Semiquantum Algorithms for Characterization and Verification

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Characterizing Quantum Systems

Characterizing quantum systems is an essential task in quantum information.

- Accurate knowledge required for high-fidelity control.
- Allows for comparing to proven and estimated thresholds.
- Characterization allows for *validating* control.

State Tomography

Common task: characterize the *state* ρ of a quantum system.
Tomographic approach: measure $p_i = \mathrm{Tr}(E_i \rho)$ for a *positive operator-valued measure* $\{E_i\}$.
Given measurement record $\{d_i\}$, what should $\hat{\rho}$ be?

- Need to ensure $\rho \geq 0$, is full-rank.
- Exponentially many parameters needed.
- How to parameterize uncertainty?

(Blume-Kohout 2010 *10/cn772j*)

Process Tomography

Can also consider learning about quantum processes, $S : \rho_i \mapsto \rho_f$.

- Even more parameters
- Negativity: difficult to separate sampling error from violation of assumptions (e.g. initially-correlated states)

(Altepeter et al. 2003 *10/dtdk4z*; Boulant et al. 2003 *10/fgvbg9*; Weinstein et al. 2004 *10/bn6sn2*)

Bayesian Approaches

Model data collection as a probability distribution, called a *likelihood function*

$$\Pr(d|\underline{x};\underline{e}).$$

d: data, $\underline{x}$: model, $\underline{e}$: experiment

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Example

Single qubit, Larmor precession at an unknown frequency ω, unknown dephasing time T_2:

$$H(\omega) = \frac{\omega}{2}\sigma_z, \quad |\psi_{\text{in}}\rangle = |+\rangle, \quad M = \{|+\rangle\langle+|, |-\rangle\langle-|\}$$

$$\Pr(d = 0|\underline{x} = (\omega, T_2); \underline{e} = (t)) = \frac{1}{2}(1 - e^{-t/T_2}) + e^{-t/T_2}\cos^2(\omega t/2)$$

Updating Knowledge

Once we have a likelihood function for our model, we can reason about

$$\Pr(\underline{x} | d, \underline{e}),$$

what we know about our model having seen some data.

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By Bayes' rule,

$$\Pr(\underline{x}|d, \underline{e}) = \frac{\Pr(d|\underline{x}; \underline{e})}{\Pr(d|\underline{e})} \Pr(\underline{x}),$$

telling us that our knowledge is intimately connected to our ability to simulate.

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Estimate $\hat{\underline{x}}$ as the expectation over $\underline{x}$,

$$\hat{\underline{x}} = \mathbb{E}[\underline{x}] = \int \underline{x}\Pr(\underline{x})\,\mathrm{d}\underline{x}.$$

Loss

Figure of merit: how well have we learned a model?
Assign to estimate $\hat{\underline{x}}$ of a "true" model $\underline{x}$ a *loss*, describing how bad $\hat{\underline{x}}$ does at estimating $\underline{x}$.

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Definition (Quadratic Loss)

$$L_{\underline{\underline{Q}}}(\hat{\underline{x}}, \underline{x}) = (\hat{\underline{x}} - \underline{x})^{\mathrm{T}} \underline{\underline{Q}} (\hat{\underline{x}} - \underline{x}),$$

where $\underline{\underline{Q}}$ is a positive semidefinite scale matrix.

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The quadratic loss generalizes the MSE for multiple parameters.

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Definition (Bayes Risk)

$$r(\underline{\hat{x}}, \pi) = \mathbb{E}_{\underline{x}\sim\pi}[R(\underline{\hat{x}}, \underline{x})]$$

Cramér-Rao Bound

The Fisher information

$$\underline{\underline{I}}(\underline{x}) = \mathbb{E}_D[(\underline{\nabla}_{\underline{x}} \log \Pr(D|\underline{x}))(\underline{\nabla}_{\underline{x}} \log \Pr(D|\underline{x}))^{\mathrm{T}}]$$

describes how much information about $\underline{x}$ is obtained by sampling data.

(Ferrie, *Granade* and Cory 2013 *10/tfx*)

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The Cramér-Rao bound tells how well any unbiased estimator can do. If $\underline{\underline{Q}} = \mathbb{1}$, then

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Compare: quantum Cramér-Rao bound (Heisenberg limit). Not necessarily the limit of practical interest.

(Ferrie, *Granade* and Cory 2013 *10/tfx*)

Bayesian Cramér-Rao Bound

Integrating the Fisher information over the prior π results in a Bayesian analog, the Bayesian Cramér-Rao bound:

$$\underline{\underline{B}} := \mathbb{E}_{\underline{x}}[\underline{\underline{I}}(\underline{x})], \quad r(\pi) \geq \underline{\underline{B}}^{-1}.$$

If experiments are designed adaptively, then the current posterior is used instead of the prior.

The BCRB can be computed iteratively, making it useful for tracking optimality in an online fashion.

$$\underline{\underline{B}}_{k+1} = \underline{\underline{B}}_k + \begin{cases} \mathbb{E}_{\underline{x}\sim\pi}[\underline{\underline{I}}(\underline{x}; \underline{e}_{k+1})] & \text{(non-adaptive)} \\ \mathbb{E}_{\underline{x}|d_1,\dots,d_k}[\underline{\underline{I}}(\underline{x}; \underline{e}_{k+1})] & \text{(adaptive)} \end{cases}$$

(Gill and Levit 1995; Ferrie, *Granade* et al. 2012 *10/s87*)

Sequential Monte Carlo

SMC is a numerical algorithm for generating samples from a distribution.

$$\text{prior} \xrightarrow{\text{Bayes' Rule}} \text{posterior}$$

Bayes' rule acts as a transition kernel from prior samples to posterior samples.

Posterior samples then give Monte Carlo approximations to integrals/expectations.

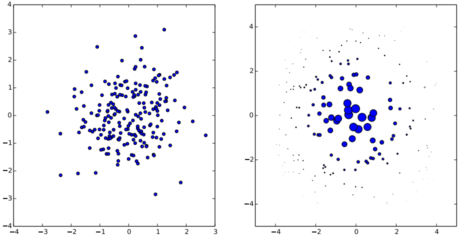
SMC Approximation

$$\Pr(\underline{x}) \approx \sum_i^n w_i \delta(\underline{x} - \underline{x}_i)$$

(Doucet and Johansen 2011; Huszár and Houlsby *10/s86*; *Granade* et al. 2012 *10/s87*)

Ambiguity and Impovrishment

The SMC approximation can represent distributions by density of *particles* (left), or by weight (right).



Using weight is less numerically stable, results in smaller *effective* number of particles.

$$n_{\text{ess}} := 1 / \sum_i w_i^2$$

Numerical Stability and Resampling

As data D is collected, $\Pr(\underline{x}_i|D) \to 0$ for initial particles $\{x_i\}$.

- Results in $n_{\text{ess}} \to 0$ as data is collected.B

Can mitigate by *resampling*: moving information from the weights to the density of SMC particles.

Resampling when $n_{\text{ess}}/n \le 0.5$ helps preserve representative sample. Moreover, monitoring n_{ess} can herald some kinds of failures.

Liu and West Algorithm

Draw new particles $\underline{x}'$ from kernel density estimate

$$\Pr(\underline{x}') \propto \sum_i w_i \exp\left((\underline{x}' - \underline{\mu}_i)^{\mathrm{T}} \underline{\underline{\Sigma}} (\underline{x}' - \underline{\mu}_i) \right)$$

$$\underline{\mu}_i = a\underline{x}_i + (1-a)\mathbb{E}[\underline{x}]$$

$$\underline{\underline{\Sigma}} = (1-a^2)\,\mathrm{Cov}[\underline{x}]$$

Set new weights to be uniform, so that $n_{\text{ess}} = n$.

- $a = 1, h = 0$: Bootstrap filter, used in state-space applications like CONDENSATION.
- $a^2 + h^2 = 1$: Ensures $\mathbb{E}[\underline{x}'] = \mathbb{E}[\underline{x}]$ and $\mathrm{Cov}(\underline{x}') = \mathrm{Cov}(\underline{x})$, but assumes unimodality.
- $a = 1, h \geq 0$: Allows for multimodality, emulating state-space with synthesized noise.

(West 1993; Isard and Blake 1998 *10/cc76f6*; Liu and West 2001)

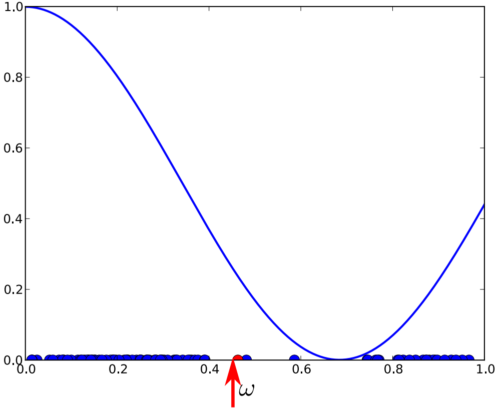
Putting it All Together: The SMC Algorithm

1. Draw $\{\underline{x}_i\} \sim \pi$, set $\{w_i\} = 1/n$.
2. For each datum $d_j \in D$:
   1. $w_i \leftarrow w_i \times \Pr(d_j | \underline{x}_i; \underline{e}_j)$.
   2. Renormalize $\{w_i\}$.
   3. If $n_{\text{ess}}/n \leq 0.5$, resample.
3. Report $\hat{\underline{x}} := \mathbb{E}[\underline{x}] \approx \sum_i w_i \underline{x}_i$.

Sequential Monte Carlo

With SMC and resampling, particles move towards the true model as data is collected.

$N = 1$



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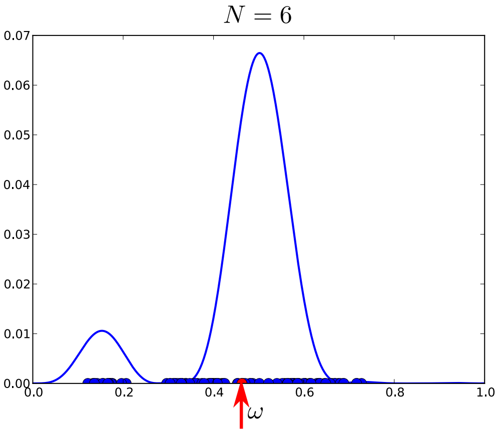

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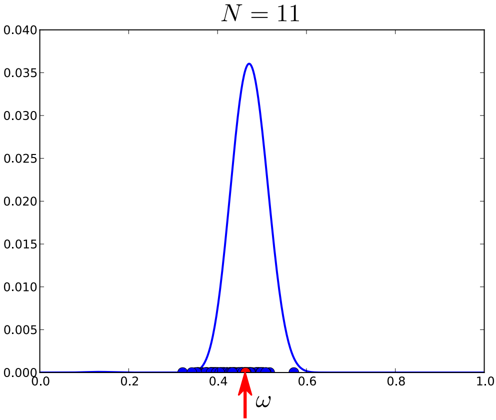

Near-Optimality for $\cos^2$

Using adaptive experiment design with Newton Conjugate-Gradient:

(*Granade* et al. 2012 *10/s87*)

Randomized Benchmarking Example

Applying sequences of random Clifford gates *twirls* errors in a gateset, such that they can be simulated using depolarizing channels.

(Knill et al. 2008 *10/cxz9vm*; Magesan et al. 2012 *10/tfz*; Magesan et al. 2012 *10/s8j*)

Randomized Benchmarking Example

SMC: interpret survival probability as likelihood. For interleaved case, the lowest-order model is:

$$\Pr(\text{survival}|A, B, \tilde{p}, p_{\text{ref}}; m, \text{mode}) = \begin{cases} A p_{\text{ref}}^m + B & \text{reference} \\ A(\tilde{p} p_{\text{ref}})^m + B & \text{interleaved} \end{cases}$$

A, B: state preparation and measurement
m: sequence length
p_{ref}: reference depolarizing parameter
$\tilde{p}$: depolarizing parameter for gate of interest

(*Granade*, Ferrie and Cory 2014 *1404.5275*)

Randomized Benchmarking Example

Using SMC, useful conclusions can be reached with significantly less data than with least-squares fitting.

(*Granade*, Ferrie and Cory 2014 *1404.5275*)

Method of Hyperparameters

If "true" model $\underline{x} \sim \Pr(\underline{x}|\underline{y})$, for some *hyperparameters* $\underline{y}$, can est. $\underline{y}$ directly:

$$\Pr(d|\underline{y};\underline{e}) = \int \Pr(d|\underline{x},\underline{y};\underline{e}) \Pr(\underline{x}|\underline{y};\underline{e}) \, \mathrm{d}\underline{x}.$$

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Example

For Larmor precession with $\omega \sim \mathrm{Cauchy}(\omega_0, T_2^{-1})$,

$$\Pr(d|(\omega_0, T_2^{-1}); t) = \mathrm{e}^{-tT_2^{-1}} \cos^2(\omega_0 t/2) + (1 - \mathrm{e}^{-tT_2^{-1}})/2.$$

Let $\underline{y} = (\omega_0, T_2^{-1})$.

(*Granade* et al. 2012 *10/s87*)

State-Space SMC

Alternatively, can move particles at each timestep $\underline{x}(t_k) \sim \Pr(\underline{x}(t_k)|\underline{x}(t_{k-1}))$.

This represents *tracking* of a stochastic process.

Confidence and Credible Regions

Characterizing uncertainty of estimates is critical for many applications:

Definition (Confidence Region)

X_α is an α-confidence region if $\Pr_D(\underline{x}_0 \in X_\alpha(D)) \geq \alpha$.

Definition (Credible Region)

X_α is an α-credible region if $\Pr_{\underline{x}}(\underline{x} \in X_\alpha | D) \geq \alpha$.

Credible regions can be calculated from posterior $\Pr(\underline{x}|D)$ by demanding

$$\int_{X_\alpha} \mathrm{d}\Pr(\underline{x}|D) \geq \alpha.$$

(*Granade* et al. 2012 *10/s87*; Ferrie 2014 *10/tb4*)

High Posterior Density

Want credible regions that are *small* (most powerful).

- Posterior covariance ellipses (PCE)— good for approximately normal posteriors
- Convex hull— very general, but verbose description
- Minimum volume enclosing ellipses (MVEE)— good approximation to hull

(*Granade* et al. 2012 *10/s87*; Ferrie 2014 *10/tb4*)

Comparison of HPD Estimators

For multimodal distributions, clustering algorithms can be used to exclude regions of small support. For a noisy coin model (heads probability p, visibility η):

Left, no clustering. Right, DBSCAN.

Plot courtesy of Chris Ferrie. (Ferrie 2014 *10/tb4*)

Hyperparameters and Region Estimation

In some hyperparameter models, can also express as region estimator on underlying parameters.

Figure : Larmor precession model w/ $\omega \sim \mathrm{N}(\mu, \sigma^2)$, three exp. design strategies

Critically, the covariance region for ω is not smaller than the true covariance given by the hyperparameter σ^2.

(*Granade* et al. 2012 *10/s87*)

Bayes Factors and Model Selection

In SMC update $w_i \mapsto w_i \times \Pr(d|\underline{x};\underline{e})/\mathcal{N}$,

$$\mathcal{N} \approx \Pr(d|\underline{e}).$$

Running SMC updaters for distinct models A and B, collecting normalizations $\mathcal{N}_A$ and $\mathcal{N}_B$ at each step gives

$$\mathrm{BF} = \frac{\mathcal{N}_A}{\mathcal{N}_B} \approx \frac{\Pr(d|A;\underline{e})}{\Pr(d|B;\underline{e})}$$

For full data record, can multiply normalization records to select A versus B.

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tdk*)

For example, deciding between linear- (left) and complete-graph (right) Ising models:

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tdk*)

Main cost to SMC: simulation calls. n each Bayes update.

Simulation and learning are intimately connected: if we can simulate, then we can learn.

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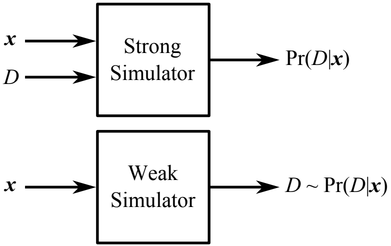
Big Idea

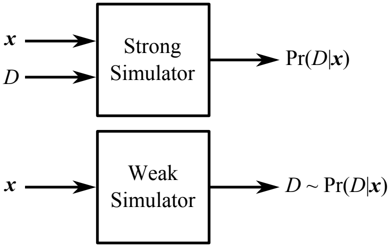
Use quantum simulation to learn about unknown quantum systems.

Weak and Strong Simulation



(Ferrie and Granade 2014 *10/tdj*)

Weak and Strong Simulation



Quantum simulation produces data, not likelihoods. Must sample to estimate likelihood.

(Ferrie and Granade 2014 *10/tdj*)

Adaptive Likelihood Estimation

Solution

Treat estimating the likelihood as a secondary estimation problem.

(Ferrie and Blume-Kohout 2012 *10/tf2*, Ferrie and Granade 2014 *10/tdj*)

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2-outcome model: hedged binomial estimator finds the probability p_0 of a "0" outcome by repeatedly sampling a weak simulator.

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Adaptive Likelihood Estimation

Solution

Treat estimating the likelihood as a secondary estimation problem.

2-outcome model: hedged binomial estimator finds the probability p_0 of a "0" outcome by repeatedly sampling a weak simulator.

Variance well-known, so collect until a fixed *tolerance* is reached.

We will show that SMC is robust to likelihood estimation errors.

(Ferrie and Blume-Kohout 2012 *10/tf2*, Ferrie and Granade 2014 *10/tdj*)

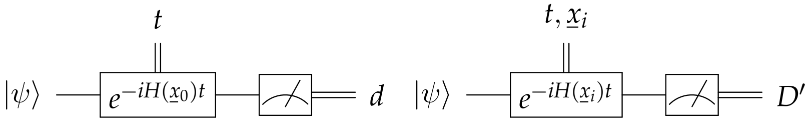
Quantum Likelihood Evaluation

First approach: compare classical outcomes of unknown and trusted quantum systems.

Evolve state $|\psi\rangle$ for time t then measure, getting d.

For each particle $\underline{x}_i$, repeatedly sample from quantum simulation of $\mathrm{e}^{-\mathrm{i}t\underline{x}_i}$, getting D'.

Unknown System Simulator



Estimated likelihood $\hat{\ell}_i := |\{d' \in D' | d' = d\}|$. SMC update:

$$w_i \mapsto w_i \hat{\ell}_i / \sum_i w_i \hat{\ell}_i.$$

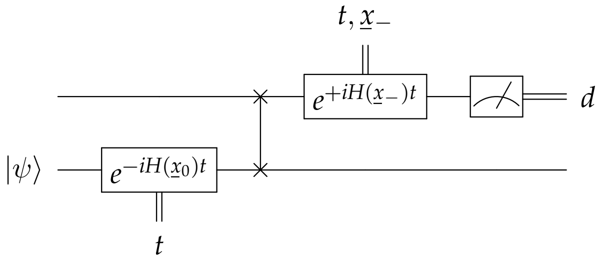
(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

QLE can work, but as $t \to \infty$, $\Pr(d|\underline{x}; t)$ equilibriates. Thus, $t \geq t_{\text{eq}}$ is uninformative.

By CRB, error then scales as $\mathrm{O}(1/N t_{\text{eq}}^2)$.

Interactive QLE

Solution: couple unknown system is to a quantum simulator, then invert evolution by hypothesis $\underline{x}_-$.



Echo

If $\underline{x}_- \approx \underline{x}_0$, then $\left|\langle\psi|\mathrm{e}^{-\mathrm{i}t(H(\underline{x}_0)-H(\underline{x}_-))}|\psi\rangle\right|^2 \approx 1$.

(Wiebe, *Granade*, Ferrie and Cory 2014 10/tf3)

Alternate Interpretation

QHL finds $\hat{\underline{x}}$ such that $H(\hat{\underline{x}})$ most closely approximates "unknown" system H_0.

Gives an α-credible bound on error introduced by replacing $H_0 \to H(\hat{\underline{x}})$.

Posterior Guess Heuristic

Inversion connects the model and experiment spaces. Use to come up with a heuristic for experiment designs.

- Choose $\underline{x}_e, \underline{x}_e' \sim \Pr(\underline{x})$, the most recent posterior.
- Choose $t = 1/\|\underline{x}_e - \underline{x}_e'\|$.
- Return $\underline{e} = (\underline{x}_e, t)$.

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

Ising Model on Spin Chains

Hamiltonian: nearest-neighbor Ising models on a chain of nine qubits.

Interactivity allows for dramatic improvements over QLE.

$\mathcal{P}$: adaptive likelihood estimation tolerance.

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

Ising Model on the Complete Graph

With IQLE, can also learn on complete interaction graphs. We show the performance as a function of the depolarization strength $\mathcal{N}$.

$\mathcal{N}$: depolarizing noise following SWAP gate.

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tdk*)

Ising Model with the Wrong Graph

Simulate with spin chains, suppose "true" system is complete, with non-NN couplings $O(10^{-4})$.

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tdk*)

Scaling Parameter

dim $\underline{x}$, not dim $\mathcal{H}$, determines scaling of IQLE.

Figure : 4 qubit (red) and 6 qubit (blue) complete graph IQLE

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

Scaling and Dimensionality

In both the spin-chain and complete graph cases, the quadratic loss on average decays exponentially, $L_{\underset{=}{Q}} \propto e^{-\gamma N}$, for some rate constant γ.

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

Scaling and Dimensionality

In both the spin-chain and complete graph cases, the quadratic loss on average decays exponentially, $L_{\underline{\underline{Q}}} \propto e^{-\gamma N}$, for some rate constant γ. Consider $\gamma = \gamma(\dim \underline{x})$:

This suggests that, with access to a quantum simulator, learning *may* scale efficiently.

(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

SMC + IQLE:

- Possibly scalable with quantum resources.
- Robust to finite sampling.
- Robust to approximate models.

Still requires simulator be at least as large as system of interest.

Information Locality

To go further, we want to *localize* our experiment, such that we can simulate on a smaller system.

Measure on X, simulate on W, and ignore all terms with support over Y.

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To go further, we want to *localize* our experiment, such that we can simulate on a smaller system.

Measure on X, simulate on W, and ignore all terms with support over Y.

Gives *approximate* model that can be used to learn Hamiltonian restricted to X.

Local and Global Particle Clouds

To reconstruct the entire system, we need to combine data from different partitions.

Separate out one partition W_k at a time, maintain a *global* cloud of particles.

Local and Global Particle Clouds

Initialize $\{\underline{x}_i\}$ over entire system. Then, for each simulated subregister W_k:

1. Make "local" particle cloud $\{\underline{x}_i|_{W_k}\}$ by slicing $\{\underline{x}_i\}$.
2. Run SMC+IQLE with $\{\underline{x}_i|_{W_k}\}$ as a prior.
3. Ensure that the final "local" cloud has been resampled (has equal weights).
4. Overwrite parameters in "global" cloud $\{\underline{x}_i\}$ corresponding to post-resampling $\{\underline{x}_i|_{W_k}\}$.

In this way, all parameters are updated by an SMC run.

Q50 Example

Goal: characterize a 50-qubit Ising model (complete graph) with unknown ZZ couplings.

All Hamiltonian terms commute, but initial state doesn't. Let A_X be observable, $A_{X'}$ be sim. observable.

$$\|A_X(t) - A_{X'}(t)\| \leq \|A_X(t)\|(\mathrm{e}^{2\|H|_Y\|t} - 1)$$
$$\Rightarrow t \leq \ln\left(\frac{\delta}{\|A_X(t)\|} + 1\right)(2\|H|_Y\|)^{-1},$$

where δ is the tolerable likelihood error.

Example Q50 Run

$|X_k| = 4$, $|W_k| = 8$, $n = 20,000$, $N = 500$, exp. decaying interactions.
NB: 1225 parameter model, L_2 error of 0.3%.

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Lieb-Robinson Bounds

More generally, for $[H|_W, H_Y] \neq 0$, use *Lieb-Robinson bound*.
If interactions between X and Y decay sufficiently quickly, then there exists C, μ and v s. t. for any observables $A_X(t)$, B_Y:

$$\|[A_X(t), B_Y]\| \leq C\|A_X(t)\|\|B_Y\||X||Y|(\mathrm{e}^{v|t|} - 1)\mathrm{e}^{-\mu d(X,Y)}$$

This *guarantees* that error due to truncation is bounded if we choose small t.

(Hastings and Koma 2006 *10/cddqgz*; Nachtergale and Sims 2006 *10/d9xwfg*)

Lieb-Robinson Bounds

Can find bound in terms of Hamiltonian by considering H site-by-site.

Let H_j be the Hamiltonian term containing distance-j interactions between W and Y, acting on sites Ω_j.

$$\|A(t) - \mathrm{e}^{\mathrm{i}H|_W t} A \mathrm{e}^{-\mathrm{i}H|_W t}\| \leq \sum_j C\|A\|\|H_j\||X||\Omega_j|\mathrm{e}^{-\mu j}(\mathrm{e}^{v|t|} - 1)$$

Trotterization

Can improve the Lieb-Robinson bound by "shaking" between simulator and system. Using $r \approx vt$ SWAP gates, error is $\mathrm{O}(t)$.

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- Using robustness of SMC, can truncate simulation $\rightarrow$ bootstrapping.

Further Information

Slides, a journal reference for this work, a full bibliography and a software implementation can be found at *http://www.cgranade.com/research/talks/msr-2014/*.

Thank you for your kind attention!