Computing the Permanent with (Fractional) Belief Propagation

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What is Permanent?

.. odd relative of determinant ...

$$\mathrm{Det}\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

$$\mathrm{Perm}\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = a_{11}a_{22} + a_{12}a_{21}$$

partition function of the dimer model over bi-partite graph

- First #-P (sharp-P) problem, Valiant (1979) & #-P complete
- Fully-Polynomial-Randomized-Algorithmic Scheme (FPRAS) -Jerram, Sinclair, Vigoda (2004) ... but a good polynomial approximate scheme is not known
- Low bound = van der Waerden (1926) conjecture: for any $n \times n$ double-stochastic p, $\mathrm{Perm}(p) \geq n^n/n!$ ... proved by Falikman (1981), Egorychev (1981), Gurvits (2008), Laurent, Schjriver (2009)

Our Main Result:

Fractional Belief Propagation is an approximation for Permanent

- which is CONVEX
- which is MONOTONE (function of the fractional parameter)
- it SANDWICHES the permanent (from below =BP and above ="chopped" MF)
- allows $\mathrm{Perm} = \mathrm{FBP} * \mathrm{Perm}$ exact relation

built on other "BP for permanents" recent stories

- Bethe Free Energy is CONVEX [Vontobel '11]
- BP gives a LOW BOUND [Gurvits '11]

Outline

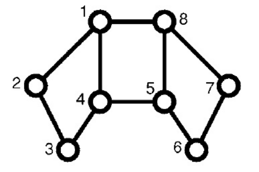
1. Graphical Models. Free Energy Functional. Belief Propagation.
   - Graphical Models
   - Bethe Free Energy & Belief Propagation (approx)
2. The Story of Permanent: Learning Flows. BP+ $\to$ FBP+.
   - Particle Tracking (Fluid Mechanics): Learning the Flow
   - BP and Loop Series (re-summed) for Permanents
   - Fractional BP: perm=FBP*perm.
3. Conclusions and Path Forward

Graphical Models = The Language

Forney style - Variables on Edges

$$\mathcal{P}(\boldsymbol{\sigma}) = Z^{-1}\prod_a f_a(\boldsymbol{\sigma}_a)$$

$$\underbrace{Z = \sum_{\boldsymbol{\sigma}}\prod_a f_a(\boldsymbol{\sigma}_a)}_{\text{partition function}}$$



$f_a \geq 0$

$\sigma_{ab} = \sigma_{ba} = \pm 1$

Boolean, for example

$\boldsymbol{\sigma}_1 = (\sigma_{12}, \sigma_{14}, \sigma_{18})$

$\boldsymbol{\sigma}_2 = (\sigma_{12}, \sigma_{23})$

Objects of Interest

- Most Probable Configuration = Maximum Likelihood = Ground State: $\arg\max \mathcal{P}(\boldsymbol{\sigma})$
- Marginal Probability: e.g. $\mathcal{P}(\sigma_{ab}) \equiv \sum_{\boldsymbol{\sigma}\setminus\sigma_{ab}} \mathcal{P}(\boldsymbol{\sigma})$
- Partition Function = weighted counting : Z

Exact Free Energy: from Discreet to Continious

$$P(\boldsymbol{\sigma}) = \frac{\prod_a f_a(\boldsymbol{\sigma}_a)}{Z}, \quad Z \equiv \sum_{\boldsymbol{\sigma}} \prod_a f_a(\boldsymbol{\sigma}_a)$$

Exact Variational Principle

J.W. Gibbs 1903 (or earlier)
also known as Kullback-Leibler (1951) in CS and IT

$$F\{b(\boldsymbol{\sigma})\} = -\sum_{\boldsymbol{\sigma}} b(\boldsymbol{\sigma}) \sum_a \ln f_a(\boldsymbol{\sigma}_a) + \sum_{\boldsymbol{\sigma}} b(\boldsymbol{\sigma}) \ln b(\boldsymbol{\sigma})$$

$$-\log Z = \min_{\{b\}} F\{b(\boldsymbol{\sigma})\}\Big|_{\sum_{\boldsymbol{\sigma}} b(\boldsymbol{\sigma})=1}$$

"Variational" Ansatz

- Mean-Field: $p(\boldsymbol{\sigma}) \approx b(\boldsymbol{\sigma}) = \prod_{(a,b)} b_{ab}(\sigma_{ab})$ exact in asymptotic
- Belief Propagation:

$$p(\boldsymbol{\sigma}) \approx b(\boldsymbol{\sigma}) = \frac{\prod_a b_a(\boldsymbol{\sigma}_a)}{\prod_{(a,b)} b_{ab}(\sigma_{ab})} \quad \text{(exact on a tree)}$$

$$\forall\ a;\ c \in a: \quad \sum_{\boldsymbol{\sigma}_a} b_a(\boldsymbol{\sigma}_a) = 1, \quad b_{ac}(\sigma_{ac}) = \sum_{\boldsymbol{\sigma}_a \setminus \sigma_{ac}} b_a(\boldsymbol{\sigma}_a)$$

Bethe Free Energy: variational approach
(Yedidia,Freeman,Weiss '01 - inspired by Bethe '35, Peierls '36)

$$F = \underbrace{-\sum_a \sum_{\boldsymbol{\sigma}_a} b_a(\boldsymbol{\sigma}_a)\ln f_a(\boldsymbol{\sigma}_a)}_{\text{self-energy}} + \underbrace{\sum_a \sum_{\boldsymbol{\sigma}_a} b_a(\boldsymbol{\sigma}_a)\ln b_a(\boldsymbol{\sigma}_a) - \sum_{(a,c)} b_{ac}(\sigma_{ac})\ln b_{ac}(\sigma_{ac})}_{\text{configurational entropy}}$$

$$\forall\ a;\ c\in a:\quad \sum_{\boldsymbol{\sigma}_a} b_a(\boldsymbol{\sigma}_a)=1,\quad b_{ac}(\sigma_{ac})=\sum_{\boldsymbol{\sigma}_a\setminus\sigma_{ac}} b_a(\boldsymbol{\sigma}_a)$$

$$\Rightarrow \min_b F \Rightarrow \text{Belief-Propagation Equations: } \left.\frac{\delta F}{\delta b}\right|_{\text{constr.}} = 0$$

Belief-Propagation as an approximation: iterative $\Rightarrow$ Gallager '61; MacKay '98

- Exact on a tree
- Trading optimality for reduction in complexity: $\sim 2^L \to \sim L$
- (BP = solving equations on the graph) $\neq$ (Message Passing = iterative BP)
- Convergence of MP to minimum of Bethe Free energy can be enforced
- $Z_{BP} \gtrless Z_{\text{exact}}$: BP is not a truly variational substitution ($\sum_{\boldsymbol{\sigma}} b(\boldsymbol{\sigma}) = 1$ is not guaranteed)

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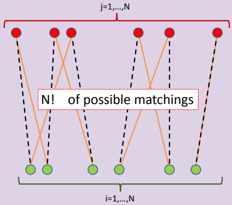
Learning via Statistical Inference

Two images



And after all we actually don't need matching.

Our goal is to LEARN THE FLOW.

Particle Image Velocimetry & Lagrangian Particle Tracking [standard solution]

- Take snapshots often = Avoid trajectory overlap
- Consequence = A lot of data
- Gigabit/s to monitor a two-dimensional slice of a $10cm^3$ experimental cell with a pixel size of $0.1mm$ and exposition time of $1ms$
- Still need to "learn" velocity (diffusion) from matching

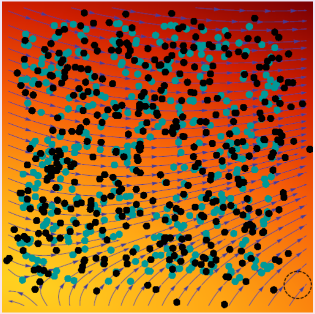
New twist

- Take fewer snapshots = Let particles overlap
- Put extra efforts into Learning/Inference
- Use the turbulence/physics community knowledge of Lagrangian evolution
- Focus on learning (rather than matching)

Inference & Learning by Passing Messages Between Images

- PNAS 10.1073/pnas.0910994107, MC, L.Kroc, F. Krzakala, L. Zdeborova, M. Vergassola

- Observe N identical particles in consequential images, $\mathbf{x} = (x_a^{(i)} | a = 1, \cdots, N; i = 1, 2)$
- Have a low parametric model for the probability of a particle to travel from $x_a^{(1)}$ to $x_b^{(2)}$: $p_{ab} = f(x_a^{(1)}, x_b^{(2)}; \lambda)$
- Maximum Likelihood estimator is the permanent: $\mathcal{P}(\mathbf{x}|\lambda) = \sum_{\boldsymbol{\sigma}} \mathcal{P}(\boldsymbol{\sigma}, \mathbf{x}|\lambda) = \text{perm}(p)$
- Optimal Learning: $\arg\max_\lambda \text{perm}(p)$



- Max-Product is exact for max perfect matching [Bayati, Shah, Sharma 2006]
- Other encouraging experiments with BP for permanents [Huang, Jebara 2009]

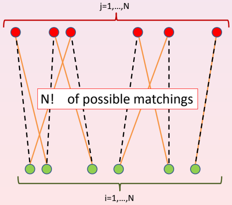
Permanent as Counting over a Graphical Model

$$\mathrm{perm}(\mu) = \underbrace{\sum_{\pi\in S_N} \mu_{a\pi(a)}}_{\text{sum over permutations}} = \overbrace{\sum_{\boldsymbol{\sigma}} \prod_{a\in\mathcal{G}_0^{(\mathrm{N}\times\mathrm{N})}} f_a^{\mathrm{dimer}}(\boldsymbol{\sigma}_a)}^{\text{partition function of a GM}}$$

$$\forall a\in\mathcal{G}_0^{(\mathrm{N}\times\mathrm{N})}: \quad f_a^{\mathrm{dimer}}(\boldsymbol{\sigma}_a) = \begin{cases} \sum_{b\sim a}\mu_{ab}\sigma_{ab}, & \sum_{b\sim a}\sigma_{ab}=1; \\ 0, & \sum_{b\sim a}\sigma_{ab}\neq 1; \end{cases}$$

$$\boldsymbol{\sigma} = (\sigma_{ab}=0,1|\{a,b\}\in\mathcal{G}^{(\mathrm{N}\times\mathrm{N})})$$
$$\forall a\in\mathcal{G}_0^{(\mathrm{N}\times\mathrm{N})}: \quad \boldsymbol{\sigma}_a = (\sigma_{ab}=0,1|b\sim a)$$

$\mathcal{G}^{(\mathrm{N}\times\mathrm{N})} = (\mathcal{G}_0^{(\mathrm{N}\times\mathrm{N})}, \mathcal{G}_1^{(\mathrm{N}\times\mathrm{N})})$ is the bi-partite graph



Bethe Free Energy for Permanents

$$\mathcal{F}^{(BP)}_{\text{perm}}(\beta) = -\sum_{\{a,b\}} \beta_{ab}\log(\mu_{ab}) + \sum_{\{a,b\}} \left(\beta_{ab}\log(\beta_{ab}) - (1-\beta_{ab})\log(1-\beta_{ab})\right)$$

$$\mathcal{D}_{\text{perm}} = \left(\beta = (\beta_{ab}\in[0;1] | \{a,b\}\in\mathcal{G}_0^{(N\times N)}) \middle| \forall a: \quad \sum_{b\sim a}\beta_{ab} = 1\right)$$

Convexity of the Bethe Free Energy [Vontobel 2011]

$\mathcal{F}^{(BP)}_{\text{perm}}(\beta)$ is convex over $\mathcal{D}_{\text{perm}}$

Belief Propagation Equations

$$\forall a: \quad \sum_{b\sim a}\beta^{(BP)}_{ab} = 1, \quad \forall\{a,b\}: \quad \beta^{(BP)}_{ab}(1-\beta^{(BP)}_{ab}) = \frac{\mu_{ab}}{u_a u_b}$$

- u_a are potentials=Lagrangian multipliers

Loop Series for Permanents (in three ways)

- assuming $\beta^{(BP)}$ lies in the interior of $\mathcal{D}_{\text{perm}}$

sum over generalized loops [Loop Calculus of MC, V. Chernyak '06]

$$\frac{\text{perm}(\mu)}{Z^{(BP)}_{\text{perm}}} = 1 + \sum_{\alpha\in\Upsilon_{\text{perm}}} \left(\prod_{a\in\alpha_0}(1-q_a(\alpha))\right)\left(\prod_{\{a,b\}\in\alpha_1}\frac{\beta^{(BP)}_{ab}}{1-\beta^{(BP)}_{ab}}\right)$$

mixed derivative

$$\frac{\text{perm}(\mu)}{Z^{(BP)}_{\text{perm}}} = \prod_a \frac{\partial}{\partial\eta_a}\left(e^{\sum_a\eta_a}\left(\prod_{\{a,b\}}\left(1+e^{-\eta_a-\eta_b}\frac{\beta^{(BP)}_{ab}}{1-\beta^{(BP)}_{ab}}\right)\right)\right)\Bigg|_{\eta\to 0}$$

perm=BP*perm [Y. Watanabe, MC '09]

$$\frac{\text{perm}(\mu)}{Z^{(BP)}_{\text{perm}}} = \frac{\text{perm}\left(\beta^{(BP)}.*(1-\beta^{(BP)})\right)}{\prod_{\{a,b\}}(1-\beta^{(BP)}_{ab})}$$

- follows directly from the BP Eqs.
- can also be derived from LS

Fractional BP for Permanents

[A.Yedidia and MC 2011]

Bethe Free Energy for permanents $\gamma \in [-1;1]$

$$\mathcal{F}^{(\gamma)}_{\text{perm}}(\beta) = -\sum_{\{a,b\}} \beta_{ab} \log \mu_{ab} + \sum_{\{a,b\}} \left(\beta_{ab} \log(\beta_{ab}) + \gamma(1-\beta_{ab}) \log(1-\beta_{ab})\right)$$

- $\beta^{(\gamma)} = \arg\min_{\beta \in \mathcal{D}_{\text{perm}}} \mathcal{F}^{(\gamma)}_{\text{perm}}(\beta)$
- BP: $\gamma = -1$; MF: $\gamma = 1$

- Fractional BP of [Yedidia, Freeman, Weiss 2005] for permanents
- only modify coefficients (FBP), not regions (would be GBP than)

Fractional BP equations: β is non-negative double stochastic +

$$\forall \{a,b\}: \quad \frac{\beta^{(\gamma)}_{ab}}{(1-\beta^{(\gamma)}_{ab})^{\gamma}} = \frac{\mu_{ab}}{u_a u_b}$$

- $\gamma > 0$: $\beta^{(\gamma)}$ is in the interior of $\mathcal{D}_{\text{perm}}$
- $\gamma \le 0$: $\beta^{(\gamma)}$ may be on the boundary of $\mathcal{D}_{\text{perm}}$
- $\beta^{(\gamma)}$ is on the boundary $\Rightarrow$ the sub-set of $\beta_{ab} = 1$ forms a partial perfect matching
- $\mu \to \mu^{1/T}$, $T > 0 \Rightarrow \exists T_c > 0$ such that at $0 < T < T_c$, $\beta^{(\gamma)}$ is a perfect matching (full or partial)
- $\mathcal{F}^{(\gamma)}_{\text{perm}}(\beta^{(\gamma)})$ is continuous in γ, decreases monotonically with γ increase

perm=FBP*perm and Bounds [A. Yedidia and MC 2011]

perm=FBP*perm: assuming $\beta^{(\gamma)}$ lies in the interior of $\mathcal{D}_{\text{perm}}$

$$\frac{\text{perm}(\mu)}{Z^{(\gamma)}_{\text{perm}}} = \text{perm}\left(\beta^{(\gamma)}./(1-\beta^{(\gamma)})^{\gamma}\right)\left(\prod_{\{a,b\}}(1-\beta^{(\gamma)}_{ab})^{\gamma}\right)$$

- follows directly from the FBP Eqs.

Sandwich Inequality

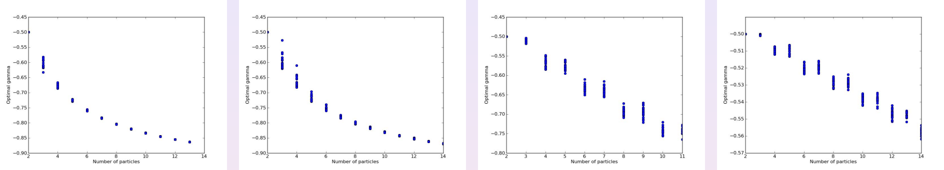
$$Z^{(\text{BP})}_{\text{perm}} = Z^{(\gamma=-1)}_{\text{perm}} =\leq \text{perm}(\mu) \leq Z^{(\gamma=0)}_{\text{perm}}$$

- $\text{perm}(\mu) \geq Z^{(\gamma=-1)}_{\text{perm}} \Leftarrow$ Gurvits 2011. For $\beta^{(\gamma)}$ in the interior, follows from perm=BP*perm + [Schrijver 1998]: $\text{perm}(\beta.*(1-\beta)) \leq \prod_{\{a,b\}}(1-\beta_{ab})$
- $\text{perm}(\mu) \leq Z^{(\gamma=0)}_{\text{perm}}$ follows from the perm=FBP*perm at $\gamma=0$ + $\text{perm}(\beta)\leq 1$ if β is non-negative, double-stochastic.

Upper Bound Conjecture by Gurvits 2011

- (translated to our language) $Z^{(\gamma=-1/2)}_{\text{perm}}$ gives the upper-bound, achieved at μ which is block-diagonal $= 2\times 2$ blocks of $1/2$
- The conjecture was confirmed in ▸ our simulations, even though for many random ensembles the $Z^{(\gamma=-1/2)}_{\text{perm}}$ is a serious overshoot

Experiments with Permanents



- $[0;1]$ uniform, "$\exp -1$" (exponential distributed), $[0;1/20]$-shifted and $[0;1/2000]$-shifted (random around the "Gurvits" matrix $=2\times 2$ blocks of $1/2$) ensembles. Full (small) matrix.
- Compared with exact (Zero-suppressed Decision Diagrams)
- Optimal γ vs $\#$ of particles (size of the matrix) is shown

Perm=FBP*Perm

Conclusions

- Fractional BP with a properly tuned parameter is well behaved (convex, monotone)
- It "sandwiches" the permanent well
- It allows exact Perm $=$ FBP $*$ Perm relation

Path Forward

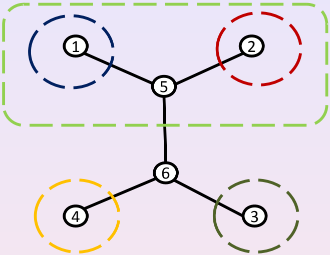
- How to find optimal (or just good enough) value of the fractional parameter?
- Is the fractional parameter "locked" for interesting ensembles?
- Does Perm $=$ FBP $*$ Perm allow a loop interpretation?
- More general matchings (bi-matchings, paths, clusters, etc)
- Generalized BP $=$ introduce regions in addition to massaging entropy (Fractional BP)
- Learning (mixed optimization, counting $+$) with FBP & GBP

Complexity & Algorithms

- How many operations are required to evaluate a graphical model of size N?
- What is the exact algorithm with the least number of operations?
- If one is ready to trade optimality for efficiency, what is the best (or just good) approximate algorithm he/she can find for a given (small) number of operations?
- Given an approximate algorithm, how to decide if the algorithm is good or bad? What is the measure of success?
- How one can systematically improve an approximate algorithm?

- Linear (or Polynomial) in N is EASY, Exponential is DIFFICULT

BP is Exact on a Tree — Bethe '35, Peierls '36



$$Z_{51}(\sigma_{51}) = f_1(\sigma_{51}), \quad Z_{52}(\sigma_{52}) = f_2(\sigma_{52}),$$
$$Z_{63}(\sigma_{63}) = f_3(\sigma_{63}), \quad Z_{64}(\sigma_{64}) = f_4(\sigma_{64})$$
$$Z_{65}(\sigma_{56}) = \sum_{\boldsymbol{\sigma}_5 \setminus \sigma_{56}} f_5(\boldsymbol{\sigma}_5) Z_{51}(\sigma_{51}) Z_{52}(\sigma_{52})$$
$$Z = \sum_{\boldsymbol{\sigma}_6} f_6(\boldsymbol{\sigma}_6) Z_{63}(\sigma_{63}) Z_{64}(\sigma_{64}) Z_{65}(\sigma_{65})$$

$$Z_{ba}(\sigma_{ab}) = \sum_{\boldsymbol{\sigma}_a \setminus \sigma_{ab}} f_a(\boldsymbol{\sigma}_a) Z_{ac}(\sigma_{ac}) Z_{ad}(\sigma_{ad}) \Rightarrow Z_{ab}(\sigma_{ab}) = A_{ab} \exp(\eta_{ab}\sigma_{ab})$$

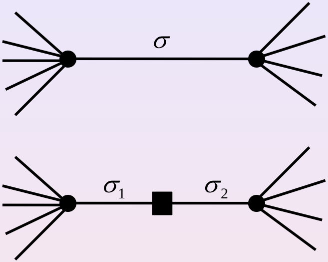
Belief Propagation Equations

$$\sum_{\boldsymbol{\sigma}_a} f_a(\boldsymbol{\sigma}_a) \exp\Big(\sum_{c\in a} \eta_{ac}\sigma_{ac}\Big) \left(\sigma_{ab} - \tanh\left(\eta_{ab} + \eta_{ba}\right)\right) = 0$$

e.g. Thouless-Anderson-Palmer (1977) Eqs.

Bethe Approximation

Local Gauge Freedom [preamble]



$\forall \sigma_1, \sigma_2 = \pm 1, \quad \forall \eta_1, \eta_2 \in \mathcal{C}$

$$\delta(\sigma_1, \sigma_2) = \frac{1 + \sigma_1\sigma_2}{2} \text{ [substitution]}$$

$$= \frac{\exp\left(\eta_1\sigma_1 + \eta_2\sigma_2\right)}{2\cosh(\eta_1 + \eta_2)} \left(1 + \sigma_1\sigma_2 \exp\left(-(\eta_1 + \eta_2)(\sigma_1 + \sigma_2)\right)\right)$$

Dance in Turbulence [movie]

Learn the flow from tracking particles

Direct Derivation of LS for Permanent from BP-Eqs.

$$\underbrace{\forall a: \quad \sum_{b\sim a} \beta_{ab}^{(BP)} = 1 \ (*), \quad \forall \{a,b\}: \quad \beta_{ab}^{(BP)}(1-\beta_{ab}^{(BP)}) = \frac{\mu_{ab}}{u_a u_b} \ (**)}$$

$\sum_{\{a,b\}} \beta_{ab}^{(BP)} \log(\text{Eq.}(**)) \Rightarrow$

$$\sum_{\{a,b\}} \beta_{ab}^{(BP)} \log(u_a u_b) = \sum_a \log(u_a)$$

$$= \sum_{\{a,b\}} \left(\beta_{ab}^{(BP)} \log(\mu_{ab}/\beta_{ab}^{(BP)}) - \beta_{ab}^{(BP)} \log(1-\beta_{ab}^{(BP)})\right)$$

$$= \log(Z_{\text{perm}}^{(BP)}) - \sum_{\{a,b\}} \log(1-\beta_{ab}^{(BP)})$$

$\text{perm}(\text{Eq.}(**)) \Rightarrow$

$$\text{perm}(\mu) = \text{perm}(\beta^{(BP)} .* (1-\beta^{(BP)})) \prod_a u_a$$

Combining $\Rightarrow$

$$\frac{\text{perm}(\mu)}{Z_{\text{perm}}^{(BP)}} = \frac{\text{perm}\left(\beta^{(BP)} .* (1-\beta^{(BP)})\right)}{\prod_{\{a,b\}}(1-\beta_{ab}^{(BP)})},$$

Perm=BP*Perm

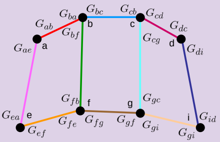
Outline

BP does not account for Loops

Questions:

- Is BP just a heuristic in a loopy case?
- Why does it (often) work so well?
- Does exact inference allow an expression in terms of BP?
- Can one correct BP systematically?

Local Gauge, G, Transformations — Chertkov, Chernyak '06



$$Z=\sum_{\boldsymbol{\sigma}}\prod_a f_a(\boldsymbol{\sigma}_a),\ \ \boldsymbol{\sigma}_a=(\sigma_{ab},\sigma_{ac},\cdots)$$

$\sigma_{ab}=\sigma_{ba}=\pm 1$; allows generalization to q-ary case

$$f_a(\boldsymbol{\sigma}_a=(\sigma_{ab},\cdots))\to \sum_{\sigma'_{ab}} G_{ab}(\sigma_{ab},\sigma'_{ab})\, f_a(\sigma'_{ab},\cdots)$$

$$\sum_{\sigma_{ab}} G_{ab}(\sigma_{ab},\sigma')G_{ba}(\sigma_{ab},\sigma'')=\delta(\sigma',\sigma'')$$

The G-gauge Invariance! [global]

$$Z=\sum_{\boldsymbol{\sigma}}\prod_a f_a(\boldsymbol{\sigma}_a)=\sum_{\boldsymbol{\sigma}}\prod_a\left(\sum_{\boldsymbol{\sigma}'_a} f_a(\boldsymbol{\sigma}'_a)\prod_{b\in a} G_{ab}(\sigma_{ab},\sigma'_{ab})\right)$$

Reminiscent of

- Re-parametrizations [pairwise models] of Wainwright, Jaakola, Willsky '03 [term by term]
- Holographic Transformations of Valiant '03 [global]

Belief Propagation as a Gauge Fixing

Chertkov, Chernyak '06

$$Z=\sum_{\boldsymbol{\sigma}}\prod_a f_a(\boldsymbol{\sigma}_a)=\sum_{\boldsymbol{\sigma}}\prod_a\left(\sum_{\boldsymbol{\sigma}'_a} f_a(\boldsymbol{\sigma}'_a)\prod_{b\in a} G_{ab}(\sigma_{ab},\sigma'_{ab})\right)$$

$$Z=\underbrace{Z_0(G)}_{\substack{\text{ground state}\\ \boldsymbol{\sigma}=+\mathbf{1}}}+\underbrace{\sum_{\text{all possible colorings of the graph}} Z_c(G)}_{\boldsymbol{\sigma}\neq+\mathbf{1},\quad \text{excited states}}$$

Belief Propagation Gauge $\forall a\ \&\ \forall b\in a:$

$$\sum_{\boldsymbol{\sigma}'_a} f_a(\boldsymbol{\sigma}')G^{(bp)}_{ab}(\sigma_{ab}=-1,\sigma'_{ab})\prod_{c\in a}^{c\neq b} G^{(bp)}_{ac}(+1,\sigma'_{ac})=0$$

No loose BLUE=colored edges at any vertex of the graph!

Belief Propagation as a Gauge Fixing (II)

$\forall a \;\&\; \forall b \in a:$

$$\left\{\begin{array}{l}\sum\limits_{\boldsymbol{\sigma}'_a} f_a(\boldsymbol{\sigma}') G^{(bp)}_{ab}(-1,\sigma'_{ab}) \prod\limits_{c\in a}^{c\neq b} G^{(bp)}_{ac}(+1,\sigma'_{ac}) = 0\\ \sum_{\sigma_{ab}} G_{ab}(\sigma_{ab},\sigma') G_{ba}(\sigma_{ab},\sigma'') = \delta(\sigma',\sigma'')\end{array}\right. \Rightarrow \left\{\begin{array}{l} G^{(bp)}_{ba}(+1,\sigma'_{ab}) = \rho_a^{-1} \overbrace{\sum\limits_{\boldsymbol{\sigma}'_a\setminus\sigma'_{ab}} f_a(\boldsymbol{\sigma}') \prod\limits_{c\in a}^{c\neq b} G^{(bp)}_{ac}(+1,\sigma'_{ac})}^{sum-product}\\ \rho_a = \sum\limits_{\boldsymbol{\sigma}'_a} f_a(\boldsymbol{\sigma}') \prod\limits_{c\in a} G^{(bp)}_{ac}(+1,\sigma'_{ac})\end{array}\right.$$

Belief Propagation in terms of Messages

$$G^{(bp)}_{ab}(+1,\sigma) = \frac{\exp(\sigma\eta_{ab})}{\sqrt{2\cosh(\eta_{ab}+\eta_{ba})}}, \quad G^{(bp)}_{ab}(-1,\sigma) = \sigma\frac{\exp(-\sigma\eta_{ba})}{\sqrt{2\cosh(\eta_{ab}+\eta_{ba})}} \Longrightarrow$$

$$\sum_{\boldsymbol{\sigma}_a} f_a(\boldsymbol{\sigma}_a)\exp\left(\sum_{c\in a}\sigma_{ac}\eta_{ac}\right)\left(\sigma_{ab}-\tanh\left(\eta_{ab}+\eta_{ba}\right)\right) = 0$$

$$b^{(G)}_a(\boldsymbol{\sigma}_a) = \frac{f_a(\boldsymbol{\sigma}_a)\prod\limits_{b\sim a} G_{ab}(0,\sigma_{ab})}{\sum_{\boldsymbol{\sigma}_a} f_a(\boldsymbol{\sigma}_a)\prod_{b\sim a} G_{ab}(0,\sigma_{ab})}, \quad b^{(G)}_{ab}(\sigma_{ab}) = G_{ab}(0,\sigma_{ab})G_{ba}(0,\sigma_{ab})$$

Variational Principle and Gauge Fixing

$$Z=\underbrace{Z_0(G)}_{\sigma=+1}+\sum_{\sigma\neq+1} Z_c(G),\quad Z_0(G)\Rightarrow \underbrace{Z_0(\epsilon),\quad \epsilon_{ab}(\sigma_{ab})=G_{ab}(+1,\sigma_{ab})}_{\text{depends only on the ground state gauges}}$$

"Variational" formulation of Belief Propagation

$$\left.\frac{\partial Z_0(\epsilon)}{\partial \epsilon_{ab}(\sigma_{ab})}\right|^{(bp)}=0 \quad\Leftrightarrow\quad \text{Belief Propagation Equations}$$

$\mathcal{F}_0(\epsilon)=-\ln Z_0(\epsilon)$ is the Bethe Free Energy
of *Yedidia, Freeman, Weiss '01*

Third Way [Wainwright, Jaakola, Willsky '03]

Re-parametrization = Substitution

$$\forall \boldsymbol{\sigma}: \quad \prod_a f_a(\boldsymbol{\sigma}_a) = Z^{(G)}(\mathbf{0}) \left(\prod_{\{a,b\}} b_{ab}^{(G)}(\sigma_{ab})\right) \prod_a \left(\frac{b_a^{(G)}(\boldsymbol{\sigma}_a)}{\prod_{b\sim a} b_{ab}^{(G)}(\sigma_{ab})}\right)$$

$$Z = \sum_{\boldsymbol{\sigma}} \prod_a f_a(\boldsymbol{\sigma}_a) = Z^{(G)}(\mathbf{0}) \mathbb{E}_{\text{edge}} \left[\prod_a \left(\frac{b_a^{(G)}(\boldsymbol{\sigma}_a)}{\prod_{b\sim a} b_{ab}^{(G)}(\sigma_{ab})}\right)\right]$$

$$b_{\text{edge}}^{(G)}(\boldsymbol{\sigma}) = \prod_{\{a,b\}} b_{ab}^{(G)}(\sigma_{ab})$$

From General Reparametrization/Gauge to BP

$$\forall a,\ \forall b \sim a,\ \forall \sigma_{ab}: \quad \sum_{\boldsymbol{\sigma}_a \setminus \sigma_{ab}} b_a^{(BP)}(\boldsymbol{\sigma}_a) = b_{ab}^{(BP)}(\sigma_{ab})$$

my interpretation of [Sudderth, Wainwright, Willsky '09]

General Remarks

- Gauge Fixing and Re-parametrization are equivalent over the binary MRF (variables on vertices, pair-wise interaction)
- q-ary generalizations are different
- ... suggest Loop Series for the Partition Function ⇒

Loop Series:

Chertkov,Chernyak '06

Exact (!!) expression in terms of BP

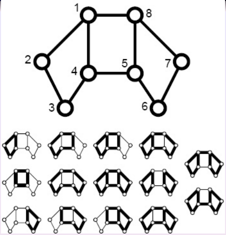
$$Z = \sum_{\boldsymbol{\sigma}_\sigma} \prod_a f_a(\boldsymbol{\sigma}_a) = Z_0 \left(1 + \sum_C r(C)\right)$$

$$r(C) = \frac{\prod_{a \in C} \mu_a}{\prod_{(ab) \in C} (1 - m_{ab}^2)} = \prod_{a \in C} \tilde{\mu}_a$$

$C \in$ Generalized Loops $=$ sub-graphs without loose ends

$$m_{ab} = \sum_{\boldsymbol{\sigma}_a} b_a^{(bp)}(\boldsymbol{\sigma}_a)\sigma_{ab}$$

$$\mu_a = \sum_{\boldsymbol{\sigma}_a} b_a^{(bp)}(\boldsymbol{\sigma}_a) \prod_{b \in a, C} (\sigma_{ab} - m_{ab})$$



- The Loop Series is finite
- All terms in the series are calculated within BP
- BP is exact on a tree
- BP is a Gauge fixing condition [Valiant talk]. Other choices of Gauges would lead to different representations.
- LS is a generalization of "high-temperature" expansion [Jerrum talk].

Have been busy since ...

- Heuristics based on Loop Series for Improving BP (Graphical Codes) [MC, Chernyak '06-'08]
- Loop Tower (Loop Series beyond binary) [Chernyak, MC '07]
- Estimating Corrections to BP via Loop Series. Counting Independent Sets [Chandrasekaran, MC, Gamarnik, Shah, Shin '09]
- There are other interesting choices of Gauges. Matching and Fermion Models (new relations). [Chernyak, MC '08]
- Planar and Surface GM which are Easy [Chernyak, MC '08 + Chernyak, MC, Loebl in progress]
- Orbit Products for Gaussian GM (det=BP*det) [Johnson, Chernyak, MC '09-]
- The Story of Permanent [MC, Kroc, Krzakala, Vergassola, Zdeborova '08-'11] + [Watanabe, MC '10] + [A.Yedidia, MC '11]