Quantum Bootstrapping

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Ioint work with:

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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 50 qubits?

Computational limits affect many aspects of building large quantum systems:

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- Design of control sequences
- Verification of control

Here, we focus mostly on characterization and verification. Control design will be addressed as a *calibration* problem.

Bootstrapping to Q50

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

Use small quantum simulators to characterize and verify large devices, bootstrap up to Q50 scale.

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- Learning control distortions

Modeling Experiments

Likelihood Function

Model data collection as a probability distribution:

Pr(data|model; experiment)

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The likelihood function *describes* an experiment and its possible outcomes.

Born's Rule: Quintessential Likelihood

Can interpret Born's Rule as the likelihood for state-learning experiments:

$$Pr(click|\psi;\phi) = |\langle \phi|\psi\rangle|^2$$

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$$\begin{aligned} \Pr(\text{click}|\psi;\phi) &= |\left\langle \phi | \psi \right\rangle|^2 \\ \text{data} & \text{click or no click} \\ \text{model} & \text{preparation } |\psi\rangle \\ \text{experiment} & \text{measurement } \left\langle \phi | \right. \end{aligned}$$

Hamiltonian Learning Likelihood

Consider Larmor precession at an unknown ω and T_2 :

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

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

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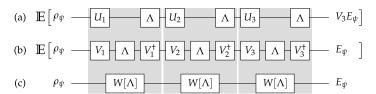
$$\Pr(d = 0 | \text{model} = (\omega, T_2); \exp = t) = \frac{1 - e^{-t/T_2}}{2} + e^{-t/T_2} \cos^2(\omega t/2)$$

Parameterize model as $\underline{x} = (\omega, T_2)$, experiment as $\underline{e} = (t)$.

Let's consider another example of a likelihood function before we move on.

Randomized Benchmarking Likelihood

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



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
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 \Longrightarrow Simulation is a resource for learning.

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In many cases, difficult to perform analytically...

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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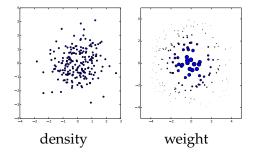
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QInfer Open-source implementation for quantum info.

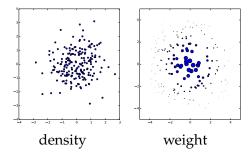
(Doucet and Johansen 2011; Huszár and Houlsby 10/s86; Granade et al. 2012 10/s87)

Ambiguity and Impovrishment

Ambiguity in SMC approximation:



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

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

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

 \blacksquare \Rightarrow $n_{\rm ess} \rightarrow 0$ 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 x' from kernel density estimate:

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

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

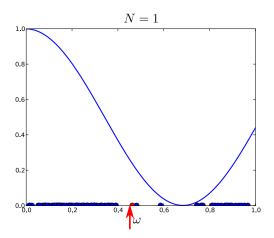
- $\blacksquare a = 1, h = 0$: Bootstrap filter, used in state-space applications like Condensation.
- $\blacksquare a^2 + h^2 = 1$: Ensures $\mathbb{E}[x'] = \mathbb{E}[x]$ and $Cov(\underline{x}') = Cov(\underline{x})$, but assumes unimodality.
- $\blacksquare a = 1, h > 0$: Allows for multimodality,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

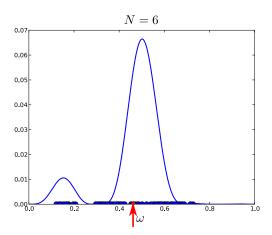
Sequential Monte Carlo

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



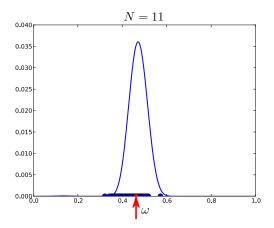
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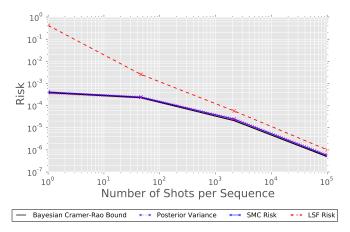
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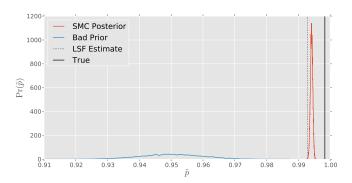
Before bootstrapping, a few examples of SMC w/ classical resources:

Randomized Benchmarking Results

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

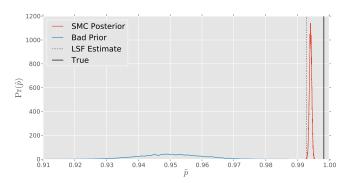


SMC is robust, even with a quite bad prior (6.9σ) .



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 \blacksquare Monitoring $n_{\rm ess}$ can herald failures due to a bad prior.

Would like to learn hyperfine coupling $\underline{\underline{A}}$ between e^- spin $\underline{\underline{S}}$ and ^{13}C spin $\underline{\underline{I}}$.

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

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

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

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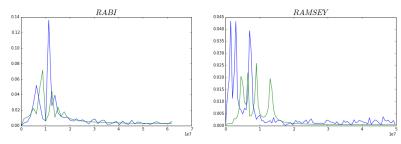
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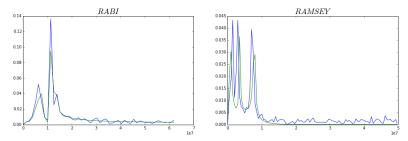
$$\alpha, \beta : \text{visibility parameters}$$

- 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.

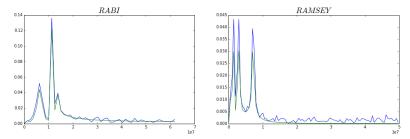
As a test, attempt to learn $\underline{\delta B}$, $\Delta_{\rm zfs}$ $\delta \omega_{\rm Rabi}$ and A_N (coupling to nitrogen spin).



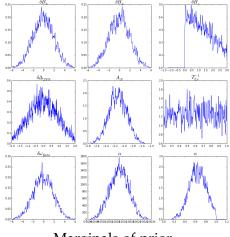
Simulation with prior mean



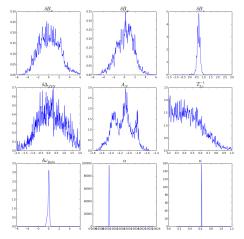
Simulation with posterior mean, 20 averages



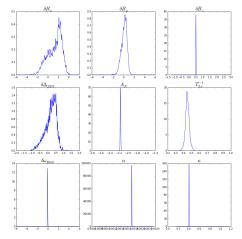
Simulation with posterior mean, 486 averages



Marginals of prior



Marginals of posterior, 20 averages



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SMC and Hamiltonian Learning as Vector Metrology

In the previous example, δB_x and δB_y manifest as effective Hamiltonian by Floquet theory.

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In the previous example, δB_x and δB_y manifest as effective Hamiltonian by Floquet theory.

Each experiment carries phase information about δB .

SMC uses this to learn vector quantities: we do not require that each component of $\underline{\delta B}$ be measured seperately.

Towards Bootstrapping

SMC uses simulation as a resource for learning.

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

Towards Bootstrapping

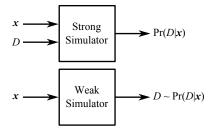
SMC uses *simulation* as a resource for *learning*.

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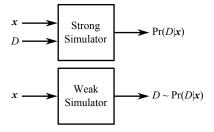
Big Idea

Use quantum simulation to extend SMC past classical resources.

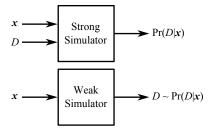
Weak and Strong Simulation



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



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Potential application for analog[ue] simulators?

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.

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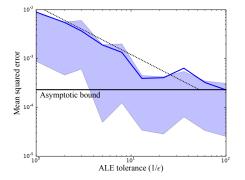
Treat estimating the likelihood as a secondary estimation problem:

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)

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

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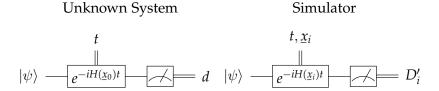
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where $\beta \approx 0.509$, $k := |\{d' \in D' | d' = d\}|$, $K = |\{D'\}|$.

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:

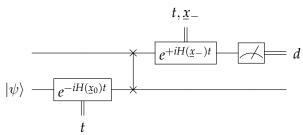
$$w_i \mapsto w_i \hat{\ell}_i / \sum_i w_i \hat{\ell}_i$$
.

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

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

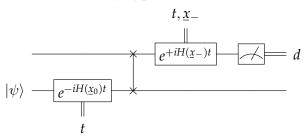
Interactive OLE

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



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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 $e = (x_-, t)$.

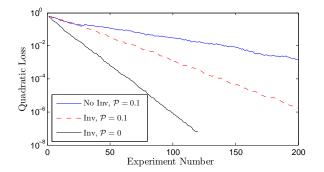
Alternate Interpretation

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.

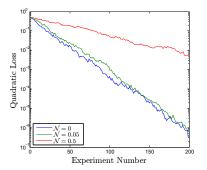
Interactivity allows for dramatic improvements over QLE.



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

Ising Model on the Complete Graph

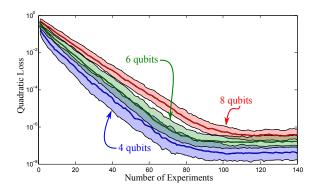
With IQLE, can also learn on complete interaction graphs. We show the performance as a function of the depolarization strength \mathcal{N} .



 \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.

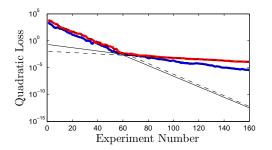


Figure: 4 qubit (red) and 6 qubit (blue) complete graph IQLE

In spin-chain and complete graph, average error decays

exponentially,

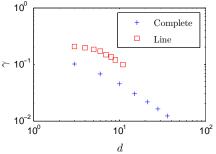
$$L(N) \propto e^{-\gamma N}$$

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)

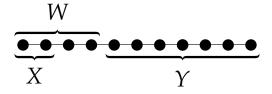
SMC + IOLE:

- 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

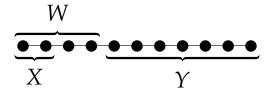
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Measure on X, simulate on W, and ignore all terms with support over Y.

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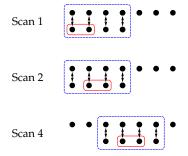


Measure on X, simulate on W, and ignore all terms with support over Y.

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 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.

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

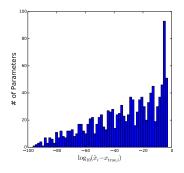
All Hamiltonian terms commute, but initial state doesn't. Let A_X be observable, $A_{X'}$ be sim. observable.

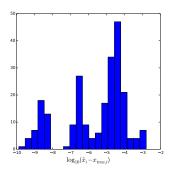
$$||A_X(t) - A_{X'}(t)|| \le ||A_X(t)|| (e^{2||H|_Y||t} - 1)$$

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

where δ is the tolerable likelihood error.

Example Q50 Run

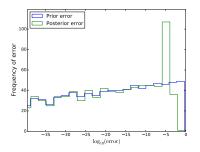




$$|X_k| = 4$$
, $|W_k| = 8$, $n = 20,000$, $N = 500$, exp. decaying interactions.

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

Example Q50 Run

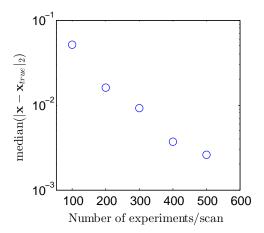


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Scaling With *N*

We expect from non-truncated quantum Hamiltonian learning that the error decays exponentially with more data. This remains the case even with truncation.



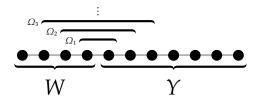
More generally, for $[H|_W, H_Y] \neq 0$, use Lieb-Robinson bound. If interactions between *X* and *Y* decay sufficiently quickly, then there exists C, μ and v s. t. for any observables $A_X(t)$, B_Y :

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

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

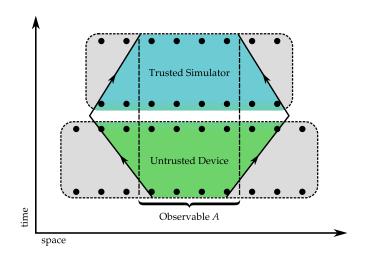
Lieb-Robinson Bounds

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



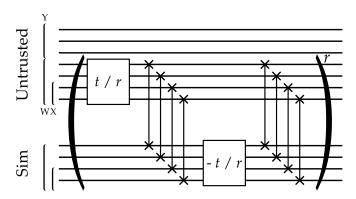
Let H_i be the Hamiltonian term containing distance-iinteractions between W and Y, acting on sites Ω_i .

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



"Shaking"

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



Bootstrapping Algorithm

Consider H an affine map H(C) of control settings C:

$$H(\underline{C}) = \underline{C} \cdot (H_1, H_2, \dots, H_M) + H_0. \tag{1}$$

E.g.: cross-talk.

We can learn this with truncated IOLE:

- Learn H(0) to estimate \hat{H}_0 .
- Learn $H(\underline{e}_i)$ for $j \in \{1, ..., M\}$.
- Subtract H_0 from each of the learned Hamiltonians to estimate the other terms.
- Use the pseudoinverse to derive control settings to generate desired Hamiltonians.

Example: Controlling NN Ising Couplings

Consider H(C) such that C_i nominally controls the coupling $H_i = \sigma_z^{(i)} \sigma_z^{(i+1)}$. For a 50-qubit device, dim C = 49, so this is a $(49+1) \times 1225 \approx 61 \times 10^3$ parameter model.

We collect 200 bits of data per scan, for a total of $50 \times 49 \times 200 = 490 \times 10^3$ bits of data. We use 20×10^3 particles, for a total of 10 million likelihood calls.

Results for Bootstrapping 50-Qubit Simulator

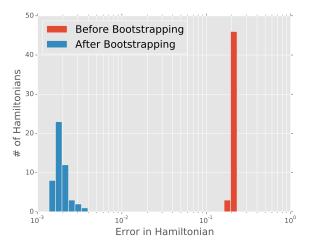


Figure: Frequencies of error $||H(\hat{\underline{C}}_i) - H_i||_2$ for Q50 bootstrapping.

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/usydney-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 On average, how well can we learn?

Cramér-Rao Bound

Fisher Information

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

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

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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

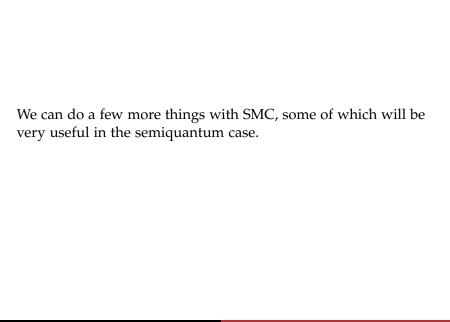
Expectation of Fisher information over prior π : the *Bayesian* Cramér-Rao bound.

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

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

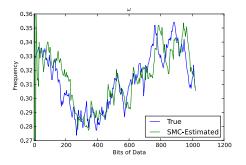
The BCRB can be computed iteratively: useful for tracking optimality online.

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



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 $Pr_D(\underline{x}_0 \in X_{\alpha}(D)) \geq \alpha$.

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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

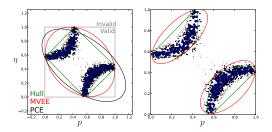
Want credible regions that are *small* (most powerful).

- 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.

Bayes Factors and Model Selection

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?

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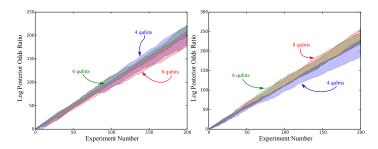
Collecting normalizations \mathcal{N}_A and \mathcal{N}_B for models A, B at each step gives

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

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

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

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



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

(Granade et al. 2012 10/s87)

Hyperparameters and Region Estimation

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

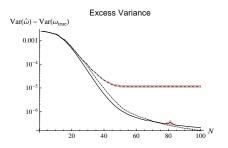


Figure : Larmor precession model w/ $\omega \sim N(\mu, \sigma^2)$, three exp. design strategies

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)