Structured Variational Inference

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Structured Variational Approximation

- Approximate inference methods based on belief propagation optimize an approximate energy functional over the class of pseudo marginals
  - But the pseudo marginals do not correspond to a globally coherent joint distribution Q
- The structured variational approach aims to optimize the energy functional over a family $\mathcal{Q}$ of coherent distributions Q
  - This family is chosen to be computationally tractable
    - Hence it is not sufficiently expressive to capture all of the information in P_Φ

Inference as Maximization

- We address the following maximization problem in Structured Variational Inference:

> Find Q ε $\mathcal{Q}$
>
> Maximizing $F[\tilde{P}_\Phi, Q]$
>
> where $\mathcal{Q}$ is a given family of distributions

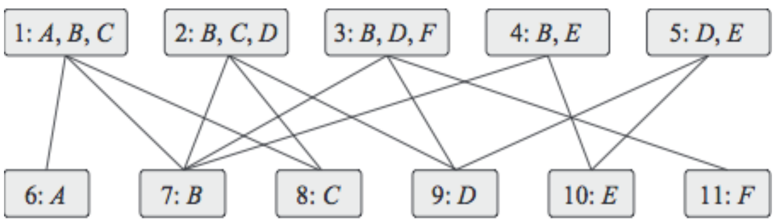
- We use the exact energy functional $F[P_\Phi, Q]$
    - which satisfies $\boldsymbol{D}(Q||P_\Phi) = \ln Z$ - $F[P_\Phi, Q]$
  - Thus maximizing the energy functional corresponds directly to obtaining a better approximation to P_Φ in terms of $\boldsymbol{D}(Q||P_\Phi)$

Parameter of Maximization

- Main parameter in maximization problem is choice of family Q
  - This choice introduces a trade-off
    - Families that are simpler, i.e., BNs and MNs of small tree width allow more efficient inference
    - If Q is too restrictive then it cannot represent distributions that are good approximations of P_Φ
      - Giving rise to a poor approximation Q
- Family is chosen to have enough structure
  - Hence called *structured variational approximation*
    - Variational calculus since we maximize over functions
    - Unlike belief propagation guaranteed to lower bound the log-partition function and guaranteed to converge

The Mean Field Approximation

- First approach considered is the mean field approximation
- It resembles the Bethe approximation to the mean field functional



Bethe bipartite graph; first layer of large clusters and second layer of univariate clusters

- The resulting algorithm performs message passing where the messages are over single variables
  - The form of the updates is different

Mean Field Class of Distributions

- The mean field algorithm finds the distribution Q which is closest to P_Φ in terms of $\boldsymbol{D}(Q||P_\Phi)$
- within the class of distributions representable as the product of independent marginals

$$Q(\chi) = \prod_i Q(X_i)$$

- Trade-off:
  - A fully factored distribution loses information
  - But we can easily evaluate any query
    - By a product of terms that involve variables in query
  - To represent Q we only need marginals of variables

Derivation of Mean Field Algorithm

- We consider the energy functional in the form

$$F\left[\tilde{P}_\Phi, Q\right] = E_Q\left[\ln \tilde{P}\left(\chi\right)\right] + H_Q\left(\chi\right) = \sum_{\phi \in \Phi} E_Q\left[\ln \phi\right] + H_Q\left(\chi\right)$$

  – where Q has the form of $Q(\chi) = \prod_i Q(X_i)$

A functional takes a function as input and produces a value as output, e.g., entropy

- We then characterize fixed points for each Q
- Thereby derive an iterative algorithm to find such fixed points
  – In fixed point iteration $x_{n+1} = f(x_n)$, $n = 0,1,2..$

Example of fixed pt: Newton's roots

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Computing the Energy Functional

- The functional contains two terms: $F\left[\tilde{P}_{\Phi},Q\right]=\sum_{\phi\in\Phi}E_{Q}\left[\ln\phi\right]+H_{Q}\left(\chi\right)$
  1. The first is a sum of terms of the form $E_{U_\Phi \sim Q}[\ln \phi]$ where we need to evaluate

$$E_{U_\phi \sim Q}\left[\ln\phi\right]=\sum_{\boldsymbol{u}_\phi}Q(\boldsymbol{u}_\phi)\ln\phi(\boldsymbol{u}_\phi)$$
$$=\sum_{\boldsymbol{u}_\phi}\left(\prod_{Xi\in\boldsymbol{U}_\phi}Q(x_i)\right)\ln\phi(\boldsymbol{u}_\phi)$$

Notation: $P_{\Phi}\left(\chi\right)=\frac{1}{Z}\prod_{\phi\in\Phi}\phi\left(U_\phi\right)$

where $U_\phi = Scope\ (\phi)$

   - We can use the form of Q to compute $Q(u_\phi)$ as a product of marginals (performed in linear in no. of values of U_ϕ
  2. The term $H_Q(\chi)$ also decomposes in this case

If $Q(\chi)=\prod_i Q(X_i)$ then $H_Q(\chi)=\sum_i H_Q(X_i)$

Entropy definition:

$$H_Q(X_i)=E_Q\left[\ln\frac{1}{Q(X_i)}\right]$$

- Thus energy functional is a sum of expectations
  - Each one over a small set of variables

Complexity of Energy Functional

- Energy functional for a fully factored distribution Q can be written as a sum of expectations:

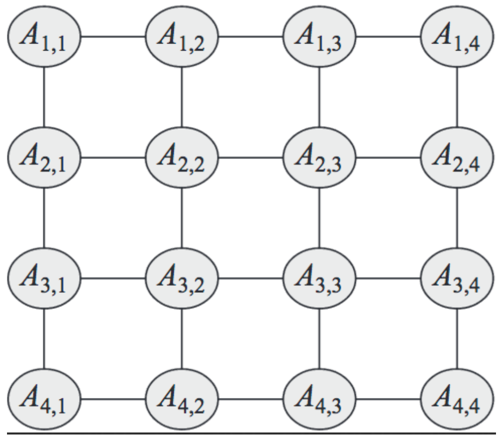
$$F\left[\tilde{P}_\Phi, Q\right] = \sum_{\boldsymbol{u}_\phi} \left(\prod_{Xi \in \boldsymbol{U}_\phi} Q(x_i) \right) \ln \phi(\boldsymbol{u}_\phi) + \sum_i E_Q\left[\ln \frac{1}{Q(X_i)} \right]$$

  - Each one over a small set of variables
  - Complexity depends on size of the factors in P_ϕ
    - Not on the topology of the network

$$P_\Phi(\chi) = \frac{1}{Z} \prod_{\phi \in \Phi} \phi(U_\phi)$$

- Thus the energy functional in this case can be represented/manipulated effectively
  - even when exact inference requires exponential time

Ex: Mean field energy for 4x4 grid



- Energy functional has the form

$$\boxed{\begin{aligned} F\left[\tilde{P}_{\Phi}, Q\right] = & \sum_{i \in \{1,2,3\}, j \in \{1,2,3,4\}} E_Q[\ln \phi(A_{i,j}, A_{i+1,j}) \\ & + \sum_{i \in \{1,2,3,4\}, j \in \{1,2,3\}} E_Q[\ln \phi(A_{i,j}, A_{i,j+1}) \\ & + \sum_{i \in \{1,2,3,4\}, j \in \{1,2,3,4\}} H_Q(A_{i,j}) \end{aligned}}$$

  - It involves only expectations over single variables and pairs of neighboring variables
    - The expression has the same form for an n x n grid
      - Thus although tree width for an n x n grid is exponential in n, the energy functional can be computed in $O(n^2)$, i.e., linear in no. of variables n^2

Maximizing Energy Functional: Fixed-point Characterization

- Task is to find distribution Q for which energy functional is maximized

Mean-Field

Find $Q \in \mathcal{Q}$

Maximizing $F[\tilde{P}_\Phi, Q]$

Subject to $Q(\chi) = \prod_i Q(X_i)$

$$\sum_{x_i} Q(x_i) = 1 \quad \forall i$$

  – We use Lagrange multipliers to characterize stationary points of $F[\tilde{P}_\Phi, Q]$
    - The structure of Q allows us to consider the optimal value of each component given the rest

Mean Field Theorem: maximum of $Q(X_i)$

- *Thm*: $Q(X_i)$ is a local max of Mean-Field given $\{Q(X_j)\}_{j \neq i}$ iff

$$Q(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi \in \Phi} E_{\chi \sim \Phi}\left[\ln \phi \mid x_i \right] \right\}$$

where Z_i is a local normalizing constant and $E_{\chi \sim Q}[\ln \boldsymbol{\phi} | x_i]$ is the conditional expectation given value x_i

$$E_{\chi \sim Q}[\ln \phi \mid x_i] = \sum_{\boldsymbol{u}_\phi} Q(\boldsymbol{u}_\phi \mid x_i) \ln(\boldsymbol{u}_\phi)$$

- Proof:

1. Objective function is: $F\left[\tilde{P}_\Phi, Q\right] = \sum_{\phi \in \Phi} E_Q\left[\ln \phi\right] + H_Q\left(\chi\right)$
2. Restricting attention to $Q(X_i)$ terms: $F_i\left[Q\right] = \sum_{\phi \in \Phi} E_{U_\phi \sim Q}\left[\ln \phi\right] + H_Q\left(X_i\right)$
3. To optimize $Q(X_i)$ define Lagrangian of terms in $F[\tilde{P}_\Phi, Q]$

$$L_i\left[Q\right] = \sum_{\phi \in \Phi} E_{U_\phi \sim Q}\left[\ln \phi\right] + H_Q(X_i) + \lambda\left(Q(x_i) - 1\right)$$

4. For derivatives use lemma: If $Q(\chi) = \prod_i Q(X_i)$ then for any function f with scope U: $\dfrac{\partial}{\partial Q(x_i)} E_{U \sim Q}\left[f(U)\right] = E_{U \sim Q}\left[f(U) \mid x_i\right]$
5. Using lemma & standard derivatives of entropy:

$$\frac{\partial}{\partial Q(x_i)} L_i = \sum_{\phi \in \Phi} E_{\chi \sim Q}\left[\ln \phi \mid x_i\right] - \ln Q(x_i) - 1 + \lambda$$

6. Set derivatives to 0 & rearrange: $\ln Q(x_i) = \lambda - 1 + \sum_{\phi \in \Phi} E_{\chi \sim Q}\left[\ln \phi \mid x_i\right]$
7. Take exponents of both sides, and λ constant.
8. Solution: $Q(X_i)$ is maximum since $\Sigma E_{U\varphi}$ is linear & H_Q is concave ■

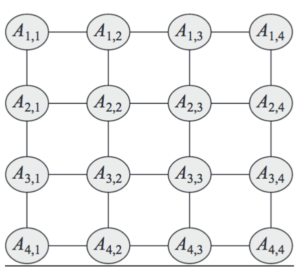
Corollary of Mean-Field Theorem

- To convert $Q(x_i)=\frac{1}{Z_i}\exp\left\{\sum_{\phi\in\Phi} E_{\chi\sim\Phi}\left[\ln\phi \mid x_i\right]\right\}$ into update algorithm
  - Observe that if $X_i \notin \text{Scope}(\phi)$ then $E_{U_\phi\sim Q}\left[\ln\phi \mid x_i\right]=E_{U_\phi\sim Q}\left[\ln\phi_i\right]$
    - i.e., expectation of such factors are independent of x_i

Cor. In mean field approx. $Q(X_i)$ is a local maximum iff

$$Q(x_i)=\frac{1}{Z_i}\exp\left\{\sum_{\phi:X_i\in Scope\{\phi\}} E_{(U_\phi-\{X_i\})\sim\Phi}\left[\ln\phi(U_\phi,x_i)\right]\right\}$$

- This representation shows that $Q(X_i)$ have to be consistent with expectation of the potentials in which it appears
  - In grid network, it implies that $Q(A_{i,j})$ is the product of four terms



$$Q(a_{i,j})=\frac{1}{Z_{i,j}}\exp\left\{\begin{array}{l}\sum_{a_{i-1,j}} Q(a_{i-1,j})\ln\left(\phi(a_{i-1,j},a_{i,j})\right)+\\ \sum_{a_{i,j-1}} Q(a_{i,j-1})\ln\left(\phi(a_{i,j-1},a_{i,j})\right)+\\ \sum_{a_{i+1,j}} Q(a_{i+1,j})\ln\left(\phi(a_{i+1,j},a_{i,j})\right)+\\ \sum_{a_{i,j+1}} Q(a_{i,j+1})\ln\left(\phi(a_{i,j},a_{i,j+1})\right)\end{array}\right\}$$

Each term is a geometric average of one of the potentials involving $A_{i,j}$

From Mean Field to Update Algorithm

- We now have tools for algorithm to find max $\boxed{F[\tilde{P}_\Phi, Q]}$
  - They are: $\boxed{Q(x_i) = \frac{1}{Z_i}\exp\left\{\sum_{\phi: X_i \in Scope\{\phi\}} E_{(U_\phi - \{X_i\}) \sim \Phi}\left[\ln \phi(U_\phi, x_i)\right]\right\}}$ and $\boxed{Q(a_{i,j}) = \frac{1}{Z_{i,j}}\exp\left\{\begin{array}{l} \sum_{a_{i-1,j}} Q(a_{i-1,j}) \ln\left(\phi(a_{i-1,j}, a_{i,j})\right) + \\ \sum_{a_{i,j-1}} Q(a_{i,j-1}) \ln\left(\phi(a_{i,j-1}, a_{i,j})\right) + \\ \sum_{a_{i+1,j}} Q(a_{i+1,j}) \ln\left(\phi(a_{i+1,j}, a_{i,j})\right) + \\ \sum_{a_{i,j+1}} Q(a_{i,j+1}) \ln\left(\phi(a_{i,j}, a_{i,j+1})\right) \end{array}\right\}}$
  - Term within exponential
    - is easily evaluated by
      - interactions between neighbors of $A_{i,j}$ and values they can take
    - RHS has expectations of variables not involving X_i
  - Resulting $Q(X_i)$ is optimal given all other values
    - Simply evaluate exponent terms for each value of x_i, normalize results to sum to 1 and assign them to $Q(X_i)$
    - Consequently we reach optimal $Q(X_i)$ in one easy step
  - To optimize relative to all variables, embed step in iterated coordinate ascent algorithm
      - Optimize single marginal at a time, given fixed choices of others

Algorithm: Mean-Field Approximation

- **Procedure** Mean-Field {Φ, //factors that define P_Φ,
  Q_0 //initial choice of Q }

1. $Q \leftarrow Q_0$

2. Unprocessed $\leftarrow \chi$

3. while *Unprocessed* $\neq \emptyset$

4. Choose X_i from *Unprocessed*

5. $Q_{\text{old}}(X_i) \leftarrow Q(X_i)$

6. for $x_i \in Val(X_i)$ **do**

7. $Q(x_i) \leftarrow$ $\boxed{\exp\left\{ \sum_{\phi: X_i \in Scope\{\phi\}} E_{(U_\phi - \{X_i\}) \sim \Phi}\left[\ln \phi(U_\phi, x_i)\right]\right\}}$

8. Normalize $Q(X_i)$ to sum to one

9. if $Q_{\text{old}}(X_i) \neq Q(X_i)$ **then**

10. Unprocessed $\leftarrow$ *Unprocessed* $\cup \left(\cup_{\phi: X_i \in Scope[\phi]} Scope[\phi]\right)$

11. Unprocessed $\leftarrow$ *Unprocessed*-$\{X_i\}$

- **return** Q

Observations about Algorithm

- A single optimization of $Q(X_i)$ does not suffice.
  - A subsequent modification of another marginal $Q(X_i)$ may result in a different optimal parameterization for $Q(X_i)$
  - Thus algorithm repeats the steps until convergence
- Each iteration of Mean-Field results in a better approximation Q to the target density P_Φ guaranteeing convergence
- The convergence points are local maxima
  - Not necessarily global

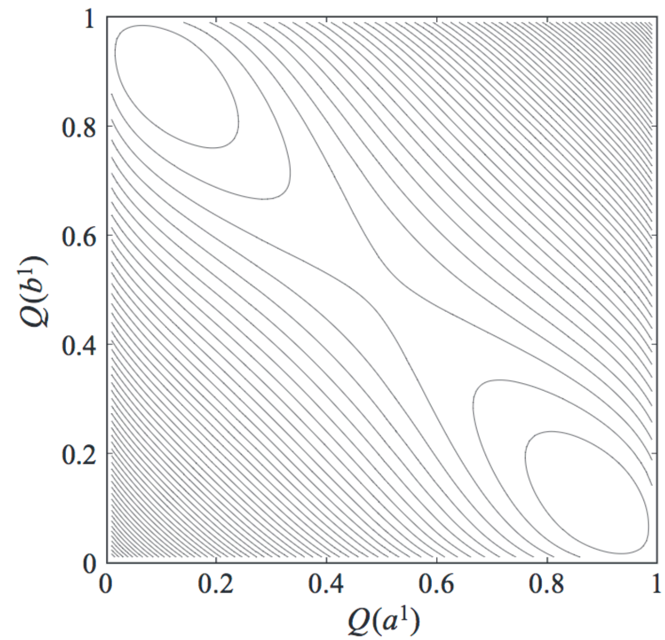
Ex: Mean-Field Energy Functional

- A distribution P_Φ

  $P(a,b) = 0.5 - \varepsilon$ if $a \neq b$

  $P(a,b) = \varepsilon$ if $a = b$

  – Which is a Noisy XOR



- Mean field Energy $F[\tilde{P}_\Phi, Q]$
- As XOR, P_Φ cannot be approximated by a product of marginals
- But energy potential surface has two peaks at $a \neq b$

Structured Approximations

- Although Mean Field Algorithm provides an easy approximation method, we are forcing Q to be a very simple distribution
  - All variables being independent of each other in Q leads to very poor approximations
- If we use a Q that can capture some dependencies in P_Φ we can get a better approximation
  - Thus explore approximations inbetween mean field and exact inference
  - Using network structures of different complexity

Fixed-point characterization

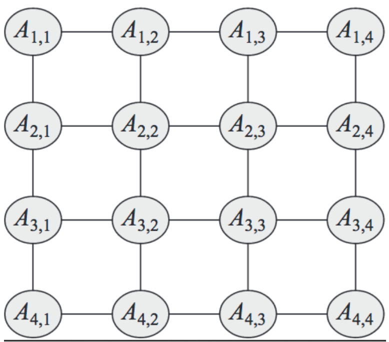
- Focus on using MNs instead of BNs
- Parameterized Gibbs distributions
  - Not restricted to factors over maximal cliques
- Form of variational approximation
  - Q is from a Gibbs parametric family
  - We are given a set of potential scopes $\{C_j \subseteq \chi : j = 1, \ldots, J\}$
  - We choose an approximation Q that has the form

$$Q(\chi) = \frac{1}{Z_Q} \prod_{j=1}^{J} \Psi_j$$

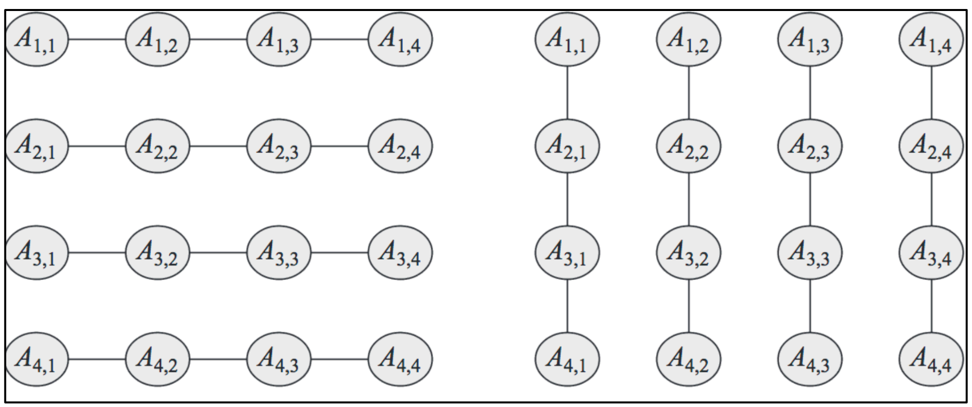
    - where Ψ_j is a factor with scope $Scope[\Psi_j] = C_j$

Ex: Grid Network

- Given:



  - There are many possible approximate network structures, two of them are:



Both a collection of independent chain structures

Inference is linear

Not much worse than mean field

Method of Structured Variational

- Decide on form of potentials ϕ for family Q
- We consider energy functional $F\left[\tilde{P}_{\Phi}, Q\right] = \sum_{\phi \in \Phi} E_Q\left[\ln \phi\right] + H_Q\left(\chi\right)$ for a distribution Q in this family
  - Characterize the stationary points of functional
  - Use those to derive iterative optimization algorithm
- Evaluating terms that involve $E_{U_\phi \sim Q}\left[\ln \phi\right]$ requires performing expectations wrt variables in $Scope[\phi]$
  - Complexity of expectation depends on structure of approximating distribution
    - Assume we can solve this problem using exact inference