Minimising Action of a Discrete Path via Gradient Descent

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1 Introduction

The action for a path, given by $S[x]$, is a scalar functional that encodes information regarding the trajectory of a particle obeying some Lagrangian. The **Principle of Least Action** states that the classical path $\bar{x}(t)$ is one that minimises the action functional

$$\left.\frac{\delta S}{\delta x}\right|_{x=\bar{x}} = 0,$$

which is a variational problem. The classical path is constructed by fixing the endpoints, given by boundary conditions, and varying the path between these fixed endpoints until we find one that minimises the action. This contradicts the more usual method of solving a dynamical system, where the initial conditions completely specify the exact solution to a system. In Hamiltonian dynamics, the action quantity is also known as Hamilton's Principle function, which is a solution to the time-dependent Hamilton-Jacobi equation.

In this project, we will attempt to solve the variation problem numerically by implementing the method of gradient descent. The solver is initialised by fixing the endpoints of the trajectory that is being sought and generating random points in between. We will then implement a gradient descent method to optimise the intermediary points by minimising the loss function as given by the action of this discretised path, under the influence of a harmonic potential. The end goal of this project is to solve for the path of a particle under the influence of a cubic anharmonic potential.

2 Background Physics

2.1 Harmonic Oscillator as a Toy Model

The toy model under consideration for the early stages of this project is

$$S[x] = \int_{t_a}^{t_b} \frac{1}{2} m \left(\dot{x}^2 - \omega^2 x^2\right) \, dt \tag{1}$$

where m and ω are the mass of particle and frequency of the potential, respectively. We can cheat and solve for the trajectory of this particle by considering the Euler-Lagrange equation. Instead, we will showcase the variational principle by explicitly varying the action and invoking the principle of least action. We impose the trivial boundary conditions $x(t_a = 0) = 0 = x(t_b = \tau)$ for simplicity – later we will consider a non-trivial set of boundary conditions, which leads to a richer family of solution. Varying the action looks something like this

$$\begin{aligned}
\delta S &= \int_0^\tau m \left(\dot{x}\delta\dot{x} - \omega^2 x \delta x\right) \, dt \\
&= m \left(\overset{0 \text{ fixed boundaries}}{\cancel{\left.\dot{x}\delta x\right|_0^\tau}} - \int_0^\tau (\ddot{x} + \omega x^2)\delta x \, dt \right) \\
&\overset{!}{=} 0 \text{ by Hamilton's Principle.}
\end{aligned}$$

Since the last equality has to hold $\forall \delta x$, the path that minimises the action is one that also satisfies the differential equation given by $\ddot{x} + \omega x^2 = 0$, yielding the usual harmonic oscillator

$$\begin{aligned}
x(t) &= A \sin \omega_n t + \cancelto{0 \text{ by boundary condition}}{B \cos \omega_n t} \\
&= A \sin n \frac{\pi t}{\tau}
\end{aligned}$$

with the discretisation condition given by $\omega_n = \frac{\pi}{\tau} n$. Notice that since the variational problem does not require an initial condition, this leaves the amplitude A as an unspecified constant. This could be problematic for classifying solutions of our numerical solver later as there could be a degenerate family of solutions, all differing by the scale factor A. Let's then define an L_2-type norm given by[1]

$$\int_0^\tau x(t)^2 \, dt = 1,$$

[1] later we might use this condition as a constraint in our loss function to help narrow down the solutions landscape.

allowing us to specify the amplitude $A := \sqrt{\frac{2}{\tau}}$.[2] The problem with this normalisation is that the amplitude explicitly depends on the end time of the variation, which is clearly only valid in the finite domain $[0, \tau]$. An alternative, more variational friendly definition is proposed below.

Definition 1 (SHO Amplitude Normalisation)**.** *The normalisation condition for a path that minimises the SHO action in the time interval* $[0, \tau]$ *is*

$$\lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau x(t)^2 \, dt = 1.$$

This definition respects causality and the finite bound of the variational principle. Notice that this definition is similar to the definition of the average power of a signal, hence one can interpret this definition as a method of preserving the scale invariance property of the SHO.

2.2 Fourier Basis Expansion

3 Computational Setup

3.1 Finite Discretisation of the Action

4 Ideas

Use average power-style norm to define the amplitude for the harmonic oscillator model. This respects causality and the finite bound time interval of the variational principle. Then impose this as a soft constraint in the loss function.

Leverage JAX's autodiff for forward, backward propagations in action basis transformations, action calculations and loss function minimisation.

Practical strategy: Start with 1–3 coefficients and informed initialisation. Once solver is stable, increase coefficient count. Try both uniform and biased initialisations for the same system and compare: If both converge to same minimum → solution likely stable. If they don't → inspect the loss landscape (multi-modal? poorly regularised?).

[2] the dependence of the amplitude on the "variational end time" τ seems precocious