

1 Energy-based Model

Definition 1. *[Energy-based Model]*

Let \mathcal{M} a measure space, and $E: \mathbb{R}^m \rightarrow (\mathcal{M} \rightarrow \mathbb{R})$. Then define probabilistic model based on E as

$$p_E(x; \theta) = \frac{\exp(-E(x; \theta))}{\int_{\mathcal{M}} dx' \exp(-E(x'; \theta))}, \quad (1)$$

where $\theta \in \mathbb{R}^m$ and $x \in \mathcal{M}$.

We call this an energy-based model, where $E(\cdot; \theta)$ is called a energy function parameterized by θ .

Theorem 2. *[Universality]*

For any probability density $q: \mathcal{M} \rightarrow \mathbb{R}$ and for $\forall C \in \mathbb{R}$, define, for $\forall x \in \text{supp}(q)$,

$$E_q(x) := -\ln q(x) + C, \quad (2)$$

then, for $\forall x \in \text{supp}(q)$,

$$q(x) = \frac{\exp(-E_q(x))}{\int_{\text{supp}(q)} dx' \exp(-E_q(x'))}. \quad (3)$$

That is, for any probability density, there exists an energy function (up to constant) that can describe the probability density.

Proof. Directly,

$$\begin{aligned} q(x) &= \frac{\exp(-E_q(x))}{\int_{\text{supp}(q)} dx' \exp(-E_q(x'))} \\ \{E_q := \dots\} &= \frac{q(x)}{\int_{\text{supp}(q)} dx' q(x')} \\ \left\{ \int_{\text{supp}(q)} dx' q(x') = 1 \right\} &= q(x). \end{aligned}$$

□

Theorem 3. *[Maximum Entropy Principle]*

For any probability density $p_D: \mathcal{M} \rightarrow \mathbb{R}$, we have

$$p_E(x) = \text{argmax}_p H[X], \quad (4)$$

s.t. constrains

$$\mathbb{E}_{x \sim p_D} \left[\frac{\partial E}{\partial \theta^\alpha}(x; \theta) \right] = \mathbb{E}_{x \sim p} \left[\frac{\partial E}{\partial \theta^\alpha}(x; \theta) \right] \quad (5)$$

are satisfied.

Theorem 4. *[Activity Rule]*

The local maximum of $p_E(\cdot; \theta)$ is the local minimum of $E(\cdot; \theta)$, and vice versa.

Theorem 5. *[Learning Rule]*

For any probability density $p_D: \mathcal{M} \rightarrow \mathbb{R}$, define Lagrangian $L(\theta; p_D) := -\int_{\mathcal{M}} dx p_D(x) \ln p_E(x; \theta)$. Then, the gradient of Lagrangian w.r.t. component θ^α is

$$\frac{\partial L}{\partial \theta^\alpha}(\theta; p_D) = \int_{\mathcal{M}} dx p_D(x) \frac{\partial E}{\partial \theta^\alpha}(x; \theta) - \int_{\mathcal{M}} dx p_E(x; \theta) \frac{\partial E}{\partial \theta^\alpha}(x; \theta), \quad (6)$$

or in more compact format,

$$\frac{\partial L}{\partial \theta^\alpha}(\theta; p_D) = \mathbb{E}_{x \sim p_D} \left[\frac{\partial E}{\partial \theta^\alpha}(x; \theta) \right] - \mathbb{E}_{x \sim p_E(x; \theta)} \left[\frac{\partial E}{\partial \theta^\alpha}(x; \theta) \right]. \quad (7)$$

2 Effective Theory

Definition 6. [Effective Energy]

Suppose exists $(\mathcal{V}, \mathcal{H})$, s.t. $\mathcal{M} = \mathcal{V} \oplus \mathcal{H}$. Re-denote $E(x; \theta) \rightarrow E(v, h; \theta)$ and $p_E(x; \theta) \rightarrow p_E(v, h; \theta)$. Then, define effective energy $E_{\text{eff}}: \mathcal{V} \rightarrow \mathbb{R}$ as

$$E_{\text{eff}}(v; \theta) := -\ln \int_{\mathcal{H}} dh \exp(-E(v, h; \theta)). \quad (8)$$

Theorem 7. [Effective Theory]

Recall that $p_{E_{\text{eff}}}(v; \theta) := \int_{\mathcal{H}} dh p(v, h; \theta)$. Then,

$$p_{E_{\text{eff}}}(v; \theta) = \frac{\exp(-E_{\text{eff}}(v; \theta))}{\int_{\mathcal{V}} dv' \exp(-E_{\text{eff}}(v'; \theta))}. \quad (9)$$

Lemma 8. [Gradient of Effective Energy]

$$\frac{\partial E_{\text{eff}}}{\partial \theta^\alpha}(v, \theta) = \int_{\mathcal{H}} dh p(h|v; \theta) \frac{\partial E}{\partial \theta^\alpha}(v, h; \theta). \quad (10)$$

Theorem 9. [Learning Rule of Effective Theory]

For any probability density $p_D: \mathcal{V} \rightarrow \mathbb{R}$, define Lagrangian $L(\theta; p_D) := -\int_{\mathcal{V}} dv p_D(v) \ln p(v; \theta)$. Then, the gradient of Lagrangian w.r.t. component θ^α is

$$\frac{\partial L}{\partial \theta^\alpha}(\theta; p_D) = \int_{\mathcal{V}} dv \int_{\mathcal{H}} dh p_D(v) p(h|v; \theta) \frac{\partial E}{\partial \theta^\alpha}(v, h; \theta) - \int_{\mathcal{V}} dv \int_{\mathcal{H}} dh p(v, h; \theta) \frac{\partial E}{\partial \theta^\alpha}(v, h; \theta),$$

or in more compact format,

$$\frac{\partial L}{\partial \theta^\alpha}(\theta; p_D) = \mathbb{E}_{v \sim p_D, h \sim p_E(h|v; \theta)} \left[\frac{\partial E}{\partial \theta^\alpha}(v, h; \theta) \right] - \mathbb{E}_{v, h \sim p_E(v, h; \theta)} \left[\frac{\partial E}{\partial \theta^\alpha}(v, h; \theta) \right]. \quad (11)$$

3 Examples

3.1 Boltzmann Machine

Definition 10. [Boltzmann Machine]

Let $\mathcal{M} = \{0, 1\}^n$, $W \in \mathbb{R}^{(n \times n)}$, $b \in \mathbb{R}^n$, $\theta := (W, b)$. Given dataset $D := \{x_i | x_i \in \mathcal{M}, i = 1, \dots, N\}$, denote expectation as \hat{x} . Then a Boltzmann machine is defined by energy function

$$E(x; W, b) := -\frac{1}{2} \sum_{\alpha, \beta} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) - \sum_{\alpha} b_{\alpha} x^{\alpha}. \quad (12)$$

Remark 11. [MaxEnt Principle of BM]

Relating to MaxEnt principle, the observable that the model simulates is

$$\forall (\alpha, \beta), \mathbb{E}_{x \sim P_D} [(x^\alpha - \hat{x}^\alpha)(x^\beta - \hat{x}^\beta)], \quad (13)$$

for which it shall also simulate

$$\forall \alpha, \mathbb{E}_{x \sim P_D} [\hat{x}^\alpha]. \quad (14)$$

Theorem 12. [Activity Rule of BM]

For $\forall \alpha$,

$$p_E(x_\alpha = 1 | x_{\setminus \alpha}) = \sigma \left(\sum_{\alpha \neq \beta} W_{(\alpha\beta)}(x^\beta - \hat{x}^\beta) + c_\alpha \right), \quad (15)$$

where $W_{(\alpha\beta)} := (W_{\alpha\beta} + W_{\beta\alpha})/2$ and $c_\alpha := b_\alpha + (1/2 - \hat{x}^\alpha)W_{\alpha\alpha}$. The sigmoid function $\sigma := 1/(1 + e^{-x})$. This relation is held for arbitrary replacement of the vector \hat{x} .

Proof. Directly, for $\forall \gamma$,

$$\begin{aligned} & \ln p(x_\gamma = 1 | x_{\setminus \gamma}) - \ln p(x_\gamma = 0 | x_{\setminus \gamma}) \\ [\alpha = \beta = \gamma] &= \frac{1}{2} W_{\gamma\gamma} (1 - \hat{x}^\gamma)^2 - \frac{1}{2} W_{\gamma\gamma} (-\hat{x}^\gamma)^2 \\ [\alpha \neq \gamma, \beta = \gamma] &+ \frac{1}{2} \sum_{\alpha \neq \gamma} W_{\alpha\gamma} (x^\alpha - \hat{x}^\alpha) (1 - \hat{x}^\gamma) - \frac{1}{2} \sum_{\alpha \neq \gamma} W_{\alpha\gamma} (x^\alpha - \hat{x}^\alpha) (-\hat{x}^\gamma) \\ [\alpha = \gamma, \beta \neq \gamma] &+ \frac{1}{2} \sum_{\beta \neq \gamma} W_{\gamma\beta} (1 - \hat{x}^\gamma) (x^\beta - \hat{x}^\beta) - \frac{1}{2} \sum_{\beta \neq \gamma} W_{\gamma\beta} (-\hat{x}^\gamma) (x^\beta - \hat{x}^\beta) \\ [\alpha, \beta \neq \gamma] &+ \frac{1}{2} \sum_{\alpha, \beta \neq \gamma} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) - \frac{1}{2} \sum_{\alpha, \beta \neq \gamma} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) \\ [\alpha = \gamma] &+ b^\gamma - 0 \\ [\alpha \neq \gamma] &+ \sum_{\alpha \neq \gamma} b_\gamma x^\gamma - \sum_{\alpha \neq \gamma} b_\gamma x^\gamma \\ &= \frac{1}{2} W_{\gamma\gamma} - W_{\gamma\gamma} \hat{x}^\gamma \\ &+ \frac{1}{2} \sum_{\alpha \neq \gamma} W_{\alpha\gamma} (x^\alpha - \hat{x}^\alpha) \\ &+ \frac{1}{2} \sum_{\beta \neq \gamma} W_{\gamma\beta} (x^\beta - \hat{x}^\beta) \\ &+ 0 \\ &+ b_\gamma \\ &+ 0 \\ &= \left(\frac{1}{2} - \hat{x}^\gamma \right) W_{\gamma\gamma} + \sum_{\alpha \neq \gamma} W_{(\gamma\alpha)} (x^\alpha - \hat{x}^\alpha) + b_\gamma \end{aligned}$$

Thus

$$p(x_\gamma = 1 | x_{\setminus \gamma}) = \sigma \left[\sum_{\alpha \neq \gamma} \frac{1}{2} (W_{\alpha\gamma} + W_{\gamma\alpha}) (x^\alpha - \hat{x}^\alpha) + \left(b_\gamma + \left(\frac{1}{2} - \hat{x}^\gamma \right) W_{\gamma\gamma} \right) \right]. \quad \square$$

3.2 Restricted Boltzmann Machine

Definition 13. [Restricted Boltzmann Machine]

Let $\mathcal{V} = \{0, 1\}^{m_1}$ and $\mathcal{H} = \{0, 1\}^{m_2}$, $\mathcal{M} = \mathcal{V} \times \mathcal{H}$. Let $U \in \mathbb{R}^{(m_1 \times m_2)}$, $b \in \mathbb{R}^{m_1}$, $c \in \mathbb{R}^{m_2}$. Then a restricted Boltzmann machine is defined by energy function¹

$$E(v, h; U, b, c) := - \sum_{\alpha, i} U_{\alpha i} (v^\alpha - \hat{v}^\alpha) (h^i - \hat{h}^i) - \sum_{\alpha} b_\alpha v^\alpha - \sum_i c_i h^i. \quad (16)$$

Remark 14. [Relation with Boltzmann machine]

¹. We use latin letters for latent variables.

By replacements in Boltzmann machine,

$$x \rightarrow (v, h), \quad (17)$$

$$b \rightarrow (b, c), \quad (18)$$

and

$$W \rightarrow \begin{pmatrix} 0 & U \\ U^T & 0 \end{pmatrix}, \quad (19)$$

we obtain the restricted Boltzmann machine.

Theorem 15. *[Activity Rule of RBM]*

We have

$$p(v_\alpha = 1 | v_{\setminus \alpha}, h_i) = \sigma \left(\sum_i U_{\alpha i} (h^i - \hat{h}^i) + b_\alpha \right), \quad (20)$$

and

$$p(h_i = 1 | v_\alpha, h_{\setminus i}) = \sigma \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) + c_i \right). \quad (21)$$

Theorem 16. *[Effective Energy of RBM]*

We have

$$E_{\text{eff}}(v; U, b, c) = \sum_\alpha \left(\sum_i U_{\alpha i} v^\alpha \hat{h}^i - b_\alpha v^\alpha \right) - \sum_i s \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) + c_i \right), \quad (22)$$

where soft-plus s is defined as

$$s(x) := \ln(1 + e^x). \quad (23)$$

Proof. Directly,

$$\begin{aligned} E_{\text{eff}}(v) &= -\ln \left(\prod_i \sum_{h^i=0,1} \right) \exp(-E(v, h)) \\ \{\text{Definition}\} &= -\ln \left(\prod_i \sum_{h^i=0,1} \right) \exp \left(\sum_{\alpha, i} U_{\alpha \beta} (v^\alpha - \hat{v}^\alpha) (h^i - \hat{h}^i) + \sum_\alpha b_\alpha v^\alpha + \sum_i c_i h^i \right) \\ \{\text{Extract } bv\} &= -\sum_\alpha b_\alpha v^\alpha - \ln \left(\prod_i \sum_{h^i=0,1} \right) \exp \left[\sum_{\alpha, i} U_{\alpha \beta} (v^\alpha - \hat{v}^\alpha) (h^i - \hat{h}^i) + \sum_i c_i h^i \right] \\ \{\text{Combine}\} &= -\sum_\alpha b_\alpha v^\alpha - \ln \left(\prod_i \sum_{h^i=0,1} \right) \exp \left[\sum_i \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) \right) (h^i - \hat{h}^i) + \sum_i c_i h^i \right] \\ \{\exp \sum = \prod \exp\} &= -\sum_\alpha b_\alpha v^\alpha - \ln \prod_i \left[\sum_{h^i=0,1} \exp \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) (h^i - \hat{h}^i) + c_i h^i \right) \right] \\ \{\ln \prod = \sum \ln\} &= -\sum_\alpha b_\alpha v^\alpha - \sum_i \ln \sum_{h^i=0,1} \exp \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) (h^i - \hat{h}^i) + c_i h^i \right). \end{aligned}$$

Since

$$\begin{aligned} & \sum_{h^i=0,1} \exp \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) (h^i - \hat{h}^i) + c_i h^i \right) \\ &= \exp \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) (1 - \hat{h}^i) + c_i \right) + \exp \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) (-\hat{h}^i) \right) \\ \{\text{Extract}\} &= \exp \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) (-\hat{h}^i) \right) \left[\exp \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) + c_i \right) + 1 \right], \end{aligned}$$

we have

$$\begin{aligned}
E_{\text{eff}}(v) & \\
\{\text{Previous}\} &= -\sum_{\alpha} b_{\alpha} v^{\alpha} - \sum_i \ln \sum_{h^i=0,1} \exp\left(\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha})(h^i - \hat{h}^i) + c_i h^i\right) \\
\{\text{Plugin}\} &= -\sum_{\alpha} b_{\alpha} v^{\alpha} + \sum_i \sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) \hat{h}^i \\
&\quad - \sum_i \ln \left[\exp\left(\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i\right) + 1 \right] \\
\{s(x) := \dots\} &= -\sum_{\alpha} b_{\alpha} v^{\alpha} + \sum_{\alpha, i} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) \hat{h}^i - \sum_i s\left(\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i\right) \\
\{\text{Extract Const}\} &= -\sum_{\alpha} b_{\alpha} v^{\alpha} + \sum_{\alpha, i} U_{\alpha i} v^{\alpha} \hat{h}^i - \sum_i s\left(\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i\right) + \text{Const} \\
\{\text{Combine}\} &= \sum_{\alpha} \left(\sum_i U_{\alpha i} v^{\alpha} \hat{h}^i - b_{\alpha} v^{\alpha} \right) - \sum_i s\left(\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i\right) + \text{Const}.
\end{aligned}$$

The constant, which will be eliminated by Z , can be omitted. \square

4 Perturbation Theory

4.1 Perturbation of Boltzmann Machine

Define $p_i(x)$ by Taylor expansion $p_E(x) = p_0(x) + p_1(x) + \dots + p_n(x) + \mathcal{O}(W^{n+1})$. Denote $\sigma_{\alpha} := \sigma(b_{\alpha})$.

4.1.1 0th-order

Lemma 17. [0th-order of Boltzmann Machine]

We have

$$p_0(x) = \prod_{\alpha} p_{\alpha}(x^{\alpha}), \quad (24)$$

where

$$p_{\alpha}(x) := \frac{\exp(b_{\alpha} x)}{1 + \exp(b_{\alpha})}. \quad (25)$$

Proof. Since $E_0(x; W, b) := -\sum_{\alpha} b_{\alpha} x^{\alpha}$,

$$\begin{aligned}
p_0(x) &= \frac{\exp(\sum_{\alpha} b_{\alpha} x^{\alpha})}{\sum_{x'^1 \in \{0,1\}} \dots \sum_{x'^n \in \{0,1\}} \exp(\sum_{\alpha} b_{\alpha} x'^{\alpha})} \\
\{\exp \sum = \prod \exp\} &= \prod_{\alpha} \frac{\exp(b_{\alpha} x^{\alpha})}{\sum_{x'^{\alpha} \in \{0,1\}} \exp(b_{\alpha} x'^{\alpha})} \\
&= \prod_{\alpha} \frac{\exp(b_{\alpha} x^{\alpha})}{1 + \exp(b_{\alpha})} \\
&= \prod_{\alpha} p_{\alpha}(x).
\end{aligned}$$

\square

Lemma 18. We have

$$\frac{\partial p_{\alpha}}{\partial b_{\alpha}}(x) = p_{\alpha}(x)(x - \sigma_{\alpha}). \quad (26)$$

Proof. Directly,

$$\begin{aligned}
\frac{\partial}{\partial b_\alpha} p_\alpha(x) &= \frac{\partial}{\partial b_\alpha} \frac{\exp(b_\alpha x)}{1 + \exp(b_\alpha)} \\
&= \frac{\exp(b_\alpha x)x}{1 + \exp(b_\alpha)} - \frac{\exp(b_\alpha x)[\exp(b_\alpha)]}{[1 + \exp(b_\alpha)]^2} \\
&= \frac{\exp(b_\alpha x)}{1 + \exp(b_\alpha)} \left[x - \frac{\exp(b_\alpha)}{1 + \exp(b_\alpha)} \right] \\
&= p_\alpha(x)(x - \sigma(b_\alpha)).
\end{aligned}$$

□

Lemma 19. For $\forall \alpha$, the mean of p_α $V^\alpha := \sum_x p_0(x) x^\alpha$ is

$$V^\alpha = \sigma^\alpha. \quad (27)$$

Proof. Since $(\partial p_\alpha / \partial b_\alpha)(x) = p_\alpha(x)(x - \sigma(b_\alpha))$,

$$\begin{aligned}
\sum_x \frac{\partial}{\partial b_\alpha} p_\alpha(x) &= \sum_x p_\alpha(x)x - \sum_x p_\alpha(x)\sigma(b_\alpha) \\
\frac{\partial}{\partial b_\alpha} \sum_x p_\alpha(x) &= \sum_x p_\alpha(x)x - \left(\sum_x p_\alpha(x) \right) \sigma(b_\alpha) \\
0 &= \sum_x p_\alpha(x)x - \sigma(b_\alpha).
\end{aligned}$$

□

Lemma 20. Variance $V^{\alpha_1 \alpha_2} := \sum_x p_0(x) (x - \sigma^{\alpha_1})(x - \sigma^{\alpha_2}) = \sum_x p_0(x) \prod_{i=1}^2 (x - \sigma^{\alpha_i})$ is

$$V^{\alpha_1 \alpha_2} = \delta^{\alpha_1 \alpha_2} \sigma^{\alpha_1} (1 - \sigma^{\alpha_1}). \quad (28)$$

Proof. Since $(\partial p_\alpha / \partial b_\alpha)(x) = p_\alpha(x)(x - \sigma(b_\alpha))$,

$$\begin{aligned}
\frac{\partial^2 p_0}{\partial b_\beta \partial b_\alpha}(x) &= \frac{\partial}{\partial b_\beta} [p_0(x)(x - \sigma^\alpha)] \\
&= p_0(x)(x - \sigma^\alpha)(x - \sigma^\beta) - \delta^{\alpha\beta} p_0(x) \sigma^\alpha (1 - \sigma^\alpha).
\end{aligned}$$

Thus,

$$\begin{aligned}
\sum_x \frac{\partial^2 p_0}{\partial b_\beta \partial b_\alpha}(x) &= \sum_x p_0(x)(x - \sigma^\alpha)(x - \sigma^\beta) - \sum_x \delta^{\alpha\beta} p_0(x) \sigma^\alpha (1 - \sigma^\alpha) \\
0 &= \sum_x p_0(x)(x - \sigma^\alpha)(x - \sigma^\beta) - \delta^{\alpha\beta} \sigma^\alpha (1 - \sigma^\alpha) \\
\sum_x p_0(x)(x - \sigma^\alpha)(x - \sigma^\beta) &= \delta^{\alpha\beta} \sigma^\alpha (1 - \sigma^\alpha).
\end{aligned}$$

□

Lemma 21. 3-momentum $V^{\alpha_1 \alpha_2 \alpha_3} := \sum_x p_0(x) \prod_{i=1}^3 (x - \sigma^{\alpha_i})$ is

$$V^{\alpha_1 \alpha_2 \alpha_3} = \delta^{\alpha_1 \alpha_2 \alpha_3} \sigma^{\alpha_1} (1 - \sigma^{\alpha_1}) (1 - 2\sigma^{\alpha_1}). \quad (29)$$

Lemma 22. 4-momentum $V^{\alpha_1 \dots \alpha_4} := \sum_x p_0(x) \prod_{i=1}^4 (x - \sigma^{\alpha_i})$ is

$$V^{\alpha_1 \dots \alpha_4} = V_c^{\alpha_1 \dots \alpha_4} + \sum_{\text{all pairs}} V^{\alpha_{m_1} \alpha_{m_2}} V^{\alpha_{n_1} \alpha_{n_2}}, \quad (30)$$

where “connected” part

$$V_c^{\alpha_1 \dots \alpha_4} := \delta^{\alpha_1 \dots \alpha_4} \sigma^{\alpha_1} (1 - \sigma^{\alpha_1}) [1 - 6\sigma^{\alpha_1} + 6(\sigma^{\alpha_1})^2], \quad (31)$$

and $(m_1, m_2), (n_1, n_2)$ runs over all (three) pairs.

4.1.2 1st-order

Lemma 23. For $\forall \alpha$,

$$\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W). \quad (32)$$

Proof. The gradient of loss gives

$$\begin{aligned} \sum_x p_D(x) x^\alpha &= \hat{x}^\alpha = \sum_x p_E(x) x^\alpha \\ \{\text{Taylor expand}\} &= \sum_x p_0(x) x^\alpha + \mathcal{O}(W) \\ \left\{ \sum_x p_0(x) x^\alpha = \sigma^\alpha \right\} &= \sigma^\alpha + \mathcal{O}(W). \end{aligned}$$

□

Theorem 24.

$$\frac{p_1(x)}{p_0(x)} = \frac{1}{2} W_{\alpha\beta} (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta}. \quad (33)$$

Proof. Directly,

$$\begin{aligned} p_E(x) &= \frac{\exp(b_\alpha x^\alpha + \frac{1}{2} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta))}{Z} \\ \{\text{Extract } b_\alpha x^\alpha\} &= \frac{\exp(b_\alpha x^\alpha) \exp(\frac{1}{2} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta))}{Z} \\ \{\text{Expand to } \mathcal{O}(W)\} &= \frac{\exp(b_\alpha x^\alpha) \{1 + \frac{1}{2} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) + \dots\}}{Z_0 (1 + Z_1 + \dots)} \\ \{p_0(x) = \dots\} &= p_0(x) \frac{\{1 + \frac{1}{2} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) + \dots\}}{1 + Z_1 + \dots} \\ \left\{ \frac{1}{1+\epsilon} \sim 1 - \epsilon \right\} &= p_0(x) \left\{ 1 + \frac{1}{2} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) + \dots \right\} \{1 - Z_1 + \dots\} \\ \{\text{Expand}\} &= p_0(x) \left\{ 1 + \frac{1}{2} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) - Z_1 + \dots \right\} \\ &=: p_0(x) + p_1(x) + \dots \end{aligned}$$

Thus

$$\begin{aligned} \frac{p_1(x)}{p_0(x)} &= \frac{1}{2} W_{\alpha\beta} (x^\alpha - \hat{x}^\alpha) (x^\beta - \hat{x}^\beta) - Z_1 \\ \{\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W)\} &= \frac{1}{2} W_{\alpha\beta} (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) - Z_1. \end{aligned}$$

Now we compute Z_1 . Since

$$\begin{aligned} 1 &= \sum_x p_E(x) = \sum_x p_0(x) \left\{ 1 + \frac{1}{2} W_{\alpha\beta} (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) - Z_1 \right\} \\ \left\{ \sum_x p_0(x) = 1 \right\} &= 1 + \frac{1}{2} W_{\alpha\beta} \left[\sum_x p_0(x) (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) \right] - Z_1 \\ \{V^{\alpha\beta} := \dots\} &= 1 + \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} - Z_1 \end{aligned}$$

we have

$$Z_1 = \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta}.$$

Then,

$$\begin{aligned} \frac{p_1(x)}{p_0(x)} &= \frac{1}{2} W_{\alpha\beta} (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) - Z_1 \\ \{Z_1 = \dots\} &= \frac{1}{2} W_{\alpha\beta} (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta}. \end{aligned}$$

□

Lemma 25. Up to $\mathcal{O}(W)$, for $\forall \gamma$,

$$\sum_x p_E(x) x^\gamma = V^\gamma + \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\gamma}. \quad (34)$$

Proof. Directly,

$$\begin{aligned} \sum_x p_E(x) x^\gamma &= \sum_x p_0(x) x^\gamma + \sum_x p_1(x) x^\gamma \\ \{p_1(x) = \dots\} &= \sum_x p_0(x) x^\gamma + \sum_x p_0(x) \left[\frac{1}{2} W_{\alpha\beta} (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) - \frac{1}{2} W_{\alpha\alpha} \sigma^\alpha (1 - \sigma^\alpha) \right] x^\gamma \\ \{\text{Expand}\} &= \sum_x p_0(x) x^\gamma \\ &\quad + \frac{1}{2} W_{\alpha\beta} \sum_x p_0(x) (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) x^\gamma \\ &\quad - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \sum_x p_0(x) x^\gamma \\ &= \sum_x p_0(x) x^\gamma \\ \{\text{Combine}\} &+ \frac{1}{2} W_{\alpha\beta} \sum_x p_0(x) (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) (x^\gamma - \sigma^\gamma) + \frac{1}{2} W_{\alpha\beta} \sum_x p_0(x) (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) \sigma^\gamma \\ &\quad - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \sum_x p_0(x) x^\gamma \\ &= V^\gamma \\ &\quad + \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\gamma} + \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \sigma^\gamma \\ \{V^\gamma = \sigma^\gamma\} &- \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \sigma^\gamma \\ &= V^\gamma + \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\gamma}. \end{aligned}$$

□

Lemma 26. Up to $\mathcal{O}(W)$, for $\forall (\mu, \nu)$,

$$\sum_x p_E(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) = V^{\mu\nu} + W_{(\alpha\beta)} V^{\alpha\mu} V^{\beta\nu} + \frac{1}{2} W_{\alpha\beta} V_c^{\alpha\beta\mu\nu}. \quad (35)$$

Proof. Directly,

$$\begin{aligned} \sum_x p_E(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) \\ \{p_E = p_0 + p_1\} &= \sum_x p_0(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) + \sum_x p_1(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) \\ &= \sum_x p_0(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) \\ \{p_1(x) = \dots\} &+ \sum_x p_0(x) \left[\frac{1}{2} W_{\alpha\beta} (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \right] (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) \\ &= \sum_x p_0(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) \\ \{\text{Expand}\} &+ \frac{1}{2} W_{\alpha\beta} \sum_x p_0(x) (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) \\ &\quad - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \sum_x p_0(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu) \end{aligned}$$

$$\begin{aligned}
\{\hat{x} = \dots\} &= \sum_x p_0(x) \left(x^\mu - \sigma^\mu - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\mu} \right) \left(x^\nu - \sigma^\nu - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\nu} \right) \\
\{\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W)\} &+ \frac{1}{2} W_{\alpha\beta} \sum_x p_0(x) (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) (x^\mu - \sigma^\mu) (x^\nu - \sigma^\nu) \\
\{\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W)\} &- \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \sum_x p_0(x) (x^\mu - \sigma^\mu) (x^\nu - \sigma^\nu) \\
[\text{Expand}] &= \sum_x p_0(x) (x^\mu - \sigma^\mu) (x^\nu - \sigma^\nu) \\
&- \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\nu} \sum_x p_0(x) (x^\mu - \sigma^\mu) \\
&- \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\mu} \sum_x p_0(x) (x^\nu - \sigma^\nu) \\
&+ \frac{1}{2} W_{\alpha\beta} \sum_x p_0(x) (x^\alpha - \sigma^\alpha) (x^\beta - \sigma^\beta) (x^\mu - \sigma^\mu) (x^\nu - \sigma^\nu) \\
&- \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} \sum_x p_0(x) (x^\mu - \sigma^\mu) (x^\nu - \sigma^\nu) \\
\{V^{\mu\nu} = \dots\} &= V^{\mu\nu} \\
\{\sigma^\mu = V^\mu = \dots\} &- 0 \\
\{\sigma^\nu = V^\nu = \dots\} &- 0 \\
\{V^{\alpha\beta\mu\nu} = \dots\} &+ \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\mu\nu} \\
\{V^{\mu\nu} = \dots\} &- \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} V^{\mu\nu} \\
&= V^{\mu\nu} \\
\{V^{\alpha\beta\mu\nu} = V_c^{\alpha\beta\mu\nu} + \dots\} &+ \frac{1}{2} W_{\alpha\beta} (V_c^{\alpha\beta\mu\nu} + V^{\alpha\beta} V^{\mu\nu} + V^{\alpha\mu} V^{\beta\nu} + V^{\alpha\nu} V^{\beta\mu}) \\
&- \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta} V^{\mu\nu} \\
&= V^{\mu\nu} + \frac{1}{2} W_{\alpha\beta} (V_c^{\alpha\beta\mu\nu} + V^{\alpha\mu} V^{\beta\nu} + V^{\alpha\nu} V^{\beta\mu}) \\
\{\text{Combine}\} &= V^{\mu\nu} + W_{(\alpha\beta)} V^{\alpha\mu} V^{\beta\nu} + \frac{1}{2} W_{\alpha\beta} V_c^{\alpha\beta\mu\nu}.
\end{aligned}$$

□

Theorem 27. *[Perturbation Solutions of BM]*

1. Define $\hat{c}^\mu := \sigma^{-1}(\hat{x}^\mu)$ and $\hat{C}^{\mu\nu} := \sum_x p_D(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu)$. Let W symmetric. By loss gradient, we have

$$\hat{x}^\alpha = \sum_x p_E(x) x^\alpha; \quad (36)$$

$$\hat{C}^{\mu\nu} = \sum_x p_E(x) (x^\mu - \hat{x}^\mu) (x^\nu - \hat{x}^\nu). \quad (37)$$

2. From these, we get, up to $\mathcal{O}(W)$, for $\forall \mu$,

$$\hat{C}^{\mu\mu} = \hat{x}^\mu (1 - \hat{x}^\mu) + \mathcal{O}(W^2), \quad (38)$$

$$b^\mu = \hat{c}^\mu - W_{\mu\mu} \left(\frac{1}{2} - \hat{x}^\mu \right); \quad (39)$$

and for $\forall \mu, \nu$ with $\mu \neq \nu$,

$$W_{\mu\nu} = \frac{\hat{C}^{\mu\nu}}{\hat{x}^\mu (1 - \hat{x}^\mu) \hat{x}^\nu (1 - \hat{x}^\nu)}. \quad (40)$$

Proof. Here we prove the second declaration.

When $\mu \neq \nu$, we have

$$\begin{aligned}\hat{C}^{\mu\nu} &= \sum_x p_E(x)(x^\mu - \hat{x}^\mu)(x^\nu - \hat{x}^\nu) \\ \{V^{\mu\nu} \propto \delta^{\mu\nu}\} &= W_{(\alpha\beta)} V^{\alpha\mu} V^{\beta\nu} \\ \{W \text{ symmetric}\} &= W_{\alpha\beta} V^{\alpha\mu} V^{\beta\nu} \\ \{V^{\alpha_1\alpha_2} = \delta^{\alpha_1\alpha_2} \sigma^{\alpha_1}(1 - \sigma^{\alpha_1})\} &= W_{\mu\nu} \sigma^\mu(1 - \sigma^\mu) \sigma^\nu(1 - \sigma^\nu) \\ \{\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W)\} &= W_{\mu\nu} \hat{x}^\mu(1 - \hat{x}^\mu) \hat{x}^\nu(1 - \hat{x}^\nu)\end{aligned}$$

thus, for $\forall \mu \neq \nu$,

$$W_{\mu\nu} = \frac{\hat{C}^{\mu\nu}}{\hat{x}^\mu(1 - \hat{x}^\mu) \hat{x}^\nu(1 - \hat{x}^\nu)}.$$

And for $\mu = \nu$,

$$\begin{aligned}\hat{C}^{\mu\mu} &= \sum_x p_E(x)(x^\mu - \hat{x}^\mu)(x^\mu - \hat{x}^\mu) \\ \{W_{\mu\nu} \text{ symmetric}\} &= V^{\mu\mu} + W_{\alpha\beta} V^{\alpha\mu} V^{\beta\mu} + \frac{1}{2} W_{\alpha\beta} V_c^{\alpha\beta\mu\mu} \\ &= \sigma^\mu(1 - \sigma^\mu) \\ &\quad + W_{\alpha\beta} \delta^{\alpha\mu} \delta^{\beta\mu} [\sigma^\mu(1 - \sigma^\mu)]^2 \\ &\quad + \frac{1}{2} W_{\alpha\beta} \delta^{\alpha\beta\mu\mu} \sigma^\mu(1 - \sigma^\mu) [1 - 6\sigma^\mu + 6(\sigma^\mu)^2] \\ &= \sigma^\mu(1 - \sigma^\mu) \\ &\quad + W_{\mu\mu} [\sigma^\mu(1 - \sigma^\mu)]^2 \\ &\quad + \frac{1}{2} W_{\mu\mu} \sigma^\mu(1 - \sigma^\mu) [1 - 6\sigma^\mu + 6(\sigma^\mu)^2] \\ \{\hat{x} = \sigma + \dots\} &= \left(\hat{x}^\mu - \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\mu} \right) \left(1 - \hat{x}^\mu + \frac{1}{2} W_{\alpha\beta} V^{\alpha\beta\mu} \right) \\ &\quad + W_{\mu\mu} [\sigma^\mu(1 - \sigma^\mu)]^2 \\ &\quad + \frac{1}{2} W_{\mu\mu} \sigma^\mu(1 - \sigma^\mu) [1 - 6\sigma^\mu + 6(\sigma^\mu)^2] \\ \{\text{Expand}\} &= \hat{x}^\mu(1 - \hat{x}^\mu) + W_{\alpha\beta} V^{\alpha\beta\mu} \left(\hat{x}^\mu - \frac{1}{2} \right) \\ &\quad + W_{\mu\mu} [\sigma^\mu(1 - \sigma^\mu)]^2 \\ &\quad + \frac{1}{2} W_{\mu\mu} \sigma^\mu(1 - \sigma^\mu) [1 - 6\sigma^\mu + 6(\sigma^\mu)^2] \\ \{V^{\alpha\beta\mu} = \dots\} &= \hat{x}^\mu(1 - \hat{x}^\mu) + W_{\mu\mu} \sigma^\mu(1 - \sigma^\mu)(1 - 2\sigma^\mu) \left(\hat{x}^\mu - \frac{1}{2} \right) \\ &\quad + W_{\mu\mu} [\sigma^\mu(1 - \sigma^\mu)]^2 \\ &\quad + \frac{1}{2} W_{\mu\mu} \sigma^\mu(1 - \sigma^\mu) [1 - 6\sigma^\mu + 6(\sigma^\mu)^2] \\ &= \hat{x}^\mu(1 - \hat{x}^\mu) + W_{\mu\mu} \hat{x}^\mu(1 - \hat{x}^\mu)(1 - 2\hat{x}^\mu) \left(\hat{x}^\mu - \frac{1}{2} \right) \\ [\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W)] &+ W_{\mu\mu} [\hat{x}^\mu(1 - \hat{x}^\mu)]^2 \\ [\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W)] &+ \frac{1}{2} W_{\mu\mu} \hat{x}^\mu(1 - \hat{x}^\mu) [1 - 6\hat{x}^\mu + 6(\hat{x}^\mu)^2] \\ \{\text{Combine}\} &= \hat{x}^\mu(1 - \hat{x}^\mu) \\ &\quad + W_{\mu\mu} \hat{x}^\mu(1 - \hat{x}^\mu) \times \\ &\quad \times \left\{ (1 - 2\hat{x}^\mu) \left(\hat{x}^\mu - \frac{1}{2} \right) + \hat{x}^\mu(1 - \hat{x}^\mu) + \frac{1}{2} [1 - 6\hat{x}^\mu + 6(\hat{x}^\mu)^2] \right\} \\ \{\text{Simplify}\} &= \hat{x}^\mu(1 - \hat{x}^\mu),\end{aligned}$$

Thus,

$$\hat{C}^{\mu\nu} = \hat{x}^\mu(1 - \hat{x}^\mu) + \mathcal{O}(W^2).$$

Finally, we have, for $\forall \mu$,

$$\begin{aligned}\hat{x}^\mu &= V^\mu + \frac{1}{2}W_{\alpha\beta}V^{\alpha\beta\mu} \\ &= \sigma^\mu + \frac{1}{2}W_{\alpha\beta}\delta^{\alpha\beta\mu}\sigma^\alpha(1-\sigma^\alpha)(1-2\sigma^\alpha) \\ &= \sigma^\mu + W_{\mu\mu}\sigma^\mu(1-\sigma^\mu)\left(\frac{1}{2}-\sigma^\mu\right). \\ \{\hat{x}^\alpha = \sigma^\alpha + \mathcal{O}(W)\} &= \sigma^\mu + W_{\mu\mu}\hat{x}^\mu(1-\hat{x}^\mu)\left(\frac{1}{2}-\hat{x}^\mu\right)\end{aligned}$$

Thus

$$\sigma^\mu = \hat{x}^\mu - W_{\mu\mu}\hat{x}^\mu(1-\hat{x}^\mu)\left(\frac{1}{2}-\hat{x}^\mu\right).$$

Since $\sigma^\mu := \sigma(b_\mu)$ and $\sigma'(\hat{c}^\mu) = \sigma(\hat{c}^\mu)(1-\sigma(\hat{c}^\mu)) = \hat{x}^\mu(1-\hat{x}^\mu)$, we have

$$\begin{aligned}\sigma(b_\mu) &= \sigma(\hat{c}^\mu) - \sigma'(\hat{c}^\mu)W_{\mu\mu}\left(\frac{1}{2}-\hat{x}^\mu\right) \\ &= \sigma\left(\hat{c}^\mu - W_{\mu\mu}\left(\frac{1}{2}-\hat{x}^\mu\right)\right) + \mathcal{O}(W^2).\end{aligned}$$

Thus

$$b_\mu = \hat{c}^\mu - W_{\mu\mu}\left(\frac{1}{2}-\hat{x}^\mu\right).$$

□

Corollary 28. *[Solution without Self-interaction]*

If set, for $\forall \mu$, $W_{\mu\mu} = 0$, then, up to $\mathcal{O}(W)$, we have the perurbation solution of Boltzmann machine as follow.

For $\forall \mu$,

$$b_\mu = \hat{c}^\mu, \tag{41}$$

and for $\forall \mu, \nu$ with $\mu \neq \nu$,

$$W_{\mu\nu} = \frac{\hat{C}^{\mu\nu}}{\hat{x}^\mu(1-\hat{x}^\mu)\hat{x}^\nu(1-\hat{x}^\nu)}. \tag{42}$$

Lemma 29. Let X^μ , $\mu = 1, \dots, N$ random variables. Then we have matrix

$$\frac{\text{Cov}(X^\mu, X^\nu)}{\text{Var}(X^\mu)\text{Var}(X^\nu)}$$

positive semi-definite.

Proof. Directly, define $Z^\mu := X^\mu / \text{Var}[X^\mu]$. Then, we have

$$\mathbb{E}[Z^\mu] = \frac{\mathbb{E}[X^\mu]}{\text{Var}[X^\mu]}.$$

Then,

$$\begin{aligned}\frac{\text{Cov}(X^\mu, X^\nu)}{\text{Var}(X^\mu)\text{Var}(X^\nu)} &= \frac{\mathbb{E}[(X^\mu - \mathbb{E}[X^\mu])(X^\nu - \mathbb{E}[X^\nu])]}{\text{Var}(X^\mu)\text{Var}(X^\nu)} \\ &= \mathbb{E}\left[\frac{(X^\mu - \mathbb{E}[X^\mu])}{\text{Var}(X^\mu)} \frac{(X^\nu - \mathbb{E}[X^\nu])}{\text{Var}(X^\nu)}\right] \\ &= \mathbb{E}[(Z^\mu - \mathbb{E}[Z^\mu])(Z^\nu - \mathbb{E}[Z^\nu])] \\ &= \text{Cov}(Z^\mu, Z^\nu),\end{aligned}$$

which, as a covariance matrix, is positive semi-definite. □

Corollary 30. *[Solution with Positive Semi-definiteness]*

1. If set, for $\forall \mu$,

$$W_{\mu\mu} = \frac{1}{\hat{x}^\mu(1-\hat{x}^\mu)}, \tag{43}$$

then $W_{\mu\nu}$ is positive semi-defined.

2. In this case, we find, for $\forall \mu$,

$$\sigma^\mu = 2\hat{x}^\mu - \frac{1}{2}. \quad (44)$$

In addition, we shall check whether $\sigma^\mu \in (0, 1)$ or not.

Proof. Here we prove the declarations one by one.

1. Directly,

$$W_{\mu\mu} = \frac{1}{\hat{x}^\mu(1-\hat{x}^\mu)}$$

$$\{\hat{C}^{\mu\nu} = \hat{x}^\mu(1-\hat{x}^\mu) + \mathcal{O}(W^2)\} = \frac{\hat{C}^{\mu\mu}}{[\hat{x}^\mu(1-\hat{x}^\mu)]^2}.$$

Together with $W_{\mu\neq\nu}$, we find, for $\forall(\mu, \nu)$,

$$W_{\mu\nu} = \frac{\text{Cov}[X^\mu, X^\nu]}{\text{Var}[X^\mu] \text{Var}[X^\nu]},$$

where we used $\text{Var}[X^\mu] = \hat{x}^\mu(1-\hat{x}^\mu)$. This is positive semi-definite.

2. In this case,

$$\begin{aligned} \sigma^\mu &= \hat{x}^\mu - W_{\mu\mu}\hat{x}^\mu(1-\hat{x}^\mu)\left(\frac{1}{2} - \hat{x}^\mu\right) \\ \{W_{\mu\mu} = \dots\} &= \hat{x}^\mu - \frac{1}{\hat{x}^\mu(1-\hat{x}^\mu)}\hat{x}^\mu(1-\hat{x}^\mu)\left(\frac{1}{2} - \hat{x}^\mu\right) \\ &= \hat{x}^\mu - \left(\frac{1}{2} - \hat{x}^\mu\right) \\ &= 2\hat{x}^\mu - \frac{1}{2}. \end{aligned}$$

3. Since perturbation demands

$$|\sigma^\mu - \hat{x}^\mu| \ll \hat{x}^\mu,$$

we get

$$|\sigma^\mu - \hat{x}^\mu| = \left| \hat{x}^\mu - \frac{1}{2} \right| \ll \hat{x}^\mu. \quad \square$$

4.2 Perturbation of Restricted Boltzmann Machine

Lemma 31. [Perturbation of RBM]

For $\forall i$, let $\hat{h}^i \equiv 1/2$ and $c_i \equiv 0$, then we have

$$E_{\text{eff}}(v; U, b, c) = -\frac{1}{2}W_{\alpha\beta}^{\text{eff}}(v^\alpha - \hat{v}^\alpha)(v^\beta - \hat{v}^\beta) - b_\alpha^{\text{eff}}v^\alpha + \mathcal{O}(U^3 + c^3), \quad (45)$$

where

$$W_{\alpha\beta}^{\text{eff}} := \frac{1}{4} \sum_i U_{\alpha i} U_{\beta i}, \quad (46)$$

and

$$b_\alpha^{\text{eff}} := b_\alpha - \sum_i U_{\alpha i} v^\alpha \left(\hat{h}^i - \frac{1}{2} - \frac{c_i}{4} \right). \quad (47)$$

That is, restricted Boltzmann machine reduces to a Boltzmann machine.

Proof. Recall that

$$E_{\text{eff}}(v; U, b, c) = \sum_\alpha \left(\sum_i U_{\alpha i} v^\alpha \hat{h}^i - b_\alpha v^\alpha \right) - \sum_i s \left(\sum_\alpha U_{\alpha i} (v^\alpha - \hat{v}^\alpha) + c_i \right), \quad (48)$$

where soft-plus s is defined as

$$s(x) := \ln(1 + e^x). \quad (49)$$

Taylor expansion of soft-plus is

$$s(x) = 0 + \frac{x}{2} + \frac{x^2}{8} + \mathcal{O}(x^3).$$

Thus

$$\begin{aligned} E_{\text{eff}}(v) &= \sum_{\alpha} \left(\sum_i U_{\alpha i} v^{\alpha} \hat{h}^i - b_{\alpha} v^{\alpha} \right) \\ \{\text{Taylor expand}\} &- \frac{1}{2} \sum_i \left[\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i \right] - \frac{1}{8} \sum_i \left[\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i \right]^2 \\ &+ \mathcal{O}(U^3 + c^3) \\ \{\text{Expand}\} &= \sum_{\alpha, i} U_{\alpha i} v^{\alpha} \hat{h}^i - \sum_{\alpha} b_{\alpha} v^{\alpha} \\ &- \frac{1}{2} \sum_{\alpha, i} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) - \frac{1}{2} \sum_i c_i \\ &- \frac{1}{8} \sum_{\alpha, \beta} \left(\sum_i U_{\alpha i} U_{\beta i} \right) (v^{\alpha} - \hat{v}^{\alpha})(v^{\beta} - \hat{v}^{\beta}) - \frac{1}{4} \sum_{\alpha, i} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) c_i - \frac{1}{8} \sum_i c_i^2 \\ &+ \mathcal{O}(U^3 + c^3) \\ \left[\propto \sum_{\alpha, i} U_{\alpha i} v^{\alpha} \right] &= \sum_{\alpha, i} U_{\alpha i} v^{\alpha} \left(\hat{h}^i - \frac{1}{2} - \frac{c_i}{4} \right) \\ &- \sum_{\alpha} b_{\alpha} v^{\alpha} \\ &- \frac{1}{8} \sum_{\alpha, \beta} \left(\sum_i U_{\alpha i} U_{\beta i} \right) (v^{\alpha} - \hat{v}^{\alpha})(v^{\beta} - \hat{v}^{\beta}) \\ [\text{Without } v] + \text{Const} &+ \mathcal{O}(U^3 + c^3) \\ &= -\frac{1}{2} \sum_{\alpha, \beta} \left[\frac{1}{4} \left(\sum_i U_{\alpha i} U_{\beta i} \right) \right] (v^{\alpha} - \hat{v}^{\alpha})(v^{\beta} - \hat{v}^{\beta}) \\ &- \sum_{\alpha} \left[b_{\alpha} - \sum_i U_{\alpha i} v^{\alpha} \left(\hat{h}^i - \frac{1}{2} - \frac{c_i}{4} \right) \right] v^{\alpha} \\ &+ \text{Const} \\ &+ \mathcal{O}(U^3 + c^3). \end{aligned}$$

Omitting the constant, which will be eliminated by Z , we have

$$E_{\text{eff}}(v) = -\frac{1}{2} W_{\alpha\beta}^{\text{eff}} (v^{\alpha} - \hat{v}^{\alpha})(v^{\beta} - \hat{v}^{\beta}) - b_{\alpha}^{\text{eff}} v^{\alpha} + \mathcal{O}(U^3), \quad (50)$$

where

$$b_{\alpha}^{\text{eff}} := b_{\alpha} - \sum_i U_{\alpha i} v^{\alpha} \left(\hat{h}^i - \frac{1}{2} - \frac{c_i}{4} \right),$$

and

$$W_{\alpha\beta}^{\text{eff}} := \frac{1}{4} \sum_i U_{\alpha i} U_{\beta i}. \quad (51) \quad \square$$

Theorem 32. *[Perturbation Equations of RBM]*

Up to $\mathcal{O}(U^2)$, we have, for $\forall \mu$,

$$b_{\mu} - \sum_i U_{\mu i} v^{\mu} \left(\hat{h}^i - \frac{1}{2} - \frac{c_i}{4} \right) = \hat{c}^{\mu} - \frac{1}{4} \sum_i U_{\mu i} U_{\mu i} \left(\frac{1}{2} - \hat{x}^{\mu} \right),$$

and for $\forall \mu, \nu$ with $\mu \neq \nu$,

$$\frac{1}{4} \sum_i U_{\mu i} U_{\nu i} = \frac{\hat{C}^{\mu\nu}}{\hat{x}^\mu(1-\hat{x}^\mu) \hat{x}^\nu(1-\hat{x}^\nu)}.$$

Remark 33. [Perturbation Solution of RBM]

1. This perturbation equations of RBM may not have a solution. Indeed, if $i = 1$ only, then $U_{\alpha i} \rightarrow U_{\alpha 1} =: u_\alpha$. We have, for $\forall \mu, \nu$ with $\mu \neq \nu$,

$$\frac{1}{4} u_\mu u_\nu = \frac{\hat{C}^{\mu\nu}}{\hat{x}^\mu(1-\hat{x}^\mu) \hat{x}^\nu(1-\hat{x}^\nu)}.$$

There are $n(n-1)/2$ equations but with n d.o.f.s, thus cannot be solved.

2. There is inner (gauge) symmetry. Indeed, if let $\hat{h}^i = 1/2$ and $c_i = 0$ for $\forall i = 1, \dots, m$, then for any orthogonal $m \times m$ matrix E , $U \rightarrow UE$ leaves the equations invariant.

4.3 Validation of Perturbations

Remark 34. [Validation of Perturbations 1]

Based on the dimension analysis, it's suspected that the condition of validation of perturbation solution in the corollary 28 is

$$W_{\mu\nu} = \frac{\text{Cov}(X^\mu, X^\nu)}{\text{Var}(X^\mu)\text{Var}(X^\nu)} \ll \frac{1}{\sqrt{\text{Var}(X^\mu)\text{Var}(X^\nu)}}. \quad (52)$$

That is, the Pearson coefficients is tiny: for $\forall \mu, \nu$ with $\mu \neq \nu$,

$$\frac{\text{Cov}(X^\mu, X^\nu)}{\sqrt{\text{Var}(X^\mu)\text{Var}(X^\nu)}} \ll 1 \quad (53)$$

Remark 35. [Validation of Perturbations 2]

For making the perturbation stated in corollary 30 valid, the dataset shall have the properties, for $\forall \alpha$,

$$\hat{x}^\alpha \approx 0.5 \quad (54)$$

and for $\forall \alpha, \beta$ with $\alpha \neq \beta$,

$$\hat{C}^{\alpha\beta} \approx 0. \quad (55)$$

Given a dataset of X^a , we construct a “soften version” of it, Y^a , s.t. this Y^a satisfies these properties.

Definition 36. [Zoom-in Trick]

Given Bernoulli random variable X , and a parameter $\delta \in [0, 0.5)$, we duplicate it to i.i.d. Bernoulli random variables Y_1, \dots, Y_m , s.t. for $\forall i$

$$p(y_i = 1 | x = 0) = \delta, \quad (56)$$

and

$$p(y_i = 1 | x = 1) = 1 - \delta. \quad (57)$$

Lemma 37. We have, for $\forall i$,

$$p(y_i = 1) = 0.5 + (2p - 1)(0.5 - \delta), \quad (58)$$

where $p := p(x = 1)$.

Theorem 38. [Zoom-in Trick]

Let $\epsilon := 0.5 - \delta > 0$. We have, for $\forall(\alpha, i)$,

$$\lim_{\epsilon \rightarrow 0} \hat{y}^{(\alpha, i)} = 0,$$

and for $\forall(\alpha, i), (\beta, j)$ with $(\alpha, i) \neq (\beta, j)$,

$$\lim_{\epsilon \rightarrow 0} \hat{C}^{(\alpha, i)(\beta, j)} = 0.$$

Specifically for the first limit, we have $\hat{y}^{(\alpha, i)} \sim \mathcal{N}(\mu, \sigma)$ where

$$\mu := 0.5 + (2\hat{x}^\alpha - 1)(0.5 - \delta), \quad (59)$$

and

$$\sigma := \sqrt{\frac{0.25 - [(2\hat{x}^\alpha - 1)(0.5 - \delta)]^2}{N}},$$

with N the data-size.

Proof. The first limit can be derived from the $\hat{y}^{(\alpha, i)} \sim \mathcal{N}(\mu, \sigma)$.

The second limit can be proved by considering the limit case, where $\delta \rightarrow 0.5$. In this situation, for $\forall(\alpha, i)$, $y^{(\alpha, i)} \sim \text{Bernoulli}(0.5)$. Thus all independent, leading to $\hat{C}^{(\alpha, i)(\beta, j)} = 0$. \square

Appendix A Perturbations by Temperature

Let $\beta := 1/T$. Then inserting temperature is replacements $U \rightarrow \beta U$, $b \rightarrow \beta b$, $c \rightarrow \beta c$, and $E_{\text{eff}}(v) \rightarrow -\beta^{-1} E_{\text{eff}}(v)$.

Thus,

$$\begin{aligned} E_{\text{eff}}(v; \beta) &= \sum_{\alpha} \left(\sum_i U_{\alpha i} v^{\alpha} \hat{h}^i - b_{\alpha} v^{\alpha} \right) - \beta^{-1} \sum_i s \left(\beta \sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + \beta c_i \right) \\ &= \sum_{\alpha} \left(\sum_i U_{\alpha i} v^{\alpha} \hat{h}^i - b_{\alpha} v^{\alpha} \right) \\ [\text{Taylor expand}] &- \frac{1}{2} \sum_i \left[\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i \right] - \frac{\beta}{8} \sum_i \left[\sum_{\alpha} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) + c_i \right]^2 + \mathcal{O}(\beta^2) \\ &= \sum_{\alpha, i} U_{\alpha i} v^{\alpha} \hat{h}^i - \sum_{\alpha} b_{\alpha} v^{\alpha} \\ &\quad - \frac{1}{2} \sum_{\alpha, i} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) \\ &\quad - \frac{\beta}{8} \sum_i \sum_{\alpha, \beta} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) U_{\beta i} (v^{\beta} - \hat{v}^{\beta}) - \frac{\beta}{4} \sum_{\alpha, i} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) c_i \\ &\quad + \text{Const} \\ &\quad + \mathcal{O}(\beta^2) \\ &= \sum_{\alpha, i} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) \left(\hat{h}^i - \frac{\beta}{4} c_i - \frac{1}{2} \right) \\ &\quad - \frac{\beta}{8} \sum_i \sum_{\alpha, \beta} U_{\alpha i} (v^{\alpha} - \hat{v}^{\alpha}) U_{\beta i} (v^{\beta} - \hat{v}^{\beta}) - \sum_{\alpha} b_{\alpha} v^{\alpha} \\ &\quad + \text{Const} \\ &\quad + \mathcal{O}(\beta^2). \end{aligned}$$

Let $\hat{h}^i \equiv 1/2$ and $c_i \equiv 0$ for $\forall i$, and omit the constant, then

$$E_{\text{eff}}(v; \beta) = - \sum_{\alpha, \beta} \left(\frac{\beta}{8} \sum_i U_{\alpha i} U_{\beta i} \right) (v^{\alpha} - \hat{v}^{\alpha}) (v^{\beta} - \hat{v}^{\beta}) - \sum_{\alpha} b_{\alpha} v^{\alpha} + \mathcal{O}(\beta^2). \quad (60)$$

Thus,

$$W_{\alpha\beta}^{\text{eff}} \rightarrow \frac{\beta}{8} \sum_i U_{\alpha i} U_{\beta i},$$

and

$$b_{\alpha}^{\text{eff}} \rightarrow b_{\alpha}. \tag{61}$$

$$\frac{p_1(x)}{p_0(x)} = \beta E(x) - \beta \sum_{\alpha} \left(\frac{W_{\alpha\alpha}}{4} + \frac{b_{\alpha}}{2} \right) + \mathcal{O}(\beta^2).$$