Lecture FYS4411, April 12, 2024

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$$P(x,h;\theta) = \frac{f(x,h;\theta)}{Z(\theta)}$$

$$Z(\theta) = \sum_{x}\sum_{h} f(x,h;\theta)$$

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

Energy model

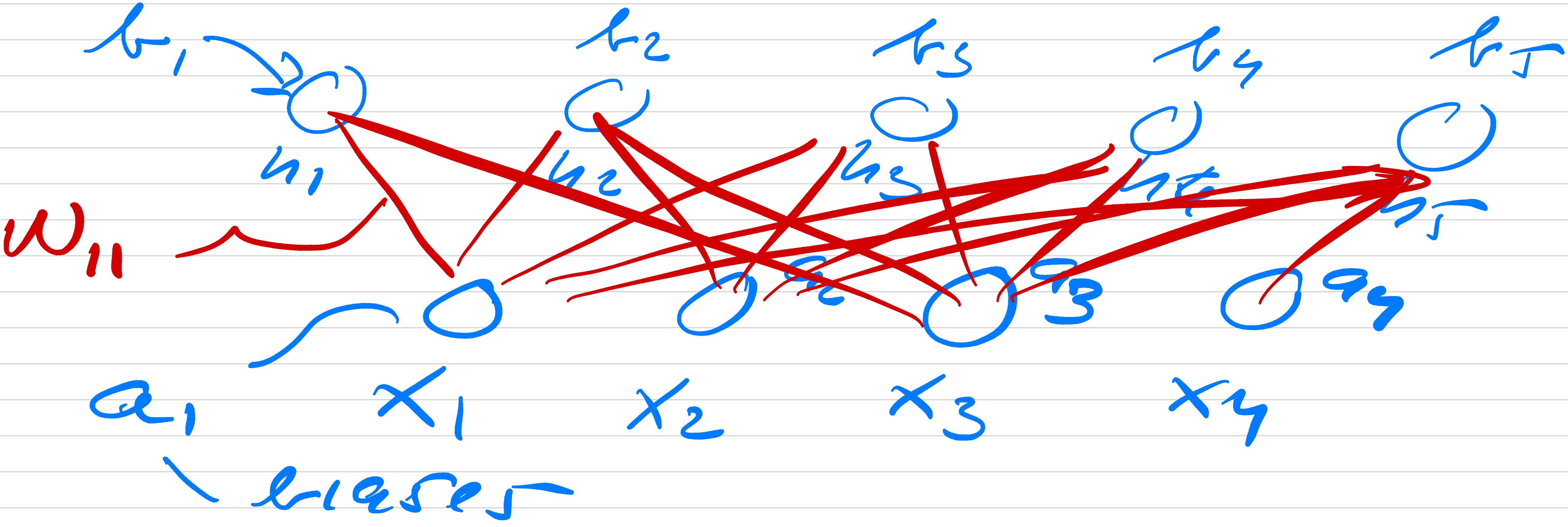
$$\tilde{E}_{BB} = -\left(\sum_{i=1}^{M} a_i x_i + \sum_{j=1}^{N} b_j h_j + \sum_{ij}^{MN} x_i w_{ij} h_j\right)$$

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

RBM

$$a \in \mathbb{R}^M \qquad b \in \mathbb{R}^N$$

$$W \in \mathbb{R}^{M \times N}$$



$$\tilde{E}_{BB}(x, h) = -(a^T x + b^T h + x^T W h)$$

$x_i = \{0, 1\}$ Binary

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

$$Z(\theta) = \sum_{x h} e^{a^T x + b^T h + x^T W h}$$

$$|\psi_T|^2 \sim p(x;\hat{\theta})$$

$$p(x;\theta) = \frac{1}{Z(\theta)} \sum_h e^{a^T x + b^T h + x^T W h}$$

$$= \frac{e^{a^T x}}{Z(\theta)} \sum_h e^{b^T h + x^T W h}$$

$$= \frac{e^{a^T x}}{Z(\theta)} \sum_h e^{\sum_{j=1}^{N} (b_j' + x^T W_{*j}) h_j}$$

$$= -\!\!\!\;|\!\!\;- \sum_h \prod_{j=1}^{N} e^{(b_j' + x^T W_{*j}) h_j'}$$

$$= \frac{1}{Z(\theta)} e^{a^T x} \left(\sum_{h_1=\{0,1\}} e^{(b_1 + x^T W_{*1}) h_1} \right)$$

$$\times \left(\sum_{h_2=\{0,1\}} e^{(b_2 + x^T W_{*2}) h_2} \right)$$

$$\times \cdots \times \left(\sum_{h_N=\{0,1\}} e^{(b_N + x^T W_{*N}) h_N} \right)$$

$$1 + e^{b_N + x^T W_{*N}}$$

$$\lim_{r_{12}\to 0}\left(-\frac{1}{r_{12}}\frac{d}{dr_{12}} + \frac{1}{r_{12}}\right)\psi(r_{12}) = 0$$

$$\frac{d}{dr_{12}}\psi(r_{12}) = \psi(r_{12})$$

$$\psi(r_{12}) \propto e^{r_{12}}$$

$l = 0$, $\uparrow \sqrt{4\pi}$

Hydrogen : $L_\alpha(r)\, e^{-r}\, P_{nlm}(\theta,\varphi)$

α

Laguerre

$$\psi_T(\vec{r}_1, \vec{r}_2) = C\, e^{-\alpha^2(r_1^2 + r_2^2)}$$

$$\times\, e^{\frac{r_{12}}{1+\beta r_{12}}}$$

$$e^{\beta r_{12}}$$

$$e^{-r}$$