Deep learning dynamics from physical principles

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Abstract

Let $T > 0$. Which potential energy functions U yield T-isochronism for the one-dimensional physical system $\ddot{x} = -U'(x)$? Under mild assumptions, one can check that the only symmetric potentials satisfying this property are harmonic : $U(x) \propto x^2$. We propose to recover this result experimentally by training a neural differential equation [1] to satisfy global T-periodicity.

1 Isochronism problem

Isochronism is the property for a physical system of having a period that is independent of the motion's amplitude. Such a property allows one to measure time reliably, be it by the means of a pendulum or of a quartz crystal [2]. Consider a one-dimensional physical system

$$\ddot{x} = -U'(x), \tag{1}$$

where we chose a unitary mass without loss of generality. It is well known that the quadratic potential $U(x) = \frac{1}{2}\omega x^2$ yields a harmonic, isochronic motion of period $T = 2\pi/\omega$. We are interested in the following question : given a fixed time $T > 0$, are there other such symmetric functions U ?

In mathematical terms, for which symmetric functions U do the dynamics (1) yield T-periodicity $X(T) = X(0)$ for **all the trajectories** $X = (x, \dot{x})^\top$ *i.e.* for all initial conditions $X(0)$? It turns out that under mild assumptions, the harmonic potential is the only solution [2] :

$$U(x) \propto x^2. \tag{2}$$

We first introduce neural differential equations (neural ODEs), then apply them to tackle our problem experimentally. Finally, we present a mathematical proof of the result.

2 Neural differential equations

Residual neural nets learn residual functions of the activations: $x_{t+1} = x_t + f_\Theta(x_t)$. In the continuum limit, if the weights are assumed to be constant along the depth of the network t, the activations are solutions of the autonomous system [1]:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f_\Theta(x). \tag{3}$$

Therefore, the values of the activations (x_t) are trajectories of the flow f_Θ along depth t. Then, minimizing a loss function of the trajectories and the weights $L[x_\Theta, \Theta]$ amounts to optimizing the weights of a parametric differential equation (3). This is allowed by sensitivity analysis of differential equations, typically by the means of automatic differentiation or by the adjoint method [3]. We give a representation of neural ODEs in figure 2.

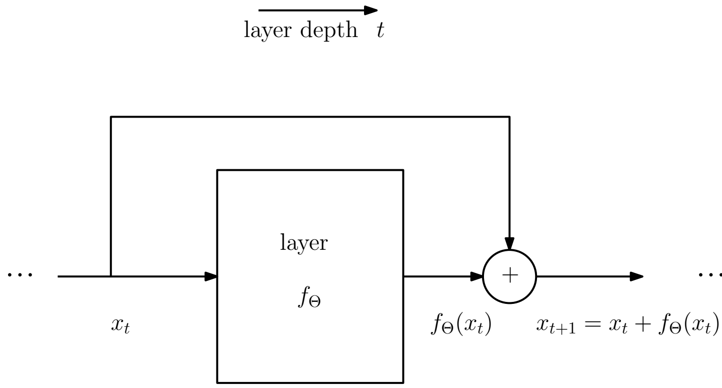

Figure 1: ResNet architecture. The layer f_Θ learns the residual of the activations.

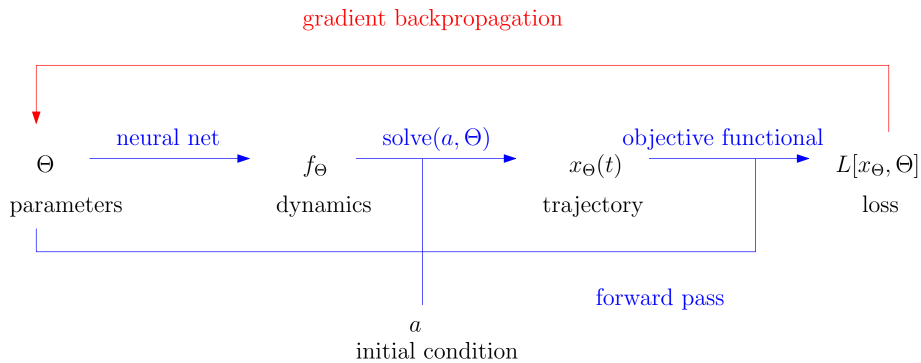

Figure 2: Training a neural ODE. Backpropagating the gradient through the integration step is performed by automatic differentiation through the solver or the adjoint method [1].

3 Learning the flow

As stated before, neural ODEs allow us to train the flow of an ODE by imposing a loss function on its trajectory. We hence parametrize the dynamics (1) in the following way

$$\ddot{x} = f_\Theta(x), \tag{4}$$

where the neural network $f_\Theta(x)$ approximates the force field $f(x) = -U'(x)$. Our objective is to yield T-periodic trajectories, so we want to optimize

$$\min_\Theta \|X_\Theta(T) - X_\Theta(0)\|^2 . \tag{5}$$

Experimental setup In our experiment, we trained our network to the objective (5) on a dataset of $N = 100$ random points of the phase portrait $X_i \sim \mathcal{N}(0, 1), \quad 1 \le i \le N$ and with $T = 2\pi$. We take for f_Θ a 2-layer fully connected architecture with width 16 and tanh nonlinearity. We used the Python package `torchdyn` [4] which is built on `torchdiffeq` [1].

Results Our results are summarized in figure 3. The circular trajectories centered on the origin in the phase space show that the potential converged to $U(x) = \frac{1}{2}x^2$. Hence, the phase portrait is that of a harmonic oscillator with angular frequency $\omega = 1$, which does equal $2\pi/T$. We further check that the flow converges to the restoring force $f(x) = -x$. Note that we didn't impose any f_Θ to be an odd function, or any symmetry assumption.

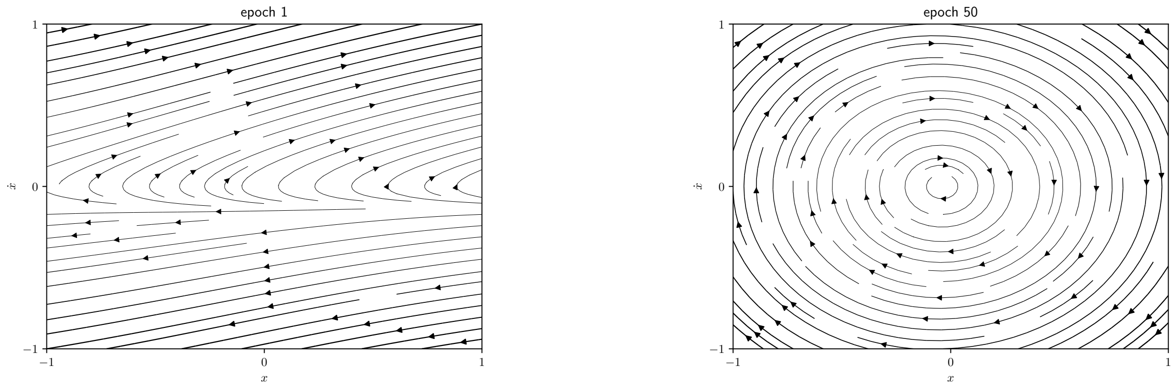

Figure 3: Evolution of the phase portrait after 60 training epochs.

4 Theoretical derivation

We prove here that harmonic potentials (2) are the only symmetric potentials yielding isochronism. Our computations are inspired by, yet different from that of [2], as ours focuses on symmetric potentials.

Let $U(x)$ denote the potential energy. We assume that U is a symmetric function, and is increasing on $\mathbb{R}_+$ (and hence decreasing on $\mathbb{R}_-$). It hence admits a global minimum at 0.

Any solution of (1) has constant energy

$$E = \frac{1}{2}\dot{x}^2 + U(x). \tag{6}$$

Hence, the momentum $\dot{x}$ is a function of the position x

$$\dot{x} = \pm\sqrt{2}\sqrt{E - U(x)}. \tag{7}$$

Assume that all trajectories following the dynamics (1) are T-periodic. The two extreme points of the trajectory are symmetric with restpect to 0 because the potential is symmetric. The turning points are $x = \pm y$, where the amplitude

$$y = y(E) > 0 \tag{8}$$

is solution of

$$\dot{x} = 0 \qquad \text{at} \qquad x = \pm y(E), \tag{9}$$

or equivalently

$$U(\pm y(E)) = E. \tag{10}$$

Since the travel time from 0 to y is equal to that from y to 0, the quarter of the period equals

$$\begin{aligned} T/4 &= \int_0^{y(E)} \mathrm{d}t \qquad (11) \\ &= \frac{\sqrt{2}}{2}\int_0^{y(E)} \frac{\mathrm{d}x}{\sqrt{E - U(x)}}. \qquad (12) \end{aligned}$$

Changing variable to $u(x) = U(x)/E$ yields

$$T/4 = \frac{\sqrt{2}}{2} \int_0^1 x'(uE)\sqrt{uE} \frac{\mathrm{d}u}{\sqrt{u(1-u)}}, \tag{13}$$

where $x(U)$ is the inverse function of $U(x)$. Let $g(U) = x'(U)\sqrt{U}$. Since there is a one-to-one correspondance (10) between the oscillator amplitude y and the energy of the system E, isochronism means that the integral

$$\int_0^1 g(uE) \frac{\mathrm{d}u}{\sqrt{u(1-u)}} \tag{14}$$

is constant with respect to $E \in \mathbb{R}_+^*$, which implies that g is constant. Indeed, if $v = \inf\{u, g(u) \neq g(0)\} < +\infty$, taking $E = v + \varepsilon$ with small $\varepsilon > 0$ and $E \to 0$ yield different values for the integral (14).

Therefore $x'(U) \propto 1/\sqrt{U}$ and

$$U(x) \propto x^2. \tag{15}$$

5 Discussion

This work showcases an application of neural ODEs, which allow to find the flow of an ODE by imposing a loss on its trajectories.

Although our experimental results could suggest that the assumption of U being symmetric might be irrelevant, it is shown in [2] that the result does not hold for any U. Hence the minimization of (5) has more than one solution, and (2) is one of them.

References

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