Applied Machine Learning

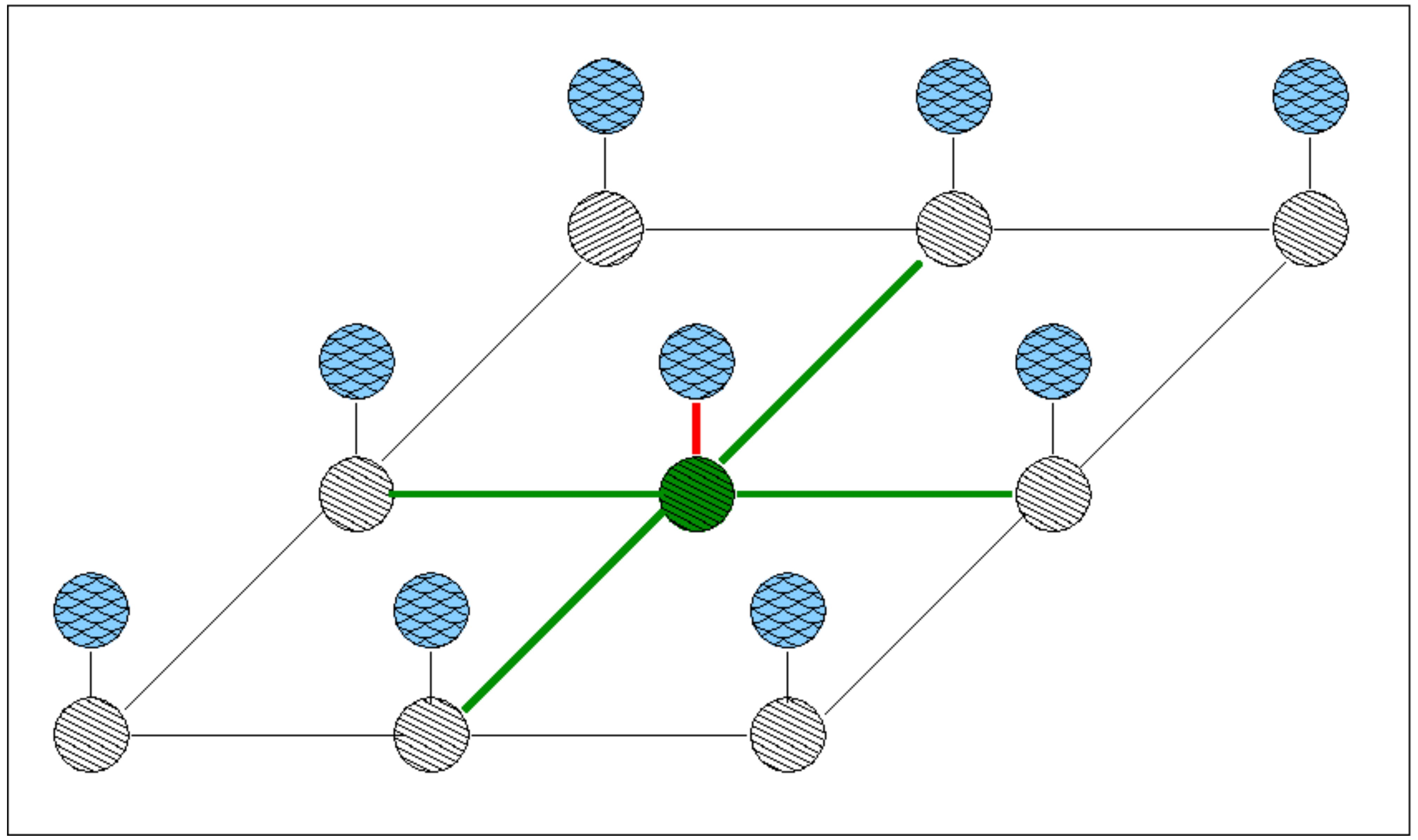
Boltzmann Machines

Boltzmann Machines

- Boltzmann Machines
- Variational Inference Approach
- Mean Field Inference Algorithm

Boltzmann Machines

- U: Set of nodes H (hidden) and X (Observed)
  - Binary $\{-1,1\}$
- Edges
  - (U_i, U_j): Coupling. $N(i)$: Neighbors of i
  - θ: Weights: Intensity of coupling
- Energy:
  - $E(U|\theta) = -\sum_i \sum_{j \in N(i)} \theta_{i,j} U_i U_j$
    - $U_i U_j = \begin{cases} 1 & U_i = Uj \\ -1 & U_i \neq Uj \end{cases}$
    - $\theta > 0$: lower energy for pairs with same value
    - $\theta < 0$: lower energy for pairs of different values



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- Log joint probability
  - $\log P(U \mid \theta) = -E(U \mid \theta) - \log Z(\theta)$
    - normalizing constant: $Z(\theta) = \sum_{U \in -1,1} e^{-E(U|\theta)}$
- Find H that maximizes
  - $P(H \mid X, \theta) \quad = \quad \frac{e^{-E(H,X|\theta)}}{\sum_H e^{-E(H,X|\theta)}}$
  - $\log P(H \mid X, \theta) = -E(H, X \mid \theta) - \log \sum_{H} e^{-E(H,X|\theta)}$
  - $\text{argmax}_H \left(\sum_{i,j} a_{i,j} h_i h_j \right) + \sum_j b_j h_j$
    $s.t.\ h_i \in -1,1$

Variational Inference
KL Divergence

- Use $Q(H; X, \hat{\theta})$ similar to $P(H|X, \theta)$ and easier to deal with
  - find parameters $\hat{\theta}$ for Q
- Similarity measure
  - Kullback-Leibler (KL) Divergence between $P(X)$ and $Q(X)$
    - $\mathbb{D}\left(P||Q\right) = \int P(X) log \frac{P(X)}{Q(X)} dx$
    - Downsides
      - Not symmetric: $\mathbb{D}\left(P\|Q\right) \neq \mathbb{D}\left(Q\|P\right)$
      - Not triangle inequality: $\mathbb{D}\left(P\|Q\right) \nleq \mathbb{D}\left(P\|R\right) + \mathbb{D}\left(P\|Q\right)$
    - Non-negative: $\mathbb{D}\left(P\|Q\right) \geq 0$

- Entropy of $P(X)$: constant
  $H(P) = -\int P(X) \log P(X) dx = -\mathbb{E}_P[\log P]$
- $$\begin{aligned} \mathbb{D}\left(P\|Q\right) &= \int P(X) log \frac{P(X)}{Q(X)} dX \\ &= \int P(X)(\log P(X) - \log Q(X)) dx \\ &= \int P(X) \log P(X) dx - \int P(X) \log Q(X) dx \end{aligned}$$
- $= \quad \mathbb{E}_P[\log P] - \mathbb{E}_P[\log Q]$
- $$\begin{aligned} -\mathbb{E}_P[\log Q] &= \mathbb{E}_P[\log P] - \mathbb{D}\left(P\|Q\right) \\ &= -H(P) - \mathbb{D}\left(P\|Q\right) \end{aligned}$$
- $$\begin{aligned} \mathcal{L}(\theta) &= \sum_i \log Q(X_i|\theta) \\ \mathcal{L}(\theta) &\approx \int P(X) \log Q(X|\theta) dX \end{aligned}$$
- $\approx \quad \mathbb{E}_P[\log Q(X|\theta)] \quad \approx \quad -H(P) - \mathbb{D}\left(P\|Q\right)$
- $-H(P) \quad \approx \quad \mathcal{L}(\theta) + \mathbb{D}\left(P\|Q\right)$

Variational Inference
From $\mathscr{L}(\theta)$ To $\mathbb{D}\left(P \| Q\right)$

- Use $Q(H; X, \hat{\theta})$ similar to $P(H \mid X, \theta)$ and easier to deal with
  - find parameters $\hat{\theta}$ for Q
- Similarity measure
  - Kullback-Leibler (KL) Divergence between $P(X)$ and $Q(X)$
    - $\mathbb{D}\left(P || Q\right) = \int P(X) log \frac{P(X)}{Q(X)} dx$
    - Downsides
      - Not symmetric: $\mathbb{D}\left(P \| Q\right) \neq \mathbb{D}\left(Q \| P\right)$
      - Not triangle inequality: $\mathbb{D}\left(P \| Q\right) \nleq \mathbb{D}\left(P \| R\right) + \mathbb{D}\left(P \| Q\right)$
    - Non-negative: $\mathbb{D}\left(P \| Q\right) \geq 0$

- Entropy of $P(X)$
  $H(P) = -\int P(X) \log P(X) dx = -\mathbb{E}_P[\log P]$
- $-H(P) \quad \approx \quad \mathscr{L}(\theta) + \mathbb{D}\left(P \| Q\right)$
  - constant
    - $\mathscr{L}(\theta)$ at maximum when $\mathbb{D}\left(P \| Q\right)$ at minimum
  - Maximizing $\mathscr{L}(\theta)$ can be achieved by minimizing $\mathbb{D}\left(P \| Q\right)$

Variational Inference
Minimizing KL Divergence

- Minimizing $\mathbb{D}\left(Q(H) \| P(H|X)\right)$
- $$\begin{aligned}\mathbb{D}\left(Q(H) \| P(H|X)\right) &= \mathbb{E}_Q[\log Q] - \mathbb{E}_Q[\log P(H|X)] \\ &= \mathbb{E}_Q[\log Q] - \mathbb{E}_Q[\log P(H,X)] + \mathbb{E}_Q[\log P(X)] \\ &= \mathbb{E}_Q[\log Q] - \mathbb{E}_Q[\log P(H,X)] + \log P(X)\end{aligned}$$
- Variational Free Energy under Q:
  - $\mathsf{E}_Q = \mathbb{E}_Q[\log Q] - \mathbb{E}_Q[\log P(H,X)]$
- $\mathbb{D}\left(Q(H) \| P(H|X)\right) \quad = \quad \mathsf{E}_Q + \log P(X)$

- $\log P(X) \quad = \quad \mathbb{D}\left(Q(H) \| P(H|X)\right) - \mathsf{E}_Q$
  - constant
    - If Variational Free Energy decreases
    - LK Divergence $\mathbb{D}\left(Q(H) \| P(H|X)\right)$ decreases
- Minimizing variational free energy E_Q minimizes $\mathbb{D}\left(Q(H) \| P(H|X)\right)$

Variational Inference
Minimizing Free Variational Energy

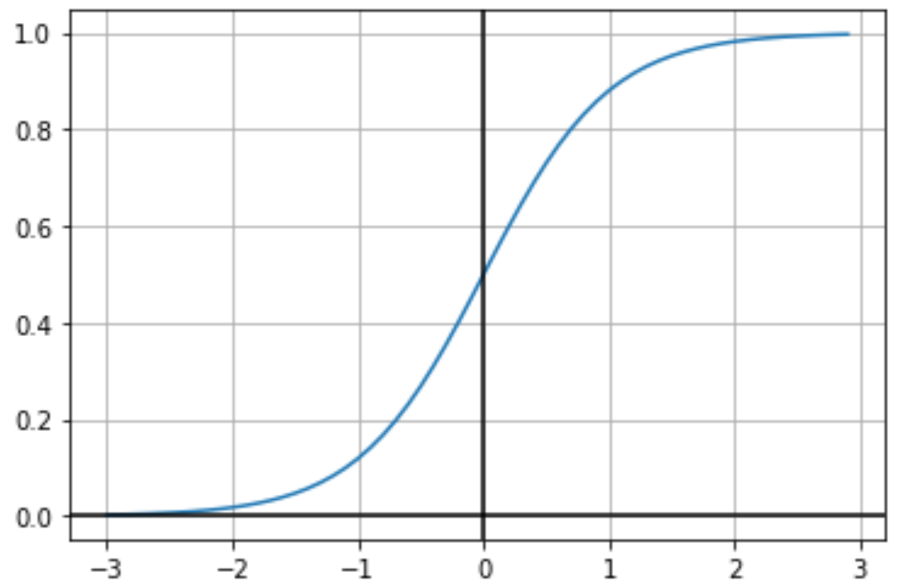
- Approximate distribution Q for Boltzmann Machine
  - Hidden variables $H_i \in \{-1,1\}$
  - $Q(H) = q_1(H_1)q_2(H_2)\ldots q_N(H_N)$
    - $q_i(H_i) = \pi_i^{\frac{1+H_i}{2}}(1-\pi_i)^{\frac{1-H_i}{2}}$
      - Values of $q_i(H_i)$: $\begin{cases} \pi_i & H_1 = 1 \\ 1-\pi_i & H_1 = -1 \end{cases}$
      - $\pi_i = P(H_i = 1)$
  - Assume that only one q_i is unknown
    - $Q_{\hat{i}} = q_1(H_1)\ldots q_{i-1}(H_{i-1})q_{i+1}(H_{i+1})\ldots q_N(H_N)$
    - find q_i that minimizes free variational energy

- Free variational energy
  $\mathsf{E}_Q = \mathbb{E}_Q[\log Q] - \mathbb{E}_Q[\log P(H,X)]$
  - $$\begin{aligned} \mathbb{E}_Q[\log Q] &= \mathbb{E}_{q_1(H_1)\ldots q_N(H_N)}[\log q_1(H_1) + \log q_N(H_N)] \\ &= \mathbb{E}_{q_1(H_1)}[\log q_1(H_1)] + \ldots \mathbb{E}_{q_N(H_N)}[\log q_N(H_N)] \end{aligned}$$
  - $$\begin{aligned} \mathbb{E}_Q[\log P(H,X)] &= q_i(-1)p_{i,-1} + q_i(1)p_{i,1} \\ p_{i,-1} &= \mathbb{E}_{Q_{\hat{i}}}[\log P(H_1,\ldots,H_i=-1,\ldots,H_N,X)] \\ p_{i,1} &= \mathbb{E}_{Q_{\hat{i}}}[\log P(H_1,\ldots,H_i=1,\ldots,H_N,X)] \end{aligned}$$
- Choose q_i that minimizes:
  - $$q_i(-1)\log q_i(-1) + q_i(1)\log q_i(1) - (q_i(-1)p_{i,-1} + q_i(1)p_{i,1})$$
    $$\text{s.t. } q_i(1) + q(-1) = 1$$

Boltzmann Machines - Mean Field Inference

- Choose q_i that minimizes:
  - $$q_i(-1)\log q_i(-1) + q_i(1)\log q_i(1) - (q_i(-1)p_{i,-1} + q_i(1)p_{i,1})$$ $$\text{s.t. } q_i(1) + q(-1) = 1$$
  - $$\begin{aligned} p_{i,-1} &= \mathbb{E}_{Q_{\hat{i}}}[\log P(H_1,\ldots,H_i=-1,\ldots,H_N,X)] \\ p_{i,1} &= \mathbb{E}_{Q_{\hat{i}}}[\log P(H_1,\ldots,H_i=1,\ldots,H_N,X)] \end{aligned}$$
- Using a Lagrange Multiplier:
  - $$\begin{aligned} q_i(-1) &= \frac{e^{p_{i,-1}}}{e^{p_{i,-1}} + e^{p_{i,1}}} \\ q_i(1) &= \frac{e^{p_{i,1}}}{e^{p_{i,-1}} + e^{p_{i,1}}} \end{aligned}$$
- Remember:
  - $\log P(U|\theta) = -E(U|\theta) - \log Z$
  - $E(U|\theta) = -\sum_i \sum_{j\in N(i)} \theta_{i,j} U_i U_j$

- $$\begin{aligned} p_{i,-1} &= \mathbb{E}_{Q_{\hat{i}}}[\textstyle\sum_{j\in N(i)\cap H}\theta_{i,j}(-1)H_j + \sum_{j\in N(i)\cap X}\theta_{i,j}(-1)X_j + K_{\hat{i}}] \\ &= \textstyle\sum_{j\in N(i)\cap H}\theta_{i,j}(-1)\mathbb{E}_{Q_{\hat{i}}}[H_j] + \sum_{j\in N(i)\cap X}\theta_{i,j}(-1)X_j + K_{\hat{i}} \end{aligned}$$
- $p_{i,-1} = \sum_{j\in N(i)\cap H}\theta_{i,j}(-1)(2\pi_j - 1) + \sum_{j\in N(i)\cap X}\theta_{i,j}(-1)X_j + K_{\hat{i}}$
- $p_{i,1} = \sum_{j\in N(i)\cap H}\theta_{i,j}(1)(2\pi_j - 1) + \sum_{j\in N(i)\cap X}\theta_{i,j}(1)X_j + K_{\hat{i}}$
- Parameters:
  - $p_i = \sum_{j\in N(i)\cap H}\theta_{i,j}(2\pi_j - 1) + \sum_{j\in N(i)\cap X}\theta_{i,j}X_j$
  - $\pi_i = \dfrac{e^{p_i}}{e^{p_i} + e^{-p_i}}$



- Mean Field Inference
  - While (π_i's change more than some ϵ)
    - update each π_i as defined above
  - Estimated $H_i = \begin{cases} 1 & \pi_i >= 0.5 \\ -1 & \pi_i < 0.5 \end{cases}$

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