FYS4411/9411, APRIL 27, 2023

BM

- deep generative models
  - optimize $p(x;\theta)$

$$\hat{\theta} = \arg\max_{\theta} \log p(x;\theta)$$

  - unsupervised learning
  - Boltzmann machine

$$p(x;\theta) = \frac{\tilde{p}(x;\theta)}{Z(\theta)}$$

$$p(x;\theta) = \frac{\int dh\, e^{-\beta E(x,h;\theta)}}{Z(\theta)}$$

$$Z(\theta) = \int dh \int dx\, e^{-\beta E(x,h;\theta)}$$

The optimization involves the calculation of $\nabla_\theta \log p(x;\theta)$

$$p(x,h;\theta) = \frac{e^{-\beta E(x,h;\theta)}}{Z(\theta)}$$

marginal probabilities

$$p(x;\theta) = \int dh\, p(x,h;\theta)$$

$$p(h;\theta) = \int dx\, p(x,h;\theta)$$

$$\left(\sum_h p(x,h;\theta) \Big/ \sum_x p(x,h;\theta) \right)$$

<u>algorithm</u>

- set η learning rate
  (Newton-Raphson's root searching)
- set # of MC-cycles

while not converged
- sample a batch of examples
  $\{x_1, x_2, \ldots, x_m\}$
- compute gradient
  $\nabla_\theta = \nabla_\theta \log p(x;\theta) = g$

for $i = 1$ to # MC
  for $j = 1$ to m
    x_j given by Metropolis / Gibbs sampling
  end
end

$\theta \leftarrow \theta + \eta \nabla_\theta \log p(x;\theta)$

end while
gives $\hat{\theta}$

$$\nabla_\theta \log p(x;\theta) = \nabla_\theta \log \tilde{p}(x;\theta) - \nabla_\theta \log Z(\theta)$$

From last week

$$\nabla_\theta \log Z(\theta) = \mathbb{E}\left[\nabla_\theta \log \tilde{p}(x;\theta)\right]$$

Detailed discussion of $\nabla_\theta \log Z(\theta)$ in Goodfellow et al chapter 18

- our case

$$p(x,h;\theta) = \frac{e^{-E(x,h;\theta)}}{Z(\theta)}$$

$$|\psi_T(x;\theta)|^2 = p(x;\theta)$$

$$p(x;\theta) = \int dh\, p(x,h;\theta)$$

- minimize $\mathbb{E}[E_L(\theta)]$

$$= \int dx\, p(x;\theta)\, E_L(x;\theta)$$

$$\simeq \frac{1}{MC} \sum_i E_L(x_i;\theta)$$

Same function as in P1

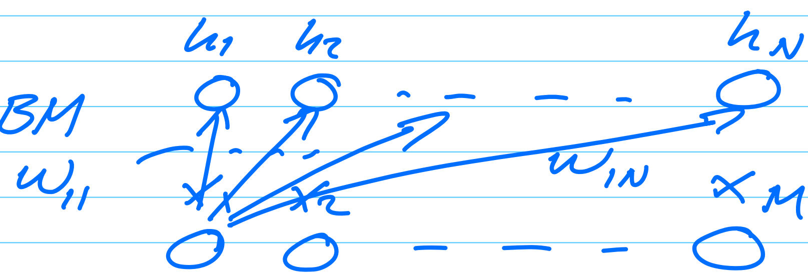
Compared with neural networks, there is no Backpropagation/automatic differentiation.

$$\nabla_\theta \mathbb{E}[E_L(\theta)] \rightarrow$$

$$\frac{\partial \langle E_L \rangle}{\partial \theta_i} = 2\left[\langle E_L \cdot \frac{1}{\psi} \frac{\partial \psi}{\partial \theta_i} \rangle - \langle E_L \rangle \langle \frac{1}{\psi} \frac{\partial \psi}{\partial \theta_i} \rangle \right]$$

$$\frac{1}{\psi} \frac{\partial \psi}{\partial \theta_i} = \frac{\partial \ln \psi}{\partial \theta_i}$$

RBM



$$p(x;\theta) = \frac{\tilde{p}(x;\theta)}{Z(\theta)}$$

$$\tilde{p}(x;\theta) = \int dh\, e^{-E(x,h;\theta)}$$

$$\left(\sum_h e^{-E(x,h;\theta)} \right.$$

biases

$$E(x, h; \theta) = \sum_{i=1}^{M} a_i x_i$$

$$+ \sum_{j=1}^{N} b_j h_j$$

$$+ \sum_{ij}^{MN} x_i w_{ij} h_j$$

weights

$$\theta = \{a, b, W\}$$

2-particles in 2-dim $\Rightarrow$

$M = 4 \quad (x_1, x_2, x_3, x_4)$

$E(x, h; \theta) = ?$

x is a continuous variable (gaussian)

h is a binary variable $\{0, 1\}$

$E(x, h; \theta)$ given by a Gaussian-Binary RBM

$$E(x, h; \theta) = \sum_{i=1}^{M} \frac{(x_i - a_i)^2}{2\sigma_i^2}$$

$(\sigma_i = 1)$

$$+ \sum_{j=1}^{N} b_j h_j + \sum_{ij} x_i w_{ij} h_j$$

Can assume

$$|\psi_T(x;\theta)|^2 =$$

$$\frac{1}{\sqrt{Z}} \sqrt{\sum_{\{h_j\}} e^{-E(x,h_j;\theta)}}$$

$$= \frac{1}{\sqrt{Z}} e^{-\sum_{i=1}^{M} (x_i - a_i)^2}$$

$$\times \prod_{j=1}^{N} \sqrt{1 + e^{b_j + \sum_{i=1}^{M} x_i w_{ij}}}$$

$$h_j = \{0, 1\}$$

$$\ln \psi_T(x;\theta) =$$

$$-\frac{1}{2} \ln Z - \sum_{i=1}^{M} \frac{(x_i - a_i)^2}{4\sigma_i^2}$$

$$+ \frac{1}{2} \sum_{j=1}^{N} \ln\left(1 + e^{b_j + \sum_{i=1}^{M} x_i w_{ij}}\right)$$

when optimizing:

$$\frac{\partial \ln \psi}{\partial a_i} = \frac{1}{2\sigma^2}(x_i - a_i)$$

$$\frac{\partial \ln \psi}{\partial b_j} = \frac{1}{2\left(e^{-b_j - \frac{1}{\sigma^2}\sum_{i=1}^{M}(x_i w_{ij})} + 1\right)}$$

$$\frac{\partial \ln \psi}{\partial w_{ij}} = \frac{x_i}{2\sigma^2\left(e^{-b_j - \frac{1}{\sigma^2}\sum_{i=1}^{M} x_i w_{ij}} + 1\right)}$$

$$\left[\quad N(\mu, \sigma) \sim e^{-\frac{(x-\mu)^2}{2\sigma^2}}\quad\right]$$

$$E_L = \frac{1}{\psi} H \psi$$

$$= \frac{1}{\psi}\left[\sum_{i=1}^{n}\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}w^2 r_i^2\right) + \sum_{i<j} v(r_{ij})\right]\psi$$

$$E_L = \frac{1}{2}\sum_{i=1}^{n}\left(-\left[\frac{\partial \ln \psi}{\partial x_i}\right]^2 - \frac{\partial^2}{\partial x_i^2}\ln \psi + w^2 r_i^2\right)$$

$$+ \sum_{i<j} v(r_{ij})$$

$$\frac{\partial \ln \psi}{\partial x_i} \qquad \frac{\partial^2 \ln \psi}{\partial x_i^2} \quad ,$$

See Jupyter-notebook for final expression.