

1 Neural ODE

1.1 Adjoint Method

Let M a manifold, and $x(t) \in C^1(\mathbb{R}, M)$ a trajectory, obeying

$$\frac{dx}{dt}(t) = f(t, x(t); \theta),$$

and

$$x(t_0) = x_0,$$

where $f \in C(\mathbb{R} \times M, T_M)$ parameterized by θ . For $\forall t_1 > t_0$, let

$$x_1 := x_0 + \int_{t_0}^{t_1} f(t, x(t); \theta) dt.$$

Then

Theorem 1. Let $\mathcal{C} \in C^1(M, \mathbb{R})$, and $\forall x(t) \in C^1(\mathbb{R}, M)$ obeying dynamics $f(t, x; \theta) \in C^1(\mathbb{R} \times M, T_M)$ with initial value $x(t_0) = x_0$. Denote

$$L := \mathcal{C}\left(x_0 + \int_{t_0}^{t_1} f(\tau, x(\tau); \theta) d\tau\right).$$

Then we have, for $\forall t \in [t_0, t_1]$ given,

$$\frac{\partial L}{\partial x^\alpha(t)} = \frac{\partial L}{\partial x_1^\alpha} - \int_t^{t_1} \frac{\partial L}{\partial x^\beta(\tau)} \frac{\partial f^\beta}{\partial x^\alpha}(\tau, x(\tau); \theta) d\tau,$$

and

$$\frac{\partial L}{\partial \theta} = - \int_{t_0}^{t_1} \frac{\partial L}{\partial x^\beta(\tau)} \frac{\partial f^\beta}{\partial \theta}(\tau, x(\tau); \theta) d\tau.$$

Proof. Suppose the $x(t)$ is layerized, the L depends on the variables (inputs and model parameters) on the i th layer can be regarded as the loss of a new model by truncating the original at the i th layer, which we call $L_i(z_i)$.

$$\begin{aligned} \frac{\partial L_i}{\partial x_i^\alpha}(x_i) &= \frac{\partial L_{i+1}}{\partial x_{i+1}^\beta}(x_{i+1}) \frac{\partial x_{i+1}^\beta}{\partial x_i^\alpha}(x_i) \\ &= \frac{\partial L_{i+1}}{\partial x_1^\beta}(x_{i+1}) \frac{\partial}{\partial x_i^\alpha}(x_i^\beta + f^\beta(t_i, x_i; \theta) \Delta t) \\ &= \frac{\partial L_{i+1}}{\partial x_{i+1}^\alpha}(x_{i+1}) + \frac{\partial L_{i+1}}{\partial x_{i+1}^\beta}(x_{i+1}) \partial_\alpha f^\beta(t_i, x_i; \theta) \Delta t. \end{aligned}$$

This hints that

$$\frac{d}{dt} \frac{\partial L}{\partial x^\alpha(t)} = - \frac{\partial L}{\partial x^\beta(t)} \frac{\partial f^\beta}{\partial x^\alpha}(t, x(t); \theta).$$

The initial value is $\partial L / \partial x_1$. Thus

$$\frac{\partial L}{\partial x(t)} = \frac{\partial L}{\partial x_1} - \int_t^{t_1} \frac{\partial L}{\partial x^\beta(\tau)} \frac{\partial f^\beta}{\partial x^\alpha}(\tau, x(\tau); \theta) d\tau.$$

Varying θ will vary the $L_i(x_i)$ from two aspects, the effect from $\partial L_{i+1}/\partial\theta$ and the Δx_{i+1} caused by $\Delta\theta$.

$$\begin{aligned}\frac{\partial L_i}{\partial\theta}(x_i) &= \frac{\partial L_{i+1}}{\partial\theta}(x_{i+1}) + \frac{\partial L_{i+1}}{\partial x_{i+1}} \frac{\partial x_{i+1}}{\partial\theta} \\ &= \frac{\partial L_{i+1}}{\partial\theta}(x_{i+1}) + \frac{\partial L_{i+1}}{\partial x_{i+1}} \frac{\partial}{\partial\theta}(x_i^\beta + f^\beta(t_i, x_i; \theta)\Delta t) \\ &= \frac{\partial L_{i+1}}{\partial\theta}(x_{i+1}) + \frac{\partial L_{i+1}}{\partial x_{i+1}} \frac{\partial f^\beta}{\partial\theta}(t_i, x_i; \theta)\Delta t.\end{aligned}$$

This hints that

$$\frac{d}{dt} \frac{\partial L}{\partial\theta} = - \frac{\partial L}{\partial x^\alpha(t)} \frac{\partial f^\beta}{\partial\theta}(t, x(t), \theta).$$

The initial value is 0 since $\mathcal{C}(\cdot)$ is explicitly independent on θ . Thus

$$\frac{\partial L}{\partial\theta} = - \int_{t_0}^t \frac{\partial L}{\partial x^\beta(\tau)} \frac{\partial f^\beta}{\partial\theta}(\tau, x(\tau); \theta) d\tau. \quad \square$$

2 Hopfield Network

2.1 Discrete-time Hopfield Network

Definition 2. *[Discrete-time Hopfield Network]*

Let $t \in \mathbb{N}$ and $x \in \{-1, +1\}^d$, $W \in \mathbb{R}^d \times \mathbb{R}^d$ with $W_{\alpha\beta} = W_{\beta\alpha}$ and $W_{\alpha\alpha} = 0$, and $b \in \mathbb{R}^d$. Define discrete-time dynamics

$$x^\alpha(t+1) = \text{sign}(W_{\alpha\beta} x^\beta(t) + b^\alpha).$$

Lemma 3. Let (x, W, b) a discrete-time Hopfield network. Define $\mathcal{E}(x) := -(1/2)W_{\alpha\beta} x^\alpha x^\beta - b_\alpha x^\alpha$. Then $\mathcal{E}(x(t+1)) - \mathcal{E}(x(t)) \leq 0$.

Proof. Consider async-updation of Hopfield network, that is, change the component at dimension $\hat{\alpha}$, i.e. $x'_{\hat{\alpha}} = \text{sign}[W_{\hat{\alpha}\beta} x^\beta + b_{\hat{\alpha}}]$, then

$$\begin{aligned}\mathcal{E}(x') - \mathcal{E}(x) &= -\frac{1}{2}W_{\alpha\beta} x'^\alpha x'^\beta - b_\alpha x'^\alpha + \frac{1}{2}W_{\alpha\beta} x^\alpha x^\beta + b_\alpha x^\alpha \\ &= -2(x'^{\hat{\alpha}} - x^{\hat{\alpha}})(W_{\hat{\alpha}\beta} x^\beta + b_{\hat{\alpha}}),\end{aligned}$$

which employs conditions $W_{\alpha\beta} = W_{\beta\alpha}$ and $W_{\alpha\alpha} = 0$. Next, we prove that, combining with $x'_{\hat{\alpha}} = \text{sign}[W_{\hat{\alpha}\beta} x^\beta + b_{\hat{\alpha}}]$, this implies $\mathcal{E}(x') - \mathcal{E}(x) \leq 0$.

If $(x'^{\hat{\alpha}} - x^{\hat{\alpha}}) > 0$, then $x'^{\hat{\alpha}} = 1$ and $x^{\hat{\alpha}} = -1$. Since $x'_{\hat{\alpha}} = \text{sign}[W_{\hat{\alpha}\beta} x^\beta + b_{\hat{\alpha}}]$, $W_{\hat{\alpha}\beta} x^\beta + b_{\hat{\alpha}} > 0$. Then $\mathcal{E}(x') - \mathcal{E}(x) < 0$. Contrarily, if $(x'^{\hat{\alpha}} - x^{\hat{\alpha}}) < 0$, then $x'^{\hat{\alpha}} = -1$ and $x^{\hat{\alpha}} = 1$, implying $W_{\hat{\alpha}\beta} x^\beta + b_{\hat{\alpha}} < 0$. Also $\mathcal{E}(x') - \mathcal{E}(x) < 0$. Otherwise, $\mathcal{E}(x') - \mathcal{E}(x) = 0$. So, we conclude $\mathcal{E}(x') - \mathcal{E}(x) \leq 0$. \square

Theorem 4. Let (x, W, b) a discrete-time Hopfield network. Then $\exists t_\star < +\infty$, s.t. $x(t+1) = x(t)$.

Proof. Since the states of the network are finite, the \mathcal{E} is lower bounded. Thus $\exists t_\star < +\infty$, s.t. $x(t+1) = x(t)$. \square

2.2 Continuous-time Hopfield Network

Definition 5. *[Continuous-time Hopfield Network]*

Let $t \in \mathbb{N}$ and $x \in [-1, +1]^d$, $W \in \mathbb{R}^d \times \mathbb{R}^d$ with $W_{\alpha\beta} = W_{\beta\alpha}$, and $b \in \mathbb{R}^d$. Define dynamics

$$\tau \frac{dx^\alpha}{dt}(t) = -x^\alpha(t) + f(W_{\alpha\beta} x^\beta(t) + b^\alpha),$$

where τ a constant and $f: \mathbb{R} \rightarrow [-1, 1]$ being increasing. The $(x, W, b; \tau, f)$ is called a continuous-time Hopfield network.

Remark 6. With

$$\tau \frac{x^\alpha(t + \Delta t) - x^\alpha(t)}{\Delta t} = -x^\alpha(t) + f(W_{\alpha\beta} x^\beta(t) + b^\alpha).$$

Setting $\Delta t = \tau$ gives and $f(\cdot) = \text{sign}(\cdot)$ gives

$$x^\alpha(t + \tau) = \text{sign}(W_{\alpha\beta} x^\beta(t) + b^\alpha),$$

which is the same as the discrete-time Hopfield network.

Lemma 7. Let $(x, W, b; \tau, f)$ a continuous-time Hopfield network. Define $a^\alpha := W_{\alpha\beta} x^\beta + b^\alpha$ and $y^\alpha := f(a^\alpha)$, then

$$\mathcal{E}(y) := -\frac{1}{2} W_{\alpha\beta} y^\alpha y^\beta - b_\alpha y^\alpha + \sum_\alpha \int^{y^\alpha} f^{-1}(y^\alpha) dy^\alpha.$$

Then $\mathcal{E}(y(x(t + dt))) - \mathcal{E}(y(x(t))) \leq 0$.

Proof. The dynamics of a^α is

$$\begin{aligned} \tau \frac{da^\alpha}{dt} &= \tau W_{\alpha\beta} \frac{dx^\beta}{dt} \\ &= W_{\alpha\beta} [-x^\beta(t) + f(a^\beta)] \\ &= -(W_{\alpha\beta} x^\beta(t) + b^\alpha) + b^\alpha + W_{\alpha\beta} y^\beta \\ &= W_{\alpha\beta} y^\beta + b^\alpha - a^\alpha. \end{aligned}$$

Since W is symmetric, we have $\partial \mathcal{E} / \partial y^\alpha = -W_{\alpha\beta} y^\beta - b_\alpha + f^{-1}(y_\alpha)$. Then

$$\begin{aligned} \frac{d\mathcal{E}}{dt} &= \frac{dy^\alpha}{dt} (-W_{\alpha\beta} y^\beta - b_\alpha + f^{-1}(y_\alpha)) \\ &= \frac{dy^\alpha}{dt} (-W_{\alpha\beta} y^\beta - b_\alpha + a_\alpha) \\ &= -\frac{dy^\alpha}{dt} (W_{\alpha\beta} y^\beta + b_\alpha - a_\alpha) \end{aligned}$$

Notice that, the second term of rhs is exactly the dynamics of a_α , then

$$\begin{aligned} \frac{d\mathcal{E}}{dt} &= -\tau \frac{dy^\alpha}{dt} \frac{da_\alpha}{dt} \\ &= -\tau \frac{dy^\alpha}{da^\alpha} \left(\frac{da^\alpha}{dt} \frac{da_\alpha}{dt} \right) \\ &= -\tau f'(a^\alpha) \left(\frac{da^\alpha}{dt} \frac{da_\alpha}{dt} \right). \end{aligned}$$

Since f is increasing and $\tau > 0$, $d\mathcal{E}/dt \leq 0$. \square

Remark 8. The condition $W_{\alpha\alpha} = 0$ for $\forall \alpha$ is not essential for this lemma. Indeed, this condition is absent in the proof. This differs from the case of discrete-time.¹

Theorem 9. Let $(x, W, b; \tau, f)$ a continuous-time Hopfield network. Then for $\forall \epsilon > 0$, $\exists t_\star < +\infty$, s.t. $\|dx/dt\| < \epsilon$.

Proof. The function $E := \mathcal{E} \circ y$ is lower bounded since y , i.e. function $f: \mathbb{R} \rightarrow [-1, 1]$, is bounded. This E is a Lyapunov function for the continuous-time Hopfield network. \square

Corollary 10. Let $(x, W, b; \tau, f)$ a continuous-time Hopfield network. And $D := \{x_n | x_n \in \mathbb{R}^d, n = 1, \dots, N\}$ a dataset². If add constraint $W_{\alpha\alpha} = 0$ for $\forall \alpha$, then we can train the Hopfield network by seeking a proper parameters (W, b) , s.t. its stable point covers the dataset as much as possible, by³

Algorithm 1

Given $1 > \Delta t > 0$, and regularizer R ,
for step = 0, ..., S:
 for $x_n \in D$:
 $y(W, b) := x(t_0 + \Delta t; W, b)$ by solving the ODE of Hopfield network with IV $x(t_0) := x_n$
 loss(W, b) := $\|y(W, b) - x_n\|$
 update (W, b) by minimizing loss via gradient descent method.

Proof. For $\forall x_n \in D$, we try to find (W, b) , s.t. $dx/dt = 0$ at x_n , i.e.

$$x_n^\alpha = f(W_{\alpha\beta}^\alpha x_n^\beta + b^\alpha).$$

When $W_{\alpha\alpha} = 0$ for $\forall \alpha$, $f(W_{\alpha\beta}^\alpha x_n^\beta + b^\alpha)$ thus has no information of x_n^α , it has to predict the x_n^α by the interaction between x_n^α and the other x 's components. [...] \square

1. With experiments, we find that adding condition $W_{\alpha\alpha} = 0$ for $\forall \alpha$ significantly restricts the capacity of Hopfield network for learning, as well as its robustness.

2. We use Greek alphabet for component in \mathbb{R}^d and Latin alphabet for element in dataset.

3. This algorithm generalizes the algorithm 42.9 of Mackay. Directly using $y^\alpha(W, b) := f(W_{\alpha\beta}^\alpha x^\beta + b^\alpha)$ instead performs significantly worse than this approach. [Why?]