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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.

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

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  $\mu_{F,y_F}$  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

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Optimization

Tree-reweighted message passing Mean Fie

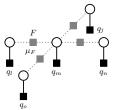
$$\operatorname{argmax}_{q \in Q} \left\{ -\sum_{i \in \mathcal{V}} \sum_{y_i \in \mathcal{Y}_i} q_i(y_i) \log q_i(y_i) - \sum_{F \in \mathcal{F}} \sum_{y_F \in \mathcal{Y}_F} \left(\prod_{i \in N(F)} q_i(y_i)\right) E_F(y_F; x_F) \right\}$$

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 hard in general.

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

- Sebastian Nowozin and Christoph H. Lampert. Structured Prediction and Learning in Computer Vision. In Foundations and Trends in Computer Graphics and Vision, Volume 6, Number 3-4. Note: Chapter 3.
- Daphne Koller and Nir Friedman. Probabilistic Graphical Models: Principles and Techniques. The MIT Press, 2009. Note: Chapter 11.
  Philipp Krähenbühl and Vladlen Koltun. Efficient Inference in Fully
- Philipp Krähenbühl and Vladlen Koltun. Efficient Inference in Fully Connected CRFs with Gaussian Edge Potentials. In Proceedings of Advances in Neural Information Processing Systems, pp. 109–117, Granada, Spain, Dec 2011. MIT Press.