An Introduction to LP Relaxations for MAP Inference

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With thanks to David Sontag (MIT) for use of some of his slides and illustrations

For more information, see http://mlg.eng.cam.ac.uk/adrian/

High level overview of our 3 lectures

- 1. Directed and undirected graphical models (last Wed)
- 2. LP relaxations for MAP inference (today)
- 3. Junction tree algorithm for exact inference, belief propagation, variational methods for approximate inference (Wed next week)

Further reading / viewing:

- Murphy, Machine Learning: a Probabilistic Perspective
- Barber, Bayesian Reasoning and Machine Learning
- Bishop, Pattern Recognition and Machine Learning
- Koller and Friedman, Probabilistic Graphical Models https://www.coursera.org/course/pgm
- Wainwright and Jordan, Graphical Models, Exponential Families, and Variational Inference

Example of MAP inference: image denoising

Inference is combining prior beliefs with observed evidence to form a prediction.



 \longrightarrow MAP inference

Example of MAP inference: protein side-chain placement

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



- 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)

- Background on undirected graphical models
- Basic LP relaxation
- Tighter relaxations
- Message passing and dual decomposition

We'll comment on

• When is an LP relaxation tight

Background: undirected graphical models

- Powerful way to represent relationships across variables
- Many applications including: computer vision, social network analysis, deep belief networks, protein folding...
- In this talk, focus on pairwise models with discrete variables (sometimes *binary*)



Example: Grid for computer vision

Background: undirected graphical models

- Discrete variables X_1, \ldots, X_n with $X_i \in \{0, \ldots, k_i 1\}$
- Potential functions, will somehow write as vector $\boldsymbol{\theta}$
- Write x = (...x₁,...,x_n,...) for one 'overcomplete configuration' of all variables, θ · x for its total score
- Probability distribution given by

$$p(x) = \frac{1}{Z} \exp(\theta \cdot x)$$

- To ensure probabilities sum to 1, need normalizing constant or partition function Z = ∑_x exp (θ · x)
- We are interested in *maximum a posteriori (MAP) inference* i.e., find a global configuration with highest probability

$$x^* \in rg \max p(x) = rg \max \theta \cdot x$$

Background: how do we write potentials as a vector θ ?

- $\theta \cdot x$ means the total score of a configuration x, where we sum over all potential functions
- If we have potential functions θ_c over some subsets c ∈ C of variables, then we want ∑_{c∈C} θ_c(x_c), where x_c means a configuration of variables just in the subset c
- $\theta_c(x_c)$ provides a measure of local compatibility, a table of values

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- $\theta_c(x_c)$ provides a measure of local compatibility, a table of values
- If we only have some unary/singleton potentials θ_i and edge/pairwise potentials θ_{ij} then we can write the total score as

$$\sum_{i} \theta_i(x_i) + \sum_{(i,j)} \theta_{ij}(x_i, x_j)$$

 Indices? Usually assume either no unary potentials (absorb them into edges) or one for every variable, leading to a graph topology (V, E) with total score

$$\sum_{i\in V=\{1,\ldots,n\}}\theta_i(x_i) + \sum_{(i,j)\in E}\theta_{ij}(x_i,x_j)$$

Background: overcomplete representation

The overcomplete representation conveniently allows us to write

$$\theta \cdot x = \sum_{i \in V} \theta_i(x_i) + \sum_{(i,j) \in E} \theta_{ij}(x_i, x_j)$$

• Concatenate singleton and edge terms into big vectors

• There are many possible values of *x* how

how many?

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• Concatenate singleton and edge terms into big vectors

• There are many possible values of x

how many? $\prod_{i \in V} k_i$

Background: Binary pairwise models

- $\theta \cdot x$ is the score of a configuration x
- Probability distribution given by

$$p(x) = \frac{1}{Z} \exp(\theta \cdot x)$$

- For MAP inference, want $x^* \in \arg \max p(x) = \arg \max \theta \cdot x$
- Want to optimize over {0,1} coordinates of 'overcomplete configuration space' corresponding to all 2ⁿ possible settings
- \bullet The convex hull of these defines the marginal polytope $\mathbb M$
- Each point μ ∈ M corresponds to a probability distribution over the 2ⁿ configurations, giving a vector of marginals

Background: the marginal polytope (all valid marginals)



Background: overcomplete and minimal representations

- The overcomplete representation is highly redundant,
 e.g. µ_i(0) + µ_i(1) = 1 ∀i
- How many dimensions if *n* binary variables with *m* edges?

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- The overcomplete representation is highly redundant,
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- How many dimensions if *n* binary variables with *m* edges? 2n + 4m
- Instead, we sometimes pick a minimal representation
- What's the minimum number of dimensions we need?

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- The overcomplete representation is highly redundant,
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- How many dimensions if n binary variables with m edges? 2n + 4m
- Instead, we sometimes pick a minimal representation
- What's the minimum number of dimensions we need? n + m
- For example, we could use $q = (q_1, \ldots, q_n, \ldots, q_{ij}, \ldots)$ where $q_i = \mu_i(1) \ \forall i, q_{ij} = \mu_{ij}(1, 1) \ \forall (i, j)$, then

$$\mu_i = \begin{pmatrix} 1 - q_i \\ q_i \end{pmatrix}, \mu_j = \begin{pmatrix} 1 - q_j \\ q_j \end{pmatrix}, \quad \mu_{ij} = \begin{pmatrix} 1 + q_{ij} - q_i - q_j & q_j - q_{ij} \\ q_i - q_{ij} & q_{ij} \end{pmatrix}$$

Note many other possible minimal representations

LP relaxation: MAP as an *integer linear program* (ILP)

• MAP inference as a discrete optimization problem is to identify a configuration with maximum total score

$$\begin{aligned} x^* &\in \arg\max_{x} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j) \\ &= \arg\max_{x} \theta \cdot x \\ &= \arg\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i) \mu_i(x_i) + \sum_{ij \in E} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) \mu_{ij}(x_i, x_j) \\ &= \arg\max_{\mu} \theta \cdot \mu \qquad \text{s.t. } \mu \text{ is integral} \end{aligned}$$

• Any other constraints?

What are the constraints?

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

$$egin{array}{rcl} \mu_i(x_i) &\in \{0,1\} &orall i\in V, x_i\ \sum_{x_i} \mu_i(x_i) &= 1 &orall i\in V\ \mu_{ij}(x_i,x_j) &\in \{0,1\} &orall ij\in E, x_i, x_j\ \sum_{x_i,x_j} \mu_{ij}(x_i,x_j) &= 1 &orall ij\in E \end{array}$$

• Enforce that these assignments are consistent:

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

MAP as an integer linear program (ILP)

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

subject to:

$$\mu_i(x_i) \in \{0,1\} \quad \forall i \in V, x_i \quad (\text{edge terms?})$$

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

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

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

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

Linear programming (LP) relaxation for MAP

Integer linear program was:

$$\mathrm{MAP}(\theta) = \max_{\mu} \theta \cdot \mu$$

subject to

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

Now relax integrality constraints, allow variables to be between 0 and 1:

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

Basic LP relaxation for MAP

$$LP(\theta) = \max_{\mu} \theta \cdot \mu$$

s.t. $\mu_i(x_i) \in [0, 1] \quad \forall i \in V, x_i$
$$\sum_{x_i} \mu_i(x_i) = 1 \quad \forall i \in V$$

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

- Linear programs can be solved efficiently: simplex, interior point, ellipsoid algorithm
- Since the LP relaxation maximizes over a larger set, its value can only be higher

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

The local polytope

$$\begin{split} \mathrm{LP}(\theta) &= \max_{\mu} \theta \cdot \mu \\ \mathrm{s.t.} \quad \mu_i(x_i) &\in [0, 1] \quad \forall i \in V, x_i \\ \sum_{x_i} \mu_i(x_i) &= 1 \quad \forall i \in V \\ \mu_i(x_i) &= \sum_{x_j} \mu_{ij}(x_i, x_j) \quad \forall ij \in E, x_i \\ \mu_j(x_j) &= \sum_{x_j} \mu_{ij}(x_i, x_j) \quad \forall ij \in E, x_j \end{split}$$

- All these constraints are linear
- Hence define a polytope in the space of marginals
- Here we enforced only local (pairwise) consistency, which defines the *local polytope*
- If instead we had optimized over the marginal polytope, which enforces global consistency, then we would have MAP(θ) =LP(θ), i.e. the LP is tight why? why don't we do this?

- \bullet Enforcing consistency of pairs of variables leads to the local polytope \mathbb{L}_2
- The marginal polytope enforces consistency over all variables $\mathbb{M} = \mathbb{L}_n$
- Natural to consider the Sherali-Adams hierarchy of successively tighter relaxations \mathbb{L}_r $2 \le r \le n$ which enforce consistency over clusters of r variables
- $\bullet\,$ Just up from the local polytope is the triplet polytope $\mathsf{TRI}{=}\,\mathbb{L}_3$

Stylized illustration of polytopes







triplet polytope \mathbb{L}_3 triplet consistency



local polytope \mathbb{L}_2 pair consistency

More accurate \leftrightarrow Less accurate

More computationally intensive \leftrightarrow Less computationally intensive

Stylized illustration of polytopes







triplet polytope \mathbb{L}_3 triplet consistency



local polytope \mathbb{L}_2 pair consistency

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 Can be shown that for binary variables, TRI=CYC, the cycle polytope, which enforces consistency over all cycles In general, TRI ⊆ CYC, open problem if TRI = CYC [SonPhD §3]

- For a model without cycles, local polytope L₂=M marginal polytope, hence the basic LP ('first order') is always tight
- More generally, if a model has treewidth r then LP+ \mathbb{L}_{r+1} is tight [WaiJor04] STRUCTURE
- Separately, if we allow any structure but restrict the class of potential functions, interesting results are known POTENTIALS
- For example, the basic LP is tight if all potentials are supermodular
- Fascinating recent work [KolThaZiv15]: if we do not restrict structure, then for any given family of potentials, either the basic LP relaxation is tight or the problem class is NP-hard!
- Identifying HYBRID conditions is an exciting current research area

When is MAP inference (relatively) easy?



STRUCTURE

POTENTIALS

Both can be handled efficiently by the basic LP relaxation, LP+L2
 For models which are not attractive but are 'close to attractive', LP+LOC is often not tight - but using an LP relaxation with higher order clusters, empirically the result is tight (Sontag et al., 2008)

Example: Image foregound-background segmentation





- Learning potentials from data, most edges are attractive but a few are repulsive: the model is 'close to attractive'
- LP+LOC enforces pairwise consistency, often not tight
- The LP relaxation over the triplet polytope TRI usually is tight

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Almost attractive and almost balanced models

Blue edges are attractive, dashed red edges are repulsive





almost attractive



balanced (attractive up to flipping)



almost balanced

- LP+TRI is tight for any almost balanced model
- Submodels can be pasted together in certain ways while preserving LP tightness
 - Can paste submodels on any one variable
 - Can paste on an edge provided it uses special variable *s* from each submodel



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not almost balanced

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• Stronger results using graph minors (W. UAI 2016)



Figure 2-6: Illustration of the cutting-plane algorithm. (a) Solve the LP relaxation. (b) Find a violated constraint, add it to the relaxation, and repeat. (c) Result of solving the tighter LP relaxation. (d) Finally, we find the MAP assignment.

SonPhD


SonPhD

We want to add constraints that are both *valid* and *useful*

- Valid: does not cut off any integer points
- Useful: leads us to update to a better solution

Local search

- Start from an arbitrary assignment (e.g., random).
- Choose a variable.
- Branch-and-bound
 - Exhaustive search over space of assignments, pruning branches that can be provably shown not to contain a MAP assignment
 - Can use the LP relaxation or its dual to obtain upper bounds
 - Lower bound obtained from value of any assignment found
- Branch-and-cut (most powerful method; used by CPLEX & Gurobi)
 - Same as branch-and-bound; spend more time getting tighter bounds
 - Adds cutting-planes to cut off fractional solutions of the LP relaxation, making the upper bound tighter

- Can be a computationally efficient way to obtain or approximate a MAP solution, takes advantage of the graph structure
- Classic example is 'max-product' belief propagation (BP)
- Sufficient conditions are known s.t. this will always converge to the solution of the basic LP, includes that the basic LP is tight [ParkShin-UAI15]
- In general, however, this may not converge to the LP solution (even for supermodular potentials)
- Other methods have been developed, many relate to dual decomposition...

Dual decomposition and reparameterizations

• Consider the MAP problem for pairwise Markov random fields:

$$MAP(\theta) = \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j).$$

 If we push the maximizations *inside* the sums, the value can only *increase*:

$$\mathrm{MAP}(\theta) \leq \sum_{i \in V} \max_{x_i} \theta_i(x_i) + \sum_{ij \in E} \max_{x_i, x_j} \theta_{ij}(x_i, x_j)$$

- Note that the right-hand side can be easily evaluated
- One can always reparameterize a distribution by operations like

$$\begin{array}{lll} \theta_i^{\mathrm{new}}(x_i) &=& \theta_i^{\mathrm{old}}(x_i) + f(x_i) \\ \theta_{ij}^{\mathrm{new}}(x_i, x_j) &=& \theta_{ij}^{\mathrm{old}}(x_i, x_j) - f(x_i) \end{array}$$

for **any** function $f(x_i)$, without changing the distribution/energy

Dual decomposition



Dual decomposition

• Define:

$$\begin{split} \tilde{\theta}_i(x_i) &= \theta_i(x_i) + \sum_{ij \in E} \delta_{j \to i}(x_i) \\ \tilde{\theta}_{ij}(x_i, x_j) &= \theta_{ij}(x_i, x_j) - \delta_{j \to i}(x_i) - \delta_{i \to j}(x_j) \end{split}$$

• It is easy to verify that

$$\sum_{i} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j) = \sum_{i} \tilde{\theta}_i(x_i) + \sum_{ij \in E} \tilde{\theta}_{ij}(x_i, x_j) \quad \forall \mathbf{x}$$

• Thus, we have that:

$$\mathrm{MAP}(\theta) = \mathrm{MAP}(\tilde{\theta}) \leq \sum_{i \in V} \max_{x_i} \tilde{\theta}_i(x_i) + \sum_{ij \in E} \max_{x_i, x_j} \tilde{\theta}_{ij}(x_i, x_j)$$

- Every value of δ gives a different upper bound on the value of the MAP
- The tightest upper bound can be obtained by minimizing the RHS with respect to δ

• We obtain the following **dual** objective: $L(\delta) =$

$$\sum_{i \in V} \max_{x_i} \left(\theta_i(x_i) + \sum_{ij \in E} \delta_{j \to i}(x_i) \right) + \sum_{ij \in E} \max_{x_i, x_j} \left(\theta_{ij}(x_i, x_j) - \delta_{j \to i}(x_i) - \delta_{i \to j}(x_j) \right),$$

$$DUAL-LP(\theta) = \min_{\delta} L(\delta)$$

• This provides an upper bound on the MAP assignment

 $MAP(\theta) \leq DUAL-LP(\theta) \leq L(\delta)$

• How can find δ which give tight bounds?

Solving the dual efficiently

• Many ways to solve the dual linear program, i.e. minimize with respect to δ :

$$\sum_{i \in V} \max_{x_i} \left(\theta_i(x_i) + \sum_{ij \in E} \delta_{j \to i}(x_i) \right) + \sum_{ij \in E} \max_{x_i, x_j} \left(\theta_{ij}(x_i, x_j) - \delta_{j \to i}(x_i) - \delta_{i \to j}(x_j) \right),$$

- One option is to use the subgradient method
- Can also solve using **block coordinate-descent**, which gives algorithms that look very much like max-sum belief propagation



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Max-product linear programming (MPLP) algorithm

Input: A set of potentials $\theta_i(x_i), \theta_{ij}(x_i, x_j)$

Output: An assignment x_1, \ldots, x_n that approximates a MAP solution **Algorithm:**

- Initialize $\delta_{i \to j}(x_j) = 0$, $\delta_{j \to i}(x_i) = 0$, $\forall ij \in E, x_i, x_j$
- Iterate until small enough change in L(δ):
 For each edge ij ∈ E (sequentially), perform the updates:

$$\begin{split} \delta_{j \to i}(x_i) &= -\frac{1}{2} \delta_i^{-j}(x_i) + \frac{1}{2} \max_{x_j} \left[\theta_{ij}(x_i, x_j) + \delta_j^{-i}(x_j) \right] \quad \forall x_i \\ \delta_{i \to j}(x_j) &= -\frac{1}{2} \delta_j^{-i}(x_j) + \frac{1}{2} \max_{x_i} \left[\theta_{ij}(x_i, x_j) + \delta_i^{-j}(x_i) \right] \quad \forall x_j \end{split}$$

where $\delta_i^{-j}(x_i) = \theta_i(x_i) + \sum_{ik \in E, k \neq j} \delta_{k \to i}(x_i)$

• Return $x_i \in \arg \max_{\hat{x}_i} \widetilde{ heta}_i^{\delta}(\hat{x}_i)$

Inputs:

• A set of factors $\theta_i(x_i), \theta_f(\boldsymbol{x}_f)$.

Output:

• An assignment x_1, \ldots, x_n that approximates the MAP.

Algorithm:

- Initialize $\delta_{fi}(x_i) = 0$, $\forall f \in F, i \in f, x_i$.
- Iterate until small enough change in $L(\delta)$ (see Eq. 1.2): For each $f \in F$, perform the updates

$$\delta_{fi}(x_i) = -\delta_i^{-f}(x_i) + \frac{1}{|f|} \max_{\boldsymbol{x}_{f\setminus i}} \left[\theta_f(\boldsymbol{x}_f) + \sum_{\hat{i}\in f} \delta_{\hat{i}}^{-f}(x_{\hat{i}}) \right],$$
(1.16)

simultaneously for all $i \in f$ and x_i . We define $\delta_i^{-f}(x_i) = \theta_i(x_i) + \sum_{\hat{f} \neq f} \delta_{\hat{f}i}(x_i)$.

• Return $x_i \in \arg \max_{\hat{x}_i} \bar{\theta}_i^{\delta}(\hat{x}_i)$ (see Eq. 1.6).

Performance on stereo vision inference task:



Dual decomposition = basic LP relaxation

• Recall we obtained the following **dual** linear program: $L(\delta) =$

$$\sum_{i \in V} \max_{x_i} \left(\theta_i(x_i) + \sum_{ij \in E} \delta_{j \to i}(x_i) \right) + \sum_{ij \in E} \max_{x_i, x_j} \left(\theta_{ij}(x_i, x_j) - \delta_{j \to i}(x_i) - \delta_{i \to j}(x_j) \right),$$

 $DUAL-LP(\theta) = \min_{\delta} L(\delta)$

We showed two ways of upper bounding the value of the MAP assignment:

$$MAP(\theta) \leq Basic LP(\theta)$$
 (1)

$$MAP(\theta) \leq DUAL-LP(\theta) \leq L(\delta)$$
 (2)

• Although we derived these linear programs in seemingly very different ways, in turns out that:

Basic $LP(\theta) = DUAL-LP(\theta)$ [SonGloJaa11]

• The dual LP allows us to upper bound the value of the MAP assignment without solving an LP to optimality



(Dual) LP relaxation (Primal) LP relaxation Integer linear program

 $MAP(\theta) \leq Basic LP(\theta) = DUAL-LP(\theta) \leq L(\delta)$

- LP relaxations yield a powerful approach for MAP inference
- Naturally lead to
 - considerations of polytope or cutting planes
 - dual decomposition and message passing
- Close relationship to methods for marginal inference
- Help build understanding as well as develop new algorithmic tools
- Exciting current research

Thank you

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