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

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We want to build a quantum computer.

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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

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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.

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- 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

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Example

Larmor precession at an unknown ω 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

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

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Given a likelihood, we can reason about

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what we know having seen some data.

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 \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

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

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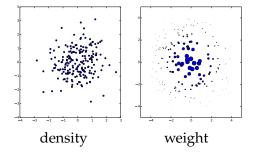
$$\Pr(\underline{x}) \approx \sum_{i}^{n} w_{i} \delta(\underline{x} - \underline{x}_{i})$$

QInfer Open-source implementation for quantum info.

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

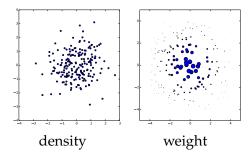
Ambiguity and Impovrishment

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_{ess} can herald some kinds of failures.

Liu and West Algorithm

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

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

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

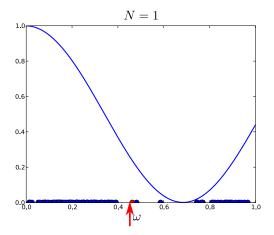
- $\blacksquare a = 1, h = 0$: Bootstrap filter, used in state-space applications like Condensation.
- $\blacksquare a^2 + h^2 = 1$: Ensures $\mathbb{E}[x'] = \mathbb{E}[x]$ and $Cov(\underline{x}') = Cov(\underline{x})$, but assumes unimodality.
- $\blacksquare a = 1, h > 0$: Allows for multimodality,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

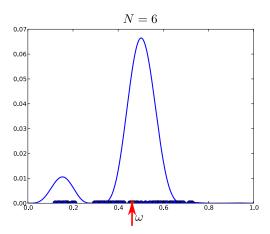
With SMC and resampling, particles move towards the true

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



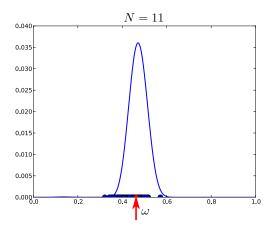
Sequential Monte Carlo

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Sequential Monte Carlo

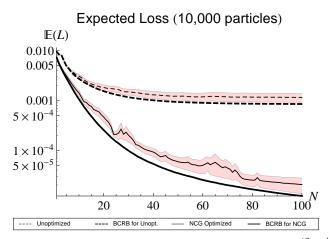
With SMC and resampling, particles move towards the true model as data is collected.



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

Near-Optimality for cos²

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

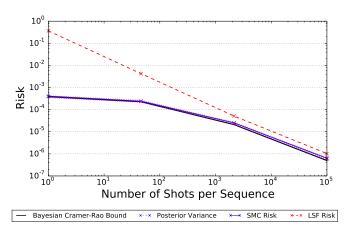
Interpret survival probability as likelihood. For interleaved case, the lowest-order model is:

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

- A, B state preparation and measurement
 - *m* sequence length
- p_{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.



SMC in Nitrogen Vacancy Centers

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

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

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

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

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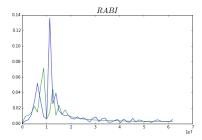
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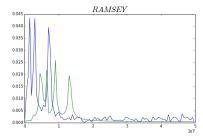
- Analytic estimate sensitive to error δB in static field.
- Use multiple \underline{B} settings to decorrelate $\underline{\delta B}$, \underline{A} .
- Each experiment informs about multiple parameters

Introduction Bayes QHL Bootstrapping Conclusions Overview SMC Algorithm Examples More SMC

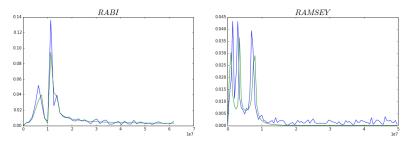
Preliminary Results from Rabi Experiment

As a test, attempt to learn δB , Δ_{zfs} $\delta \omega_{Rabi}$ and A_N (coupling to nitrogen spin).

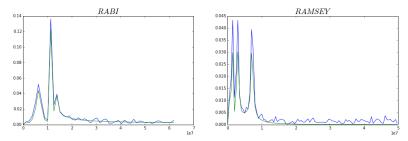




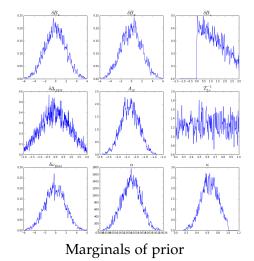
Simulation with prior mean

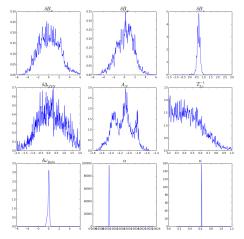


Simulation with posterior mean, 20 averages

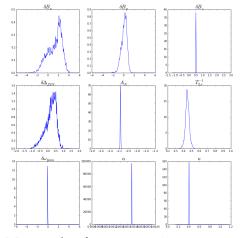


Simulation with posterior mean, 486 averages





Marginals of posterior, 20 averages

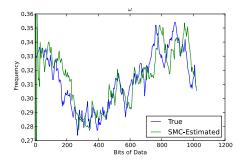


Marginals of posterior, 486 averages

We can do a few more things with SMC, some of which will be very useful in the semiquantum case.

State-Space SMC

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 $\Pr_{D}(\underline{x}_{0} \in X_{\alpha}(D)) \geq \alpha$.

Confidence and Credible Regions

Characterizing uncertainty of estimates is critical for many applications:

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

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

High Posterior Density

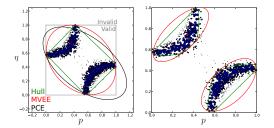
Want credible regions that are *small* (most powerful).

- 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 η):



Left, no clustering. Right, DBSCAN.

Drunk Under the Streetlights

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

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

Is this useful?

Bayes Factors and Model Selection

Drunk Under the Streetlights

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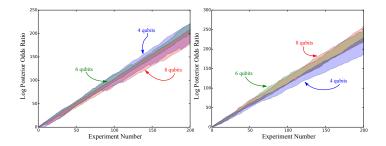
Is this useful?

Collecting normalizations \mathcal{N}_A and \mathcal{N}_B for models A, B at each step gives (assuming uniform prior over A, B)

Bayes factor =
$$\frac{\Pr(D|A;\underline{e})}{\Pr(D|B;\underline{e})} \approx \frac{\prod_{d \in D} \mathcal{N}_A(d)}{\prod_{d \in D} \mathcal{N}_B(d)}$$

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

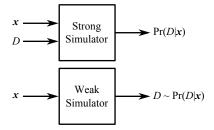
SMC uses *simulation* as a resource for *learning*.

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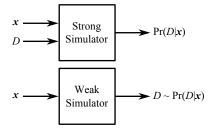
Big Idea

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.

Introduction Bayes QHL Bootstrapping Conclusions Weak Sim

Adaptive Likelihood Estimation

Solution

Treat estimating the likelihood as a secondary estimation problem:

Learn likelihood of untrusted system from frequencies of trusted system.

Introduction Bayes QHL Bootstrapping Conclusions Weak Sim. Likelihood Results

Adaptive Likelihood Estimation

Solution

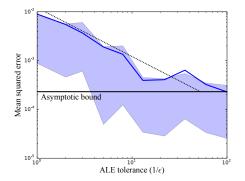
Treat estimating the likelihood as a secondary estimation problem:

Learn likelihood of untrusted system from frequencies of trusted system.

SMC is robust to likelihood estimation errors.

Performance of SMC+ALE

Ex: Simple 'photodetector' model $Pr(0|p) = \alpha p + (1-p)\beta$



 α, β known bright, dark references

(Ferrie and Granade 2014 10/tdj)

Given:

d result of measurement

D' set of samples from weak simulator

Hedged binomial estimate of likelihood ℓ 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 ℓ from frequency k/K:

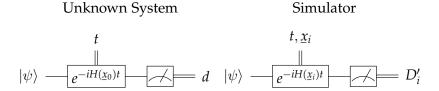
$$\hat{\ell} = \frac{k + \beta}{K + 2\beta},$$

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 ℓ_i from D'_i .

SMC update:

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

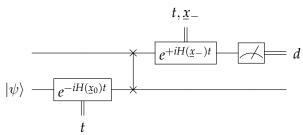
(Wiebe, Granade, Ferrie and Cory 2014 10/tf3)

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

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

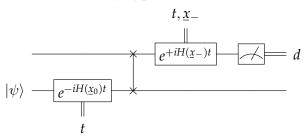
Interactive OLE

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



Interactive OLE

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



Echo

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

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 $e = (x_-, t)$.

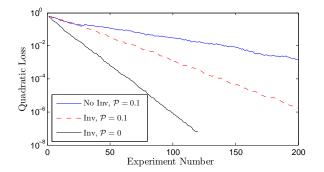
Alternate Interpretation

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

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

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

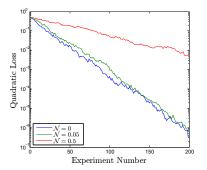
Interactivity allows for dramatic improvements over QLE.



 \mathcal{P} : adaptive likelihood estimation tolerance. (Wiebe, Granade, Ferrie and Cory 2014 10/tf3)

Ising Model on the Complete Graph

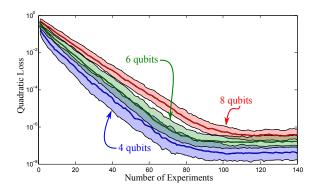
With IQLE, can also learn on complete interaction graphs. We show the performance as a function of the depolarization strength \mathcal{N} .



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

Ising Model with the Wrong Graph

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



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

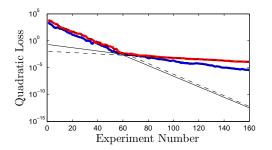


Figure: 4 qubit (red) and 6 qubit (blue) complete graph IQLE

In spin-chain and complete graph, average error decays

exponentially,

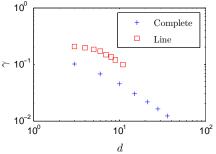
$$L(N) \propto e^{-\gamma N}$$

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)

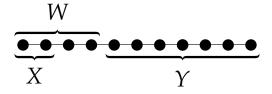
SMC + IOLE:

- 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

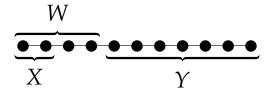
To go further, we want to *localize* our experiment, such that we can simulate on a smaller system.



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

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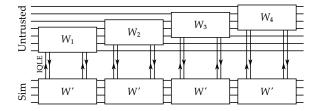


Measure on X, simulate on W, and ignore all terms with support over Y.

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.

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

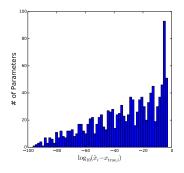
All Hamiltonian terms commute, but initial state doesn't. Let A_X be observable, $A_{X'}$ be sim. observable.

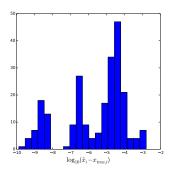
$$||A_X(t) - A_{X'}(t)|| \le ||A_X(t)|| (e^{2||H|_Y||t} - 1)$$

$$\Rightarrow t \le \ln\left(\frac{\delta}{||A_X(t)||} + 1\right) (2||H|_Y||)^{-1},$$

where δ is the tolerable likelihood error.

Example Q50 Run

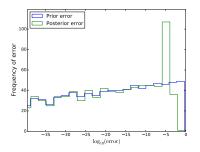




$$|X_k| = 4$$
, $|W_k| = 8$, $n = 20,000$, $N = 500$, exp. decaying interactions.

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

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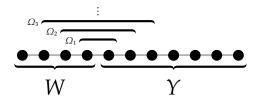
More generally, for $[H|_W, H_Y] \neq 0$, use Lieb-Robinson bound. If interactions between *X* and *Y* decay sufficiently quickly, then there exists C, μ and v s. t. for any observables $A_X(t)$, B_Y :

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

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

Lieb-Robinson Bounds

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

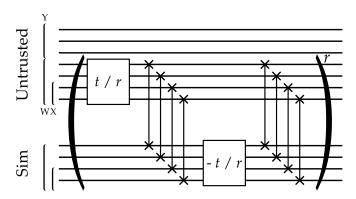


Let H_i be the Hamiltonian term containing distance-iinteractions between W and Y, acting on sites Ω_i .

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

"Shaking"

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



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Learning *g* is also important to bootstrapping. Suppose:

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

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Learning Controls with IQLE

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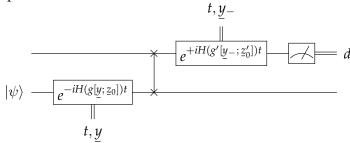
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Doesn't help with all distortions, but covers a range of important cases.

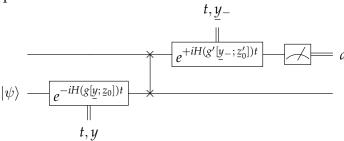
IQLE Setup

Experiment:



IQLE Setup

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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 $g'[y_i'; \underline{z}_0'] = g[y; \underline{z}_i]$.

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

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

Control/Distortion Duality

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

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).

Extend to learning time-dependent distortions?

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Can quantum resources be applied to *design* control?

Introduction Bayes QHL Bootstrapping Conclusions

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- 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 http://www.cgranade.com/research/talks/lfqis-2014/.



Thank you for your kind attention!

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

Loss How well have we learned?

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Cramér-Rao Bound

Fisher Information

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

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

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

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

Bayesian Cramér-Rao Bound

Expectation of Fisher information over prior π : the *Bayesian* Cramér-Rao bound.

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

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:

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

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

(Granade et al. 2012 10/s87)

Hyperparameters and Region Estimation

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

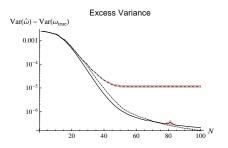


Figure : Larmor precession model w/ $\omega \sim N(\mu, \sigma^2)$, three exp. design strategies

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

(Granade et al. 2012 10/887)