

Probabilistic Graphical Models

Variational Inference

Eric Xing Lecture 13, February 24, 2014



Reading: See class website

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Inference Problems

- Compute the likelihood of observed data
- Compute the marginal distribution $p(x_A)$ over a particular subset of nodes $A \subset V$
- Compute the conditional distribution $p(x_A|x_B)$ for disjoint subsets A and B
- Compute a mode of the density $\hat{x} = \arg \max_{x \in \mathcal{X}^m} p(x)$
- Methods we have



Individual computations independent



(Forward-backward , Max-product /BP, Junction Tree)

Sharing intermediate terms

Sum-Product Revisited

• Tree-structured GMs

$$p(x_1, \cdots, x_m) = \frac{1}{Z} \prod_{s \in V} \psi_s(x_s) \prod_{(s,t) \in E} \psi_{st}(x_s, x_t)$$



• Message Passing on Trees:

$$M_{t \to s}(x_s) \leftarrow \kappa \sum_{x'_t} \left\{ \psi_{st}(x_s, x'_t) \psi_t(x'_t) \prod_{u \in N(t) \setminus s} M_{u \to t}(x'_t) \right\}$$

• On trees, converge to a unique fixed point after a finite number of iterations

Junction Tree Revisited

• General Algorithm on Graphs with Cycles







• Steps:

-> Triangularization

=> Construct JTs

=> Message Passing on Clique Trees



Local Consistency

- Given a set of functions $\{\tau_C, C \in C\}$ and $\{\tau_S, S \in S\}$ associated with the cliques and separator sets
- They are locally consistent if:

$$\sum_{\substack{x'_S \\ x'_S = x_S}} \tau_S(x'_S) = 1, \ \forall S \in \mathcal{S}$$
$$\sum_{\substack{x'_C \mid x'_S = x_S}} \tau_C(x'_C) = \tau_S(x_S), \ \forall C \in \mathcal{C}, \ S \subset C$$

• For junction trees, local consistency is equivalent to global consistency!



An Ising model on 2-D image

- Nodes encode hidden information (patchidentity).
- They receive local information from the image (brightness, color).
- Information is propagated though the graph over its edges.
- Edges encode 'compatibility' between nodes.



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Why Approximate Inference?

• Why can't we just run junction tree on this graph?



 $p(X) = \frac{1}{Z} \exp\left\{\sum_{i < i} \theta_{ij} X_i X_j + \sum_i \theta_{i0} X_i\right\}$

- If NxN grid, tree width at least N
- N can be a huge number(~1000s of pixels)
 - If N~O(1000), we have a clique with 2¹⁰⁰ entries

Approaches to inference

- Exact inference algorithms
 - The elimination algorithm
 - Message-passing algorithm (sum-product, belief propagation)
 - The junction tree algorithms

• Approximate inference techniques

- Variational algorithms
 - Loopy belief propagation
 - Mean field approximation
- Stochastic simulation / sampling methods
- Markov chain Monte Carlo methods



Loopy Belief Propogation

Recap: Belief Propagation



BP on trees always converges to exact marginals (cf. Junction tree algorithm)

k

k

k



Beliefs and messages in FG





What if the graph is loopy?



Belief Propagation on loopy graphs



Compatibilities (interactions)

• May not converge or converge to a wrong solution

k

k

k

k

 $b_i(x_i) \propto \psi_i(x_i) \prod M_k(x_k)$

Loopy Belief Propagation

- A fixed point iteration procedure that tries to minimize F_{bethe}
- Start with random initialization of messages and beliefs
 - While not converged do

 $b_i(x_i) \propto \prod_{a \in N(i)} m_{a \to i}(x_i) \qquad b_a(X_a) \propto f_a(X_a) \prod_{i \in N(a)} m_{i \to a}(x_i)$ $m_{i \to a}^{new}(x_i) = \prod m_{c \to i}(x_i) \qquad m_{a \to i}^{new}(x_i) = \sum f_a(X_a) \prod m_{j \to a}(x_j)$

 $X_a \setminus x_i$

 $j \in N(a) \setminus i$

- At convergence, stationarity properties are guaranteed
- However, not guaranteed to converge!

 $c \in N(i) \setminus a$



Loopy Belief Propagation

- If BP is used on graphs with loops, messages may circulate indefinitely
- But let's run it anyway and hope for the best ... ©
- Empirically, a good approximation is still achievable
 - Stop after fixed # of iterations
 - Stop when no significant change in beliefs
 - If solution is not oscillatory but converges, it usually is a good approximation

Loopy-belief Propagation for Approximate Inference: An Empirical Study Kevin Murphy, Yair Weiss, and Michael Jordan. *UAI '99 (Uncertainty in AI).*]

So what is going on?

• Is it a dirty hack that you bet your luck?



Approximate Inference

• Let us call the actual distribution P

$$P(X) = 1/Z \prod_{f_a \in F} f_a(X_a)$$

- We wish to find a distribution *Q* such that *Q* is a "good" approximation to *P*
- Recall the definition of KL-divergence

$$KL(Q_1 || Q_2) = \sum_X Q_1(X) \log(\frac{Q_1(X)}{Q_2(X)})$$

- KL(Q₁||Q₂)>=0
- KL(Q₁||Q₂)=0 iff Q₁=Q₂
- We can therefore use KL as a scoring function to decide a good Q
- But, $KL(Q_1||Q_2) \neq KL(Q_2||Q_1)$

Which KL?

- Computing KL(*P*||*Q*) requires inference!
- But KL(*Q*||*P*) can be computed without performing inference on *P*

$$KL(Q || P) = \sum_{X} Q(X) \log(\frac{Q(X)}{P(X)})$$
$$= \sum_{X} Q(X) \log Q(X) - \sum_{X} Q(X) \log P(X)$$
$$= -H_Q(X) - E_Q \log P(X)$$

• Using
$$P(X) = 1/Z \prod_{f_a \in F} f_a(X_a)$$

 $KL(Q \parallel P) = -H_Q(X) - E_Q \log(1/Z \prod_{f_a \in F} f_a(X_a))$
 $= -H_Q(X) - \log 1/Z - \sum_{f_a \in F} E_Q \log f_a(X_a)$

Optimization function

$$KL(Q \parallel P) = \boxed{-H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a) + \log Z}$$

$$\overbrace{F(P,Q)}$$

- We will call F(P,Q) the "Free energy" *
- F(P, P) = ?
- F(P,Q) >= F(P,P)

*Gibbs Free Energy

The Energy Functional

• Let us look at the functional

$$F(P,Q) = -H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a)$$

- $\sum_{f_a \in F} E_Q \log f_a(X_a)$ can be computed if we have marginals over each f_a
- $H_Q = -\sum_X Q(X) \log Q(X)$ is harder! Requires summation over all possible values
- Computing *F*, is therefore hard in general.
- Approach 1: Approximate F(P,Q) with easy to compute F(P,Q)



Tree Energy Functionals

• Consider a tree-structured distribution



- The probability can be written as: $b(\mathbf{x}) = \prod b_a(\mathbf{x}_a) \prod b_i(x_i)^{1-d_i}$
- $H_{tree} = -\sum_{a} \sum_{\mathbf{x}_{a}} b_{a}(\mathbf{x}_{a}) \ln b_{a}(\mathbf{x}_{a}) + \sum_{i} (d_{i} \mathbf{1}) \sum_{\mathbf{x}_{i}} b_{i}(\mathbf{x}_{i}) \ln b_{i}(\mathbf{x}_{i})$ $F_{Tree} = \sum_{a} \sum_{\mathbf{x}_{a}} b_{a}(\mathbf{x}_{a}) \ln \frac{b_{a}(\mathbf{x}_{a})}{f_{a}(\mathbf{x}_{a})} + \sum_{i} (\mathbf{1} d_{i}) \sum_{\mathbf{x}_{i}} b_{i}(\mathbf{x}_{i}) \ln b_{i}(\mathbf{x}_{i})$

 $= F_{12} + F_{23} + \ldots + F_{67} + F_{78} - F_1 - F_5 - F_2 - F_6 - F_3 - F_7$

• involves summation over edges and vertices and is therefore easy to compute

Bethe Approximation to Gibbs Free Energy

• For a general graph, choose $\hat{F}(P,Q) = F_{Betha}$

$$H_{Bethe} = -\sum_{a} \sum_{\mathbf{x}_{a}} b_{a}(\mathbf{x}_{a}) \ln b_{a}(\mathbf{x}_{a}) + \sum_{i} (d_{i} - 1) \sum_{\mathbf{x}_{i}} b_{i}(\mathbf{x}_{i}) \ln b_{i}(\mathbf{x}_{i})$$
$$F_{Bethe} = \sum_{a} \sum_{\mathbf{x}_{a}} b_{a}(\mathbf{x}_{a}) \ln \frac{b_{a}(\mathbf{x}_{a})}{f_{a}(\mathbf{x}_{a})} + \sum_{i} (1 - d_{i}) \sum_{\mathbf{x}_{i}} b_{i}(\mathbf{x}_{i}) \ln b_{i}(\mathbf{x}_{i}) = -\langle f_{a}(\mathbf{x}_{a}) \rangle - H_{betha}$$

Called "Bethe approximation" after the physicist Hans Bethe



 $F_{\textit{bethe}} = F_{12} + F_{23} + ... + F_{67} + F_{78} - F_1 - F_5 - 2F_2 - 2F_6 ... - F_8$

- Equal to the exact Gibbs free energy when the factor graph is a tree
- In general, H_{Bethe} is **not** the same as the H of a tree

Bethe Approximation



• Pros:

- Easy to compute, since entropy term involves sum over pairwise and single variables
- Cons:
 - $F(P,Q) = F_{bethe}$ may or may not be well connected to F(P,Q)
 - It could, in general, be greater, equal or less than F(P,Q)

• Optimize each $b(\mathbf{x}_a)$'s.

- For discrete belief, constrained opt. with Lagrangian multiplier
- For continuous belief, not yet a general formula
- Not always converge



Bethe Free Energy for FG



$$F_{Betha} = \sum_{a} \sum_{\mathbf{x}_{a}} b_{a}(\mathbf{x}_{a}) \ln \frac{b_{a}(\mathbf{x}_{a})}{f_{a}(\mathbf{x}_{a})} + \sum_{i} (\mathbf{1} - d_{i}) \sum_{\mathbf{x}_{i}} b_{i}(\mathbf{x}_{i}) \ln b_{i}(\mathbf{x}_{i})$$

$$H_{Bethe} = -\sum_{a} \sum_{\mathbf{x}_{a}} b_{a}(\mathbf{x}_{a}) \ln b_{a}(\mathbf{x}_{a}) + \sum_{i} (d_{i} - \mathbf{1}) \sum_{\mathbf{x}_{i}} b_{i}(\mathbf{x}_{i}) \ln b_{i}(\mathbf{x}_{i})$$

$$F_{Bethe} = -\langle f_a(\mathbf{x}_a) \rangle - H_{betha}$$

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Minimizing the Bethe Free Energy

•
$$L = F_{Bethe} + \sum_{i} \gamma_{i} \{1 - \sum_{x_{i}} b_{i}(x_{i})\}$$
$$+ \sum_{a} \sum_{i \in N(a)} \sum_{x_{i}} \lambda_{ai}(x_{i}) \left\{ b_{i}(x_{i}) - \sum_{X_{a} \setminus x_{i}} b_{a}(X_{a}) \right\}$$

• Set derivative to zero

Constrained Minimization of the Bethe Free Energy

$$L = F_{Bethe} + \sum_{i} \gamma_{i} \{ \sum_{x_{i}} b_{i}(x_{i}) - 1 \}$$
$$+ \sum_{a} \sum_{i \in N(a)} \sum_{x_{i}} \lambda_{ai}(x_{i}) \left\{ \sum_{X_{a} \setminus x_{i}} b_{a}(X_{a}) - b_{i}(x_{i}) \right\}$$

$$\frac{\partial L}{\partial b_i(x_i)} = 0 \qquad \Longrightarrow \qquad b_i(x_i) \propto \exp\left(\frac{1}{d_i - 1} \sum_{a \in N(i)} \lambda_{ai}(x_i)\right)$$
$$\frac{\partial L}{\partial b_a(X_a)} = 0 \qquad \Longrightarrow \qquad b_a(X_a) \propto \exp\left(-E_a(X_a) + \sum_{i \in N(a)} \lambda_{ai}(x_i)\right)$$

Bethe = BP on FG



The "belief" is the BP approximation of © Eric Xing @ CMU, 2005-2014

BP Message-update Rules

Using
$$b_{a \to i}(x_i) = \sum_{X_a \setminus x_i} b_a(X_a)$$
, we get

$$m_{a \to i}(x_i) = \sum_{X_a \setminus x_i} f_a(X_a) \prod_{j \in N(a) \setminus i} \prod_{b \in N(j) \setminus a} m_{b \to j}(x_j)$$

(A sum product algorithm)





The Theory Behind LBP



- For a distribution *p*(X/θ) associated with a complex graph, computing the marginal (or conditional) probability of arbitrary random variable(s) is intractable
- Variational methods
 - formulating probabilistic inference as an optimization problem:

$$q^* = \arg\min_{q \in S} \left\{ F_{Betha}(p,q) \right\}$$

$$F_{Bethe} = \sum_{a} \sum_{\mathbf{x}_{a}} b_{a}(\mathbf{x}_{a}) \ln \frac{b_{a}(\mathbf{x}_{a})}{f_{a}(\mathbf{x}_{a})} + \sum_{i} (\mathbf{1} - d_{i}) \sum_{\mathbf{x}_{i}} b_{i}(\mathbf{x}_{i}) \ln b_{i}(\mathbf{x}_{i}) = -\langle f_{a}(\mathbf{x}_{a}) \rangle - H_{bethe}$$

q: a (tractable) probability distribution

The Theory Behind LBP



• But we do not optimize $q(\mathbf{X})$ explicitly, focus on the set of beliefs

•
$$e.g., b = \{b_{i,j} = \tau(x_i, x_j), b_i = \tau(x_i)\}$$

- Relax the optimization problem
 - approximate objective:
 - relaxed feasible set:

 $H_{q} \approx F(b)$ $\mathcal{M} \to \mathcal{M}_{o} \quad (\mathcal{M}_{o} \supseteq \mathcal{M})$

$$b^* = \arg\min_{b \in \mathcal{M}_p} \left\{ \left\langle E \right\rangle_b + F(b) \right\}$$

- The loopy BP algorithm: ^{*v*}
 - a fixed point iteration procedure that tries to solve b*

The Theory Behind LBP

• But we do not optimize $q(\mathbf{X})$ explicitly, focus on the set of beliefs

•
$$e.g., b = \{b_{i,j} = \tau(x_i, x_j), b_i = \tau(x_i)\}$$

- Relax the optimization problem
 - approximate objective:
 - relaxed feasible set:

$$H_{Betha} = H(b_{i,j}, b_i)$$

$$\mathcal{M}_o = \left\{ \tau \ge \mathbf{0} \mid \sum_{x_i} \tau(x_i) = \mathbf{1}, \sum_{x_i} \tau(x_i, x_j) = \tau(x_j) \right\}$$

$$b^* = \arg\min_{b \in \mathcal{M}_a} \left\{ \left\langle E \right\rangle_b + F(b) \right\}$$

- The loopy BP algorithm: ^{be}
 - a fixed point iteration procedure that tries to solve *b**





Mean Field Approximation

Naïve Mean Field

• Fully factorized variational distribution

$$q(x) = \prod_{s \in V} q(x_s)$$



Naïve Mean Field for Ising Model

Optimization Problem

Update

$$\max_{\mu \in [0,1]^m} \left\{ \sum_{s \in V} \theta_s \mu_s + \sum_{(s,t) \in E} \theta_{st} \mu_s \mu_t + \sum_{s \in V} H_s(\mu_s) \right\}$$

Rule

$$\mu_s \leftarrow \sigma \Big(\theta_s + \sum_{t \in N(s)} \theta_{st} \mu_t \Big)$$

- $\mu_t = p(X_t = 1) = \mathbb{E}_p[X_t]$ resembles "message" sent from node t to s
- $\{\mathbb{E}_p[X_t], t \in N(s)\}$ forms the "mean field" applied to s from its neighborhood

Mean field methods



- Optimize $q(\mathbf{X}_H)$ in the space of tractable families
 - *i.e.*, subgraph of G_p over which exact computation of H_q is feasible
- Tightening the optimization space
 - exact objective: H_q tightened feasible set: $Q \to \mathcal{T}$ $(\mathcal{T} \subseteq Q)$

$$q^* = \arg\min_{q\in\mathcal{T}} \langle E \rangle_q - H_q$$
Cluster-based approx. to the Gibbs free energy (Wiegerinck 2001, Xing et al 03,04)



Exact: G[p(X)] (intractable) Clusters: $G[\{q_c(X_c)\}]$



Mean field approx. to Gibbs free energy

- Given a disjoint clustering, $\{C_1, \ldots, C_l\}$, of all variables
- Let $q(\mathbf{X}) = \prod q_i(\mathbf{X}_{C_i}),$
- Mean-field free energy

$$G_{\rm MF} = \sum_{i} \sum_{\mathbf{x}_{C_i}} \prod_{i} q_i \left(\mathbf{x}_{C_i} \right) E(\mathbf{x}_{C_i}) + \sum_{i} \sum_{\mathbf{x}_{C_i}} q_i \left(\mathbf{x}_{C_i} \right) \ln q_i \left(\mathbf{x}_{C_i} \right)$$

e.g., $G_{\rm MF} = \sum_{i < j} \sum_{x_i x_j} q(x_i) q(x_j) \phi(x_i x_j) + \sum_i \sum_{x_i} q(x_i) \phi(x_i) + \sum_i \sum_{x_i} q(x_i) \ln q(x_i)$ (naïve mean field)

- Will **never** equal to the exact Gibbs free energy no matter what clustering is used, but it does **always** define a lower bound of the likelihood
- Optimize each $q_i(x_c)$'s.
 - Variational calculus ...
 - Do inference in each $q_i(x_c)$ using any tractable algorithm

The Generalized Mean Field theorem



Theorem: The optimum GMF approximation to the cluster marginal is isomorphic to the cluster posterior of the original distribution given internal evidence and its generalized mean fields:

$$q_i^*(\mathbf{X}_{H,C_i}) = p(\mathbf{X}_{H,C_i} | \mathbf{x}_{E,C_i}, \langle \mathbf{X}_{H,MB_i} \rangle_{q_{i\neq i}})$$

GMF algorithm: Iterate over each q_i

A generalized mean field algorithm [xing et al. UAI 2003]





A generalized mean field algorithm [xing et al. UAI 2003]





Convergence theorem



Theorem: The GMF algorithm is guaranteed to converge to a local optimum, and provides a lower bound for the likelihood of evidence (or partition function) the model.

The naive mean field approximation



- Approximate $p(\mathbf{X})$ by fully factorized $q(\mathbf{X}) = P_i q_i(X_i)$
- For Boltzmann distribution $p(X) = \exp\{\sum_{i < j} q_{ij} X_i X_j + q_{io} X_i\}/Z$:

mean field equation:

$$q_{i}(X_{i}) = \exp\left\{\theta_{i0}X_{i} + \sum_{j \in \mathcal{N}_{i}} \theta_{ij}X_{i}\langle X_{j}\rangle_{q_{j}} + A_{i}\right\}$$

$$= p(X_{i} |\{\langle X_{j}\rangle_{q_{j}} : j \in \mathcal{N}_{i}\})$$

- $\langle X_j \rangle_{q_j}$ resembles a "message" sent from node *j* to *i*
- { $\langle X_j \rangle_{q_j} : j \in \mathcal{N}_i$ } forms the "mean field" applied to X_i from its neighborhood

Example 1: Generalized MF approximations to Ising models



Cluster marginal of a square block C_k :

$$q(X_{C_k}) \propto \exp\left\{\sum_{i,j\in C_k} \theta_{ij} X_i X_j + \sum_{i\in C_k} \theta_{i0} X_i + \sum_{\substack{i\in C_k, j\in MB_k, \\ k'\in MBC_k}} \theta_{ij} X_i \langle X_j \rangle_{q(X_{C_k})}\right\}$$

Virtually a reparameterized Ising model of small size. © Eric Xing @ CMU, 2005-2014

GMF approximation to Ising models



Repulsive coupling: negatively weighted

Example 2: Sigmoid belief network









Example 3: Factorial HMM







Automatic Variational Inference



fHMM

Mean field approx.

Structured variational approx.

- Currently for each new model we have to
 - derive the variational update equations
 - write application-specific code to find the solution
- Each can be time consuming and error prone
- Can we build a general-purpose inference engine which automates these procedures?

Cluster-based MF (e.g., GMF)

- a general, iterative message passing algorithm
- clustering completely defines approximation
 - preserves dependencies
 - flexible performance/cost trade-off
 - clustering automatable
- recovers model-specific structured VI algorithms, including:
 - fHMM, LDA
 - variational Bayesian learning algorithms
- easily provides new structured VI approximations to complex models