Classical and Quantum Algorithms for Cosmology

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Classical - The Metropolis-Hastings Algorithm

Suppose we have a probability distribution $P(\vec{x})$ which is difficult to sample from, but for which we know some function $f(\vec{x}) \propto P(\vec{x})$. The MH algorithm is a Markov Chain Monte Carlo algorithm which provides a way to produce a sequence of points to approximate $P(\vec{x})$. The general procedure is as follows:

1. At step n, randomly choose a new point of parameters $\vec{x}_{n+1}$.
2. Compute $f(\vec{x}_{n+1})$ and $\alpha = \frac{f(\vec{x}_{n+1})}{f(\vec{x}_n)} = \frac{P(\vec{x}_{n+1})}{P(\vec{x}_n)}$.
3. If $\alpha \geq 1$, move to the new point. Otherwise, move to the new point with probability α.

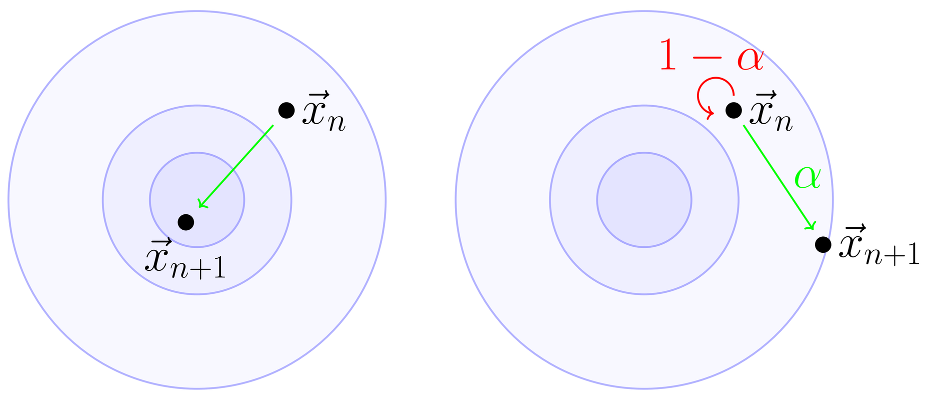

Figure 1: Illustration of the nth step of the MH algorithm. Here, the underlying distribution is a 2-D Gaussian.

4. After sufficient iterations, the points $\{f(\vec{x}_0), \ldots f(\vec{x}_N)\}$ can be used to approximate $P(\vec{x})$, as the algorithm collects points that contribute most to the distribution.

In Cosmology - Constraining parameters

One of two primary branches of contemporary cosmology is investigation of cosmological parameters (such as the 6 parameters that define the Λ-CDM model); here we discuss Cobaya (COde for BAYesian Analysis) [1] [2] which uses Bayesian inference to address this task. In Bayesian inference, one considers a model $\mathcal{M}$ parameterized by θ, and a dataset $\mathcal{D}$ to model using $\mathcal{M}$. We wish to find the posterior probability $P(\theta|\mathcal{D},\mathcal{M})$ of the parameters θ given $\mathcal{D}$ and $\mathcal{M}$. This can be computed via Bayes' theorem:

$$P(\theta|\mathcal{D},\mathcal{M}) = \frac{\mathcal{L}(D|\mathcal{M}(\theta))\pi(\theta|\mathcal{M})}{P(\mathcal{D}|\mathcal{M})} \tag{1}$$

Where $\mathcal{L}(D|\mathcal{M}(\theta))$ is the likelihood of the data given some set of model parameters, $\pi(\theta|\mathcal{M})$ is the prior, and $P(\mathcal{D}|\mathcal{M})$ the evidence. The likelihood is obtained by comparison of theoretical models (e.g. model code that takes in cosmological parameters to produce CMB observables) and experimental likelihoods (e.g. obtained by observations of the CMB). $P(\theta|\mathcal{D},\mathcal{M})$ is sampled in Cobaya using the MH algorithm above.

Demonstration - Cobaya Results

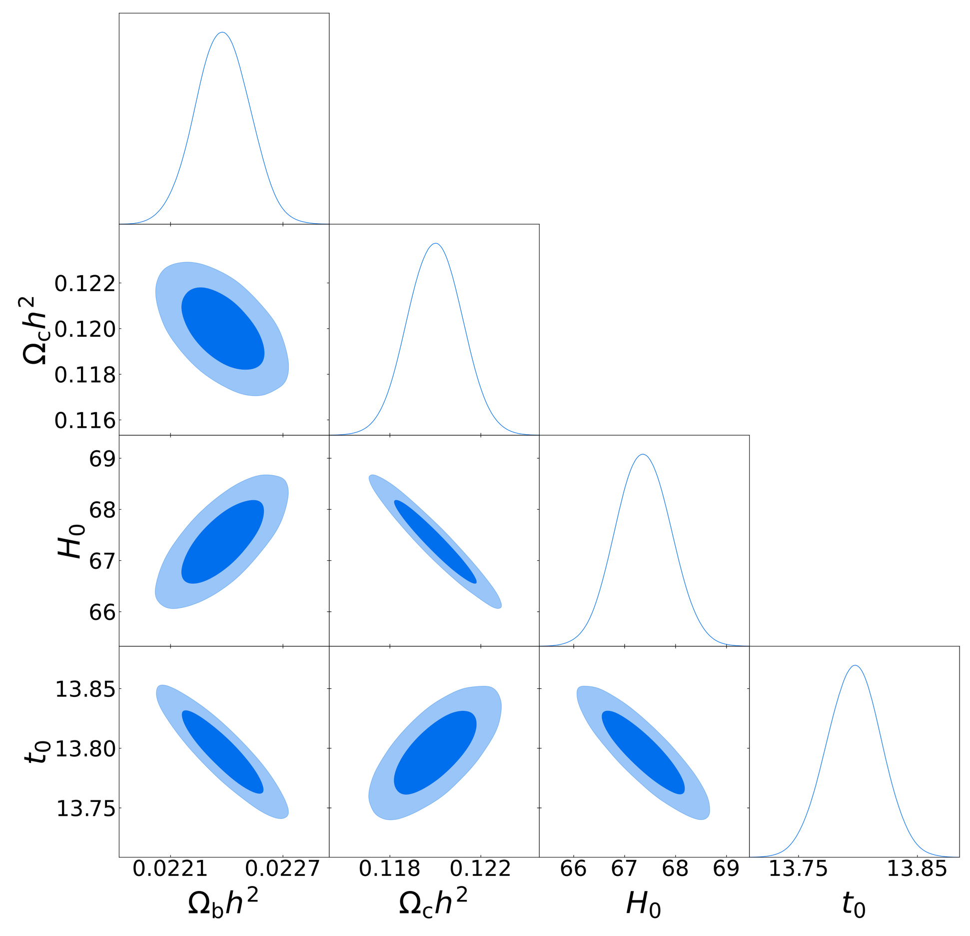

Figure 2: Distributions for parameters $\Omega_b h^2$ (baryon density) $\Omega_c h^2$ (dark matter density) H_0 (Hubble constant) and t_0 (age of the universe) as obtained using Cobaya [1][2] with CAMB theory code [3][4] and Planck 2018 Experimental CMB data [5][6].

Using Cobaya, we can constrain the 6 core cosmological parameters in the Λ-CDM cosmological model (such as baryon/dark matter density and t_0) as well as derived parameters (like H_0). Although we only display a standard Λ-CDM run here as a proof-of-concept, Cobaya can be used to test novel cosmological theories and to constrain parameters in these theories according to likelihoods obtained from CMB observations.

Quantum - The VQE Algorithm

In quantum mechanics, often of interest is the ground state energy E_0 of a given Hamiltonian H. A tool to find this is the variational theorem, which says that for any state $|\psi\rangle$:

$$\langle\psi|H|\psi\rangle \geq E_0 \tag{2}$$

with equality if $|\psi\rangle$ is the ground state of the Hamiltonian. Due to the exponential scaling of the number of parameters needed to specify a general (entangled) quantum state, evaluating the LHS of (2) in general is a difficult problem. Fortunately, it is one that quantum computers are well-suited to address, as states can be prepared efficiently. The Variational Quantum Eigensolver algorithm that can be performed is as follows:

1. Prepare a variational ansatz state $|\psi(\vec{p})\rangle$ with parameters $\vec{p}$ (on the quantum device).
2. Measure the energy $\langle\psi(\vec{p})|H|\psi(\vec{p})\rangle$ (on the quantum device).
3. Based on this measurement, update $\vec{p}$ (using a classical computer). Repeat until $\langle\psi(\vec{p})|H|\psi(\vec{p})\rangle$ is minimized to approximate E_0.

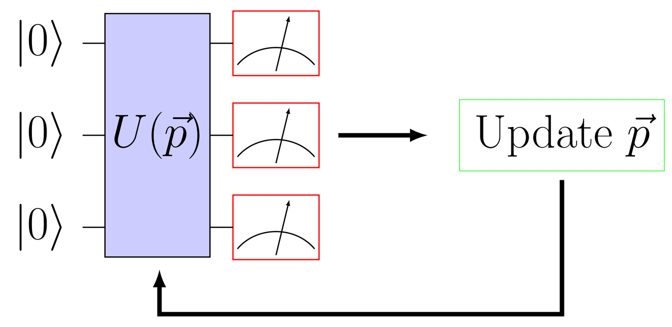

Figure 3: Illustration of VQE. We have a VQE ciruit, where the ansatz state is prepared (blue) and measured (red) on a quantum computer. The parameters are then optimized on classically (green) and we repeat until the energy is minimized.

In Cosmology - Inflationary Dynamics

In theories of cosmic inflation, we consider an inflaton field $\phi(\vec{r},t)$ with associated potential energy $V(\phi)$. One such model is that of Starobinsky inflation, with potential:

$$V(\phi) = M_1^4(1 - e^{\phi/M_2})^2. \tag{3}$$

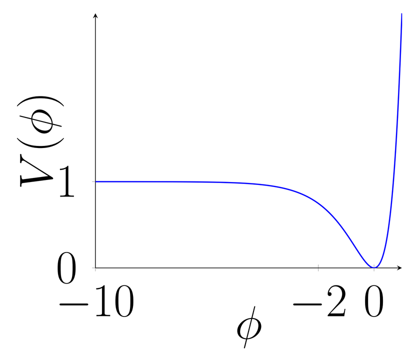

Figure 4: Plot of the Starobinsky Potential (with $M_1 = M_2 = 1$).

The VQE method can be applied to this potential to find E_0 of this potential, which can be used to predict inflationary dynamics (in this case, $E_0 > 0$ indicating an additional exponential expansion period from the model) [7].

In Cosmology - Dark Matter Dynamics

In ultra-light boson dark matter models and the $m \to \infty$ limit of CDM models,the time-evolution of a wavefunction ψ representing dark matter is governed by the Schrodinger-Poisson Equations:

$$i\frac{\partial}{\partial t}\psi = -\frac{\nabla^2}{2}\psi + aV\psi \tag{4}$$

$$\nabla^2 V = |\psi|^2 - 1 \tag{5}$$

these can be solved using VQE, yielding exponential speedup over classical simulations [8].

Disclaimer - The NISQ Era

Currently, we only have Noisy Intermediate-Scale Quantum (NISQ) devices at our disposal, with a demonstration of true "quantum supremacy" still in the works. It is notable that the work in [7], [8] lack any demonstration on physical quantum devices, instead choosing to simulate their quantum algorithms classically. Given more time, it would be interesting to carry out these algorithms and see how the results fare on current-generation quantum devices. Nevertheless, such proofs-of-concepts give hope that quantum computers may become part of the cosmologist's toolkit in the near future.

References

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