Probabilistic Graphical Models

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Approximate marginal inference

- Given the joint $p(x_1, \ldots, x_n)$ represented as a graphical model, how do we perform **marginal inference**, e.g. to compute $p(x_1)$?
- We showed in Lecture 5 that doing this exactly is NP-hard
- Nearly all *approximate inference* algorithms are either:
  1. Monte-carlo methods (e.g., likelihood reweighting, MCMC)
  2. Variational algorithms (e.g., mean-field, TRW, loopy belief propagation)
- These next two lectures will be on variational methods

Variational methods

- **Goal**: Approximate difficult distribution $p(\mathbf{x})$ with a new distribution $q(\mathbf{x})$ such that:
  1. $p(\mathbf{x})$ and $q(\mathbf{x})$ are "close"
  2. Computation on $q(\mathbf{x})$ is easy
- How should we measure distance between distributions?
- The **Kullback-Leibler divergence** (KL-divergence) between two distributions p and q is defined as

$$D(p\|q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}.$$

  (measures the expected number of extra bits required to describe *samples from* $p(\mathbf{x})$ using a code based on q instead of p)
- As you showed in your homework, $D(p \,\|\, q) \geq 0$ for all p, q, with equality if and only if $p = q$
- Notice that KL-divergence is **asymmetric**

KL-divergence *(see Section 8.5 of K&F)*

$$D(p\|q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}.$$

- Suppose p is the true distribution we wish to do inference with
- What is the difference between the solution to

$$\arg\min_q D(p\|q)$$

(called the *M-projection* of q onto p) and

$$\arg\min_q D(q\|p)$$

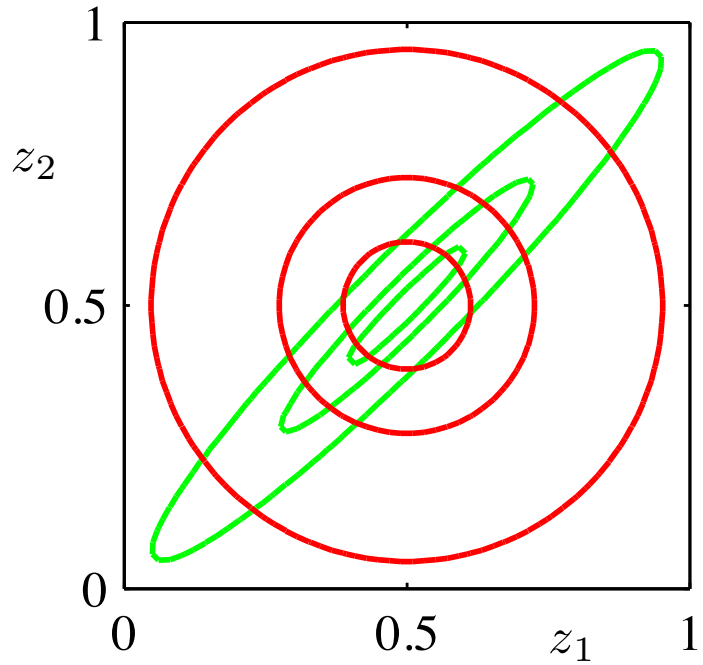
(called the *I-projection*)?

- These two will differ only when q is minimized over a restricted set of probability distributions $Q = \{q_1, \ldots\}$, and in particular when $p \notin Q$

KL-divergence – M-projection

$$q^* = \arg\min_{q \in Q} D(p\|q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}.$$

For example, suppose that $p(\mathbf{z})$ is a 2D Gaussian and Q is the set of all Gaussian distributions with diagonal covariance matrices:



p=Green, q=Red

KL-divergence – I-projection

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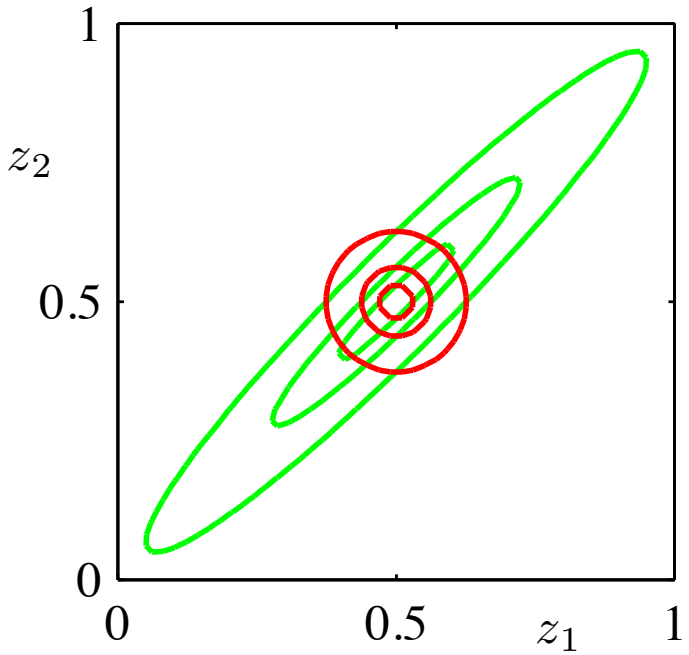
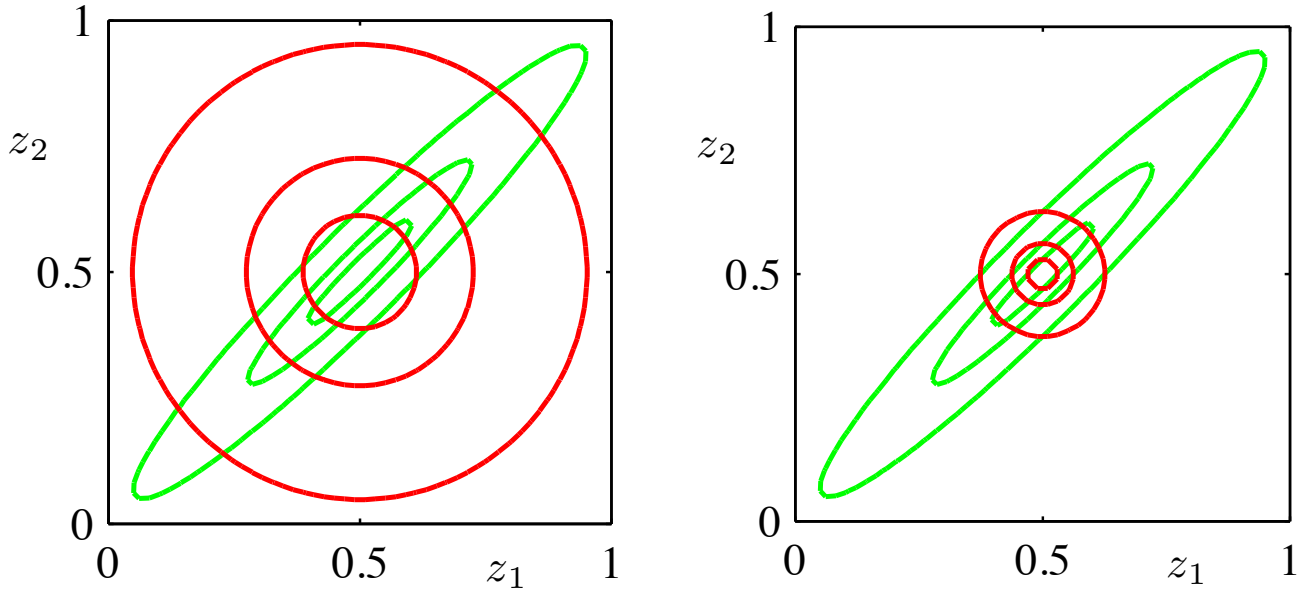
For example, suppose that $p(\mathbf{z})$ is a 2D Gaussian and Q is the set of all Gaussian distributions with diagonal covariance matrices:



p=Green, q=Red

KL-divergence (single Gaussian)

In this simple example, both the M-projection and I-projection find an approximate $q(\mathbf{x})$ that has the correct mean (i.e. $E_p[\mathbf{z}] = E_q[\mathbf{z}]$):

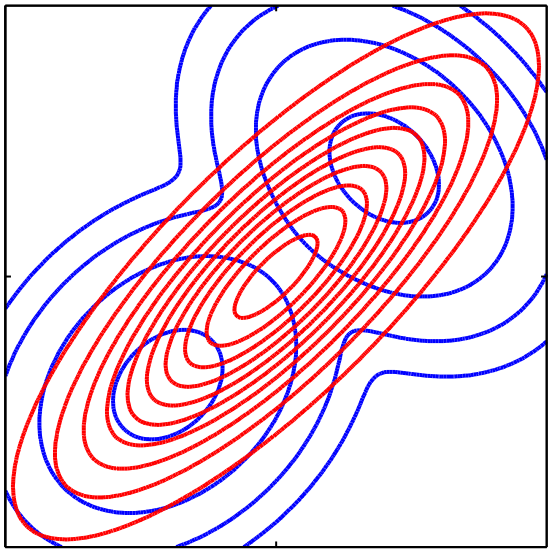


What if $p(\mathbf{x})$ is multi-modal?

KL-divergence – M-projection (mixture of Gaussians)

$$q^* = \arg\min_{q \in Q} D(p\|q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}.$$

Now suppose that $p(\mathbf{x})$ is mixture of two 2D Gaussians and Q is the set of all 2D Gaussian distributions (with arbitrary covariance matrices):

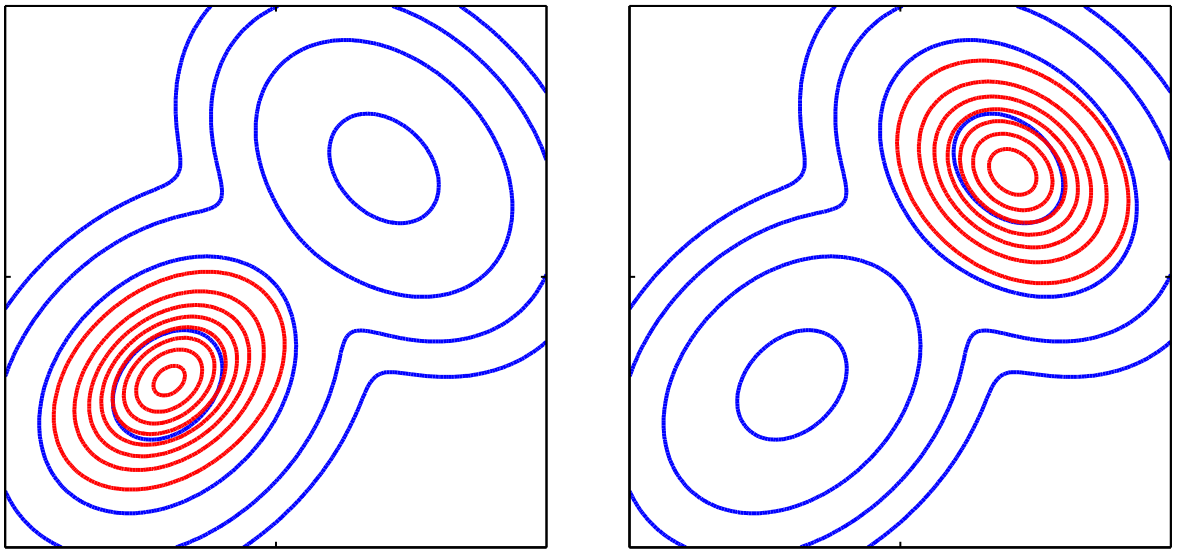


p=Blue, q=Red

M-projection yields distribution $q(\mathbf{x})$ with the correct mean and covariance.

KL-divergence – I-projection (mixture of Gaussians)

$$q^* = \arg\min_{q \in Q} D(q\|p) = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})}.$$



p=Blue, q=Red (two equivalently good solutions!)

Unlike the M-projection, the I-projection does not necessarily yield the correct moments.

Finding the M-projection is the same as exact inference

M-projection is:

$$q^* = \arg\min_{q \in Q} D(p\|q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}.$$

- Recall the definition of probability distributions in the exponential family:

$$q(\mathbf{x}; \eta) = h(\mathbf{x}) \exp\{\eta \cdot \mathbf{f}(\mathbf{x}) - \ln Z(\eta)\}$$

  $\mathbf{f}(\mathbf{x})$ are called the *sufficient statistics*

- In the exponential family, there is a one-to-one correspondance between distributions $q(\mathbf{x}; \eta)$ and marginal vectors $E_q[\mathbf{f}(\mathbf{x})]$
- Suppose that Q is an exponential family ($p(\mathbf{x})$ can be arbitrary)
- It can be shown (see Thm 8.6) that the expected sufficient statistics, with respect to $q^*(\mathbf{x})$, are *exactly* the corresponding marginals under $p(\mathbf{x})$:

$$E_{q^*}[\mathbf{f}(\mathbf{x})] = E_p[\mathbf{f}(\mathbf{x})]$$

- Thus, solving for the M-projection is just as hard as the original inference problem

Most variational inference algorithms make use of the I-projection

Variational methods

- Suppose that we have an arbitrary graphical model:

$$p(\mathbf{x};\theta) = \frac{1}{Z(\theta)} \prod_{\mathbf{c}\in C} \phi_c(\mathbf{x_c}) = \exp\Big(\sum_{\mathbf{c}\in C} \theta_c(\mathbf{x_c}) - \ln Z(\theta)\Big)$$

- All of the approaches begin as follows:

$$\begin{aligned}
D(q\|p) &= \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln p(\mathbf{x}) - \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{1}{q(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \big(\sum_{\mathbf{c}\in C} \theta_c(\mathbf{x_c}) - \ln Z(\theta)\big) - H(q(\mathbf{x})) \\
&= -\sum_{\mathbf{c}\in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x_c}) + \sum_{\mathbf{x}} q(\mathbf{x}) \ln Z(\theta) - H(q(\mathbf{x})) \\
&= -\sum_{\mathbf{c}\in C} E_q[\theta_c(\mathbf{x_c})] + \ln Z(\theta) - H(q(\mathbf{x})).
\end{aligned}$$

Variational approach

- Since $D(q\|p) \geq 0$, we have

$$-\sum_{\mathbf{c}\in C} E_q[\theta_c(\mathbf{x_c})] + \ln Z(\theta) - H(q(\mathbf{x})) \geq 0,$$

  which implies that

$$\ln Z(\theta) \geq \sum_{\mathbf{c}\in C} E_q[\theta_c(\mathbf{x_c})] + H(q(\mathbf{x})).$$

- Thus, *any* approximating distribution $q(\mathbf{x})$ gives a lower bound on the log-partition function
- Recall that $D(q\|p) = 0$ if and only if $p = q$.Thus, if we allow ourselves to optimize over *all* distributions, we have:

$$\ln Z(\theta) = \max_q \sum_{\mathbf{c}\in C} E_q[\theta_c(\mathbf{x_c})] + H(q(\mathbf{x})).$$

Mean-field algorithms

$$\ln Z(\theta) = \max_q \sum_{\mathbf{c} \in C} E_q[\theta_c(\mathbf{x_c})] + H(q(\mathbf{x})).$$

- Although this function is concave and thus in theory should be easy to optimize, we need some compact way of representing $q(\mathbf{x})$
- Mean-field algorithms assume a factored representation of the joint distribution:

$$q(\mathbf{x}) = \prod_{i \in V} q_i(x_i)$$

- The objective function to use for variational inference then becomes:

$$\max_{\{q_i(x_i) \geq 0, \sum_{x_i} q_i(x_i) = 1\}} \sum_{\mathbf{c} \in C} \sum_{\mathbf{x_c}} \theta_c(\mathbf{x_c}) \prod_{i \in \mathbf{c}} q_i(x_i) + \sum_{i \in V} H(\mathbf{q_i})$$

- Key difficulties: **(1)** highly non-convex optimization problem, and **(2)** factored distribution is usually too big of an approximation

Convex relaxation

$$\ln Z(\theta) = \max_q \sum_{\mathbf{c} \in C} E_q[\theta_c(\mathbf{x_c})] + H(q(\mathbf{x})).$$

- Assume that $p(\mathbf{x})$ is in the exponential family, and let $\mathbf{f}(\mathbf{x})$ be its sufficient statistic vector
- Let Q be the exponential family with sufficient statistics $\mathbf{f}(\mathbf{x})$
- Define $\mu_q = E_q[\mathbf{f}(\mathbf{x})]$ be the *marginals* of $q(\mathbf{x})$
- We can re-write the objective as

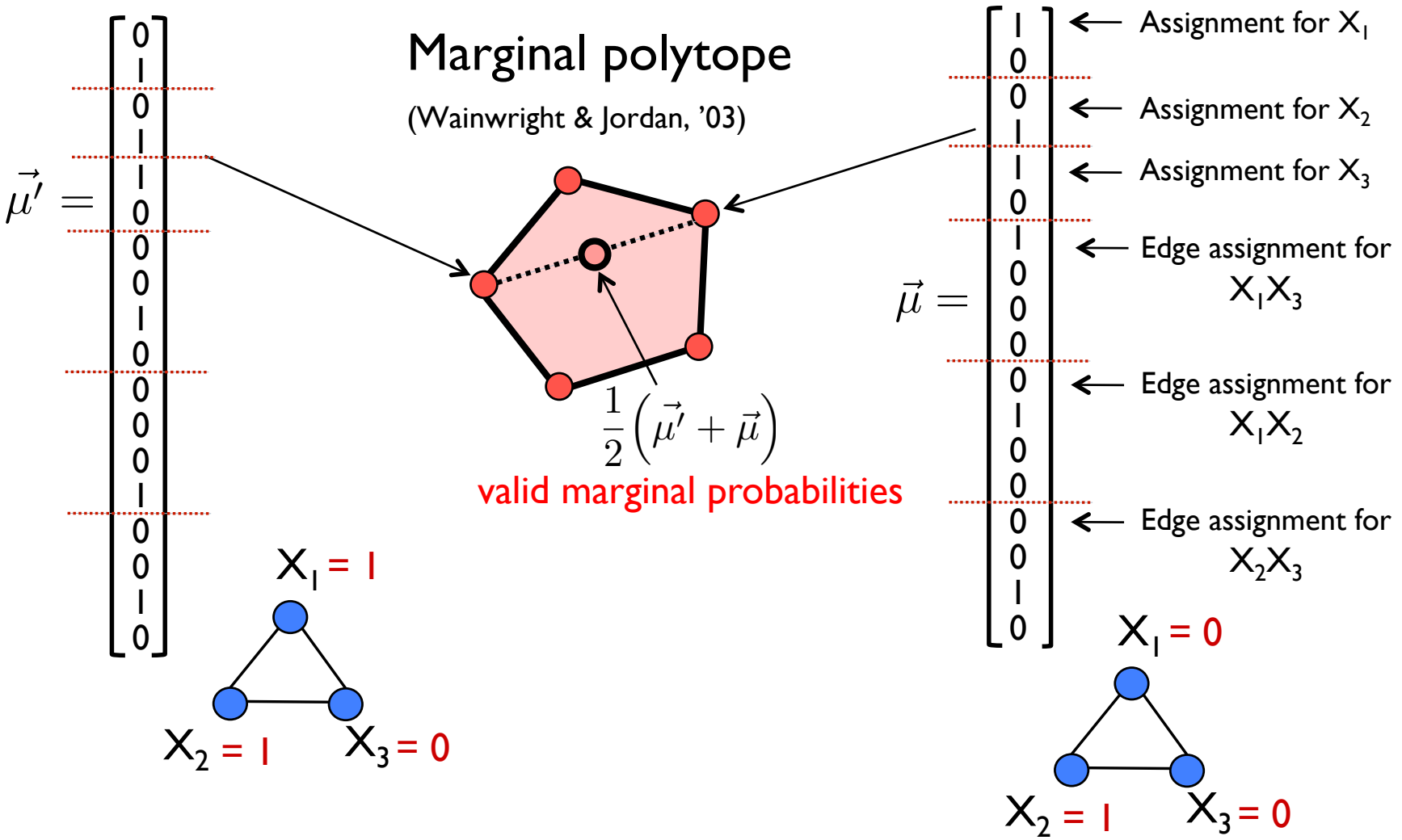
$$\ln Z(\theta) = \max_q \sum_{\mathbf{c} \in C} \sum_{\mathbf{x_c}} \theta_c(\mathbf{x_c}) \mu_q^c(\mathbf{x_c}) + H(\mu_q),$$

  where we define $H(\mu_q)$ to be the entropy of the *maximum entropy distribution* with marginals μ_q

- Next, instead of optimizing over distributions $q(\mathbf{x})$, optimize over valid marginal vectors μ. We obtain:

$$\ln Z(\theta) = \max_{\mu \in M} \sum_{\mathbf{c} \in C} \sum_{\mathbf{x_c}} \theta_c(\mathbf{x_c}) \mu_c(\mathbf{x_c}) + H(\mu)$$

Marginal polytope (same as from Lecture 7!)



Convex relaxation

$$\ln Z(\theta) = \max_{\mu \in M} \sum_{\mathbf{c} \in C} \sum_{\mathbf{x_c}} \theta_c(\mathbf{x_c}) \mu_c(\mathbf{x_c}) + H(\mu)$$

- We still haven't achieved anything, because:
  1. The marginal polytope M is complex to describe (in general, exponentially many vertices and facets)
  2. $H(\mu)$ is very difficult to compute or optimize over
- We now make two approximations:
  1. We replace M with a *relaxation* of the marginal polytope, e.g. the local consistency constraints M_L
  2. We replace $H(\mu)$ with a concave function $\tilde{H}(\mu)$ which upper bounds $H(\mu)$, i.e. $H(\mu) \leq \tilde{H}(\mu)$
- As a result, we obtain the following **upper bound** on the log-partition function, which is concave and easy to optimize:

$$\ln Z(\theta) \leq \max_{\mu \in M_L} \sum_{\mathbf{c} \in C} \sum_{\mathbf{x_c}} \theta_c(\mathbf{x_c}) \mu_c(\mathbf{x_c}) + \tilde{H}(\mu)$$

Local consistency polytope (same as from Lecture 7!)

- Force every "cluster" of variables to choose a local assignment:

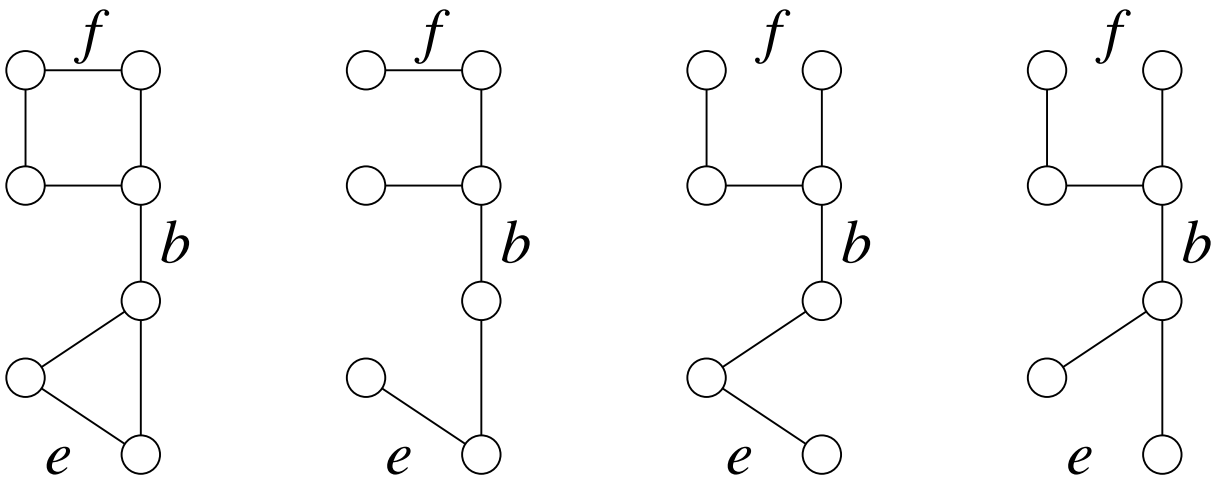
$$\begin{aligned}
\mu_i(x_i) &\geq 0 \quad \forall i \in V, x_i \\
\sum_{x_i} \mu_i(x_i) &= 1 \quad \forall i \in V \\
\mu_{ij}(x_i, x_j) &\geq 0 \quad \forall ij \in E, x_i, x_j \\
\sum_{x_i, x_j} \mu_{ij}(x_i, x_j) &= 1 \quad \forall ij \in E
\end{aligned}$$

- Enforce that these local assignments are globally consistent:

$$\begin{aligned}
\mu_i(x_i) &= \sum_{x_j} \mu_{ij}(x_i, x_j) \quad \forall ij \in E, x_i \\
\mu_j(x_j) &= \sum_{x_i} \mu_{ij}(x_i, x_j) \quad \forall ij \in E, x_j
\end{aligned}$$

Tree reweighted entropy

One particularly powerful concave entropy approximation is the **tree-reweighted** approximation from Jaakkola, Wainwright, & Wilsky (2005)



Obtaining true bounds on the marginals

- We showed how to obtain *upper* and *lower* bounds on the partition function
- These can be used to obtain upper and lower bounds on marginals
- Let $Z(\theta_{x_i})$ denote the partition function of the distribution on $\mathbf{X}_{\mathbf{V}\setminus i}$ where $X_i = x_i$
- Suppose that $L_{x_i} \leq Z(\theta_{x_i}) \leq U_{x_i}$
- Then,

$$\begin{aligned} p(x_i;\theta) &= \frac{\sum_{\mathbf{x}_{\mathbf{V}\setminus i}} \exp(\theta(\mathbf{x}_{\mathbf{V}\setminus i}, x_i))}{\sum_{\hat{x}_i} \sum_{\mathbf{x}_{\mathbf{V}\setminus i}} \exp(\theta(\mathbf{x}_{\mathbf{V}\setminus i}, \hat{x}_i))} \\ &= \frac{Z(\theta_{x_i})}{\sum_{\hat{x}_i} Z(\theta_{\hat{x}_i})} \\ &\leq \frac{U_{x_i}}{\sum_{\hat{x}_i} L_{\hat{x}_i}}. \end{aligned}$$

- Similarly, $p(x_i;\theta) \geq \frac{L_{x_i}}{\sum_{\hat{x}_i} U_{\hat{x}_i}}$.