Supplementary Material: Classification of Sets using Restricted Boltzmann Machines

Jérôme Louradour
A2iA SA
40 bis, rue Fabert
75007 Paris, France

Hugo Larochelle *
Département d'informatique
Université de Sherbrooke
Sherbrooke, Canada

Abstract

We provide here some additional details relatively to our submission, regarding the derivation of the free-energy functions for the two ClassSetRBMs.

Derivation of the free-energy for ClassSetRBM$^{\mathrm{XOR}}$

We provide here the derivation of the free-energy for ClassSetRBM$^{\mathrm{XOR}}$. To simplify the derivation, we assume hidden layer sizes of $H = 1$. The generalization to arbitrary size is trivial, since the necessary sums factorize for each hidden unit, for the same reason that the conditional over $\mathbf{H}$ given $\mathbf{X}$ and $\mathbf{y}$ factorizes into each of the j^{th} hidden unit sets $\{h_j^s\}$.

$$
\begin{aligned}
p(\mathbf{y} = \mathbf{e}_c|\mathbf{x}) &= \sum_{\mathbf{H}} p(\mathbf{y} = \mathbf{e}_c, \mathbf{H}|\mathbf{x}) \\
&= \frac{\sum_{\mathbf{H}} \exp(-E(\mathbf{X}, \mathbf{y}, \mathbf{H}))}{\sum_{\mathbf{H}'} \sum_{c'=1\ldots C} \exp(-E(\mathbf{X}, \mathbf{e}_{c'}, \mathbf{H}'))}
\end{aligned}
\tag{1}
$$

where

$$
\begin{aligned}
& \sum_{\mathbf{H}} \exp(-E(\mathbf{X}, \mathbf{y}, \mathbf{H})) \\
= & \sum_{\mathbf{H}} \exp\left(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \sum_s \mathbf{c}^\top \mathbf{h}^{(s)} + \sum_s \left({\mathbf{h}^{(s)}}^\top \mathbf{W}\mathbf{x}^{(s)} + {\mathbf{h}^{(s)}}^\top \mathbf{U}\mathbf{y}\right)\right) \\
= & \exp(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)}) \sum_{\mathbf{H}} \exp\left(\sum_s \mathbf{c}^\top \mathbf{h}^{(s)} + \sum_s \left({\mathbf{h}^{(s)}}^\top \mathbf{W}\mathbf{x}^{(s)} + {\mathbf{h}^{(s)}}^\top \mathbf{U}\mathbf{y}\right)\right) \\
= & \exp(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)}) \left(\exp(0) + \sum_s \exp\left(c_1 + \mathbf{W}_1.\mathbf{x}^{(s)} + \mathbf{U}_1.\mathbf{y}\right)\right) \\
= & \exp(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)}) \left(1 + \exp(\mathbf{U}_1.\mathbf{y}) \sum_s \exp\left(c_1 + \mathbf{W}_1.\mathbf{x}^{(s)}\right)\right)
\end{aligned}
\tag{2}
$$

* This work was done while Hugo was at University of Toronto

where at line 2 we used the mutual exclusivity constraint $\sum_s h_1^{(s)} \in \{0, 1\}$ over $\mathbf{H}$. Hence we can write

$$
\begin{aligned}
\log \sum_{\mathbf{H}} \exp(-E(\mathbf{X}, \mathbf{y}, \mathbf{H})) &= \mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \mathrm{softplus}\left(\mathbf{U}_{1\cdot}\mathbf{y} + \log\left(\sum_s \exp\left(c_1 + \mathbf{W}_{1\cdot}\mathbf{x}^{(s)}\right)\right)\right) \\
&= \mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \mathrm{softplus}\left(\mathbf{U}_{1\cdot}\mathbf{y} + \mathrm{softmax}_1(\mathbf{X})\right)
\end{aligned}
$$

where we use the definition of $\mathrm{softmax}_j(\mathbf{X})$ for the ClassSetRBM$^{\mathrm{XOR}}$ (see Section 3.1 of submission). Going back to Equation 1:

$$
\begin{aligned}
p(\mathbf{y} = \mathbf{e}_c|\mathbf{x}) &= \frac{\sum_{\mathbf{H}} \exp(-E(\mathbf{X}, \mathbf{y}, \mathbf{H}))}{\sum_{\mathbf{H}'} \sum_{c'=1\ldots C} \exp(-E(\mathbf{X}, \mathbf{e}_{c'}, \mathbf{H}'))} \\
&= \frac{\exp\left(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \mathrm{softplus}\left(\mathbf{U}_{1\cdot}\mathbf{y} + \mathrm{softmax}_1(\mathbf{X})\right)\right)}{\sum_{c'=1\ldots C} \exp\left(\mathbf{d}^\top \mathbf{e}_{c'} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \mathrm{softplus}\left(\mathbf{U}_{1\cdot}\mathbf{e}_{c'}, + \mathrm{softmax}_1(\mathbf{X})\right)\right)} \\
&= \frac{\exp\left(\mathbf{d}^\top \mathbf{y} + \mathrm{softplus}\left(\mathbf{U}_{1\cdot}\mathbf{y} + \mathrm{softmax}_1(\mathbf{X})\right)\right)}{\sum_{c'=1\ldots C} \exp\left(\mathbf{d}^\top \mathbf{e}_{c'} + \mathrm{softplus}\left(\mathbf{U}_{1\cdot}\mathbf{e}_{c'}, + \mathrm{softmax}_1(\mathbf{X})\right)\right)} \\
&= \frac{\exp\left(-F^{\mathrm{XOR}}(\mathbf{X}, \mathbf{y})\right)}{\sum_{c'=1\ldots C} \exp\left(-F^{\mathrm{XOR}}(\mathbf{X}, \mathbf{e}_{c'})\right)}
\end{aligned}
$$

where we recover $F^{\mathrm{XOR}}(\mathbf{X}, \mathbf{y}) = -\mathbf{d}^\top \mathbf{y} - \mathrm{softplus}\left(\mathbf{U}_{1\cdot}\mathbf{y} + \mathrm{softmax}_1(\mathbf{X})\right)$ for $H = 1$. Because of the hidden unit factorization property, we get the general free-energy function $F^{\mathrm{XOR}}(\mathbf{X}, \mathbf{y}) = -\mathbf{d}^\top \mathbf{y} - \sum_{j=1}^{H} \mathrm{softplus}\left(\mathbf{U}_{j\cdot}\mathbf{y} + \mathrm{softmax}_j(\mathbf{X})\right)$ for arbitrary values of H.

Derivation of the free-energy for ClassSetRBM$^{\mathrm{OR}}$

Again, we provide the derivation of the free-energy for ClassSetRBM$^{\mathrm{XOR}}$. Here, we can also simplify the derivation by we assuming hidden layers of size $H = 1$.

$$
\begin{aligned}
p(\mathbf{y} = \mathbf{e}_c|\mathbf{x}) &= \sum_{\mathbf{G}} \sum_{\mathbf{H}} p(\mathbf{y} = \mathbf{e}_c, \mathbf{H}, \mathbf{G}|\mathbf{x}) \\
&= \frac{\sum_{\mathbf{G}} \sum_{\mathbf{H}} \exp(-E(\mathbf{X}, \mathbf{y}, \mathbf{H}, \mathbf{G}))}{\sum_{\mathbf{G}'} \sum_{\mathbf{H}'} \sum_{c'=1\ldots C} \exp(-E(\mathbf{X}, \mathbf{e}_{c'}, \mathbf{H}', \mathbf{G}'))} \qquad (3)
\end{aligned}
$$

where

$$
\begin{aligned}
& \sum_{\mathbf{G}} \sum_{\mathbf{H}} \exp(-E(\mathbf{X}, \mathbf{y}, \mathbf{H}, \mathbf{G})) \\
= \;& \sum_{\mathbf{G}} \sum_{\mathbf{H}} \exp \left(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \sum_s \mathbf{c}^\top \mathbf{h}^{(s)} + \sum_s \left(\mathbf{h}^{(s)\top} \mathbf{W} \mathbf{x}^{(s)} + \mathbf{g}^{(s)\top} \mathbf{U} \mathbf{y} \right) \right) \\
= \;& \exp(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)}) \sum_{\mathbf{G}} \sum_{\mathbf{H}} \exp \left(\sum_s \mathbf{c}^\top \mathbf{h}^{(s)} + \sum_s \left(\mathbf{h}^{(s)\top} \mathbf{W} \mathbf{x}^{(s)} + \mathbf{g}^{(s)\top} \mathbf{U} \mathbf{y} \right) \right) \\
= \;& \exp(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)}) \left(\exp(0) \left(\sum_{\mathbf{H}} \exp \left(\mathbf{c}^\top \mathbf{h}^{(s)} + \mathbf{h}^{(s)\top} \mathbf{W} \mathbf{x}^{(s)} \right) \right) \right. \qquad (4) \\
& \qquad \left. + \sum_s \exp(\mathbf{U}_1 . \mathbf{y}) \left(\sum_{\mathbf{H} \text{ s.t. } h_1^{(s)}=1} \exp \left(\mathbf{c}^\top \mathbf{h}^{(s)} + \mathbf{h}^{(s)} \mathbf{W} \mathbf{x}^{(s)} \right) \right) \right) \\
= \;& \exp(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)}) \left(\exp(0) \prod_{s'} \left(1 + \exp \left(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s')} \right) \right) \right. \qquad (5) \\
& \qquad \left. + \sum_s \exp(\mathbf{U}_1 . \mathbf{y} + c_1 + \mathbf{W}_1 . \mathbf{x}^{(s)}) \prod_{s' \neq s} \left(1 + \exp \left(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s')} \right) \right) \right) \\
= \;& \exp(\mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)}) \left(\prod_{s'} \left(1 + \exp \left(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s')} \right) \right) \right) \left(1 + \exp(\mathbf{U}_1 . \mathbf{y}) \sum_s \frac{\exp(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s)})}{1 + \exp(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s)})} \right)
\end{aligned}
$$

where at line 4 we used the mutual exclusivity constraint $\sum_s g_1^{(s)} \in \{0, 1\}$ over $\mathbf{G}$, and at line 5 we used the inequality constraint between $\mathbf{H}$ and $\mathbf{G}$, $h_1^{(s)} \geq g_1^{(s)} \; \forall \, s$. Hence we can write

$$
\begin{aligned}
& \log \sum_{\mathbf{G}} \sum_{\mathbf{H}} \exp(-E(\mathbf{X}, \mathbf{y}, \mathbf{H}, \mathbf{G})) \\
= \;& \mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \sum_{s'} \text{softplus}(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s')}) + \text{softplus} \left(\mathbf{U}_1 . \mathbf{y} + \log \sum_s \frac{\exp(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s)})}{1 + \exp(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s)})} \right) \\
= \;& \mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \sum_{s'} \text{softplus}(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s')}) + \text{softplus} \left(\mathbf{U}_1 . \mathbf{y} + \log \sum_s \exp(\text{softminus}(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s)})) \right) \\
= \;& \mathbf{d}^\top \mathbf{y} + \sum_s \mathbf{b}^\top \mathbf{x}^{(s)} + \sum_{s'} \text{softplus}(c_1 + \mathbf{W}_1 . \mathbf{x}^{(s')}) + \text{softplus} \left(\mathbf{U}_1 . \mathbf{y} + \text{softmax}_1(\mathbf{X}) \right)
\end{aligned}
$$

where we use the definition of $\mathrm{softmax}_j(\mathbf{X})$ for the ClassSetRBM$^{\mathrm{OR}}$ (see Section 3.2 of submission). Going back to Equation 3:

$$\begin{aligned} p(\mathbf{y}=\mathbf{e}_c|\mathbf{x}) &= \frac{\sum_{\mathbf{H}}\sum_{\mathbf{G}}\exp(-E(\mathbf{X},\mathbf{y},\mathbf{H},\mathbf{G}))}{\sum_{\mathbf{H}'}\sum_{\mathbf{G}'}\sum_{c'=1\ldots C}\exp(-E(\mathbf{X},\mathbf{e}_{c'},\mathbf{H}',\mathbf{G}'))} \\ &= \frac{\exp\left(\mathbf{d}^\top\mathbf{y} + \mathrm{softplus}\left(\mathbf{U}_1.\mathbf{y} + \mathrm{softmax}_1(\mathbf{X})\right)\right)}{\sum_{c'=1\ldots C}\exp(\mathbf{d}^\top\mathbf{e}_{c'} + \mathrm{softplus}\left(\mathbf{U}_1.\mathbf{e}_{c'} + \mathrm{softmax}_1(\mathbf{X})\right))} \\ &= \frac{\exp\left(-F^{\mathrm{OR}}(\mathbf{X},\mathbf{y})\right)}{\sum_{c'=1\ldots C}\exp\left(-F^{\mathrm{OR}}(\mathbf{X},\mathbf{e}_{c'})\right)} \end{aligned}$$

where we recover $F^{\mathrm{OR}}(\mathbf{X},\mathbf{y}) = -\mathbf{d}^\top\mathbf{y} - \mathrm{softplus}\left(\mathbf{U}_1.\mathbf{y} + \mathrm{softmax}_1(\mathbf{X})\right)$ for $H = 1$. Again, because of the hidden unit factorization property of ClassSetRBM$^{\mathrm{OR}}$, we get the general free-energy function $F^{\mathrm{OR}}(\mathbf{X},\mathbf{y}) = -\mathbf{d}^\top\mathbf{y} - \sum_{j=1}^{H}\mathrm{softplus}\left(\mathbf{U}_j.\mathbf{y} + \mathrm{softmax}_j(\mathbf{X})\right)$ for arbitrary values of H.