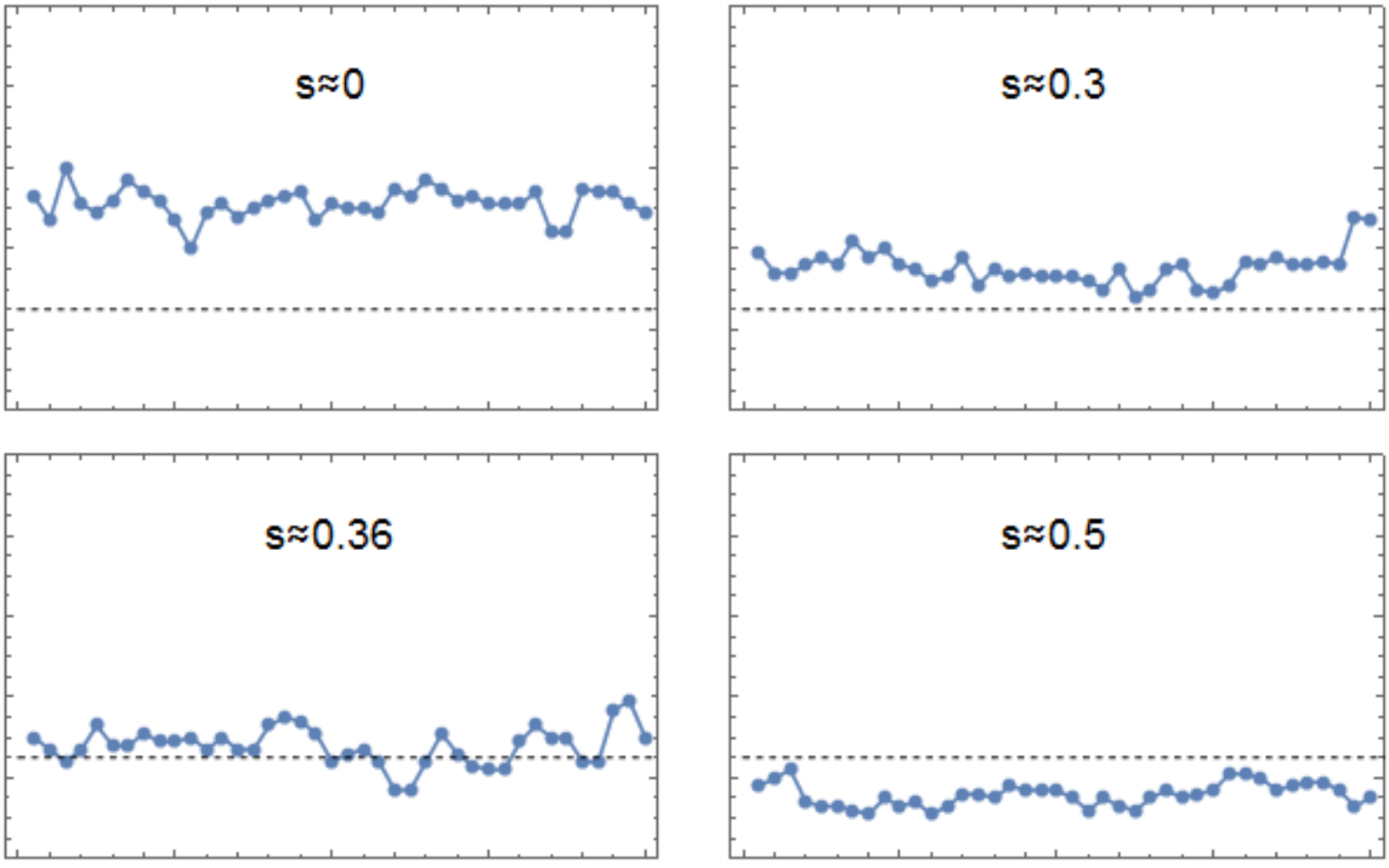
  - $\tilde{\mathcal{O}}(n^{17})$ with single-site Metropolis updates



  - $\tilde{\mathcal{O}}(n^{7})$ with worldline heat-bath updates



Visualizing SQA for the spike system

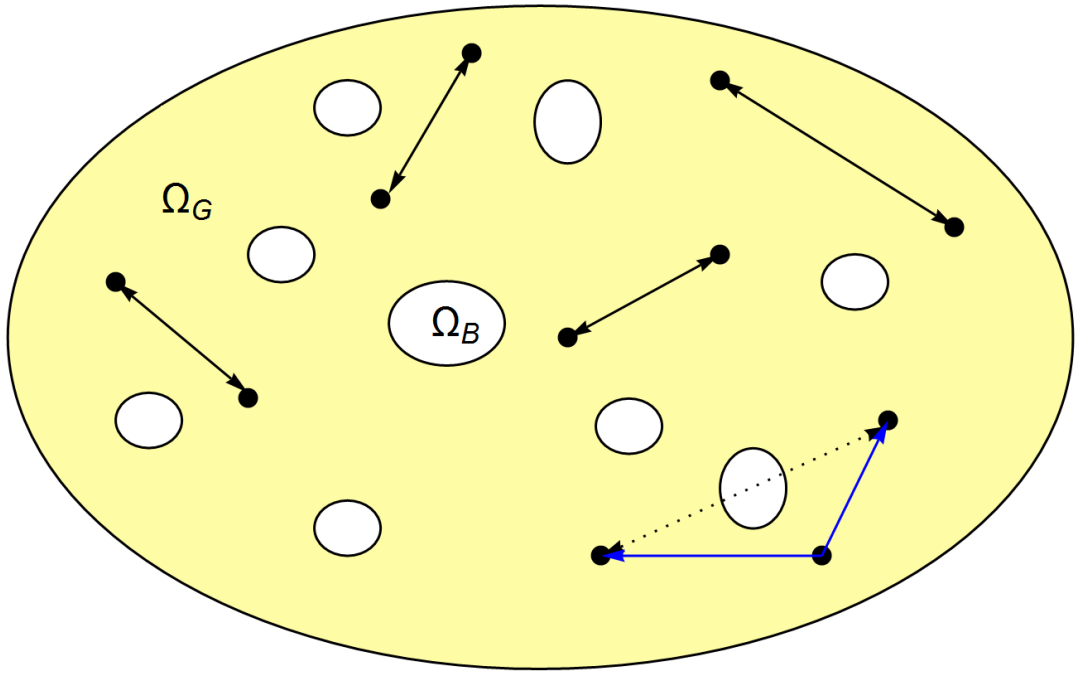


Proof ideas

- Compare the SQA Markov chain with and w/o the spike term
- For "worst-case" configurations the spike distribution π may be very different from the spikeless distribution $\tilde{\pi}$
- Use expectation values of the quantum system to see that for "typical configurations" $\pi \approx \tilde{\pi}$ when $a + b < 1/2$.
- Use canonical paths for the spikeless system to construct canonical paths for the spike system within the typical subset, and show that leaks outside of this subset are rare.
- Quasi-equilibration of SQA within a subset of the state space, adiabatic path guarantees warm starts in this subset.

Most-paths comparison method

- **Idea:** $(z_1, ..., z_L) \in \{0,1\}^{n \times L}$ which do not spend too much time on the spike will have $\pi(z_1, ..., z_L) \approx \tilde{\pi}(z_1, ..., z_L)$.



- Use "most" of the canonical paths for the spikeless system to build paths for the spike system with congestion $R = \mathcal{O}(\tilde{R})$ inside a subset Ω_G of large measure, $\pi(\Omega_G) > 1 - 1/\mathrm{poly}(n)$.

Summary and Conclusion

- We've shown that SQA can inherit some of the quantum advantages of QA and given the first proof of an exponential separation in the asymptotic performance of SA and SQA.

- Can we apply the ideas in the proof to better understand the stationary distribution and convergence properties of SQA in more general systems?

- Besides path integral SQA, there are other "quantum Monte Carlo" methods for stoquastic Hamiltonians. However, there are obstructions to using any existing QMC method to simulate stoquastic QA in full generality.

- *Thank you for your attention!*