Today's lecture

Approximate inference in graphical models.

- Forward and Backward KL divergence

- Variational Inference

- Mean Field: Naive and Structured

- Marginal Polytope

- Local Polytope

- Relaxation methods

- Loopy BP

- LP relaxations for MAP inference

Figures from D. Sontag, Murphy's book

Approximate marginal inference

- Given the joint $p(x_1, \cdots, x_n)$ represented as a graphical model, we want to perform **marginal inference**, e.g., $p(x_i|e)$

Approximate marginal inference

- Given the joint $p(x_1, \cdots, x_n)$ represented as a graphical model, we want to perform **marginal inference**, e.g., $p(x_i|e)$
- We showed in last lecture that doing this exactly is NP-hard

Approximate marginal inference

- Given the joint $p(x_1, \cdots, x_n)$ represented as a graphical model, we want to perform **marginal inference**, e.g., $p(x_i|e)$

- We showed in last lecture that doing this exactly is NP-hard

- We also covered variable elimination (VE), which can solve these type of queries for any graphical model, but $\cdots$

Approximate marginal inference

- Given the joint $p(x_1, \cdots, x_n)$ represented as a graphical model, we want to perform **marginal inference**, e.g., $p(x_i|e)$

- We showed in last lecture that doing this exactly is NP-hard

- We also covered variable elimination (VE), which can solve these type of queries for any graphical model, but $\cdots$

- Almost all approximate inference algorithms in practice are
  - Variational algorithms (e.g., mean-field, loopy belief propagation)
  - Sampling methods (e.g., Gibbs sampling, MCMC)

Variational Methods

- **Goal:** Approximate a difficult distribution $p(\mathbf{x}|\mathbf{e})$ with a new distribution $q(\mathbf{x})$

Variational Methods

- **Goal:** Approximate a difficult distribution $p(\mathbf{x}|\mathbf{e})$ with a new distribution $q(\mathbf{x})$
  - $p(\mathbf{x}|\mathbf{e})$ and $q(\mathbf{x})$ should be "close"

Variational Methods

- **Goal:** Approximate a difficult distribution $p(\mathbf{x}|\mathbf{e})$ with a new distribution $q(\mathbf{x})$
  - $p(\mathbf{x}|\mathbf{e})$ and $q(\mathbf{x})$ should be "close"
  - Computation on $q(\mathbf{x})$ should be easy

Variational Methods

- **Goal:** Approximate a difficult distribution $p(\mathbf{x}|\mathbf{e})$ with a new distribution $q(\mathbf{x})$
    - $p(\mathbf{x}|\mathbf{e})$ and $q(\mathbf{x})$ should be "close"
    - Computation on $q(\mathbf{x})$ should be easy
- How should we measure distance between distributions?

Variational Methods

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

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

Variational Methods

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

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

- It measures the expected number of extra bits (nats) required to describe samples from $p(\mathbf{x})$ using a code based on q instead of p

Variational Methods

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

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

- It measures the expected number of extra bits (nats) required to describe samples from $p(\mathbf{x})$ using a code based on q instead of p
- $D(p||q) \geq 0$ for all p, q, with equality if and only if $p = q$

Variational Methods

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

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

- It measures the expected number of extra bits (nats) required to describe samples from $p(\mathbf{x})$ using a code based on q instead of p
- $D(p||q) \geq 0$ for all p, q, with equality if and only if $p = q$
- The KL-divergence is asymmetric

KL-divergence

- Suppose p is the true distribution

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

KL-divergence

- Suppose p is the true distribution

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

- This is difficult to optimize because the expectations w.r.t. p are typically intractable

KL-divergence

- Suppose p is the true distribution

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

- This is difficult to optimize because the expectations w.r.t. p are typically intractable

- We can reverse the KL

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

KL-divergence

- Suppose p is the true distribution

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

- This is difficult to optimize because the expectations w.r.t. p are typically intractable
- We can reverse the KL

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

- Typically the expectation w.r.t. q will be tractable, but $\cdots$

KL-divergence

- Suppose p is the true distribution

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

- This is difficult to optimize because the expectations w.r.t. p are typically intractable
- We can reverse the KL

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

- Typically the expectation w.r.t. q will be tractable, but $\cdots$
- $\cdots$ computing $p(\mathbf{x})$ is still hard, due to the partition function

KL-divergence

- Suppose p is the true distribution

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

- This is difficult to optimize because the expectations w.r.t. p are typically intractable

- We can reverse the KL

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

- Typically the expectation w.r.t. q will be tractable, but $\cdots$

- $\cdots$ computing $p(\mathbf{x})$ is still hard, due to the partition function

- What can we do?

Variational Inference

- Let's look at the unnormalized distribution

$$J(q) \;=\; \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{\tilde{p}(\mathbf{x})}$$

Variational Inference

- Let's look at the unnormalized distribution

$$J(q) = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{\tilde{p}(\mathbf{x})}$$

$$= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{Z \cdot p(\mathbf{x})}$$

Variational Inference

- Let's look at the unnormalized distribution

$$
\begin{aligned}
J(q) &= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{\tilde{p}(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{Z \cdot p(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} - \log Z
\end{aligned}
$$

Variational Inference

- Let's look at the unnormalized distribution

$$
\begin{aligned}
J(q) &= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{\tilde{p}(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{Z \cdot p(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} - \log Z \\
&= KL(q||p) - \log Z
\end{aligned}
$$

Variational Inference

- Let's look at the unnormalized distribution

$$
\begin{aligned}
J(q) &= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{\tilde{p}(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{Z \cdot p(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} - \log Z \\
&= KL(q||p) - \log Z
\end{aligned}
$$

- Since Z is constant, by minimizing $J(q)$, we will force q to become close to p

Variational Inference

- Let's look at the unnormalized distribution

$$
\begin{aligned}
J(q) &= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{\tilde{p}(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{Z \cdot p(\mathbf{x})} \\
&= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} - \log Z \\
&= KL(q||p) - \log Z
\end{aligned}
$$

- Since Z is constant, by minimizing $J(q)$, we will force q to become close to p
- The KL is always non-negative, so we see that $J(q)$ is an upper bound on the negative log likelihood (NLL)

$$
J(q) = KL(q||p) - \log Z \geq -\log Z = -\log p(\mathcal{D})
$$

Alternative Interpretations

- (1). We can alternatively write

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x})] + \mathbb{E}_q[-log\, \tilde{p}(\mathbf{x})]$$

Alternative Interpretations

- (1). We can alternatively write

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x})] + \mathbb{E}_q[-log\,\tilde{p}(\mathbf{x})] = -\mathbb{H}(q) + \mathbb{E}_q[E(\mathbf{x})]$$

  which is the expected energy minus the entropy.

Alternative Interpretations

- (1). We can alternatively write

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x})] + \mathbb{E}_q[-log\,\tilde{p}(\mathbf{x})] = -\mathbb{H}(q) + \mathbb{E}_q[E(\mathbf{x})]$$

  which is the expected energy minus the entropy.

- In physics, $J(q)$ is called the **variational free energy** or **Helmholtz free energy**

Alternative Interpretations

- (1). We can alternatively write

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x})] + \mathbb{E}_q[-log\,\tilde{p}(\mathbf{x})] = -\mathbb{H}(q) + \mathbb{E}_q[E(\mathbf{x})]$$

which is the expected energy minus the entropy.

- In physics, $J(q)$ is called the **variational free energy** or **Helmholtz free energy**

- (2). Another alternative:

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x}) - \log p(\mathbf{x})p(\mathcal{D})]$$

Alternative Interpretations

- (1). We can alternatively write

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x})] + \mathbb{E}_q[-log\,\tilde{p}(\mathbf{x})] = -\mathbb{H}(q) + \mathbb{E}_q[E(\mathbf{x})]$$

which is the expected energy minus the entropy.

- In physics, $J(q)$ is called the **variational free energy** or **Helmholtz free energy**

- (2). Another alternative:

$$
\begin{aligned}
J(q) &= \mathbb{E}_q[\log q(\mathbf{x}) - \log p(\mathbf{x})p(\mathcal{D})] \\
&= \mathbb{E}_q[\log q(\mathbf{x}) - \log p(\mathbf{x}) - \log p(\mathcal{D})]
\end{aligned}
$$

Alternative Interpretations

- (1). We can alternatively write

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x})] + \mathbb{E}_q[-log\,\tilde{p}(\mathbf{x})] = -\mathbb{H}(q) + \mathbb{E}_q[E(\mathbf{x})]$$

which is the expected energy minus the entropy.

- In physics, $J(q)$ is called the **variational free energy** or **Helmholtz free energy**

- (2). Another alternative:

$$\begin{aligned}
J(q) &= \mathbb{E}_q[\log q(\mathbf{x}) - \log p(\mathbf{x})p(\mathcal{D})] \\
&= \mathbb{E}_q[\log q(\mathbf{x}) - \log p(\mathbf{x}) - \log p(\mathcal{D})] \\
&= \mathbb{E}_q[-\log p(\mathcal{D})] + KL(q||p)
\end{aligned}$$

Alternative Interpretations

- (1). We can alternatively write

$$J(q) = \mathbb{E}_q[\log q(\mathbf{x})] + \mathbb{E}_q[-\log \tilde{p}(\mathbf{x})] = -\mathbb{H}(q) + \mathbb{E}_q[E(\mathbf{x})]$$

  which is the expected energy minus the entropy.

- In physics, $J(q)$ is called the **variational free energy** or **Helmholtz free energy**

- (2). Another alternative:

$$
\begin{aligned}
J(q) &= \mathbb{E}_q[\log q(\mathbf{x}) - \log p(\mathbf{x})p(\mathcal{D})] \\
&= \mathbb{E}_q[\log q(\mathbf{x}) - \log p(\mathbf{x}) - \log p(\mathcal{D})] \\
&= \mathbb{E}_q[-\log p(\mathcal{D})] + KL(q||p)
\end{aligned}
$$

- This is the expected NLL plus a penalty term that measures how far apart the two distributions are

KL-divergence

- Before we do something let's inspect again

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

KL-divergence

- Before we do something let's inspect again

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

- What is the difference between the solution to

$$\arg \min_{q} KL(p||q)$$

and

$$\arg \min_{q} KL(q||p)$$

KL-divergence

- Before we do something let's inspect again

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

- What is the difference between the solution to

$$\arg\min_{q} KL(p\|q)$$

and

$$\arg\min_{q} KL(q\|p)$$

- They differ only when q is minimized over a restricted set of probability distribution $Q = \{q_1, \cdots\}$, and $p \neq q$. Why?

- Minimizing $KL(p||q)$ or $KL(q||p)$ will give different results

Forward or Reverse KL

- Minimizing $KL(p||q)$ or $KL(q||p)$ will give different results
- **I projection**, or **Information projection**

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

Forward or Reverse KL

- Minimizing $KL(p||q)$ or $KL(q||p)$ will give different results
- **I projection**, or **Information projection**

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

This is infinite if $p(\mathbf{x}) = 0$ and $q(\mathbf{x}) > 0$. Thus we must ensure that if $p(\mathbf{x}) = 0$ then $q(\mathbf{x}) = 0$

Forward or Reverse KL

- Minimizing $KL(p||q)$ or $KL(q||p)$ will give different results
- **I projection**, or **Information projection**

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

  This is infinite if $p(\mathbf{x}) = 0$ and $q(\mathbf{x}) > 0$. Thus we must ensure that if $p(\mathbf{x}) = 0$ then $q(\mathbf{x}) = 0$
- Thus the reverse KL is **zero forcing** and q will under-estimate the support of p

Forward or Reverse KL

- Minimizing $KL(p||q)$ or $KL(q||p)$ will give different results
- **I projection**, or **Information projection**

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

  This is infinite if $p(\mathbf{x}) = 0$ and $q(\mathbf{x}) > 0$. Thus we must ensure that if $p(\mathbf{x}) = 0$ then $q(\mathbf{x}) = 0$
- Thus the reverse KL is **zero forcing** and q will under-estimate the support of p
- **M projection** or **moment projection**

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

Forward or Reverse KL

- Minimizing $KL(p||q)$ or $KL(q||p)$ will give different results

- **I projection**, or **Information projection**

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

This is infinite if $p(\mathbf{x}) = 0$ and $q(\mathbf{x}) > 0$. Thus we must ensure that if $p(\mathbf{x}) = 0$ then $q(\mathbf{x}) = 0$

- Thus the reverse KL is **zero forcing** and q will under-estimate the support of p

- **M projection** or **moment projection**

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

- This is infinite if $q(\mathbf{x}) = 0$ and $p(\mathbf{x}) > 0$. This is **zero avoiding**, and the forward KL over-estimates the support of p

KL divergence - M projection

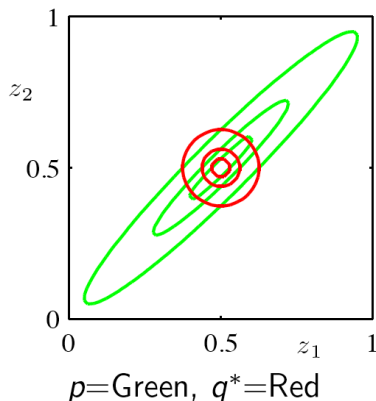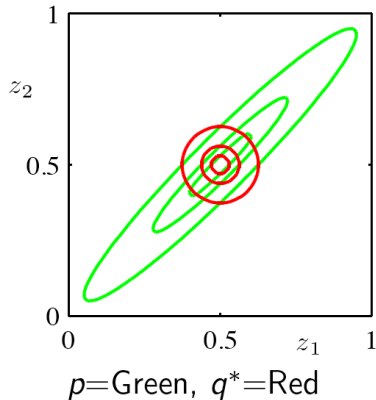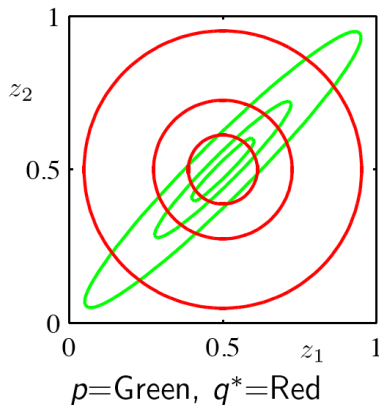$$q^* = arg \min_{q \in Q} KL(p||q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}$$

$p(\mathbf{x})$ is a 2D Gaussian and Q is the set of all Gaussian distributions with diagonal covariance matrices

p=Green, q^*=Red
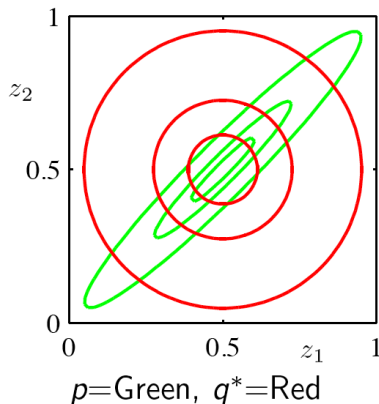
$$q^* = arg \min_{q \in Q} KL(q||p) = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})}$$

$p(\mathbf{x})$ is a 2D Gaussian and Q is the set of all Gaussian distributions with diagonal covariance matrices
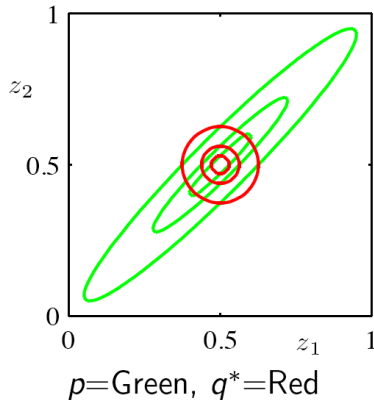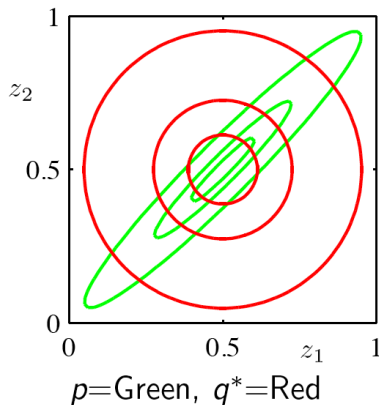

p=Green, q^*=Red

KL Divergence (single Gaussian)

- In this example, both the M-projection and I-projection find an approximate $q(\mathbf{x})$ that has the correct mean (i.e., $\mathbb{E}_p(\mathbf{z}) = \mathbb{E}_q(\mathbf{x})$)

p=Green, q^*=Red

p=Green, q^*=Red

KL Divergence (single Gaussian)

- In this example, both the M-projection and I-projection find an approximate $q(\mathbf{x})$ that has the correct mean (i.e., $\mathbb{E}_p(\mathbf{z}) = \mathbb{E}_q(\mathbf{x})$)
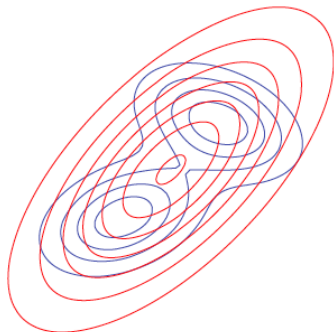

p=Green, q^*=Red

p=Green, q^*=Red

What if $p(\mathbf{x})$ is multimodal?

M projection (Mixture of Gaussians)

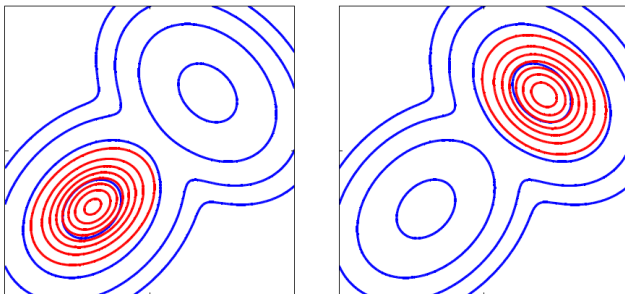$$q^* = arg \min_{q \in Q} KL(p||q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}$$

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

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

I projection (Mixture of Gaussians)

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

p=Blue, q^*=Red (two local minima!)

The I-projection does not necessarily yield the correct moments

Mean Field

- One of the most popular variational inference algorithms [Opper & Saad 01]

Mean Field

- One of the most popular variational inference algorithms [Opper & Saad 01]
- Assume that the posterior fully factorizes

$$q(\mathbf{x}) = \prod_i q_i(x_i)$$

Mean Field

- One of the most popular variational inference algorithms [Opper & Saad 01]
- Assume that the posterior fully factorizes

$$q(\mathbf{x}) = \prod_i q_i(x_i)$$

- Our goal is to

$$\min_{q_1, \cdots, q_D} KL(q||p)$$

where we optimize over the parameters of each marginal distribution q_i

Mean Field

- One of the most popular variational inference algorithms [Opper & Saad 01]
- Assume that the posterior fully factorizes

$$q(\mathbf{x}) = \prod_i q_i(x_i)$$

- Our goal is to

$$\min_{q_1, \cdots, q_D} KL(q||p)$$

  where we optimize over the parameters of each marginal distribution q_i

- Minimize the upper bound $J(q) \geq -\log p(\mathcal{D})$ or alternatively we want to maximize the lower bound

$$L(q) = -J(q) = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})} \leq \log p(\mathcal{D})$$

Mean Field

- One of the most popular variational inference algorithms [Opper & Saad 01]
- Assume that the posterior fully factorizes

$$q(\mathbf{x}) = \prod_i q_i(x_i)$$

- Our goal is to

$$\min_{q_1, \cdots, q_D} KL(q||p)$$

  where we optimize over the parameters of each marginal distribution q_i

- Minimize the upper bound $J(q) \geq -\log p(\mathcal{D})$ or alternatively we want to maximize the lower bound

$$L(q) = -J(q) = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{\tilde{p}(\mathbf{x})}{q(\mathbf{x})} \leq \log p(\mathcal{D})$$

- We can do the maximization one node at a time, in an iterative fashion

Mean Field Updates

- Focus on q_j (holding all other terms constant)

$$L(q_j) = \sum_{\mathbf{x}} \prod_i q_i(\mathbf{x}) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right]$$

Mean Field Updates

- Focus on q_j (holding all other terms constant)

$$
\begin{aligned}
L(q_j) &= \sum_{\mathbf{x}} \prod_i q_i(\mathbf{x}) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} \sum_{\mathbf{x}_{-j}} q_j(\mathbf{x}_j) \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right]
\end{aligned}
$$

Mean Field Updates

- Focus on q_j (holding all other terms constant)

$$
\begin{aligned}
L(q_j) &= \sum_{\mathbf{x}} \prod_i q_i(\mathbf{x}) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} \sum_{\mathbf{x}_{-j}} q_j(\mathbf{x}_j) \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \log \tilde{p}(\mathbf{x}) - \\
&\quad \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\sum_{k \neq j} \log q_k(x_k) + \log q_j(\mathbf{x}_j) \right]
\end{aligned}
$$

Mean Field Updates

- Focus on q_j (holding all other terms constant)

$$
\begin{aligned}
L(q_j) &= \sum_{\mathbf{x}} \prod_i q_i(\mathbf{x}) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} \sum_{\mathbf{x}_{-j}} q_j(\mathbf{x}_j) \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \log \tilde{p}(\mathbf{x}) - \\
&\quad\; \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\sum_{k \neq j} \log q_k(x_k) + \log q_j(\mathbf{x}_j) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log f_j(\mathbf{x}_j) - \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log q_j(\mathbf{x}_j) + \text{const}
\end{aligned}
$$

Mean Field Updates

- Focus on q_j (holding all other terms constant)

$$
\begin{aligned}
L(q_j) &= \sum_{\mathbf{x}} \prod_i q_i(\mathbf{x}) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} \sum_{\mathbf{x}_{-j}} q_j(\mathbf{x}_j) \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \log \tilde{p}(\mathbf{x}) - \\
&\qquad \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\sum_{k \neq j} \log q_k(x_k) + \log q_j(\mathbf{x}_j) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log f_j(\mathbf{x}_j) - \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log q_j(\mathbf{x}_j) + \text{const}
\end{aligned}
$$

where
$$
\log f_j(\mathbf{x}_j) = \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \log \tilde{p}(\mathbf{x}) = \mathbb{E}_{-q_j}[\log \tilde{p}(\mathbf{x})]
$$

Mean Field Updates

- Focus on q_j (holding all other terms constant)

$$
\begin{aligned}
L(q_j) &= \sum_{\mathbf{x}} \prod_i q_i(\mathbf{x}) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} \sum_{\mathbf{x}_{-j}} q_j(\mathbf{x}_j) \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\log \tilde{p}(\mathbf{x}) - \sum_k \log q_k(\mathbf{x}_k) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \log \tilde{p}(\mathbf{x}) - \\
&\quad\quad \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\sum_{k \neq j} \log q_k(x_k) + \log q_j(\mathbf{x}_j) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log f_j(\mathbf{x}_j) - \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log q_j(\mathbf{x}_j) + \text{const}
\end{aligned}
$$

where

$$
\log f_j(\mathbf{x}_j) = \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \log \tilde{p}(\mathbf{x}) = \mathbb{E}_{-q_j}[\log \tilde{p}(\mathbf{x})]
$$

- So we average out all the variables except x_j, and can rewrite $L(q_j)$ as

$$
L(q_j) = -KL(q_j || f_j)
$$

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

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

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

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

- We can compute the KL

$$KL(q \| p) = \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})}$$

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

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

- We can compute the KL

$$
\begin{aligned}
KL(q||p) &= \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln p(\mathbf{x}) - \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{1}{q(\mathbf{x})}
\end{aligned}
$$

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

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

- We can compute the KL

$$
\begin{aligned}
KL(q\|p) &= \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln p(\mathbf{x}) - \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{1}{q(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \left(\sum_{c \in C} \theta_c(\mathbf{x}_c) - \ln Z(\theta) \right) - H(q(\mathbf{x}))
\end{aligned}
$$

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

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

- We can compute the KL

$$
\begin{aligned}
KL(q\|p) &= \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln p(\mathbf{x}) - \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{1}{q(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \left(\sum_{c \in C} \theta_c(\mathbf{x}_c) - \ln Z(\theta)\right) - H(q(\mathbf{x})) \\
&= -\sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x}_c) + \sum_{\mathbf{x}} q(\mathbf{x}) \ln Z(\theta) - H(q(\mathbf{x}))
\end{aligned}
$$

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

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

- We can compute the KL

$$
\begin{aligned}
KL(q\|p) &= \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln p(\mathbf{x}) - \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{1}{q(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \left(\sum_{c \in C} \theta_c(\mathbf{x}_c) - \ln Z(\theta)\right) - H(q(\mathbf{x})) \\
&= -\sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x}_c) + \sum_{\mathbf{x}} q(\mathbf{x}) \ln Z(\theta) - H(q(\mathbf{x})) \\
&= -\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x}))
\end{aligned}
$$

- The partition function can be considered as constant when minimizing over q

Mean Field for Variational Inference

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

# Mean Field for Variational Inference

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

- 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 for Variational Inference

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

- 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**: assume a factored representation of the joint distribution
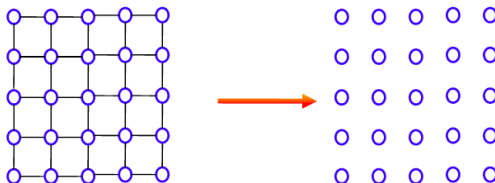
$$q(\mathbf{x}) = \prod_{i \in V} q_i(x_i)$$

This is called "naive" mean field

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in c} q_i(x_i)$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

- The joint entropy decomposes as a sum of local entropies

$$H(q) = -\sum_{\mathbf{x}} q(\mathbf{x}) \ln q(\mathbf{x})$$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

- The joint entropy decomposes as a sum of local entropies

$$
\begin{aligned}
H(q) &= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln q(\mathbf{x}) \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln \prod_{i \in V} q_i(x_i) = -\sum_{\mathbf{x}} q(\mathbf{x}) \sum_{i \in V} \ln q_i(x_i)
\end{aligned}
$$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

- The joint entropy decomposes as a sum of local entropies

$$
\begin{aligned}
H(q) &= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln q(\mathbf{x}) \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln \prod_{i \in V} q_i(x_i) = -\sum_{\mathbf{x}} q(\mathbf{x}) \sum_{i \in V} \ln q_i(x_i) \\
&= -\sum_{i \in V} \sum_{\mathbf{x}} q(\mathbf{x}) \ln q_i(x_i)
\end{aligned}
$$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

- The joint entropy decomposes as a sum of local entropies

$$
\begin{aligned}
H(q) &= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln q(\mathbf{x}) \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln \prod_{i \in V} q_i(x_i) = -\sum_{\mathbf{x}} q(\mathbf{x}) \sum_{i \in V} \ln q_i(x_i) \\
&= -\sum_{i \in V} \sum_{\mathbf{x}} q(\mathbf{x}) \ln q_i(x_i) \\
&= -\sum_{i \in V} \sum_{\mathbf{x}_i} q_i(x_i) \ln q_i(x_i) \sum_{\mathbf{x}_{-i}} q(\mathbf{x}_{-i}|x_i) = \sum_{i \in V} H(q_i)
\end{aligned}
$$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

- The joint entropy decomposes as a sum of local ones $H(q) = \sum_{i \in V} H(q_i)$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

  since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

- The joint entropy decomposes as a sum of local ones $H(q) = \sum_{i \in V} H(q_i)$

- Putting these together, we obtain

$$\max_q \sum_{c \in C} \sum_{\mathbf{x}_c} \theta_c(\mathbf{x}_c) \prod_{i \in c} q_i(x_i) + \sum_{i \in V} H(q_i)$$

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

since $q(\mathbf{x}_c) = \prod_{i \in C} q_i(x_i)$

- The joint entropy decomposes as a sum of local ones $H(q) = \sum_{i \in V} H(q_i)$

- Putting these together, we obtain

$$\max_q \sum_{c \in C} \sum_{\mathbf{x}_c} \theta_c(\mathbf{x}_c) \prod_{i \in c} q_i(x_i) + \sum_{i \in V} H(q_i)$$

subject to the constraints

$$q_i(x_i) \geq 0 \qquad \forall i \in V, x_i$$

$$\sum_{x_i} q_i(x_i) = 1 \qquad \forall i \in V$$

Naive Mean Field for Pairwise MRFs

- For pairwise MRFs we have

$$\max_q \sum_{ij \in E} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) q_i(x_i) q_j(x_j) - \sum_{i \in V} \sum_{x_i} q_i(x_i) \ln q_i(x_i) \qquad (1)$$

Naive Mean Field for Pairwise MRFs

- For pairwise MRFs we have

$$\max_q \sum_{ij \in E} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) q_i(x_i) q_j(x_j) - \sum_{i \in V} \sum_{x_i} q_i(x_i) \ln q_i(x_i) \qquad (1)$$

- This is a non-concave optimization problem, with many local maxima!

Naive Mean Field for Pairwise MRFs

- For pairwise MRFs we have

$$\max_q \sum_{ij \in E} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) q_i(x_i) q_j(x_j) - \sum_{i \in V} \sum_{x_i} q_i(x_i) \ln q_i(x_i) \qquad (1)$$

- This is a non-concave optimization problem, with many local maxima!

- We can do block coordinate ascent
  1. For each $i \in V$
     - Fully maximize Eq. (1) wrt $\{q_i(x_i), \forall x_i\}$
  2. repeat until convergence

Naive Mean Field for Pairwise MRFs

- For pairwise MRFs we have

$$\max_q \sum_{ij \in E} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) q_i(x_i) q_j(x_j) - \sum_{i \in V} \sum_{x_i} q_i(x_i) \ln q_i(x_i) \qquad (1)$$

- This is a non-concave optimization problem, with many local maxima!

- We can do block coordinate ascent
  1. For each $i \in V$
     - Fully maximize Eq. (1) wrt $\{q_i(x_i), \forall x_i\}$
  2. repeat until convergence

- Constructing the Lagrangian, taking the derivatives and setting to zero yields the update

$$q_i(x_i) \leftarrow \frac{1}{Z_i} \exp \left\{ \theta_i(x_i) + \sum_{j \in N(i)} \sum_{x_j} q_j(x_j) \theta_{ij}(x_i, x_j) \right\}$$

Naive Mean Field for Pairwise MRFs

- For pairwise MRFs we have

$$\max_q \sum_{ij \in E} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) q_i(x_i) q_j(x_j) - \sum_{i \in V} \sum_{x_i} q_i(x_i) \ln q_i(x_i) \tag{1}$$

- This is a non-concave optimization problem, with many local maxima!

- We can do block coordinate ascent
  1. For each $i \in V$
     - Fully maximize Eq. (1) wrt $\{q_i(x_i), \forall x_i\}$
  2. repeat until convergence

- Constructing the Lagrangian, taking the derivatives and setting to zero yields the update

$$q_i(x_i) \leftarrow \frac{1}{Z_i} \exp \left\{ \theta_i(x_i) + \sum_{j \in N(i)} \sum_{x_j} q_j(x_j) \theta_{ij}(x_i, x_j) \right\}$$

- See *Mean field example for the Ising Model*, Murphy 21.3.2

Structured mean-field approximations

- Rather than assuming a fully-factored distribution for q, we can use a structured approximation, such as a spanning tree

Structured mean-field approximations

- Rather than assuming a fully-factored distribution for q, we can use a structured approximation, such as a spanning tree

- For example, for a factorial HMM, a good approximation may be a product of chain-structured models (see Murphy 21.4.1)
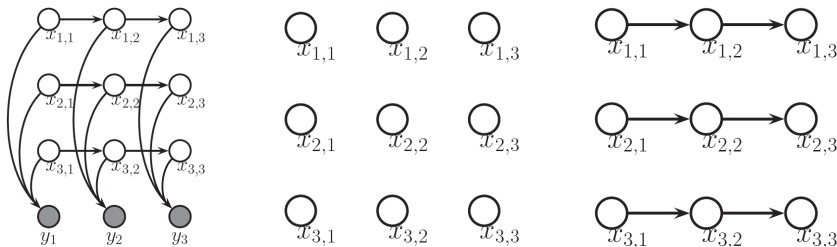
# Approximate Inference via Loopy BP

- Mean field inference approximates posterior as product of marginal distributions

- Allows use of different forms for each variable: useful when inferring statistical parameters of models, or regression weights

- An alternative approximate inference algorithm is **loopy belief propagation**

- Same algorithm shown to do exact inference in trees last class

- In loopy graphs, BP not guaranteed to give correct results, may not converge, but often works well in practice

Algorithm 22.1: Loopy belief propagation for a pairwise MRF

1 Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
2 Initialize messages $m_{s \to t}(x_t) = 1$ for all edges $s - t$;
3 Initialize beliefs $\mathrm{bel}_s(x_s) = 1$ for all nodes s;
4 **repeat**
5   Send message on each edge
     $m_{s \to t}(x_t) = \sum_{x_s} \left(\psi_s(x_s) \psi_{st}(x_s, x_t) \prod_{u \in \mathrm{nbr}_s \setminus t} m_{u \to s}(x_s) \right)$;
6   Update belief of each node $\mathrm{bel}_s(x_s) \propto \psi_s(x_s) \prod_{t \in \mathrm{nbr}_s} m_{t \to s}(x_s)$;
7 **until** *beliefs don't change significantly*;
8 Return marginal beliefs $\mathrm{bel}_s(x_s)$;

Loopy BP for Factor Graph
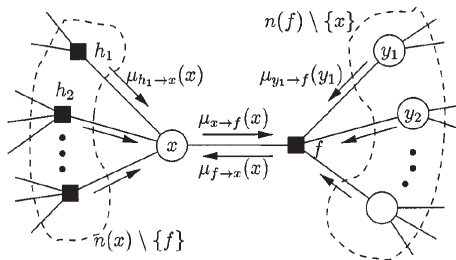
$$m_{i \to f}(x_i) = \prod_{h \in M(i) \setminus f} m_{h \to i}(x_i)$$

$$m_{f \to i}(x_i) = \sum_{\mathbf{x}_c \setminus x_i} f(\mathbf{x}_c) \prod_{j \in N(f) \setminus i} m_{j \to f}(x_j)$$

$$\mu_i(x_i) \propto \prod_{f \in M(i)} m_{f \to i}(x_i)$$

Convergence of LBP

- Can we predict when will converge?

Convergence of LBP

- Can we predict when will converge?
  - Unroll messages across time in a *computation tree*: T iterations of LBP is exact computation in tree of height $T + 1$
  - if leaves' effect on root diminishes over time will converge

Convergence of LBP

- Can we predict when will converge?
  - Unroll messages across time in a *computation tree*: T iterations of LBP is exact computation in tree of height $T + 1$
  - if leaves' effect on root diminishes over time will converge
- Can we make it more likely to converge?

Convergence of LBP

- Can we predict when will converge?
  - Unroll messages across time in a *computation tree*: T iterations of LBP is exact computation in tree of height $T + 1$
  - if leaves' effect on root diminishes over time will converge

- Can we make it more likely to converge?
  - Damp the messages to avoid oscillations
  - Can we speed up convergence?

Convergence of LBP

- Can we predict when will converge?
    - Unroll messages across time in a *computation tree*: T iterations of LBP is exact computation in tree of height $T + 1$
    - if leaves' effect on root diminishes over time will converge

- Can we make it more likely to converge?
    - Damp the messages to avoid oscillations
    - Can we speed up convergence?

- Change from synchronous to asynchronous updates

Convergence of LBP

- Can we predict when will converge?
  - Unroll messages across time in a *computation tree*: T iterations of LBP is exact computation in tree of height $T + 1$
  - if leaves' effect on root diminishes over time will converge

- Can we make it more likely to converge?
  - Damp the messages to avoid oscillations
  - Can we speed up convergence?

- Change from synchronous to asynchronous updates
  - Update sets of nodes at a time, e.g., spanning trees (*tree reparameterization)*

LBP as Variational Inference

- More theoretical analysis of LBP from variational point of view: (Wainwright & Jordan, 2008)

LBP as Variational Inference

- More theoretical analysis of LBP from variational point of view: (Wainwright & Jordan, 2008)

- Dense tome

LBP as Variational Inference

- More theoretical analysis of LBP from variational point of view: (Wainwright & Jordan, 2008)

- Dense tome

- Simplify by considering pairwise UGMs, discrete variables

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

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

- We can compute the KL

$$
\begin{aligned}
KL(q\|p) &= \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \ln p(\mathbf{x}) - \sum_{\mathbf{x}} q(\mathbf{x}) \ln \frac{1}{q(\mathbf{x})} \\
&= -\sum_{\mathbf{x}} q(\mathbf{x}) \left(\sum_{c \in C} \theta_c(\mathbf{x}_c) - \ln Z(\theta)\right) - H(q(\mathbf{x})) \\
&= -\sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x}_c) + \sum_{\mathbf{x}} q(\mathbf{x}) \ln Z(\theta) - H(q(\mathbf{x})) \\
&= -\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x}))
\end{aligned}
$$

- The partition function is a constant when minimizing over q

The log-partition Function

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

$$-\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x})) \geq 0$$

The log-partition Function

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

$$-\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x})) \geq 0$$

which implies

$$\ln Z(\theta) \geq \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

The log-partition Function

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

$$-\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x})) \geq 0$$

which implies

$$\ln Z(\theta) \geq \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

- Thus, any approximating distribution q(x) gives a lower bound on the log-partition function

The log-partition Function

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

$$-\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x})) \geq 0$$

which implies

$$\ln Z(\theta) \geq \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

- Thus, any approximating distribution q(x) gives a lower bound on the log-partition function

- Recall that $KL(p||q) = 0$ if an only if $p = q$. Thus, if we optimize over all distributions we have

$$\ln Z(\theta) = \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

The log-partition Function

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

$$-\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x})) \geq 0$$

which implies

$$\ln Z(\theta) \geq \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

- Thus, any approximating distribution q(x) gives a lower bound on the log-partition function

- Recall that $KL(p||q) = 0$ if an only if $p = q$. Thus, if we optimize over all distributions we have

$$\ln Z(\theta) = \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

- This casts exact inference as a variational optimization problem

Rewriting Objective in terms of Moments

$$\ln Z(\theta) \;\;=\;\; \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

Rewriting Objective in terms of Moments

$$
\begin{aligned}
\ln Z(\theta) &= \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
\end{aligned}
$$

Rewriting Objective in terms of Moments

$$
\begin{aligned}
\ln Z(\theta) &= \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x})\theta_c(\mathbf{x}_c) + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
\end{aligned}
$$

Rewriting Objective in terms of Moments

$$
\begin{aligned}
\ln Z(\theta) &= \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x})\theta_c(\mathbf{x}_c) + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
\end{aligned}
$$

- Assume that $p(\mathbf{x})$ is in the exponential family, and let $\mathbf{f}(\mathbf{x})$ be its sufficient statistic vector

$$
\begin{aligned}
\ln Z(\theta) &= \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
\end{aligned}
$$

- Assume that $p(\mathbf{x})$ is in the exponential family, and let $\mathbf{f}(\mathbf{x})$ be its sufficient statistic vector
- Define $\mu_q = \mathbb{E}[\mathbf{f}(\mathbf{x})]$ to be the marginals of $q(\mathbf{x})$

Rewriting Objective in terms of Moments

$$
\begin{aligned}
\ln Z(\theta) &= \max_{q} \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x})) \\
&= \max_{q} \sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x})) \\
&= \max_{q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
\end{aligned}
$$

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

$$
\ln Z(\theta) = \max_{\mu \in M} \max_{q : \mathbb{E}_q[\mathbf{f}(\mathbf{x})] = \mu} \sum_{c \in C} \sum_{\mathbf{x}_c} \mu_c(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
$$

Rewriting Objective in terms of Moments

$$
\begin{aligned}
\ln Z(\theta) &= \max_q \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x})) \\
&= \max_q \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
\end{aligned}
$$

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

$$
\ln Z(\theta) = \max_{\mu \in M} \max_{q : \mathbb{E}_q[\mathbf{f}(\mathbf{x})] = \mu} \sum_{c \in C} \sum_{\mathbf{x}_c} \mu_c(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))
$$

where M is the **marginal polytope**, having all valid marginal vectors

Rewriting Objective in terms of Moments

- We next push the max inside

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

$$H(\mu) = \max_{q : \mathbb{E}_q[\mathbf{f}(\mathbf{x})] = \mu} H(q)$$

Rewriting Objective in terms of Moments

- We next push the max inside

$$
\begin{aligned}
\ln Z(\theta) &= \max_{\mu \in M} \sum_{c \in C} \sum_{\mathbf{x}_c} \theta_c(\mathbf{x}_c) \mu_c(\mathbf{x}_c) + H(\mu) \\
H(\mu) &= \max_{q : \mathbb{E}_q[\mathbf{f}(\mathbf{x})] = \mu} H(q)
\end{aligned}
$$

- For discrete random variables, the marginal polytope M is the set of all mean parameters for the given model that can be generated from a valid prob. distribution

Rewriting Objective in terms of Moments

- We next push the max inside

$$
\begin{aligned}
\ln Z(\theta) &= \max_{\mu \in M} \sum_{c \in C} \sum_{\mathbf{x}_c} \theta_c(\mathbf{x}_c) \mu_c(\mathbf{x}_c) + H(\mu) \\
H(\mu) &= \max_{q : \mathbb{E}_q[\mathbf{f}(\mathbf{x})] = \mu} H(q)
\end{aligned}
$$

- For discrete random variables, the marginal polytope M is the set of all mean parameters for the given model that can be generated from a valid prob. distribution

$$
M = \left\{ \mu \in \Re^d \mid \exists p \text{ s.t. } \mu = \sum_{x \in \mathcal{X}^m} p(\mathbf{x}) \mathbf{f}(\mathbf{x}) \text{ for some } p(\mathbf{x}) \geq 0, \sum_{x \in \mathcal{X}^m} p(\mathbf{x}) = 1 \right\}
$$

Rewriting Objective in terms of Moments

- We next push the max inside

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

$$H(\mu) = \max_{q:\mathbb{E}_q[\mathbf{f}(\mathbf{x})]=\mu} H(q)$$

- For discrete random variables, the marginal polytope M is the set of all mean parameters for the given model that can be generated from a valid prob. distribution

$$M = \left\{ \mu \in \Re^d \mid \exists p \text{ s.t. } \mu = \sum_{x \in \mathcal{X}^m} p(\mathbf{x})\mathbf{f}(\mathbf{x}) \text{ for some } p(\mathbf{x}) \geq 0, \sum_{x \in \mathcal{X}^m} p(\mathbf{x}) = 1 \right\}$$

$$= \text{conv}\{\mathbf{f}(\mathbf{x}), \mathbf{x} \in \mathcal{X}^m\}$$

with conv the convex hull (it has exponential number of facets)

Rewriting Objective in terms of Moments

- We next push the max inside

$$
\begin{aligned}
\ln Z(\theta) &= \max_{\mu \in M} \sum_{c \in C} \sum_{\mathbf{x}_c} \theta_c(\mathbf{x}_c) \mu_c(\mathbf{x}_c) + H(\mu) \\
H(\mu) &= \max_{q:\mathbb{E}_q[\mathbf{f}(\mathbf{x})]=\mu} H(q)
\end{aligned}
$$

- For discrete random variables, the marginal polytope M is the set of all mean parameters for the given model that can be generated from a valid prob. distribution

$$
\begin{aligned}
M &= \left\{ \mu \in \Re^d \mid \exists p \text{ s.t. } \mu = \sum_{x \in \mathcal{X}^m} p(\mathbf{x}) \mathbf{f}(\mathbf{x}) \text{ for some } p(\mathbf{x}) \geq 0, \sum_{x \in \mathcal{X}^m} p(\mathbf{x}) = 1 \right\} \\
&= \operatorname{conv} \{ \mathbf{f}(\mathbf{x}), \mathbf{x} \in \mathcal{X}^m \}
\end{aligned}
$$

  with conv the convex hull (it has exponential number of facets)

- For a discrete-variable MRF, the sufficient statistic vector $\mathbf{f}(\mathbf{x})$ is simply the concatenation of indicator functions for each clique of variables that appear together in a potential function

Rewriting Objective in terms of Moments

- We next push the max inside

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

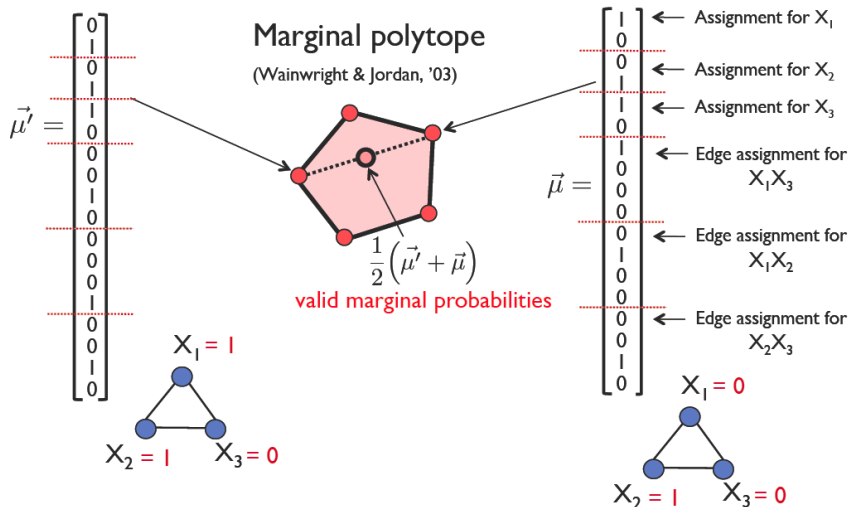$$H(\mu) = \max_{q: \mathbb{E}_q[\mathbf{f}(\mathbf{x})] = \mu} H(q)$$

- For discrete random variables, the marginal polytope M is the set of all mean parameters for the given model that can be generated from a valid prob. distribution

$$M = \left\{ \mu \in \Re^d | \exists p \text{ s.t. } \mu = \sum_{x \in \mathcal{X}^m} p(\mathbf{x})\mathbf{f}(\mathbf{x}) \text{ for some } p(\mathbf{x}) \geq 0, \sum_{x \in \mathcal{X}^m} p(\mathbf{x}) = 1 \right\}$$

$$= \text{conv} \{\mathbf{f}(\mathbf{x}), \mathbf{x} \in \mathcal{X}^m\}$$

  with conv the convex hull (it has exponential number of facets)

- For a discrete-variable MRF, the sufficient statistic vector $\mathbf{f}(\mathbf{x})$ is simply the concatenation of indicator functions for each clique of variables that appear together in a potential function

- For example, if we have a pairwise MRF on binary variables with $m = |V|$ variables and $|E|$ edges, $d = 2m + 4|E|$

Marginal Polytope for Discrete MRFs

Marginal polytope
(Wainwright & Jordan, '03)

$\vec{\mu}' =$ [vector]

$\vec{\mu} =$ [vector]

← Assignment for X_1

← Assignment for X_2

← Assignment for X_3

← Edge assignment for $X_1 X_3$

← Edge assignment for $X_1 X_2$

← Edge assignment for $X_2 X_3$

$\frac{1}{2}\left(\vec{\mu}' + \vec{\mu}\right)$

valid marginal probabilities

$X_1 = 1$

$X_2 = 1$ $X_3 = 0$

$X_1 = 0$

$X_2 = 1$ $X_3 = 0$

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

We still haven't achieved anything, because:

Relaxation

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

We still haven't achieved anything, because:

- The marginal polytope M is complex to describe (in general, exponentially many vertices and facets)

Relaxation

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

We still haven't achieved anything, because:

- The marginal polytope M is complex to describe (in general, exponentially many vertices and facets)

- $H(\mu)$ is very difficult to compute or optimize over

Relaxation

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

We still haven't achieved anything, because:

- The marginal polytope M is complex to describe (in general, exponentially many vertices and facets)
- $H(\mu)$ is very difficult to compute or optimize over

We now make two approximations:

Relaxation

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

We still haven't achieved anything, because:

- The marginal polytope M is complex to describe (in general, exponentially many vertices and facets)
- $H(\mu)$ is very difficult to compute or optimize over

We now make two approximations:

- We replace M with a relaxation of the marginal polytope, e.g. the local consistency constraints M_L

Relaxation

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

We still haven't achieved anything, because:

- The marginal polytope M is complex to describe (in general, exponentially many vertices and facets)
- $H(\mu)$ is very difficult to compute or optimize over

We now make two approximations:

- We replace M with a relaxation of the marginal polytope, e.g. the local consistency constraints M_L
- We replace $H(\mu)$ with a function $\tilde{H}(\mu)$ which approximates $H(\mu)$

Local Consistency Constraints

- For every "cluster" of variables to choose a local assignment

Local Consistency Constraints

- For every "cluster" of variables to choose a local assignment

$$\begin{aligned}
\mu_i(x_i) &\in \{0,1\} \qquad \forall i \in V, x_i \\
\sum_{x_i} \mu_i(x_i) &= 1 \qquad \forall i \in V
\end{aligned}$$

Local Consistency Constraints

- For every "cluster" of variables to choose a local assignment

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

Local Consistency Constraints

- For every "cluster" of variables to choose a local assignment

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

- Enforce that these local assignments are globally consistent

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

Local Consistency Constraints

- For every "cluster" of variables to choose a local assignment

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

- Enforce that these local assignments are globally consistent

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

- The local consistency polytope, M_L is defined by these constraints

Local Consistency Constraints

- For every "cluster" of variables to choose a local assignment

$$\mu_i(x_i) \in \{0,1\} \qquad \forall i \in V, x_i$$

$$\sum_{x_i} \mu_i(x_i) = 1 \qquad \forall i \in V$$

$$\mu_{ij}(x_i, x_j) \in \{0,1\} \qquad \forall i,j \in E, x_i, x_j$$

$$\sum_{x_i, x_j} \mu_{ij}(x_i, x_j) = 1 \qquad \forall i,j \in E$$

- Enforce that these local assignments are globally consistent

$$\mu_i(x_i) = \sum_{x_j} \mu_{ij}(x_i, x_j) \qquad \forall ij \in E, x_i$$

$$\mu_j(x_j) = \sum_{x_i} \mu_{ij}(x_i, x_j) \qquad \forall ij \in E, x_j$$

- The local consistency polytope, M_L is defined by these constraints
- The μ_i and μ_{ij} are called pseudo-marginals

polytope for a tree-structured MRF, and the pseudomarginals are the marginals. marginal polytope, i.e., $M \subseteq M_L$

Mean-field vs relaxation

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

Mean-field vs relaxation

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

- **Relaxation** algorithms work directly with pseudo-marginals which may not be consistent with any joint distribution

Mean-field vs relaxation

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

- **Relaxation** algorithms work directly with pseudo-marginals which may not be consistent with any joint distribution
- **Mean-field** algorithms assume a factored representation of the joint distribution
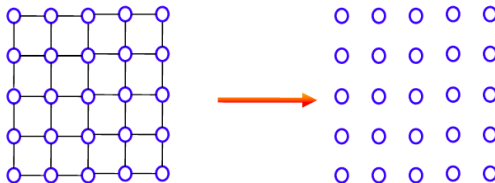
$$q(\mathbf{x}) = \prod_{i \in V} q_i(x_i)$$

Naive Mean-Field

- Using the same notation naive mean-field is:

$$(*) \max_{\mu} \sum_{c \in C} \sum_{\mathbf{x}_c} \mu_c(\mathbf{x}_c) \theta_c(\mathbf{x}_c) + \sum_{i \in V} H(\mu_i) \qquad \text{subject to}$$

$$\mu_i(x_i) \geq 0, \qquad \forall i \in V, x_i$$

$$\sum_{x_i} \mu_i(x_i) = 1 \qquad \forall i \in V$$

$$\mu_c(\mathbf{x}_c) = \prod_{i \in c} \mu_i(x_i)$$

Naive Mean-Field

- Using the same notation naive mean-field is:

$$(*) \max_{\mu} \sum_{c \in C} \sum_{\mathbf{x}_c} \mu_c(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + \sum_{i \in V} H(\mu_i) \qquad \text{subject to}$$

$$\mu_i(x_i) \geq 0, \qquad \forall i \in V, x_i$$

$$\sum_{x_i} \mu_i(x_i) = 1 \qquad \forall i \in V$$

$$\mu_c(\mathbf{x}_c) = \prod_{i \in c} \mu_i(x_i)$$

- Corresponds to optimizing over an inner bound on the marginal polytope:
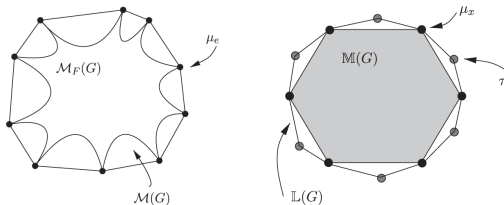
Naive Mean-Field

- Using the same notation naive mean-field is:

$$(*) \max_{\mu} \sum_{c \in C} \sum_{\mathbf{x}_c} \mu_c(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + \sum_{i \in V} H(\mu_i) \qquad \text{subject to}$$

$$\mu_i(x_i) \geq 0, \qquad \forall i \in V, x_i$$

$$\sum_{x_i} \mu_i(x_i) = 1 \qquad \forall i \in V$$

$$\mu_c(\mathbf{x}_c) = \prod_{i \in c} \mu_i(x_i)$$

- Corresponds to optimizing over an inner bound on the marginal polytope:
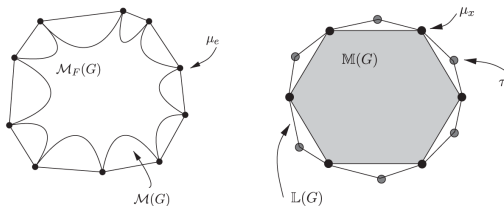
- We obtain a lower bound on the partition function, i.e., $(*) \leq \ln Z(\theta)$

MAP Inference

- Recall the MAP inference task

$$\arg \max_{\mathbf{x}} p(\mathbf{x}), \qquad p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

we assume any evidence has been subsumed into the potentials

MAP Inference

- Recall the MAP inference task

$$\arg\max_{\mathbf{x}} p(\mathbf{x}), \qquad p(\mathbf{x}) = \frac{1}{Z}\prod_{c\in C}\phi_c(\mathbf{x}_c)$$

we assume any evidence has been subsumed into the potentials

- As the partition function is a constant we can alternatively

$$\arg\max_{\mathbf{x}}\prod_{c\in C}\phi_c(\mathbf{x}_c)$$

This is the **max product** inference task

# MAP Inference

- Recall the MAP inference task

$$\arg\max_{\mathbf{x}} p(\mathbf{x}), \qquad p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

we assume any evidence has been subsumed into the potentials

- As the partition function is a constant we can alternatively

$$\arg\max_{\mathbf{x}} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

This is the **max product** inference task

- Since the log is monotonic, let $\theta_c(\mathbf{x}_c) = \log \phi_c(\mathbf{x}_c)$

$$\arg\max_{\mathbf{x}} \sum_{c \in C} \theta_c(\mathbf{x}_c)$$

This is called the **max-sum**

Application: protein side-chain placement

- Find "minimum energy" configuration of amino acid side-chains along fixed carbon backbone:


(Yanover, Meltzer, Weiss '06)

Application: protein side-chain placement

- Find "minimum energy" configuration of amino acid side-chains along fixed carbon backbone:

(Yanover, Meltzer, Weiss '06)
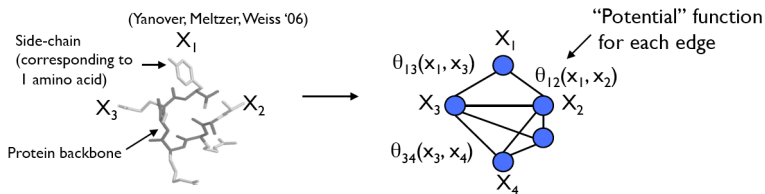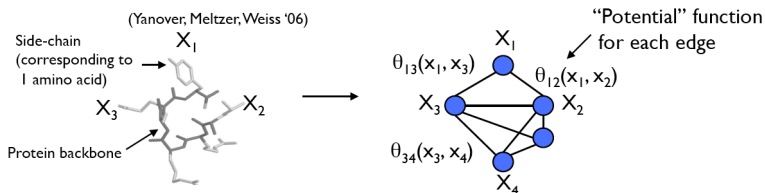
- Orientations of the side-chains are represented by discretized angles called rotamers

Application: protein side-chain placement

- Find "minimum energy" configuration of amino acid side-chains along fixed carbon backbone:

(Yanover, Meltzer, Weiss '06)
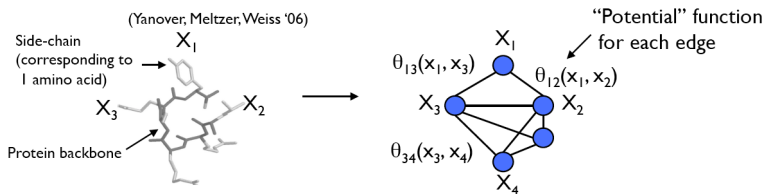
- Orientations of the side-chains are represented by discretized angles called rotamers

- Rotamer choices for nearby amino acids are energetically coupled (attractive and repulsive forces)
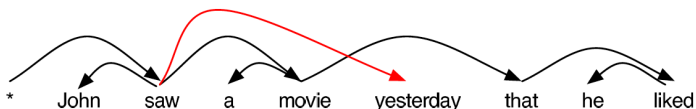
- Given a sentence, predict the dependency tree that relates the words

* John saw a movie yesterday that he liked

Application: Dependency parser

- Given a sentence, predict the dependency tree that relates the words

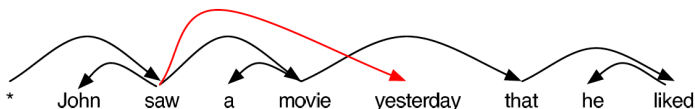- Arc from head word of each phrase to words that modify it

- Given a sentence, predict the dependency tree that relates the words

- Arc from head word of each phrase to words that modify it
- May be non-projective: each word and its descendants may not be a contiguous subsequence

Application: Dependency parser

- Given a sentence, predict the dependency tree that relates the words

- Arc from head word of each phrase to words that modify it
- May be non-projective: each word and its descendants may not be a contiguous subsequence
- m words $\Rightarrow m(m-1)$ binary arc selection variables $x_{ij} \in \{0, 1\}$

Application: Dependency parser

- Given a sentence, predict the dependency tree that relates the words

- Arc from head word of each phrase to words that modify it
- May be non-projective: each word and its descendants may not be a contiguous subsequence
- m words $\Rightarrow m(m-1)$ binary arc selection variables $x_{ij} \in \{0, 1\}$
- We represent the problem as

$$\max_{\mathbf{x}} \theta_T(\mathbf{x}) + \sum_{ij} \theta_{ij}(x_{ij}) + \sum_i \theta_{i|}(\mathbf{x}_{i|})$$
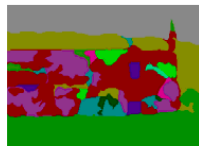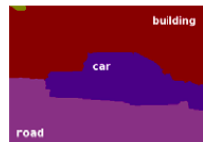
with $\mathbf{x}_{|i} = \{x_{ij}\}_{j \neq i}$ (all outgoing edges)

Application: Semantic Segmentation

- Use Potts to encode that neighboring pixels are likely to have the same discrete label and hence belong to the same segment
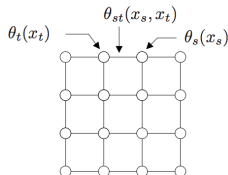
$$p(\mathbf{x}, \theta) = \max_{\mathbf{x}} \sum_i \theta_i(x_i) + \sum_{i,j} \theta_{i,j}(x_i, x_j)$$

MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = arg \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = arg \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

- To turn this into an integer linear program (ILP) we introduce indicator variables

MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = \arg \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

- To turn this into an integer linear program (ILP) we introduce indicator variables

  1. $\mu_i(x_i)$, one for each $i \in V$ and state x_i

MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = arg \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

- To turn this into an integer linear program (ILP) we introduce indicator variables

  1. $\mu_i(x_i)$, one for each $i \in V$ and state x_i
  2. $\mu_{ij}(x_i, x_j)$, one for each edge $ij \in E$ and pair of states x_i, x_j

MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = arg \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

- To turn this into an integer linear program (ILP) we introduce indicator variables

  1. $\mu_i(x_i)$, one for each $i \in V$ and state x_i
  2. $\mu_{ij}(x_i, x_j)$, one for each edge $ij \in E$ and pair of states x_i, x_j

- The objective function is then

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = \arg\max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

- To turn this into an integer linear program (ILP) we introduce indicator variables

  1. $\mu_i(x_i)$, one for each $i \in V$ and state x_i
  2. $\mu_{ij}(x_i, x_j)$, one for each edge $ij \in E$ and pair of states x_i, x_j

- The objective function is then

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i) \mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j) \mu_{ij}(x_i, x_j)$$

- What is the dimension of μ, if binary variables?

MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = \arg\max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

- To turn this into an integer linear program (ILP) we introduce indicator variables

  1. $\mu_i(x_i)$, one for each $i \in V$ and state x_i
  2. $\mu_{ij}(x_i, x_j)$, one for each edge $ij \in E$ and pair of states x_i, x_j

- The objective function is then

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

- What is the dimension of μ, if binary variables?
- Are these two problems equivalent?

Constraints

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

Constraints

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

- For every "cluster" of variables to choose a local assignment

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

Constraints

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

- For every "cluster" of variables to choose a local assignment

$$\mu_i(x_i) \in \{0,1\} \qquad \forall i \in V, x_i$$
$$\sum_{x_i} \mu_i(x_i) = 1 \qquad \forall i \in V$$
$$\mu_{ij}(x_i, x_j) \in \{0,1\} \qquad \forall i,j \in E, x_i, x_j$$
$$\sum_{x_i, x_j} \mu_{ij}(x_i, x_j) = 1 \qquad \forall i,j \in E$$

- Enforce that these local assignments are globally consistent

$$\mu_i(x_i) = \sum_{x_j} \mu_{ij}(x_i, x_j) \qquad \forall ij \in E, x_i$$
$$\mu_j(x_j) = \sum_{x_i} \mu_{ij}(x_i, x_j) \qquad \forall ij \in E, x_j$$

MAP as an integer linear program (ILP)

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

subject to:

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

MAP as an integer linear program (ILP)

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

subject to:

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

- Many extremely good off-the-shelf solvers, such as CPLEX and Gurobi

MAP as an integer linear program (ILP)

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

subject to:

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

- Many extremely good off-the-shelf solvers, such as CPLEX and Gurobi
- But it might be too slow...

Linear Programing Relaxation for MAP

$$MAP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

subject to:

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

- Relax integrality constraints, allowing the variables to be between 0 and 1

$$\mu_i(x_i) \in [0,1] \ \forall i \in V, x_i \qquad \mu_{ij}(x_i, x_j) \in [0,1] \ \forall ij \in E, x_i, x_j$$

Linear Programing Relaxation for MAP

$$LP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

$$\mu_i(x_i) \quad \in \quad [0,1] \quad \forall i \in V, x_i$$

$$\mu_{ij}(x_i, x_j) \quad \in \quad [0,1] \quad \forall i, j \in E, x_i, x_j$$

$$\sum_{x_i} \mu_i(x_i) \quad = \quad 1 \quad \forall i \in V$$

$$\mu_i(x_i) \quad = \quad \sum_{x_j} \mu_{ij}(x_i, x_j) \quad \forall ij \in E, x_i$$

$$\mu_j(x_j) \quad = \quad \sum_{x_i} \mu_{ij}(x_i, x_j) \quad \forall ij \in E, x_j$$

Linear Programing Relaxation for MAP

$$LP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

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

- Linear programs can be solved relatively efficient via Simplex method, interior point, ellipsoid algorithm

Linear Programing Relaxation for MAP

$$LP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

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

- Linear programs can be solved relatively efficient via Simplex method, interior point, ellipsoid algorithm

- Since the LP relaxation maximizes over a larger set of solutions, its value can only be higher

$$MAP(\theta) \leq LP(\theta)$$

Linear Programing Relaxation for MAP

$$LP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i) \mu_i(x_i) + \sum_{ij}(x_i, x_j) \mu_{ij}(x_i, x_j)$$

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

- Linear programs can be solved relatively efficient via Simplex method, interior point, ellipsoid algorithm
- Since the LP relaxation maximizes over a larger set of solutions, its value can only be higher

$$MAP(\theta) \leq LP(\theta)$$

- LP relaxation is tight for tree-structured MRFs

Linear Programing Relaxation for MAP

$$LP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

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

- Linear programs can be solved relatively efficient via Simplex method, interior point, ellipsoid algorithm
- Since the LP relaxation maximizes over a larger set of solutions, its value can only be higher

$$MAP(\theta) \leq LP(\theta)$$

- LP relaxation is tight for tree-structured MRFs
- Faster algorithms by deriving the dual (dual variables represent messages)

Linear Programing Relaxation for MAP

$$LP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

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

- Linear programs can be solved relatively efficient via Simplex method, interior point, ellipsoid algorithm
- Since the LP relaxation maximizes over a larger set of solutions, its value can only be higher

$$MAP(\theta) \leq LP(\theta)$$

- LP relaxation is tight for tree-structured MRFs
- Faster algorithms by deriving the dual (dual variables represent messages)
- Zero limit temperature of the variational inference for Marginals

Loopy Belief Propagation (Max Product)

- Introducing Lagrange multipliers and solving we get (see Murphy 22.3.5.4)

$$M_{i \to j}(x_i) \propto \max_{x_j} \left[\exp\{\theta_{ij}(x_i, x_j) + \theta_j(x_j)\} \prod_{u \in N(j) \setminus i} M_{u \to j}(x_j) \right]$$

Loopy Belief Propagation (Max Product)

- Introducing Lagrange multipliers and solving we get (see Murphy 22.3.5.4)

$$M_{i \to j}(x_i) \propto \max_{x_j} \left[\exp\{\theta_{ij}(x_i, x_j) + \theta_j(x_j)\} \prod_{u \in N(j) \setminus i} M_{u \to j}(x_j) \right]$$

- Thus we pass messages for a fixed number of iterations, or until the messages do not change too much

Loopy Belief Propagation (Max Product)

- Introducing Lagrange multipliers and solving we get (see Murphy 22.3.5.4)

$$M_{i \to j}(x_i) \propto \max_{x_j} \left[\exp\{\theta_{ij}(x_i, x_j) + \theta_j(x_j)\} \prod_{u \in N(j) \setminus i} M_{u \to j}(x_j) \right]$$

- Thus we pass messages for a fixed number of iterations, or until the messages do not change too much

- We decode the local scoring functions by

$$\mu_s(x_s) \quad \propto \quad \exp(\theta_s(x_s)) \prod_{t \in N(s)} M_{t \to s}(x_s)$$

Loopy Belief Propagation (Max Product)

- Introducing Lagrange multipliers and solving we get (see Murphy 22.3.5.4)

$$M_{i \to j}(x_i) \propto \max_{x_j} \left[\exp\{\theta_{ij}(x_i, x_j) + \theta_j(x_j)\} \prod_{u \in N(j) \setminus i} M_{u \to j}(x_j) \right]$$

- Thus we pass messages for a fixed number of iterations, or until the messages do not change too much

- We decode the local scoring functions by

$$\mu_s(x_s) \quad \propto \quad \exp(\theta_s(x_s)) \prod_{t \in N(s)} M_{t \to s}(x_s)$$

- We then compute the maximal value of $\mu_s(x_s)$

Loopy Belief Propagation (Max Product)

- Introducing Lagrange multipliers and solving we get (see Murphy 22.3.5.4)

$$M_{i \to j}(x_i) \propto \max_{x_j} \left[\exp\{\theta_{ij}(x_i, x_j) + \theta_j(x_j)\} \prod_{u \in N(j) \setminus i} M_{u \to j}(x_j) \right]$$

- Thus we pass messages for a fixed number of iterations, or until the messages do not change too much

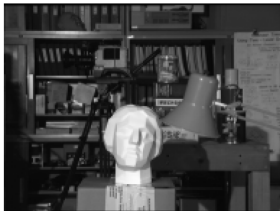- We decode the local scoring functions by

$$\mu_s(x_s) \quad \propto \quad \exp(\theta_s(x_s)) \prod_{t \in N(s)} M_{t \to s}(x_s)$$

- We then compute the maximal value of $\mu_s(x_s)$

- What if two solutions that have the same score?

Stereo Estimation

- Tsukuba images from Middlebury stereo database

Left   Right

Stereo Estimation

- Tsukuba images from Middlebury stereo database

Left

Right

- MRF for each pixel, with states the disparity
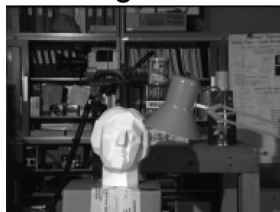
Stereo Estimation

- Tsukuba images from Middlebury stereo database

Left   Right

- MRF for each pixel, with states the disparity
- Our unary is the matching term

$$\theta_i(d_i) = |L(x + d_i, y) - R(x, y)|$$

where pixel $p_i = (x, y)$

Stereo Estimation

- Tsukuba images from Middlebury stereo database

Left   Right

- MRF for each pixel, with states the disparity
- Our unary is the matching term

$$\theta_i(d_i) = |L(x + d_i, y) - R(x, y)|$$

where pixel $p_i = (x, y)$

- The pairwise factor θ_{ij} between neighboring pixels favor smoothness

Stereo Estimation

- If we only use the unary terms. How would you do inference in this case?

Stereo Estimation

- If we only use the unary terms. How would you do inference in this case?

- If full graphical model

| left, | right, | up, | down sweeps |

[Credit: Coughlan BP Tutorial]

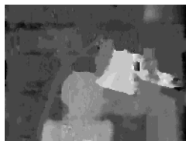Subsequent iterations:

2

3

4

5

... 20

Note:

Little change after first few iterations.

Model can be improved to give better results

-- this is just a simple example to illustrate BP.

[Credit: Coughlan BP Tutorial]