概率图模型理论及应用

Theory and Applications of Probabilistic Graphical Models

(Lesson 11 - variational)

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课前摘要

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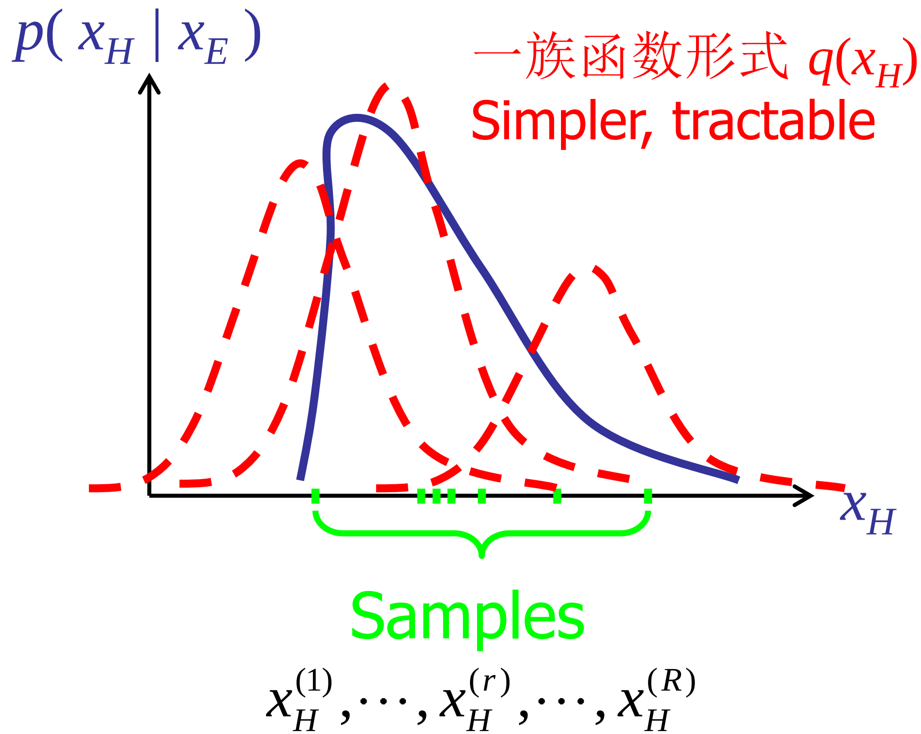
课程章节

- 第一章 引言（1）
- 第二章 图模型的表示理论（2）
  - Semantics (DGM, UGM)
  - HMM, CRF
- 第三章 图模型的推理理论（6）
  - 精确推理：variable-elimination，cluster-tree，triangulate
  - 连续变量：Kalman
  - 采样近似：sampling
  - 变分近似：variational
- 第四章 图模型的学习理论（3）
  - 参数学习：maxlikelihoodEstimate，RFLearning，BayesEstimate
  - 结构学习：StructureLearning
- 第五章 一个综合例子（1）

近似求解分布函数 $p(x_H \mid x_E)$

- 采样近似
  - 样本数足够多可任意近似
  - 适用任意分布函数
  - 速度慢，不适应大规模问题

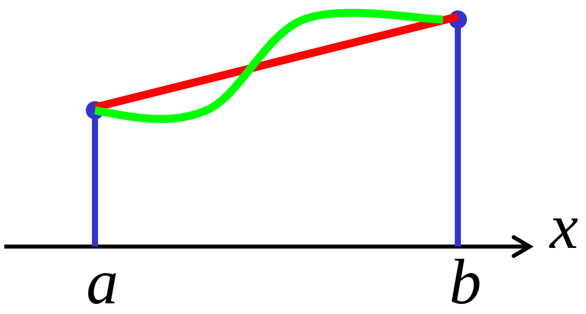


- 变分近似
  - 速度较快
  - 可应用于大规模问题
  - 较难分析近似误差
  - **将条件分布的求解 形式化成 一个最优化问题**

$$\hat{q}(x_H) = \arg\min_q \underbrace{KL\left(q(x_H) \,\|\, p(x_H \mid x_E)\right)}_{J(q(x_H))}$$

变分方法是一种经典的泛函最优化方法

- 泛函最优化
  - 例：求平面内两点之间具有最短长度的曲线



$$\max_{f} J(f) = \int_a^b \sqrt{1+\dot{f}^2}\,dx$$

$$f \in \{[a,b]\text{上的连续函数集合，} f(a), f(b)\text{固定}\}$$

- 泛函微分(Frechet微分)

$$\delta J(f;h) = \lim_{\alpha \to 0} \frac{J(f+\alpha h) - J(f)}{\alpha} = \frac{\partial J}{\partial f} \circ h$$

D. G. Luenberger，“最优化的矢量方法”，O244 35

变分近似推理

- 变分方法是一种经典的泛函最优化方法
- 变分近似推理：变分优化方法用于推理问题
- Block approach
  - 变分均值场方法（Variational mean field）
  - 结构变分方法（Structured variational approach）
  - 变分贝叶斯方法（Variational Bayesian）用于贝叶斯参数估计
- Sequential approach
  - Local variational method

Variational Inference for $p(x_H \mid x_E)$

用一个简单的好操作的函数 $q(x_H)$ 去近似真实函数 $p(x_H \mid x_E)$

$$\hat{q}(x_H) = \arg\min_q KL\left(q(x_H) \| p(x_H \mid x_E)\right)$$

Three steps …

① Use Kullback-Leibler distance $KL(q||p)$ as a measure of 'difference' between $p(x_H|x_E)$ and $q(x_H)$.

② Choose a family of <u>variational distributions</u> (变分分布) $q(x_H)$.

③ Find $q(x_H)$ which minimises KL distance.

① Minimise the KL distance

$$KL(q \| p) = \sum_{x_H} q(x_H) \log \frac{q(x_H)}{p(x_H \mid x_E)}$$

fixed maximise minimise

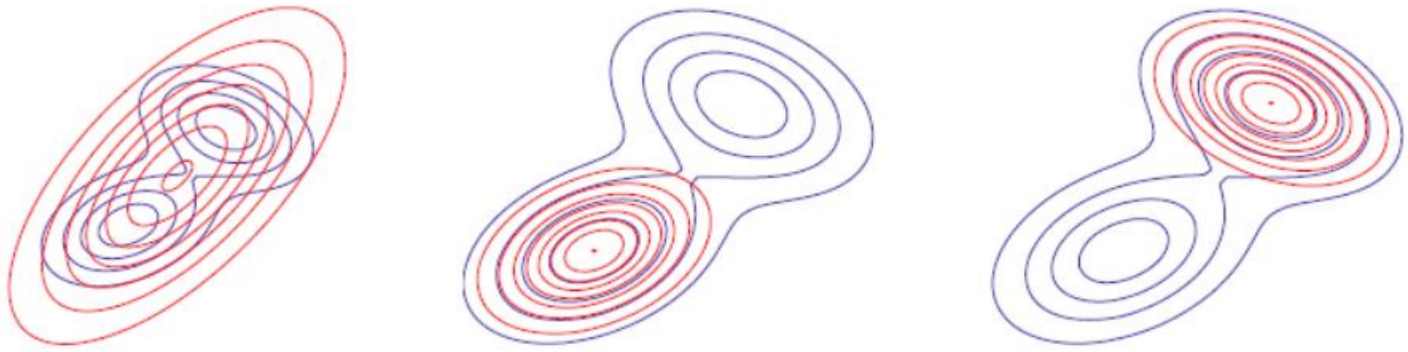
$$\log p(x_E) = L(q) + KL(q \| p)$$

$$L(q) = \sum_{x_H} q(x_H) \log \frac{p(x_H, x_E)}{q(x_H)}$$ Minus Free Energy

$$-L(q) = -\sum_{x_H} q(x_H) \log p(x_H, x_E) - \sum_{x_H} q(x_H) \log \frac{1}{q(x_H)}$$

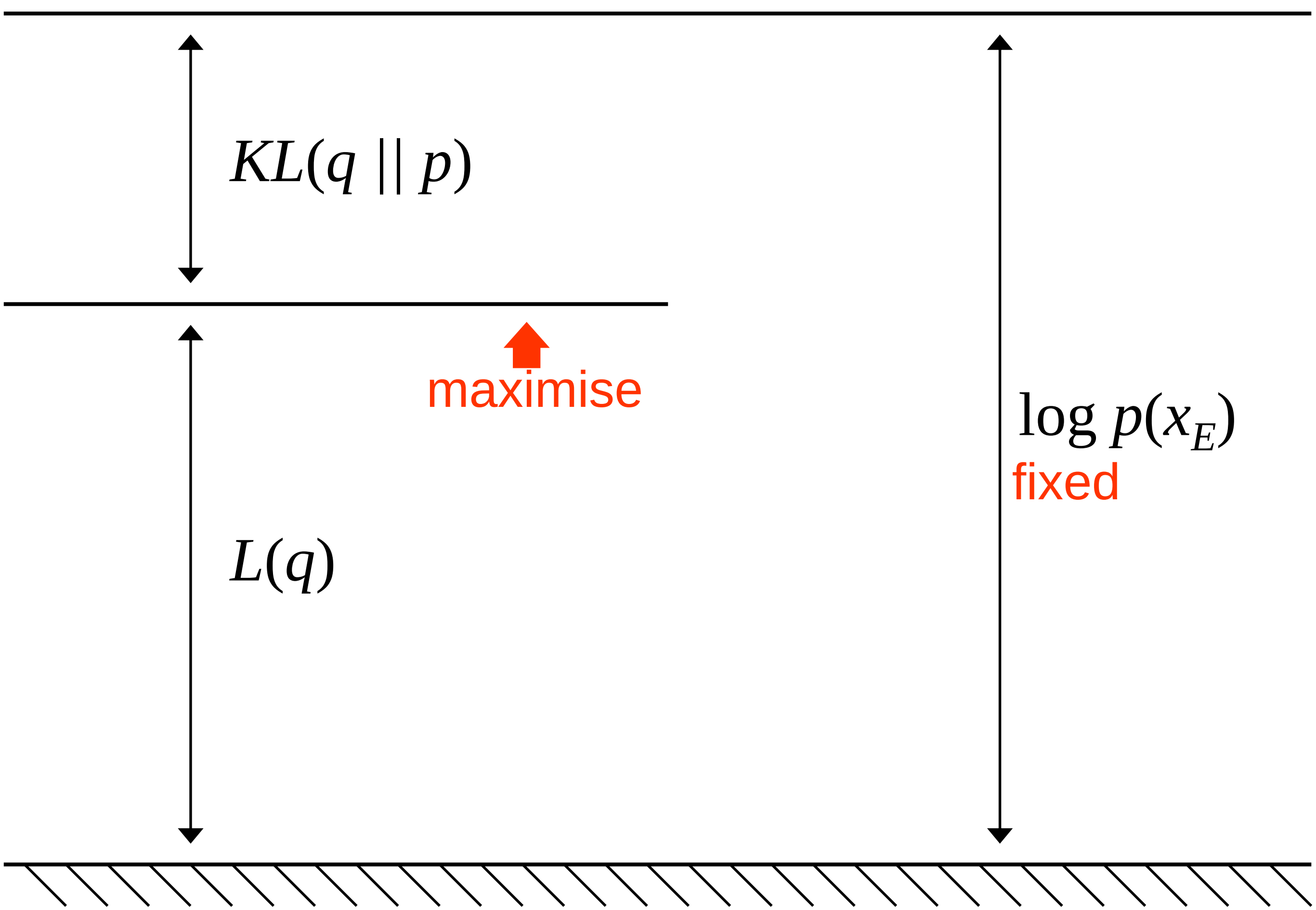
$KL(p \| q)$ Expectation Propagation (Minka, 2001), PRML 10.7

Discussion (Mackay book / Murphy book)

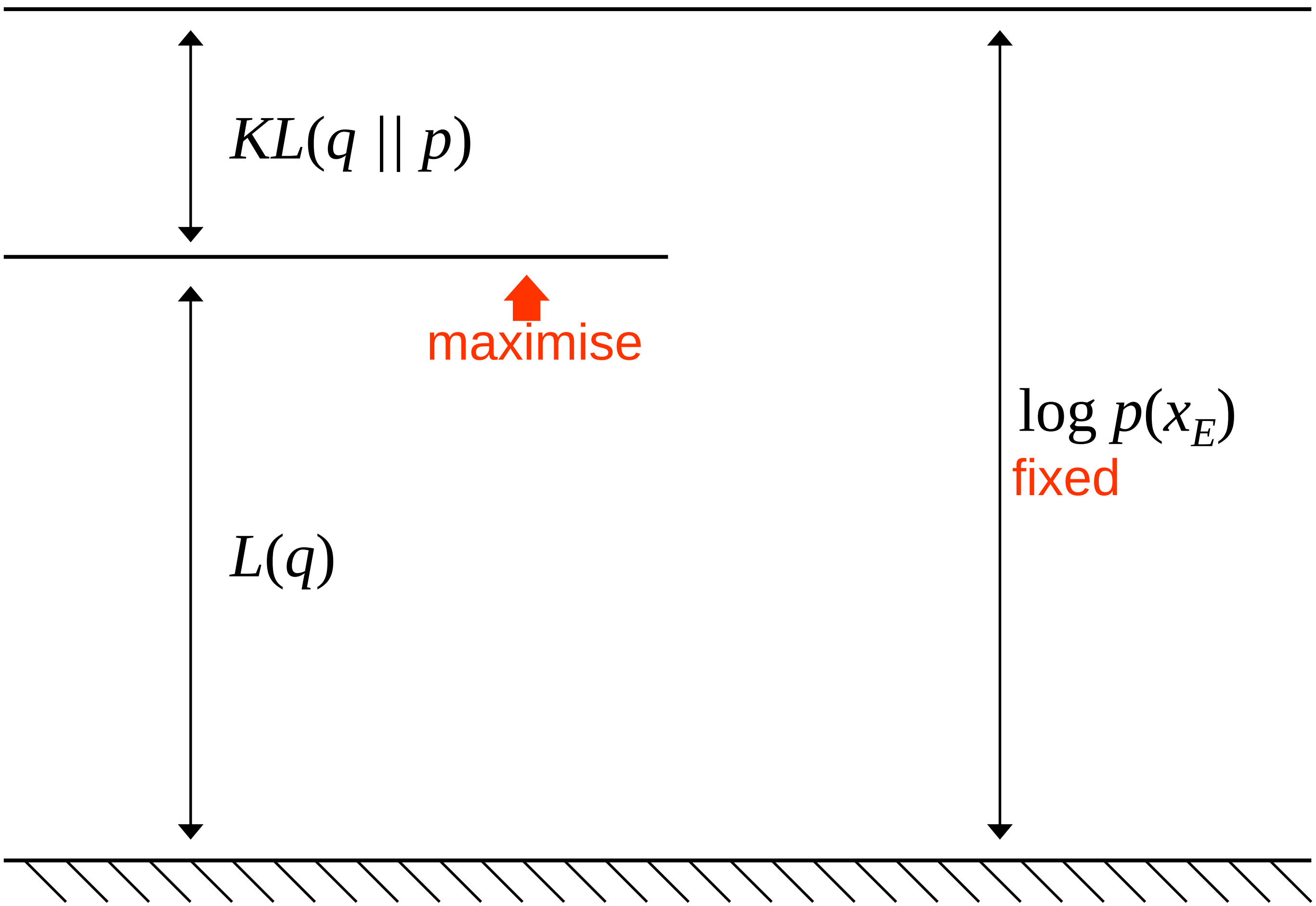

(a) (b) (c)

- Exclusive KL / Reverse KL: $\mathrm{KL}(q||p) = \int q \log \frac{q}{p}$
  - Zero forcing (迫零) for q: if p=0 we must ensure q=0.
  - q will typically under-estimate the support of p.
  - q locks on to one of the two modes.
- Inclusive KL / Forwards KL: $\mathrm{KL}(p||q) = \int p \log \frac{p}{q}$
  - Zero avoiding (避零) for q: if p>0 we must ensure q>0.
  - tends to find q that has higher entropy than the original
  - q tends to “cover” p

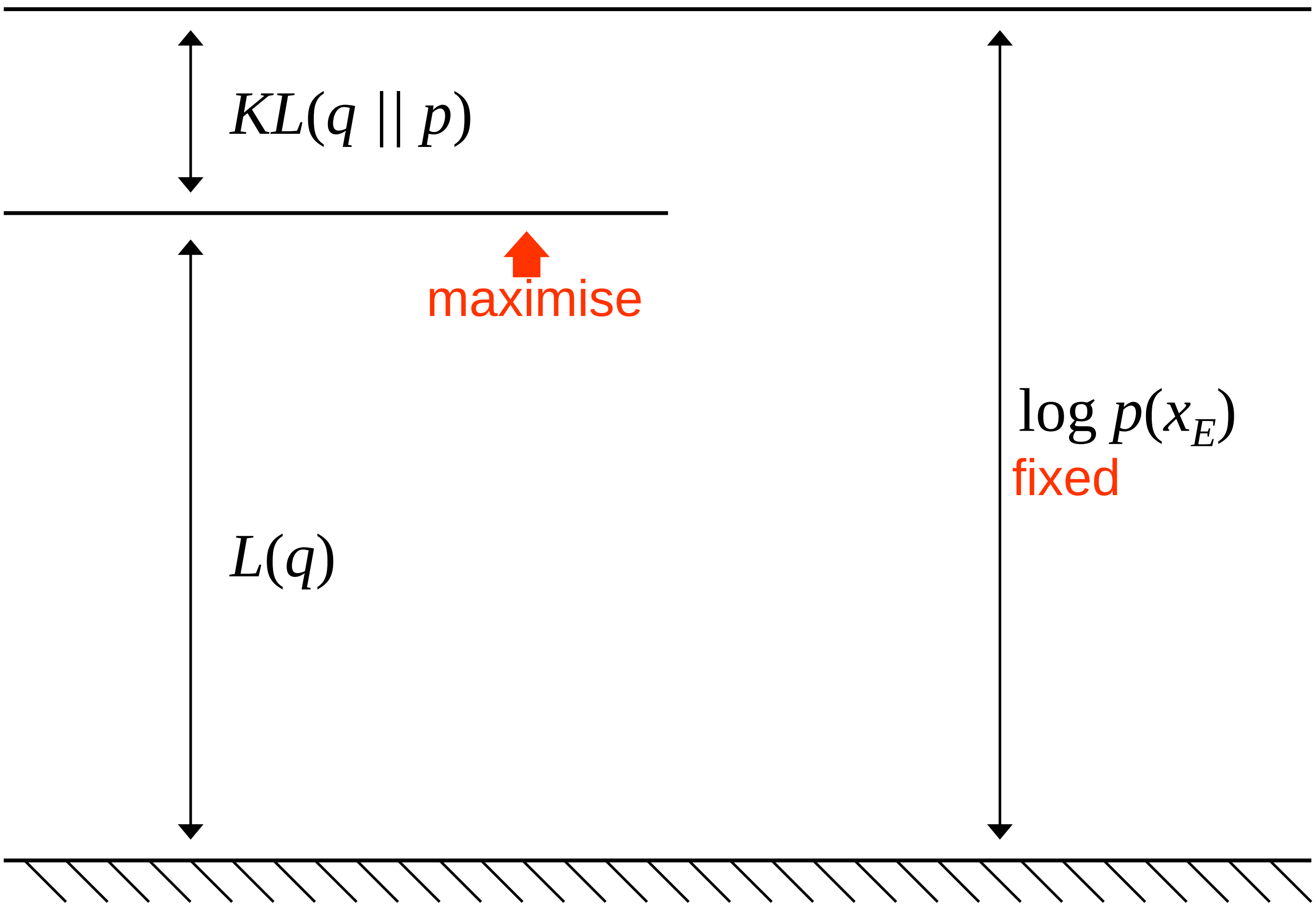
① Minimise the KL distance



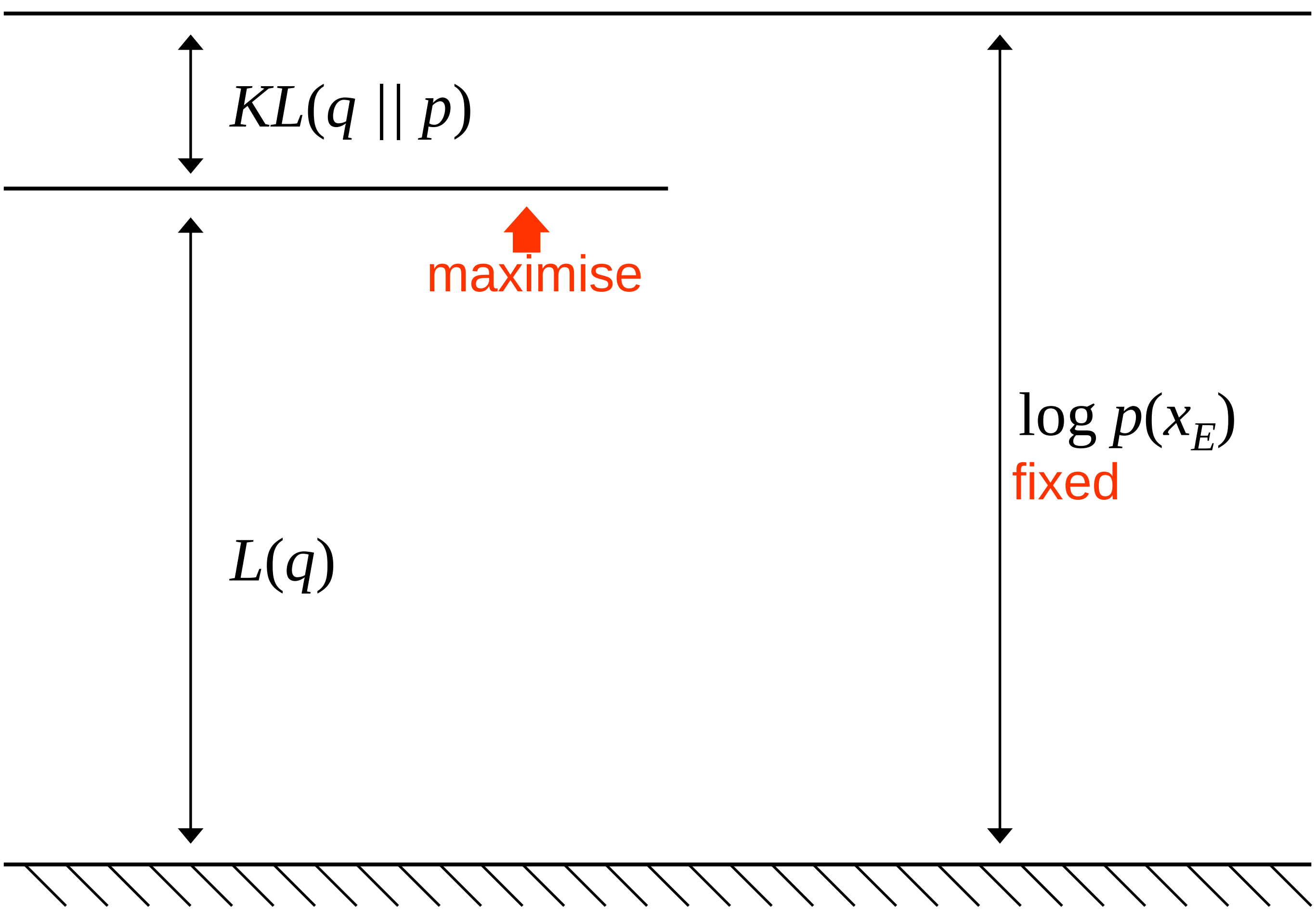
① Minimise the KL distance



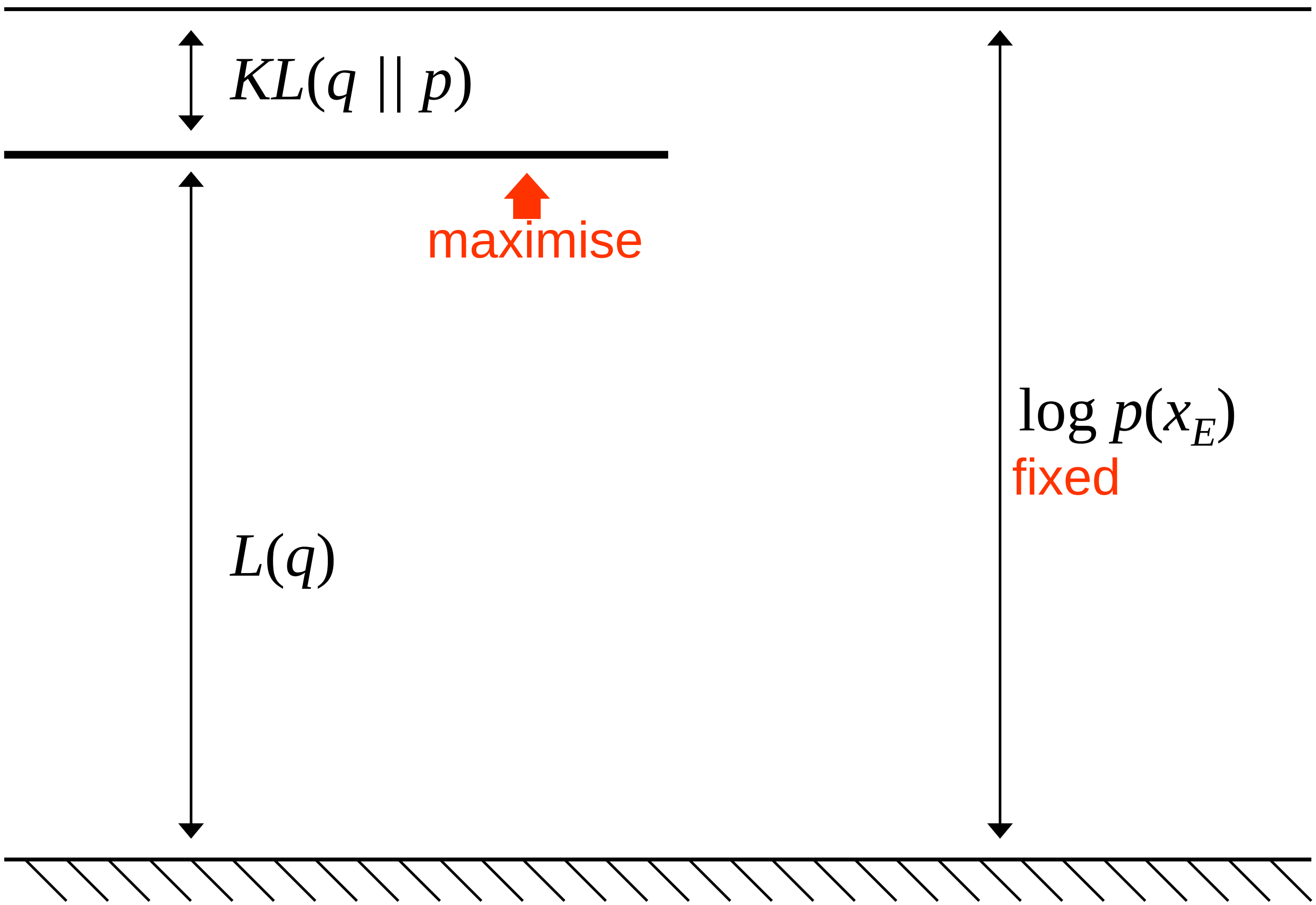
① Minimise the KL distance



① Minimise the KL distance



① Minimise the KL distance



① Minimise the KL distance

$$KL(q \| p) = \sum_{x_H} q(x_H) \log \frac{q(x_H)}{p(x_H | x_E)}$$

fixed maximise minimise

$$\log p(x_E) = L(q) + KL(q \| p)$$

$$L(q) = \sum_{x_H} q(x_H) \log \frac{p(x_H, x_E)}{q(x_H)} = H(q) + \underbrace{\sum_{x_H} q(x_H) \log p(x_H, x_E)}$$

$$\arg\max L(q) = ?$$

q: 任意

$$E_q\left[\log p(x_H, x_E)\right]$$

$$\arg\max L(q) = ?$$

q: 形式受限

$$\langle \log p(x_H, x_E) \rangle_q$$

选择一族形式受限的 q 分布函数

② Choose a family of variational distributions $q(x_H)$

- 变分均值场方法假设 $q(x_H)=\prod_{i\in H} q(x_i)$
  - 假设变分分布下 x_H 的各分量统计独立
  - $q(x_H)$ 称为均值场变分分布（mean field distribution）
  - 变分边缘分布函数—variational marginal $q(x_i)$ 的函数形式无约束

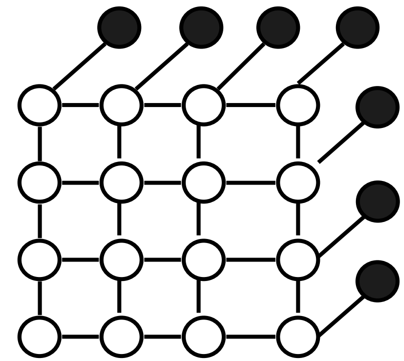
② Choose a family of variational distributions $q(x_H)$

- 图像去噪
  - 给定带噪观测图像 y，恢复原始干净图像 x

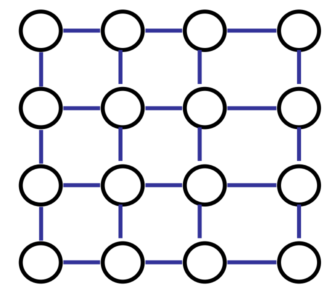
$$p(x, y) \propto \exp\left\{\beta \sum_{i-j} x_i x_j + \gamma \sum_{i} x_i y_i \right\} \qquad \beta > 0, \gamma > 0$$

x_i \ x_j	-1	1
-1	e^{β}	$e^{-\beta}$
1	$e^{-\beta}$	e^{β}

x_i \ y_i	-1	1
-1	e^{γ}	$e^{-\gamma}$
1	$e^{-\gamma}$	e^{γ}



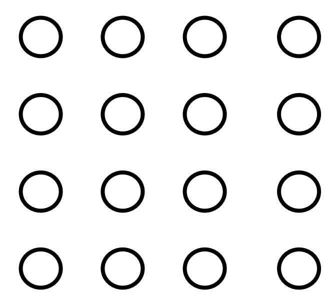
$p(x_{1:16}, y_{1:16})$的无向图表示



真实后验分布$p(x_{1:16}|y_{1:16})$的无向图表示

$$p(x_i \mid y_{1:16}) = ?$$

$$p(x_{1:16} \mid y_{1:16}) \approx q(x_{1:16}) = \prod_{i=1}^{16} q(x_i)$$



变分分布$q(x_{1:16})$的无向图表示

③ Find $q(x_H)$ which minimises KL distance.

$$\underset{q:\text{ 形式受限}}{\arg\max}\, L(q) = ?$$ 泛函最优化，求泛函微分

- 变分均值场方法假设 $q(x_H) = \prod_{i\in H} q(x_i)$
  - $q(x_i)$ 无约束，可分别独立变动/调整，逐个优化

针对$q(x_k)$的最优化：将 $L(q)$ 视为 $q(x_k)$ 的函数，与 $q(x_k)$ 无关项并入常数

$$L(q) = H(q) + \sum_{x_H} q(x_H)\log p(x_H, x_E)$$

$$= H(q(x_k)) + \sum_{x_k}\sum_{x_{H\setminus k}} q(x_k)\prod_{i\neq k} q(x_i)\log p(x_H, x_E) + \text{常数}$$

定义一个新的分布 $\log \tilde{p}(x_k) = \sum_{x_{H\setminus k}}\prod_{i\neq k} q(x_i)\log p(x_H, x_E) + \text{常数}$

$$\max_{q(x_k)} L(q) = H(q(x_k)) + \sum_{x_k} q(x_k)\log \tilde{p}(x_k) + \text{常数}$$

$$= -\min_{q(x_k)} KL(q(x_k)\,\|\,\tilde{p}(x_k)) + \text{常数}$$

③ Find $q(x_H)$ which minimises KL distance.

- 变分均值场方法 $q(x_H)=\prod_{i\in H} q(x_i)$

单个边缘分布的最优解 $\log q(x_k)=\log\tilde{p}(x_k)$

$$=\sum_{x_{H\setminus k}}\prod_{i\neq k} q(x_i)\log p(x_H,x_E)+\text{常数}$$

$$=\sum_{x_{H\setminus k}} q(x_{H\setminus k}\mid x_k)\times\log p(x_H,x_E)=E_q\left[\log p(x_H,x_E)\middle| x_k\right]+\text{常数}$$

均值场更新公式： $\log q(x_k)=E_q\left[\log p(x_H,x_E)\mid x_k\right]+const,\ k\in H$

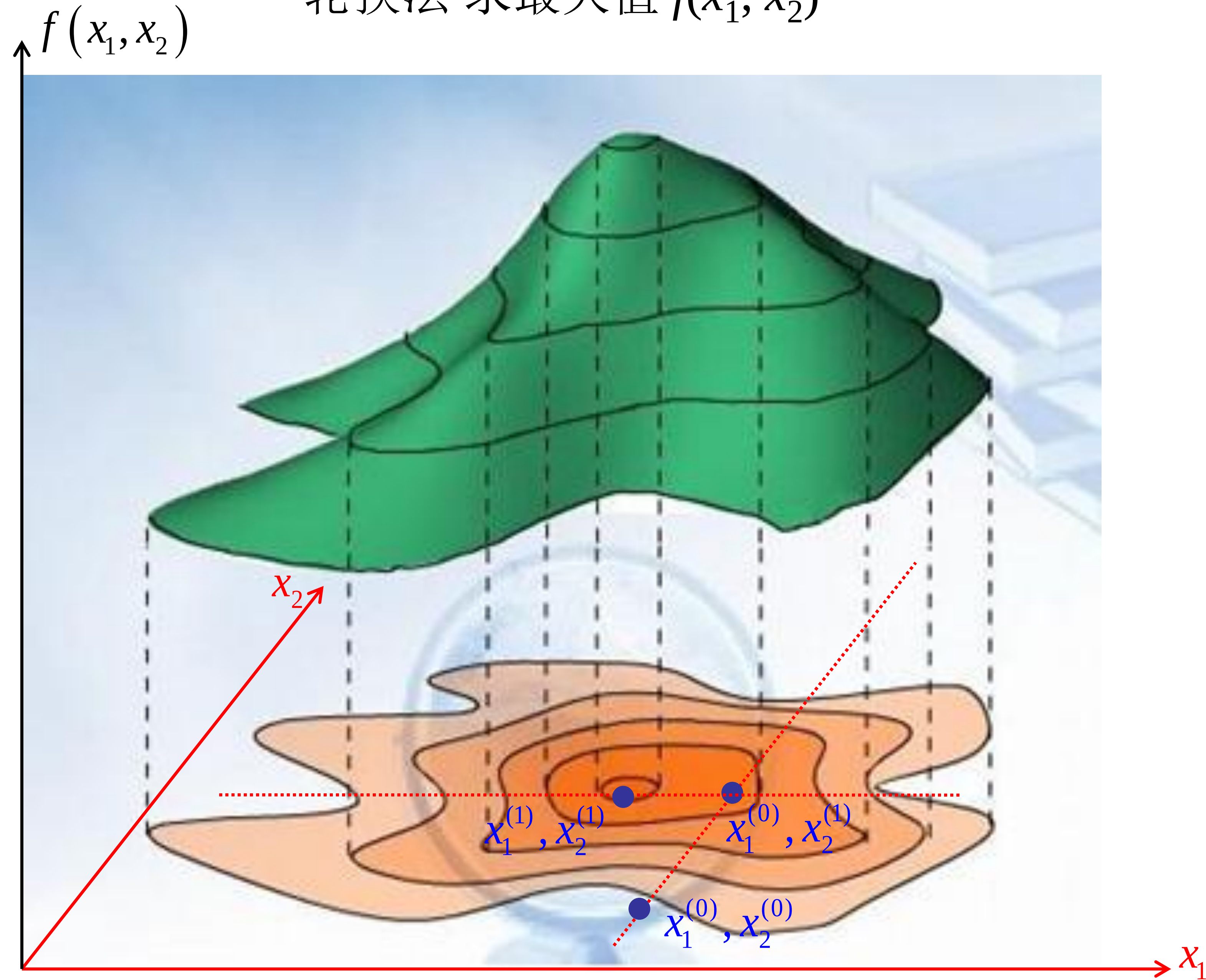
$$q(x_k)\propto\exp\left\{E_q\left[\log p(x_H,x_E)\mid x_k\right]\right\}$$

轮换法求解： $q^{(0)}(x_1),q^{(0)}(x_2),q^{(0)}(x_3),\cdots,q^{(0)}(x_K)$

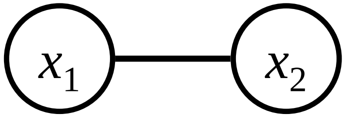
$q^{(1)}(x_1),q^{(0)}(x_2),q^{(0)}(x_3),\cdots,q^{(0)}(x_K)$

$q^{(1)}(x_1),q^{(1)}(x_2),q^{(0)}(x_3),\cdots,q^{(0)}(x_K)$

轮换法 求最大值 $f(x_1, x_2)$

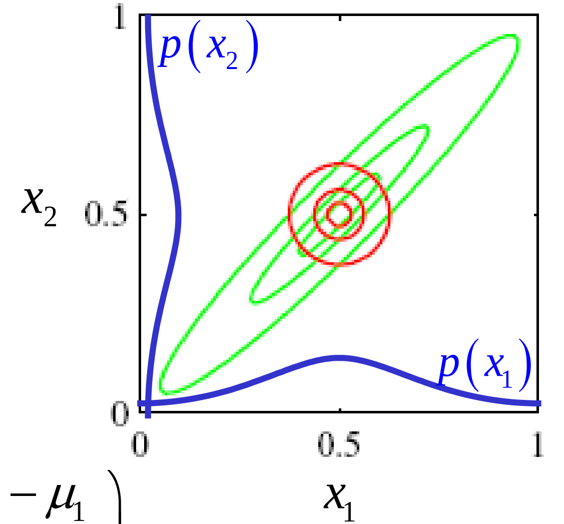


A simple example



$$p(x_1, x_2) = N\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \middle| \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} K_{11} & K_{21} \\ K_{21} & K_{22} \end{pmatrix}^{-1}\right)$$

$q(x_1)$ $\quad$ $q(x_2)$



$$\log p(x_1, x_2) = -\frac{D}{2}\log 2\pi + \frac{1}{2}\log|K| - \frac{1}{2}\begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix}^T \begin{pmatrix} K_{11} & K_{21} \\ K_{21} & K_{22} \end{pmatrix}\begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix}$$

套公式 $\log q(x_k) = E_q\left[\log p(x_H, x_E) \mid x_k\right] + const$ 最小化$KL\left(p(x_1, x_2), q(x_1)q(x_2)\right)$

$$\log q(x_1) = \sum_{x_2} q(x_2)\log p(x_1, x_2) + const$$

$$= -\frac{1}{2}(x_1 - \mu_1)^2 K_{11} - (x_1 - \mu_1)K_{12}\left(\langle x_2\rangle_q - \mu_2\right) + const$$

$$N(x \mid g, h, K) = \exp\left\{g + h\cdot x - \frac{1}{2}K\cdot x^2\right\}$$

x_1的二次项： $-\frac{1}{2}K_{11}\cdot x_1^2$

x_1的一次项： $x_1\cdot\mu_1 K_{11} - x_1\cdot K_{12}\left(\langle x_2\rangle_q - \mu_2\right)$

$$\mu = K^{-1}h$$

$$\Sigma = K^{-1}$$

$$q(x_1) = N\left(x_1 \mid \mu_1 - K_{11}^{-1}K_{12}\left(\langle x_2\rangle_q - \mu_2\right), K_{11}^{-1}\right)$$

A simple example

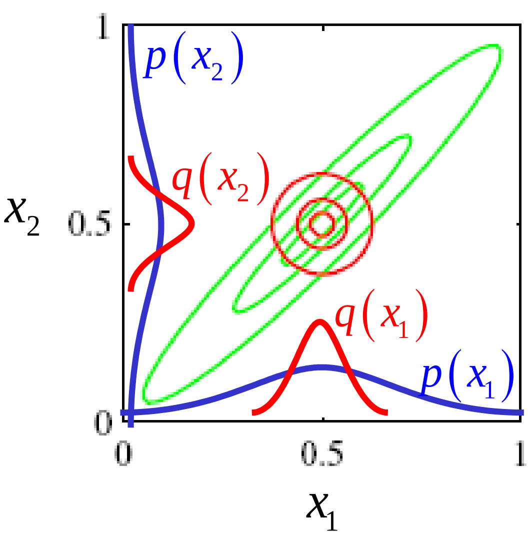
$$p(x_1, x_2) = N\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \middle| \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} K_{11} & K_{21} \\ K_{21} & K_{22} \end{pmatrix}^{-1}\right) \qquad q(x_1) \qquad q(x_2)$$

$$q^{(0)}(x_1), q^{(0)}(x_2)$$
$$\downarrow$$
$$q^{(1)}(x_1), q^{(0)}(x_2)$$
$$\downarrow$$
$$q^{(1)}(x_1), q^{(1)}(x_2)$$

最小化$KL\left(p(x_1, x_2), q(x_1)q(x_2)\right)$，最优解是：

$$\log q(x_1) = \sum_{x_2} q(x_2) \log p(x_1, x_2) + const$$
$$\log q(x_2) = \sum_{x_1} q(x_1) \log p(x_1, x_2) + const$$

$$\rightarrow \begin{cases} q(x_1) = N\left(x_1 \mid \mu_1 - K_{11}^{-1}K_{12}\left(\langle x_2 \rangle_q - \mu_2\right), K_{11}^{-1}\right) \\ q(x_2) = N\left(x_2 \mid \mu_2 - K_{22}^{-1}K_{21}\left(\langle x_1 \rangle_q - \mu_1\right), K_{22}^{-1}\right) \end{cases}$$



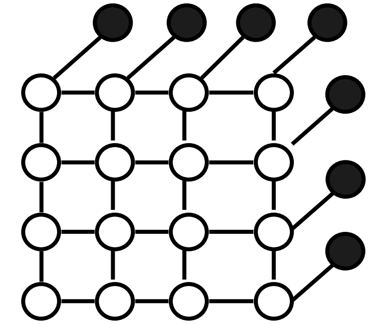
$$q(x_1, x_2) = q(x_1)q(x_2)$$

位于正确的均值位置，但是方差低估了

一般来说，均值场方法给出偏紧凑的近似分布

❖ 图像去噪

- 给定带噪观测图像 y，恢复原始干净图像 x

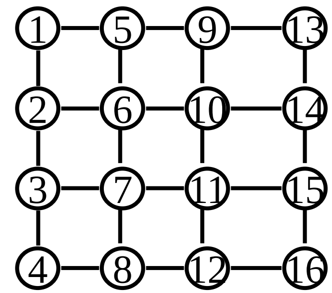


$$p\left(x_{1:16}, y_{1:16}\right) \propto \exp\left\{\beta \sum_{i-j} x_i x_j + \gamma \sum_i x_i y_i\right\} \quad \beta > 0, \gamma > 0$$

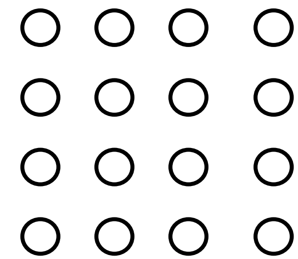
x_i \ x_j	-1	1
-1	e^{β}	$e^{-\beta}$
1	$e^{-\beta}$	e^{β}

x_i \ y_i	-1	1
-1	e^{γ}	$e^{-\gamma}$
1	$e^{-\gamma}$	e^{γ}

$$p\left(x_{1:16} \mid y_{1:16}\right) = ?$$



$$q\left(x_{1:16}\right) = \prod_{i=1}^{16} q\left(x_i\right)$$



套公式 $\log q\left(x_k\right) = E_q\left[\log p\left(x_H, x_E\right) \mid x_k\right] + const$

$$\log q\left(x_i\right) = E_q\left[\beta \sum_{i-j} x_i x_j + \gamma \sum_i x_i y_i \,\middle|\, x_i\right] + const$$

$$\log q\left(x_1\right) = ?$$

$$\log q\left(x_2\right) = ?$$

均值场变分推理 vs Gibbs采样

均值场变分分布计算公式：

$$\log q(x_k) = E_q\left[\log p(x_H, x_E) \mid x_k\right] + const$$

轮换求解：

$$q(x_1), q(x_2), q(x_3), \cdots, q(x_K)$$

$$\hat{q}(x_1), q(x_2), q(x_3), \cdots, q(x_K)$$

$$\hat{q}(x_1), \hat{q}(x_2), q(x_3), \cdots, q(x_K)$$

Gibbs采样公式：

$$x_k - sampling\ from\ p\left(x_k \mid x_{H\backslash\{k\}}, x_E\right)$$

$$x_k - sampling\ from\ p(x_H, x_E)$$

轮换采样：

$$x_1,\ x_2,\ x_3,\ \cdots,\ x_K$$

$$\hat{x}_1,\ x_2,\ x_3,\ \cdots,\ x_K$$

$$x_1,\ \hat{x}_2,\ x_3,\ \cdots,\ x_K$$

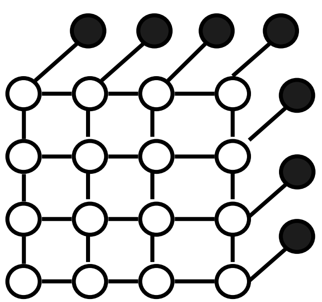
Mean field equations

均值场方程（k=1, …, K）的计算与两种图结构有关

$$\log q_k(x_k) = E_q\left[\log p(x_H, x_E) \mid x_k\right] + const \;= E_q\left[\sum_C \log\phi_C(x_C) \middle| x_k\right] + const$$

$$= \sum_C E_q\left[\log\phi_C(x_C) \middle| x_k\right] + const$$

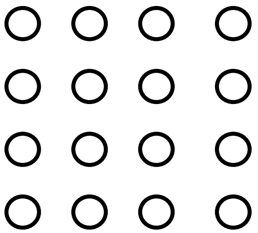
原概率分布 $p(x_H, x_E)$ 的结构



$$= \sum_C \sum_{x_{C\cap(H\setminus k)}} q\left(x_{C\cap(H\setminus k)} \mid x_k\right) \log\phi_C(x_C) + const$$

变分分布 $q(x_H)$ 的结构

$C\cap(H\setminus k)$: 簇 C 中除 k 外的所有隐变量



变分近似推理

- 变分方法是一种经典的泛函最优化方法
- 变分近似推理：变分优化方法用于推理问题
- Block approach
  - 变分均值场方法（Variational mean field）
  - **结构变分方法（Structured variational approach）**
  - 变分贝叶斯方法（Variational Bayesian）用于贝叶斯参数估计
- Sequential approach
  - Local variational method

Structured variational approach

找出一些子结构（substructure），
子结构内部方便做精确推理，子结构之间做均值场近似

- 假设 $q(x_H)=\prod_i q(x_{h_i})$ $\bigcup_i h_i = H,\ h_i \cap h_j = 0 \text{ for } i \neq j$
  - 变分边缘分布函数—variational marginal $q(x_{hi})$ 的函数形式无约束
  - 可分别独立变动/调整，逐个优化

$$\log q(x_{h_i}) = E_q\left[\log p(x_H, x_E) \mid x_{h_i}\right] + const$$

$$= \sum_C E_q\left[\log \phi_C(x_C) \mid x_{h_i}\right] + const$$

原概率分布 $p(x_H, x_E)$ 的结构

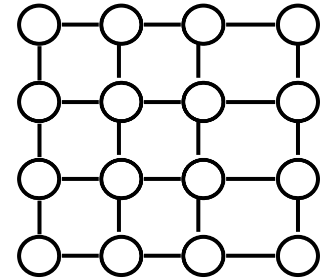
$$= \sum_C \sum_{x_{C\cap(H\setminus h_i)}} q\left(x_{C\cap(H\setminus h_i)} \mid x_{h_i}\right) \log \phi_C(x_C) + const$$

$C\cap(H\setminus h_i)$: 簇 C 中除 h_i 外的所有隐变量

变分分布 $q(x_H)$ 的结构

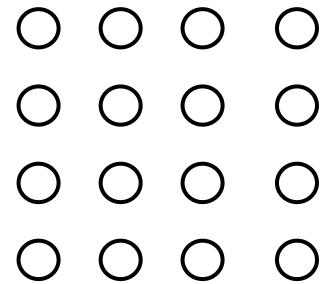
- 图像去噪
  - 给定带噪观测图像 y，恢复原始干净图像 x

$$p(x,y) \propto \exp\left\{\beta\sum_{i-j} x_i x_j + \gamma\sum_i x_i y_i\right\} \quad \beta>0,\gamma>0$$



真实后验分布$p(x_{1:16}|y_{1:16})$的无向图表示

- 均值场变分近似分布 $q(x_H)=\prod_{i\in H} q(x_i)$



均值场变分分布$q(x_{1:16})$的无向图表示

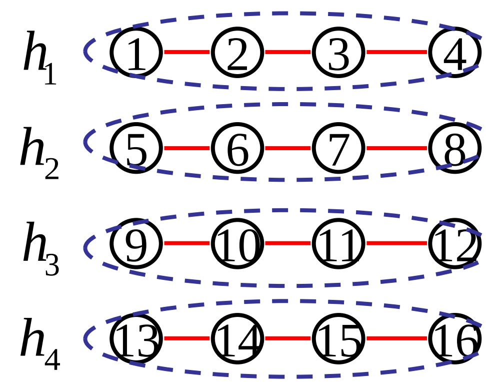
- 结构变分近似分布 $q(x_H)=\prod_{i=1}^{4} q(x_{h_i})$

套公式 $\log q(x_{h_i}) = E_q\left[\log p(x_H, x_E) \mid x_{h_i}\right] + const$

$$\log q(x_{h_i}) = E_q\left\{\beta\sum_{i-j} x_i x_j + \gamma\sum_i x_i y_i \middle| x_{h_i}\right\} + const$$

$$\log q(x_{h_1}) = ?$$

$$\log q(x_{h_2}) = ?$$



结构变分分布的无向图表示

变分近似推理

- 变分方法是一种经典的泛函最优化方法
- 变分近似推理：变分优化方法用于推理问题
- Block approach
  - 变分均值场方法（Variational mean field）
  - 结构变分方法（Structured variational approach）
  - 变分贝叶斯方法（Variational Bayesian）用于贝叶斯参数估计
- Sequential approach
  - Local variational method

M.J. Wainwright, M.I. Jordan.
“Graphical models, exponential families, and variational inference”,
Foundations and Trends in Machine Learning, vol.1, pp.1–305, 2008.

Connect to Deep Learning

Auto-Encoding Variational Bayes

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ICLR 14

Variational Inference using Implicit Distributions

Ferenc Huszár [1]

arxiv Feb.2017; Twitter, London, U.K.

课程章节

- 第一章 引言（1）
- 第二章 图模型的表示理论（2）
  - Semantics (DGM, UGM)
  - HMM, CRF
- 第三章 图模型的推理理论（6）
  - 精确推理：variable-elimination，cluster-tree，triangulate
  - 连续变量：Kalman
  - 采样近似：sampling
  - 变分近似：variational
- 第四章 图模型的学习理论（3）
  - 参数学习：maxlikelihoodEstimate，RFLearning，BayesEstimate
  - 结构学习：StructureLearning
- 第五章 一个综合例子（1）