

Neural Ordinary Differential Equations

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This is a note on the paper “Neural Ordinary Differential Equations” by Chen et al.[CRBD18].

1 Introduction

- Many existing neural networks models creates a sequence of hidden states $\mathbf{h}_0, \mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_T$ by adding something to the previous state:

$$\mathbf{h}_{t+1} = \mathbf{h}_t + \mathbf{f}(\mathbf{h}_t, t, \boldsymbol{\theta})$$

Such models include such as residual networks [HZRS15], recurrent neural networks, and normalizing flows [RM15, DKB14].

- What if we take the limit as the number of time step goes to infinity? We will have a differential equation:

$$\frac{d\mathbf{h}(t)}{dt} = \mathbf{f}(\mathbf{h}(t), t, \boldsymbol{\theta}).$$

- To use the network, we simply say that $\mathbf{h}(0)$ is the input layer, and the output is $\mathbf{h}(T)$ at some time T . The output can be found by solving the initial value problem, and this can be done by any black-box differential equation solver.

2 How to train a neural ODE model

- The problem with the above approach is that it is unclear how to train such a neural ODE model.
 - The computation of the solution can require a lot of time steps. Differentiating through these time steps to compute the gradient would requires saving a lot of information in memory.
- The good news is that there is a method to compute the gradient using constant memory (i.e., does not depend on the number of time steps). This is called the **adjoint sensitivity method**. It requires, however, an ODE solve, which can be done, again, by any ODE solver.

2.1 Problem Setup

- Let the hidden state be a vector in \mathbb{R}^n . We typically denote it by \mathbf{z} .
- Let the neural network’s parameters be a vector in \mathbb{R}^m , and we typically denote it by $\boldsymbol{\theta}$.
- We will work on a state space vector $\mathbf{r} = (\mathbf{z}, t, \boldsymbol{\theta}) \in \mathbb{R}^{n+1+m}$.
- We will want to see how \mathbf{r} evolves through time. We denote the \mathbf{r} at time t with $\mathbf{r}_t = (\mathbf{z}_t, t, \boldsymbol{\theta})$. Note that $\boldsymbol{\theta}$ does not vary with t .

- It also makes sense to talk about the function that sends t to \mathbf{r}_t . We denote this by $\mathbf{R} : \mathbb{R} \rightarrow \mathbb{R}^{n+1+m}$, and we can write

$$\mathbf{r}_t = \mathbf{R}(t) = (\mathbf{Z}(t), T(t), \boldsymbol{\Theta}(t)) = (\mathbf{z}_t, t, \boldsymbol{\theta}).$$

Note that T is the identity function, and $\boldsymbol{\Theta}$ is a constant function.

- The act of solving the neural ODE is a function that maps \mathbf{r}_t to some $\mathbf{r}_{t+\Delta t}$ for some $\Delta t \geq 0$. Let us denote this function by $\mathbf{s}_{\Delta t}^+ : \mathbb{R}^{n+1+m} \rightarrow \mathbb{R}^{n+1+m}$. (The letter \mathbf{s} stands for “solve.”) We have that

$$\mathbf{s}_{\Delta t}^+(\mathbf{z}_t, t, \boldsymbol{\theta}) = (\mathbf{z}_{t+\Delta t}, t, \boldsymbol{\theta}) = \begin{bmatrix} \mathbf{z}_{t+\Delta t} \\ t + \Delta t \\ \boldsymbol{\theta} \end{bmatrix} = \begin{bmatrix} \mathbf{z}_t + \int_t^{t+\Delta t} \mathbf{f}(\mathbf{z}_u, u, \boldsymbol{\theta}) du \\ t + \Delta t \\ \boldsymbol{\theta} \end{bmatrix}.$$

- The above function runs the ODE for a fixed time interval Δt . However, we can also talk about running the ODE until a fixed time t_1 . We denote this by

$$\mathbf{s}_{\rightarrow t_1}^+(\mathbf{z}_t, t, \boldsymbol{\theta}) = \mathbf{s}_{t_1-t}^+(\mathbf{z}_t, t, \boldsymbol{\theta}) = \begin{bmatrix} \mathbf{z}_t + \int_t^{t_1} \mathbf{f}(\mathbf{z}_u, u, \boldsymbol{\theta}) du \\ t + \Delta t \\ \boldsymbol{\theta} \end{bmatrix}.$$

- When optimizing a neural network, we need a loss function. In our case, the loss function is given by $L : \mathbb{R}^{n+1+m} \rightarrow \mathbb{R}$ that maps a state vector to a real number. When we write $L(\mathbf{r}) = L(\mathbf{z}, t, \boldsymbol{\theta})$, it is typical to say that the function only depends on \mathbf{z} , the produced hidden state. So,

$$L(\mathbf{r}) = L(\mathbf{z}, t, \boldsymbol{\theta}) = L(\mathbf{z}).$$

- When training a neural ODE, we start with the input state vector \mathbf{r}_t . We then solve the ODE to get the state \mathbf{r}_{t_1} . We then evaluate $L(\mathbf{r}_{t_1})$ to compute the loss. Let $\mathcal{L} : \mathbb{R}^{n+1+m} \rightarrow \mathbb{R}$ be the function that maps the input state to the final loss. This function is thus given by

$$\mathcal{L}(\mathbf{z}_t, t, \boldsymbol{\theta}) = L(\mathbf{s}_{\rightarrow t_1}^+(\mathbf{z}_t, t, \boldsymbol{\theta})).$$

- To train the neural network, we need the gradient

$$\nabla_{\S 3} \mathcal{L}(\mathbf{z}_{t_0}, t_0, \boldsymbol{\theta})$$

where t_0 is the time we designate for the input, typically 0. Here, we use the notations for multivariable derivatives from [Khu22] to avoid confusion. $\nabla_{\S 3} \mathcal{L}$ denotes the gradient with respect to the third block of arguments of \mathcal{L} , which is the network parameters $\boldsymbol{\theta}$.

2.2 Adjoint Sensitivity Method

- Define the **adjoint** to be the function $\mathbf{a} : \mathbb{R} \rightarrow \mathbb{R}^{1 \times (n+1+m)}$ such that

$$\mathbf{a} : t \mapsto \nabla \mathcal{L}(\mathbf{z}_t, t, \boldsymbol{\theta}).$$

In other words,

$$\mathbf{a}(t) = \mathcal{L}(\mathbf{R}(t)) = L(\mathbf{s}_{\rightarrow t_1}^+(\mathbf{R}(t)))$$

or $\mathbf{a} = \mathcal{L} \circ \mathbf{R} = L \circ \mathbf{s}_{\rightarrow t_1}^+ \circ \mathbf{R}$.

- With the adjoint function, our end goal is to evaluate

$$\mathbf{a}_{\S 3}(t_0) = \mathbf{a}(t_0)[\cdot, \S 3] = \nabla \mathcal{L}(\mathbf{z}_{t_0}, t_0, \boldsymbol{\theta})[\cdot, \S 3] = \nabla_{\S 3} \mathcal{L}(\mathbf{z}_{t_0}, t_0, \boldsymbol{\theta}).$$

- The adjoint sensitivity method relies on the fact that we can express $d\mathbf{a}/dt$ in terms for \mathbf{a} and \mathbf{f} .

Theorem 1. *We have that*

$$\frac{d\mathbf{a}(t)}{dt} = -\mathbf{a}(t) \begin{bmatrix} \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 2} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ \mathbf{0} & 0 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}$$

In particular,

$$\begin{aligned} \frac{d\mathbf{a}_{\S 1}(t)}{dt} &= -\mathbf{a}_{\S 1}(t) \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}), \\ \frac{d\mathbf{a}_{\S 3}(t)}{dt} &= -\mathbf{a}_{\S 1}(t) \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}). \end{aligned}$$

Proof. We have that

$$\frac{d\mathbf{a}(t)}{dt} = \lim_{\varepsilon \rightarrow 0} \frac{\mathbf{a}(t + \varepsilon) - \mathbf{a}(t)}{\varepsilon}.$$

To prove the theorem, we shall write $\mathbf{a}(t)$ in terms of $\mathbf{a}(t + \varepsilon)$.

Consider the function \mathcal{L} . We have that, for any $\varepsilon > 0$ such that $t + \varepsilon < t_1$,

$$\mathcal{L}(\mathbf{z}_t, t, \boldsymbol{\theta}) = \mathcal{L}(\mathbf{z}_{t+\varepsilon}, t + \varepsilon, \boldsymbol{\theta}).$$

This is because both $(\mathbf{z}_t, t, \boldsymbol{\theta})$ and $(\mathbf{z}_{t+\varepsilon}, t + \varepsilon, \boldsymbol{\theta})$ are on the trajectory to the final state vector $(\mathbf{z}_{t_1}, t_1, \boldsymbol{\theta})$. So, starting running the ODE from either points would lead to the same result. As a result, we may say that

$$\mathcal{L} = \mathcal{L} \circ \mathbf{s}_{\varepsilon}^+$$

if ε is small enough. Applying the chain rule, we have that

$$\begin{aligned} \nabla \mathcal{L}(\mathbf{z}_t, t, \boldsymbol{\theta}) &= \nabla \mathcal{L}(\mathbf{s}_{\varepsilon}^+(\mathbf{z}_t, t, \boldsymbol{\theta})) \nabla \mathbf{s}_{\varepsilon}^+(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ \nabla \mathcal{L}(\mathbf{z}_t, t, \boldsymbol{\theta}) &= \nabla \mathcal{L}(\mathbf{z}_{t+\varepsilon}, t + \varepsilon, \boldsymbol{\theta}) \nabla \mathbf{s}_{\varepsilon}^+(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ \mathbf{a}(t) &= \mathbf{a}(t + \varepsilon) \nabla \mathbf{s}_{\varepsilon}^+(\mathbf{z}_t, t, \boldsymbol{\theta}). \end{aligned}$$

Now,

$$\begin{aligned} \mathbf{s}_{\varepsilon}^+(\mathbf{z}_t, t, \boldsymbol{\theta}) &= \begin{bmatrix} \mathbf{z}_t + \int_t^{t+\varepsilon} \mathbf{f}(\mathbf{z}_u, u, \boldsymbol{\theta}) du \\ t + \varepsilon \\ \boldsymbol{\theta} \end{bmatrix} = \begin{bmatrix} \mathbf{z}_t + \varepsilon \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) + O(\varepsilon^2) \\ t + \varepsilon \\ \boldsymbol{\theta} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{z}_t \\ t \\ \boldsymbol{\theta} \end{bmatrix} + \varepsilon \begin{bmatrix} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ 1 \\ \mathbf{0} \end{bmatrix} + O(\varepsilon^2). \end{aligned}$$

So,

$$\nabla \mathbf{s}_{\varepsilon}^+(\mathbf{z}_t, t, \boldsymbol{\theta}) = I + \varepsilon \begin{bmatrix} \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 2} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ \mathbf{0} & 0 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} + O(\varepsilon^2).$$

This gives

$$\mathbf{a}(t) = \mathbf{a}(t + \varepsilon) + \varepsilon \mathbf{a}(t + \varepsilon) \begin{bmatrix} \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 2} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ \mathbf{0} & 0 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} + O(\varepsilon^2),$$

and so

$$\frac{\mathbf{a}(t + \varepsilon) - \mathbf{a}(t)}{\varepsilon} = -\mathbf{a}(t + \varepsilon) \begin{bmatrix} \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 2} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ \mathbf{0} & 0 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} + O(\varepsilon).$$

Taking the limit as $\varepsilon \rightarrow 0$, we have that

$$\frac{d\mathbf{a}(t)}{dt} = -\mathbf{a}(t) \begin{bmatrix} \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 2} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) & \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) \\ \mathbf{0} & 0 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}$$

as required. □

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- In a typical traning process, we start from $\mathbf{r}_{t_0} = (\mathbf{z}_{t_0}, t_0, \boldsymbol{\theta})$, and we solve the neural SDE forward in time to obtain $\mathbf{r}_{t_1} = (\mathbf{z}_{t_1}, t_1, \boldsymbol{\theta})$. We assume that we do not save any intermediate information in the forward solving process. Now, we need to compute the gradient $\mathbf{a}_{\S 3}(t_0) = \nabla_{\S 3} \mathcal{L}(\mathbf{z}_{t_0}, t_0, \boldsymbol{\theta})$.

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- The idea is then to start at time t_1 and jointly solve the following differential equations backward in time to t_0 :

$$\begin{aligned} \frac{d\mathbf{z}_t}{dt} &= \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}), \\ \frac{d\mathbf{a}_{\S 1}(t)}{dt} &= -\mathbf{a}_{\S 1}(t) \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}), \\ \frac{d\mathbf{a}_{\S 3}(t)}{dt} &= -\mathbf{a}_{\S 1}(t) \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}). \end{aligned}$$

In other words, we would like to compute the following integrals:

$$\begin{aligned} \mathbf{z}_{t_0} &= \mathbf{z}_{t_1} + \int_{t_1}^{t_0} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) dt, \\ \mathbf{a}_{\S 1}(t_0) &= \mathbf{a}_{\S 1}(t_1) - \int_{t_1}^{t_0} \mathbf{a}_{\S 1}(\mathbf{z}_t, t, \boldsymbol{\theta}) \nabla_{\S 1} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) dt, \\ \mathbf{a}_{\S 3}(t_0) &= \mathbf{a}_{\S 3}(t_1) - \int_{t_1}^{t_0} \mathbf{a}_{\S 1}(\mathbf{z}_t, t, \boldsymbol{\theta}) \nabla_{\S 3} \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}) dt. \end{aligned}$$

The initial conditions include \mathbf{z}_{t_1} , which we just computed using the forward process. The other initial conditions are:

$$\begin{aligned} a_{\S 1}(t_1) &= \nabla_{\S 1} \mathcal{L}(\mathbf{z}_{t_1}, t_1, \boldsymbol{\theta}) = \nabla_{\S 1} L(\mathbf{z}_{t_1}, t_1, \boldsymbol{\theta}) = \nabla L(\mathbf{z}_{t_1}), \\ a_{\S 3}(t_1) &= \nabla_{\S 3} \mathcal{L}(\mathbf{z}_{t_1}, t_1, \boldsymbol{\theta}) = \nabla_{\S 3} L(\mathbf{z}_{t_1}, t_1, \boldsymbol{\theta}) = \mathbf{0}. \end{aligned}$$

The last line follows from the fact that we assumed that L does not depend on $\boldsymbol{\theta}$. All of these values are easy to compute.

- To solve the ODEs, we can use any black-box ODE solver. The interface for such a solver requires us to provide (1) an initial state vector, and (2) a function that computes the time derivative of the state vector given the time and the state vector. `##### HEAD`

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`##### 59f7aea97bc71b38541aa8ae8fede48971e0efd5` Here, our state vector would be $\mathbf{q}^{(t)} \in \mathbb{R}^{n+n+m}$. It would be divided into three blocks $\mathbf{q}^{(t)} = (\mathbf{q}_{\S 1}^{(t)}, \mathbf{q}_{\S 2}^{(t)}, \mathbf{q}_{\S 3}^{(t)})$, and the blocks would correspond to \mathbf{z}_t , $\mathbf{a}_{\S 1}(t)^T$, and $\mathbf{a}_{\S 3}(t)^T$, respectively. The initial state vector would be

$$\mathbf{q}^{(t_1)} = \begin{bmatrix} \mathbf{z}_{t_1} \\ \nabla(L(\mathbf{z}_{t_1}))^T \\ \mathbf{0} \end{bmatrix}.$$

The derivative would be given by

$$\frac{d\mathbf{q}^{(t)}}{dt} = \begin{bmatrix} \mathbf{f}(\mathbf{q}_{\S 1}^{(t)}, t, \boldsymbol{\theta}) \\ -(\mathbf{q}_{\S 2}^{(t)})^T \nabla_{\S 1} \mathbf{f}(\mathbf{q}_{\S 1}^{(t)}, t, \boldsymbol{\theta}) \\ -(\mathbf{q}_{\S 2}^{(t)})^T \nabla_{\S 3} \mathbf{f}(\mathbf{q}_{\S 1}^{(t)}, t, \boldsymbol{\theta}) \end{bmatrix}.$$

Note that both $(\mathbf{q}_{\S 2}^{(t)})^T \nabla_{\S 1} \mathbf{f}(\mathbf{q}_{\S 1}^{(t)}, t, \boldsymbol{\theta})$ and $(\mathbf{q}_{\S 2}^{(t)})^T \nabla_{\S 3} \mathbf{f}(\mathbf{q}_{\S 1}^{(t)}, t, \boldsymbol{\theta})$ are both vector-Jacobian products (i.e., they are directional derivatives). They can thus be evaluated efficiently using automatic differentiation at the cost proportional to the evaluation of $\mathbf{f}(\mathbf{q}_{\S 1}^{(t)}, t, \boldsymbol{\theta})$.

- All in all, the adjoint sensitivity method allows us to compute the gradient without backpropagating through the operations of the forward solver. If we use forward-mode automatic differentiation, then the required memory is proportional to the size of the intermediate tensor vectors. There’s no dependence on the network’s depth at all. Hence, neural ODE is a very memory efficient architecture.

3 Continuous Normalizing Flows

- **Normalizing flows** refer to a body of techniques for modeling probability distributions that work by transforming a simple probability distribution (such as an isotropic Gaussian) to a more complicated one by compositing multiple simple transformations [KPB21].
- More concretely, we may start with $\mathbf{z}_0 \sim p(\mathbf{z}_0)$ where $p(\mathbf{z}_0)$ is simple. We can now make the probability distribution more complex by applying a bijective function \mathbf{g}_1 to get

$$\mathbf{z}_1 = \mathbf{g}_1(\mathbf{z}_0).$$

We have that

$$p(\mathbf{z}_1) = p(\mathbf{z}_0) |\det \nabla \mathbf{g}_1(\mathbf{z}_0)|^{-1}$$

or

$$\log p(\mathbf{z}_1) = \log p(\mathbf{z}_0) - \log |\det \nabla \mathbf{g}_1(\mathbf{z}_0)|.$$

- In most normalizing flow techniques, multiple transformations are used:

$$\mathbf{z}_k = (\mathbf{g}_k \circ \mathbf{g}_{k-1} \circ \cdots \circ \mathbf{g}_2 \circ \mathbf{g}_1)(\mathbf{z}_0) = \mathbf{g}_k(\mathbf{g}_{k-1}(\cdots \mathbf{g}_2(\mathbf{g}_1(\mathbf{z}_0)))) ,$$

which implies

$$\log p(\mathbf{z}_k) = \log p(\mathbf{z}_0) - \sum_{i=1}^k |\det \nabla \mathbf{g}_i(\mathbf{z}_{i-1})|. \quad (1)$$

This above expression allows us to (1) compute the probability, and (2) train the normalizing flow model with maximum likelihood.

- Normalizing flows can be casted into the neural ODE framework if we require that all transformations have the same form

$$\mathbf{z}_{t+1} = \mathbf{g}_{t+1}(\mathbf{z}_t) = \mathbf{z}_t + \mathbf{f}(\mathbf{z}_t, t, \boldsymbol{\theta}).$$

As usual, we take the limit as $t \leftarrow \infty$ to obtain

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{f}(\mathbf{z}, t, \boldsymbol{\theta}),$$

which gives us a continuous normalizing flow.

- To compute probability and to train our neural ODE model, we need an expression like (1). This is given by the following theorem.

Theorem 2 (Instantaneous change of variables). *Let $\mathbf{z}(t)$ be a finite continuous random variable with probability $p(\mathbf{z}(t))$ dependent on time. Let $d\mathbf{z}/dt = \mathbf{f}(\mathbf{z}(t), t)$ be a differential equation governing the value of \mathbf{z} . Assuming that \mathbf{f} is ununiformly Lipschitz continuous in \mathbf{z} and continuous in t . Then,*

$$\frac{d \log p(\mathbf{z}(t))}{dt} = -\text{tr}(\nabla_{\mathbf{z}} \mathbf{f}(\mathbf{z}(t), t)).$$

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