Simultaneous Stoquasticity

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Stoquastic Hamiltonians

Stoquastic Hamiltonian

A Hamiltonian whose off-diagonal entries are all real and non-positive.

- This is a basis dependent property
- In mathematics these are known as Z-matrices or negative Metzler matrices
- By the Perron-Frobenius theorem, the ground state is entirely real

$$\begin{pmatrix} d_1 & & & \\ & \ddots & & - \\ & & \ddots & \\ - & & & d_N \end{pmatrix}$$

The Sign Problem (Using Path-Integral Quantum Monte Carlo as an example)

Consider a Partition Function

$$\mathcal{Z} = \sum_{x} \langle x| e^{-\beta\left(\hat{H}_d + \hat{H}_o\right)} |x\rangle$$

Use a Suzuki-Trotter expansion in diagonal basis

$$\mathcal{Z} = \lim_{T\to\infty} \sum_{\{x_i\}} \prod_{i=1}^{T} \langle x_{i+1}| e^{-\frac{\beta}{T}(\hat{H}_o + \hat{H}_d)} |x_i\rangle$$

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We want to interpret these as classical Boltzmann probabilities

$$p(\{x_i\}) = \frac{1}{\mathcal{Z}} \prod_{i=1}^{T} e^{-\frac{\beta}{T} H_d(x_i)} \langle x_{i+1}| \, e^{-\frac{\beta}{T}\hat{H}_o} \, |x_i\rangle$$

For stoquastic Hamiltonians, the $p(\{x_i\})$ are positive

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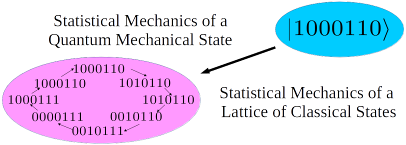
$$p(\{x_i\}) = \frac{1}{\mathcal{Z}} \prod_{i=1}^{T} e^{-\frac{\beta}{T} H_d(x_i)} \langle x_{i+1}| \left(I - \frac{\beta}{T}\hat{H}_o\right) |x_i\rangle$$

For stoquastic Hamiltonians, the $p(\{x_i\})$ are positive

Implications of the Sign Problem



- Simulating sign-problem Hamiltonians requires exponential slow-downs
- Non-stoquastic ≠ Sign Problem

- Mostly[1,2], simulating stoquastic Hamiltonians is classically efficient
- Stoquasticity is tied into computational complexity

[1] M. B. Hastings, The power of adiabatic quantum computation with no sign problem, Quantum **5**, 597 (2021).

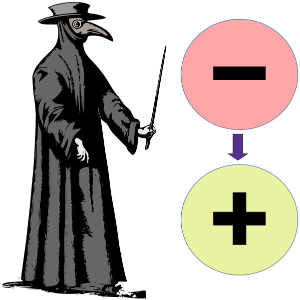
[2] J. Bringewatt and M. Jarret, Effective gaps are not effective: Quasipolynomial classical simulation of obstructed stoquastic Hamiltonians, Phys. Rev. Lett. **125**, 170504 (2020).

Curing Non-Stoquasticity

Curing

Finding a (local) basis in which the sign problem does not exist.

- Such a basis always exists (the eigenbasis)
- A local stoquastic basis might not exist
- Curing the sign problem is NP-Hard
- Mitigation and Avoidance algorithms exist



Quantum Annealing with Stoquasticity

Quantum Annealing

Adiabatic Quantum Annealing with a local stoquastic basis is no more powerful than classical computing

There are some caveats here

1. Adiabatic - Diabatic annealing can get around this
2. Local - Hastings has one example with a non-local basis
3. Basis - Annealing takes place in the same basis throughout

The Quantum Advantage rests either with locality or the basis interaction between the annealing Hamiltonians

Core Question

Simultaneous Stoquasticity

Assume I have a set of Hamiltonians

$$S = \{H_1, H_2, \dots H_m\}$$

- m – Number of Hamiltonians in set
- d – Dimension of Hamiltonians

Does there exist a basis in which all $H_j \in S$ are stoquastic

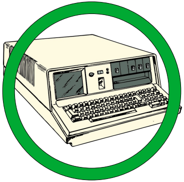
$$\begin{pmatrix} d_1^* & & & \\ & \ddots & & - \\ & & \ddots & \\ - & & & d_N^* \end{pmatrix}$$

$$U H_j U^\dagger = H_j^*$$

Analogy to Simultaneous Diagonalizability

Our problem is analogous to simultaneous Diagonalizability

$$\left[H_i, H_j\right] = 0 \qquad \forall \;\; H_i, H_j \in S$$

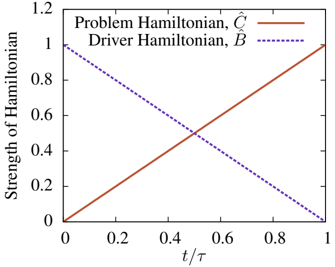


- Shared Eigenbasis
- No quantum advantage
- We want a condition like this
- Anything we do can apply to this similarity setting as well

Why is This Useful

Quantum Annealing

- Can the entire anneal be stoquastic
- Quantum annealing with stoquastic Hamiltonians seemingly lacks advantage*
- This can be useful in Monte Carlo simulation
- The question came up in some optimal control work

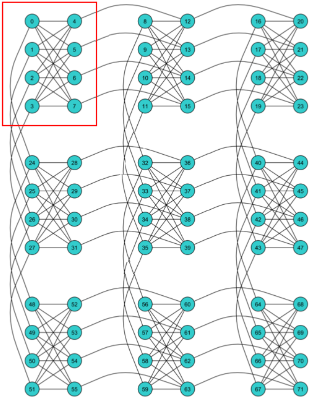


Quantum Complexity

- Stoquasticity plays into several complexity classes

What are the Limitations

Locality



- Our work currently doesn't consider locality
- Locality could be spatial or connectivity
- Monte Carlo and complexity results require locality
- Locality is the next extension

Feasibility **Geometricity**

Results

$$S = \{H_1, \cdots, H_m\} \quad \& \quad S' = \{H'_1, \cdots, H'_m\}$$

Theorem (Existence)

The ordered sets S and S' are simultaneously unitarily similar iff $\mathrm{Tr}[w(S)] = \mathrm{Tr}[w(S')]$ for all words w in S, S'.

Theorem (Quick No-Go)

Every eigenvalue $\lambda \neq 0$ of $i[H_i, H_j]$ there is another eigenvalue $-\lambda$ of $i[H_i, H_j]$ (paired eigenvalue condition) for all $H_i \neq H_j \in S$.

Theorem (Frequency)

For almost every S with $m \geqslant 2$, $d \geqslant 3$, S is not simultaneously stoquasticizable.

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Lie Algebras

Structure of $\mathfrak{su}(d)$

Generalized Gell-Mann Basis

$$\hat{\lambda}_{jk}^{(x)} = |j\rangle\langle k| + |k\rangle\langle j|, \quad (1 \leqslant j < k \leqslant d)$$

$$\hat{\lambda}_{jk}^{(y)} = -i\,|j\rangle\langle k| + i\,|k\rangle\langle j|, \quad (1 \leqslant j < k \leqslant d)$$

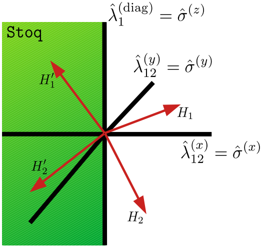
$$\hat{\lambda}_{j}^{(\text{diag})} = \sqrt{\frac{2}{j(j+1)}}\text{diag}(\underbrace{1,\cdots,1}_{j},-j,0,\cdots,0)$$

Generalized Bloch Vectors

$$H = \vec{b}\cdot\vec{\lambda}$$

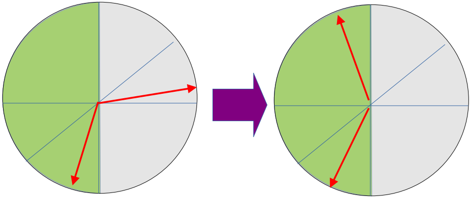
Stoquastic:

$$\{b^{(y)} = 0, b^{(x)} \leqslant 0\}$$



Simultaneous Stoquasticity in $\mathfrak{su}(2)$

$SU(2)$ is a double-cover of $SO(3)$



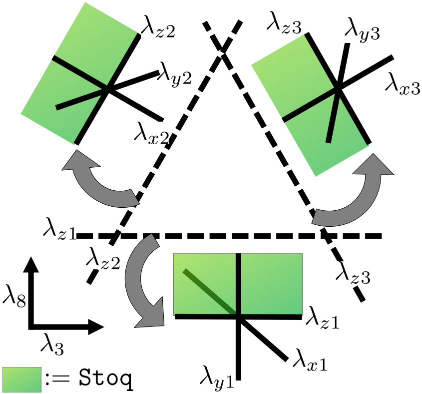
- Stoquasticity is the negative half-xz-plane
- It is always possible to rotate two vectors into a half-plane
- Simultaneous stoquasticity is always possible with $m = 2$

The Bloch Sphere is Misleading

$SU(d)$ does not have nice relationships with SO

- Normal rotations do not apply
- Structure constants mix weirdly

λ_{xj}	λ_{yj}	λ_{zj}
λ_{xj}	λ_{yj}	λ_{zk}
λ_{xj}	λ_{xk}	λ_{yi}
λ_{yj}	λ_{yk}	λ_{yi}



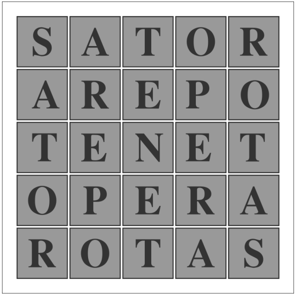
Complete Conditions

Words and Invariants

A word is some product of operators

$$w = \hat{B}^3\ \hat{C}\ \hat{B}\ \hat{C}^2 \qquad \ell = 7$$

- Words can be used to make up commutators
- $\mathrm{Tr}\,(w)$ is an invariant under unitary rotations
- Provably the traces of all words describe every invariant property of a matrix



Unitary Similarity

$$S = \{H_1, \cdots, H_m\} \quad \& \quad S' = \{H'_1, \cdots, H'_m\}$$

Theorem (Existence)

The ordered sets S *and* S' *are simultaneously unitarily similar iff* $\mathrm{Tr}[w(S)] = \mathrm{Tr}[w(S')]$ *for all words* w *in* S, S'.

- This is the known foundation of unitary similarity
- We only need to check finitely many words

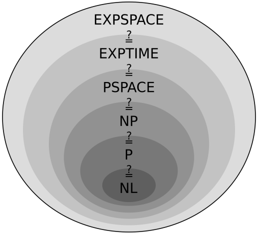
$$\ell_{max} = cd\sqrt{\frac{2(cd)^2}{cd-1} + \frac{1}{4}} + \frac{cd}{2} - 2 \in \mathcal{O}\left((\sqrt{m}d)^{3/2}\right)$$

$$\text{w/ } (c^2 - 3c + 2 \geqslant 2m)$$

System of Equations

We get a system of conditions for simultaneous stoquasticity:

$$\begin{aligned}
\mathrm{Tr}[w(S)] &= \mathrm{Tr}[w(S')], && \forall\, |w| \leqslant \ell_{\max} \\
\mathrm{Re}(H'_{jk}) &\leqslant 0, && \forall j \neq k, H' \in S' \\
\mathrm{Im}(H'_{jk}) &= 0, && \forall j \neq k, H' \in S'
\end{aligned}$$



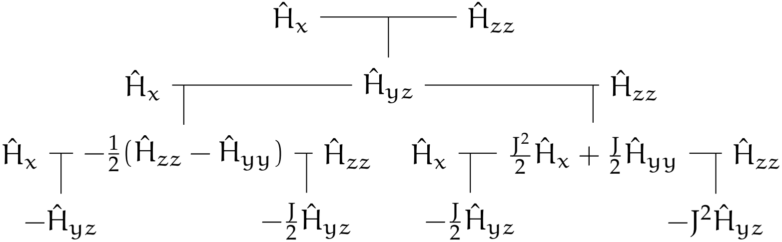
This has $\mathcal{O}\left(m^{\mathcal{O}((\sqrt{m}d)^{3/2})}\right)$ equality constraints and $md(d-1)/2$ inequality constraints

- Many of these are redundant
- Determining if a solution exists is NP-Hard

Simplified Condition

Dynamical Lie Algebra (DLA)

Lie algebra generated from your Hamiltonians via nested commutation



For $n = 3$ Transverse Field Ising model

- The relative tree structure is invariant
- Incredibly useful for control theory

One Step Up

Go one step up the DLA

$$\left[\hat{H}_0, \hat{H}_1\right] = 2i\hat{H}_2$$

1. The eigenvalues are all invariant
2. If $\hat{H}_0$ and $\hat{H}_1$ can be simultaneously stoquastic, $\hat{H}_2$ is composed only of $\lambda^{(y)}$ in that basis
3. Then $\hat{H}_2$ is skew-symmetric and must have paired eigenvalues

λ_1	$-a$
λ_2	$-b$
λ_3	$-c$
λ_4	0
λ_5	c
λ_6	b
λ_7	a

Limitations

- This is a necessary but not sufficient condition
- This condition can be met by Hamiltonians that are not Simultaneously stoquastic*
- We are not looking at enough invariants
- This would be equivalent to the words if we looked at the entire DLA
- Related to the Cartan decomposition of $\mathfrak{su}(p)$

Frequency of Satisfying Conditions

Structure of $\mathfrak{su}(d)$

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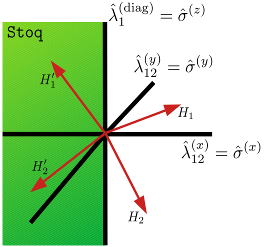


Word Invariants with Bloch Vectors

We can express the trace invariants in terms of Bloch vectors

$$\mathrm{Tr}[w(S)] = \mathrm{Tr}\left[\prod_{j=1}^{|w|}\sum_{\mu_j=1}^{d^2-1} b_{\mu_j}^{(w_j)}\hat{\lambda}_{\mu_j}\right]$$

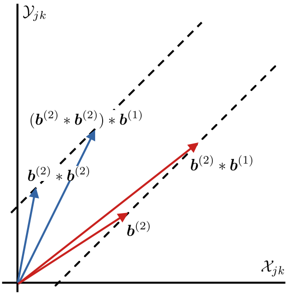
- This allows us to look at all possible invariants of a system in terms of combinations of Bloch vectors.
- All possible Bloch vectors generated by a set of Hamiltonians' invariants is denoted by $\mathcal{B}$
- We can show that a necessary condition for simultaneous stoquasticity is that $\dim(\mathrm{span}(\mathcal{B})) \leqslant (d^2+d-1)/2$

Dimension of Full Space

We can show that for almost all pairs of Hamiltonians

$$\dim(\mathrm{span}(\mathcal{B})) = (d^2 + d - 1)$$

So almost all pairs of Hamiltonians have spans larger than can fit into simultaneous stoquasticizability



- Cool ideas, but the proof is too long
- Equivalent to saying that almost all pairs of Hamiltonians have a DLA $= \mathfrak{su}(d)$ - full controllability
- A similar proof can be made for simultaneous diagonalizability

Conclusion

Summary

- Simultaneous Stoquasticity is rare
- Unpaired eigenvalues of $\left[\hat{B}, \hat{C}\right]$ imply no stoquasticity
- Stoquasticity is basis dependent but simultaneous stoquasticizability is basis independent
- Bloch vectors are a powerful geometric tool