20 심층 생성 모형

20.1 볼츠만 기계

$$P(\boldsymbol{x}) = \frac{\exp(-E(\boldsymbol{x}))}{Z}.$$

$$E(\boldsymbol{x}) = -\boldsymbol{x}^\top \boldsymbol{U}\boldsymbol{x} - \boldsymbol{b}^\top \boldsymbol{x}.$$

$$E(\boldsymbol{v},\boldsymbol{h}) = -\boldsymbol{v}^\top \boldsymbol{R}\boldsymbol{v} - \boldsymbol{v}^\top \boldsymbol{W}\boldsymbol{h} - \boldsymbol{h}^\top \boldsymbol{S}\boldsymbol{h} - \boldsymbol{b}^\top \boldsymbol{v} - \boldsymbol{c}^\top \boldsymbol{h}.$$

20.2 제한 볼츠만 기계

$$P(\mathrm{v}=\boldsymbol{v},\mathrm{h}=\boldsymbol{h})=\frac{1}{Z}\exp(-E(\boldsymbol{v},\boldsymbol{h})).$$

$$E(\boldsymbol{v},\boldsymbol{h})=-\boldsymbol{b}^\top\boldsymbol{v}-\boldsymbol{c}^\top\boldsymbol{h}-\boldsymbol{v}^\top\boldsymbol{W}\boldsymbol{h}.$$

$$Z=\sum_{\boldsymbol{v}}\sum_{\boldsymbol{h}}\exp\{-E(\boldsymbol{v},\boldsymbol{h})\}.$$

20.2.1 조건부 분포

$$P(\boldsymbol{h}|\boldsymbol{v}) = \frac{P(\boldsymbol{h},\boldsymbol{v})}{P(\boldsymbol{v})}$$

$$= \frac{1}{P(\boldsymbol{v})}\frac{1}{Z}\exp\left\{\boldsymbol{b}^\top\boldsymbol{v} + \boldsymbol{c}^\top\boldsymbol{h} + \boldsymbol{v}^\top\boldsymbol{W}\boldsymbol{h}\right\}$$

$$= \frac{1}{Z'}\exp\left\{\boldsymbol{c}^\top\boldsymbol{h} + \boldsymbol{v}^\top\boldsymbol{W}\boldsymbol{h}\right\}$$

$$= \frac{1}{Z'}\exp\left\{\sum_{j=1}^{n_h} c_j h_j + \sum_{j=1}^{n_h}\boldsymbol{v}^\top\boldsymbol{W}_{:,j}\boldsymbol{h}_j\right\}$$

$$= \frac{1}{Z'}\prod_{j=1}^{n_h}\exp\left\{c_j h_j + \boldsymbol{v}^\top\boldsymbol{W}_{:,j}\boldsymbol{h}_j\right\}.$$

$$P(h_j = 1|\boldsymbol{v}) = \frac{\tilde{P}(h_j = 1|\boldsymbol{v})}{\tilde{P}(h_j = 0|\boldsymbol{v}) + \tilde{P}(h_j = 1|\boldsymbol{v})}$$

$$= \frac{\exp\left\{c_j + \boldsymbol{v}^\top\boldsymbol{W}_{:,j}\right\}}{\exp\{0\} + \exp\left\{c_j + \boldsymbol{v}^\top\boldsymbol{W}_{:,j}\right\}}$$

$$= \sigma\left(c_j + \boldsymbol{v}^\top\boldsymbol{W}_{:,j}\right).$$

$$P(\boldsymbol{h}|\boldsymbol{v}) = \prod_{j=1}^{n_h}\sigma\left((2\boldsymbol{h}-1)\odot(\boldsymbol{c} + \boldsymbol{W}^\top\boldsymbol{v})\right)_j.$$

$$P(\boldsymbol{v}|\boldsymbol{h}) = \prod_{i=1}^{n_v}\sigma\left((2\boldsymbol{v}-1)\odot(\boldsymbol{b} + \boldsymbol{W}\boldsymbol{h})\right)_i.$$

20.3 심층 믿음망

$$P(\boldsymbol{h}^{(l)}, \boldsymbol{h}^{(l-1)}) \propto \exp\left(\boldsymbol{b}^{(l)\top}\boldsymbol{h}^{(l)} + \boldsymbol{b}^{(l-1)\top}\boldsymbol{h}^{(l-1)} + \boldsymbol{h}^{(l-1)\top}\boldsymbol{W}^{(l)}\boldsymbol{h}^{(l)}\right),$$

$$P(h_i^{(k)} = 1 \mid \boldsymbol{h}^{(k+1)}) = \sigma\left(b_i^{(k)} + \boldsymbol{W}_{:,i}^{(k+1)\top}\boldsymbol{h}^{(k+1)}\right) \forall i, \forall k \in 1, \ldots, l-2,$$

$$P(v_i = 1 \mid \boldsymbol{h}^{(1)}) = \sigma\left(b_i^{(0)} + \boldsymbol{W}_{:,i}^{(1)\top}\boldsymbol{h}^{(1)}\right) \forall i.$$

$$\mathbf{v} \sim \mathcal{N}\left(\boldsymbol{v}; \boldsymbol{b}^{(0)} + \boldsymbol{W}^{(1)\top}\boldsymbol{h}^{(1)}, \boldsymbol{\beta}^{-1}\right)$$

$$\mathbb{E}_{\mathbf{v} \sim p_{\text{자료}}} \mathbb{E}_{\mathbf{h}^{(1)} \sim p^{(1)}(\boldsymbol{h}^{(1)} \mid \boldsymbol{v})} \log p^{(2)}(\boldsymbol{h}^{(1)})$$

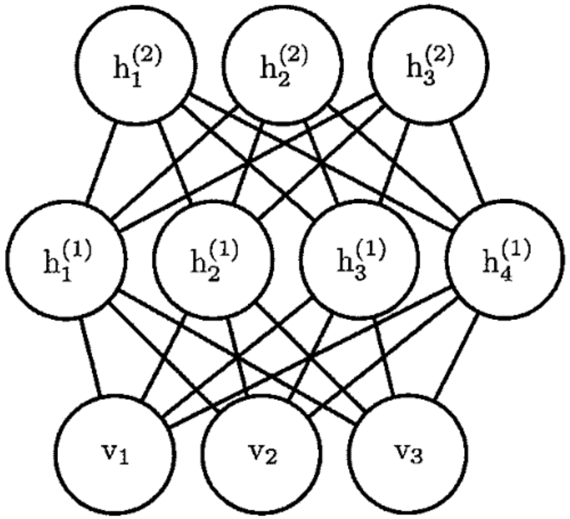
$$\boldsymbol{h}^{(1)} = \sigma\left(b^{(1)} + \boldsymbol{v}^\top \boldsymbol{W}^{(1)}\right),$$

$$\boldsymbol{h}^{(l)} = \sigma\left(b_i^{(l)} + \boldsymbol{h}^{(l-1)\top}\boldsymbol{W}^{(l)}\right), \quad \forall l \in 2, \ldots, m.$$

20.4 심층 볼츠만 기계

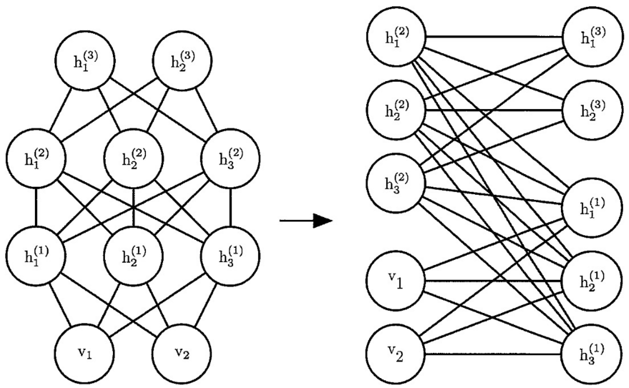
$$P\big(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}, \boldsymbol{h}^{(3)}\big) = \frac{1}{Z(\boldsymbol{\theta})} \exp\big(-E(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}, \boldsymbol{h}^{(3)}; \boldsymbol{\theta})\big).$$

$$E(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}, \boldsymbol{h}^{(3)}; \boldsymbol{\theta}) = -\boldsymbol{v}^\top \boldsymbol{W}^{(1)} \boldsymbol{h}^{(1)} - \boldsymbol{h}^{(1)\top} \boldsymbol{W}^{(2)} \boldsymbol{h}^{(2)} - \boldsymbol{h}^{(2)\top} \boldsymbol{W}^{(3)} \boldsymbol{h}^{(3)}.$$



20.4 심층 볼츠만 기계

$$P(v_i = 1 \mid \boldsymbol{h}^{(1)}) = \sigma\Big(\boldsymbol{W}_{i,:}^{(1)} \boldsymbol{h}^{(1)}\Big),$$



$$P\left(h_i^{(1)} = 1 \mid \boldsymbol{v}, \boldsymbol{h}^{(2)}\right) = \sigma\Big(\boldsymbol{v}^\top \boldsymbol{W}_{:,i}^{(1)} + \boldsymbol{W}_{i,:}^{(2)} \boldsymbol{h}^{(2)}\Big),$$

$$P\left(h_k^{(2)} = 1 \mid \boldsymbol{h}^{(1)}\right) = \sigma\Big(\boldsymbol{h}^{(1)\top} \boldsymbol{W}_{:,k}^{(2)}\Big).$$

20.5 실숫값 자료에 대한 볼츠만 기계

- 원래 볼츠만 기계는 이진 자료에 사용할 목적으로 개발되었다.
- 그러나 이미지나 음성을 모형화하는 등의 여러 응용에서는 실숫값들에 관한 확률분포를 표현할 수 있어야한다.

20.5.1 가우스-베르누이 RBM

$$p(\boldsymbol{v} \mid \boldsymbol{h}) = \mathcal{N}(\boldsymbol{v}; \boldsymbol{W}\boldsymbol{h}, \boldsymbol{\beta}^{-1}).$$

$$\log \mathcal{N}(\boldsymbol{v}; \boldsymbol{W}\boldsymbol{h}, \boldsymbol{\beta}^{-1}) = -\frac{1}{2}(\boldsymbol{v} - \boldsymbol{W}\boldsymbol{h})^\top \boldsymbol{\beta}(\boldsymbol{v} - \boldsymbol{W}\boldsymbol{h}) + f(\boldsymbol{\beta})$$

$$\frac{1}{2}\boldsymbol{h}^\top \boldsymbol{W}^\top \boldsymbol{\beta} \boldsymbol{W}\boldsymbol{h}$$

$$\frac{1}{2}h_i \sum_j \beta_j W_{j,i}^2.$$

$$E(\boldsymbol{v}, \boldsymbol{h}) = \frac{1}{2}\boldsymbol{v}^\top (\boldsymbol{\beta} \odot \boldsymbol{v}) - (\boldsymbol{v} \odot \boldsymbol{\beta})^\top \boldsymbol{W}\boldsymbol{h} - \boldsymbol{b}^\top \boldsymbol{h}.$$

20.6 합성곱 볼츠만 기계

- 이미지와 같은 격자 형태의 데이터를 처리하기 위해 합성곱 연산을 사용하는 볼츠만 기계의 확장형

20.7 구조적 출력 또는 순차열 출력을 위한 볼츠만 기계

- 복잡한 출력 구조(예: 순차열 또는 트리 구조)를 가진 문제를 처리하기 위해 설계된 볼츠만 기계의 변형형

20.8 기타 볼츠만 기계

- 훈련 판정기준을 달리 두어서 확장할 수 있음
- 실제 응용에 쓰이는 대부분의 볼츠만 기계의 에너지 함수에는 이차 상호작용만 있음

20.9 확률적(무작위) 연산에 대한 역전파

$$\mathrm{y} \sim \mathcal{N}(\mu, \sigma^2).$$

$$y = \mu + \sigma z.$$

$$\mathbf{y} \sim p(\mathbf{y} | \boldsymbol{\omega})$$

$$\boldsymbol{y} = f(\boldsymbol{z}; \boldsymbol{\omega})$$

20.9.1 이산 확률적 연산에 대한 역전파

$$\boldsymbol{y} = f(\boldsymbol{z};\boldsymbol{\omega}).$$

$$\mathbb{E}_z[J(\boldsymbol{y})] = \sum_{\boldsymbol{y}} J(\boldsymbol{y})p(\boldsymbol{y}),$$

$$\partial\mathbb{E}\,\frac{[J(\boldsymbol{y})]}{\partial\boldsymbol{\omega}} = \sum_{y} J(\boldsymbol{y})\frac{\partial p(\boldsymbol{y})}{\partial\boldsymbol{\omega}}$$

$$= \sum_{y} J(\boldsymbol{y})p(\boldsymbol{y})\frac{\partial \log p(\boldsymbol{y})}{\partial\boldsymbol{\omega}}$$

$$\approx \frac{1}{m}\sum_{\mathbf{y}^{(i)} \sim p(\boldsymbol{y}),\, i=1}^{m} J(\boldsymbol{y}^{(i)})\frac{\partial \log p(\boldsymbol{y}^{(i)})}{\partial\boldsymbol{\omega}}.$$

20.9.1 이산 확률적 연산에 대한 역전파

$$E_{p(\boldsymbol{y})}\left[\frac{\partial \log p(\boldsymbol{y})}{\partial \boldsymbol{\omega}}\right] = \sum_{\boldsymbol{y}} p(\boldsymbol{y}) \frac{\partial \log p(\boldsymbol{y})}{\partial \boldsymbol{\omega}}$$

$$= \sum_{\boldsymbol{y}} \frac{\partial p(\boldsymbol{y})}{\partial \boldsymbol{\omega}}$$

$$= \frac{\partial}{\partial \boldsymbol{\omega}} \sum_{\boldsymbol{y}} p(\boldsymbol{y}) = \frac{\partial}{\partial \boldsymbol{\omega}} 1 = 0$$

$$E_{p(\boldsymbol{y})}\left[(J(\boldsymbol{y}) - b(\boldsymbol{\omega})) \frac{\partial \log p(\boldsymbol{y})}{\partial \boldsymbol{\omega}}\right] = E_{p(\boldsymbol{y})}\left[J(\boldsymbol{y}) \frac{\partial \log p(\boldsymbol{y})}{\partial \boldsymbol{\omega}}\right] - b(\boldsymbol{\omega}) E_{p(\boldsymbol{y})}\left[\frac{\partial \log p(\boldsymbol{y})}{\partial \boldsymbol{\omega}}\right]$$

$$= E_{p(\boldsymbol{y})}\left[J(\boldsymbol{y}) \frac{\partial \log p(\boldsymbol{y})}{\partial \boldsymbol{\omega}}\right]$$

$$b^*(\boldsymbol{\omega})_i = \frac{E_{p(\boldsymbol{y})}\left[J(\boldsymbol{y}) \frac{\partial \log p(\boldsymbol{y})}{\partial \omega_i}^2\right]}{E_{p(\boldsymbol{y})}\left[\frac{\partial \log p(\boldsymbol{y})}{\partial \omega_i}^2\right]}.$$

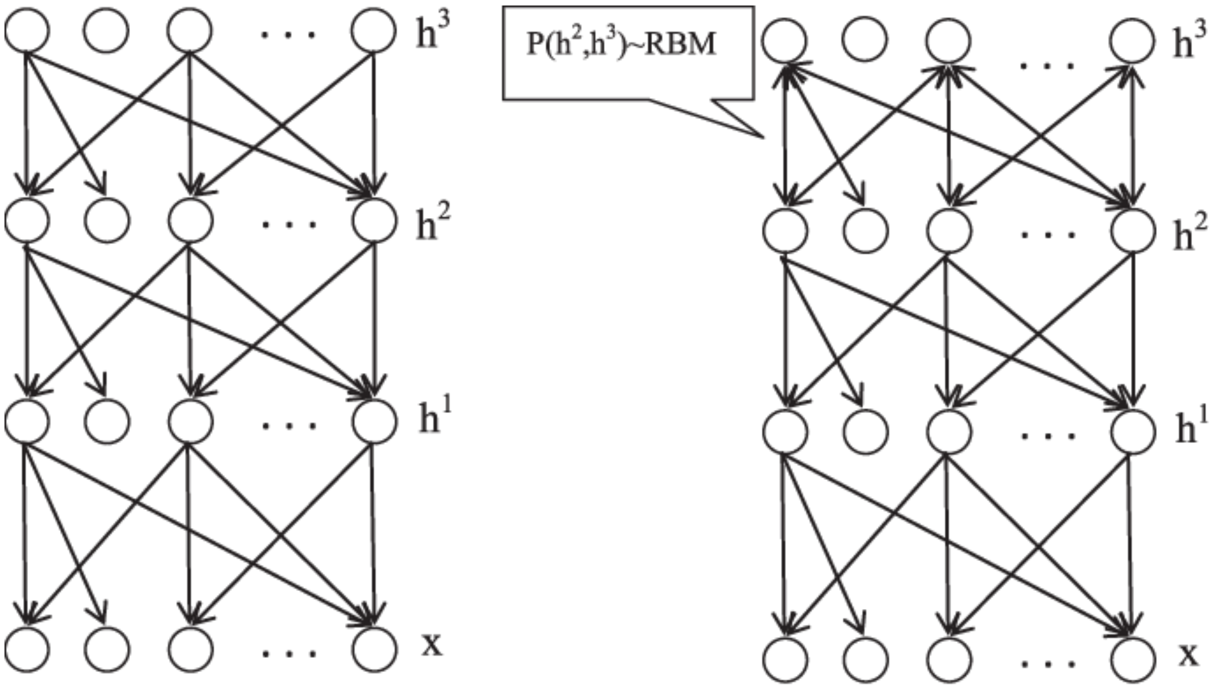
$$(J(\boldsymbol{y}) - b(\boldsymbol{\omega})_i) \frac{\partial \log p(\boldsymbol{y})}{\partial \omega_i}.$$

20.10 유향 생성망

- 딥러닝 공동체와 관련이 있던 표준적인 유향 그래프 모형 몇 가지를 살펴볼 예정

20.10.1 S자형 믿음망

$$p(s_i) = \sigma\left(\sum_{j<i} W_{j,i} s_j + b_i\right).$$



Sigmoid Belief Networks

Deep Belief Networks

20.10.2 미분 가능 생성자망

$$\boldsymbol{x} = g(\boldsymbol{z}) = \mu + \boldsymbol{L}\boldsymbol{z}.$$

$$p_z(\boldsymbol{z}) = p_x(g(\boldsymbol{z}))\left|\det\left(\frac{\partial g}{\partial \boldsymbol{z}}\right)\right|.$$

$$p_x(\boldsymbol{x}) = \frac{p_z(g^{-1}(\boldsymbol{x}))}{\left|\det\left(\frac{\partial g}{\partial \boldsymbol{z}}\right)\right|}.$$

$$p(\mathrm{x}_i = 1 \mid \boldsymbol{z}) = g(\boldsymbol{z})_i.$$

$$p(\boldsymbol{x}) = \mathbb{E}_z p(\boldsymbol{x} \mid \boldsymbol{z}).$$

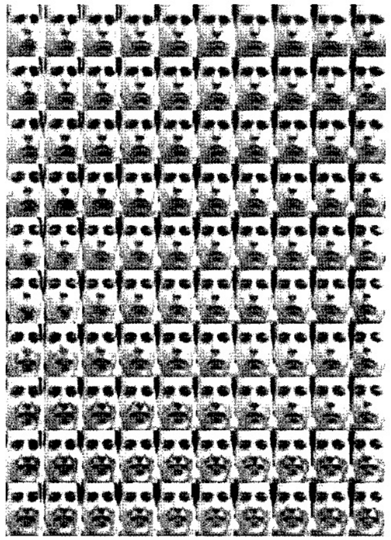
20.10.3 변분 자동부호기

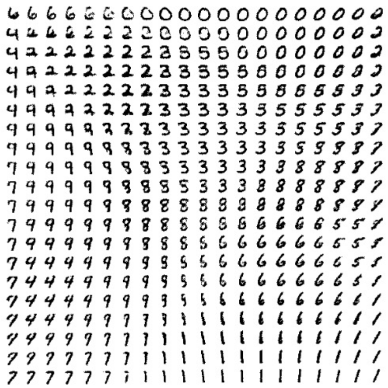
$$\mathcal{L}(q) = \mathbb{E}_{z \sim q(z|x)} \log p_{\text{모형}}(z, x) + \mathcal{H}(q(\mathbf{z}|x))$$

$$= \mathbb{E}_{z \sim q(z|x)} \log p_{\text{모형}}(x|z) - D_{\mathrm{KL}}(q(\mathbf{z}|x) \| p_{\text{모형}}(\mathbf{z}))$$

$$\leq \log p_{\text{모형}}(x).$$

$$\mathcal{L}_k(x, q) = \mathbb{E}_{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(k)} \sim q(z|x)} \left[\log \frac{1}{k} \sum_{i=1}^{k} \frac{p_{\text{모형}}(x, z^{(i)})}{q(z^{(i)}|x)} \right].$$





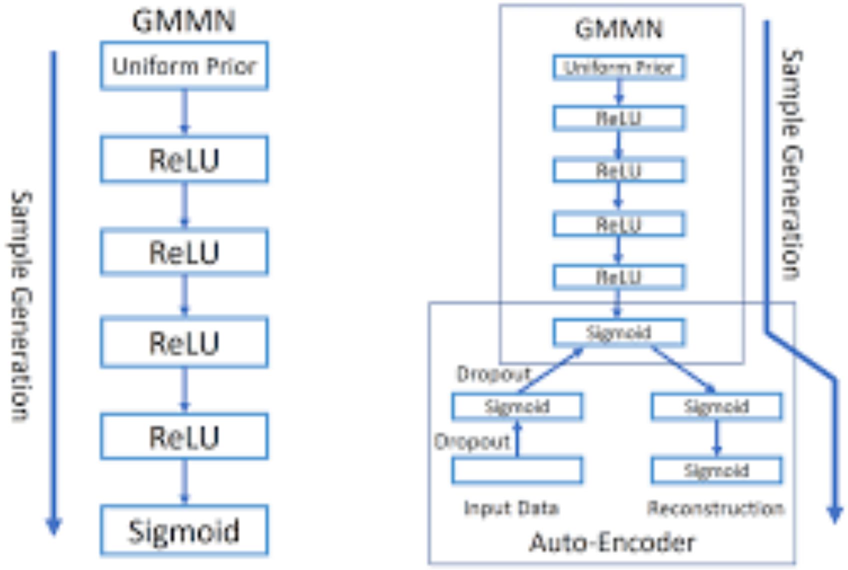
20.10.4 생성 대립 신경망(GAN)

$$g^* = \arg\min_g \max_d v(g, d).$$

$$v(\boldsymbol{\theta}^{(g)}, \boldsymbol{\theta}^{(d)}) = \mathbb{E}_{\mathbf{x} \sim p_{\text{자료}}} \log d(\boldsymbol{x}) + \mathbb{E}_{\boldsymbol{x} \sim p_{\text{모형}}} \log(1 - d(\boldsymbol{x})).$$

20.10.5 생성 적률 부합망

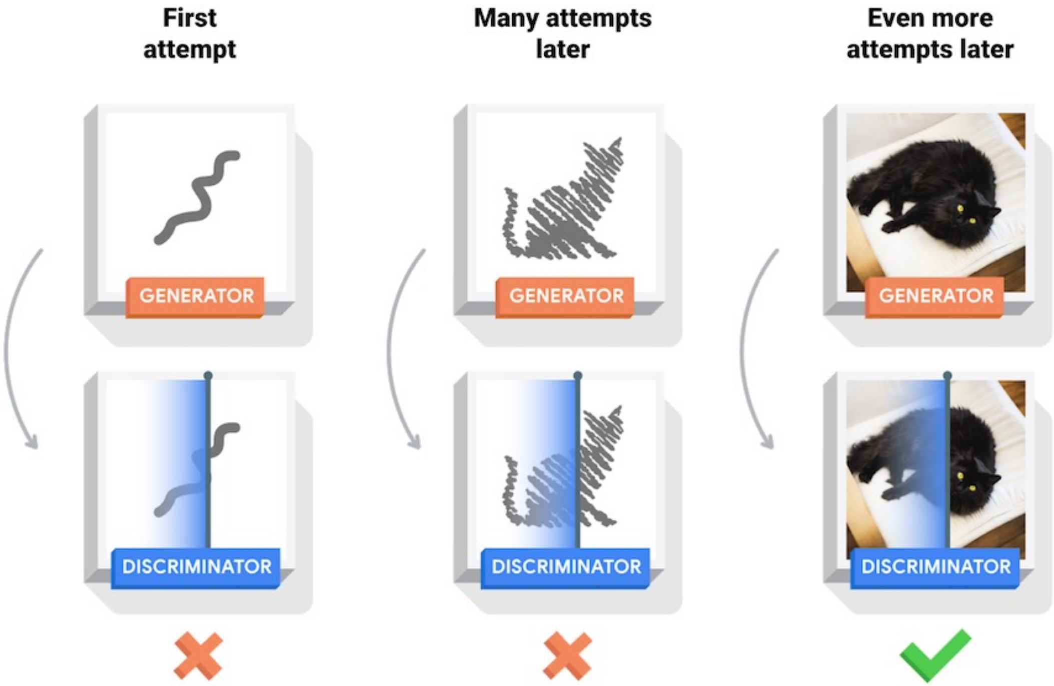
$$\mathbb{E}_{\boldsymbol{x}} \prod_i x_i^{n_i}$$



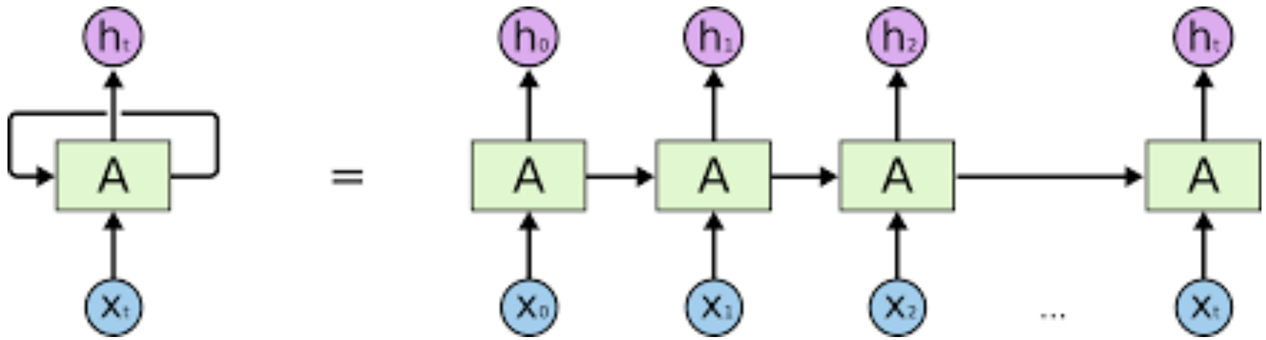
(a) GMMN

(b) GMMN + AE

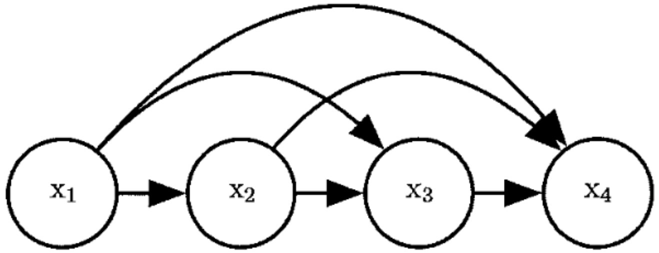
20.10.6 합성곱 생성망

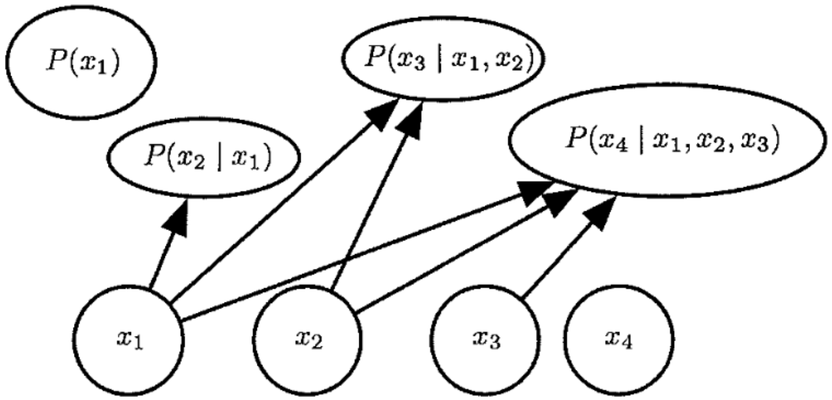


20.10.7 자기회귀망

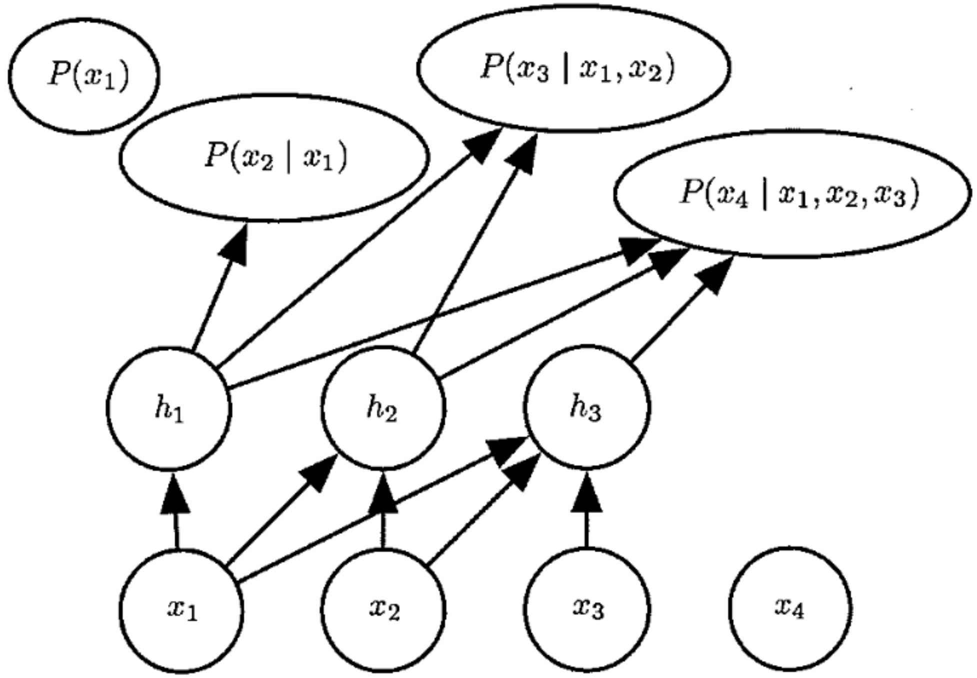


20.10.8 선형 자기회귀망

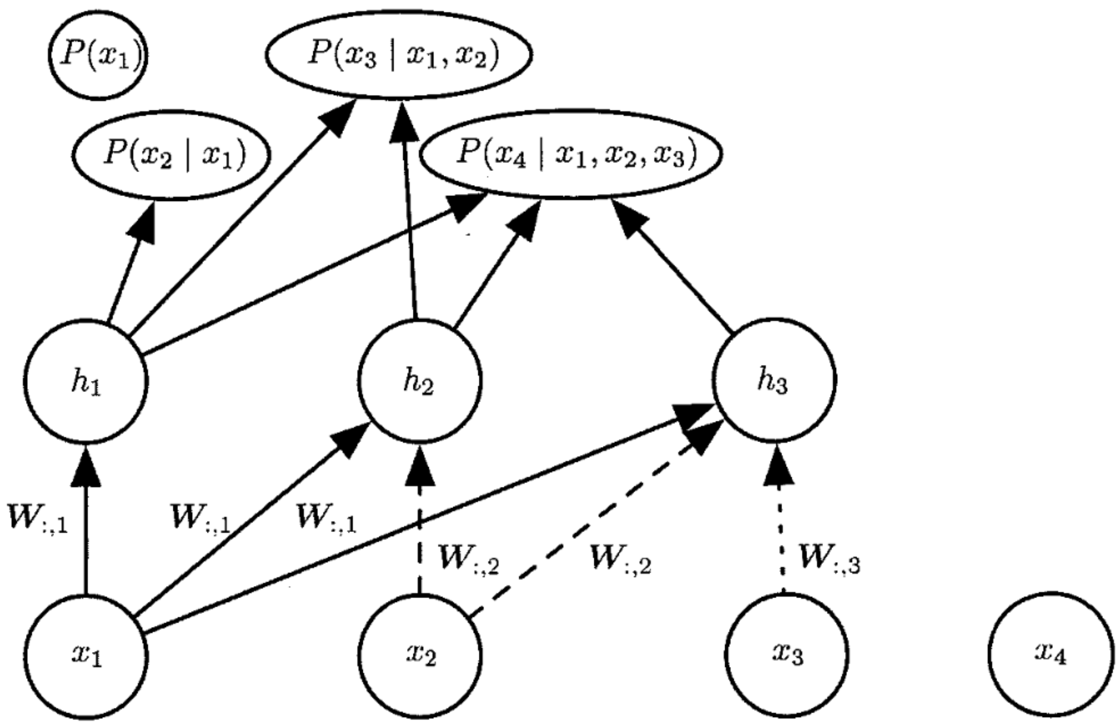




20.10.9 신경 자기회귀망



20.10.10 NADE

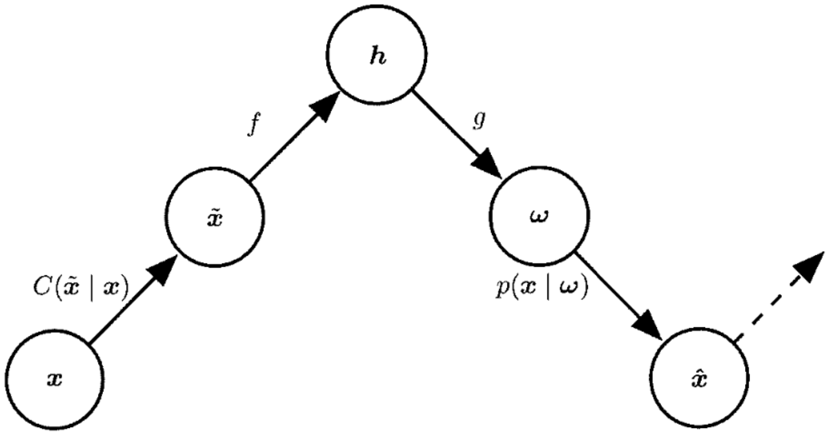


$P(x_1)$
$P(x_3 \mid x_1, x_2)$
$P(x_2 \mid x_1)$
$P(x_4 \mid x_1, x_2, x_3)$
h_1
h_2
h_3
$W_{:,1}$
$W_{:,1}$
$W_{:,1}$
$W_{:,2}$
$W_{:,2}$
$W_{:,3}$
x_1
x_2
x_3
x_4

20.11 자동부호기의 표본추출

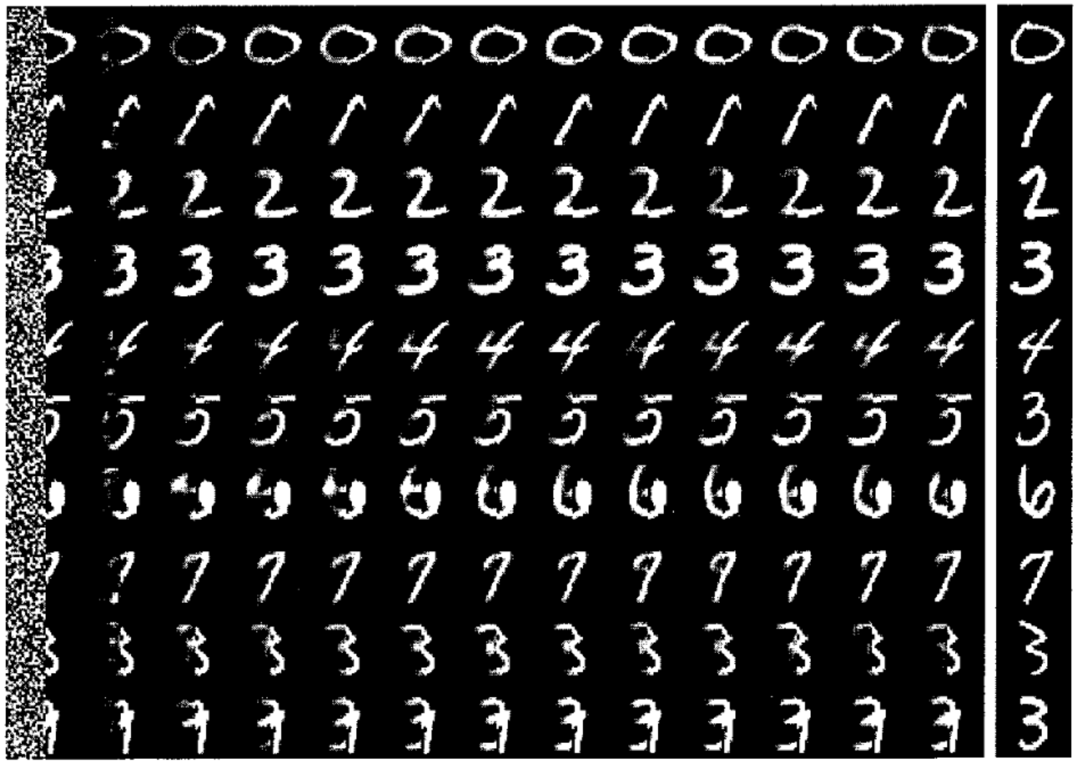
- 표본을 추출하기 위해서는 대부분의 autoencoder들은 MCMC 표집을 사용해야 함

20.11.1 임의의 잡음 제거 자동부호기를 위한 마르코프 연쇄



1. 이전 상태 $\boldsymbol{x}$에서 시작해서 손상 입력(잡음)을 주입하고, $C(\tilde{\boldsymbol{x}}|\boldsymbol{x})$로부터 $\tilde{\boldsymbol{x}}$를 추출한다.
2. $\tilde{\boldsymbol{x}}$를 $\boldsymbol{h} = f(\tilde{\boldsymbol{x}})$로 부호화한다.
3. $\boldsymbol{h}$를 복호화해서 $p(\mathbf{x}|\boldsymbol{\omega} = g(\boldsymbol{h})) = p(\mathbf{x}|\tilde{\boldsymbol{x}})$의 매개변수 $\boldsymbol{\omega} = g(\boldsymbol{h})$를 구한다.
4. $p(\mathbf{x}|\boldsymbol{\omega} = g(\boldsymbol{h})) = p(\mathbf{x}|\tilde{\boldsymbol{x}})$에서 다음 상태 $\boldsymbol{x}$를 추출한다.

20.11.2 고정과 조건부 표집



20.12 생성 확률적 신경망