FYS4411, APRIL 7, 2022

P2: – Boltzmann machines
– Neural Networks

P1: $\psi_T(\vec{R};\vec{\alpha})$

$$= \left[\prod_{i=1}^{N} \varphi_i(\vec{r}_i;\vec{\alpha})\right] \psi_C(\vec{R};\vec{\alpha})$$

alternative 1:

Boltzmann machines (BM)

NN = neural network

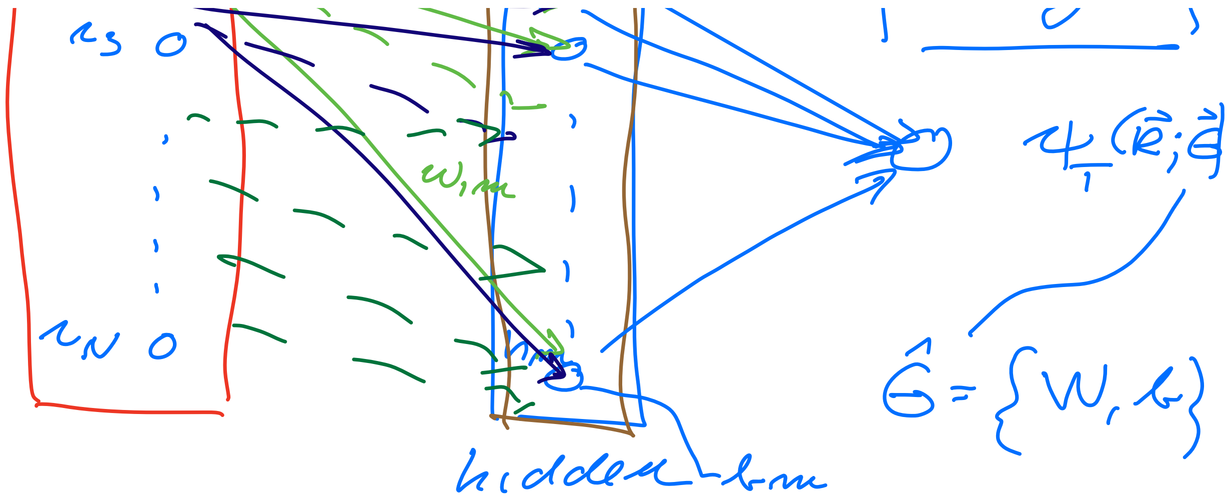
alternative 2:

$\psi_T(\vec{R};\vec{\alpha})$: NN or BM

Boltzmann machines

Basics of a NN

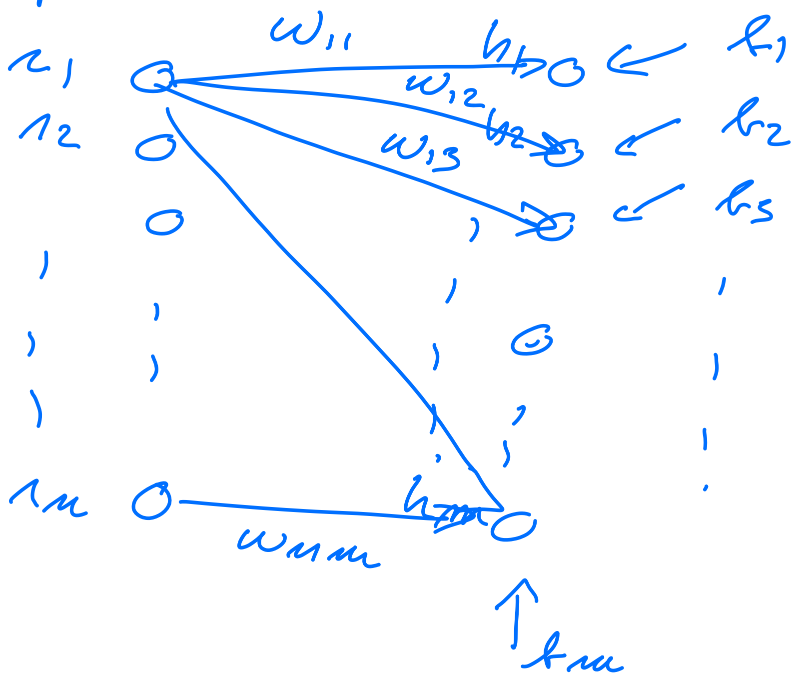
input layer : $\vec{R}$ (1-Dim)



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

Boltzmann machines

input layer hidden layer



unknown parameters

$W \in \mathbb{R}^{n \times m}$

$\begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} \end{bmatrix}$

$$W = \begin{bmatrix} & \vdots & \\ w_{m1} & \cdots & w_{mm} \end{bmatrix}$$

$$b^T = [b_1, b_2, \ldots b_m]$$

$$|\psi_T(\vec{R}; \Theta)|^2 \qquad \Theta = \{W, b\}$$

$$= P(\vec{R}; \Theta) = \frac{1}{Z} e^{-\frac{1}{T} E(\vec{R}; \Theta)}$$

(alternative 2)

$$P(\vec{R}; \Theta) \rightarrow P(x, h)$$

input values   hidden nodes

$$Z = \iint dx\,dh\; e^{-\frac{1}{T} E(x,h)}$$

$$|\psi_T(x)|^2 = \int dh\; P(x, h)$$

marginal probability

$$E(x, h) = ?$$

Binary-Binary BM

$$E(x, h) = -\sum^{n} x_i a_i - \sum^{m} b_i h_i$$

$i=1$) $\quad\quad j=1$)

$$\left(x_i = \{0,1\} \qquad h_j = \{0,1\} \right)$$

$$- \sum_{ij}^{nm} w_{ij} x_i h_j$$

Gaussian-binary

$$E(x,h) = \sum_{i=1}^{n} \frac{(x_i - a_i)^2}{2\sigma_i^2} - \sum_{j=1}^{m} b_j h_j - \sum_{ij}^{nm} \frac{x_i w_{ij} h_j}{\sigma_{ij}^2}$$

$$\sigma_{ij}^2 = \sigma_i^2 = 1$$