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Self-supervised hamiltonian mechanics neural networks

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Abstract

We developed a method to derive the hamiltonian of an unknown system by machine learning the motions of the system. We modified the training process of Greydanus et al.'s hamiltonian neural network to make it be capable of learning from a dataset without the change-of-state ground truth. In other word, the learning process is self-supervised. This improvement can extend the application of the hamiltonian neural network because it is sometimes difficult to accurately measure the change of state of the system. Our model can now be able to learn the free particle system and the harmonic oscillator system.

Keywords— hamiltonian, machine learning, mechanics

Contents

1 Introduction

Neural networks excel in learning from given datasets. Besides image classification and strategy decision, its ability also makes it capable to derive the infomation (mathematical descriptions) about a physics system. If a neural network can learn a physics system according to the motion of it, there can be a lot of applications that can be done with it because deriving the motion of a system only requires measuring, but deriving the abstract mathematical form of a system requires induction, which is more difficult. Thus, we want to develop a machine learning method in physics.

One of the most often used description of mechanics systems is the hamiltonian. When one observes the motion of a system, he may be curious about what is the hamiltonian of it if such a hamiltonian exists.

Here there have been several approaches to do this, such as the hamiltonian neural network (HNN) [4], the lagrangian neural network [3], and the neural ODE [2]. Like what we are going to do, they optimize a neural network that reads the state $\mathbf{x}$ of a system as the input and outputs the change of state w.r.t. time $\mathrm{d}\mathbf{x}/\mathrm{d}t$ of the system.

In this process, they have a common property: they train the neural network in a supervised mode, which means there are $\mathrm{d}\mathbf{x}/\mathrm{d}t$ ground truth in the dataset. However, in a physics experiment, measuring the change rate of the state is probably more difficult than directly measuring the state. Thus, we want to introduce a method to optimize the neural network in a self-supervised way.

Here in the paper, we will show how to use self-supervised learning for learning the hamiltonian of a system (based on Greydanus et al.'s HNN [4]), and compare the result with ours (learning using a dataset without $\dot{\mathbf{x}}$ ground truth) and theirs (learning using the same dataset with ground truth).

2 Canonical equation and ODE

To build a common sense of the physics theories it is going to involve, the canonical equation is introduced.

The canonical equation is a set of ordinary differential equations (ODE) whose solution depicts the motion of the system. The equation in mathematical form is [5][1, p. 65][7, p. 132]

$$\dot{\mathbf{q}} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}}, \tag{1}$$

where $\mathbf{q} \in \mathbb{R}^n$ is the **generalized coordinates**, $\mathbf{p} \in \mathbb{R}^n$ is the **generalized momentum**, and $\mathcal{H}$ is the **hamiltonian** of the system, which is a scalar function w.r.t. t, $\mathbf{q}$, and $\mathbf{p}$. n is the number of degrees of freedom (DOF). A hamiltonian is specific for a specific system.

The tuple $\mathbf{x} := (\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2n}$ is called the **canonical coordinates**. In computer programs, it is convenient to write Equation 1 in form of

$$\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}), \tag{2}$$

which is the common form of ODE. Here in our specific case,

$$\mathbf{f}(t, \mathbf{x}) := \boldsymbol{\omega}\nabla_{\mathbf{x}}\mathcal{H}, \tag{3}$$

where the notion $\boldsymbol{\omega}\nabla_{\mathbf{x}}$ denotes the **symplectic gradient** w.r.t. $\mathbf{x}$, whose first n components is the gradient w.r.t. the last n components of $\mathbf{x}$, and the last n components is the negative gradient w.r.t. the first n components of $\mathbf{x}$.

One of properties of the symplectic gradient is that, moving along the symplectic gradient field of a scalar does not change the value of the scalar function, which means that the value of $\mathcal{H}$ is conserved if $\partial\mathcal{H}/\partial t = 0$ [1, p. 67][7, p. 132]. In fact, the physical meaning of $\mathcal{H}$ is the energy, so its conservation is obvious.

According to Equation 3, the difference between $\mathbf{x}$ at 2 different times is an integral

$$\mathbf{x}(t_2) = \mathbf{x}(t_1) + \int_{t_1}^{t_2} \mathbf{f}(t, \mathbf{x}(t))\,\mathrm{d}t. \tag{4}$$

The integral can be calculated using the torchdiffeq Python package [2].

3 Training with proposed loss

Our goal is to derive the function $(t, \mathbf{x}) \mapsto \mathcal{H}$ according to the dataset containing a series of samples in form of $(t, \mathbf{x})$ on a series of possible motions of the system. To make our work simpler, we assume that $\partial\mathcal{H}/\partial t = 0$, which fits with most cases.

The dataset does not contain the $\dot{\mathbf{x}}$ infomation, which acts as the ground truth in the supervised model [4]. Our model is self-supervised, and thus does not need the $\dot{\mathbf{x}}$ infomation.

The model uses the loss inspired from Equation 4

$$\mathcal{L} := \operatorname{MSE}\left(\mathbf{x}(t_1) + \int_{t_1}^{t_2} \boldsymbol{\omega}\nabla_{\mathbf{x}}\mathcal{H}\mathrm{d}t, \mathbf{x}(t_2)\right), \tag{5}$$

where $(t_1, \mathbf{x}(t_1))$ and $(t_1, \mathbf{x}(t_1))$ are 2 samples from the same motion of the system. The complete process of a traning circle is shown in Figure 1b. For comparison, the train circle of the supervised HNN is shown in Figure 1a.

The Adam optimizer [6] is used for optimizing the neural network.

3.1 The structure of the neural network

The structure of the neural network is a simple multilayer perceptron (MLP), which is the same as that adopted in Greydanus et al.'s HNN [4].

There are 3 layers of linear mapping, the last of which outputs the value of hamiltonian. Between 2 linear layers, there is a nonlinearity layer, as which we adopted tanh.

The hidden dimension (the input size and output size of the 2nd linear mapping) is taken as 200 in the following experiments in Section 5.

4 Few-parameters optimization

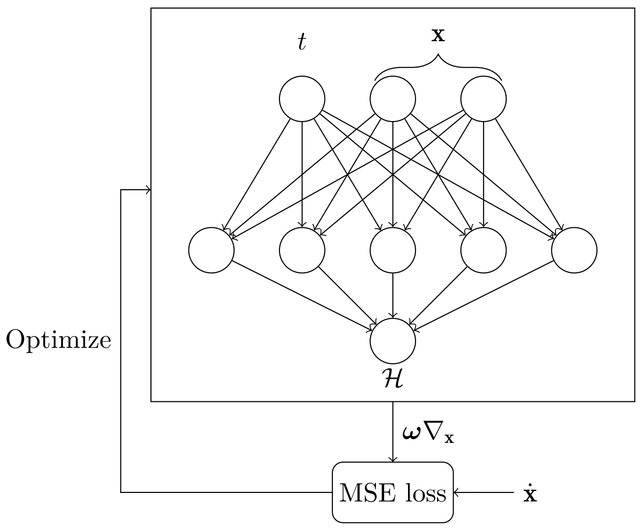
If the form of the hamiltonian is previously known, and there are just a few parameters in the formula of the hamiltonian to be decided, the few-parameters optimization.

For example, there is a harmonic oscillator with its frequency unknown. Its hamiltonian is

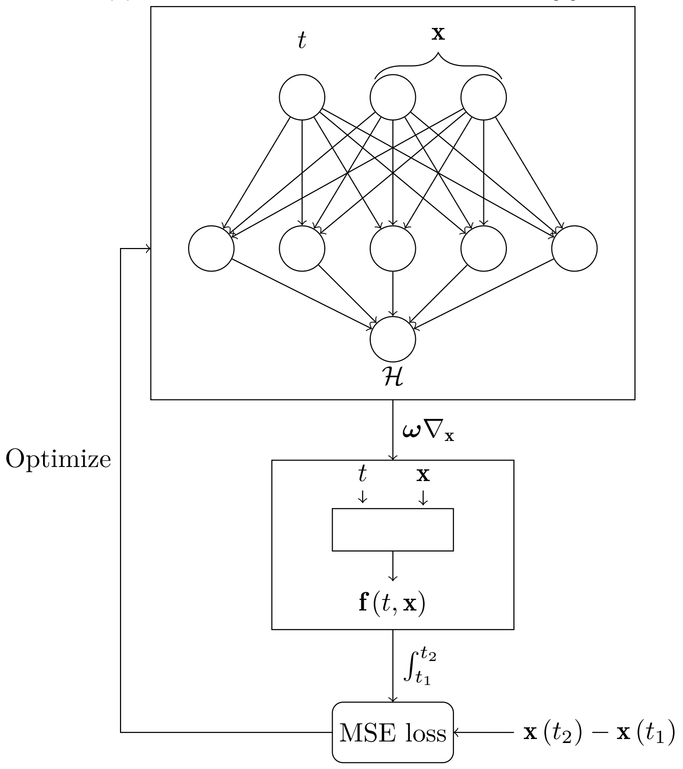
$$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2, \tag{6}$$

where ω is the only parameter that should be optimized.

We can use the procedure explained in Section 3 to optimize the parameter.



(a) The train circle of a supervised HNN [4]



t
$\mathbf{x}$
$\mathcal{H}$
$\boldsymbol{\omega}\nabla_{\mathbf{x}}$
Optimize
t
$\mathbf{x}$
$\mathbf{f}(t,\mathbf{x})$
$\int_{t_1}^{t_2}$
MSE loss
$\mathbf{x}(t_2) - \mathbf{x}(t_1)$

(b) The train circle of a self-supervised HNN

Figure 1: The train circle of the neural network

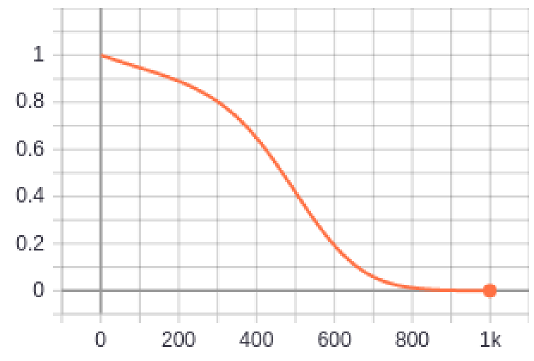
Here we have gone on an experiment. Use the ground truth $\omega = 2$, and initialize the parameter as $\omega = 1$. Use a dataset with only 2 datas $\mathbf{x}(0) = (1, 0)$, and $\mathbf{x}\left(\frac{\pi}{2}\right) = (-1, 0)$. After we trained it for 1000 epoches with learn rate 1×10^{-3}, the parameter is optimized to the true value 2.

The change in loss and ω during the training is shown in Figure 2.

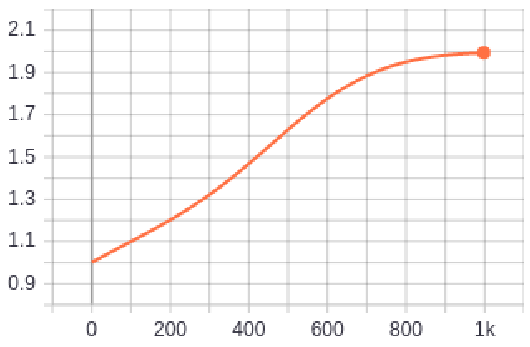
Although the few-parameters optimization experiment does not have much value because we often do not know the form of the hamiltonian before we train the model, this experiment shows that the method introduced in Section 3 is feasible.

However, this method has some flaw. If we take the initial value of ω as 5.0, the final value of ω is not correct. This is because the loss has multiple minimals w.r.t. ω [8, p. 121], one of which is 2, taken when $\omega = 4$. Specially, in some cases, the wrong minimal of loss can be 0, so we cannot judge whether the result of the optimized parameter is correct by looking at whether the loss is 0.

This reminds us that the method has its limitations. To avoid the wrong result, the dataset should be comprehensive enough. After some trials, we found that the best strategy is to switch to another data when the loss converges. After switching the data several times, the parameters should converge to a correct value.

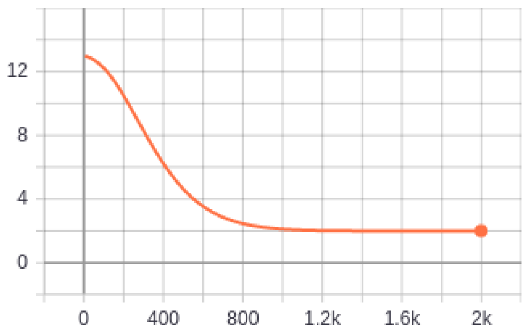


(a) The change in loss during the training

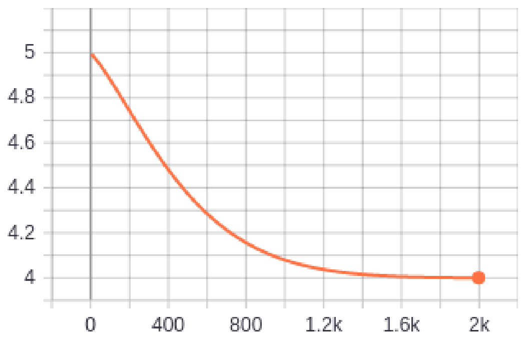


(b) The change in ω during the training

Figure 2: The process of training using the few-parameters optimization (abscissa is the epoch number)



(a) The change in loss during the training, converging to a non-zero value



(b) The change in ω during the training, converging to a wrong answer

Figure 3: The process of training using the few-parameters optimization, but coming out with a bad result

5 Experiments

5.1 Free particle

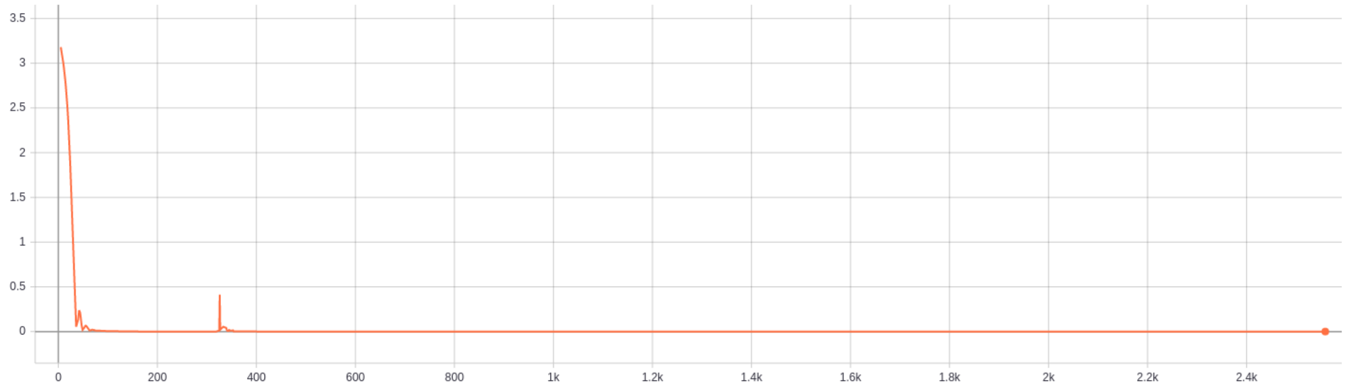


Figure 4: The loss change during the training of the model of free particle

A free particle is a system with 1 DOF whose hamiltonian is [7, p. 133][1, p. 66]

$$\mathcal{H}(t, q, p) := \frac{p^2}{2m},$$

where m is the mass of the particle. To be simple, we take $m := 1/2$.

The model of a free particle is the simplest model. We take this model as the first task to test the basic capability of our idea.

The dataset is generated using a ODE solver. The dataset has totally 16 datas. Every data consists of the size of considered time interval (lies in the range $(0, 2)$), a series of 200 different initial conditions (lies in the range $(-1, 1)^2$) to be learned as a batch, and the corresponding state of the system at the end of the time interval.

Every data is learned for 160 epoches. When a data is finished, the neural network moves on to the next data. Thus there are totally 2560 steps. The loss change in shown in Figure 4.

5.2 Harmonic oscillator

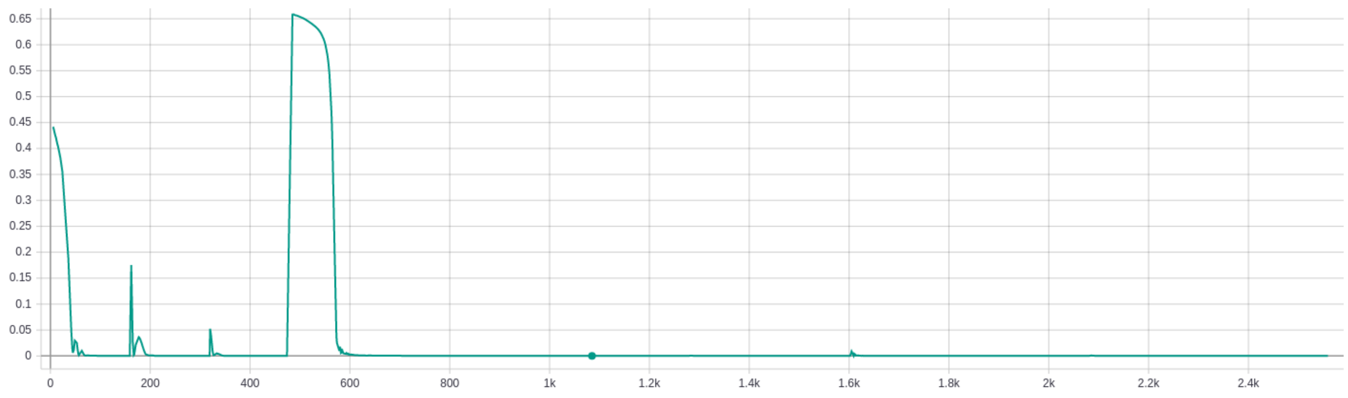


Figure 5: The loss change during the training of the model of a harmonic oscillator

A harmonic oscillator is a system with 1 DOF whose hamiltonian is [7, p. 157]

$$\mathcal{H}(t, q, p) := \frac{p^2}{2m} + \frac{1}{2}kq^2,$$

where m is the mass of the particle, and k is a parameter. To be simple, we take $m := 1/2$ and $k := 2$.

The dataset is generated using a ODE solver. The dataset has totally 16 datas. Every data consists of the size of considered time interval (lies in the range $(0, 2)$), a series of 200 different initial conditions (lies in the range $(-0.71, 0.71)^2$) to be learned as a batch, and the corresponding state of the system at the end of the time interval.

Every data is learned for 160 epoches. When a data is finished, the neural network moves on to the next data. Thus there are totally 2560 steps. The loss change in shown in Figure 5.

The loss may suddenly jump to a high value when the neural network switches to a different data because it may have converged to a wrong minimal of loss when it learns with the last data.

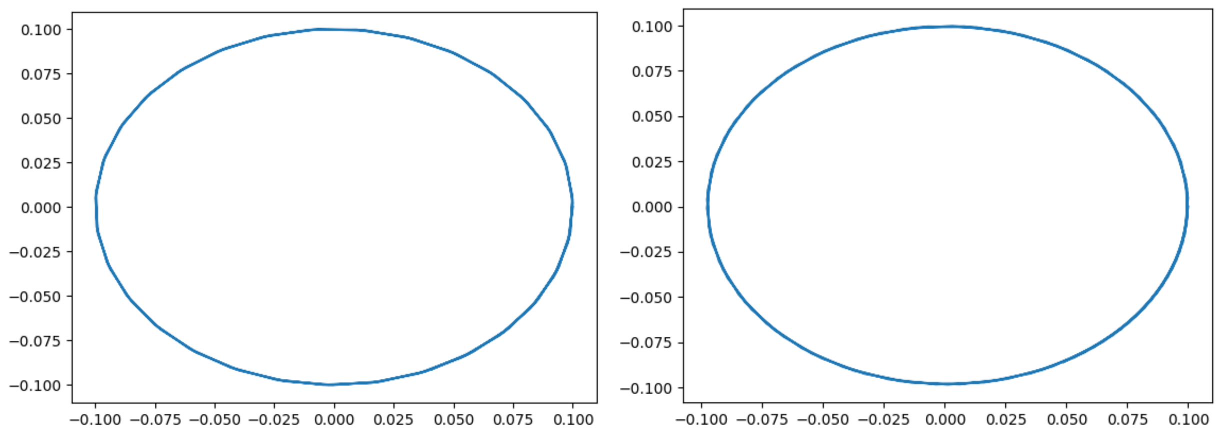
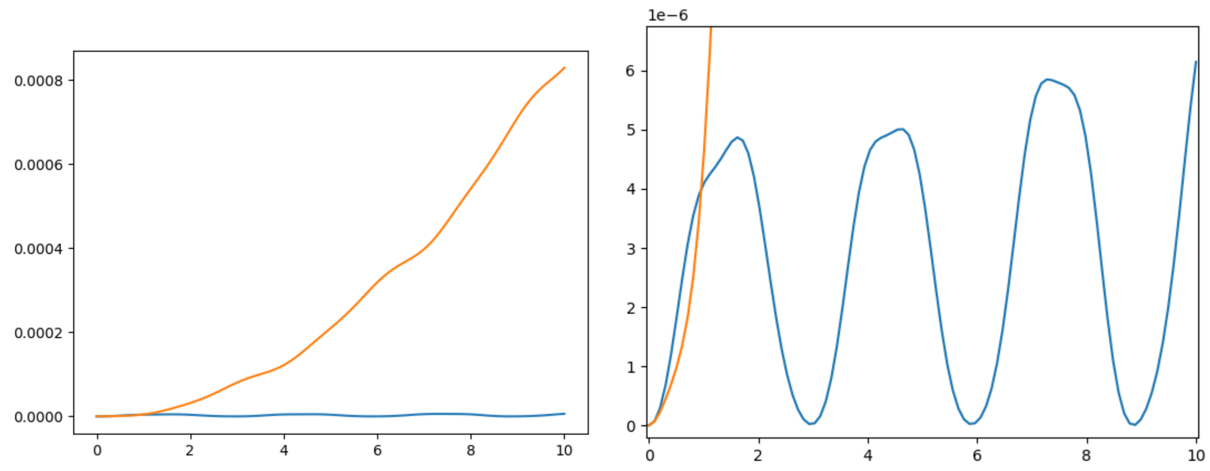

(a) The result given by the trained model (b) The ground truth

Figure 6: The comparation of the result given by the trained model and the ground truth



(a) Overview of how the two estimation erros change (b) Details of estimation errors

Figure 7: The comparation of the estimation of the result given by Greydanus et al.'s HNN and that given by ours, where the yellow line is theirs, and the blue one is ours

Taking the initial condition $\mathbf{x} = (0.1, 0)$ to test the trained model and compare it with the ground truth, the result can be seen in Figure 6. The figure shows the trajectory of the motion in space of $\mathbf{x}$, which is the phase path [7, p. 146][1, p. 68]. As can be seen, it can give the correct result: the phase path is a circle [1, p. 17].

Here we can compare the result of the self-supervised HNN with the original Greydanus et al.'s HNN. The graph of MSE between $\mathbf{x}$ predicted by HNN and the actual $\mathbf{x}$ w.r.t. t is shown in Figure 7. As can be seen, loss of ours is much less than that of theirs despite that ours did not use the $\dot{\mathbf{x}}$ ground truth in the dataset. However, the cost is that our neural networks require much more time (48 minutes on a device with GeForce RTX 2070 SUPER) to train than theirs (less than 1 minute on the same device).

6 Possible further improvements

The model is currently not capable enough to learn complex systems quickly (like those with more than one DOF). In other words, the original neural network model does not fit with the self-supervised learning pattern when it comes to complex systems. The problem can be solved if an improved neural network customized to hamiltonian learning is developed, but whether such an improvement exists is not sure.

The other possible improvement is to make the $\mathbf{x}$ not necessarily be the canonical coordinates but be the arbitrary generalized coordinates. This can be useful because it is sometimes difficult to derive the generalized momentum of a system during a physics experiment. The HNN is not capable of this, but the lagrangian neural network (LNN) is for this [3]. However, there are also some difficulties in using the lagrangian neural network with the self-supervised learning pattern.

7 Conclusion

We have developed a method to use Greydanus et al.'s HNN [4] to learn a hamiltonian mechanics system using self-supervised machine learning. Besides most of the advantages of theirs (can conserve the energy and has reversibility), the self-supervised learning pattern can make it more capable when it comes to applications.

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