Fachgebiet Maschinelles Lernen Institut für Softwaretechnik und theoretische Informatik Fakultät IV, Technische Universität Berlin Prof. Dr. Klaus-Robert Müller

Email: klaus-robert.mueller@tu-berlin.de

Exercise Sheet 15

Exercise 1: RBM with Ternary Hidden Units (20 + 10 P)

We consider a variant of the restricted Boltzmann machine with ternary hidden units $h \in \{-1,0,1\}^H$. Input features remain binary, i.e. $x \in \{0,1\}^d$, like for the classical RBM. The probability model is given by:

$$p(\boldsymbol{x}, \boldsymbol{h}|\theta) = \frac{1}{\mathcal{Z}} \exp\left(\sum_{j=1}^{H} \boldsymbol{w}_{j}^{\top} \boldsymbol{x} \cdot h_{j} + \sum_{j=1}^{H} h_{j} b_{j}\right)$$

where $\theta = (\boldsymbol{w}_j, b_j)_{j=1}^H$ are the parameters of the model, and where and \mathcal{Z} is the partition function that normalizes the probability distribution to 1.

(a) Show that this modified RBM can also be expressed as a product of experts

$$p(\boldsymbol{x}|\theta) = \frac{1}{\mathcal{Z}} \prod_{j=1}^{H} g_j(\boldsymbol{x}, \theta_j),$$

with

$$g_j(\boldsymbol{x}, \theta_j) = 1 + 2 \cosh(\boldsymbol{w}_j^{\top} \boldsymbol{x} + b_j),$$

where cosh is the hyperbolic cosine function.

(b) Show that the gradient of the log-likelihood assigned to some data point x_n by the modified RBM has the form

$$\forall_{j=1}^{H}: \frac{\partial \log p(\boldsymbol{x}_{n}|\boldsymbol{\theta})}{\partial \boldsymbol{w}_{j}} = \boldsymbol{x}_{n} \cdot \sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x}_{n} + b_{j}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\theta})} [\boldsymbol{x} \cdot \sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})]$$

$$\forall_{j=1}^{H}: \frac{\partial \log p(\boldsymbol{x}_{n}|\boldsymbol{\theta})}{\partial b_{i}} = \sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x}_{n} + b_{j}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\theta})} [\sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})]$$

where
$$\sigma(t) = \frac{\sinh(t)}{0.5 + \cosh(t)}$$
.

Exercise 2: Product of Gaussian Mixture Models (20 + 10 P)

Consider the product of experts:

$$p(\boldsymbol{x}|\theta) = \frac{1}{\mathcal{Z}} \prod_{j=1}^{H} g_j(\boldsymbol{x}, \theta_j)$$

where each expert is a Gaussian mixture model in d-dimensions, and where each element of the mixture is Gaussian with identity covariance:

$$\forall_{j=1}^{H}: g_{j}(\boldsymbol{x}, \theta_{j}) = \sum_{k=1}^{C} \alpha_{jk} \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2} \|\boldsymbol{x} - \boldsymbol{\mu}_{jk}\|^{2}\right).$$

(a) Show that $p(\mathbf{x}|\theta)$ can be rewritten as a mixture of C^H elements, where each mixture element (indexed by the vector $\mathbf{k} \in \{1, \dots, C\}^H$) has center

$$m_{oldsymbol{k}} = rac{1}{H} \sum_{j=1}^{H} oldsymbol{\mu}_{jk_j}.$$

(b) Give the centers m_k of the mixture model equivalent to a product of two mixture models, where each mixture model in the product has 2 elements, where the first mixture has the two-dimensional centers $\mu_{11} = \binom{2}{0}$ and $\mu_{12} = \binom{4}{0}$, and where the second mixture has the two-dimensional centers $\mu_{21} = \binom{0}{2}$ and $\mu_{22} = \binom{0}{4}$.

Exercise 3: Programming (40 P)

Download the programming files on ISIS and follow the instructions.

Exercise 1: RBM with Ternary Hidden Units (20 + 10 P)

We consider a variant of the restricted Boltzmann machine with ternary hidden units $\mathbf{h} \in \{-1,0,1\}^H$. Input features remain binary, i.e. $\mathbf{x} \in \{0,1\}^d$, like for the classical RBM. The probability model is given by:

$$p(\boldsymbol{x}, \boldsymbol{h} | \theta) = \frac{1}{\mathcal{Z}} \exp \left(\sum_{j=1}^{H} \boldsymbol{w}_{j}^{\top} \boldsymbol{x} \cdot h_{j} + \sum_{j=1}^{H} h_{j} b_{j} \right)$$

where $\theta = (\boldsymbol{w}_j, b_j)_{j=1}^H$ are the parameters of the model, and where and \mathcal{Z} is the partition function that normalizes the probability distribution to 1.

(a) Show that this modified RBM can also be expressed as a product of experts

$$p(\boldsymbol{x}|\theta) = \frac{1}{\mathcal{Z}} \prod_{j=1}^{H} g_j(\boldsymbol{x}, \theta_j),$$

with

$$g_j(\boldsymbol{x}, \theta_j) = 1 + 2 \cosh(\boldsymbol{w}_j^{\top} \boldsymbol{x} + b_j),$$

where cosh is the hyperbolic cosine function.

$$P(x | \Theta) = \sum_{h \in \{4,0,4\}^{H}} P(x,h | \Theta) = \sum_{h \in \{4,0,4\}^{H}} \frac{1}{2} \cdot exp(\sum_{j=4}^{H} w_{j}^{T} x \cdot h_{j} + \sum_{j=4}^{H} h_{j}b_{j})$$

$$= \sum_{h \in \{4,0,4\}^{H}} \frac{1}{2} \cdot exp(\sum_{j=4}^{H} [(w_{j}^{T} x + b_{j})h_{j}])$$

$$= \sum_{h \in \{4,0,4\}^{H}} \frac{1}{2} \cdot exp((w_{j}^{T} x + b_{j})h_{j})$$

$$= \sum_{j=4}^{H} \prod_{h \in \{4,0,4\}^{H}} exp((w_{j}^{T} x + b_{j})h_{j})$$

$$= \sum_{j=4}^{H} \prod_{h \in \{4,0,4\}^{H}} exp((w_{j}^{T} x + b_{j})h_{j})$$

$$= \sum_{j=4}^{H} \prod_{h \in \{4,0,4\}^{H}} (A + exp(-(w_{j}^{T} x + b_{j})) + exp(w_{j}^{T} x + b_{j}))$$

$$= \sum_{j=4}^{H} \prod_{h \in \{4,0,4\}^{H}} (A + exp(-(w_{j}^{T} x + b_{j})) + exp(w_{j}^{T} x + b_{j}))$$

$$\begin{split} p(\boldsymbol{x}|\boldsymbol{\theta}) &= \sum_{\boldsymbol{h} \in \{-1,0,1\}^H} p(\boldsymbol{x},\boldsymbol{h}|\boldsymbol{\theta}) \\ &= \sum_{\boldsymbol{h} \in \{-1,0,1\}^H} \frac{1}{Z} \exp\left(\sum_{j=1}^H \boldsymbol{w}_j^\top \boldsymbol{x} \cdot h_j + \sum_{j=1}^H h_j b_j\right) \\ &= \sum_{\boldsymbol{h} \in \{-1,0,1\}^H} \frac{1}{Z} \exp\left(\sum_{j=1}^H (\boldsymbol{w}_j^\top \boldsymbol{x} + b_j) \cdot h_j\right) \\ &= \frac{1}{Z} \sum_{\boldsymbol{h} \in \{-1,0,1\}^H} \prod_{j=1}^H \exp\left((\boldsymbol{w}_j^\top \boldsymbol{x} + b_j) \cdot h_j\right) \\ &= \frac{1}{Z} \sum_{h_1 \in \{-1,0,1\}} \dots \sum_{h_H \in \{-1,0,1\}} \prod_{j=1}^H \exp\left((\boldsymbol{w}_j^\top \boldsymbol{x} + b_j) \cdot h_j\right) \\ &= \frac{1}{Z} \prod_{j=1}^H \sum_{h_j \in \{-1,0,1\}} \exp\left((\boldsymbol{w}_j^\top \boldsymbol{x} + b_j) \cdot h_j\right) \\ &= \frac{1}{Z} \prod_{j=1}^H \left(1 + \exp(\boldsymbol{w}_j^\top \boldsymbol{x} + b_j) + \exp(-(\boldsymbol{w}_j^\top \boldsymbol{x} + b_j))\right) \\ &= \frac{1}{Z} \prod_{j=1}^H \left(\frac{1 + 2 \cosh(\boldsymbol{w}_j^\top \boldsymbol{x} + b_j)}{g_j(\boldsymbol{x},\boldsymbol{\theta}_j)}\right) \end{split}$$

(b) Show that the gradient of the log-likelihood assigned to some data point x_n by the modified RBM has the form

 $= \underbrace{1}_{J_{1}}^{H} \underbrace{g(x, \theta_{j})}_{J_{2}} \qquad \qquad \underbrace{2}_{K = \underbrace{1}_{J_{2}, A}}^{H} \underbrace{\frac{H}{I}}_{J_{2}} \underbrace{g_{j}(x, \theta_{j})}_{J_{2}}$

$$\forall_{j=1}^{H}: \frac{\partial \log p(\boldsymbol{x}_{n}|\boldsymbol{\theta})}{\partial \boldsymbol{w}_{j}} = \boldsymbol{x}_{n} \cdot \sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x}_{n} + b_{j}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\theta})} [\boldsymbol{x} \cdot \sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})]$$

$$\forall_{j=1}^{H}: \frac{\partial \log p(\boldsymbol{x}_{n}|\boldsymbol{\theta})}{\partial b_{j}} = \sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x}_{n} + b_{j}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\theta})} [\sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})]$$

where $\sigma(t) = \frac{\sinh(t)}{0.5 + \cosh(t)}$.

$$P(X_{N} | \Theta) = \frac{1}{2} \prod_{i=1}^{N} (A + 2 \cosh(W_{i}^{T} X_{N} + b_{j} I))$$

$$= \frac{1}{2} \log_{2} (A + 2 \cosh(W_{i}^{T} X_{N} + b_{j} I)) - \log_{2} = \sum_{j=1}^{N} \log_{2} (G_{j}(X_{i} \Theta_{j})) - \log_{2$$

 $= \frac{\Lambda}{2} \cdot \sum_{X \in \mathcal{T}_{b,A}, A} \left(\prod_{i \neq j} g_{j}(x, \Theta_{i}) \right) \cdot 2 s_{i, b}(w_{j}^{T} X + b_{j}) \cdot X$

$$= \frac{\sum_{x_{m} \in \{a_{m}\}^{3}} \sum_{x_{m} \in \{a_{m}\}^{3}}$$

(b) We build upon the PoE formulation from exercise 1(a), which we rewrite as follows:

$$p(\boldsymbol{x}|\boldsymbol{\theta}) = \frac{1}{\mathcal{Z}} \prod_{j=1}^{H} \left(1 + 2 \cosh(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j}) \right) = \frac{1}{\mathcal{Z}} \exp\left(\log \prod_{j=1}^{H} (1 + 2 \cosh(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})) \right)$$

$$= \frac{1}{\mathcal{Z}} \exp\left(f(\boldsymbol{x}, \boldsymbol{\theta}) \right) = \frac{\exp\left(f(\boldsymbol{x}, \boldsymbol{\theta}) \right)}{\sum_{\boldsymbol{x} \in \{0,1\}^{d}} \exp\left(f(\boldsymbol{x}, \boldsymbol{\theta}) \right)},$$

where in the last step we expanded the normalization constant \mathcal{Z} . Therefore, the log-likelihood has the following form:

$$\log p(\boldsymbol{x}_n|\boldsymbol{\theta}) = f(\boldsymbol{x}_n,\boldsymbol{\theta}) - \log \sum_{\boldsymbol{x} \in \{0,1\}^d} \exp \big(f(\boldsymbol{x},\boldsymbol{\theta})\big)$$

We use this form to compute the gradient as follows:

$$\nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{x}_{n}|\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}_{n},\boldsymbol{\theta}) - \nabla_{\boldsymbol{\theta}} \log \sum_{\boldsymbol{x} \in \{0,1\}^{d}} \exp \left(f(\boldsymbol{x},\boldsymbol{\theta}) \right)$$

$$= \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}_{n},\boldsymbol{\theta}) - \frac{1}{\sum_{\boldsymbol{x} \in \{0,1\}^{d}} \exp \left(f(\boldsymbol{x},\boldsymbol{\theta}) \right)} \cdot \sum_{\boldsymbol{x} \in \{0,1\}^{d}} \exp \left(f(\boldsymbol{x},\boldsymbol{\theta}) \right) \cdot \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x},\boldsymbol{\theta})$$

$$= \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}_{n},\boldsymbol{\theta}) - \sum_{\boldsymbol{x} \in \{0,1\}^{d}} \frac{\exp \left(f(\boldsymbol{x},\boldsymbol{\theta}) \right)}{\sum_{\boldsymbol{y} \in \{0,1\}^{d}} \exp \left(f(\boldsymbol{y},\boldsymbol{\theta}) \right)} \cdot \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x},\boldsymbol{\theta})$$

$$= \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}_{n},\boldsymbol{\theta}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\theta})} [\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x},\boldsymbol{\theta})]$$

That is,

$$\nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{x}_n | \boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}_n, \boldsymbol{\theta}) - \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x} | \boldsymbol{\theta})} [\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta})]$$
(1)

Remember our definition of $f(x, \theta)$:

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \log \prod_{j=1}^{H} (1 + 2 \cosh(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})) = \sum_{j=1}^{H} \log(1 + 2 \cosh(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j}))$$
(2)

Therefore, the corresponding gradients are given as:

$$\nabla_{\boldsymbol{w}_{j}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \underbrace{\frac{2 \sinh(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})}{1 + 2 \cosh(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})}}_{\sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j})} \boldsymbol{x} = \sigma(\boldsymbol{w}_{j}^{\top} \boldsymbol{x} + b_{j}) \cdot \boldsymbol{x}$$
(3)

$$\frac{\partial f(\boldsymbol{x}, \boldsymbol{\theta})}{\partial b_j} = \underbrace{\frac{2 \sinh(\boldsymbol{w}_j^{\top} \boldsymbol{x} + b_j)}{1 + 2 \cosh(\boldsymbol{w}_j^{\top} \boldsymbol{x} + b_j)}}_{\sigma(\boldsymbol{w}_j^{\top} \boldsymbol{x} + b_j)} = \sigma(\boldsymbol{w}_j^{\top} \boldsymbol{x} + b_j)$$
(4)

Inserting (3) and (4) into (1) gives our target form.

Exercise 2: Product of Gaussian Mixture Models (20+10 P)

Consider the product of experts:

$$p(\boldsymbol{x}|\theta) = \frac{1}{\mathcal{Z}} \prod_{j=1}^{H} g_j(\boldsymbol{x}, \theta_j)$$

where each expert is a Gaussian mixture model in d-dimensions, and where each element of the mixture is Gaussian with identity covariance:

$$\forall_{j=1}^{H}: g_{j}(\boldsymbol{x}, \theta_{j}) = \sum_{k=1}^{C} \alpha_{jk} \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2} \|\boldsymbol{x} - \boldsymbol{\mu}_{jk}\|^{2}\right).$$

(a) Show that $p(\mathbf{x}|\theta)$ can be rewritten as a mixture of C^H elements, where each mixture element (indexed by the vector $\mathbf{k} \in \{1, \dots, C\}^H$) has center

$$\boldsymbol{m_k} = \frac{1}{H} \sum_{i=1}^{H} \boldsymbol{\mu}_{jk_j}.$$

$$P(x|\theta) = \frac{1}{4} + \frac{1}{12} \cdot \frac{12} \cdot \frac{1}{12} \cdot \frac{1}{12} \cdot \frac{1}{12} \cdot \frac{1}{12} \cdot \frac{1}{12} \cdot \frac{1}$$

(b) Give the centers m_k of the mixture model equivalent to a product of two mixture models, where each mixture model in the product has 2 elements, where the first mixture has the two-dimensional centers $\mu_{11} = \binom{2}{0}$ and $\mu_{12} = \binom{4}{0}$, and where the second mixture has the two-dimensional centers $\mu_{21} = \binom{0}{2}$ and $\mu_{22} = \binom{0}{4}$.

$$m{m_k} = rac{1}{H} \sum_{j=1}^{H} m{\mu}_{jk_j}.$$
 index k is a vector !

$$R = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \qquad MR = \frac{1}{2} \cdot \left(\mu_{1} R_{1} + \mu_{2} R_{2} \right) = \frac{1}{2} \left(\mu_{1} \Lambda + \mu_{2} \Lambda \right) = \frac{1}{2} \left[\begin{pmatrix} 2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 2 \end{pmatrix} \right] = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$R = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$
 $M_{k} = \frac{1}{2} \left(\mu_{AA} + \mu_{22} \right) = \frac{1}{2} \left[\begin{pmatrix} 2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \psi \end{pmatrix} \right] = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$

$$R = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \qquad MR = \begin{pmatrix} 2 \\ 5 \\ 1 \end{pmatrix} \mu_{AA} + \mu_{AA} = \begin{pmatrix} 2 \\ 5 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$k = {2 \choose 2}$$
 $M_K = \frac{1}{2} [M_{A2} + M_{22}] = {2 \choose 2}$