Robust Online Hamiltonian Learning

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Motivation

Accurate characterization of the dynamics of a quantum system is important for many applications in quantum information processing, including robust control design and simulation. Our goal here is to provide an algorithm to estimate parameters of unknown Hamiltonians, as well to quantify our uncertainty in those estimates. We do so by applying the methods of Bayesian inference and adaptive experiment design.

We benchmark our algorithm using several different models, the simplest being that of a single qubit undergoing Larmor precession at an unknown frequency ω.

$$\Pr(\text{data} = 0 | \text{model} = \omega;\ t) = \cos^2(\omega t / 2)$$

Here, t is a *control parameter* that we can vary to adaptively query the dynamics of the model.

Inference and Decision Theory

We infer parameters of a model by using *Bayes' Rule*:

$$\Pr(\boldsymbol{x}|D;C) = \frac{\Pr(D|\boldsymbol{x};C)}{\Pr(D|C)} \Pr(\boldsymbol{x})$$

We judge the quality of an estimate by the *squared error* loss:

$$L(\hat{\boldsymbol{x}}, \boldsymbol{x}) = (\boldsymbol{x} - \hat{\boldsymbol{x}})^T (\boldsymbol{x} - \hat{\boldsymbol{x}})$$

Ultimately, the performance of any algorithm is measured by the quadratic loss averaged over the distribution of parameters. This quantity is called the Bayes risk:

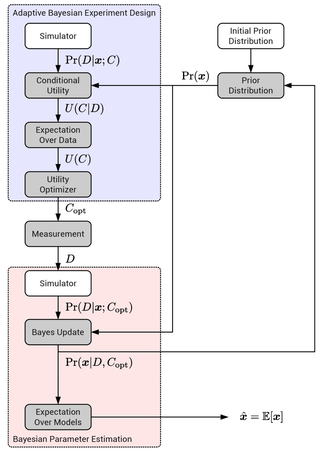
$$r(\pi) = \mathbb{E}_{x,D|C}[L(\hat{x}, x)]$$

The utility of a hypothetical experiment C is then the expected negative of the risk function. Our algorithm adaptively designs experiments that efficiently provide information about the system by optimizing control parameters with respect to this utility.

Sequential Monte Carlo Algorithm

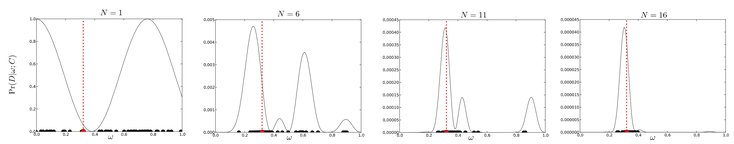
We use the *sequential Monte Carlo* (SMC) algorithm to efficiently approximate expectation values over posterior distributions. This algorithm works by approximating the true distribution over models as a weighted sum of delta functions (often called "particles"):

$$\Pr(\boldsymbol{x}|D,C) = \sum_i w_i \delta(\boldsymbol{x} - \boldsymbol{x}_i)$$



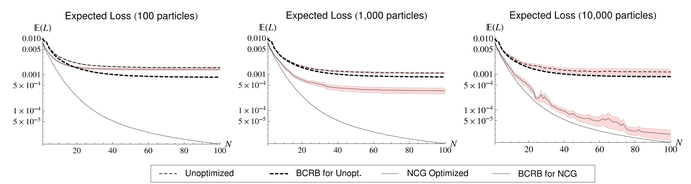
Expectation values can now be computed as finite sums, and the Bayes update step can be computed with one calculation per SMC particle.

In order to explore the parameter space, we occasionally *resample*, moving particles and resetting their weights so as to preserve expectation values.



This figure demonstrates the flow of probability mass and particles as the algorithm processes data. The red dot and line represent the randomly selected "true" model while the black dots are the SMC particles (the weights are uniform here).

Results for Known T_2



Left to right: the performance, as a function of the number of measurements N, of the SMC algorithm for n = 100, 1000 and 10 000 particles. For all cases, $T_2 = 100\pi$. The dashed lines indicate data taken without local optimization, while the solid lines indicate trials in which initial guesses were optimized using the Newton Conjugate Gradient (NCG) method. For each data set, the corresponding thick line indicates the Bayesian Cramer Rao Bound (BCRB). Errors in estimating the performance are indicated by red shaded regions around each curve. **As expected, the performance of the SMC algorithm improves as the number of particles increases.**

Extension to Unknown T_2

We also consider models based on *hyperparameters* of some underlying distribution. For example, in the precession model, if the "true" ω is itself drawn from a Lorentz distribution with location ω_0 and scale γ, then we obtain the unknown-T_2 model:

$$\Pr(0|\text{model} = (\omega_0, \gamma); t) = \frac{1}{2} + \frac{1}{2} e^{-t\gamma} \cos(\omega t)$$

Conclusions

Our work provides a simple algorithm that applies Bayesian inference to learn a Hamiltonian in an online fashion; that is to say, that our algorithm learns the Hamiltonian parameters as the experiment proceeds rather than collecting data and inferring the Hamiltonian through post-processing. This eliminates the need to store and process gigabytes of data that are recovered from even relatively short experiments. Our work has several advantages over existing approaches to learning Hamiltonian parameters. First, it can be used to estimate the optimal parameterization of the dynamics of an arbitrary quantum system within a space of model Hamiltonians. Second, it can be used to provide a region estimate of the Hamiltonian parameters. The importance of this is obvious: it allows us to not only learn the unknown parameters but also quantify our uncertainty in them. Third, our analysis of the algorithm shows a clear trade o between the experimental time and the computational time needed to parameterize the Hamiltonian.

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References

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For more information and a software implementation, please visit http://www.cgranade.com/research/rohl or scan the code at left.