

Sparse Classification RBM

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Mathematical Formulation

$$E(y, \mathbf{X}, \mathbf{h}) = E(y, x_1, \dots, x_C, \mathbf{h}) = - \sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} \mathbf{e}_{x_i} + \mathbf{b}^{(i)T} \mathbf{e}_{x_i}) - \mathbf{h}^T \mathbf{c} - dy - \mathbf{h}^T \mathbf{U} y$$

$$p(y, \mathbf{X}, \mathbf{h}) = p(y, x_1, \dots, x_C, \mathbf{h}) = \frac{\exp(-E(y, x_1, \dots, x_C, \mathbf{h}))}{Z}$$

$$Z = \sum_y \sum_{\mathbf{X}} \sum_{\mathbf{h}} p(y, \mathbf{X}, \mathbf{h})$$

$$\mathbf{e}_y = (1_{i=y})_{1 \leq i \leq C}$$

$$y \in \{0, 1\}$$

$$x_i \in \{1, \dots, k_i\}, 1 \leq i \leq C$$

$$h_i \in \{0, 1\}, 1 \leq i \leq H$$

Parameter Set: $\theta = \{\mathbf{W}, \mathbf{b}, \mathbf{d}, \mathbf{c}, \mathbf{U}\}$

Model Explanation

y : click ($y=1$) or no click ($y=0$).

x_i : feature value of the i -th feature class (there are total of C feature classes).

h_i : i -th hidden unit value.

Derivation of Properties

$$p(\mathbf{h}|y, \mathbf{X}) = \prod_j p(h_j|y, \mathbf{X})$$

$$\begin{aligned} p(\mathbf{h}|y, \mathbf{X}) &= \frac{p(y, \mathbf{X}, \mathbf{h})}{p(y, \mathbf{X})} = \frac{p(y, \mathbf{X}, \mathbf{h})}{\sum_{\mathbf{h}'} p(y, \mathbf{X}, \mathbf{h}')} = \frac{\exp[-E(y, \mathbf{X}, \mathbf{h})]}{\sum_{\mathbf{h}'} \exp[-E(y, \mathbf{X}, \mathbf{h}')] } \\ &= \frac{\exp\{\sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} \mathbf{e}_{x_i} + \mathbf{b}^{(i)T} \mathbf{e}_{x_i}) + \mathbf{h}^T \mathbf{c} + dy + \mathbf{h}^T \mathbf{U} y\}}{\sum_{\mathbf{h}'} \exp\{\sum_{1 \leq i \leq C} (\mathbf{h}'^T \mathbf{W}^{(i)} \mathbf{e}_{x_i} + \mathbf{b}^{(i)T} \mathbf{e}_{x_i}) + \mathbf{h}'^T \mathbf{c} + dy + \mathbf{h}'^T \mathbf{U} y\}} \\ &= \frac{\exp(dy) \exp(\sum_{1 \leq i \leq C} \mathbf{b}^{(i)T} \mathbf{e}_{x_i})}{\exp(dy) \exp(\sum_{1 \leq i \leq C} \mathbf{b}^{(i)T} \mathbf{e}_{x_i})} \frac{\exp\{\mathbf{h}^T [\sum_{1 \leq i \leq C} \mathbf{W}^{(i)} \mathbf{e}_{x_i} + \mathbf{c} + \mathbf{U} y]\}}{\sum_{\mathbf{h}'} \exp\{\mathbf{h}'^T [\sum_{1 \leq i \leq C} \mathbf{W}^{(i)} \mathbf{e}_{x_i} + \mathbf{c} + \mathbf{U} y]\}} \\ &= \frac{\exp\{\sum_{1 \leq j \leq H} [h_j (\sum_{1 \leq i \leq C} W_{j, x_i}^{(i)} + c_i + U_i y)]\}}{\sum_{\mathbf{h}'} \exp\{\sum_{1 \leq j \leq H} [h'_j (\sum_{1 \leq i \leq C} W_{j, x_i}^{(i)} + c_i + U_i y)]\}} \end{aligned}$$

$$\begin{aligned}
&= \frac{\prod_{1 \leq j \leq H} \exp[h_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]}{\sum_{\mathbf{h}'} \prod_{1 \leq j \leq H} \exp[h'_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]} \\
&= \frac{\prod_{1 \leq j \leq H} \exp[h_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]}{\sum_{h'_1} \dots \sum_{h'_H} \prod_{1 \leq j \leq H} \exp[h'_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]} \\
&= \frac{\prod_{1 \leq j \leq H} \exp[h_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]}{\left\{ \sum_{h'_1 \in \{0,1\}} \exp[h'_1(\sum_{1 \leq i \leq C} W_{1,x_i}^{(i)} + c_1 + U_1 y)] \right\} \dots \left\{ \sum_{h'_H \in \{0,1\}} \exp[h'_H(\sum_{1 \leq i \leq C} W_{H,x_i}^{(i)} + c_H + U_H y)] \right\}} \\
&= \frac{\prod_{1 \leq j \leq H} \exp[h_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]}{\left\{ 1 + \exp[(\sum_{1 \leq i \leq C} W_{1,x_i}^{(i)} + c_1 + U_1 y)] \right\} \dots \left\{ 1 + \exp[(\sum_{1 \leq i \leq C} W_{H,x_i}^{(i)} + c_H + U_H y)] \right\}} \\
&= \prod_{1 \leq j \leq H} \frac{\exp[h_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]}{1 + \exp[(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_j + U_j y)]} \\
&= \prod_{1 \leq j \leq H} p(h_j | y, \mathbf{X})
\end{aligned}$$

$$p(h_j = 1 | y, \mathbf{X}) = \sigma\left(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_j + U_j y\right)$$

$$\begin{aligned}
p(h_j = 1 | y, \mathbf{X}) &= \sum_{\mathbf{h}' \in \{..., h_j=1, ...\}} p(\mathbf{h}' | y, \mathbf{X}) \\
&= \sum_{\mathbf{h}' \in \{..., h_j=1, ...\}} \prod_{1 \leq k \leq H} \frac{\exp[h_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]}{1 + \exp[(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_j + U_j y)]} \\
&= \frac{\exp[h_j(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y)]}{1 + \exp[(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_j + U_j y)]} \prod_{1 \leq k \leq H, k \neq j} \sum_{h_k \in \{0,1\}} \frac{\exp[h_k(\sum_{1 \leq i \leq C} W_{k,x_i}^{(i)} + c_k + U_k y)]}{1 + \exp[(\sum_{1 \leq i \leq C} W_{k,x_i}^{(i)} + c_k + U_k y)]} \\
&= \frac{\exp[\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_i + U_i y]}{1 + \exp[(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_j + U_j y)]} \\
&= \sigma\left(\sum_{1 \leq i \leq C} W_{j,x_i}^{(i)} + c_j + U_j y\right)
\end{aligned}$$

$$p(y | \mathbf{X}) = \frac{\exp\{-F(y, \mathbf{X})\}}{\sum_{y''} \exp\{-F(y'', \mathbf{X})\}}$$

Note that:

$$\begin{aligned}
\sum_{\mathbf{h}'} p(y, \mathbf{X}, \mathbf{h}') &= \frac{1}{Z} \sum_{\mathbf{h}'} \exp(-E(y, \mathbf{X}, \mathbf{h}')) \\
&= \frac{1}{Z} \sum_{\mathbf{h}'} \exp\left\{ \sum_{1 \leq i \leq C} (\mathbf{h}'^T \mathbf{W}^{(i)} \mathbf{e}_{x_i} + \mathbf{b}^{(i)T} \mathbf{e}_{x_i}) + \mathbf{h}'^T \mathbf{c} + dy + \mathbf{h}'^T \mathbf{U} y \right\}
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{Z} \sum_{\mathbf{h}'} \{ \exp(dy) \} \{ \exp(\sum_{1 \leq i \leq C} \mathbf{b}^{(i)\top} \mathbf{e}_{x_i}) \} \left\{ \exp \left[\mathbf{h}'^\top \left(\sum_{1 \leq i \leq C} \mathbf{w}^{(i)} \mathbf{e}_{x_i} + \mathbf{c} + \mathbf{U}y \right) \right] \right\} \\
&= \frac{1}{Z} \{ \exp(\sum_{1 \leq i \leq C} \mathbf{b}^{(i)\top} \mathbf{e}_{x_i}) \} \{ \exp(dy) \} \sum_{\mathbf{h}'} \left\{ \exp \left[\mathbf{h}'^\top \left(\sum_{1 \leq i \leq C} \mathbf{w}^{(i)} \mathbf{e}_{x_i} + \mathbf{c} + \mathbf{U}y \right) \right] \right\} \\
&= \frac{1}{Z} \{ \exp(\sum_{1 \leq i \leq C} \mathbf{b}^{(i)\top} \mathbf{e}_{x_i}) \} \{ \exp(dy) \} \prod_{1 \leq k \leq H} \sum_{h_k \in \{0,1\}} \left\{ \exp \left[h_k \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y \right) \right] \right\} \\
&= \frac{1}{Z} \{ \exp(\sum_{1 \leq i \leq C} \mathbf{b}^{(i)\top} \mathbf{e}_{x_i}) \} \{ \exp(dy) \} \prod_{1 \leq k \leq H} \left\{ 1 + \exp \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y \right) \right\}
\end{aligned}$$

Hence:

$$\begin{aligned}
p(y|\mathbf{X}) &= \frac{p(y, \mathbf{X})}{p(\mathbf{X})} = \frac{\sum_{\mathbf{h}'} p(y, \mathbf{X}, \mathbf{h}')}{\sum_{y''} \sum_{\mathbf{h}''} p(y'', \mathbf{X}, \mathbf{h}'')} \\
&= \frac{\{ \exp(dy) \} \prod_{1 \leq k \leq H} \left\{ 1 + \exp \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y \right) \right\}}{\sum_{y''} \{ \exp(dy'') \} \prod_{1 \leq k \leq H} \left\{ 1 + \exp \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y'' \right) \right\}} \\
&= \frac{\exp \left\{ dy + \ln \left[\prod_{1 \leq k \leq H} \left\{ 1 + \exp \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y \right) \right\} \right] \right\}}{\sum_{y''} \exp \left\{ dy'' + \ln \left[\prod_{1 \leq k \leq H} \left\{ 1 + \exp \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y'' \right) \right\} \right] \right\}} \\
&= \frac{\exp \left\{ dy + \sum_{1 \leq k \leq H} \ln \left[1 + \exp \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y \right) \right] \right\}}{\sum_{y''} \exp \left\{ dy'' + \sum_{1 \leq k \leq H} \ln \left[1 + \exp \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y'' \right) \right] \right\}} \\
&= \frac{\exp \left\{ dy + \sum_{1 \leq k \leq H} \text{softplus} \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y \right) \right\}}{\sum_{y''} \exp \left\{ dy'' + \sum_{1 \leq k \leq H} \text{softplus} \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y'' \right) \right\}} \\
&= \frac{\exp \left\{ dy + \sum_{1 \leq k \leq H} \text{softplus} \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k y \right) \right\}}{\exp \left\{ \sum_{1 \leq k \leq H} \text{softplus} \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k \right) \right\} + \exp \left\{ d + \sum_{1 \leq k \leq H} \text{softplus} \left(\sum_{1 \leq i \leq C} w_{k,x_i}^{(i)} + c_k + \mathbf{U}_k \right) \right\}} \\
&= \frac{\exp \{-F(y, \mathbf{X})\}}{\sum_{y''} \exp \{-F(y'', \mathbf{X})\}}
\end{aligned}$$

$$p(y|\mathbf{h}) = \frac{\exp\{dy + \mathbf{h}^\top \mathbf{U}y\}}{1 + \exp\{d + \mathbf{h}^\top \mathbf{U}\}}$$

Note that

$$\begin{aligned}
\sum_{\mathbf{X}} p(y, \mathbf{X}, \mathbf{h}) &= \frac{1}{Z} \sum_{\mathbf{X}} \exp \left\{ \sum_{1 \leq i \leq C} (\mathbf{h}^\top \mathbf{w}^{(i)} + \mathbf{b}^{(i)\top}) \mathbf{e}_{x_i} \right\} \exp\{\mathbf{h}^\top \mathbf{c}\} \exp\{dy + \mathbf{h}^\top \mathbf{U}y\} \\
&= \frac{1}{Z} \exp\{\mathbf{h}^\top \mathbf{c}\} \exp\{dy + \mathbf{h}^\top \mathbf{U}y\} \sum_{\mathbf{X}} \exp \left\{ \sum_{1 \leq i \leq C} (\mathbf{h}^\top \mathbf{w}^{(i)} + \mathbf{b}^{(i)\top}) \mathbf{e}_{x_i} \right\}
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{Z} \exp\{\mathbf{h}^T \mathbf{c}\} \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}\} \prod_{1 \leq i \leq C} \sum_{\mathbf{x}_i} \exp\{(\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i}\} \\
&= \frac{1}{Z} \exp\{\mathbf{h}^T \mathbf{c}\} \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}\} K(\mathbf{h})
\end{aligned}$$

Hence:

$$\begin{aligned}
p(\mathbf{y}|\mathbf{h}) &= \frac{p(\mathbf{y}, \mathbf{h})}{p(\mathbf{h})} = \frac{\sum_{\mathbf{x}'} p(\mathbf{y}, \mathbf{x}', \mathbf{h})}{\sum_{\mathbf{y}''} \sum_{\mathbf{x}''} p(\mathbf{y}'', \mathbf{x}'', \mathbf{h})} \\
&= \frac{\exp\{\mathbf{h}^T \mathbf{c}\} \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}\} K(\mathbf{h})}{\sum_{\mathbf{y}''} \exp\{\mathbf{h}^T \mathbf{c}\} \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}''\} K(\mathbf{h})} = \frac{\exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}\}}{\sum_{\mathbf{y}''} \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}''\}} = \frac{\exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}\}}{1 + \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U}\}}
\end{aligned}$$

$$p(\mathbf{y} = 1|\mathbf{h}) = \sigma(\mathbf{d} + \mathbf{h}^T \mathbf{U})$$

$$p(\mathbf{X}|\mathbf{h}) = \prod_{1 \leq i \leq C} p(x_i|\mathbf{h})$$

Note that:

$$\begin{aligned}
\sum_{\mathbf{y}'} p(\mathbf{y}', \mathbf{X}, \mathbf{h}) &= \frac{1}{Z} \sum_{\mathbf{y}'} \exp\left\{\sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} \mathbf{e}_{\mathbf{x}_i} + \mathbf{b}^{(i)T} \mathbf{e}_{\mathbf{x}_i}) + \mathbf{h}^T \mathbf{c} + \mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}'\right\} \\
&= \frac{1}{Z} \sum_{\mathbf{y}'} \exp\left\{\sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i}\right\} \exp\{\mathbf{h}^T \mathbf{c}\} \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}'\} \\
&= \frac{1}{Z} \left[\exp\left\{\sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i}\right\} \exp\{\mathbf{h}^T \mathbf{c}\} \right] \sum_{\mathbf{y}'} \exp\{\mathbf{d} + \mathbf{h}^T \mathbf{U} \mathbf{y}'\} \\
&= \frac{1}{Z} [1 + \exp(\mathbf{d} + \mathbf{h}^T \mathbf{U})] \exp\{\mathbf{h}^T \mathbf{c}\} \exp\left\{\sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i}\right\}
\end{aligned}$$

Hence:

$$\begin{aligned}
p(\mathbf{X}|\mathbf{h}) &= \frac{p(\mathbf{X}, \mathbf{h})}{p(\mathbf{h})} = \frac{\sum_{\mathbf{y}'} p(\mathbf{y}', \mathbf{X}, \mathbf{h})}{\sum_{\mathbf{x}''} \sum_{\mathbf{y}''} p(\mathbf{y}'', \mathbf{x}'', \mathbf{h})} \\
&= \frac{\exp\{\sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i}\}}{\sum_{\mathbf{x}''} \exp\left\{\sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i''}\right\}} \\
&= \frac{\prod_{1 \leq i \leq C} \exp\{(\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i}\}}{\prod_{1 \leq i \leq C} \sum_{\mathbf{x}_i'' \in \{1, \dots, C_i\}} \exp\{(\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{\mathbf{x}_i''}\}} \\
&= \prod_{1 \leq i \leq C} p(x_i|h)
\end{aligned}$$

$$p(x_i = k|\mathbf{h}) = \frac{\exp(\sum_{1 \leq j \leq H} h_j W_{j,k}^{(i)})}{\sum_{1 \leq q \leq C_i} \exp(\sum_{1 \leq j \leq H} h_j W_{j,q}^{(i)})}$$

$$\begin{aligned} p(x_i = k|\mathbf{h}) &= \frac{\exp\{(\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{x_i}\}}{\sum_{x_i'' \in \{1, \dots, C_i\}} \exp\{(\mathbf{h}^T \mathbf{W}^{(i)} + \mathbf{b}^{(i)T}) \mathbf{e}_{x_i}\}} \\ &= \frac{\exp(\sum_{1 \leq j \leq H} h_j W_{j,k}^{(i)})}{\sum_{1 \leq q \leq C_i} \exp(\sum_{1 \leq j \leq H} h_j W_{j,q}^{(i)})} \end{aligned}$$

Derivation of Learning Algorithm

Generative Learning

$$\frac{\partial \ln p(y, \mathbf{X})}{\partial \theta} = -\mathbb{E}_{p(\mathbf{h}|y, \mathbf{X})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] + \mathbb{E}_{p(y, \mathbf{X}, \mathbf{h})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right]$$

$$\begin{aligned} \frac{\partial \ln p(y, \mathbf{X})}{\partial \theta} &= \frac{\partial}{\partial \theta} \left\{ \ln \sum_{\mathbf{h}'} \exp(-E(y, \mathbf{X}, \mathbf{h}')) - \ln Z \right\} \\ &= - \sum_{\mathbf{h}'} \left[\frac{\exp(-E(y, \mathbf{X}, \mathbf{h}'))}{\sum_{\mathbf{h}''} \exp(-E(y, \mathbf{X}, \mathbf{h}''))} \frac{\partial E(y, \mathbf{X}, \mathbf{h}')}{\partial \theta} \right] + \sum_{y', \mathbf{X}', \mathbf{h}'} \left[\frac{\exp(-E(y', \mathbf{X}', \mathbf{h}'))}{Z} \frac{\partial E(y', \mathbf{X}', \mathbf{h}')}{\partial \theta} \right] \\ &= - \sum_{\mathbf{h}'} p(\mathbf{h}'|y, \mathbf{X}) \frac{\partial E(y, \mathbf{X}, \mathbf{h}')}{\partial \theta} + \sum_{y', \mathbf{X}', \mathbf{h}'} p(y', \mathbf{X}', \mathbf{h}') \frac{\partial E(y', \mathbf{X}', \mathbf{h}')}{\partial \theta} \end{aligned}$$

Discriminative Learning

$$\frac{\partial \ln p(y|\mathbf{X})}{\partial \theta} = -\mathbb{E}_{p(\mathbf{h}|y, \mathbf{X})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] + \mathbb{E}_{p(y, \mathbf{h}|\mathbf{X})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right]$$

$$\begin{aligned} \frac{\partial \ln p(y|\mathbf{X})}{\partial \theta} &= \frac{\partial}{\partial \theta} \ln \left[\frac{\frac{1}{Z} \sum_{\mathbf{h}'} p(y, \mathbf{X}, \mathbf{h}')}{\frac{1}{Z} \sum_{y'} \sum_{\mathbf{h}'} p(y', \mathbf{X}, \mathbf{h}')} \right] \\ &= \frac{\partial}{\partial \theta} \left\{ \ln \left[\sum_{\mathbf{h}'} p(y, \mathbf{X}, \mathbf{h}') \right] - \ln \left[\sum_{y'} \sum_{\mathbf{h}'} p(y', \mathbf{X}, \mathbf{h}') \right] \right\} \\ &= - \sum_{\mathbf{h}'} \left\{ \frac{p(y, \mathbf{X}, \mathbf{h}')}{\sum_{\mathbf{h}''} p(y, \mathbf{X}, \mathbf{h}'')} \frac{\partial E(y, \mathbf{X}, \mathbf{h}')}{\partial \theta} \right\} + \sum_{y'} \sum_{\mathbf{h}'} \left\{ \frac{p(y', \mathbf{X}, \mathbf{h}')}{\sum_{y''} \sum_{\mathbf{h}''} p(y'', \mathbf{X}, \mathbf{h}'')} \frac{\partial E(y', \mathbf{X}, \mathbf{h}')}{\partial \theta} \right\} \\ &= - \sum_{\mathbf{h}'} p(\mathbf{h}'|y, \mathbf{X}) \frac{\partial E(y, \mathbf{X}, \mathbf{h}')}{\partial \theta} + \sum_{y'} \sum_{\mathbf{h}'} p(y', \mathbf{h}'|\mathbf{X}) \frac{\partial E(y', \mathbf{X}, \mathbf{h}')}{\partial \theta} \end{aligned}$$

Hybrid Learning

$$\begin{aligned}
\frac{\ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial \theta} &= \frac{\partial \ln p(y|\mathbf{X})}{\partial \theta} + \alpha \frac{\partial \ln p(y, \mathbf{X})}{\partial \theta} \\
&= -(1 + \alpha) \mathbb{E}_{p(\mathbf{h}|\mathbf{y}, \mathbf{X})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] + \mathbb{E}_{p(y, \mathbf{h}|\mathbf{X})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] + \alpha \mathbb{E}_{p(y, \mathbf{X}, \mathbf{h})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] \\
&= -(1 + \alpha) A(y, \mathbf{X}, \mathbf{h}, \theta) + B(y, \mathbf{X}, \mathbf{h}, \theta) + \alpha C(y, \mathbf{X}, \mathbf{h}, \theta)
\end{aligned}$$

Derivatives of Gradients

$$E(y, \mathbf{X}, \mathbf{h}) = E(y, x_1, \dots, x_C, \mathbf{h}) = - \sum_{1 \leq i \leq C} (\mathbf{h}^T \mathbf{W}^{(i)} \mathbf{e}_{x_i} + \mathbf{b}^{(i)T} \mathbf{e}_{x_i}) - \mathbf{h}^T \mathbf{c} - dy - \mathbf{h}^T \mathbf{U} \mathbf{y}$$

Parameter Set: $\theta = \{\mathbf{W}, \mathbf{b}, \mathbf{d}, \mathbf{c}, \mathbf{U}\}$

$$\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial W_{j,k}^{(i)}} = -h_j 1_{(x_i=k)}$$

$$\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial b_j^i} = -1_{(x_i=j)}$$

$$\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial d} = -y$$

$$\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial c_i} = -h_i$$

$$\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial U_i} = -h_i y$$

Parameter Updates

$$A(y, \mathbf{X}, \mathbf{h}, \theta)$$

$$A(y, \mathbf{X}, \mathbf{h}, W_{j,k}^{(i)}) = -p(h_j = 1|y, X) 1_{(x_i=k)}$$

$$A(y, \mathbf{X}, \mathbf{h}, b_k^i) = -1_{(x_i=k)}$$

$$A(y, \mathbf{X}, \mathbf{h}, d) = -y$$

$$A(y, \mathbf{X}, \mathbf{h}, c_j) = -p(h_j = 1|y, X)$$

$$A(y, \mathbf{X}, \mathbf{h}, U_j) = -p(h_j = 1|y, X)y$$

$$A(y, \mathbf{X}, \mathbf{h}, \theta) = \mathbb{E}_{p(\mathbf{h}|\mathbf{y}, \mathbf{X})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] = \sum_{\mathbf{h}'} p(\mathbf{h}'|\mathbf{y}, \mathbf{X}) \frac{\partial E(y, \mathbf{X}, \mathbf{h}')}{\partial \theta}$$

$$\begin{aligned}
A(y, \mathbf{X}, \mathbf{h}, W_{j,k}^{(i)}) &= - \sum_{\mathbf{h}'} p(\mathbf{h}'|\mathbf{y}, \mathbf{X}) h_j 1_{(x_i=k)} = -p(h_j = 1|y, X) 1_{(x_i=k)} \prod_{q, q \neq j} \sum_{h_q \in \{0,1\}} p(h_q|y, X) \\
&= -p(h_j = 1|y, X) 1_{(x_i=k)}
\end{aligned}$$

$$A(y, \mathbf{X}, \mathbf{h}, b_k^i) = - \sum_{\mathbf{h}'} p(\mathbf{h}'|\mathbf{y}, \mathbf{X}) 1_{(x_i=k)} = -1_{(x_i=k)}$$

$$A(y, \mathbf{X}, \mathbf{h}, d) = - \sum_{\mathbf{h}'} p(\mathbf{h}'|\mathbf{y}, \mathbf{X}) y = -y$$

$$A(y, \mathbf{X}, \mathbf{h}, c_j) = - \sum_{\mathbf{h}'} p(\mathbf{h}' | y, \mathbf{X}) h_j = -p(h_j = 1 | y, \mathbf{X})$$

$$A(y, \mathbf{X}, \mathbf{h}, U_j) = - \sum_{\mathbf{h}'} p(\mathbf{h}' | y, \mathbf{X}) h_j y = -p(h_j = 1 | y, \mathbf{X}) y$$

$$B(y, \mathbf{X}, \mathbf{h}, \theta)$$

$$B(y, \mathbf{X}, \mathbf{h}, W_{j,k}^{(i)}) = -1_{(x_i=k)} \sum_{y'} p(y' | \mathbf{X}) p(h_j = 1 | y', \mathbf{X})$$

$$B(y, \mathbf{X}, \mathbf{h}, b_k^i) = -1_{(x_i=k)}$$

$$B(y, \mathbf{X}, \mathbf{h}, d) = - \sum_{y'} p(y | \mathbf{X}) y'$$

$$B(y, \mathbf{X}, \mathbf{h}, c_j) = - \sum_{y'} p(y' | \mathbf{X}) p(h_j = 1 | y', \mathbf{X})$$

$$B(y, \mathbf{X}, \mathbf{h}, U_j) = -p(y = 1 | \mathbf{X}) p(h_j = 1 | y = 1, \mathbf{X})$$

$$B(y, \mathbf{X}, \mathbf{h}, \theta) = \mathbb{E}_{p(y, \mathbf{h} | \mathbf{X})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] = \sum_{y'} \sum_{\mathbf{h}'} p(y', \mathbf{h}' | \mathbf{X}) \frac{\partial E(y', \mathbf{X}, \mathbf{h}')}{\partial \theta}$$

$$B(y, \mathbf{X}, \mathbf{h}, W_{j,k}^{(i)}) = - \sum_{y'} \sum_{\mathbf{h}'} p(y', \mathbf{h}' | \mathbf{X}) h_j 1_{(x_i=k)} = -1_{(x_i=k)} \sum_{y'} p(y | \mathbf{X}) \sum_{\mathbf{h}'} p(\mathbf{h}' | y, \mathbf{X}) h_j$$

$$= -1_{(x_i=k)} \sum_{y'} p(y' | \mathbf{X}) p(h_j = 1 | y', \mathbf{X})$$

$$B(y, \mathbf{X}, \mathbf{h}, b_k^i) = - \sum_{y'} \sum_{\mathbf{h}'} p(y', \mathbf{h}' | \mathbf{X}) h_j 1_{(x_i=k)} = -1_{(x_i=k)}$$

$$B(y, \mathbf{X}, \mathbf{h}, d) = - \sum_{y'} \sum_{\mathbf{h}'} p(y', \mathbf{h}' | \mathbf{X}) y = - \sum_{y'} p(y' | \mathbf{X}) y' \sum_{\mathbf{h}'} p(\mathbf{h}' | y', \mathbf{X}) = - \sum_{y'} p(y | \mathbf{X}) y'$$

$$B(y, \mathbf{X}, \mathbf{h}, c_j) = - \sum_{y'} p(y | \mathbf{X}) \sum_{\mathbf{h}'} p(\mathbf{h}' | y, \mathbf{X}) h_j = - \sum_{y'} p(y' | \mathbf{X}) p(h_j = 1 | y', \mathbf{X})$$

$$B(y, \mathbf{X}, \mathbf{h}, U_j) = - \sum_{y'} y' p(y' | \mathbf{X}) \sum_{\mathbf{h}'} p(\mathbf{h}' | y', \mathbf{X}) h_j = -p(y = 1 | \mathbf{X}) p(h_j = 1 | y = 1, \mathbf{X})$$

$C(y, \mathbf{X}, \mathbf{h}, \theta)$ Using CD-k Approximation

$$C(y, \mathbf{X}, \mathbf{h}, W_{j,k}^{(i)}) = -h_j 1_{(x_i=k)}$$

$$C(y, \mathbf{X}, \mathbf{h}, b_k^i) = -1_{(\hat{x}_i=k)}$$

$$C(y, \mathbf{X}, \mathbf{h}, d) = -\hat{y}$$

$$C(y, \mathbf{X}, \mathbf{h}, c_j) = -\hat{h}_j$$

$$C(y, \mathbf{X}, \mathbf{h}, U_j) = -\hat{h}_j \hat{y}$$

$$C(y, \mathbf{X}, \mathbf{h}, \theta) = \mathbb{E}_{p(y, \mathbf{X}, \mathbf{h})} \left[\frac{\partial E(y, \mathbf{X}, \mathbf{h})}{\partial \theta} \right] = \sum_{y', \mathbf{X}', \mathbf{h}'} p(y', \mathbf{X}', \mathbf{h}') \frac{\partial E(y', \mathbf{X}', \mathbf{h}')}{\partial \theta} \approx \frac{\partial E(\hat{y}, \hat{\mathbf{X}}, \hat{\mathbf{h}})}{\partial \theta}$$

$$C(y, \mathbf{X}, \mathbf{h}, W_{j,k}^{(i)}) = -\hat{h}_j 1_{(\hat{x}_i=k)}$$

$$C(y, \mathbf{X}, \mathbf{h}, b_k^i) = -1_{(\hat{x}_i=k)}$$

$$\begin{aligned}
C(y, \mathbf{X}, \mathbf{h}, d) &= -\hat{y} \\
C(y, \mathbf{X}, \mathbf{h}, c_j) &= -\hat{h}_j \\
C(y, \mathbf{X}, \mathbf{h}, U_j) &= -\hat{h}_j \hat{y}
\end{aligned}$$

Combine All

$$\frac{\ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial \theta} = -(1 + \alpha)A(y, \mathbf{X}, \mathbf{h}, \theta) + B(y, \mathbf{X}, \mathbf{h}, \theta) + \alpha C(y, \mathbf{X}, \mathbf{h}, \theta)$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial W_{j,k}^{(i)}} = 1_{(x_i=k)} \left\{ (1 + \alpha)p(h_j = 1|y, X) - \sum_{y'} p(y'|\mathbf{X})p(h_j = 1|y', \mathbf{X}) - \alpha \hat{h}_j \right\}$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial b_j^i} = \alpha [1_{(x_i=k)} - 1_{(\hat{x}_i=k)}]$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial d} = (1 + \alpha)y - p(y = 1|\mathbf{X}) - \alpha \hat{y}$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial c_i} = (1 + \alpha)p(h_j = 1|y, X) - \sum_{y'} p(y'|\mathbf{X})p(h_j = 1|y', \mathbf{X}) - \alpha \hat{h}_j$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial U_i} = (1 + \alpha)p(h_j = 1|y, \mathbf{X})y - p(y = 1|\mathbf{X})p(h_j = 1|y = 1, \mathbf{X}) - \alpha \hat{h}_j \hat{y}$$

CD-K Updates

```

 $X^{(0)} \leftarrow X, y^{(0)} \leftarrow y$ 
For t = 0, ..., k - 1 do

    For i = 1, ..., H do sample  $h_i^{(t)} \sim p(h_i = 1|y^{(t)}, X^{(t)})$ 

    For i = 1, ..., C do sample  $x_i^{(t+1)} \sim p(x_i|y^{(t)}, h^{(t)})$ 

    Do Sample  $y^{(t+1)} \sim p(y = 1|h^{(t)})$ 

For i = 1,...H do  $h_i^{(k)} \leftarrow p(h_i = 1|y^{(k)}, X^{(k)})$ 

```

Maximum Likelihood and the Delta Rule

- Maximum Likelihood

$$\ln L(\vec{\theta}|\vec{S}) = \ln \prod_{i=1}^l p(\vec{v}^i|\vec{\theta}) = \sum_{i=1}^l \ln p(\vec{v}^i|\vec{\theta})$$

- Mini-batch Gradient Ascent (Delta Rule)

$$\overrightarrow{\theta^{t+1}} = \overrightarrow{\theta^t} + \underbrace{\eta \frac{\partial}{\partial \overrightarrow{\theta^t}} \left[\sum_{i=1}^N \ln L(\overrightarrow{\theta^t}|\vec{v}^i) \right]}_{:= \Delta \overrightarrow{\theta^t}} - \lambda \overrightarrow{\theta^t} + \nu \Delta \overrightarrow{\theta^{t-1}}$$

Learning Algorithm

//CD-k, only if $\alpha \neq 0$

$X^{(0)} \leftarrow X, y^{(0)} \leftarrow y$

For $t = 0, \dots, k-1$ do

For $j = 1, \dots, H$ do sample $h_j^{(t)} \sim p(h_j = 1 | y^{(t)}, \mathbf{X}^{(t)}) = \sigma(\sum_{1 \leq i \leq C} W_{j, x_i^{(t)}}^{(i)} + c_j + U_j y^{(t)})$ [O(C+H)]

For $i = 1, \dots, C$ do sample $x_i^{(t+1)} \sim p(x_i = k | \mathbf{h}^{(t)}) = \frac{\exp(\sum_{1 \leq j \leq H} h_j^{(t)} W_{j, k}^{(i)})}{\sum_{1 \leq q \leq C} \exp(\sum_{1 \leq j \leq H} h_j^{(t)} W_{j, q}^{(i)})}$ (Computation Intensive! O(H*V))

Do Sample $y^{(t+1)} \sim p(y = 1 | \mathbf{h}^{(t)}) = \sigma(d + \mathbf{h}^{(t)T} \mathbf{U})$ [O(H)]

For $i = 1, \dots, H$ do $h_i^{(k)} \leftarrow p(h_i = 1 | y^{(k)}, X^{(k)}) = \sigma(\sum_{1 \leq i \leq C} W_{j, x_i^{(k)}}^{(i)} + c_j + U_j y^{(k)})$ [O(H)]

//Gradient Calculation

$\hat{y} \leftarrow y^{(k)}, \hat{X} \leftarrow X^{(k)}, \hat{h} \leftarrow h^{(k)}$

$$p(h_j = 1 | y, X) = \sigma\left(\sum_{1 \leq i \leq C} W_{j, x_i}^{(i)} + c_j + U_j y\right)$$

$$p(y = 1 | X) = \frac{\exp\{dy + \sum_{1 \leq k \leq H} \text{softplus}(\sum_{1 \leq i \leq C} W_{k, x_i}^{(i)} + c_k + U_k y)\}}{\exp\{\sum_{1 \leq k \leq H} \text{softplus}(\sum_{1 \leq i \leq C} W_{k, x_i}^{(i)} + c_k)\} + \exp\{d + \sum_{1 \leq k \leq H} \text{softplus}(\sum_{1 \leq i \leq C} W_{k, x_i}^{(i)} + c_k + U_k)\}}$$

[O(H*C)]

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial W_{j, k}^{(i)}} = \mathbf{1}_{(x_i=k)} \left\{ (1 + \alpha) p(h_j = 1 | y, X) - \sum_{y'} p(y' | X) p(h_j = 1 | y', X) - \alpha \widehat{h}_j \right\}$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial b_j^i} = \alpha [1_{(x_i=k)} - 1_{(\widehat{x}_i=k)}]$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial d} = (1 + \alpha) y - p(y = 1 | X) - \alpha \widehat{y}$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial c_i} = (1 + \alpha) p(h_j = 1 | y, X) - \sum_{y'} p(y' | X) p(h_j = 1 | y', X) - \alpha \widehat{h}_j$$

$$\frac{\partial \ln \text{Hybrid}(\alpha, y, \mathbf{X})}{\partial U_i} = (1 + \alpha) p(h_j = 1 | y, X) y - p(y = 1 | X) p(h_j = 1 | y = 1, X) - \alpha \widehat{h}_j \widehat{y}$$

//Parameter Update

$$\overrightarrow{\theta^{t+1}} = \overrightarrow{\theta^t} + \eta \underbrace{\frac{\partial}{\partial \overrightarrow{\theta^t}} \left[\sum_{i=1}^N \ln L(\overrightarrow{\theta^t} | \overrightarrow{v^i}) \right]}_{:= \Delta \overrightarrow{\theta^t}} - \lambda \overrightarrow{\theta^t} + \nu \Delta \overrightarrow{\theta^{t-1}}$$

[Note, storing two sets of parameters would be memory hungry, store the differences only??]

Note:

Efficient calculation of the following is the key to the performance of CD-k!

Naïve implementation requires $O(|X| * |H|)$

$$x_i^{(t+1)} \sim p(x_i = k | \mathbf{h}^{(t)}) = \frac{\exp\left(\sum_{1 \leq j \leq H} \mathbf{h}_j^{(t)} \mathbf{w}_{j,k}^{(i)}\right)}{\sum_{1 \leq q \leq C_i} \exp\left(\sum_{1 \leq j \leq H} \mathbf{h}_j^{(t)} \mathbf{w}_{j,q}^{(i)}\right)}, 1 \leq k \leq C_i$$

Use Mini-batch + Cache Strategy??

Nonexact sampling?? MCMC??? Importance Sampling, rejection sampling etc to avoid the normalization constant? ????

What else??

SparseClassRBM Verses Logistic Regression

Note that in logistic regression, we have:

$$p(y|X) = \frac{\exp\{y(W^T x + c)\}}{1 + \exp\{W^T x + c\}}$$

And for SparseClassRBM, we have

$$p(y|X) = \frac{\exp\{dy\} \prod_{1 \leq k \leq H} \sum_{\mathbf{h}_k \in \{0,1\}} \exp\{\mathbf{h}_k [\sum_{1 \leq i \leq C} \mathbf{w}_{k,x_i}^{(i)} + c_k + U_k y]\}}{\sum_{y'} \exp\{dy'\} \prod_{1 \leq k \leq H} \sum_{\mathbf{h}_k \in \{0,1\}} \exp\{\mathbf{h}_k [\sum_{1 \leq i \leq C} \mathbf{w}_{k,x_i}^{(i)} + c_k + U_k y']\}}$$

Setting $H=1$, $\mathbf{h}_1 = 1, d=1, U = 0$, we have

$$p(y|X) = \frac{\exp\{y (\sum_{1 \leq i \leq C} \mathbf{w}_{x_i}^{(i)} + c)\}}{1 + \exp\{\sum_{1 \leq i \leq C} \mathbf{w}_{x_i}^{(i)} + c\}}$$

which is a form of logistic regression.

Therefore, we can view logistic regression as a special form of RBM with less variables.