Carleton UNIVERSITY

Canada's Capital University

Neural ODEs

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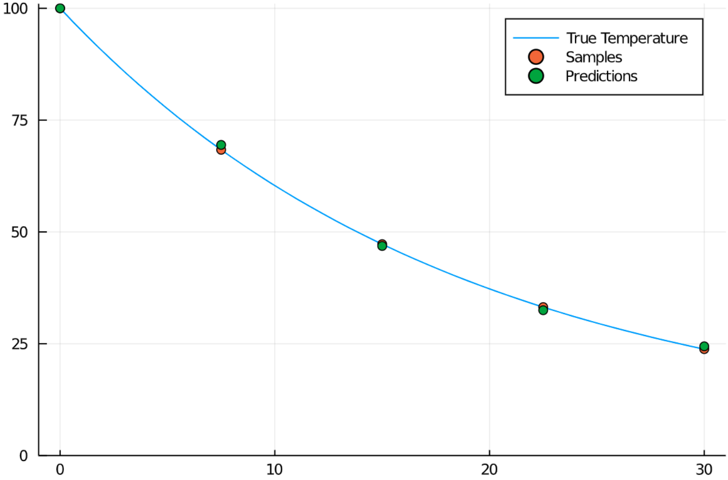
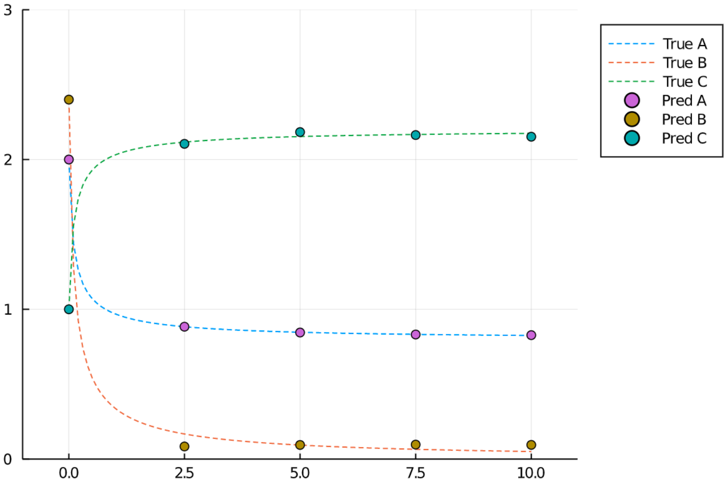
Some cool results

Newton’s Law of Cooling

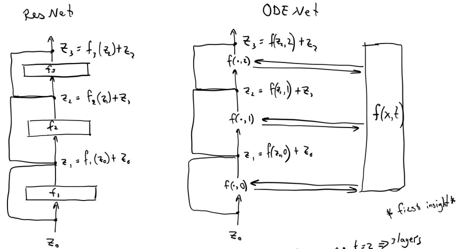


Chemical Reaction Rate Law



ML Part

Neural ODE Presentation



$F(z, \Theta)$ OR
$F(f_1, f_2, f_3, z, \Theta)$

e.g. $F(z_0, \Theta_0)$

num layers -1   e.g. $t_1 = 2 \Rightarrow 3$ layers

$F(z, t_1, \theta)$

OR $F(f, z, t_1, \theta)$

params θ

e.g. $F(f_\theta, z_0, 2, \theta_0)$

We can view z as a func. of t:

$$z(t)$$

then:

$$z_0 = z(0)$$
$$z_1 = z(1)$$
$$z_2 = z(2)$$
$$z_3 = z(3)$$

However, we don't "know" z, it's hidden.

Then we can write F as a cont. func. of t:

$z_0 = z(0)$ ⟵ we are given this as input

So that F is no longer a func. of z,
but we only need the input/'initial' value of z_0

$$F(f, z, t, \theta) = F(f, z(0), t, \theta)$$

ML Territory

Dynamical Systems Land

t_0 - "initial time"
implicitly zero for ns
before

t_1 - final time, "number of
layers" in some sense

$$\text{ODESolve}(z(0), f, t_0, t_1, \theta)$$

true output

our estimate

$$\underbrace{\hat{z}(t_1) \quad - \quad z(t_1)}_{\text{Loss}}$$

Problem: How to backprop through ODESolve? * second insight *

Dynamical Systems Part

Dynamical Systems (and ODEs)

Dynamical system is:

1) Some "state" that changes with time, e.g.

$$z(t)$$

2) Some "rule" for how that state changes:

$$\frac{dz}{dt} = f(\underset{\text{time}}{t}, \underset{\text{state}}{z}, \underset{\text{parameters}}{p})$$

Usually this is a system of ODEs
(ordinary diff. equations)

"Solution" to an ODE is a function

$$z(t)$$

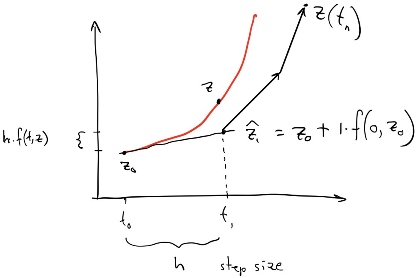
E.g. So we can find $z(5.5)$ directly, without the "rule" $\frac{dz}{dt}$.

Note: we are always given $z(0)$ – initial value
(important later)

Finding a solution to a dynamical system

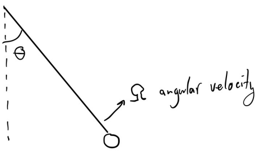
Given some dynamical system $f(t, z, p)$ with an initial condition z_0, find the solution $z(t)$.

Euler method: $z_{t+1} = z_t + h\, f(t, z_t)$



This way we can find $z(t)$ for any t.

Example : Pendulum




```
def pendulum(y, t, b, c):
    θ, Ω = y          ← state
    dydt = [Ω, -bΩ - c sin(θ)]
    return dydt
```

Assume

$b = 0.25$

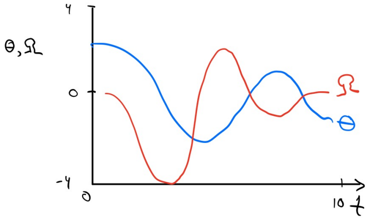
$c = 5.0$

```
y0 = [π-0.1, 0.0]
```
Initially pendulum is nearly vertical

```
t = np.linspace(0, 10, 101)
```
Solve for 101 points in $0 \le t \le 10$

```
from scipy.integrate import odeint
sol = odeint(pendulum, y0, t, args=(b, c))
```

Let's Plot sol[:,0], sol[:,1]



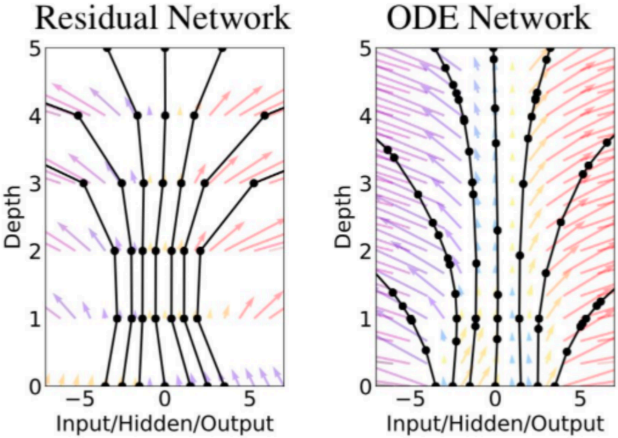
The solution

Adjoint method

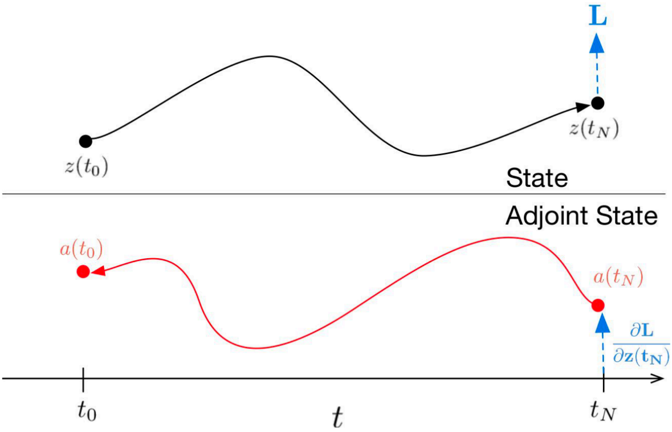
From ResNET to ODENet

Starting from the input $z(0)$ layer we can define output layer $z(T)$ to be the solution to an ODE initial value problem:

$$\frac{dz(t)}{dt} = f(z(t), t, \theta)$$



Backprop through ODE solver



Continuous time backprop

Continuous-time Backpropagation

Residual network. $a_t := \frac{\partial L}{\partial z_t}$

Forward: $z_{t+h} = z_t + hf(z_t)$

Backward: $a_t = a_{t+h} + ha_{t+h}\frac{\partial f(z_t)}{\partial z_t}$

Params: $\frac{\partial L}{\partial \theta} = ha_{t+h}\frac{\partial f(z(t),\theta)}{\partial \theta}$

Adjoint method. Define: $a(t) := \frac{\partial L}{\partial z(t)}$

Forward: $z(t+1) = z(t) + \int_t^{t+1} f(z(t))\,dt$

Backward: $\underbrace{a(t)}_{\text{adjoint state}} = a(t+1) + \int_{t+1}^{t} \underbrace{a(t)\frac{\partial f(z(t))}{\partial z(t)}}_{(1)?}dt$

Params: $\underbrace{\frac{\partial L}{\partial \theta}}_{(2)?} = \int_t^{t+1} a(t)\frac{\partial f(z(t),\theta)}{\partial \theta}\,dt$

We will show how to obtain adjoint differential equation (1) and gradients wr.t. θ (2) next!

Adjoint Method proof

Let $\mathbf{z}(t)$ follow the differential equation $\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), t, \theta)$, where θ are the parameters. We will prove that if we define an adjoint state

$$\mathbf{a}(t) = \frac{dL}{d\mathbf{z}(t)} \tag{34}$$

then it follows the differential equation

$$\frac{d\mathbf{a}(t)}{dt} = -\mathbf{a}(t)\frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)} \tag{35}$$

The adjoint state is the gradient with respect to the hidden state at a specified time t. In standard neural networks, the gradient of a hidden layer $\mathbf{h}_t$ depends on the gradient from the next layer $\mathbf{h}_{t+1}$ by chain rule

$$\frac{dL}{d\mathbf{h}_t} = \frac{dL}{d\mathbf{h}_{t+1}} \frac{d\mathbf{h}_{t+1}}{d\mathbf{h}_t}. \tag{36}$$

With a continuous hidden state, we can write the transformation after an ε change in time as

$$\mathbf{z}(t+\varepsilon) = \int_t^{t+\varepsilon} f(\mathbf{z}(t), t, \theta) dt + \mathbf{z}(t) = T_\varepsilon(\mathbf{z}(t), t) \tag{37}$$

and chain rule can also be applied

$$\frac{dL}{\partial \mathbf{z}(t)} = \frac{dL}{d\mathbf{z}(t+\varepsilon)} \frac{d\mathbf{z}(t+\varepsilon)}{d\mathbf{z}(t)} \qquad \text{or} \qquad \mathbf{a}(t) = \mathbf{a}(t+\varepsilon) \frac{\partial T_\varepsilon(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)} \tag{38}$$

The proof of (35) follows from the definition of derivative:

$$\frac{d\mathbf{a}(t)}{dt} = \lim_{\varepsilon \to 0^+} \frac{\mathbf{a}(t+\varepsilon) - \mathbf{a}(t)}{\varepsilon} \tag{39}$$

$$= \lim_{\varepsilon \to 0^+} \frac{\mathbf{a}(t+\varepsilon) - \mathbf{a}(t+\varepsilon)\frac{\partial}{\partial \mathbf{z}(t)} T_\varepsilon(\mathbf{z}(t))}{\varepsilon} \qquad \text{(by Eq 38)} \tag{40}$$

$$= \lim_{\varepsilon \to 0^+} \frac{\mathbf{a}(t+\varepsilon) - \mathbf{a}(t+\varepsilon)\frac{\partial}{\partial \mathbf{z}(t)} \left(\mathbf{z}(t) + \varepsilon f(\mathbf{z}(t), t, \theta) + \mathcal{O}(\varepsilon^2)\right)}{\varepsilon} \qquad \text{(Taylor series around } \mathbf{z}(t)\text{)} \tag{41}$$

$$= \lim_{\varepsilon \to 0^+} \frac{\mathbf{a}(t+\varepsilon) - \mathbf{a}(t+\varepsilon)\left(I + \varepsilon \frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)} + \mathcal{O}(\varepsilon^2)\right)}{\varepsilon} \tag{42}$$

$$= \lim_{\varepsilon \to 0^+} \frac{-\varepsilon \mathbf{a}(t+\varepsilon)\frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)} + \mathcal{O}(\varepsilon^2)}{\varepsilon} \tag{43}$$

$$= \lim_{\varepsilon \to 0^+} -\mathbf{a}(t+\varepsilon)\frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)} + \mathcal{O}(\varepsilon) \tag{44}$$

$$= -\mathbf{a}(t)\frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)} \tag{45}$$

Gradients w.r.t θ

We can generalize (35) to obtain gradients with respect to θ–a constant wrt. t–and and the initial and end times, t_0 and t_N. We view θ and t as states with constant differential equations and write

$$\frac{\partial \theta(t)}{\partial t} = \mathbf{0} \qquad \frac{dt(t)}{dt} = 1 \tag{47}$$

We can then combine these with z to form an augmented state[1] with corresponding differential equation and adjoint state,

$$\frac{d}{dt}\begin{bmatrix}\mathbf{z}\\ \theta\\ t\end{bmatrix}(t) = f_{aug}([\mathbf{z}, \theta, t]) := \begin{bmatrix} f([\mathbf{z}, \theta, t]) \\ \mathbf{0} \\ 1 \end{bmatrix},\ \mathbf{a}_{aug} := \begin{bmatrix}\mathbf{a}\\ \mathbf{a}_\theta \\ \mathbf{a}_t\end{bmatrix},\ \mathbf{a}_\theta(t) := \frac{dL}{d\theta(t)},\ \mathbf{a}_t(t) := \frac{dL}{dt(t)} \tag{48}$$

Note this formulates the augmented ODE as an autonomous (time-invariant) ODE, but the derivations in the previous section still hold as this is a special case of a time-variant ODE. The Jacobian of f has the form

$$\frac{\partial f_{aug}}{\partial[\mathbf{z}, \theta, t]} = \begin{bmatrix} \frac{\partial f}{\partial \mathbf{z}} & \frac{\partial f}{\partial \theta} & \frac{\partial f}{\partial t} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} (t) \tag{49}$$

where each $\mathbf{0}$ is a matrix of zeros with the appropriate dimensions. We plug this into (35) to obtain

$$\frac{d\mathbf{a}_{aug}(t)}{dt} = -\begin{bmatrix} \mathbf{a}(t) & \mathbf{a}_\theta(t) & \mathbf{a}_t(t) \end{bmatrix} \frac{\partial f_{aug}}{\partial[\mathbf{z}, \theta, t]}(t) = -\begin{bmatrix} \mathbf{a}\frac{\partial f}{\partial \mathbf{z}} & \mathbf{a}\frac{\partial f}{\partial \theta} & \mathbf{a}\frac{\partial f}{\partial t} \end{bmatrix}(t) \tag{50}$$

Full backprop algorithm

Algorithm 2 Complete reverse-mode derivative of an ODE initial value problem

Input: dynamics parameters θ, start time t_0, stop time t_1, final state $\mathbf{z}(t_1)$, loss gradient $\partial L / \partial \mathbf{z}(t_1)$

$\frac{\partial L}{\partial t_1} = \frac{\partial L}{\partial \mathbf{z}(t_1)}^{\mathsf{T}} f(\mathbf{z}(t_1), t_1, \theta)$ ▷ Compute gradient w.r.t. t_1

$s_0 = [\mathbf{z}(t_1), \frac{\partial L}{\partial \mathbf{z}(t_1)}, \mathbf{0}_{|\theta|}, -\frac{\partial L}{\partial t_1}]$ ▷ Define initial augmented state

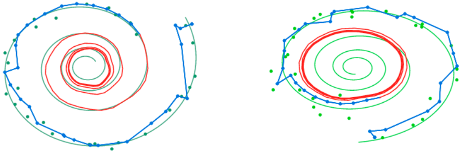
def aug_dynamics($[\mathbf{z}(t), \mathbf{a}(t), \cdot, \cdot], t, \theta$): ▷ Define dynamics on augmented state

  return $[f(\mathbf{z}(t), t, \theta), -\mathbf{a}(t)^{\mathsf{T}} \frac{\partial f}{\partial \mathbf{z}}, -\mathbf{a}(t)^{\mathsf{T}} \frac{\partial f}{\partial \theta}, -\mathbf{a}(t)^{\mathsf{T}} \frac{\partial f}{\partial t}]$ ▷ Compute vector-Jacobian products

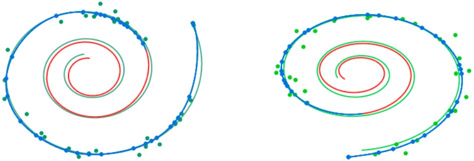
$[\mathbf{z}(t_0), \frac{\partial L}{\partial \mathbf{z}(t_0)}, \frac{\partial L}{\partial \theta}, \frac{\partial L}{\partial t_0}] = \text{ODESolve}(s_0, \text{aug\_dynamics}, t_1, t_0, \theta)$ ▷ Solve reverse-time ODE

return $\frac{\partial L}{\partial \mathbf{z}(t_0)}, \frac{\partial L}{\partial \theta}, \frac{\partial L}{\partial t_0}, \frac{\partial L}{\partial t_1}$ ▷ Return all gradients

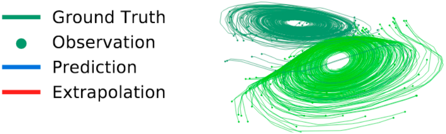
The End



(a) Recurrent Neural Network



(b) Latent Neural Ordinary Differential Equation



References

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