1 Hopfield Network

1.1 Discrete-time Hopfield Network

1.1.1 Definition

Definition 1. [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

$$x^{\alpha}(t+1) = \operatorname{sign}(W^{\alpha}{}_{\beta}x^{\beta}(t) + b^{\alpha}).$$

The (x, W, b) is called a discrete-time Hopfield network.

1.1.2 Convergence

Lemma 2. 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

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

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 $\mathcal{E}(x') - \mathcal{E}(x) \le 0$.

Theorem 3. [Convergene of Discrete-time Hopfield Network] Let (x, W, b) a discrete-time Hopfield network. Then any trajectory obeying the update rule will converge either to a fixed point or a limit circle.

Proof. Since the states of the network are finite, the \mathcal{E} is lower bounded.

1.2 Continuous-time Hopfield Network

1.2.1 Definition

Definition 4. [Continuous-time Hopfield Network]

Let $t \in [0, +\infty)$ 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

$$\tau \frac{\mathrm{d}x^{\alpha}}{\mathrm{d}t}(t) = -x^{\alpha}(t) + f(W^{\alpha}_{\beta} x^{\beta}(t) + b^{\alpha}),$$

where $\tau \in (0, +\infty)$ a constant and $f: \mathbb{R} \to [-1, 1]$ being increasing. The $(x, W, b; \tau, f)$ is called a continuous-time Hopfield network.

Remark 5. 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(.) = sign(.) gives

$$x^{\alpha}(t+\tau) = \operatorname{sign}(W^{\alpha}{}_{\beta}x^{\beta}(t) + b^{\alpha}),$$

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

1.2.2 Convergence

Lemma 6. Let $(x, W, b; \tau, f)$ a continous-time Hopfield network. Define $a^{\alpha} := W^{\alpha}_{\beta} x^{\beta} + b^{\alpha}$ and $y^{\alpha} := f(a^{\alpha})$, then

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

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

Proof. The dynamics of a^{α} is

$$\begin{split} \tau \frac{\mathrm{d} a^{\alpha}}{\mathrm{d} t} = & \tau W^{\alpha}{}_{\beta} \frac{\mathrm{d} x^{\beta}}{\mathrm{d} t} \\ = & W^{\alpha}{}_{\beta} [-x^{\beta}(t) + f(a^{\beta})] \\ = & -(W^{\alpha}{}_{\beta} x^{\beta}(t) + b^{\alpha}) + b^{\alpha} + W^{\alpha}{}_{\beta} y^{\beta} \\ = & W^{\alpha}{}_{\beta} y^{\beta} + b^{\alpha} - a^{\alpha}. \end{split}$$

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

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} = \frac{\mathrm{d}y^{\alpha}}{\mathrm{d}t} (-W_{\alpha\beta}y^{\beta} - b_{\alpha} + f^{-1}(y_{\alpha}))$$
$$= \frac{\mathrm{d}y^{\alpha}}{\mathrm{d}t} (-W_{\alpha\beta}y^{\beta} - b_{\alpha} + a_{\alpha})$$
$$= -\frac{\mathrm{d}y^{\alpha}}{\mathrm{d}t} (W_{\alpha\beta}y^{\beta} + b_{\alpha} - a_{\alpha})$$

Notice that, the second term of rhs is exactly the dynamics of a_{α} , then

$$\begin{split} \frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} &= -\tau \frac{\mathrm{d}y^{\alpha}}{\mathrm{d}t} \frac{\mathrm{d}a_{\alpha}}{\mathrm{d}t} \\ &= -\tau \frac{\mathrm{d}y^{\alpha}}{\mathrm{d}a^{\alpha}} \left(\frac{\mathrm{d}a^{\alpha}}{\mathrm{d}t} \frac{\mathrm{d}a_{\alpha}}{\mathrm{d}t} \right) \\ &= -\tau f'(a^{\alpha}) \left(\frac{\mathrm{d}a^{\alpha}}{\mathrm{d}t} \frac{\mathrm{d}a_{\alpha}}{\mathrm{d}t} \right). \end{split}$$

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

Remark 7. 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.

Theorem 8. [Convergene of Continuous-time Hopfield Network] Let $(x, W, b; \tau, f)$ a continuous-time Hopfield network. Then any trajectory along the dynamics will converge either to a fixed point or a limit circle.

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

1.2.3 Learning Rule

Corollary 9. Let $(x, W, b; \tau, f)$ a continous-time Hopfield network. And $D := \{x_n | x_n \in \mathbb{R}^d, n = 1, ..., N\}$ a dataset¹. If add constraint $W_{\alpha\alpha} = 0$ for $\forall \alpha$, then we can train the Hopfield nework by seeking a proper parameters (W, b), s.t. its stable points cover the dataset as much as possible, by²

Algorithm 1

```
W, b = init_W, init_b # e.g. by Glorot initializer
for step in range(max_step):
    for x in dataset:
        y = f(W @ x + b)
        loss = norm(x - y)
        optimizer.minimize(objective=loss, variables=(W, b))
        W = set_zero_diag(symmetrize(W))
```

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

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

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

Remark 10. This algorithm is equivalent to

Algorithm 2

```
dt = ... # e.g. 0.1
W, b = init_W, init_b
for step in range(max_step):
    for x in dataset:
        # that is, compute x(dt), with x(0) = x
        y = ode_solve(f=lambda t, x: -x + f(W @ x + b), t0=0, t1=dt, x0=x)
        loss = norm(x - y)
        optimizer.minimize(objective=loss, variables=(W, b))
        W = set_zero_diag(symmetrize(W))
```

Indeed, trying to reach y = x within a small interval will force x to be a fixed point.

1.2.4 Relation to Auto-encoder

Notice that at fixed point x_{\star} , $x_{\star}^{\alpha} = f(W_{\beta}^{\alpha} x_{\star}^{\beta} + b^{\alpha})$, which is a single-layer auto-encoder. The learning rule is also simply the learning rule of single-layer auto-encoder.

1.2.5 Stability of Fixed Points

We study the stability of fixed points. Let $z^{\alpha} := W^{\alpha}_{\beta} x^{\beta} + b^{\alpha}$. Jacobian

$$J^{\alpha}{}_{\beta} = \frac{\partial}{\partial x^{\beta}} (-x^{\alpha} + f(z^{\alpha}))$$
$$= -\delta^{\alpha}{}_{\beta} + f'(z^{\alpha})W^{\alpha}{}_{\beta}.$$

^{1.} We use Greek alphabet for component in \mathbb{R}^d and Lattin alphabet for element in dataset.

^{2.} This algorithm generalizes the algorithm 42.9 of Mackay.

If $f(x) = \tanh(x)$, and at fixed point,

$$\begin{split} J^{\alpha}{}_{\beta} = & -\delta^{\alpha}{}_{\beta} + \frac{1}{2}(1 - f^2(z^{\alpha}))W^{\alpha}{}_{\beta} \\ = & -\delta^{\alpha}{}_{\beta} + \frac{1}{2}(1 - x^{\alpha}_{\star})(1 + x^{\alpha}_{\star})W^{\alpha}{}_{\beta}. \end{split}$$

The eigen-value of J, $\lambda_J =: -1 + \lambda$, have

$$\det\!\left(\frac{1}{2}(1-x_\star^\alpha)(1+x_\star^\alpha)W^\alpha{}_\beta-\lambda\delta^\alpha{}_\beta\right)\!=\!0$$

For instance, if $x_{\star}^{\alpha} \to \pm 1$ for $\forall \alpha$, that is $\|x_{\star}^2 - 1\| \ll 1$, then, because of the linearity of this equation, we will have $\lambda \ll 1$. In this case, $\lambda_J \approx -1 < 0$, indicating the stability of the fixed point x_{\star} .

2 Variations

2.1 Dense Associative Memories

Theorem 11. Let $v \in \mathbb{R}^d$, $F \in C^1(\mathbb{R}^n, \mathbb{R})$, $W \in \mathbb{R}^n \times \mathbb{R}^d$, $b \in \mathbb{R}^n$, and $\tau > 0$. Define the dynamics

$$\tau \frac{\mathrm{d}x}{\mathrm{d}t} = -\nabla E(x) = -x + W^T \cdot \nabla F(W \cdot x + b) + v.$$

If $\nabla F(.)$ is bounded, i.e. $\exists K > 0$ s.t. $\max_{x \in \mathbb{R}^n} \{ \nabla F(x) \} < K$, then any trajectory along the dynamics will converge either to a fixed point or a limit circle.

Proof. Let $E(x) := \frac{1}{2} x_{\alpha} x^{\alpha} - v_{\alpha} x^{\alpha} - F(W^{\alpha}{}_{\beta} x^{\beta} + b^{\alpha})$, then $\tau dx/dt = -\nabla E(x)$. The -x term will dominate the $W^T \cdot \nabla F(W \cdot x + b)$ term for ||x|| > K||W||, thus converges. So E is a Lyapunov function of the dynamics.

Example 12. Let $F(x) := \sum_{\alpha} \int_{-\infty}^{x^{\alpha}} \sigma(s) ds$, where σ is sigmoid function. Then

$$\tau \frac{\mathrm{d}x}{\mathrm{d}t} = -x + W^T \cdot \sigma(W \cdot x + b) + v.$$

This coincides with the form in ref 1.

Example 13. Let $F(x) := \beta^{-1} \ln(\beta \sum_{\alpha} e^{x^{\alpha}}), b = 0$, and v = 0, then

$$\tau \frac{\mathrm{d}x}{\mathrm{d}t} = -x + W^T \cdot \mathrm{softmax}(\beta W \cdot x).$$

This coincides with the form in ref 2.

Example 14. Let $v_i := W_{i,\cdot}$, i.e. the *i*th row of the matrix W. Assume $||v_i|| = 1$ for $\forall i = 1, ..., n$. Let $F(x) := \beta^{-1} \ln(\beta \sum_{\alpha} e^{x^{\alpha}})$, and v = 0, then

$$\tau \frac{\mathrm{d}x^{\alpha}}{\mathrm{d}t} = -x^{\alpha} + \sum_{i} p_{i} v_{i}^{\alpha},$$

where $z_i := v_i \cdot x + b_i$ and then $p^i := \exp(\beta z^i) / \sum_j \exp(\beta z^j)$. The $\{(p_i, v_i) | i = 1, ..., n\}$ forms a categorical distribution.

Lemma 15. Assume example 14. The Jacobian of the dynamics is

$$J^{\alpha\beta}(x) = -\delta^{\alpha\beta} + \operatorname{Cov}_{p(x)}(v^{\alpha}, v^{\beta}),$$

where $Cov_p(\cdot,\cdot)$ denotes the covariance given distribution p.

Proof. Directly,

$$\begin{split} J^{\alpha\beta} &\equiv \frac{\partial}{\partial x_{\beta}} \bigg(-x^{\alpha} + \sum_{i} v_{i}^{\alpha} p_{i} \bigg) \\ &= -\delta^{\alpha\beta} + \sum_{i,j} v_{i}^{\alpha} \frac{\partial p_{i}}{\partial z^{j}} \frac{\partial z^{j}}{\partial x_{\beta}} \\ &= -\delta^{\alpha\beta} + \beta \sum_{i,j} v_{i}^{\alpha} v_{j}^{\beta} (p_{i} \delta_{i,j} - p_{i} p_{j}) \\ &= -\delta^{\alpha\beta} + \beta \sum_{i} p_{i} v_{i}^{\alpha} v_{i}^{\beta} - \beta \bigg(\sum_{i} p_{i} v_{i}^{\alpha} \bigg) \bigg(\sum_{j} p_{j} v_{j}^{\beta} \bigg) \\ &= -\delta^{\alpha\beta} + \beta \mathbb{E}(v^{\alpha} v^{\beta}) - \beta \mathbb{E}(v^{\alpha}) \mathbb{E}(v^{\beta}) \\ &= -\delta^{\alpha\beta} + \beta \text{Cov}_{v}(v^{\alpha}, v^{\beta}). \end{split}$$

And notice that the only variable that depends on x is p. So we insert x and gain the result. \square

For instance, at fixed point $x = v_1$, p = (1, 0, ..., 0). $Cov_{p(v_1)}(v^{\alpha}, v^{\beta}) = v_1^{\alpha}v_1^{\beta} - v_1^{\alpha}v_1^{\beta} = 0$. So $J^{\alpha\beta} = -\delta^{\alpha\beta}$ is negative defined, indicating that the fixed point is stable.

2.2 Cellular Automa

TODO

3 References

- 1. On autoencoder scoring.
- 2. Hopfield networks is All You Need.