

Semiquantum Algorithms for Characterization and Verification

Christopher Granade

www.cgranade.com/research/talks/msr-2014

Joint work with:

Nathan Wiebe Christopher Ferrie D. G. Cory

Institute for Quantum Computing
University of Waterloo, Ontario, Canada

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Microsoft Research

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 $p_i = \text{Tr}(E_i \rho)$ 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?

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

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

what we know about our model having seen some data.

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

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

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{x} of a “true” model x a *loss*, describing how bad \hat{x} does at estimating x .

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Definition (Quadratic Loss)

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

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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Estimator: function from data records D to estimates $\hat{x}(D)$.
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Definition (Bayes Risk)

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

Cramér-Rao Bound

The Fisher information

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

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

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

$$R(\hat{\underline{x}}, \underline{x}) = \text{Tr}(\text{Cov}(\hat{\underline{x}})) \geq \text{Tr}(\underline{\underline{I}}(\underline{x})^{-1}).$$

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

Bayesian Cramér-Rao Bound

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

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

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.

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

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.

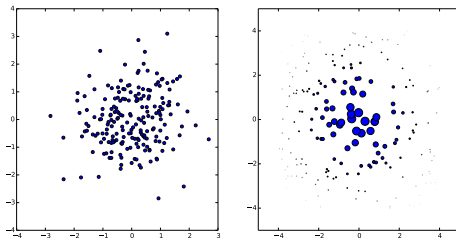
SMC Approximation

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

(Doucet and Johansen 2011; Huszár and Hounsby 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, $\Pr(\underline{x}_i|D) \rightarrow 0$ for initial particles $\{x_i\}$.

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

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

Resampling when $n_{\text{ess}}/n \leq 0.5$ 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

$$\begin{aligned}\Pr(\underline{x}') &\propto \sum_i w_i \exp \left((\underline{x}' - \underline{\mu}_i)^T \underline{\underline{\Sigma}} (\underline{x}' - \underline{\mu}_i) \right) \\ \underline{\mu}_i &= a \underline{x}_i + (1 - a) \mathbb{E}[\underline{x}] \\ \underline{\underline{\Sigma}} &= (1 - a^2) \text{Cov}[\underline{x}]\end{aligned}$$

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 $\text{Cov}(\underline{x}') = \text{Cov}(\underline{x})$, but assumes unimodality.
- $a = 1, h \geq 0$: Allows for multimodality, emulating state-space with synthesized noise.

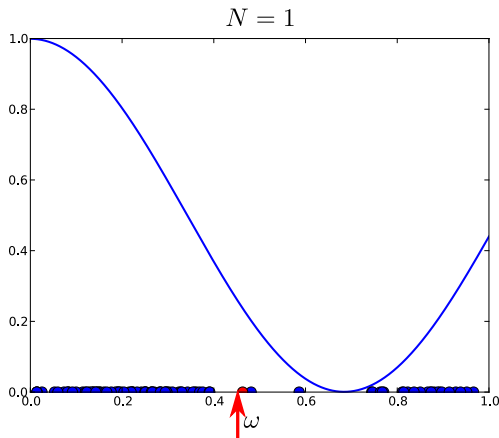
(West 1993; Liu and West 2001)

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 $\hat{\underline{x}} := \mathbb{E}[\underline{x}] \approx \sum_i w_i \underline{x}_i$.

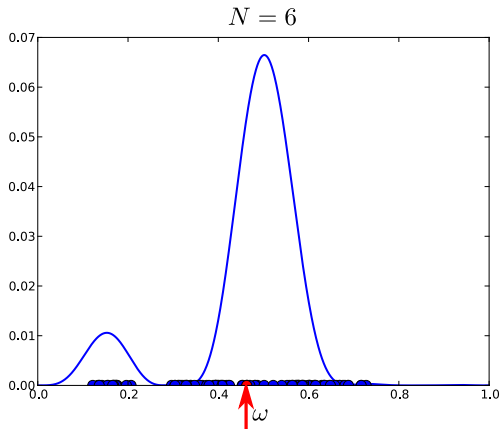
Sequential Monte Carlo

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



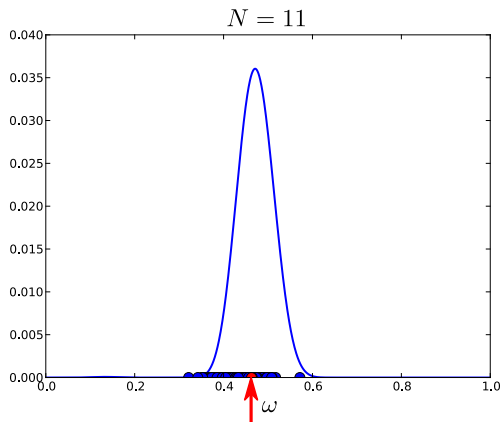
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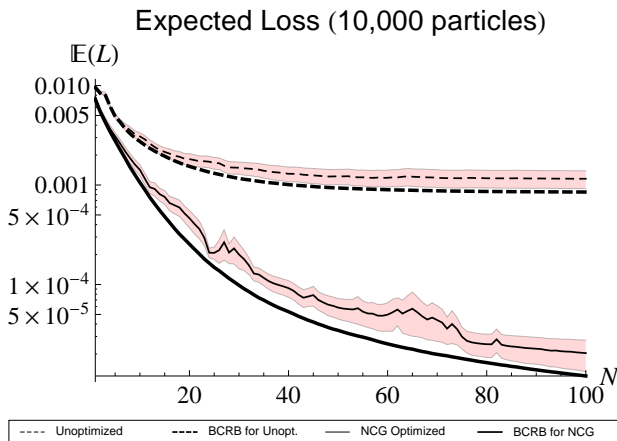
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Near-Optimality for \cos^2

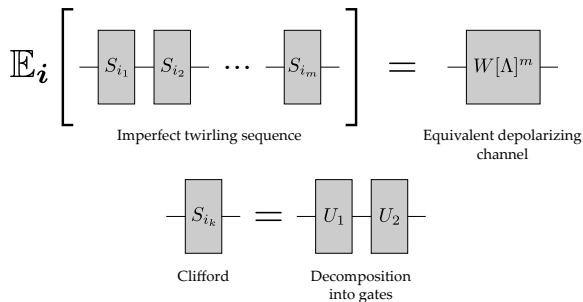
Using adaptive experiment design with Newton Conjugate-Gradient:



(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:

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

A, B : state preparation and measurement

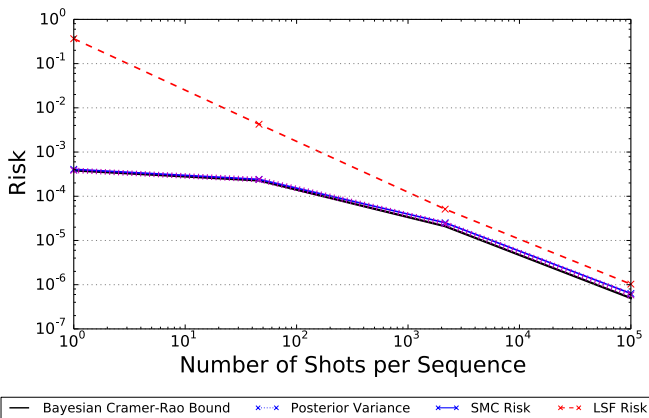
m : sequence length

p_{ref} : reference depolarizing parameter

\tilde{p} : depolarizing parameter for gate of interest

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:

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

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Example

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

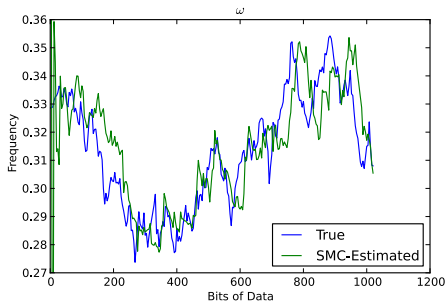
$$\Pr(d|(\omega_0, T_2^{-1}); t) = e^{-tT_2^{-1}} \cos^2(\omega_0 t/2) + (1 - e^{-tT_2^{-1}})/2.$$

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

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

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

High Posterior Density

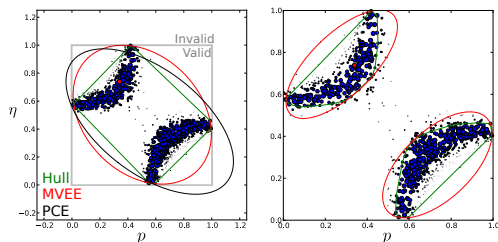
Want credible regions that are *small* (most powerful).

- 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.

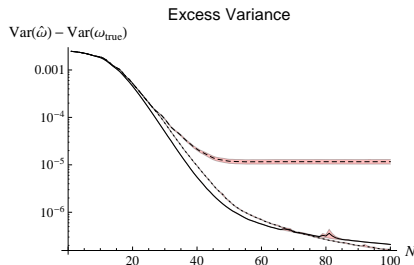


Figure : Larmor precession model w/ $\omega \sim N(\mu, \sigma^2)$, three exp. design strategies

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

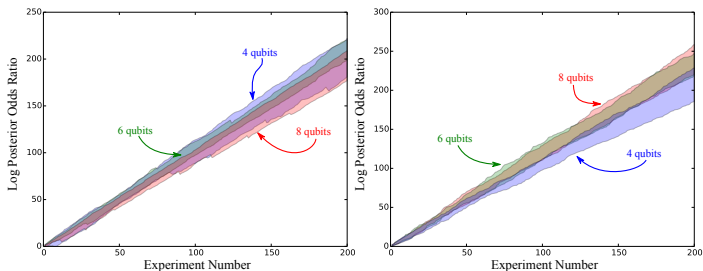
$$\mathcal{N} \approx \Pr(d|\underline{e}).$$

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

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

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

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.

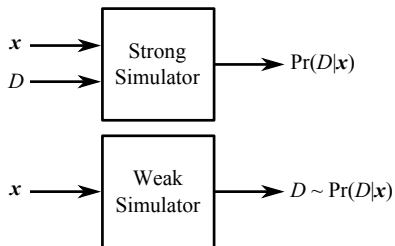
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Big Idea

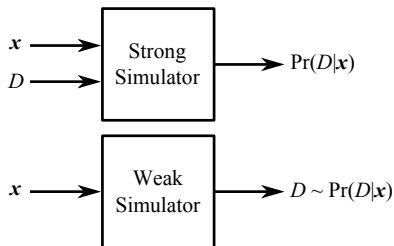
Use quantum simulation to learn about unknown quantum systems.

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.

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](#))

Adaptive Likelihood Estimation

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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.

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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.

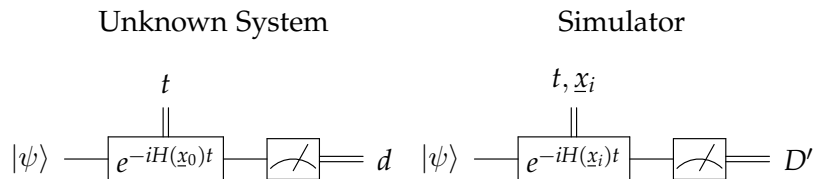
(Ferrie and Blume-Kohout 2012 [10/tf2](#), Ferrie and Granade 2014 [10/tdj](#))

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 $e^{-iH(\underline{x}_i)t}$, getting D' .



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

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

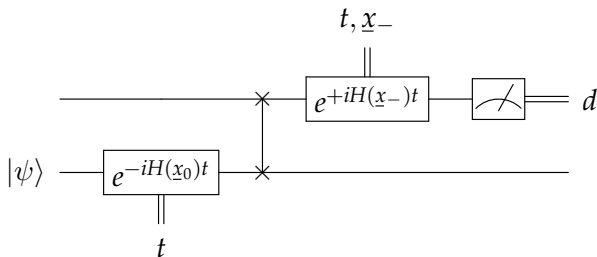
(Wiebe, Granade, Ferrie and Cory 2014 [10/tf3](#))

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

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

Interactive QLE

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



Echo

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

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

Alternate Interpretation

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

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

Posterior Guess Heuristic

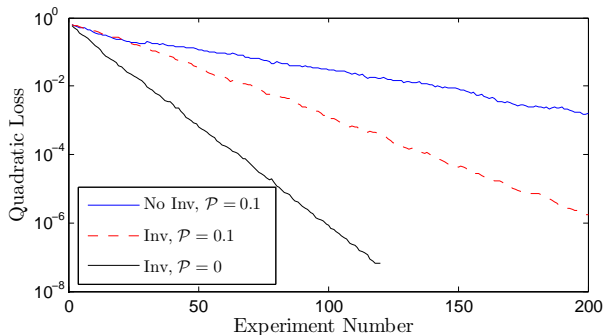
Inversion connects the model and experiment spaces. Use to come up with a heuristic for experiment designs.

- 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 $\underline{e} = (\underline{x}_e, t)$.

Ising Model on Spin Chains

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

Interactivity allows for dramatic improvements over QLE.

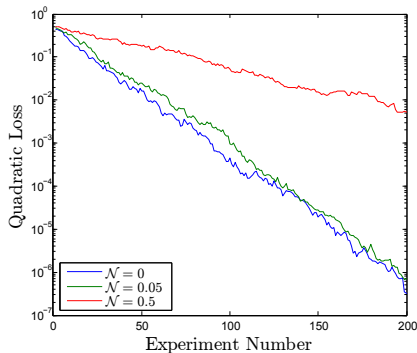


\mathcal{P} : adaptive likelihood estimation tolerance.

(Wiebe, Granade, Ferrie and Cory 2014 10/f3)

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} .

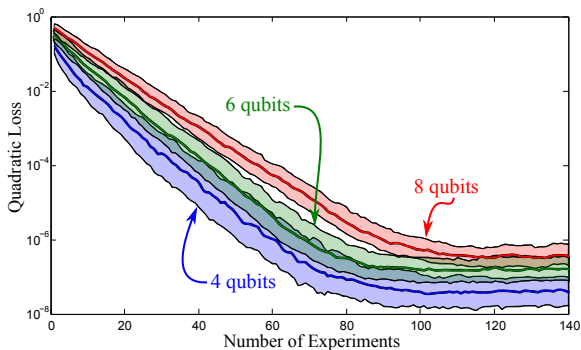


\mathcal{N} : depolarizing noise following SWAP gate.

(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.

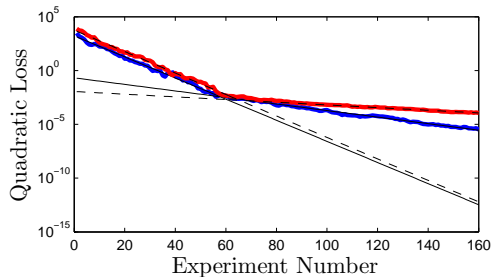


Figure : 4 qubit (red) and 6 qubit (blue) complete graph IQLE

(Wiebe, Granade, Ferrie and Cory 2014 [10/tf3](#))

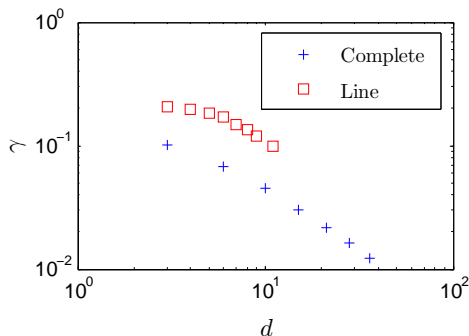
Scaling and Dimensionality

In both the spin-chain and complete graph cases, the quadratic loss on average decays exponentially, $L_Q \propto e^{-\gamma N}$, 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, $L_Q \propto e^{-\gamma N}$, 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](#))

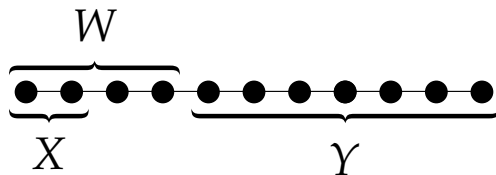
SMC + IQLE:

- 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

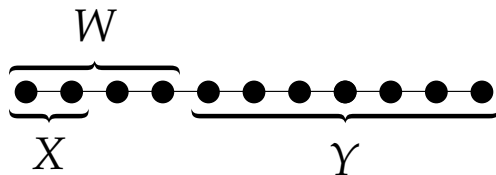
To go further, we want to *localize* our experiment, such that we can simulate on a smaller system.



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

Information Locality

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

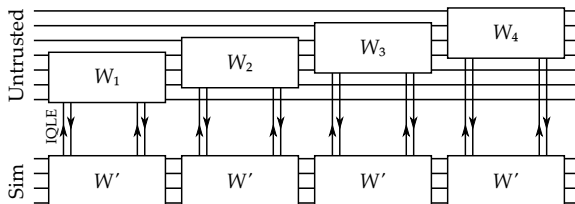


Measure on X , simulate on W , and ignore all terms with support over Y .

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

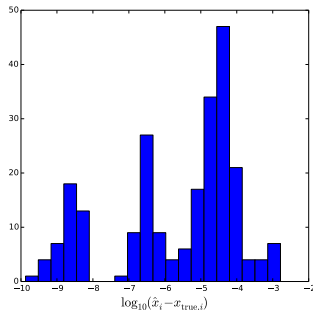
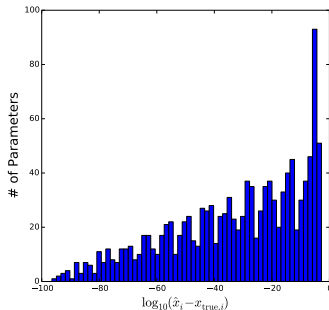
Goal: characterize a 50-qubit Ising model (complete graph) with unknown ZZ couplings.

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

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

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%.

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 $A_X(t), B_Y$:

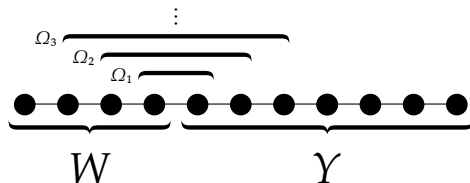
$$\|[A_X(t), B_Y]\| \leq C\|A_X(t)\|\|B_Y\|\|X\|\|Y\|(e^{v|t|} - 1)e^{-\mu d(X,Y)}$$

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.

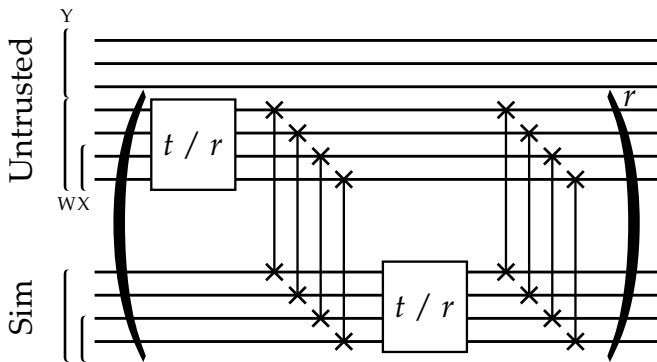


Let H_j be the Hamiltonian term containing distance- j interactions between W and Y , acting on sites Ω_j .

$$\|A(t) - e^{iH|w|t} A e^{-iH|w|t}\| \leq \sum_j C \|A\| \|H_j\| |X| |\Omega_j| e^{-\mu j} (e^{v|t|} - 1)$$

Trotterization

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



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- Robust to many practical concerns.
- Can use quantum simulation to offer potential scaling.
- 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/*](http://www.cgranade.com/research/talks/msr-2014/).



Thank you for your kind attention!