Quantum Bootstrapping

Christopher Granade

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

Joint work with:

Nathan Wiebe Christopher Ferrie D. G. Cory

Institute for Quantum Computing
University of Waterloo, Ontario, Canada

July 18, 2014

LFQIS 2014

Q100

We want to build a quantum computer.

Q100

We want to build a quantum computer.

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

Building Large Systems: Computational Limits

Computational limits affect many aspects of building large quantum systems:

- Characterization of H

Building Large Systems: Computational Limits

Computational limits affect many aspects of building large quantum systems:

- Characterization of H
- Characterization of controls

Building Large Systems: Computational Limits

Computational limits affect many aspects of building large quantum systems:

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

Building Large Systems: Computational Limits

Computational limits affect many aspects of building large quantum systems:

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

Building Large Systems: Computational Limits

Computational limits affect many aspects of building large quantum systems:

- 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.

Outline

- Bayesian inference as platform

Outline

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

Outline

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

Outline

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

Outline

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

Outline

- 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 ω and T_2:

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

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

Updating Knowledge

Given a likelihood, we can reason about

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

what we know having seen some data.

Updating Knowledge

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.

Updating Knowledge

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.

Updating Knowledge

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.

Updating Knowledge

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

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

Sequential Monte Carlo

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

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

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

SMC Approximation

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

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

Sequential Monte Carlo

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

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

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

SMC Approximation

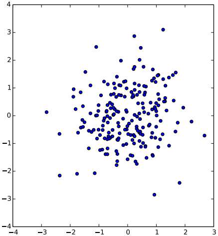
$$\Pr(\underline{x}) \approx \sum_{i}^{n} w_i \delta(\underline{x} - \underline{x}_i)$$

QInfer Open-source implementation for quantum info.

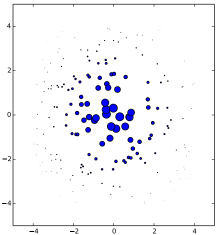
(Doucet and Johansen 2011; Huszár and Houlsby *10/s86*; *Granade* et al. 2012 *10/s87*)

Ambiguity and Impovrishment

Ambiguity in SMC approximation:



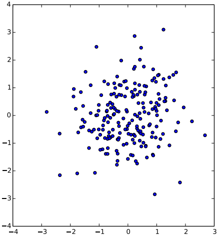
density



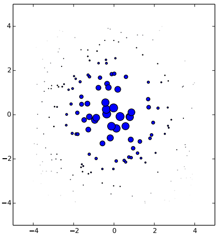
weight

Ambiguity and Impovrishment

Ambiguity in SMC approximation:



density



weight

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

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

Numerical Stability and Resampling

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

- $\Rightarrow n_{\text{ess}} \to 0$ as data is collected.

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

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

Liu and West Algorithm

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

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

$$\underline{\mu}_i := a\underline{x}_i + (1-a)\mathbb{E}[\underline{x}] \qquad \underline{\underline{\Sigma}} := h^2 \operatorname{Cov}[\underline{x}] \qquad w_i' := 1/n$$

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

Liu and West Algorithm

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

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

$$\underline{\mu}_i := a\underline{x}_i + (1-a)\mathbb{E}[\underline{x}] \qquad \underline{\underline{\Sigma}} := h^2 \operatorname{Cov}[\underline{x}] \qquad w'_i := 1/n$$

Parameters a and h can be set based on application:

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

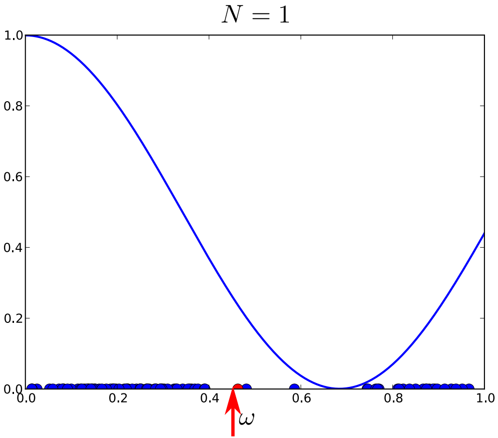
(West 1993; Isard and Blake 1998 *10/cc76f6*; Liu and West 2001)

Putting it All Together: The SMC Algorithm

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

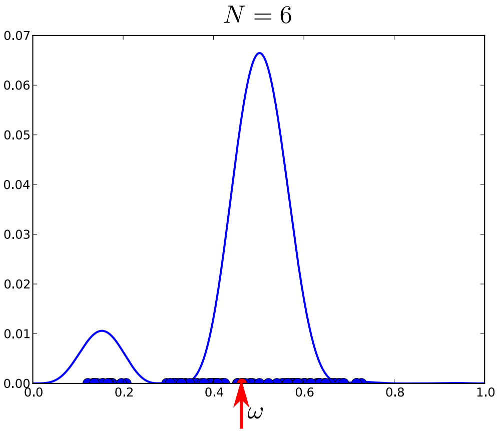
Sequential Monte Carlo

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



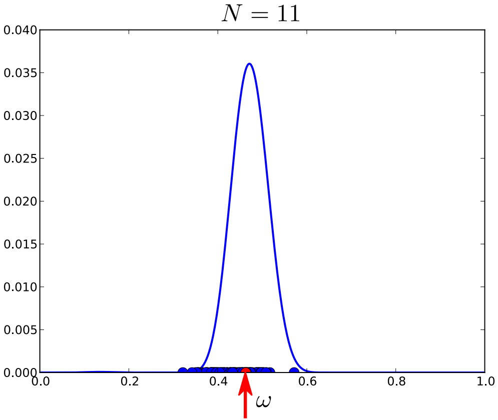
Sequential Monte Carlo

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



Sequential Monte Carlo

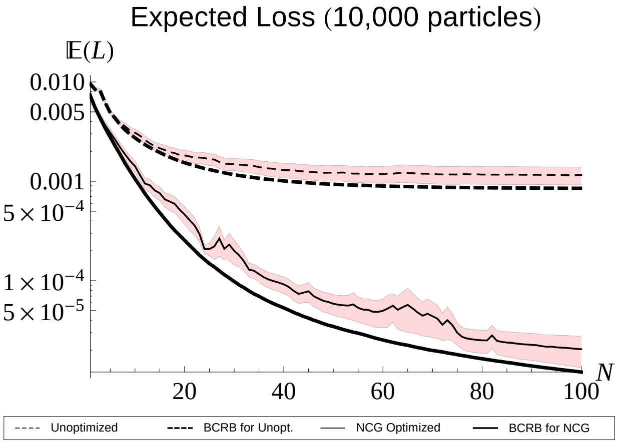
With SMC and resampling, particles move towards the true model as data is collected.



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

Near-Optimality for $\cos^2$

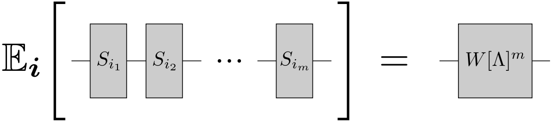
Adaptive experiment design w/ Newton Conjugate-Gradient, vs. optimum from Bayesian Cramér-Rao Bound:



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

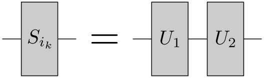
Randomized Benchmarking Example

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



Imperfect twirling sequence

Equivalent depolarizing channel



Clifford

Decomposition into gates

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

Randomized Benchmarking Example

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

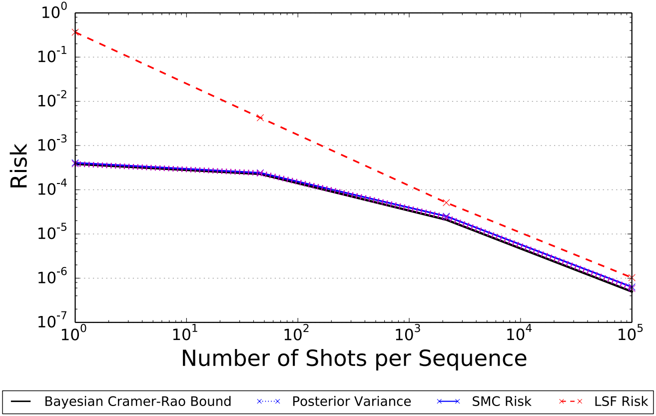
$$\Pr(\text{survival}|A, B, \tilde{p}, p_{\text{ref}}; m, \text{mode}) = \begin{cases} A p_{\text{ref}}^m + B & \text{reference} \\ A(\tilde{p} p_{\text{ref}})^m + B & \text{interleaved} \end{cases}$$

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

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

Randomized Benchmarking Example

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



(*Granade*, Ferrie and Cory 2014 1404.5275)

SMC in Nitrogen Vacancy Centers

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

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

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

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

SMC in Nitrogen Vacancy Centers

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

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

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

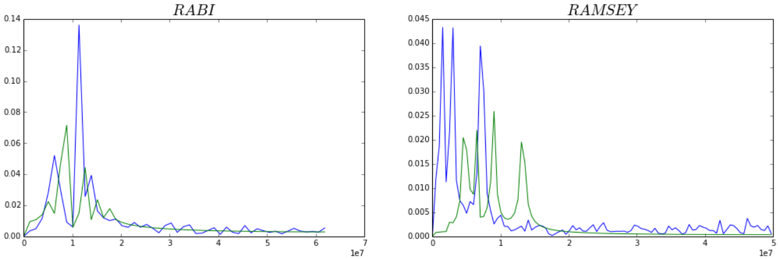
$$\alpha, \beta : \text{visibility parameters}$$

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

Preliminary Results from Rabi Experiment

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

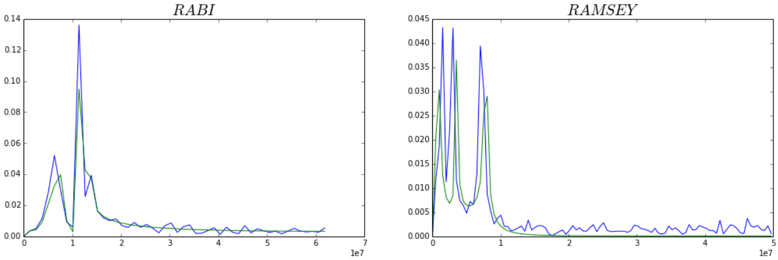
Preliminary Results from Rabi Experiment



Simulation with prior mean

Each average: 30k shots per point, 100 Rabi points + 200 Ramsey points

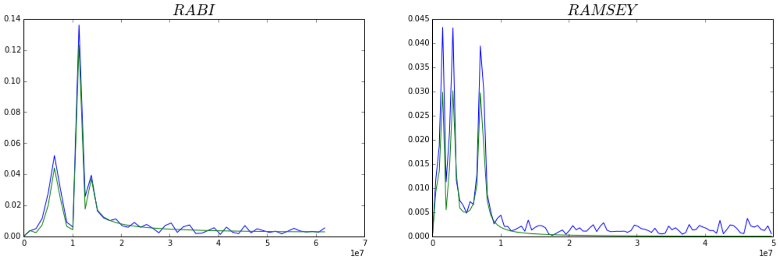
Preliminary Results from Rabi Experiment



Simulation with posterior mean, 20 averages

Each average: 30k shots per point, 100 Rabi points + 200 Ramsey points

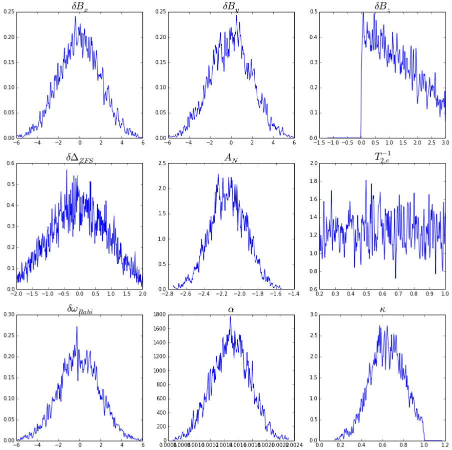
Preliminary Results from Rabi Experiment



Simulation with posterior mean, 486 averages

Each average: 30k shots per point, 100 Rabi points + 200 Ramsey points

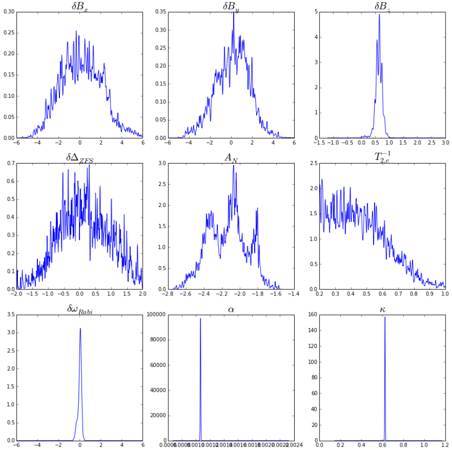
Preliminary Results from Rabi Experiment



Marginals of prior

Each average: 30k shots per point, 100 Rabi points + 200 Ramsey points

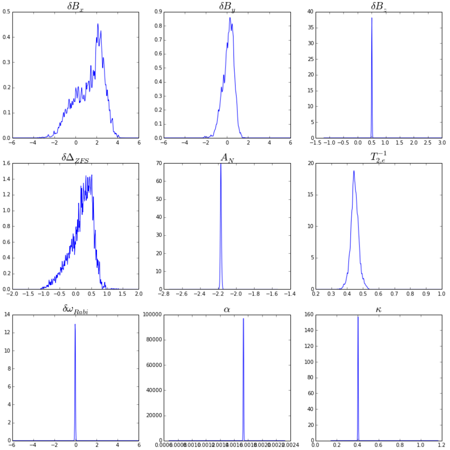
Preliminary Results from Rabi Experiment



Marginals of posterior, 20 averages

Each average: 30k shots per point, 100 Rabi points + 200 Ramsey points

Preliminary Results from Rabi Experiment



Marginals of posterior, 486 averages

Each average: 30k shots per point, 100 Rabi points + 200 Ramsey points

SMC and Hamiltonian Learning as Vector Metrology

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

SMC and Hamiltonian Learning as Vector Metrology

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

Each experiment carries phase information about $\underline{\delta B}$.

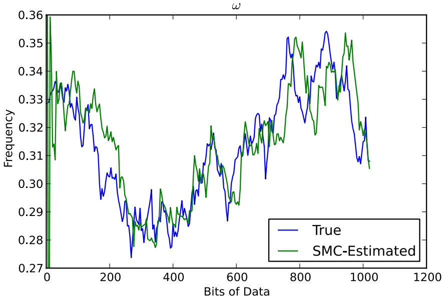
SMC uses this to learn vector quantities: we do not require that each component of $\underline{\delta B}$ be measured seperately.

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

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

Confidence and Credible Regions

Characterizing uncertainty of estimates is critical for many applications:

Definition (Credible Region)

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

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

Confidence and Credible Regions

Characterizing uncertainty of estimates is critical for many applications:

Definition (Credible Region)

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

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

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

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

High Posterior Density

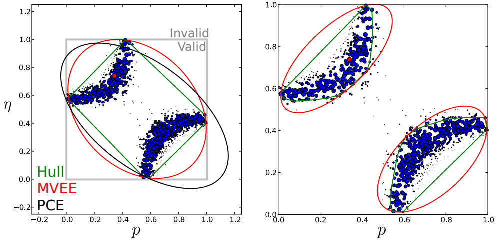
Want credible regions that are *small* (most powerful).

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

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

Comparison of HPD Estimators

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



Left, no clustering. Right, DBSCAN.

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

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?

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

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?

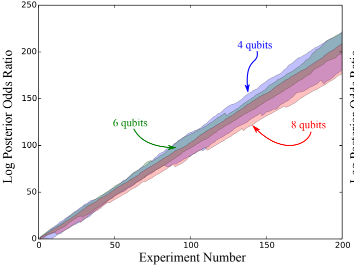
Collecting normalizations $\mathcal{N}_A$ and $\mathcal{N}_B$ for models A, B at each step gives

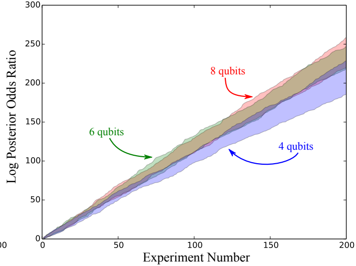
$$\text{Bayes factor} = \frac{\Pr(D|A;\underline{e})\Pr(A)}{\Pr(D|B;\underline{e})\Pr(B)} \approx \frac{\prod_{d\in D}\mathcal{N}_A(d)}{\prod_{d\in D}\mathcal{N}_B(d)} \times \frac{\Pr(A)}{\Pr(B)}$$

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:





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

Towards Bootstrapping

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

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

Towards Bootstrapping

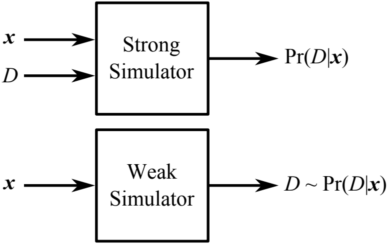
SMC uses *simulation* as a resource for *learning*.

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

Big Idea

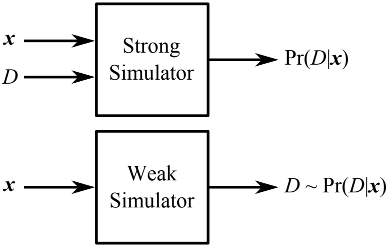
Use quantum simulation to extend SMC past classical resources.

Weak and Strong Simulation



(Ferrie and *Granade* 2014 *10/tdj*)

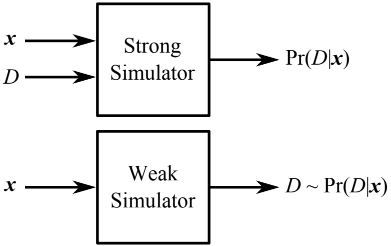
Weak and Strong Simulation



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

(Ferrie and *Granade* 2014 *10/tdj*)

Weak and Strong Analog[ue]? Simulation



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

Potential application for analog[ue] simulators?

(Ferrie and *Granade* 2014 *10/tdj*)

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

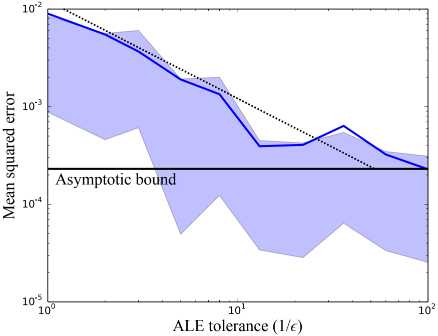
Treat estimating the likelihood as a secondary estimation problem:

Learn likelihood of untrusted system from frequencies of trusted system.

SMC is robust to likelihood estimation errors.

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

(Ferrie and Blume-Kohout 2012 *10/tf2*, 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 $\beta \approx 0.509$, $k := |\{d' \in D' | d' = d\}|$, $K = |\{D'\}|$.

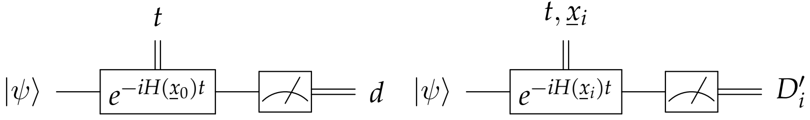
Variance well-known, so collect until a fixed *tolerance* is reached.

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

Quantum Likelihood Evaluation

Compare *classical* outcomes of unknown and trusted systems.

Unknown System Simulator



For each $\underline{x}_i$:

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

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

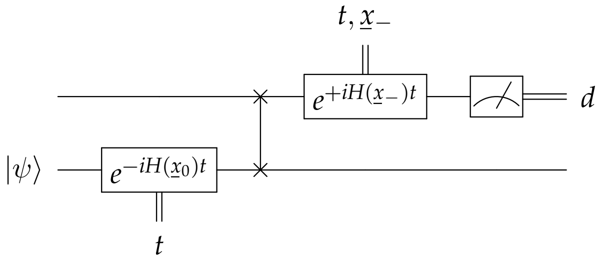
(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

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

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

Interactive QLE

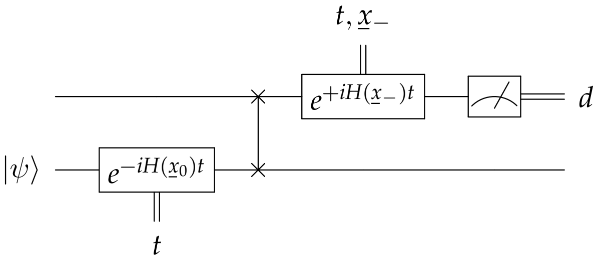
Solution: couple unknown system to a quantum simulator, then invert evolution by hypothesis $\underline{x}_-$.



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

Interactive QLE

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



Echo

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

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

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 $t = 1/\|\underline{x}_- - \underline{x}'_-\|$.
- Return $\underline{e} = (\underline{x}_-, t)$.

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

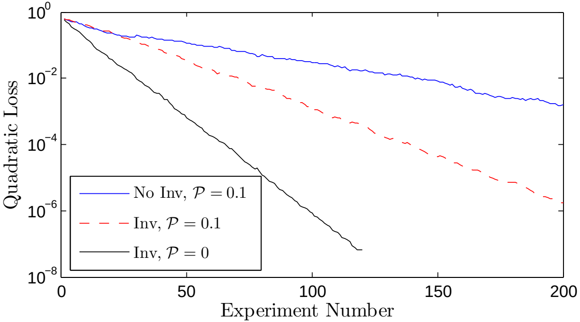
Alternate Interpretation

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

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

Ising Model on Spin Chains

Hamiltonian: nearest-neighbor Ising models on a chain of nine qubits.
Interactivity allows for dramatic improvements over QLE.

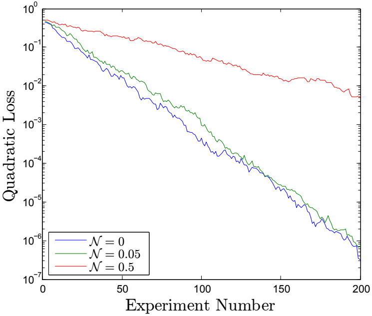


$\mathcal{P}$: adaptive likelihood estimation tolerance.

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

Ising Model on the Complete Graph

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

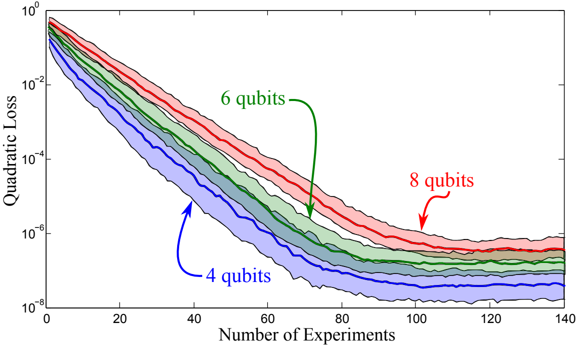


$\mathcal{N}$: depolarizing noise following SWAP gate.

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

Ising Model with the Wrong Graph

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



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

Scaling Parameter

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

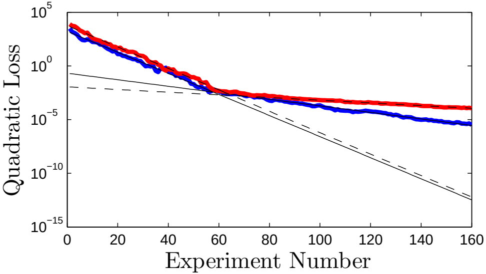


Figure : 4 qubit (red) and 6 qubit (blue) complete graph IQLE

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

Scaling and Dimensionality

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

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

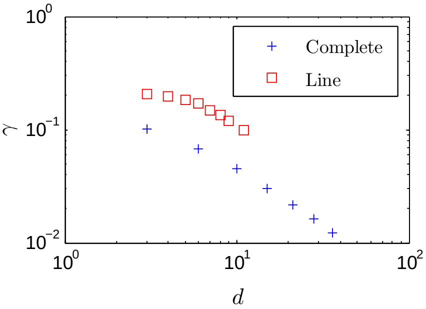
(Wiebe, *Granade*, Ferrie and Cory 2014 *10/tf3*)

Scaling and Dimensionality

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

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

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



With quantum simulation, learning *may* scale efficiently.

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

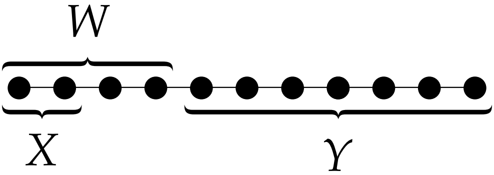
SMC + IQLE:

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

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

Information Locality

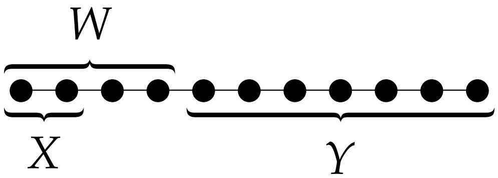
To go further, we want to *localize* our experiment, such that we can simulate on a smaller system.



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

Information Locality

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

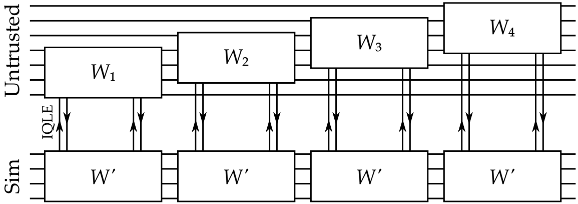


Measure on X, simulate on W, and ignore all terms with support over Y.

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

Local and Global Particle Clouds

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



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

Local and Global Particle Clouds

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

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

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

Q50 Example

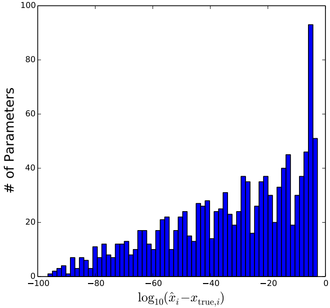
Goal: characterize a 50-qubit Ising model (complete graph) with unknown ZZ couplings.

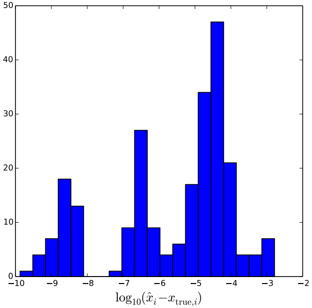
All Hamiltonian terms commute, but initial state doesn't. Let A_X be observable, $A_{X'}$ be sim. observable.

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

where δ is the tolerable likelihood error.

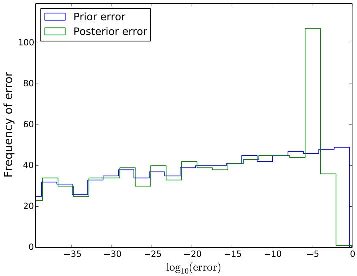
Example Q50 Run





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

Example Q50 Run



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

Lieb-Robinson Bounds

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

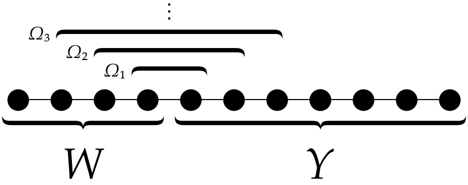
$$\|[A_X(t), B_Y]\| \leq C\|A_X(t)\|\|B_Y\||X||Y|(\mathrm{e}^{v|t|} - 1)\mathrm{e}^{-\mu d(X,Y)}$$

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

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

Lieb-Robinson Bounds

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

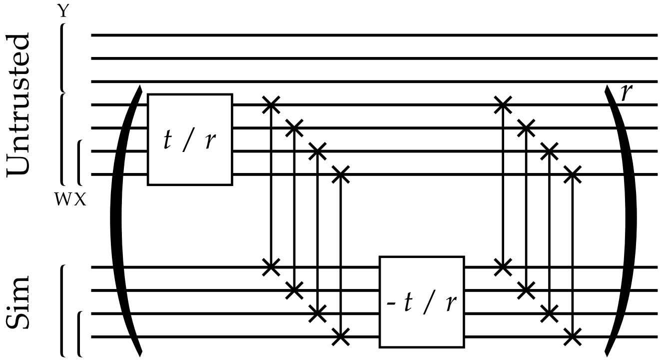


Let H_j be the Hamiltonian term containing distance-j interactions between W and Y, acting on sites Ω_j.

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

"Shaking"

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



Distortion Operators

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

$$H(t) = H(t; g[\underline{p}]),$$

where $\underline{p}$ is a pulse, $\underline{q} = g[\underline{p}]$ is the distorted pulse.

(Hincks, Granade, Borneman and Cory *forthcoming*)

Distortion Operators

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

$$H(t) = H(t; g[\underline{p}]),$$

where $\underline{p}$ is a pulse, $\underline{q} = g[\underline{p}]$ is the distorted pulse.

- Resonator transfer function

(Hincks, Granade, Borneman and Cory *forthcoming*)

Distortion Operators

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

$$H(t) = H(t; g[\underline{p}]),$$

where $\underline{p}$ is a pulse, $\underline{q} = g[\underline{p}]$ is the distorted pulse.

- Resonator transfer function
- Cross-talk of control lines

(Hincks, Granade, Borneman and Cory *forthcoming*)

Distortion Operators

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

$$H(t) = H(t; g[\underline{p}]),$$

where $\underline{p}$ is a pulse, $\underline{q} = g[\underline{p}]$ is the distorted pulse.

- Resonator transfer function
- Cross-talk of control lines
- Phase calibration / reference frame

(Hincks, Granade, Borneman and Cory *forthcoming*)

Learning Controls with IQLE

Learning g is also important to bootstrapping. Suppose:

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

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

- Trusted simulator is characterized s.t. arbitrary $g[\cdot; \underline{z}_i]$ can be simulated

Learning Controls with IQLE

Learning g is also important to bootstrapping. Suppose:

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

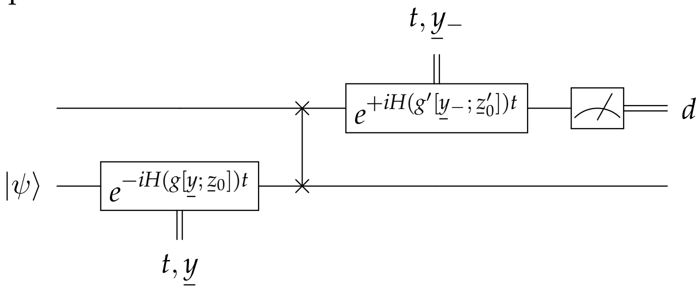
$$H = H(\underline{x}) = H(g[\underline{y}; \underline{z}])$$

- Trusted simulator is characterized s.t. arbitrary $g[\cdot; \underline{z}_i]$ can be simulated

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

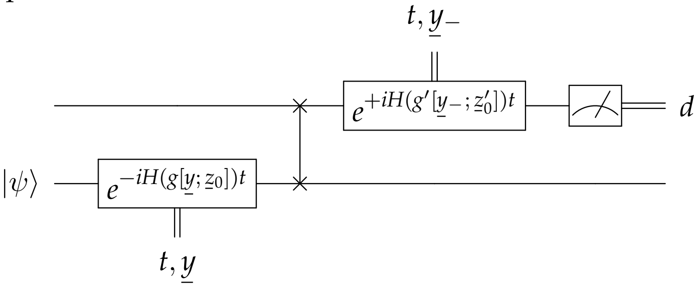
IQLE Setup

Experiment:

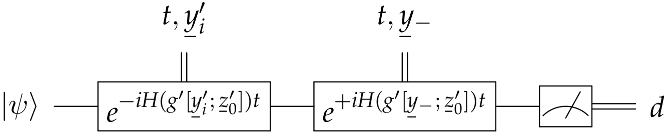


IQLE Setup

Experiment:



Simulator:



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

Control/Distortion Duality

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

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

Control/Distortion Duality

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

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

Shows duality between *hypothesis* and *simulation*.

Experiment		Simulation
hypothesis $\underline{z}_i$	$\longleftrightarrow$	fixed $\underline{z}'_0$
fixed $\underline{y}$		control $\underline{y}'_i$

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

Future: Bootstrapping for Control

Same approach can be used to model cross-talk:

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

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

Extend to learning time-dependent distortions?

Future: Bootstrapping for Control

Same approach can be used to model cross-talk:

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

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

Extend to learning time-dependent distortions?

Can quantum resources be applied to *design* control?

- 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 $\rightarrow$ bootstrapping.

Further Information

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

Thank you for your kind attention!

Decision Theory

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

Loss How well have we learned?
$L_{\underline{\underline{Q}}}(\hat{\underline{x}}, \underline{x}) := (\hat{\underline{x}} - \underline{x})^{\mathrm{T}} \underline{\underline{Q}} (\hat{\underline{x}} - \underline{x})$

Decision Theory

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

Loss How well have we learned?
$L_{\underline{\underline{Q}}}(\hat{\underline{x}}, \underline{x}) := (\hat{\underline{x}} - \underline{x})^{\mathrm{T}} \underline{\underline{Q}} (\hat{\underline{x}} - \underline{x})$

Risk On average, how well will we learn a particular model?
$R(\hat{\underline{x}}, \underline{x}) := \mathbb{E}_D[L(\hat{\underline{x}}(D), \underline{x})]$

Decision Theory

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

Loss How well have we learned?
$L_{\underline{\underline{Q}}}(\underline{\hat{x}}, \underline{x}) := (\underline{\hat{x}} - \underline{x})^{\mathrm{T}} \underline{\underline{Q}} (\underline{\hat{x}} - \underline{x})$

Risk On average, how well will we learn a particular model?
$R(\underline{\hat{x}}, \underline{x}) := \mathbb{E}_D[L(\underline{\hat{x}}(D), \underline{x})]$

Bayes risk On average, how well will we learn a range of models?
$r(\underline{\hat{x}}, \pi) = \mathbb{E}_{\underline{x} \sim \pi}[R(\underline{\hat{x}}, \underline{x})]$

Decision Theory

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

Loss How well have we learned?
$L_{\underline{\underline{Q}}}(\hat{\underline{x}}, \underline{x}) := (\hat{\underline{x}} - \underline{x})^{\mathrm{T}} \underline{\underline{Q}} (\hat{\underline{x}} - \underline{x})$

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

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?

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

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

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

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

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

Bayesian Cramér-Rao Bound

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

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

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

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

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

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

Method of Hyperparameters

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

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

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

Method of Hyperparameters

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

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

Example

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

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

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

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

Hyperparameters and Region Estimation

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

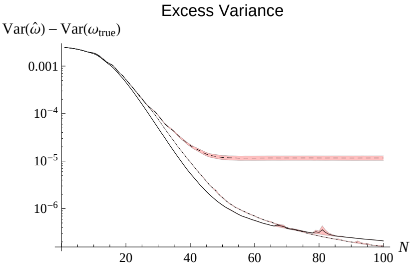


Figure : Larmor precession model w/ $\omega \sim \mathrm{N}(\mu, \sigma^2)$, three exp. design strategies

Critically, the covariance region for ω is not smaller than the true covariance given by the hyperparameter σ^2. (*Granade* et al. 2012 *10/s87*)