

A. Supplementary Materials for *Bidirectional Learning for Time-series Models with Hidden Units*

Here, we derive specific learning rules suggested by (27)-(28) as well as those with approximation with (29). These learning rule can be derived in a way similar to the learning rules (18)-(22) are derived from (17). We also provide some of the details, which are omitted in the derivation of (18)-(22).

The learning rules for \mathbf{U} and \mathbf{Z} are derived from (27)-(28) as follows:

$$\mathbf{U}^{[d]} \leftarrow \mathbf{U}^{[d]} + \eta \log p_{\theta}(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \alpha^{[s-1]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi})^{\top} \quad (32)$$

$$\mathbf{Z}^{[d]} \leftarrow \mathbf{Z}^{[d]} + \eta \log p_{\theta}(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \beta^{[s-1]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi})^{\top} \quad (33)$$

$$\mathbf{U}^{[\delta]} \leftarrow \mathbf{U}^{[\delta]} + \eta \log p_{\theta}(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \mathbf{x}^{[s-\delta]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi})^{\top} \quad (34)$$

$$\mathbf{Z}^{[\delta]} \leftarrow \mathbf{Z}^{[\delta]} + \eta \log p_{\theta}(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \mathbf{h}^{[s-\delta]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi})^{\top} \quad (35)$$

for $1 \leq \delta < d$, where $\langle \mathbf{H}^{[s]} \rangle_{\phi}$ denotes the expected values of $\mathbf{h}^{[s]}$ with respect to the conditional distribution given by the following p_{ϕ} :

$$p_{\phi}(\mathbf{h}^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) = \frac{1}{Z'} \exp(-E_{\phi}(\mathbf{h}^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]})) \quad (36)$$

for any binary vectors $\mathbf{h}^{[s]}$, where Z' is a normalization factor for the probabilities to sum up to one, and

$$E_{\phi}(\mathbf{h}^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) = - \sum_{\delta=1}^{d-1} (\mathbf{x}^{[s-\delta]})^{\top} \mathbf{U}^{[\delta]} \mathbf{h}^{[s]} - \sum_{\delta=1}^{d-1} (\mathbf{h}^{[s-\delta]})^{\top} \mathbf{Z}^{[\delta]} \mathbf{h}^{[s]} - (\alpha^{[s-1]})^{\top} \mathbf{U}^{[d]} \mathbf{h}^{[s]} - (\beta^{[s-1]})^{\top} \mathbf{Z}^{[d]} \mathbf{h}^{[s]}. \quad (37)$$

The energy in (37) can be decomposed into the energy associated with each hidden unit j as follows:

$$E_{\phi}(\mathbf{h}^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) = \sum_{j \in \mathcal{H}} E_{\phi,j}(h_j^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) \quad (38)$$

where \mathcal{H} denotes the set of hidden units, and

$$E_{\phi,j}(h_j^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) = - \sum_{\delta=1}^{d-1} (\mathbf{x}^{[s-\delta]})^{\top} \mathbf{U}_{:,j}^{[\delta]} h_j^{[s]} - \sum_{\delta=1}^{d-1} (\mathbf{h}^{[s-\delta]})^{\top} \mathbf{Z}_{:,j}^{[\delta]} h_j^{[s]} - (\alpha^{[s-1]})^{\top} \mathbf{U}_{:,j}^{[d]} h_j^{[s]} - (\beta^{[s-1]})^{\top} \mathbf{Z}_{:,j}^{[d]} h_j^{[s]}, \quad (39)$$

where $\mathbf{U}_{:,j}$ denotes a column vector corresponding to the j -th column of \mathbf{U} , and $\mathbf{Z}_{:,j}$ is defined analogously.

Then (36) can be expressed as

$$p_{\phi}(\mathbf{h}^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) = \prod_{j \in \mathcal{H}} p_{\phi,j}(h_j^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}), \quad (40)$$

where

$$p_{\phi,j}(h_j^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) = \frac{\exp(-E_{\phi,j}(h_j^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}))}{\exp(-E_{\phi,j}(h_j^{[s]} = 0 | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]})) + \exp(-E_{\phi,j}(h_j^{[s]} = 1 | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}))} \quad (41)$$

$$= \frac{\exp(-E_{\phi,j}(h_j^{[s]} | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}))}{1 + \exp(-E_{\phi,j}(h_j^{[s]} = 1 | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}))}. \quad (42)$$

The j -th element of $\langle \mathbf{H}^{[s]} \rangle_\phi$ is then given by

$$\langle H_j^{[s]} \rangle_\phi = p_{\phi,j}(h_j^{[s]} = 1 | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) \quad (43)$$

In (32)-(35), the value of $\langle \mathbf{H}^{[s]} \rangle_\phi$ is computed with the latest values of ϕ . Let $\phi^{[t-1]}$ be the value of ϕ immediately before step t . With the recursive computation of (29), the learning rules of (32)-(35) are approximated with the following learning rules:

$$\mathbf{U}^{[d]} \leftarrow \mathbf{U}^{[d]} + \eta(1 - \gamma) \log p_\theta(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \gamma^{t-1-s} \boldsymbol{\alpha}^{[s-1]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi^{[s-1]}})^\top \quad (44)$$

$$\mathbf{Z}^{[d]} \leftarrow \mathbf{Z}^{[d]} + \eta(1 - \gamma) \log p_\theta(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \gamma^{t-1-s} \boldsymbol{\beta}^{[s-1]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi^{[s-1]}})^\top \quad (45)$$

$$\mathbf{U}^{[\delta]} \leftarrow \mathbf{U}^{[\delta]} + \eta(1 - \gamma) \log p_\theta(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \gamma^{t-1-s} \mathbf{x}^{[s-\delta]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi^{[s-1]}})^\top \quad (46)$$

$$\mathbf{Z}^{[\delta]} \leftarrow \mathbf{Z}^{[\delta]} + \eta(1 - \gamma) \log p_\theta(\mathbf{x}^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) \sum_{s=\ell}^{t-1} \gamma^{t-1-s} \mathbf{h}^{[s-\delta]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi^{[s-1]}})^\top \quad (47)$$

for $1 \leq \delta < d$, where the quantity such as

$$G'_{t-1} \equiv \sum_{s=\ell}^{t-1} \gamma^{t-1-s} \boldsymbol{\alpha}^{[s-1]} (\mathbf{h}^{[s]} - \langle \mathbf{H}^{[s]} \rangle_{\phi^{[s-1]}})^\top \quad (48)$$

can be computed recursively as

$$G'_t \leftarrow \gamma G'_{t-1} + (1 - \gamma) \boldsymbol{\alpha}^{[t-1]} (\mathbf{h}^{[t]} - \langle \mathbf{H}^{[t]} \rangle_{\phi^{[t-1]}})^\top. \quad (49)$$

One may consider real-valued units as well (Dasgupta & Osogami, 2017; Osogami, 2016). For example, each of $x_i^{[t]}$ and $h_j^{[t]}$ may have a Gaussian distribution with the following density:

$$p_{\theta,i}(x_i^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{(x_i^{[t]} - E_{\theta,i}(x_i^{[t]} = 1 | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}))^2}{2\sigma_i^2}\right) \quad (50)$$

$$p_{\phi,j}(h_j^{[t]} | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}) = \frac{1}{\sqrt{2\pi\sigma_j^2}} \exp\left(-\frac{(h_j^{[t]} - E_{\phi,j}(h_j^{[t]} = 1 | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]}))^2}{2\sigma_j^2}\right), \quad (51)$$

where σ_i^2 and σ_j^2 are variance parameters, $E_{\phi,j}$ is given by (39), and $E_{\theta,i}(x_i^{[t]} = 1 | \mathbf{x}^{[<t]}, \mathbf{h}^{[<t]})$ is given by

$$E_{\theta,i}(x_i^{[s]} = 1 | \mathbf{x}^{[<s]}, \mathbf{h}^{[<s]}) = -b_i - \sum_{\delta=1}^{d-1} (\mathbf{x}^{[s-\delta]})^\top \mathbf{W}_{:,i}^{[\delta]} - \sum_{\delta=1}^{d-1} (\mathbf{h}^{[s-\delta]})^\top \mathbf{V}_{:,i}^{[\delta]} - (\boldsymbol{\alpha}^{[s-1]})^\top \mathbf{W}_{:,i}^{[d]} - (\boldsymbol{\beta}^{[s-1]})^\top \mathbf{V}_{:,i}^{[d]}. \quad (52)$$