CS 6347

Lectures 6 & 7

Approximate MAP Inference

Belief Propagation

- Efficient method for inference on a tree
- Represent the variable elimination process as a collection of messages passed between nodes in the tree
  - The messages keep track of the potential functions produced throughout the elimination process

Belief Propagation (for pairwise MRFs)

- $p(x_1, \dots, x_n) = \frac{1}{Z} \prod_{i \in V} \phi_i(x_i) \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j)$

$$m_{i \to j}(x_j) = \sum_{x_i} \phi_i(x_i) \psi_{ij}(x_i, x_j) \prod_{k \in N(i) \setminus j} m_{k \to \mathrm{i}}(x_i)$$

where $N(i)$ is the set of neighbors of node i in the graph

- Messages are passed in two phases: from the leaves up to the root and then from the root down to the leaves

Sum-Product

- To construct the marginal distributions, we look at the max-marginal produced by the algorithm

$$b_i(x_i) = \frac{1}{Z}\phi_i(x_i) \prod_{k \in N(i)} m_{k \to i}(x_i)$$

$$b_{ij}(x_i, x_j) = \frac{1}{Z}\phi_i(x_i)\phi_j(x_j)\psi_{ij}(x_i, x_j)\left(\prod_{k \in N(i) \setminus j} m_{k \to i}(x_i)\right)\left(\prod_{k \in N(j) \setminus i} m_{k \to j}(x_j)\right)$$

- Last time, we argued that, on a tree,

$$b_i(x_i) = \sum_{x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n} p(x_1, \ldots, x_n)$$

MAP Inference

- Compute the most likely assignment under the (conditional) joint distribution

$$x^* = \arg\max_x p(x)$$

- Can encode 3-SAT, maximum independent set problem, etc. as a MAP inference problem

Max-Product (for pairwise MRFs)

- $p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{i \in V} \phi_i(x_i) \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j)$

$$m_{i \to j}(x_j) = \max_{x_i} \left[\phi_i(x_i) \psi_{ij}(x_i, x_j) \prod_{k \in N(i) \setminus j} m_{k \to \mathrm{i}}(x_i) \right]$$

- Guaranteed to produced the correct answer on a tree
- Typical applications do not require computing Z

Max-Product

- To construct the maximizing assignment, we look at the max-marginal produced by the algorithm

$$\mu_i(x_i) = \frac{1}{Z}\phi_i(x_i) \prod_{k \in \mathrm{N}(i)} m_{k\to i}(x_i)$$

$$\mu_{ij}(x_i, x_j) = \frac{1}{Z}\phi_i(x_i)\phi_j(x_j)\psi_{ij}(x_i, x_j)\left(\prod_{k \in \mathrm{N}(i)\setminus j} m_{k\to i}(x_i)\right)\left(\prod_{k \in \mathrm{N}(j)\setminus i} m_{k\to j}(x_j)\right)$$

- Again, on a tree,

$$\mu_i(x_i) = \max_{x_1,\dots,x_{i-1},x_{i+1},\dots,x_n} p(x_1, \dots, x_n)$$

Reparameterization

- The messages passed in max-product and sum-product can be used to construct a **reparameterization** of the joint distribution

$$p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{i \in V} \phi_i(x_i) \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j)$$

and

$$p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{i \in V} \left[\phi_i(x_i) \prod_{k \in N(i)} m_{k \to i}(x_i) \right] \prod_{(i,j) \in E} \frac{\psi_{ij}(x_i, x_j)}{m_{i \to j}(x_j) m_{j \to i}(x_i)}$$

Reparameterization

$$p(x_1, \dots, x_n) = \frac{1}{Z} \prod_{i \in V} \left[\phi_i(x_i) \prod_{k \in N(i)} m_{k \to i}(x_i) \right] \prod_{(i,j) \in E} \frac{\psi_{ij}(x_i, x_j)}{m_{i \to j}(x_j) m_{j \to i}(x_i)}$$

- Reparameterizations do not change the partition function, the MAP solution, or the factorization of the joint distribution
  - They push "weight" around between the different factors
- Other reparameterizations are possible/useful

Max-Product Tree Reparameterization

- On a tree, the joint distribution has a special form

$$p(x_1, \dots, x_n) = \frac{1}{Z'} \prod_{i \in V} \mu_i(x_i) \prod_{(i,j) \in E} \frac{\mu_{ij}(x_i, x_j)}{\mu_i(x_i)\mu_j(x_j)}$$

- μ_i is the max-marginal distribution of the i^{th} variable and μ_{ij} is the max-marginal distribution for the edge $(i, j) \in E$

- How to express μ_{ij} as a function of the messages and the potential functions?

MAP in General MRFs

- While max-product solves the MAP problem on trees, the MAP problem in MRFs is, in general, intractable (could use it to find a maximal independent set!)
  - Don't expect to be able to solve the problem exactly
  - Will settle for "good" approximations
  - Can use max-product messages as a starting point
- This is an active area of research

Upper Bounds

$$\max_{x_1,\ldots,x_n} p(x_1, \ldots, x_n) \leq \frac{1}{Z} \prod_{i \in V} \max_{x_i} \phi_i(x_i) \prod_{(i,j) \in E} \max_{x_i, x_j} \psi_{ij}(x_i, x_j)$$

- This provides an upper bound on the optimization problem
  - Do other reparameterizations provide better bounds?

Duality

$$L(m) = \frac{1}{Z} \prod_{i \in V} \max_{x_i} \left[\phi_i(x_i) \prod_{k \in N(i)} m_{k \to i}(x_i) \right] \prod_{(i,j) \in E} \max_{x_i, x_j} \left[\frac{\psi_{ij}(x_i, x_j)}{m_{i \to j}(x_j) m_{j \to i}(x_i)} \right]$$

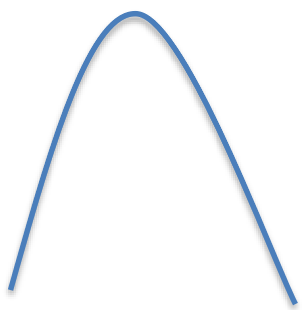
- We construct a dual optimization problem

$$\min_{m \geq 0} L(m) \geq \max_x p(x)$$

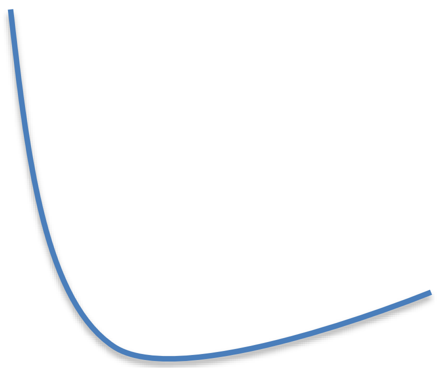
- Equivalently, we can minimize the convex function U

$$U(\log m) = -\log Z + \sum_{i \in V} \max_{x_i} \left[\log \phi_{i(x_i)} + \sum_{\{k \in N(i)\}} \log m_{k \to i}(x_i) \right]$$
$$+ \sum_{(i,j) \in E} \max_{x_i, x_j} [\log \psi_{ij}(x_i, x_j) - \log m_{i \to j}(x_j) - \log m_{j \to i}(x_i)]$$

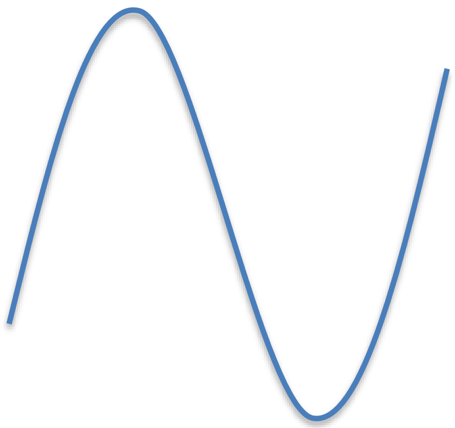
Convex and Concave Functions



Convex



Concave



Neither

Optimizing the Dual

- Minimizing $U(\log m)$
  - Block coordinate descent: improve the bound by changing only a small subset of the messages at a time (usually look like message-passing algorithms)
  - Subgradient descent: variant of gradient descent for non-differentiable functions
  - Many more optimization methods…
- Note that $\min_{m \geq 0} L(m)$ is not necessarily equal to $\max_x p(x)$, so this procedure only yields an approximation to the maximal value

Gradient Descent

- Iterative method to minimize a differentiable convex function f (for non-differentiable use subgradients)
  - Intuition: step along a direction in which the function is decreasing

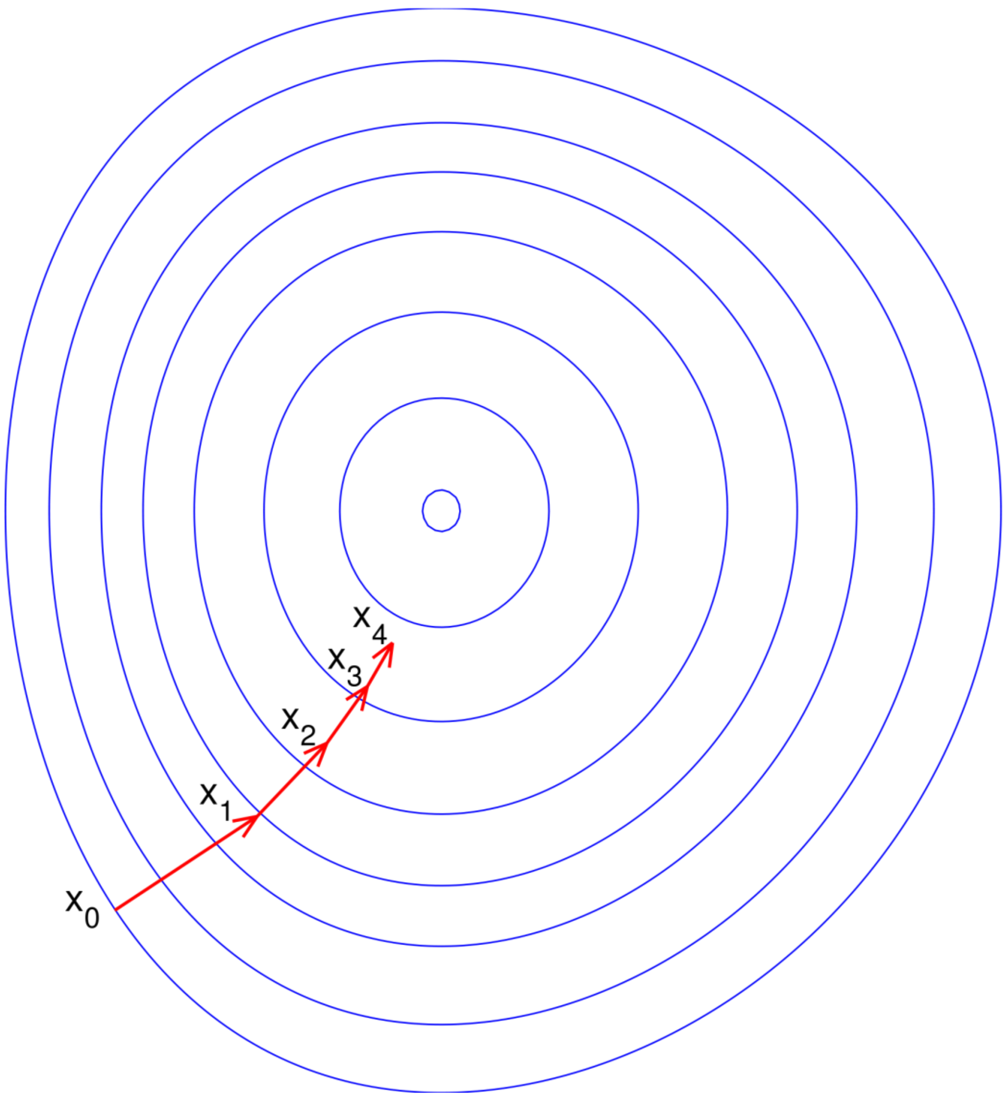
- Pick an initial point x_0

- Iterate until convergence

$$x_{t+1} = x_t - \gamma_t \nabla f(x_t)$$

where $\gamma_t = \frac{2}{2+t}$ is the t^{th} step size

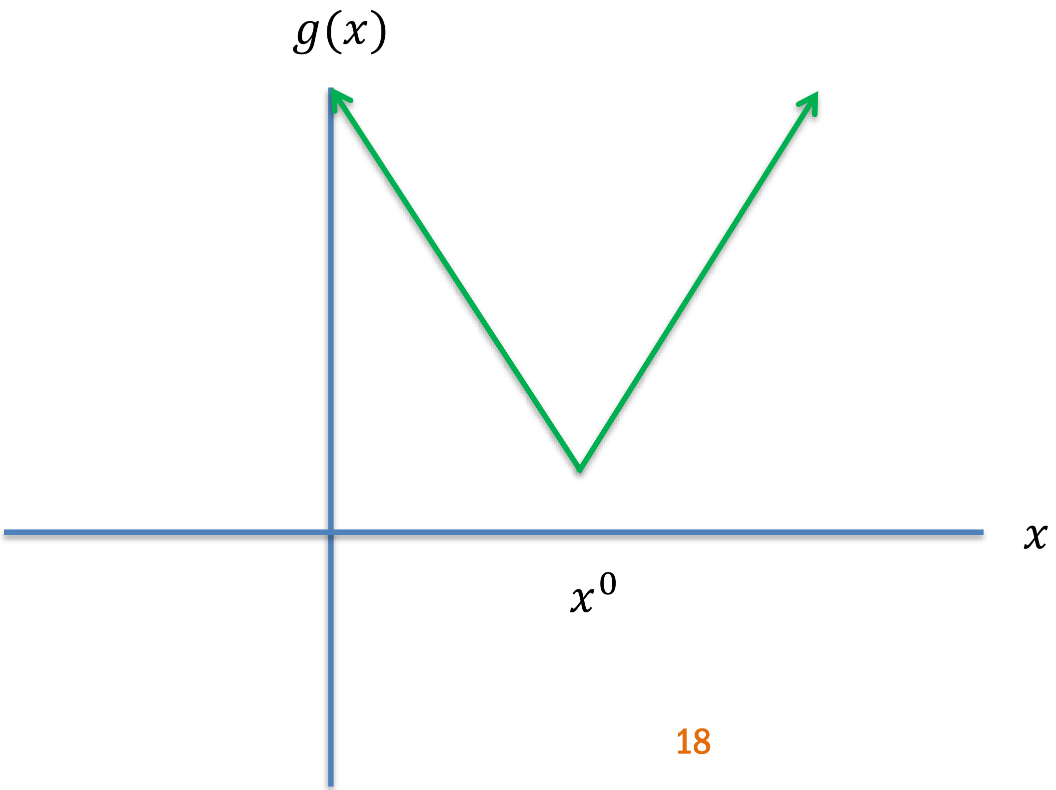
Gradient Descent



source: Wikipedia

Subgradients

- For a convex function $g(x)$, a subgradient at a point x^0 is any tangent line/plane through the point x^0 that underestimates the function everywhere



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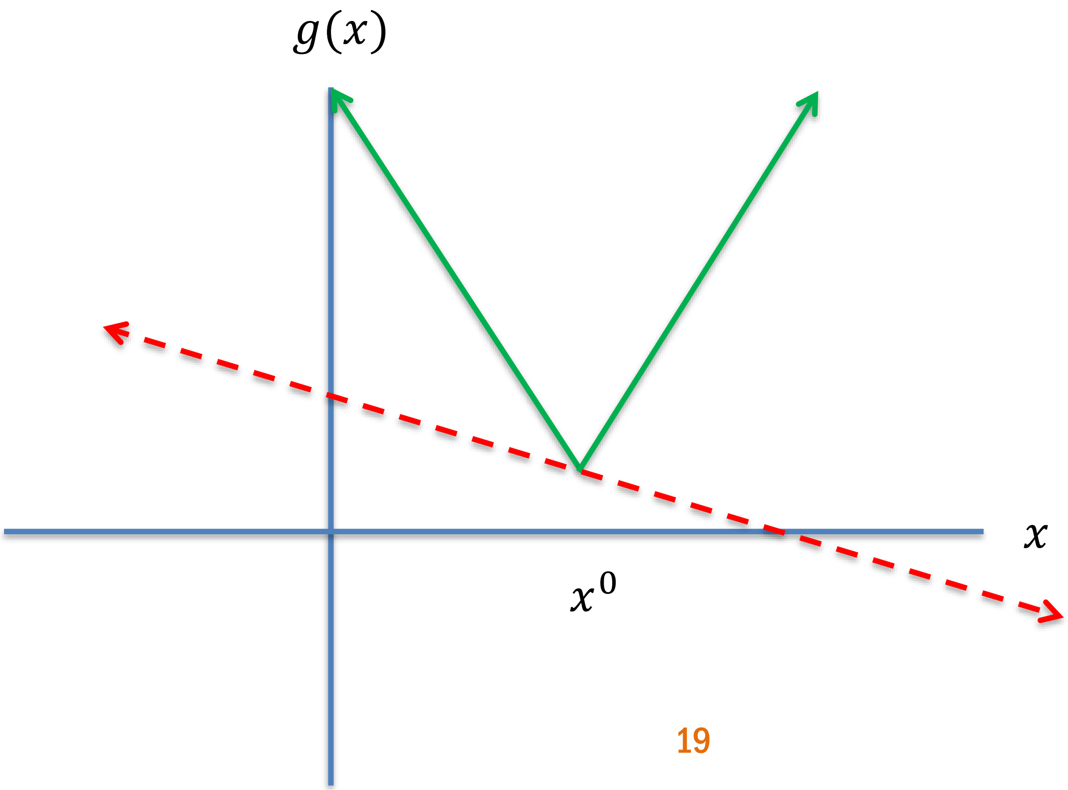

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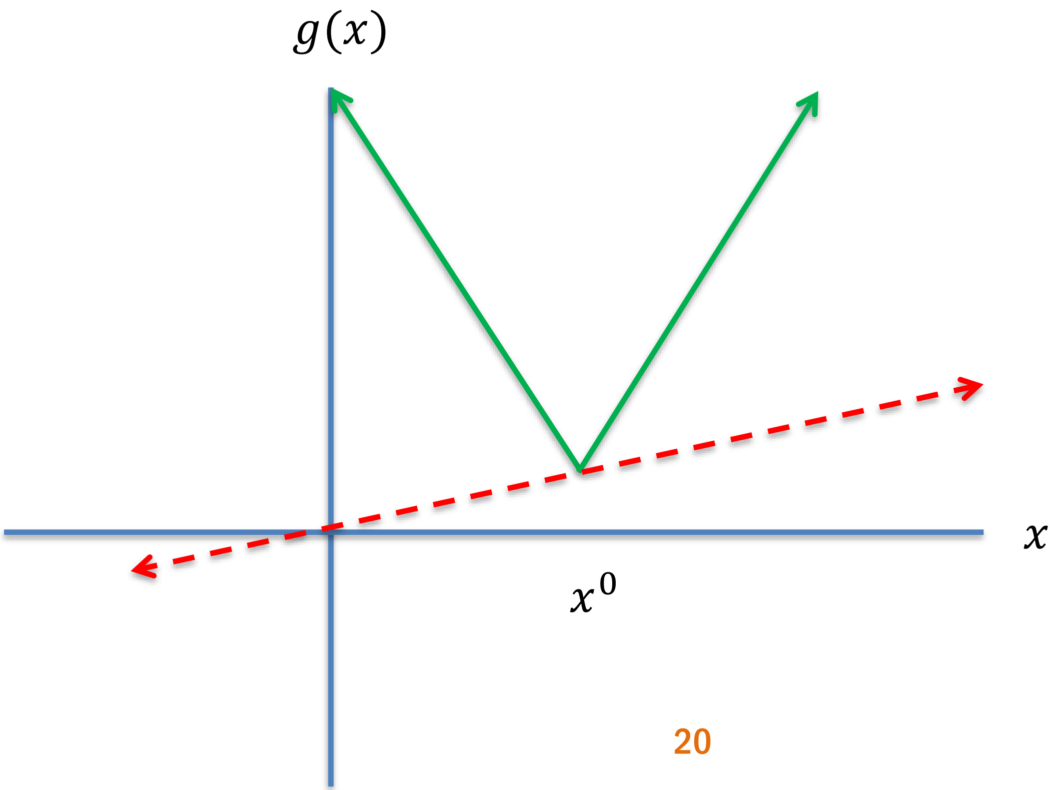

Subgradients

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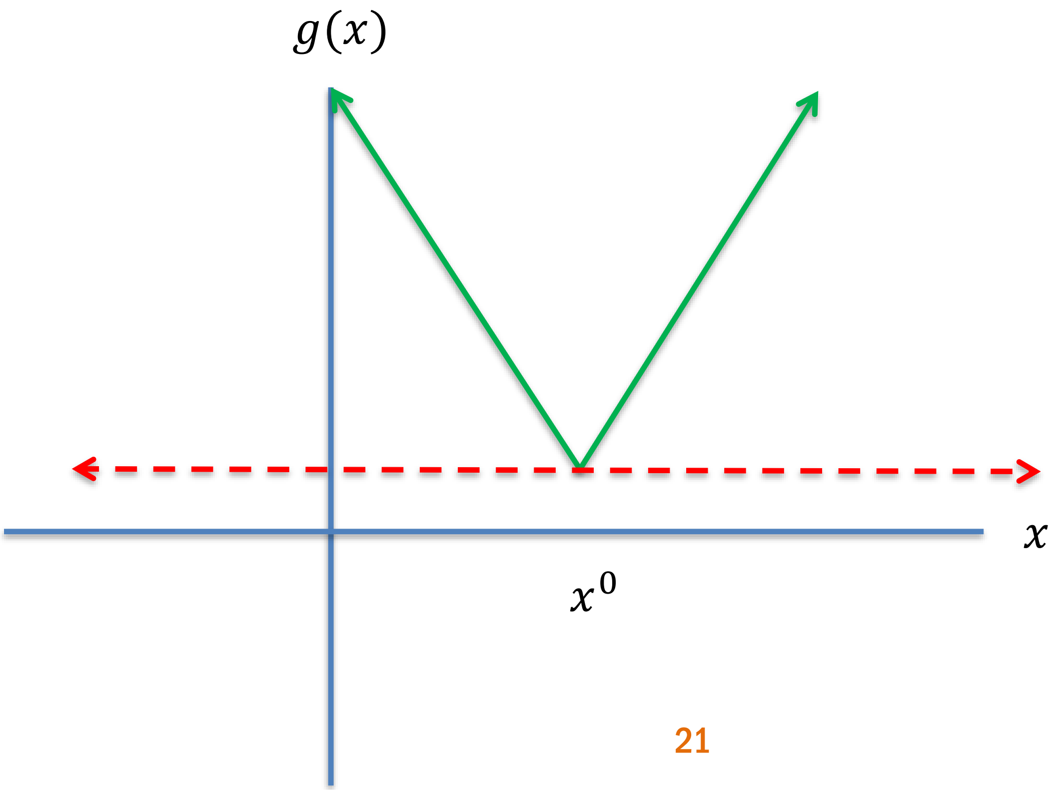

If $\vec{0}$ is a subgradient at x^0, then x^0 is a global minimum

Integer Programming

- We can also express the MAP problem as a 0,1 integer programming problem
  - Convert a maximum of a product into a maximum of a sum by taking logs
  - Introduce indicator variables, τ, to represent the chosen assignment

Integer Programming

- Introduce indicator variables for a specific assignment
  - $\tau_i(x_i) \in \{0,1\}$ for each $i \in V$ and x_i
  - $\tau_{ij}(x_i, x_j) \in \{0,1\}$ for each $(i,j) \in E$ and x_i, x_j
- The linear objective function is then

$$\max_{\tau} \sum_{i \in V} \sum_{x_i} \tau_i(x_i) \log \phi_i(x_i) + \sum_{(i,j)\in E} \sum_{x_i, x_j} \tau_{ij}(x_i, x_j) \log \psi_{ij}(x_i, x_j)$$

where the τ's are required to satisfy certain marginalization conditions

Integer Programming

$$\max_{\tau} \sum_{i \in V} \sum_{x_i} \tau_i(x_i) \log \phi_i(x_i) + \sum_{(i,j) \in E} \sum_{x_i, x_j} \tau_{ij}(x_i, x_j) \log \psi_{ij}(x_i, x_j)$$

such that

$$\sum_{x_i} \tau_i(x_i) = 1$$

For all $i \in V$

$$\sum_{x_j} \tau_{ij}(x_i, x_j) = \tau_i(x_i)$$

For all $(i,j) \in E, x_i$

$$\tau_i(x_i) \in \{0,1\}$$

For all $i \in V, x_i$

$$\tau_{ij}(x_i, x_j) \in \{0,1\}$$

For all $(i,j) \in E, x_i, x_j$

Integer Programming

$$\max_{\tau} \sum_{i\in V} \sum_{x_i} \tau_i(x_i) \log \phi_i(x_i) + \sum_{(i,j)\in E} \sum_{x_i,x_j} \tau_{ij}(x_i,x_j) \log \psi_{ij}(x_i,x_j)$$

such that

These constraints define the vertices of the **marginal polytope** (set of all valid marginal distributions)

$$\sum_{x_i} \tau_i(x_i) = 1$$ **For all** $i \in V$

$$\sum_{x_j} \tau_{ij}(x_i,x_j) = \tau_i(x_i)$$ **For all** $(i,j) \in E, x_i$

$$\tau_i(x_i) \in \{0,1\}$$ **For all** $i \in V, x_i$

$$\tau_{ij}(x_i,x_j) \in \{0,1\}$$ **For all** $(i,j) \in E, x_i, x_j$

Marginal Polytope

- Given an assignment to all of the random variables, x^*, can construct τ in the marginal polytope so that the value of the objective function is $\log p(x^*)$
  - Set $\tau_i(x_i^*) = 1$, and zero otherwise
  - Set $\tau_{ij}\left(x_i^*, x_j^*\right) = 1$, and zero otherwise
- Given a τ in the marginal polytope, can construct an x^* such that the value of the objective function at τ is equal to $\log p(x^*)$
  - Set $x_i^* = \operatorname{argmax}_{\mathrm{x_i}} \tau_i(x_i)$

An Example: Independent Sets

- What is the integer programming problem corresponding to the uniform distribution over independent sets of a graph $G = (V, E)$?

$$p(x_V) = \frac{1}{Z} \prod_{(i,j)\in E} 1_{x_i + x_j \leq 1}$$

(worked out on the board)

Linear Relaxation

- The integer program can be relaxed into a linear program by replacing the 0,1 integrality constraints with linear constraints
  - This relaxed set of constraints forms the local marginal polytope
    - The τ's no longer correspond to an achievable marginal distribution, so we call them pseudo-marginals
  - We call it a relaxation because the constraints have been relaxed: all solutions to the IP are contained as solutions of the LP
- Linear programming problems can be solved in polynomial time!

Linear Relaxation

$$\max_{\tau} \sum_{i \in V} \sum_{x_i} \tau_i(x_i) \log \phi_i(x_i) + \sum_{(i,j) \in E} \sum_{x_i, x_j} \tau_{ij}(x_i, x_j) \log \psi_{ij}(x_i, x_j)$$

such that

$$\sum_{x_i} \tau_i(x_i) = 1$$ For all $i \in V$

$$\sum_{x_j} \tau_{ij}(x_i, x_j) = \tau_i(x_i)$$ For all $(i, j) \in E, x_i$

$$\tau_i(x_i) \in [0,1]$$ For all $i \in V, x_i$

$$\tau_{ij}(x_i, x_j) \in [0,1]$$ For all $(i, j) \in E, x_i, x_j$

An Example: Independent Sets

- What is the **linear** programming problem corresponding to the uniform distribution over independent sets of a graph $G = (V, E)$?

$$p(x_V) = \frac{1}{Z} \prod_{(i,j)\in E} 1_{x_i + x_j \leq 1}$$

- The MAP LP is a relaxation of the integer programming problem
  - MAP LP could have a better solution… (example in class)

Tightness of the MAP LP

- When is it that solving the MAP LP (or equivalently, the dual optimization) is the same as solving the integer programming problem?
  - We say that there is no gap when this is the case
  - The answer can be expressed as a structural property of the graph (beyond the scope of this course)