#### Quantum Bootstrapping

#### 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

> July 14, 2014 **LFQIS 2014**

We want to build a quantum computer.

We want to build a quantum computer.

Need to push past what a classical computer can do. How do we get to 100 qubits?

Computational limits affect many aspects of building large quantum systems:

Characterization of H

Computational limits affect many aspects of building large quantum systems:

- Characterization of H
- Characterization of controls

Computational limits affect many aspects of building large quantum systems:

- Characterization of H
- Characterization of controls
- Design of control sequences

Computational limits affect many aspects of building large quantum systems:

- Characterization of H
- Characterization of controls
- Design of control sequences
- Verification of control

### Computational limits affect many aspects of building large quantum systems:

Building Large Systems: Computational Limits

- Characterization of H
- Characterization of controls
- Design of control sequences
- Verification of control

Here, we focus on characterization and verification.

#### Bootstrapping to Q100

Express challenges in terms of *simulation*, then use quantum simulators.

Use small quantum simulators to characterize and verify large devices, bootstrap up to Q100 scale.

#### Bootstrapping to Q100

Express challenges in terms of *simulation*, then use quantum simulators.

Use small quantum simulators to characterize and verify large devices, bootstrap up to Q100 scale.

■ Bayesian inference as platform

- Bayesian inference as platform
  - Sequential Monte Carlo: algorithm for Bayesian inference

- Bayesian inference as platform
  - Sequential Monte Carlo: algorithm for Bayesian inference
  - Generality and robustness of SMC

- Bayesian inference as platform
  - Sequential Monte Carlo: algorithm for Bayesian inference
  - Generality and robustness of SMC
- Hamiltonian learning w/ quantum resources

- Bayesian inference as platform
  - Sequential Monte Carlo: algorithm for Bayesian inference
  - Generality and robustness of SMC
- Hamiltonian learning w/ quantum resources
- Bootstrapping Hamiltonian learning

- Bayesian inference as platform
  - Sequential Monte Carlo: algorithm for Bayesian inference
  - Generality and robustness of SMC
- Hamiltonian learning w/ quantum resources
- Bootstrapping Hamiltonian learning
- Learning control distortions

### Bayesian Approaches to Characterization and Control

#### Likelihood Function

Model data collection as a probability distribution:

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

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

### Bayesian Approaches to Characterization and Control

#### Likelihood Function

Model data collection as a probability distribution:

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

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

#### Example

Larmor precession at an unknown  $\omega$  and  $T_2$ :

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

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

Given a likelihood, we can reason about

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

Given a likelihood, we can reason about

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

By Bayes' Rule: 
$$\Pr(\underline{x}|d,\underline{e}) = \frac{\Pr(\underline{a}|\underline{x};\underline{e})}{\Pr(\underline{d}|\underline{e})} \Pr(\underline{x}).$$
  $\Longrightarrow$  Simulation is a resource for learning.

Given a likelihood, we can reason about

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

By Bayes' Rule: 
$$\Pr(\underline{x}|d,\underline{e}) = \frac{\Pr(\underline{a}|\underline{x};\underline{e})}{\Pr(\underline{d}|\underline{e})} \Pr(\underline{x}).$$
  $\Longrightarrow$  Simulation is a resource for learning.

Given a likelihood, we can reason about

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

By Bayes' Rule: 
$$\Pr(\underline{x}|d,\underline{e}) = \frac{\Pr(\underline{a}|\underline{x};\underline{e})}{\Pr(\underline{d}|\underline{e})} \Pr(\underline{x}).$$
  $\Longrightarrow$  Simulation is a resource for learning.

Given a likelihood, we can reason about

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

what we know having seen some data.

By Bayes' Rule: 
$$\Pr(\underline{x}|d,\underline{e}) = \frac{\Pr(d|\underline{x};\underline{e})}{\Pr(d|\underline{e})} \Pr(\underline{x}).$$
  $\Longrightarrow$  Simulation is a resource for learning.

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

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

### Sequential Monte Carlo

**SMC** (aka *particle filter*): numerical algorithm for generating samples from a distribution, using a transition kernel.

$$\operatorname{prior} \stackrel{\operatorname{Bayes'} \operatorname{Rule}}{\longrightarrow} \operatorname{posterior}$$

Posterior samples then approximate  $\int /\mathbb{E}$ .

#### **SMC** Approximation

$$\Pr(\underline{x}) \approx \sum_{i}^{n} w_{i} \delta(\underline{x} - \underline{x}_{i})$$

### Sequential Monte Carlo

**SMC** (aka *particle filter*): numerical algorithm for generating samples from a distribution, using a transition kernel.

$$prior \stackrel{Bayes' \ Rule}{\longrightarrow} posterior$$

Posterior samples then approximate  $\int /\mathbb{E}$ .

#### **SMC** Approximation

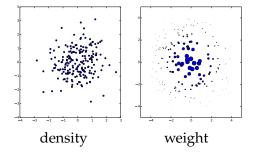
$$\Pr(\underline{x}) \approx \sum_{i}^{n} w_{i} \delta(\underline{x} - \underline{x}_{i})$$

QInfer Open-source implementation for quantum info.

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

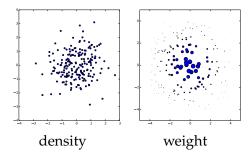
### Ambiguity and Impovrishment

#### Ambiguity in SMC approximation:



#### Ambiguity and Impovrishment

#### Ambiguity in SMC approximation:



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

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

#### Numerical Stability and Resampling

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

 $\blacksquare$   $\Rightarrow$   $n_{\rm ess} \to 0$  as data is collected.

*Resampling*: move information from weights to the density of SMC particles.

- Resampling when  $n_{\rm ess}/n \le 0.5$  preserves stability.
- Monitoring  $n_{\text{ess}}$  can herald some kinds of failures.

#### Liu and West Algorithm

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

$$\Pr(\underline{x}') \propto \sum_{i} w_{i} \exp\left((\underline{x}' - \underline{\mu}_{i})^{T} \underline{\underline{\Sigma}} (\underline{x}' - \underline{\mu}_{i})\right)$$
$$\underline{\mu}_{i} := a\underline{x}_{i} + (1 - a)\mathbb{E}[\underline{x}] \qquad \underline{\underline{\Sigma}} := h^{2} \operatorname{Cov}[\underline{x}] \qquad w'_{i} := 1/n$$

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

$$\Pr(\underline{x}') \propto \sum_{i} w_{i} \exp\left((\underline{x}' - \underline{\mu}_{i})^{T} \underline{\underline{\Sigma}} (\underline{x}' - \underline{\mu}_{i})\right)$$
$$\underline{\mu}_{i} := a\underline{x}_{i} + (1 - a)\mathbb{E}[\underline{x}] \qquad \underline{\underline{\Sigma}} := h^{2} \operatorname{Cov}[\underline{x}] \qquad w'_{i} := 1/n$$

Parameters *a* and *h* can be set based on application:

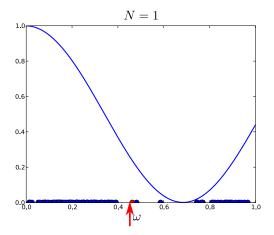
- $\blacksquare a = 1, h = 0$ : Bootstrap filter, used in state-space applications like Condensation.
- $\blacksquare a^2 + h^2 = 1$ : Ensures  $\mathbb{E}[x'] = \mathbb{E}[x]$  and  $Cov(\underline{x}') = Cov(\underline{x})$ , but assumes unimodality.
- $\blacksquare a = 1, h > 0$ : Allows for multimodality,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

### Putting it All Together: The SMC Algorithm

- 1 Draw  $\{x_i\} \sim \pi$ , set  $\{w_i\} = 1/n$ .
- **2** For each datum  $d_i \in D$ :
  - 1  $w_i \leftarrow w_i \times \Pr(d_i|x_i;e_i)$ .
  - 2 Renormalize  $\{w_i\}$ .
  - 3 If  $n_{\rm ess}/n \leq 0.5$ , resample.
- **3** Report  $\hat{x} := \mathbb{E}[x] \approx \sum_i w_i x_i$ .

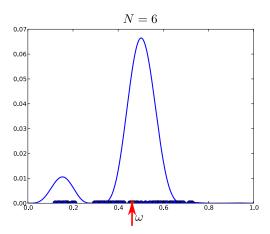
# With SMC and resampling, particles move towards the true

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



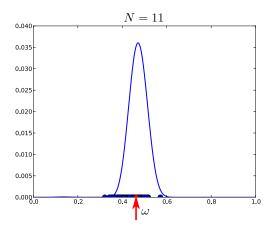
### Sequential Monte Carlo

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



### Sequential Monte Carlo

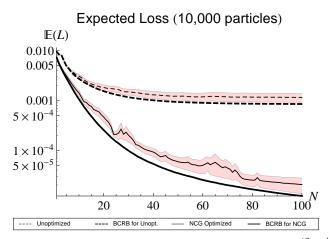
With SMC and resampling, particles move towards the true model as data is collected.



Before bootstrapping, a few examples of SMC w/ classical resources:

## Near-Optimality for cos<sup>2</sup>

Adaptive experiment design w/ Newton Conjugate-Gradient, vs. optimum from Bayesian Cramér-Rao Bound:



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

### Randomized Benchmarking Example

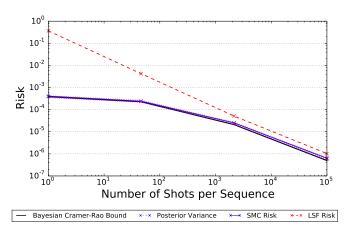
Interpret survival probability as likelihood. For interleaved case, the lowest-order model is:

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

- A, B state preparation and measurement
  - *m* sequence length
- $p_{\text{ref}}$  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.



Would like to learn hyperfine coupling <u>A</u> between  $e^-$  spin <u>S</u> and  $^{13}$ C spin I.

$$H(\underline{x}) = \Delta_{zfs}S_z^2 + \gamma(\underline{B} + \underline{\delta}\underline{B}) \cdot \underline{S} + \underline{S} \cdot \underline{\underline{A}} \cdot \underline{I}$$

$$\underline{x} = (\Delta_{zfs}, \underline{\delta}\underline{B}, \underline{\underline{A}}, \alpha, \beta, T_{2,e}^{-1}, T_{2,C}^{-1})$$

$$\alpha, \beta : \text{visibility parameters}$$

Would like to learn hyperfine coupling <u>A</u> between  $e^-$  spin <u>S</u> and  $^{13}$ C spin I.

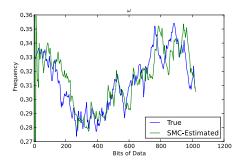
$$H(\underline{x}) = \Delta_{zfs}S_z^2 + \gamma(\underline{B} + \underline{\delta}\underline{B}) \cdot \underline{S} + \underline{S} \cdot \underline{\underline{A}} \cdot \underline{I}$$

$$\underline{x} = (\Delta_{zfs}, \underline{\delta}\underline{B}, \underline{\underline{A}}, \alpha, \beta, T_{2,e}^{-1}, T_{2,C}^{-1})$$

$$\alpha, \beta : \text{visibility parameters}$$

- Analytic estimate sensitive to error  $\delta B$  in static field.
- Use multiple  $\underline{B}$  settings to decorrelate  $\underline{\delta B}$ ,  $\underline{A}$ .

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)

 $X_{\alpha}$  is an  $\alpha$ -confidence region if  $\Pr_D(x_0 \in X_{\alpha}(D)) \geq \alpha$ .

### Confidence and Credible Regions

Characterizing uncertainty of estimates is critical for many applications:

#### Definition (Credible Region)

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

### Confidence and Credible Regions

Characterizing uncertainty of estimates is critical for many applications:

#### Definition (Credible Region)

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

Credible regions can be calculated from posterior Pr(x|D) by demanding

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

### High Posterior Density

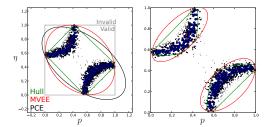
Want credible regions that are *small* (most powerful).

- 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

### Comparison of HPD Estimators

For multimodal distributions, clustering can be used to exclude regions of small support.

For a noisy coin model (heads probability p, visibility  $\eta$ ):



Left, no clustering. Right, DBSCAN.

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

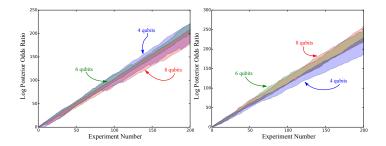
$$\mathcal{N} \approx \Pr(d|\underline{e}).$$

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

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

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:



### Towards Bootstrapping

SMC uses simulation as a resource for learning.

Simulation calls: main cost to SMC (*n* each Bayes update).

### Towards Bootstrapping

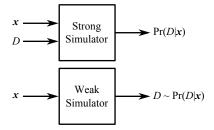
SMC uses *simulation* as a resource for *learning*.

Simulation calls: main cost to SMC (*n* each Bayes update).

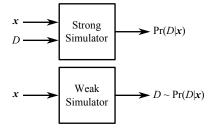
#### Big Idea

Use quantum simulation to extend SMC past classical resources.

### Weak and Strong Simulation



### 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:

Learn likelihood of untrusted system from frequencies of trusted system.

### Adaptive Likelihood Estimation

#### Solution

Treat estimating the likelihood as a secondary estimation problem:

Learn likelihood of untrusted system from frequencies of trusted system.

SMC is robust to likelihood estimation errors, given enough particles.

### ALE Example: Two-Outcome Models

Given:

d result of measurement

D' set of samples from weak simulator

Hedged binomial estimate of likelihood  $\ell$  from frequency k/K:

$$\hat{\ell} = \frac{k+\beta}{K+2\beta},$$

where  $\beta \approx 0.509$ ,  $k := |\{d' \in D' | d' = d\}|$ ,  $K = |\{D'\}|$ .

### ALE Example: Two-Outcome Models

Given:

d result of measurement

D' set of samples from weak simulator

Hedged binomial estimate of likelihood  $\ell$  from frequency k/K:

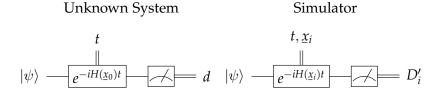
$$\hat{\ell} = \frac{k + \beta}{K + 2\beta},$$

where  $\beta \approx 0.509$ ,  $k := |\{d' \in D' | d' = d\}|$ ,  $K = |\{D'\}|$ .

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

### **Quantum Likelihood Evaluation**

Compare *classical* outcomes of unknown and trusted systems.



#### For each $x_i$ :

- repeatedly sample from quantum simulation of  $e^{-it\underline{x}_i}$ , getting  $D'_i$ .
- estimate  $\ell_i$  from  $D'_i$ .

SMC update:

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

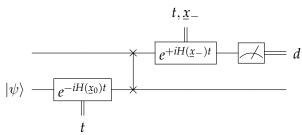
(Wiebe, Granade, Ferrie and Cory 2014 10/tf3)

QLE can work, but as  $t \to \infty$ ,  $\Pr(d|\underline{x};t) \leadsto 1/\dim \mathcal{H}$ . Thus,  $t \ge t_{\rm eq}$  is uninformative.

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

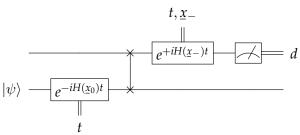
### Interactive OLE

Solution: couple unknown system is to a quantum simulator, then invert evolution by hypothesis  $x_-$ .



### Interactive OLE

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  $\left| \langle \psi | e^{-it(H(\underline{x}_{0}) - H(\underline{x}_{-}))} | \psi \rangle \right|^{2} \approx 1$ .

### Posterior Guess Heuristic

Inversion connects the model and experiment spaces. Use this duality as a heuristic for experiment design.

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

### Alternate Interpretation

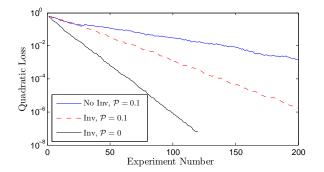
QHL finds  $\hat{x}$  such that  $H(\hat{x})$  most closely approximates "unknown" system  $H_0$ .

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

### Ising Model on Spin Chains

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

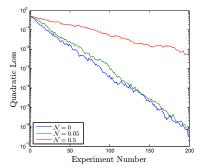
Interactivity allows for dramatic improvements over QLE.



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

### Ising Model on the Complete Graph

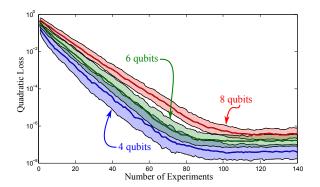
With IQLE, can also learn on complete interaction graphs. We show the performance as a function of the depolarization strength  $\mathcal{N}$ .



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

### Ising Model with the Wrong Graph

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



## Scaling Parameter

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

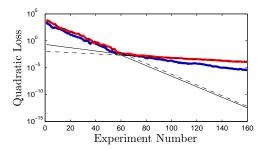


Figure: 4 qubit (red) and 6 qubit (blue) complete graph IQLE

In spin-chain and complete graph, average error decays exponentially,

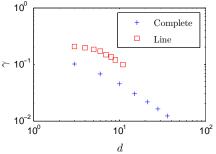
$$L(N) \propto e^{-\gamma N}$$

### Scaling and Dimensionality

In spin-chain and complete graph, average error decays exponentially,

$$L(N) \propto e^{-\gamma N}$$

Assess scaling by finding  $\gamma = \gamma(\dim x)$ :



With quantum simulation, learning may scale efficiently.

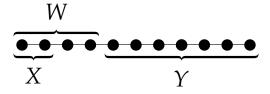
(Wiebe, Granade, Ferrie and Cory 2014 10/tf3)

- 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

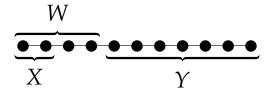
To go further, we want to *localize* our experiment, such that we can simulate on a smaller system.



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.

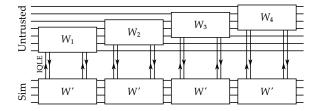


Measure on X, simulate on W, and ignore all terms with support over Y.

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.
- 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.

# O50 Example

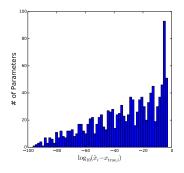
Goal: characterize a 50-qubit Ising model (complete graph) with unknown ZZ couplings.

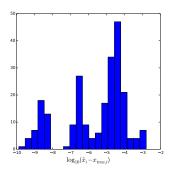
All Hamiltonian terms commute, but initial state doesn't. Let  $A_X$  be observable,  $A_{X'}$  be sim. observable.

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

where  $\delta$  is the tolerable likelihood error.

### Example Q50 Run

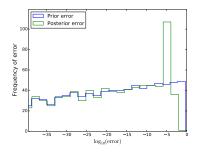




$$|X_k| = 4$$
,  $|W_k| = 8$ ,  $n = 20,000$ ,  $N = 500$ , exp. decaying interactions.

NB: 1225 parameter model,  $L_2$  error of 0.3%.

#### Example Q50 Run



 $|X_k| = 4$ ,  $|W_k| = 8$ , n = 20,000, N = 500, exp. decaying interactions.

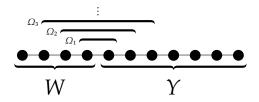
NB: 1225 parameter model,  $L_2$  error of 0.3%.

#### 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, $\mu$ and v s. t. for any observables $A_X(t)$ , $B_Y$ :

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

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

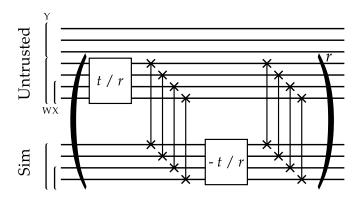
#### Can find bound in terms of Hamiltonian by considering H site-by-site.



Let  $H_i$  be the Hamiltonian term containing distance-iinteractions between W and Y, acting on sites  $\Omega_i$ .

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

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



## <u>Distorti</u>on Operators

Control affected by classical system, *distorts* controls from intended pulse.

$$H(t) = H(t; g[p]),$$

where p is a pulse, q = g[p] is the distorted pulse.

### Learning Controls with IQLE

Learning g is also important to bootstrapping. Suppose:

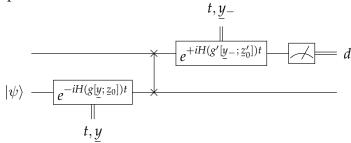
- $\blacksquare H \neq H(t)$
- $g: y \mapsto \underline{x}$  distorts static Hamiltonians
- $\blacksquare$  g parameterized by z

$$H = H(\underline{x}) = H(g[y;\underline{z}])$$

■ Trusted simulator is characterized s.t. arbitrary  $g[\cdot; z_i]$  can be simulated

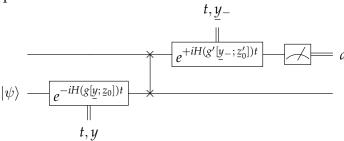
### IQLE Setup

#### **Experiment:**



### IQLE Setup

#### **Experiment:**



#### Simulator:

$$t, \underline{y}_i' \qquad t, \underline{y}_-$$
 
$$||\psi\rangle - e^{-iH(g'[\underline{y}_i';\underline{z}_0'])t} - e^{+iH(g'[\underline{y}_-;\underline{z}_0'])t}$$
 where  $g'[y_i';\underline{z}_0'] = g[y;z_i]$ .

### Control/Distortion Duality

Unknown rescaling example:  $g[y;\underline{z}] = y \odot \underline{z}$ . Straightforward to invert:

$$\underline{y}_i' = \underline{y} \odot \underline{z}_i \oslash \underline{z}_0' \quad \Longrightarrow \quad g'[\underline{y}_i'; \underline{z}_0'] = g[\underline{y}; \underline{z}_i]$$

## Control/Distortion Duality

Unknown rescaling example:  $g[\underline{y}; \underline{z}] = \underline{y} \odot \underline{z}$ . Straightforward to invert:

$$\underline{y}'_i = \underline{y} \odot \underline{z}_i \oslash \underline{z}'_0 \implies g'[\underline{y}'_i; \underline{z}'_0] = g[\underline{y}; \underline{z}_i]$$

Shows duality between hypothesis and simulation.

$$\begin{array}{ccc} \text{Experiment} & \text{Simulation} \\ \text{hypothesis} \, \underline{z_i} & \longleftrightarrow & \text{fixed} \, \underline{z_0'} \\ \text{fixed} \, y & & \text{control} \, y_i' \end{array}$$

QHL: special case  $\underline{y} = \underline{1}$ . What must we invert by to affect 1?

### Future: Bootstrapping for Control

Same approach can be used to model cross-talk:

$$\underline{z} = (\text{vec}\,\underline{\underline{G}}, \underline{\epsilon}) \quad g[y; \underline{z}] = \underline{\underline{G}}y + \underline{\epsilon}$$

Parameter count can be reduced by restricting  $\underline{\underline{G}}$  (i.e.: tridiagonal).

### Future: Bootstrapping for Control

Same approach can be used to model cross-talk:

$$\underline{z} = (\text{vec}\,\underline{G}, \underline{\epsilon}) \quad g[y; \underline{z}] = \underline{G}y + \underline{\epsilon}$$

Parameter count can be reduced by restricting  $\underline{\underline{G}}$  (i.e.: tridiagonal).

Can quantum resources be applied to *design* control?

Introduction Bayes QHL Bootstrapping Conclusions

■ Bayesian inference: simulation as a characterization/validation resource.

- Bayesian inference: simulation as a characterization/validation resource.
- Sequential Monte Carlo: numerical algorithm for inference.

- Bayesian inference: simulation as a characterization/validation resource.
- Sequential Monte Carlo: numerical algorithm for inference.
- Robust to many practical concerns.

- Bayesian inference: simulation as a characterization/validation resource.
- Sequential Monte Carlo: numerical algorithm for inference.
- Robust to many practical concerns.
- Can use quantum simulation to offer potential scaling.

- Bayesian inference: simulation as a characterization/validation resource.
- Sequential Monte Carlo: numerical algorithm for inference.
- Robust to many practical concerns.
- Can use quantum simulation to offer potential scaling.
- Using robustness of SMC, can truncate simulation → bootstrapping.

#### **Further Information**

Slides, a journal reference for this work, a full bibliography and a software implementation can be found at <a href="http://www.cgranade.com/research/talks/lfqis-2014/">http://www.cgranade.com/research/talks/lfqis-2014/</a>.



Thank you for your kind attention!

A few definitions help us evaluate estimates  $\hat{x}$  of  $\underline{x}$ :

Loss How well have we learned?

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

A few definitions help us evaluate estimates  $\hat{x}$  of  $\underline{x}$ :

Loss How well have we learned?

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

Risk On average, how well will we learn a particular model?

$$R(\hat{\underline{x}}, \underline{x}) := \mathbb{E}_D[L(\hat{\underline{x}}(D), \underline{x})]$$

A few definitions help us evaluate estimates  $\hat{x}$  of  $\underline{x}$ :

Loss How well have we learned?

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

Risk On average, how well will we learn a particular model?

$$R(\hat{\underline{x}}, \underline{x}) := \mathbb{E}_D[L(\hat{\underline{x}}(D), \underline{x})]$$

Bayes risk On average, how well will we learn a range of models?

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

A few definitions help us evaluate estimates  $\hat{x}$  of  $\underline{x}$ :

Loss How well have we learned?

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

Risk On average, how well will we learn a particular model?

$$R(\hat{\underline{x}}, \underline{x}) := \mathbb{E}_D[L(\hat{\underline{x}}(D), \underline{x})]$$

Bayes risk On average, how well will we learn a range of models?

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

Cramér-Rao Bound On average, how well can we learn?

#### Cramér-Rao Bound

#### Fisher Information

How much information about  $\underline{x}$  is obtained by sampling data?

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

#### Cramér-Rao Bound

#### Fisher Information

How much information about  $\underline{x}$  is obtained by sampling data?

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

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

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

### Bayesian Cramér-Rao Bound

Expectation of Fisher information over prior  $\pi$ : the *Bayesian* Cramér-Rao bound.

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

For adaptive experiments, the posterior is used instead of the prior.

The BCRB can be computed iteratively: useful for tracking optimality online.

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

### Method of Hyperparameters

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

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

# Method of Hyperparameters

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

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

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

(Granade et al. 2012 10/s87)

## Hyperparameters and Region Estimation

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

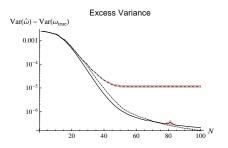


Figure : Larmor precession model w/  $\omega \sim N(\mu, \sigma^2)$ , three exp. design strategies

Critically, the covariance region for  $\omega$  is not smaller than the true covariance given by the hyperparameter  $\sigma^2$ .

(Granade et al. 2012 10/887)