

Bethe Free Energy

accts for pairwise corr
• Exact η on trees

Params $b_i(x_i) \cong P(x_i)$
 $b_{ij}(x_i, x_j) \cong P(x_i, x_j)$

Abuse notation + $b = \{b_i, b_{ij}\}$ wrt G

Def Ideally, wanna search over globally consistent marg wrt G

$\text{Marg}(G) \triangleq \{b : \{b_i\}_{i \in V}, \{b_{ij}\}_{(i,j) \in E} \text{ s.t. } \exists P(x) \text{ w.}$

$$b_i(x_i) = \sum_{x_{-i}} P(x) \quad \forall i \in V$$

$$b_{ij}(x_i, x_j) = \sum_{x_{-ij}} P(x) \quad \forall (i,j) \in E$$

but checking if $b \in \text{Marg}$ is NP-hard $\cap$

Instead,

Def $\text{Loc}(G) \triangleq \{b : \sum_{x_i} b_i(x_i) = 1 \quad \forall i \in V$



$$\sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i) \quad \forall (i,j) \in E \}$$

Local $\nRightarrow$ Global

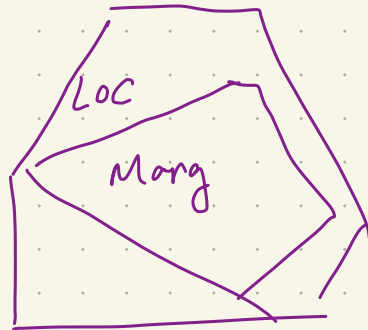
$$X = \{0, 1\}$$

$$b_i = \begin{bmatrix} .49 \\ .51 \end{bmatrix}$$

$$b_{12} = b_{23} = \begin{bmatrix} .49 & .01 \\ .01 & .49 \end{bmatrix}$$

$$b_{13} = \begin{bmatrix} .01 & .49 \\ .49 & .01 \end{bmatrix}$$

For general G



When G is a tree, $\forall$ locally consistent b
 $\exists P(x)$ which is globally consistent for b

$$\tilde{P}(x) = \prod_{i \in V} b_i(x_i) \prod_{\substack{(i,j) \\ e \in E}} \frac{b_{ij}(x_i, x_j)}{b_i(x_i) b_j(x_j)}$$

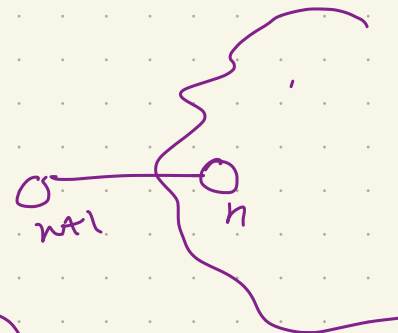
Claim: $\tilde{P}$ is consistent if G is a tree

~~PF~~ By induction on n .

$$n=1 \quad \tilde{P}(x_1) = b_1(x_1) \quad \checkmark$$

Suppose true $\forall$ trees of size $\leq n$

Fix a tree of size $n+1$. It has a leaf.



$$\begin{aligned} \tilde{P}(x_1^n, x_{n+1}) &= \tilde{P}(x_1^n) \cdot b_{n+1}(x_{n+1}) \cdot \frac{b_{n,n+1}(x_n, x_{n+1})}{b_n \cdot b_{n+1}} \\ &= \tilde{P}(x_1^n) \cdot \frac{b_{n,n+1}}{b_n} \end{aligned}$$

$$\begin{aligned} \tilde{P}(x_n, x_{n+1}) &\stackrel{\sim}{=} \sum_{x \in V \setminus \{n, n+1\}} \tilde{P}(x_1^n, x_{n+1}) = \tilde{P}(x_n) \cdot \frac{b_{n,n+1}(x_n, x_{n+1})}{b_n \cdot b_{n+1}} \cdot b_{n+1} \\ &\stackrel{IH}{=} \frac{\cancel{b_n(x_n)}}{\cancel{b_n} \cdot b_{n+1}} \cdot \frac{b_{n,n+1}}{\cancel{b_n} \cdot \cancel{b_{n+1}}} \cdot \cancel{b_{n+1}} \quad \checkmark \end{aligned}$$

Def Bethe Free Energy on a tree

$$\mathbb{F}(b) \triangleq G_{\text{tree}}(b) = -\text{Energy} + \text{Entropy}$$

$$= \sum_{(i,j) \in E} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log(f_{ij}(x_i, x_j)) - \log[b_{ij}(x_i, x_j)] + \sum_{i \in V} (\deg(i)-1) \sum_{x_i} b_i(x_i) \log b_i(x_i)$$

(Claim: if G is a tree, then

$$\sup_{b \in \text{LOC}(G)} \mathbb{F}(b) = \sup_{b \in \text{Marg}(G)} \mathbb{G}(b) = \mathbb{F}$$

This is the Bethe variational prob

(opt on a non-tree is called Bethe appx)

Bethe free energy & BP (not just trees!)

Claim: (1) fixed pts of BP are one-to-one w. stationary pts of Bethe.

(2) BP messages $\{m_{i \rightarrow j}(x_i)\}$ are the exponentials of lagrangians $\{\lambda_{ij}^*(x_i)\}$

Gibbs Free Energy for gen b is

$$G_{\text{Ftotal}}(b) = - \mathbb{E}_b \left[\underbrace{-\log(f_{\text{total}}(b))}_{\text{energy}} \right] + \mathbb{E}_b \left[\underbrace{-\log b(b)}_{\text{entropy}} \right]$$

Evaluate on

$$b(x) = \prod_{i \in V} b_i(x_i) \prod_{(i,j) \in E} \frac{b_{ij}(x_i, x_j)}{b_i(x_i) b_j(x_j)}$$

$$\text{Energy} = - \sum_{(i,j) \in E} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log f_i(x_i, x_j)$$

$$\text{Entropy} = \mathbb{E}_b \left[-\log \left[\prod_{i \in V} b_i(x_i) \prod_{(i,j) \in E} \frac{b_{ij}(x_i, x_j)}{b_i(x_i) b_j(x_j)} \right] \right]$$

$$= \sum_i \sum_{x_i} -b_i \log b_i(x_i)$$

$$- \sum_{(i,j) \in E} \sum_{x_i, x_j} b_{ij} (\log b_{ij} - \log b_i - \log b_j)$$

$$\sum_{(i,j) \in E} \sum_{x_i, x_j} b_{ij} \log b_{ij} - \sum_{i \in V} \sum_{x_i} \deg(i) b_i \log b_i$$

Pf Lagrangian mults.: λ_i for $\sum_{x_i} b_i(x_i) = 1$
 $\lambda_{i \rightarrow j}(x_i)$ for $\sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i)$

$$\text{Lag}(b, \lambda) = \#b - \lambda_i \left[\sum_{x_i} b_i(x_i) - 1 \right] - \sum_{i,j} \sum_{x_i} \lambda_{i \rightarrow j}(x_i) \left[\sum_{x_j} b_{ij}(x_i, x_j) - b_i(x_i) \right]$$

$$\nabla_{b_{ij}(x_i, x_j)} \text{Lag}(b, \lambda) = -1 - \log b_{ij}(x_i, x_j) + \log f_{ij}(x_i, x_j) - \lambda_{i \rightarrow j}(x_i) - \lambda_{j \rightarrow i}(x_j)$$

$$\nabla_{b_i(x_i)} \text{Lag}(b, \lambda) = -(1 - \deg(i)) \log(b_i(x_i) \cdot e) - \lambda_i + \sum_{j \in \delta_i} \lambda_{i \rightarrow j}(x_i)$$

setting $= 0$ & solving $\Rightarrow$

$$b_{ij}(x_i, x_j) = f_{ij}(x_i, x_j) \exp \left\{ -1 - \lambda_{i \rightarrow j}(x_i) - \lambda_{j \rightarrow i}(x_j) \right\}$$

$$b_i^*(x_i) \propto \exp \left\{ -\frac{1}{\deg(i)-1} \sum_{j \in \delta_i} \lambda_{i \rightarrow j}(x_i) \right\}$$

$$\sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i)$$

Change variables $m_{i \rightarrow j}(x_i) \propto e^{-\lambda_{i \rightarrow j}(x_i)}$

$$(1) \quad b_{ij}^* \propto m_{ij}(x_i) f_{ij}(x_i, x_j) m_{j \rightarrow i}(x_j)$$

$$(2) \quad b_i^* \propto \prod_{j \in \delta_i} (m_{i \rightarrow j}(x_j))^{\deg(i)-1}$$

$$(3) \quad \sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i)$$

To show $\equiv$

$$\prod_{k \in \mathcal{S}(i,j)} \{ \sum_{k \in \mathcal{S}(i,j)} b_{ik}^* f_k(x_i, x_k) \} = \prod_{k \in \mathcal{S}(i,j)} b_{ik}^* (x_i) =$$

$\} \} \leftarrow \textcircled{1}$
Stationarity

$\downarrow$
Local Consistency

$$b_{ik}^* (x_i) \deg(i) - 1$$

$\} \leftarrow$ stationarity of $\mathbb{F}_b$ $\textcircled{2}$

$$\prod_{k \in \mathcal{S}(i,j)} m_{i \rightarrow k}(x_i) \sum_{x_k} m_{k \rightarrow i}(x_k) f_{ik}(x_i, x_k)$$

$\downarrow$

$$\prod_{k \in \mathcal{S}(i,j)} \sum_{x_k} m_{k \rightarrow i}(x_k) f_{ik}(x_k, x_i)$$

$\propto$

$$\prod_{k \in \mathcal{S}(i)} m_{i \rightarrow k}(x_i)$$

$\downarrow$

cancelling for $k \neq j$

$$m_{i \rightarrow j}(x_i)$$

$\downarrow$

The BP update!

Naive MF

$$\max_{b \in (\Delta_{|x|-1})^n} G(b)$$

Bethe FE on tree $\nearrow$ ^{right on tree}

$$\max_{b \in \text{Loc}(T)} G(b) \leq \max_{b(\cdot) \in \Delta_{X^n-1}} G(b) \leq \sum_{T \in \mathcal{T}} \max_{b \in \text{Loc}(T)} G(b)$$

Tree-Weighted BP

Region-based FE

$$\max_{b(\cdot) \in \text{Loc}(GR)} G(b)$$

Generalized BP

(Not UB or LB)

Bethe FE on non-tree

$$\max_{b(\cdot) \in \text{Loc}(G)} G(b)$$

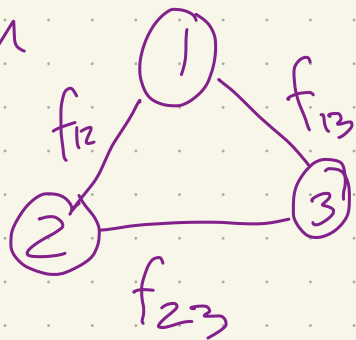
BP

Tree weighted BP

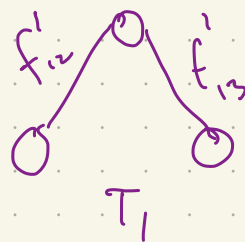
(slides have more deets)

"A new class of upper bds on the log partition fn" Wainwright, Jaakkola, Willsky

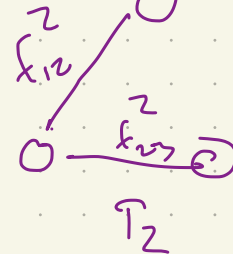
example) GM



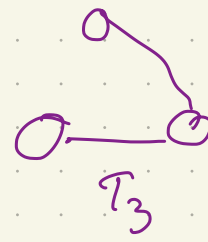
Consider all spanning trees / wts for trees



$$c_1 =$$



$$c_2 =$$



$$= c_3 = \frac{1}{3}$$

$$f_{12} = (f_{12}^{(1)})^{c_1} \cdot (f_{12}^{(2)})^{c_2}$$

$$= (f_{12}^{3/2})^{1/3} (f_{12}^{3/2})^{1/3}$$

Consider all S.T.s. $T_k \in \mathcal{T}(G)$
 φ wts. c_k s.t.

$$\sum c_k = 1 \varphi$$

$$\forall ij \quad \log f_{ij}(x_i, x_j) = \sum_{k=1}^{|\mathcal{T}(G)|} c_k \log f_{ij}^k(x_i, x_j)$$

Then, energy of G Free energy decomposes:

$$\mathbb{E}_b \left[- \sum_{i,j \in E} \log f_{ij}(x_i, x_j) \right] = \mathbb{E}_b \left[- \sum_E \sum_k c_k \log f_{ij}^k(x_i, x_j) \right]$$

↑ energy of one tree model

$$= \sum_k c_k \mathbb{E}_b \left[- \sum_{i,j \in E} \log f_{ij}^k(x_i, x_j) \right]$$

Claim: $\log Z \leq \sum_k c_k \log Z_k$

Pf

$$\log Z = \max_{b \in \Delta(|X|^n - 1)} \mathbb{E}_b \left[\sum_{(i,j) \in E} \log t_{ij}(x_i, x_j) \right] + \text{Entropy}(b)$$

$$= \max_b \sum_k c_k \mathbb{E}_b \left[\sum_{(i,j) \in E_k} \log t_{ij}^{(k)}(x_i, x_j) \right] + \text{Entropy}(b)$$

$$\leq \sum_k c_k \max_b \left\{ \mathbb{E}_b \left[\sum_{(i,j) \in E_k} \log t_{ij}^{(k)}(x_i, x_j) \right] + \text{Entropy}(b) \right\}$$

$$\xrightarrow{\text{GM on a tree } T_k!} = \sum_k c_k \max_{b \in \text{Loc}(T_k)} \left\{ \mathbb{E}_b \left[\sum_{(i,j) \in E_k} \log t_{ij}^{(k)}(x_i, x_j) \right] + \text{Entropy}(b) \right\}$$

Can be solved exactly w. BP.

Details that must be addressed (but we don't here):

- $c_k, f_{ij}^{(k)}$ must be chosen to min RHS
- # STs explodes

