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KL divergence

Assume two discrete probability distributions P and Q. One way to measure the difference between P and Q is to calculate the Kullback–Leibler (KL) divergence (a.k.a. relative entropy) defined as

$$D_{\mathrm{KL}}(P||Q) = \sum_{i} P(i) \log \frac{P(i)}{Q(i)} = \sum_{i} P(i) \log P(i) - \sum_{i} P(i) \log Q(i)$$
$$= \mathbb{E}_{P}[\log P(i)] - \mathbb{E}_{P}[\log Q(i)].$$

It is defined iff Q(i) = 0 implies P(i) = 0, for all i. If P(i) = 0, then the *i*th term is interpreted as 0. The KL divergence is always non-negative, moreover $D_{\text{KL}}(P||Q) = 0$ iff P = Q almost everywhere.

Interpretation (Information Theory): it is the amount of information lost when Q is used to approximate P. It measures the expected number of extra bits required to code samples from P using a code optimized for Q rather than the code optimized for P.

 $\begin{aligned} & \textbf{Mean Field methods} \\ & \textbf{Tree-reweighted message passing} & \textbf{Mean Field methods} \\ & \textbf{D}_{KL}(q(y) \| p(y \mid x)) = -H(q) - \sum_{y \in \mathcal{Y}} q(y) \log p(y \mid x) \\ & = -H(q) - \sum_{y \in \mathcal{Y}} q(y) \log \frac{1}{Z(x)} \prod_{F \in \mathcal{F}} \exp(-E_F(y_F; x_F)) \\ & = -H(q) + \sum_{y \in \mathcal{Y}} q(y) \sum_{F \in \mathcal{F}} E_F(y_F; x_F) + \log Z(x) \\ & = -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \sum_{\substack{y' \in \mathcal{Y}_F \\ \mu_{F,y_F}(q)}} q(y) E_F(y_F; x_F) + \log Z(x) \\ & = -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \sum_{\mu_{F,y_F}(q)} q(y) E_F(y_F; x_F) + \log Z(x) , \end{aligned}$

where $\mu_{F,y_F}(q) = \sum_{y' \in \mathcal{Y}, y'_F = y_F} q(y)$ are the marginals of q.

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Putting it together,

$$\begin{split} q^* &\in \mathop{\mathrm{argmin}}_{q \in Q} D_{\mathrm{KL}}(q(y) \| p(y \mid x)) \\ &= \mathop{\mathrm{argmin}}_{q \in Q} \left\{ -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F,y_F}(q) E_F(y_F; x_F) + \log Z(x) \right\} \\ &= \mathop{\mathrm{argmax}}_{q \in Q} \left\{ H(q) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F,y_F}(q) E_F(y_F; x_F) \right\} \\ &= \mathop{\mathrm{argmax}}_{q \in Q} \left\{ -\sum_{i \in \mathcal{V}} \sum_{y_i \in \mathcal{Y}_i} q_i(y_i) \log q_i(y_i) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \left(\prod_{i \in N(F)} q_i(y_i) \right) E_F(y_F; x_F) \right\}. \end{split}$$

Optimizing over Q means to optimize over all q_i such that $q_i(y_i) \ge 0$ and $\sum_{y_i \in \mathcal{Y}_i} q_i(y_i) = 1$ for all $i \in \mathcal{V}.$

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Motivation

Mean Field methods



For general (discrete) factor graph models, performing *probabilistic inference* is hard. Assume we are given an **intractable** distribution p(y | x). We consider an **approximate distribution** q(y), which is tractable, for p(y | x).

One way of finding the best approximating distribution is to pose it as an **optimization problem** over probability distributions: given a distribution $p(y \mid x)$ and a family Q of tractable distributions $q \in Q$ on \mathcal{Y} , we want to solve

$$\begin{split} q^* &\in \mathop{\mathrm{argmin}}_{q \in Q} D_{\mathrm{KL}}(q(y) \| p(y \mid x)) = \mathop{\mathrm{argmin}}_{q \in Q} \sum_{y \in \mathcal{Y}} q(y) \log \frac{q(y)}{p(y \mid x)} \\ &= \mathop{\mathrm{argmin}}_{q \in Q} \left\{ \underbrace{\sum_{y \in \mathcal{Y}} q(y) \log q(y)}_{-H(q)} - \sum_{y \in \mathcal{Y}} q(y) \log p(y \mid x) \right\}. \end{split}$$

The term $-\sum_{y \in \mathcal{V}} q(y) \log q(y) \stackrel{\Delta}{=} H(q)$ is called the **entropy** of the distribution q.

Gibbs inequality *

If the set Q is rich enough to contain a close approximation to $p(y \mid x)$ and we succeed at finding it, then the marginals of q^* will provide a good approximation to the true marginals of $p(y \mid x)$ that are intractable to compute.

Gibbs inequality provides a lower bound on the log partition function.

$$\begin{split} 0 \leqslant & D_{\mathrm{KL}}(q(y) \| p(y \mid x)) = -H(q) + \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F,y_F}(q) E_F(y_F; x_F) + \log Z(x) \\ \log Z(x) \geqslant & H(q) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \mu_{F,y_F}(q) E_F(y_F; x_F) \ . \end{split}$$

Set Q consists of all distributions in the form:

Tree-reweighted message passing

$$q(y) = \prod_{i \in \mathcal{V}} q_i(y_i)$$

Naive mean field

Marginals μ_{F,y_F} take the form $\mu_{F,y_F}(q) = \sum_{i=1}^{N}$

$$F_{F,y_F}(q) = \sum_{\substack{y' \in \mathcal{Y}, \\ y'_F = y_F}} q(y) = q_{N(F)}(y_F) = \prod_{i \in N(F)} q_i(y_i) \ .$$

Entropy H(q) decomposes as

$$H(q) = \sum_{i \in \mathcal{V}} H_i(q_i) = -\sum_{i \in \mathcal{V}} \sum_{y_i \in \mathcal{Y}_i} q_i(y_i) \log q_i(y_i) .$$

Proof. Exercise

Optimization

Tree-reweighted message passing Mean Fiel

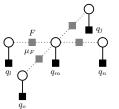
$$\operatorname{argmax}_{q \in Q} \left\{ -\sum_{i \in \mathcal{V}} \sum_{y_i \in \mathcal{Y}_i} q_i(y_i) \log q_i(y_i) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \left(\prod_{i \in N(F)} q_i(y_i)\right) E_F(y_F; x_F) \right\}$$

The entropy term is concave and the second term is non-concave due to products of variables occurring in the expression. Therefore solving this non-concave maximization problem globally is in general hard.

Remedy: block coordinate ascent

We hold all variables fixed except for a single block $q_m,\,{\rm then}$ we obtain a tractable concave maximization problem

 \rightarrow closed-form update for each q_m .



Legange multiplies
 Legange multiplies
 Description matrix

 Legange multiplies
 The description makes well in the Legangie function:

$$L_{(p, \lambda)} = \left\{ -\frac{L_{(p)}}{L_{(p)}} \frac{L_{(p)}}{L_{(p)}} \frac{L_{(p)}}{$$

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