Deep Temporal Sigmoid Belief Networks for Sequence Modeling: Supplementary Material

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A Outline of the NVIL algorithm

The outline of the NVIL algorithm for computing gradients are shown below (reproduced from [1]). $C_{\boldsymbol{\lambda}}(\boldsymbol{v}_t)$ represents the data-dependent baseline, and $\alpha = 0.8$ throughout the experiments.

Algorithm 1 Compute gradient estimates for the model parameters and recognition parameters.

$\Delta\boldsymbol{\theta} \leftarrow 0, \Delta\boldsymbol{\phi} \leftarrow 0, \Delta\boldsymbol{\lambda} \leftarrow 0$
$\mathcal{L} \leftarrow 0$
for $t \leftarrow 1$ **to** T **do**
  $\boldsymbol{h}_t \sim q_{\boldsymbol{\phi}}(\boldsymbol{h}_t|\boldsymbol{v}_t)$
  $l_t \leftarrow \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t, \boldsymbol{h}_t) - \log q_{\boldsymbol{\phi}}(\boldsymbol{h}_t|\boldsymbol{v}_t)$
  $\mathcal{L} \leftarrow \mathcal{L} + l_t$
  $l_t \leftarrow l_t - C_{\boldsymbol{\lambda}}(\boldsymbol{v}_t)$
end for
$c_b \leftarrow \text{mean}(l_1, \ldots, l_T)$
$v_b \leftarrow \text{variance}(l_1, \ldots, l_T)$
$c \leftarrow \alpha c + (1-\alpha) c_b$
$v \leftarrow \alpha v + (1-\alpha) v_b$
for $t \leftarrow 1$ **to** T **do**
  $l_t \leftarrow \frac{l_t - c}{\max(1, \sqrt{v})}$
  $\Delta\boldsymbol{\theta} \leftarrow \Delta\boldsymbol{\theta} + \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t, \boldsymbol{h}_t)$
  $\Delta\boldsymbol{\phi} \leftarrow \Delta\boldsymbol{\phi} + l_t \nabla_{\boldsymbol{\phi}} \log q_{\boldsymbol{\phi}}(\boldsymbol{h}_t|\boldsymbol{v}_t)$
  $\Delta\boldsymbol{\lambda} \leftarrow \Delta\boldsymbol{\lambda} + l_t \nabla_{\boldsymbol{\lambda}} C_{\boldsymbol{\lambda}}(\boldsymbol{v}_t)$
end for

B Learning and Inference Details on TSBN

For $t = 1, \ldots, T$, consider $\boldsymbol{v}_t \in \{0,1\}^M$, $\boldsymbol{h}_t \in \{0,1\}^J$, the model parameters $\boldsymbol{\theta}$ are specified as $\mathbf{W}_1 \in \mathbb{R}^{J\times J}$, $\mathbf{W}_2 \in \mathbb{R}^{M\times J}$, $\mathbf{W}_3 \in \mathbb{R}^{J\times M}$, $\mathbf{W}_4 \in \mathbb{R}^{M\times M}$, $\boldsymbol{b} \in \mathbb{R}^J$, and $\boldsymbol{c} \in \mathbb{R}^M$. The generative model is expressed as

$$p(h_{jt} = 1|\boldsymbol{h}_{t-1}, \boldsymbol{v}_{t-1}) = \sigma(\boldsymbol{w}_{1j}^\top \boldsymbol{h}_{t-1} + \boldsymbol{w}_{3j}^\top \boldsymbol{v}_{t-1} + b_j)\,, \tag{1}$$

$$p(v_{mt} = 1|\boldsymbol{h}_t, \boldsymbol{v}_{t-1}) = \sigma(\boldsymbol{w}_{2m}^\top \boldsymbol{h}_t + \boldsymbol{w}_{4m}^\top \boldsymbol{v}_{t-1} + c_m)\,, \tag{2}$$

The recognition model is expressed as

$$q(h_{jt} = 1|\boldsymbol{h}_{t-1}, \boldsymbol{v}_t, \boldsymbol{v}_{t-1}) = \sigma(\boldsymbol{u}_{1j}^\top \boldsymbol{h}_{t-1} + \boldsymbol{u}_{2j}^\top \boldsymbol{v}_t + \boldsymbol{u}_{3j}^\top \boldsymbol{v}_{t-1} + d_j)\,, \tag{3}$$

where the recognition parameters are specified as $\mathbf{U}_1 \in \mathbb{R}^{J\times J}$, $\mathbf{U}_2 \in \mathbb{R}^{J\times M}$, $\mathbf{U}_3 \in \mathbb{R}^{J\times M}$, and $\boldsymbol{d} \in \mathbb{R}^J$. $\boldsymbol{h}_0$ and $\boldsymbol{v}_0$, needed for $p(\boldsymbol{h}_1)$, $p(\boldsymbol{v}_1|\boldsymbol{h}_1)$ and $q(\boldsymbol{h}_1|\boldsymbol{v}_1)$, are defined as zero vectors, for conciseness.

In order to implement the NVIL algorithm described in [1], we need to calculate the lower bound and also the gradients. Specifically, we have the variational lower bound $\mathcal{L} = \sum_{t=1}^{T} \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{v})}[l_t]$, where l_t is expressed as

$$l_t = \sum_{j=1}^{J} \Big(\psi_{jt}^{(1)} h_{jt} - \log(1+\exp(\psi_{jt}^{(1)}))\Big) + \sum_{m=1}^{M} \Big(\psi_{mt}^{(2)} v_{mt} - \log(1+\exp(\psi_{mt}^{(2)}))\Big) \\ - \left[\sum_{j=1}^{J} \Big(\psi_{jt}^{(3)} h_{jt} - \log(1+\exp(\psi_{jt}^{(3)}))\Big)\right], \tag{4}$$

and we have defined

$$\psi_{jt}^{(1)} = \boldsymbol{w}_{1j}^\top \boldsymbol{h}_{t-1} + \boldsymbol{w}_{3j}^\top \boldsymbol{v}_{t-1} + b_j\,, \tag{5}$$

$$\psi_{mt}^{(2)} = \boldsymbol{w}_{2m}^\top \boldsymbol{h}_{t} + \boldsymbol{w}_{4m}^\top \boldsymbol{v}_{t-1} + c_m\,, \tag{6}$$

$$\psi_{jt}^{(3)} = \boldsymbol{u}_{1j}^\top \boldsymbol{h}_{t-1} + \boldsymbol{u}_{2j}^\top \boldsymbol{v}_{t} + \boldsymbol{u}_{3j}^\top \boldsymbol{v}_{t-1} + d_j\,. \tag{7}$$

By further defining

$$\chi_{jt}^{(1)} = h_{jt} - \sigma(\psi_{jt}^{(1)}), \quad \chi_{mt}^{(2)} = v_{mt} - \sigma(\psi_{mt}^{(2)}), \quad \chi_{jt}^{(3)} = h_{jt} - \sigma(\psi_{jt}^{(3)}), \tag{8}$$

The gradients for the model parameters $\boldsymbol{\theta}$ are expressed as

$$\frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{1jj'}} = \chi_{jt}^{(1)} h_{j't-1}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{3jm}} = \chi_{jt}^{(1)} v_{mt-1}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial b_j} = \chi_{jt}^{(1)}\,, \tag{9}$$

$$\frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{2mj}} = \chi_{mt}^{(2)} h_{jt}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{4mm'}} = \chi_{mt}^{(2)} v_{m't-1}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial c_m} = \chi_{mt}^{(2)}\,. \tag{10}$$

The gradients for the recognition parameters $\boldsymbol{\phi}$ are expressed as

$$\frac{\partial \log q_{\boldsymbol{\phi}}(\boldsymbol{h}_t|\boldsymbol{v}_t)}{\partial u_{1jj'}} = \chi_{jt}^{(3)} h_{j't-1}, \qquad \frac{\partial \log q_{\boldsymbol{\phi}}(\boldsymbol{h}_t|\boldsymbol{v}_t)}{\partial u_{2jm}} = \chi_{jt}^{(3)} v_{mt}\,, \tag{11}$$

$$\frac{\partial \log q_{\boldsymbol{\phi}}(\boldsymbol{h}_t|\boldsymbol{v}_t)}{\partial u_{3jm}} = \chi_{jt}^{(3)} v_{mt-1}, \qquad \frac{\partial \log q_{\boldsymbol{\phi}}(\boldsymbol{h}_t|\boldsymbol{v}_t)}{\partial d_j} = \chi_{jt}^{(3)}\,. \tag{12}$$

B.1 Modeling Real-valued Data

When modeling real-valued data, we substitute (2) with $p(\boldsymbol{v}_t|\boldsymbol{h}_t,\boldsymbol{v}_{t-1}) = \mathcal{N}(\boldsymbol{\mu}_t, \mathrm{diag}(\boldsymbol{\sigma}_t^2))$, where

$$\mu_{mt} = \boldsymbol{w}_{2m}^\top \boldsymbol{h}_t + \boldsymbol{w}_{4m}^\top \boldsymbol{v}_{t-1} + c_m, \quad \log \sigma_{mt} = (\boldsymbol{w}_{2m}')^\top \boldsymbol{h}_t + (\boldsymbol{w}_{4m}')^\top \boldsymbol{v}_{t-1} + c_m', \tag{13}$$

and we have $\mathbf{W}_2' \in \mathbb{R}^{M\times J}$ and $\mathbf{W}_4' \in \mathbb{R}^{M\times M}$. The recognition model remains the same as in (3). Let $\tau_{mt} = \log \sigma_{mt}$, we obtain

$$l_t = \sum_{j=1}^{J} \Big(\psi_{jt}^{(1)} h_{jt} - \log(1+\exp(\psi_{jt}^{(1)}))\Big) - \sum_{m=1}^{M} \left(\frac{1}{2}\log 2\pi + \tau_{mt} + \frac{(v_{mt}-\mu_{mt})^2}{2e^{2\tau_{mt}}}\right) \\ - \left[\sum_{j=1}^{J} \Big(\psi_{jt}^{(3)} h_{jt} - \log(1+\exp(\psi_{jt}^{(3)}))\Big)\right]. \tag{14}$$

All the gradient calculation remains the same as (9)-(12), except the following.

$$\frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{2mj}} = \chi_{mt}^{(4)} h_{jt}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{4mm'}} = \chi_{mt}^{(4)} v_{m't-1}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial c_m} = \chi_{mt}^{(4)}\,, \tag{15}$$

$$\frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{2mj}'} = \chi_{mt}^{(5)} h_{jt}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial w_{4mm'}'} = \chi_{mt}^{(5)} v_{m't-1}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial c_m'} = \chi_{mt}^{(5)}\,, \tag{16}$$

where we have defined

$$\chi_{mt}^{(4)} = \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial \mu_{mt}} = \frac{v_{mt}-\mu_{mt}}{e^{2\tau_{mt}}}, \quad \chi_{mt}^{(5)} = \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t,\boldsymbol{h}_t)}{\partial \tau_{mt}} = \frac{(v_{mt}-\mu_{mt})^2}{e^{2\tau_{mt}}} - 1\,. \tag{17}$$

B.2 Modeling Count Data

We also introduce an approach for modeling time-series data with count observations, by replacing (2) with $p(\boldsymbol{v}_t|\boldsymbol{h}_t, \boldsymbol{v}_{t-1}) = \prod_{m=1}^{M} y_{mt}^{v_{mt}}$, where

$$y_{mt} = \frac{\exp(\boldsymbol{w}_{2m}^\top \boldsymbol{h}_t + \boldsymbol{w}_{4m}^\top \boldsymbol{v}_{t-1} + c_m)}{\sum_{m'=1}^{M} \exp(\boldsymbol{w}_{2m'}^\top \boldsymbol{h}_t + \boldsymbol{w}_{4m'}^\top \boldsymbol{v}_{t-1} + c_{m'})} \,. \tag{18}$$

The recognition model still remains the same as in (3). The l_t now is expressed as

$$l_t = \sum_{j=1}^{J} \left(\psi_{jt}^{(1)} h_{jt} - \log(1 + \exp(\psi_{jt}^{(1)}))\right) + \sum_{m=1}^{M} \left(\psi_{mt}^{(2)} v_{mt} - v_{mt} \log \sum_{m'=1}^{M} \exp(\psi_{mt}^{(2)})\right) \tag{19}$$
$$- \left[\sum_{j=1}^{J} \left(\psi_{jt}^{(3)} h_{jt} - \log(1 + \exp(\psi_{jt}^{(3)}))\right)\right] .$$

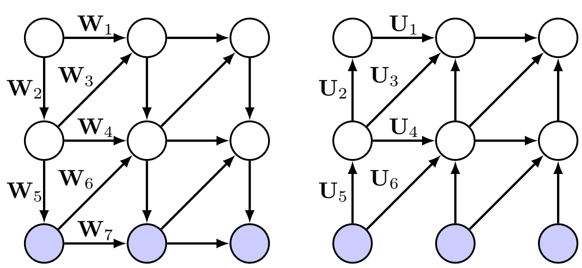
All the gradient calculations remain the same as (9)-(12), except the following

$$\frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t, \boldsymbol{h}_t)}{\partial w_{2mj}} = \chi_{mt}^{(6)} h_{jt}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t, \boldsymbol{h}_t)}{\partial w_{4mm'}} = \chi_{mt}^{(6)} v_{m't-1}, \quad \frac{\partial \log p_{\boldsymbol{\theta}}(\boldsymbol{v}_t, \boldsymbol{h}_t)}{\partial c_m} = \chi_{mt}^{(6)} . \tag{20}$$

where we have defined $\chi_{mt}^{(6)} = v_{mt} - y_{mt} \sum_{m'=1}^{M} v_{m't}$.

C Learning and Inference Details on Deep TSBN

For the ease of notation, we consider a two-hidden-layer deep TSBN here, which can be readily extended to a deep model with any depth. For $t = 1, \ldots, T$, we consider the observation as $\boldsymbol{v}_t \in \{0,1\}^M$. The top hidden layer is denoted as $\boldsymbol{z}_t \in \{0,1\}^J$.



(a) Generative model (b) Recognition model

Figure 1: Generative and recognition model of a two-layer Deep TSBN.

C.1 Using stochastic hidden layer

Denote the first stochastic hidden layer as $\boldsymbol{h}_t \in \{0,1\}^K$. The generative model is expressed as

$$p(z_{jt} = 1) = \sigma(\boldsymbol{w}_{1j}^\top \boldsymbol{z}_{t-1} + \boldsymbol{w}_{3j}^\top \boldsymbol{h}_{t-1} + b_{1j}) \,, \tag{21}$$
$$p(h_{kt} = 1) = \sigma(\boldsymbol{w}_{2k}^\top \boldsymbol{z}_t + \boldsymbol{w}_{4k}^\top \boldsymbol{h}_{t-1} + \boldsymbol{w}_{6k}^\top \boldsymbol{v}_{t-1} + b_{2k}) \,, \tag{22}$$
$$p(v_{mt} = 1) = \sigma(\boldsymbol{w}_{5m}^\top \boldsymbol{h}_t + \boldsymbol{w}_{7m}^\top \boldsymbol{v}_{t-1} + b_{3m}) \,, \tag{23}$$

where we have defined $\mathbf{W}_1 \in \mathbb{R}^{J\times J}$, $\mathbf{W}_2 \in \mathbb{R}^{K\times J}$, $\mathbf{W}_3 \in \mathbb{R}^{J\times K}$, $\mathbf{W}_4 \in \mathbb{R}^{K\times K}$, $\mathbf{W}_5 \in \mathbb{R}^{M\times K}$, $\mathbf{W}_6 \in \mathbb{R}^{K\times M}$, and $\mathbf{W}_7 \in \mathbb{R}^{M\times M}$. The bias terms are $\boldsymbol{b}_1 \in \mathbb{R}^{J\times 1}$, $\boldsymbol{b}_2 \in \mathbb{R}^{K\times 1}$ and $\boldsymbol{b}_3 \in \mathbb{R}^{M\times 1}$. The corresponding recognition model is expressed as

$$q(h_{kt} = 1) = \sigma(\boldsymbol{u}_{5k}^\top \boldsymbol{v}_t + \boldsymbol{u}_{4k}^\top \boldsymbol{h}_{t-1} + \boldsymbol{u}_{6k}^\top \boldsymbol{v}_{t-1} + c_{2k}) \tag{24}$$
$$q(\boldsymbol{z}_{jt} = 1) = \sigma(\boldsymbol{u}_{2j}^\top \boldsymbol{h}_t + \boldsymbol{u}_{1j}^\top \boldsymbol{z}_{t-1} + \boldsymbol{u}_{3j}^\top \boldsymbol{h}_{t-1} + c_{1j}) \tag{25}$$

where the recognition parameters are specified as $\mathbf{U}_1 \in \mathbb{R}^{J\times J}$, $\mathbf{U}_2 \in \mathbb{R}^{J\times K}$, $\mathbf{U}_3 \in \mathbb{R}^{J\times K}$, $\mathbf{U}_4 \in \mathbb{R}^{K\times K}$, $\mathbf{U}_5 \in \mathbb{R}^{K\times M}$ and $\mathbf{U}_6 \in \mathbb{R}^{K\times M}$. The bias terms are $\boldsymbol{c}_1 \in \mathbb{R}^{J\times 1}$ and $\boldsymbol{c}_2 \in \mathbb{R}^{K\times 1}$. Now, l_t is expressed as

$$
\begin{aligned}
l_t = & \sum_{j=1}^{J}\left(\psi_{jt}^{(1)} z_{jt} - \log(1+\exp(\psi_{jt}^{(1)}))\right) + \sum_{k=1}^{K}\left(\psi_{kt}^{(2)} h_{kt} - \log(1+\exp(\psi_{kt}^{(2)}))\right) \\
& + \sum_{m=1}^{M}\left(\psi_{mt}^{(3)} v_{mt} - \log(1+\exp(\psi_{mt}^{(3)}))\right) \\
& - \left[\sum_{k=1}^{K}\left(\psi_{kt}^{(4)} h_{kt} - \log(1+\exp(\psi_{kt}^{(4)}))\right) + \sum_{j=1}^{J}\left(\psi_{jt}^{(5)} z_{jt} - \log(1+\exp(\psi_{jt}^{(5)}))\right)\right] ,
\end{aligned}
\tag{26}
$$

and we have defined

$$
\begin{aligned}
\psi_{jt}^{(1)} &= \boldsymbol{w}_{1j}^{\top}\boldsymbol{z}_{t-1} + \boldsymbol{w}_{3j}^{\top}\boldsymbol{h}_{t-1} + b_{1j} \,, && (27)\\
\psi_{kt}^{(2)} &= \boldsymbol{w}_{2k}^{\top}\boldsymbol{z}_{t} + \boldsymbol{w}_{4k}^{\top}\boldsymbol{h}_{t-1} + \boldsymbol{w}_{6k}^{\top}\boldsymbol{v}_{t-1} + b_{2k} \,, && (28)\\
\psi_{mt}^{(3)} &= \boldsymbol{w}_{5m}^{\top}\boldsymbol{h}_{t} + \boldsymbol{w}_{7m}^{\top}\boldsymbol{v}_{t-1} + b_{3m} \,, && (29)\\
\psi_{kt}^{(4)} &= \boldsymbol{u}_{5k}^{\top}\boldsymbol{v}_{t} + \boldsymbol{u}_{4k}^{\top}\boldsymbol{h}_{t-1} + \boldsymbol{u}_{6k}^{\top}\boldsymbol{v}_{t-1} + c_{2k} \,, && (30)\\
\psi_{jt}^{(3)} &= \boldsymbol{u}_{2j}^{\top}\boldsymbol{h}_{t} + \boldsymbol{u}_{1j}^{\top}\boldsymbol{z}_{t-1} + \boldsymbol{u}_{3j}^{\top}\boldsymbol{h}_{t-1} + c_{1j} \,. && (31)
\end{aligned}
$$

All the gradients can be calculated readily as in (9)-(12).

C.2 Using deterministic hidden layer

For the generative model, denote the deterministic hidden layer as $\boldsymbol{h}_t^g \in \mathbb{R}^K$. For the recognition model, denote the deterministic hidden layer as $\boldsymbol{h}_t^r \in \mathbb{R}^K$. $\mathbf{W}_3$ and $\mathbf{U}_3$ are set to be zero matrices for the ease of gradient calculation. The generative model is expressed as

$$
\begin{aligned}
p(z_{jt}=1) &= \sigma(\boldsymbol{w}_{1j}^{\top}\boldsymbol{z}_{t-1} + b_{1j}) \,, && (32)\\
h_{kt}^{g} &= f(\boldsymbol{w}_{2k}^{\top}\boldsymbol{z}_{t} + \boldsymbol{w}_{4k}^{\top}\boldsymbol{h}_{t-1}^{g} + \boldsymbol{w}_{6k}^{\top}\boldsymbol{v}_{t-1} + b_{2k}) \,, && (33)\\
p(v_{mt}=1) &= \sigma(\boldsymbol{w}_{5m}^{\top}\boldsymbol{h}_{t} + \boldsymbol{w}_{7m}^{\top}\boldsymbol{v}_{t-1} + b_{3m}) \,, && (34)
\end{aligned}
$$

The corresponding recognition model is expressed as

$$
\begin{aligned}
h_{kt}^{r} &= f(\boldsymbol{u}_{5k}^{\top}\boldsymbol{v}_{t} + \boldsymbol{u}_{4k}^{\top}\boldsymbol{h}_{t-1} + \boldsymbol{u}_{6k}^{\top}\boldsymbol{v}_{t-1} + c_{2k}) && (35)\\
q(\boldsymbol{z}_{jt}=1) &= \sigma(\boldsymbol{u}_{2j}^{\top}\boldsymbol{h}_{t} + \boldsymbol{u}_{1j}^{\top}\boldsymbol{z}_{t-1} + c_{1j}) && (36)
\end{aligned}
$$

Hence, $\mathcal{L} = \sum_{t=1}^{T}\mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{v})}[l_t]$, and l_t is expressed as

$$
\begin{aligned}
l_t = & \sum_{j=1}^{J}\left(\psi_{jt}^{(1)} z_{jt} - \log(1+\exp(\psi_{jt}^{(1)}))\right) + \sum_{m=1}^{M}\left(\psi_{mt}^{(2)} v_{mt} - \log(1+\exp(\psi_{mt}^{(2)}))\right) \\
& - \left[\sum_{j=1}^{J}\left(\psi_{jt}^{(3)} z_{jt} - \log(1+\exp(\psi_{jt}^{(3)}))\right)\right] ,
\end{aligned}
\tag{37}
$$

and we have defined

$$
\begin{aligned}
\psi_{jt}^{(1)} &= \boldsymbol{w}_{1j}^{\top}\boldsymbol{z}_{t-1} + b_{1j} \,, && (38)\\
\psi_{mt}^{(2)} &= \boldsymbol{w}_{5m}^{\top}\boldsymbol{h}_{t}^{g} + \boldsymbol{w}_{7m}^{\top}\boldsymbol{v}_{t-1} + b_{3m} \,, && (39)\\
\psi_{jt}^{(3)} &= \boldsymbol{u}_{2j}^{\top}\boldsymbol{h}_{t}^{r} + \boldsymbol{u}_{1j}^{\top}\boldsymbol{z}_{t-1} + c_{1j} \,. && (40)
\end{aligned}
$$

The gradients *w.r.t.* $\mathbf{W}_1, \mathbf{W}_5, \mathbf{W}_7, \mathbf{U}_1$ and $\mathbf{U}_2$ can be calculated easily. In order to calculate the gradients *w.r.t.* $\mathbf{W}_2, \mathbf{W}_4, \mathbf{W}_6, \mathbf{U}_4, \mathbf{U}_5$ and $\mathbf{U}_6$, we need to obtain $\frac{\partial \mathcal{L}}{\partial h_{kt}^{g}}$ and $\frac{\partial \mathcal{L}}{\partial h_{kt}^{r}}$, which can be

Table 1: Average prediction error and the average negative log-likelihood per frame for the bouncing balls dataset. (◇) taken from [2].

MODEL	DIM	ORDER	PRED. ERR.	NEG. LOG. LIKE.
DTSBN-S	100-100	2	**2.79** ± 0.39	**69.29** ± 1.52
DTSBN-D	100-100	2	2.99 ± 0.42	70.47 ± 1.52
DTSBN-S	100-100	1	10.39 ± 0.38	78.63 ± 0.92
TSBN	100	4	3.07 ± 0.40	70.41 ± 1.55
TSBN	100	2	4.00 ± 0.45	73.32 ± 1.75
TSBN	100	1	9.48 ± 0.38	77.71 ± 0.83
HMSBN	100	1	23.94 ± 0.41	86.27 ± 0.80
AR	0	2	3.63 ± 0.42	73.80 ± 1.46
AR	0	1	11.01 ± 0.24	93.61 ± 0.67
RTRBM◇	3750	1	3.88 ± 0.33	–
SRTRBM◇	3750	1	3.31 ± 0.33	–

calculated recursively via the back-propagation through time algorithm. Specifically, $\frac{\partial \mathcal{L}}{\partial h^g_{kt}} = \frac{\partial \mathcal{Q}_1}{\partial h^g_{kt}}$ and we have defined

$$\mathcal{Q}_1 = \sum_{t=1}^{T} \sum_{m=1}^{M} \left(\psi^{(2)}_{mt} v_{mt} - \log(1 + \exp(\psi^{(2)}_{mt})) \right) . \tag{41}$$

We observe that $\mathcal{Q}_1$ can be computed recursively using

$$\mathcal{Q}_t = \sum_{\tau=t}^{T} \sum_{m=1}^{M} \left(\psi^{(2)}_{m\tau} v_{m\tau} - \log(1 + \exp(\psi^{(2)}_{m\tau})) \right) \tag{42}$$

$$= \mathcal{Q}_{t+1} + \sum_{m=1}^{M} \left(\psi^{(2)}_{mt} v_{mt} - \log(1 + \exp(\psi^{(2)}_{mt})) \right) , \tag{43}$$

where $\mathcal{Q}_{T+1} = 0$. Using the chain rule, we have

$$\frac{\partial \mathcal{Q}_t}{\partial h^g_{kt}} = \sum_{k'} \frac{\partial \mathcal{Q}_{t+1}}{\partial h^g_{k't+1}} \cdot \frac{\partial h^g_{k't+1}}{\partial h^g_{kt}} + \sum_{m=1}^{M} w_{5mk}(v_{mt} - \sigma(\psi^{(2)}_{mt})) \tag{44}$$

$$= \sum_{k'} \frac{\partial \mathcal{Q}_{t+1}}{\partial h^g_{k't+1}} \cdot f'(\psi^{(4)}_{k't+1}) w_{4k'k} + \sum_{m=1}^{M} w_{5mk}(v_{mt} - \sigma(\psi^{(2)}_{mt})) , \tag{45}$$

where we have defined

$$\psi^{(4)}_{kt} = \boldsymbol{w}_{2k}^\top \boldsymbol{z}_t + \boldsymbol{w}_{4k}^\top \boldsymbol{h}^g_{t-1} + \boldsymbol{w}_{6k}^\top \boldsymbol{v}^g_{t-1} + b_{2k} , \tag{46}$$

and

$$\frac{\partial \mathcal{Q}_T}{\partial h^g_{kt}} = \sum_{m=1}^{M} w_{5mk}(v_{mT} - \sigma(\psi^{(2)}_{mT})) . \tag{47}$$

$\frac{\partial \mathcal{L}}{\partial h^r_{kt}}$ can be calculated similarly.

D Additional Results

D.1 Generated Data

The generated, synthetic motion capture data, and polyphonic music data can be downloaded from `https://drive.google.com/drive/u/0/folders/0B1HR6m3IZSO_SWt0aS1oYmlneDQ`.

D.2 Bouncing balls dataset

Additional experimental results are shown in Table 1. AR represents an auto-regressive Markov model without latent variables [3].

Table 2: Average prediction error obtained for the MIT motion capture dataset.

MODEL	PRED. ERR.
DTSBN-S	**3.71** $\pm$ 0.03
DTSBN-D	4.19 $\pm$ 0.01
TSBN	3.86 $\pm$ 0.02
HMSBN	17.49 $\pm$ 0.20

D.3 MIT motion capture dataset

We randomly select 10% of the dataset as the test set. Quantitative results are shown in Table 2.

References

[1] A. Mnih and K. Gregor. Neural variational inference and learning in belief networks. In *ICML*, 2014.

[2] R. Mittelman, B. Kuipers, S. Savarese, and H. Lee. Structured recurrent temporal restricted boltzmann machines. In *ICML*, 2014.

[3] Christopher M Bishop. *Pattern recognition and machine learning*. springer, 2006.