



Statistical Inference with Gauges, Loops and Fermions

Michael Chertkov

Center for Nonlinear Studies & Theory Division, LANL

Oct 15, 2008

Princeton

The talk is based on joint papers with V. Chernyak (Wayne State, Detroit)

Outline

1 Intro: Graphical Models & Belief Propagation

- Examples (Physics, IT, CS)
- Bethe Free Energy & Belief Propagation (approx)

2 Loop Calculus: Exact Inference with BP

- Loops ... Questions
- Gauge Transformations and BP
- Loop Series

3 Determinants, Fermions & Loops

- Grassmanns, Determinant, Belief Propagation & Loop Series
- Monomer-Dimer Model, Cycles and Determinants

4 Future Challenges

Example (1): Statistical Physics

Ising model

$\sigma_i = \pm 1$

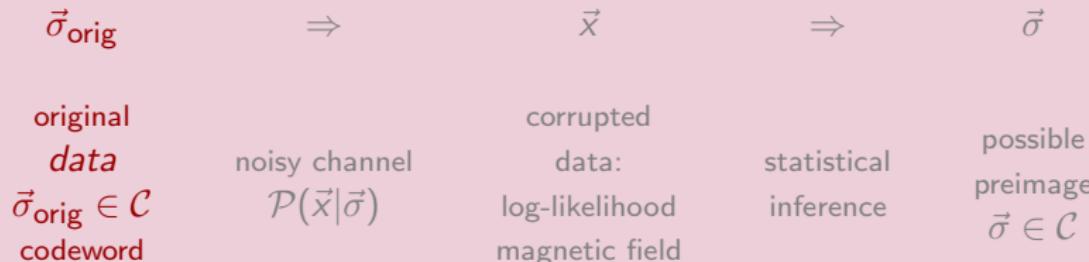
$$\mathcal{P}(\vec{\sigma}) = Z^{-1} \exp \left(\sum_{(i,j)} J_{ij} \sigma_i \sigma_j \right)$$

J_{ij} defines the graph (lattice)

- Ferromagnetic ($J_{ij} < 0$), Anti-ferromagnetic ($J_{ij} > 0$) or Frustrated/Glassy
- Magnetization (order parameter) and Ground State
- Thermodynamic Limit, $N \rightarrow \infty$
- Phase Transitions

Example (2): Information Theory, Machine Learning, etc

Probabilistic Reconstruction (Statistical Inference)



Maximum Likelihood [ground state]

Marginalization

$$\text{ML}(\vec{x}) = \arg \max_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$$

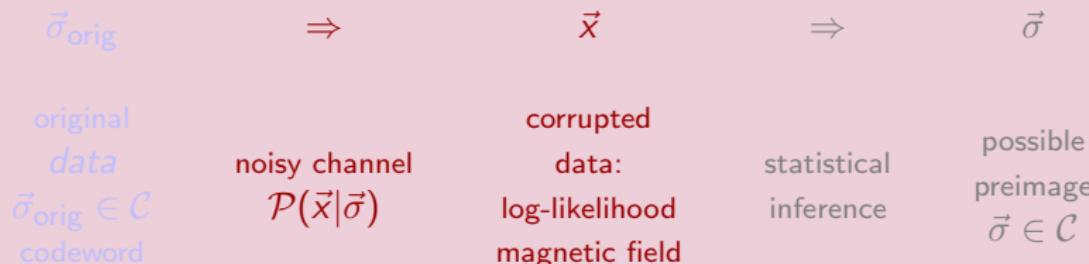
$$\sigma_i^*(\vec{x}) = \arg \max_{\sigma_i} \sum_{\vec{\sigma} \setminus \sigma_i} \mathcal{P}(\vec{x}|\vec{\sigma})$$

e.g., **decoding** in forward error correction



Example (2): Information Theory, Machine Learning, etc

Probabilistic Reconstruction (Statistical Inference)



Maximum Likelihood [ground state]

Marginalization

$$\text{ML}(\vec{x}) = \arg \max_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$$

$$\sigma_i^*(\vec{x}) = \arg \max_{\sigma_i} \sum_{\vec{\sigma} \setminus \sigma_i} \mathcal{P}(\vec{x}|\vec{\sigma})$$

e.g., **decoding** in forward error correction



Example (2): Information Theory, Machine Learning, etc

Probabilistic Reconstruction (Statistical Inference)



Maximum Likelihood [ground state]

Marginalization

$$\text{ML}(\vec{x}) = \arg \max_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$$

$$\sigma_i^*(\vec{x}) = \arg \max_{\sigma_i} \sum_{\vec{\sigma} \setminus \sigma_i} \mathcal{P}(\vec{x}|\vec{\sigma})$$

e.g., **decoding** in forward error correction



Example (2): Information Theory, Machine Learning, etc

Probabilistic Reconstruction (Statistical Inference)



Maximum Likelihood [ground state]

Marginalization

$$\text{ML}(\vec{x}) = \arg \max_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$$

$$\sigma_i^*(\vec{x}) = \arg \max_{\sigma_i} \sum_{\vec{\sigma} \setminus \sigma_i} \mathcal{P}(\vec{x}|\vec{\sigma})$$

e.g., **decoding** in forward error correction



Example (3): Combinatorial Optimization, K-SAT

$$F(\vec{x}) = \begin{aligned} & (x_1 \vee x_2 \vee \bar{x}_3) \wedge \\ & (x_5 \vee \bar{x}_1 \vee \bar{x}_4) \wedge \\ & (x_2 \vee x_7 \vee x_3) \wedge \\ & (\bar{x}_7 \vee x_5 \vee \bar{x}_5) \wedge \\ & \dots \end{aligned}$$

$1, 2, \dots, N$ – variables

$F(\vec{x})$ is a conjunction of M clauses

$x_i = 0$ (bad), 1(good)

\bar{x}_i is negation of x_i

\vee = OR \wedge = AND

\vec{x} is a “valid assignment” if $F(\vec{x}) = 1$

Probabilistic interpretation

$$P(\vec{x}) = Z^{-1} F(\vec{x}), \quad Z \equiv \sum_{\vec{x}} F(\vec{x})$$

- Finding a Valid Assignment, Counting Number of Assignments
- Graphical Representation, Sparseness
- Random, non-Random formulas
- SAT/UNSAT transition wrt $\alpha = M/N$, $M, N \rightarrow \infty$
- Focus on Algorithms for given finite instance

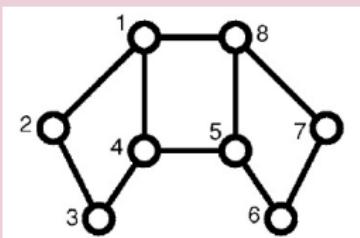


Graphical Models = The Language

Forney style - variables on the edges

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

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



$$f_a \geq 0$$

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

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

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

Objects of Interest

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



Complexity & Algorithms

- How many operations are required to calculate partition function, find a ground state, etc ... for 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 Algebraic) in N is EASY, Exponential is DIFFICULT

Easy & Difficult Problems

EASY

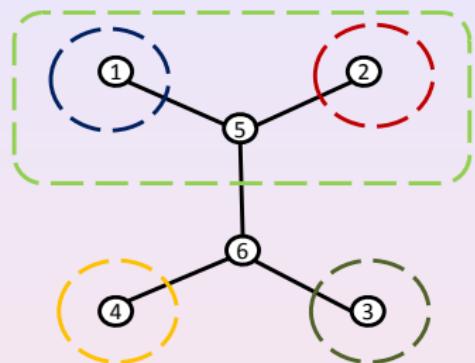
- Any graphical problems **on a tree** (Bethe-Pieirls, dynamical programming, belief propagation, and other names)
- Ground State of a Rand. Field Ferrom. Ising model on any graph
- Partition function of a planar Ising model
- Finding if 2-SAT is satisfiable
- Decoding over Binary Erasure Channel = XOR-SAT
- Some network flow problems (max-flow, min-cut, shortest path, etc)
- Minimal Perfect Matching Problem
- Some special cases of Integer Programming (TUM)

Typical graphical problem, **with loops** and factor functions of a general position, is **DIFFICULT**



BP is Exact on a Tree

Bethe '35, Peierls '36



$$Z_{15}(\sigma_{15}) = f_1(\sigma_{15}), \quad Z_{25}(\sigma_{25}) = f_2(\sigma_{25}),$$

$$Z_{36}(\sigma_{36}) = f_3(\sigma_{36}), \quad Z_{46}(\sigma_{46}) = f_4(\sigma_{46})$$

$$Z_{56}(\sigma_{56}) = \sum_{\vec{\sigma}_5 \setminus \sigma_{56}} f_5(\vec{\sigma}_5) Z_{15}(\sigma_{15}) Z_{25}(\sigma_{25})$$

$$Z = \sum_{\vec{\sigma}_6} f_6(\vec{\sigma}_6) Z_{36}(\sigma_{36}) Z_{46}(\sigma_{46}) Z_{56}(\sigma_{56})$$

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

Belief Propagation Equations

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



Variational Method in Statistical Mechanics

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

Exact Variational Principle

J.W. Gibbs 1903 (or earlier)

also known as Kullback-Leibler (1951) in CS and IT

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

$$\frac{\delta F}{\delta b(\vec{\sigma})} \Big|_{b(\vec{\sigma})=p(\vec{\sigma})} = 0 \quad \text{under} \quad \sum_{\vec{\sigma}} b(\vec{\sigma}) = 1$$

Variational Ansatz

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

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

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



Variational Method in Statistical Mechanics

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

Exact Variational Principle

J.W. Gibbs 1903 (or earlier)

also known as Kullback-Leibler (1951) in CS and IT

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

$$\frac{\delta F}{\delta b(\vec{\sigma})} \Big|_{b(\vec{\sigma})=p(\vec{\sigma})} = 0 \quad \text{under} \quad \sum_{\vec{\sigma}} b(\vec{\sigma}) = 1$$

Variational Ansatz

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

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

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



Bethe Free Energy: variational approach

(Yedidia, Freeman, Weiss '01 -

inspired by Bethe '35, Peierls '36)

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

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

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

Belief-Propagation as heuristics: iterative \Rightarrow Gallager '61; MacKay '98

- Exact on a tree
- Trading optimality for reduction in complexity: $\sim 2^L \rightarrow \sim L$
- (BP = solving equations on the graph) \neq (Message Passing = iterative BP)
- Convergence of MP to minimum of Bethe Free energy can be enforced
- $Z_{BP} \gtrless Z_{\text{exact}}$
- Relation to Linear Programming

Bethe Free Energy: variational approach

(Yedidia, Freeman, Weiss '01 -

inspired by Bethe '35, Peierls '36)

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

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

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

Belief-Propagation as heuristics: iterative \Rightarrow Gallager '61; MacKay '98

- Exact on a tree
- Trading optimality for reduction in complexity: $\sim 2^L \rightarrow \sim L$
- (BP = solving equations on the graph) \neq (Message Passing = iterative BP)
- Convergence of MP to minimum of Bethe Free energy can be enforced
- $Z_{BP} \gtrless Z_{\text{exact}}$
- Relation to Linear Programming

Outline

1 Intro: Graphical Models & Belief Propagation

- Examples (Physics, IT, CS)
- Bethe Free Energy & Belief Propagation (approx)

2 Loop Calculus: Exact Inference with BP

- Loops ... Questions
- Gauge Transformations and BP
- Loop Series

3 Determinants, Fermions & Loops

- Grassmanns, Determinant, Belief Propagation & Loop Series
- Monomer-Dimer Model, Cycles and Determinants

4 Future Challenges



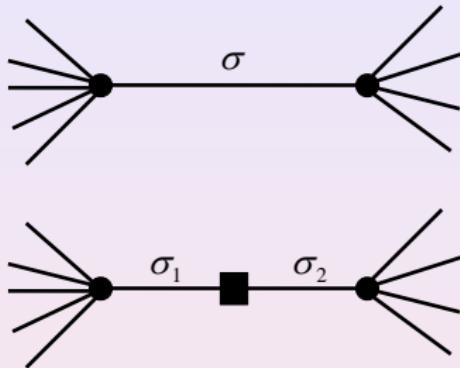
BP does not account for Loops

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 Freedom

[preamble]



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

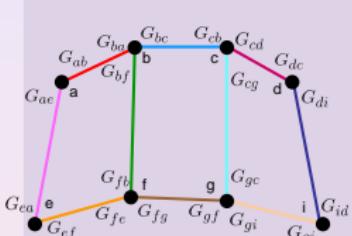
$$\begin{aligned} \delta(\sigma_1, \sigma_2) &= \frac{1 + \sigma_1 \sigma_2}{2} \\ &= \frac{\exp(\eta_1 \sigma_1 + \eta_2 \sigma_2)}{2 \cosh(\eta_1 + \eta_2)} (1 + \sigma_1 \sigma_2 \exp(-(\eta_1 + \eta_2)(\sigma_1 + \sigma_2))) \end{aligned}$$



Gauge Transformations

Chertkov, Chernyak '06

Local Gauge, G , Transformations



$$Z = \sum_{\vec{\sigma}} \prod_a f_a(\vec{\sigma}_a), \quad \vec{\sigma}_a = (\sigma_{ab}, \sigma_{ac}, \dots)$$

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

$$f_a(\vec{\sigma}_a = (\sigma_{ab}, \dots)) \rightarrow \sum_{\sigma'_{ab}} G_{ab}(\sigma_{ab}, \sigma'_{ab}) f_a(\sigma'_{ab}, \dots)$$

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

The partition function is invariant under any G -gauge!

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

Belief Propagation as a Gauge Fixing

Chertkov, Chernyak '06

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

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

Belief Propagation Gauge

$\forall a \text{ & } \forall b \in a :$

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

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

Belief Propagation as a Gauge Fixing (II)

$\forall a \text{ & } \forall b \in a :$

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

Belief Propagation in terms of **Messages**

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

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

$$b_a(\vec{\sigma}_a) = \frac{f_a(\vec{\sigma}_a) \exp \left(\sum_{b \in a} \sigma_{ab} \eta_{ab} \right)}{\sum_{\vec{\sigma}_a} f_a(\vec{\sigma}_a) \exp \left(\sum_{b \in a} \sigma_{ab} \eta_{ab} \right)}, \quad b_{ab}(\sigma) = \frac{\exp(\sigma(\eta_{ab} + \eta_{ba}))}{\sum_{\sigma} \exp(\sigma(\eta_{ab} + \eta_{ba}))}$$

Variational Principle and Gauge Fixing

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

Variational formulation of Belief Propagation

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

$\mathcal{F}_0(\epsilon) = -\ln Z_0(\epsilon)$ – Bethe Free Energy at the BP-extremum

General Remarks on Gauge Fixing

- Related to the Re-parametrization Framework of Wainwright, Jaakkola and Willsky '03
- Generalizable to q -ary alphabet Chernyak, Chertkov '07
- ... suggests Loop Series for the Partition Function \Rightarrow

Variational Principle and Gauge Fixing

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

Variational formulation of Belief Propagation

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

$\mathcal{F}_0(\epsilon) = -\ln Z_0(\epsilon)$ – Bethe Free Energy at the BP-extremum

General Remarks on Gauge Fixing

- Related to the Re-parametrization Framework of Wainwright, Jaakkola and Willsky '03
- Generalizable to q -ary alphabet Chernyak, Chertkov '07
- ... suggests Loop Series for the Partition Function \Rightarrow

Loop Series:

Exact (!!) expression in terms of BP

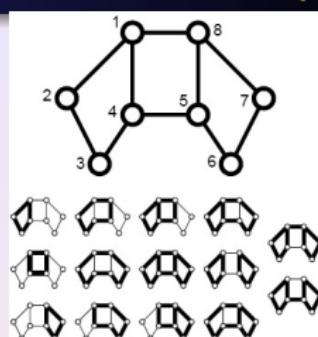
$$Z = \sum_{\vec{\sigma}} \prod_a f_a(\vec{\sigma}_a) = Z_0 \left(1 + \sum_C r(C) \right)$$

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

$C \in \text{Generalized Loops} = \text{Loops without loose ends}$

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

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



- The Loop Series is finite
 - All terms in the series are calculated **within BP**
 - BP is **exact** on a tree
 - Different series for different BP-extrema
 - Other (than BP) gauges lead to **other** representations
 - Generalizes **high-temperature** expansion

Loop Calculus & Related

- Improving Decoding of LDPC codes in the Error-floor regime [MC, Chernyak '06]
- Loop Corrections for Approximate Inference on Factor Graphs [Gómez, Mooij, Kappen '07]
- Low bound on Partition Function (Loop Series is positive): ordered state of FRFI [Sudderth, Wainwright, Willsky '08]
- Loop Calculus for Planar Problems [MC, Chernyak, Teodorescu '08]
- Counting and Learning in Matching
 - ▶ Tracking Particles in Fluid Experiment [MC, Kroc, Vergassola '08]
- Counting Independent Sets [Chandrasekar, Gamarnik, Shah '08 and Shin, MC, Shah '08]
- Determinants, Fermions and Loops ⇒

Outline

1 Intro: Graphical Models & Belief Propagation

- Examples (Physics, IT, CS)
- Bethe Free Energy & Belief Propagation (approx)

2 Loop Calculus: Exact Inference with BP

- Loops ... Questions
- Gauge Transformations and BP
- Loop Series

3 Determinants, Fermions & Loops

- Grassmanns, Determinant, Belief Propagation & Loop Series
- Monomer-Dimer Model, Cycles and Determinants

4 Future Challenges

Matrix and Monomer-Dimer Model

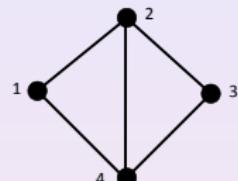
H : $N \times N$ matrix

$\mathcal{G}(H)$: nodes - $a \in \mathcal{G}_0$

undirected edges - $\{a, b\} \in \mathcal{G}_1$

directed edges - $(a, b) \in \mathcal{G}_1$

$$H = \begin{pmatrix} H_{11} & H_{12} & 0 & H_{14} \\ H_{21} & H_{22} & H_{23} & H_{24} \\ 0 & H_{32} & H_{33} & H_{34} \\ H_{41} & H_{42} & H_{43} & H_{44} \end{pmatrix}$$



Monomer-Dimer Model (on the same graph)

$$Z_{MD}(H) \equiv \sum_{\pi} \left(\prod_{a \in \mathcal{G}_0} w_a^{\pi_a} \right) \left(\prod_{\{a,b\} \in \mathcal{G}_1} w_{ab}^{\pi_{ab}} \right) \left(\prod_{a \in \mathcal{G}_0} \delta \left(\pi_a + \sum_{b \sim a} \pi_{ab}, 1 \right) \right)$$

$$\pi \equiv \pi_v \cup \pi_e, \quad \pi_v \equiv (\pi_a = 0, 1; a \in \mathcal{G}_0), \text{ and } \pi_e \equiv (\pi_{ab} = 0, 1; \{a, b\} \in \mathcal{G}_1)$$

$$w_{ab} \equiv -H_{ab}H_{ba} \text{ and } w_a \equiv H_{aa}$$

- Do $\det(H)$ and $Z_{MD}(H)$ have anything in common?
- Any relation to Loops and Belief Propagation?

Matrix and Monomer-Dimer Model

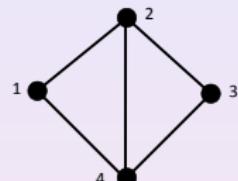
H : $N \times N$ matrix

$\mathcal{G}(H)$: nodes - $a \in \mathcal{G}_0$

undirected edges - $\{a, b\} \in \mathcal{G}_1$

directed edges - $(a, b) \in \mathcal{G}_1$

$$H = \begin{pmatrix} H_{11} & H_{12} & 0 & H_{14} \\ H_{21} & H_{22} & H_{23} & H_{24} \\ 0 & H_{32} & H_{33} & H_{34} \\ H_{41} & H_{42} & H_{43} & H_{44} \end{pmatrix}$$



Monomer-Dimer Model (on the same graph)

$$Z_{MD}(H) \equiv \sum_{\pi} \left(\prod_{a \in \mathcal{G}_0} w_a^{\pi_a} \right) \left(\prod_{\{a, b\} \in \mathcal{G}_1} w_{ab}^{\pi_{ab}} \right) \left(\prod_{a \in \mathcal{G}_0} \delta \left(\pi_a + \sum_{b \sim a} \pi_{ab}, 1 \right) \right)$$

$$\pi \equiv \pi_v \cup \pi_e, \quad \pi_v \equiv (\pi_a = 0, 1; a \in \mathcal{G}_0), \text{ and } \pi_e \equiv (\pi_{ab} = 0, 1; \{a, b\} \in \mathcal{G}_1)$$

$$w_{ab} \equiv -H_{ab}H_{ba} \text{ and } w_a \equiv H_{aa}$$

- Do $\det(H)$ and $Z_{MD}(H)$ have anything in common?
- Any relation to Loops and Belief Propagation?

Matrix and Monomer-Dimer Model

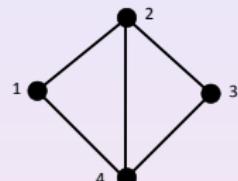
H : $N \times N$ matrix

$\mathcal{G}(H)$: nodes - $a \in \mathcal{G}_0$

undirected edges - $\{a, b\} \in \mathcal{G}_1$

directed edges - $(a, b) \in \mathcal{G}_1$

$$H = \begin{pmatrix} H_{11} & H_{12} & 0 & H_{14} \\ H_{21} & H_{22} & H_{23} & H_{24} \\ 0 & H_{32} & H_{33} & H_{34} \\ H_{41} & H_{42} & H_{43} & H_{44} \end{pmatrix}$$



Monomer-Dimer Model (on the same graph)

$$Z_{MD}(H) \equiv \sum_{\pi} \left(\prod_{a \in \mathcal{G}_0} w_a^{\pi_a} \right) \left(\prod_{\{a, b\} \in \mathcal{G}_1} w_{ab}^{\pi_{ab}} \right) \left(\prod_{a \in \mathcal{G}_0} \delta \left(\pi_a + \sum_{b \sim a} \pi_{ab}, 1 \right) \right)$$

$$\pi \equiv \pi_v \cup \pi_e, \quad \pi_v \equiv (\pi_a = 0, 1; a \in \mathcal{G}_0), \text{ and } \pi_e \equiv (\pi_{ab} = 0, 1; \{a, b\} \in \mathcal{G}_1)$$

$$w_{ab} \equiv -H_{ab}H_{ba} \text{ and } w_a \equiv H_{aa}$$

- Do $\det(H)$ and $Z_{MD}(H)$ have anything in common?
- Any relation to Loops and Belief Propagation?

Highlights of Results

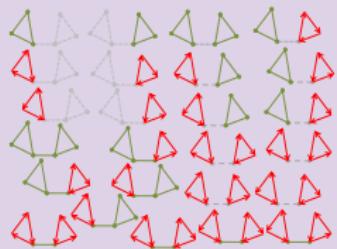
[Chernyak, Chertkov '08]

Loop Series for Determinant

$$\det(H) = Z_{\text{BP}} \left(1 + \sum_{C \in GL(\mathcal{G})} \sum_{C' \in ODC(C)} r(C, C') \right)$$

$GL(\mathcal{G})$ - set of generalized loops on \mathcal{G}
 $ODC(C)$ - set of oriented disjoint cycles on C
 $Z_{\text{BP}}, r(C, C')$ are expressed via BP solution

[BP gauge]

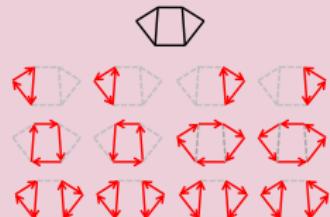


MD as Series of Determinants

[non-BP gauge]

$$Z_{\text{MD}} = \sum_{C \in ODC(\mathcal{G})} \bar{r}(C)$$

$$\bar{r}(C) = \det(H|_{\mathcal{G} \setminus C}) \prod_{(a,b) \in C} H_{ab}$$



Berezin/Grassman (super) Calculus

Berezin/Grassman (**anti-commuting**) Variables, Integrals

$$\{\bar{\theta}, \theta\} = \{\bar{\theta}_a, \theta_a\}_{a \in \mathcal{G}_0}, \quad a = 1, \dots, N$$

$$\forall a, b \in \mathcal{G}_0 : \quad \theta_a \theta_b = -\theta_b \theta_a, \quad \bar{\theta}_a \theta_b = -\theta_b \bar{\theta}_a, \quad \bar{\theta}_a \bar{\theta}_b = -\bar{\theta}_b \bar{\theta}_a$$

$$\text{Berezin measure : } \mathcal{D}\theta \mathcal{D}\bar{\theta} = \prod_{a \in \mathcal{G}_0} d\theta_a d\bar{\theta}_a$$

$$\forall a, b \in \mathcal{G}_0 : \quad \int \theta_a d\theta_a = \int \bar{\theta}_a d\bar{\theta}_a = 1, \quad \int d\theta_a = \int d\bar{\theta}_a = 0$$

... and Determinants

via Grassmanns on vertexes

$$\det H = \underbrace{\int \mathcal{D}\theta \mathcal{D}\bar{\theta} e^{S_0(\bar{\theta}, \theta)}}_{\text{Gaussian (fermi) Graphical Model}}, \quad S_0(\bar{\theta}, \theta) = \sum_{a \in \mathcal{G}_0} H_{aa} \bar{\theta}_a \theta_a + \sum_{a, b \in \mathcal{G}_0}^{a \sim b} H_{ab} \bar{\theta}_a \theta_b$$

$$\{\bar{\theta}, \theta\} = \{\bar{\theta}_a, \theta_a\}_{a \in \mathcal{G}_0} \text{ with } a = 1, \dots, N$$

via Grassmanns on edges

$$\det H = \left(\prod_{\{a, b\} \in \mathcal{G}_1} (H_{ab} H_{ba}) \right) \left(\prod_{a \in \mathcal{G}_0} H_{aa} \right) \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \prod_{a \in \mathcal{G}_0} f_a(\bar{\chi}_a, \chi_a) \prod_{\alpha \in \mathcal{G}_1} g_\alpha(\bar{\chi}_\alpha, \chi_\alpha)$$

$$g_\alpha(\bar{\chi}_\alpha, \chi_\alpha) = \exp((H_{ab})^{-1} \bar{\chi}_{ab} \chi_{ba} + (H_{ba})^{-1} \bar{\chi}_{ba} \chi_{ab}) \\ \alpha = \{a, b\}, \quad \chi_\alpha = \{\chi_{ab}, \chi_{ba}\}, \quad \bar{\chi}_\alpha = \{\bar{\chi}_{ab}, \bar{\chi}_{ba}\}$$

$$f_a(\bar{\chi}_a, \chi_a) = \exp\left(-(H_{aa})^{-1} \sum_{b \in \mathcal{G}_0}^{\sim a} \bar{\chi}_{ba} \sum_{b' \in \mathcal{G}_0}^{\sim a} \chi_{b'a}\right) \\ \chi_a = \{\chi_{ba}\}_{b \in \mathcal{G}_0, b \sim a}, \quad \bar{\chi}_a = \{\bar{\chi}_{ba}\}_{b \in \mathcal{G}_0, b \sim a}$$

Gauge Transformation

$$\det H = \left(\prod_{(a,b) \in \mathcal{G}_1} (H_{ab} H_{ba}) \right) \left(\prod_{a \in \mathcal{G}_0} H_{aa} \right) \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \prod_{a \in \mathcal{G}_0} f_a(\bar{\chi}_a, \chi_a) \prod_{\alpha \in \mathcal{G}_1} g_\alpha(\bar{\chi}_\alpha, \chi_\alpha)$$

$$g_\alpha(\bar{\chi}_\alpha, \chi_\alpha) = \exp \left(\frac{\bar{\chi}_{ab} \chi_{ba}}{H_{ab}} + \frac{\bar{\chi}_{ba} \chi_{ab}}{H_{ba}} \right)$$

γ is the local Gauge variable $\forall \alpha = \{a, b\} :$

$$g_\alpha(\gamma) = \underbrace{\frac{e^{\gamma_{ab} \bar{\chi}_{ab} \chi_{ab}} e^{\gamma_{ba} \bar{\chi}_{ba} \chi_{ba}} - H_{ab} H_{ba} \gamma_{ab} \gamma_{ba} e^{\frac{\bar{\chi}_{ab} \chi_{ab}}{H_{ab}} H_{ba} \gamma_{ba}} e^{\frac{\bar{\chi}_{ab} \chi_{ab}}{H_{ab}} H_{ba} \gamma_{ba}}}{1 - H_{ab} H_{ba} \gamma_{ab} \gamma_{ba}}}_{\text{ground state} = g_\alpha^{(0;\gamma)}} + \underbrace{\frac{\bar{\chi}_{ab} \chi_{ba}}{H_{ab}} + \frac{\bar{\chi}_{ba} \chi_{ab}}{H_{ba}}}_{\text{excited state} = g_\alpha^{(1;\gamma)}}$$

Determinant as a series – valid $\forall \gamma !!$

$$\det H = \sum_{\sigma} Z_{\sigma}^{(\gamma)}, \quad \sigma = (\sigma_{ab} = 0, 1 | \{a, b\} \in \mathcal{G}_1), \quad Z(\sigma)^{(\gamma)} \equiv$$

$$\left(\prod_{(a,b) \in \mathcal{G}_1} (H_{ab} H_{ba}) \right) \left(\prod_{a \in \mathcal{G}_0} H_{aa} \right) \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \prod_{a \in \mathcal{G}_0} f_a(\bar{\chi}_a, \chi_a) \prod_{\alpha \in \mathcal{G}_1} g_\alpha^{(\sigma_{ab}; \gamma)}(\bar{\chi}_\alpha, \chi_\alpha)$$



Belief Propagation (for fermi and bose)

$$\det H = \left(\prod_{(a,b) \in \mathcal{G}_1} (H_{ab} H_{ba}) \right) \left(\prod_{a \in \mathcal{G}_0} H_{aa} \right) \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \prod_{a \in \mathcal{G}_0} f_a(\bar{\chi}_a, \chi_a) \prod_{\alpha \in \mathcal{G}_1} g_\alpha(\bar{\chi}_\alpha, \chi_\alpha)$$

BP-fermi as γ -Gauge fixing

$$(a, b) \in \mathcal{G}_1 : \quad H_{ab} H_{ba} \gamma_{ba}^{(bp)} = H_{bb} - \sum_{a' \sim b}^{a' \neq a} (\gamma_{a'b}^{(bp)})^{-1}$$

- No loose-end constraints: $\forall a \in \mathcal{G}_0$ and $\{a, c\} \in \mathcal{G}_1$:

$$\int d\chi_a d\bar{\chi}_a f_a(\bar{\chi}_a, \chi_a) e^{\frac{\bar{\chi}_{ca} \chi_{ca}}{H_{ac} H_{ca} \gamma_{ac}}} \prod_{b \sim a}^{b \neq c} e^{\gamma_{ba} \bar{\chi}_{ba} \chi_{ba}} \Big|_{\gamma^{(bp)}} = 0$$

- Variational constraints:

$$\forall a \in \mathcal{G}_0 \text{ and } \{a, c\} \in \mathcal{G}_1 : \quad \frac{\partial Z_0}{\partial \gamma_{ca}} \Big|_{\gamma^{bp}} = 0, \quad Z_{BP;fermi} = Z_0(\gamma^{bp})$$

Belief Propagation (for fermi and bose)

$$\det H = \left(\prod_{(a,b) \in \mathcal{G}_1} (H_{ab} H_{ba}) \right) \left(\prod_{a \in \mathcal{G}_0} H_{aa} \right) \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \prod_{a \in \mathcal{G}_0} f_a(\bar{\chi}_a, \chi_a) \prod_{\alpha \in \mathcal{G}_1} g_\alpha(\bar{\chi}_\alpha, \chi_\alpha)$$

BP-fermi as γ -Gauge fixing

$$(a, b) \in \mathcal{G}_1 : H_{ab} H_{ba} \gamma_{ba}^{(bp)} = H_{bb} - \sum_{a' \sim b}^{a' \neq a} (\gamma_{a'b}^{(bp)})^{-1}$$

- No loose-end constraints: $\forall a \in \mathcal{G}_0$ and $\{a, c\} \in \mathcal{G}_1$:

$$\int d\chi_a d\bar{\chi}_a f_a(\bar{\chi}_a, \chi_a) e^{\frac{\bar{\chi}_{ca} \chi_{ca}}{H_{ac} H_{ca} \gamma_{ac}}} \prod_{b \sim a}^{b \neq c} \left. e^{\gamma_{ba} \bar{\chi}_{ba} \chi_{ba}} \right|_{\gamma^{(bp)}} = 0$$

- Variational constraints:

$$\forall a \in \mathcal{G}_0 \text{ and } \{a, c\} \in \mathcal{G}_1 : \left. \frac{\partial Z_0}{\partial \gamma_{ca}} \right|_{\gamma^{bp}} = 0, \quad Z_{BP;fermi} = Z_0(\gamma^{bp})$$

Gaussian (bose) Graphical Model

[normal c -number integrations]

$$(\det H)^{-1} = \int \prod_a \left(\frac{d\bar{\psi}_a d\psi_a}{2\pi} \right) \exp \left(-\frac{1}{2} \sum_{a \in \mathcal{G}_0} H_{aa} \bar{\psi}_a \psi_a + \sum_{a,b \in \mathcal{G}_0} H_{ab} \bar{\psi}_a \psi_b \right)$$

- BP for “bose” is equivalent to BP for “fermi”: $Z_{BP;fermi} Z_{BP;bose} = 1$

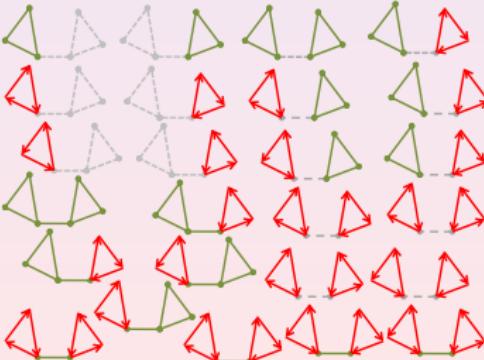
Loop Series for Determinant

$$\det(H) = Z_{BP; \text{fermi}} \left(1 + \sum_{C \in GL(\mathcal{G})} \sum_{C' \in ODC(C)} r(C, C') \right)$$

$GL(\mathcal{G})$ - set of generalized loops on \mathcal{G}

$ODC(C)$ - set of oriented disjoint cycles on C

Z_{BP} , $r(C, C')$ are expressed via BP solution



► Details for BP-fermi Loop series = ↪ ↤ ↥

Gauge Theory

$$\int \det(H(\sigma)) d\sigma = \text{Gauge Theory}$$

//

//

Monomer-Dimer

Disjoint Cycle
Series

Inversion of Det-Series
in a simple (non-BP) gauge

$$\forall (a, b) \in \mathcal{G}_1 : H_{ab}(\sigma) = \sigma_{ab} H_{ab}; \quad \forall a \in \mathcal{G}_0 : H_{aa}(\sigma) = H_{aa}$$
$$Z = 2^{-|\mathcal{G}_1|} \sum_{\sigma \in \mathcal{G}_1} \det(H(\sigma)) \equiv \int_{\mathcal{G}_1} \mathcal{D}\sigma \det(H(\sigma))$$

From Gauge Theory to Monomer-Dimer Model

From Graphical Gauge Model

$$Z = \int_{\mathcal{G}_1} \mathcal{D}\sigma \det(H(\sigma)) = \int_{\mathcal{G}_1} \mathcal{D}\sigma \int \mathcal{D}\theta \mathcal{D}\bar{\theta} \exp(S_0(\bar{\theta}, \theta; \sigma))$$

$$S_0(\bar{\theta}, \theta; \sigma) = \sum_{a \in \mathcal{G}_0} H_{aa} \bar{\theta}_a \theta_a + \sum_{\{a,b\} \in \mathcal{G}_1} \sigma_{ab} (H_{ab} \bar{\theta}_a \theta_b + H_{ba} \bar{\theta}_b \theta_a)$$

To Monomer-Dimer Model

$$Z = \int \mathcal{D}\theta \mathcal{D}\bar{\theta} \prod_{a \in \mathcal{G}_0} (1 + w_a \bar{\theta}_a \theta_a) \prod_{\{a,b\} \in \mathcal{G}_1} (1 + w_{ab} \bar{\theta}_a \theta_a \bar{\theta}_b \theta_b)$$

$$= Z_{MD} \equiv \sum_{\pi} \left(\prod_{a \in \mathcal{G}_0} w_a^{\pi_a} \right) \left(\prod_{\{a,b\} \in \mathcal{G}_1} w_{ab}^{\pi_{ab}} \right) \left(\prod_{a \in \mathcal{G}_0} \delta \left(\pi_a + \sum_{b \sim a} \pi_{ab}, 1 \right) \right)$$

$$\pi \equiv \pi_v \cup \pi_e, \quad \pi_v \equiv (\pi_a = 0, 1; a \in \mathcal{G}_0), \quad \pi_e \equiv (\pi_{ab} = 0, 1; \{a, b\} \in \mathcal{G}_1)$$

$$\forall (a, b) \in \mathcal{G}_1 : \quad w_{ab} = -H_{ab} H_{ba}; \quad \forall a \in \mathcal{G}_0 : \quad w_a = H_{aa}$$

From Gauge Theory to Determinants

From Graphical Gauge Model

$$\begin{aligned} Z &= \int_{\mathcal{G}_1} \mathcal{D}\sigma \int \mathcal{D}\theta \mathcal{D}\bar{\theta} \exp(\mathcal{S}_0(\bar{\theta}, \theta; \sigma)) \\ &= \int \mathcal{D}\theta \mathcal{D}\bar{\theta} \prod_{a \in \mathcal{G}_0} e^{w_a \bar{\theta}_a \theta_a} \prod_{\{a, b\} \in \mathcal{G}_1} \left(e^{H_{ab} \bar{\theta}_a \theta_b + H_{ba} \bar{\theta}_b \theta_a} - [H_{ab} \bar{\theta}_a \theta_b + H_{ba} \bar{\theta}_b \theta_a] \right) \end{aligned}$$

To Determinants

$$Z = \sum_{C \in \text{ODC}(\mathcal{G})} \bar{r}(C), \quad \bar{r}(C) = \det(H|_{\mathcal{G} \setminus C}) \prod_{(a,b) \in C} H_{ab}$$

Established expanding into sum over $[\dots]$, integrating and collecting H-monom

Monomer-Dimer Models and Determinants [Cycle Series]

Determinant as Series over MD on subgraphs [non-BP gauge]

$$\forall (a, b) \in \mathcal{G}_1 : \gamma_{ab} = \pm (H_{ab})^{-1} \quad [\text{no need to solve BP equations}]$$

Series over “odd” states

► Det as Series over non-BP gauges :

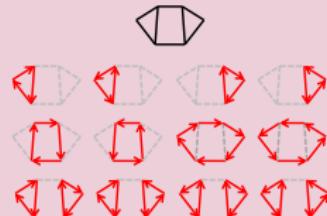
$$\det(H) = \sum_{C \in ODC(\mathcal{G})} r(C), \quad r(C) = (-1)^{|C|} \prod_{(a,b) \in C} H_{ab} Z_{MD}(\mathcal{G} \setminus C)$$

MD as Series of Determinants

[non-BP gauge]

$$Z_{MD} = \sum_{C \in ODC(\mathcal{G})} \bar{r}(C)$$

$$\bar{r}(C) = \det(H|_{\mathcal{G} \setminus C}) \prod_{(a,b) \in C} H_{ab}$$



Future Challenges (Loop Calculus +)

- Disorder Average, Relation to Cavity, Replica Calculations
- Efficient Approximate Algorithms
- Relation & Complementarity to MCMC, Mixing Time
- Phase Transitions in Glasses (Physics) and SAT (CS, IT)
- Dynamical Graphical Models (non-equilibrium)

Fermion-Gauge Approach

- Extension to Surface Graphs (embedded into surfaces with nonzero genus)
- Easy planar and surface models
- From loops,cycles to walks/paths (e.g. in relation with Walk-Sum and ζ -functions)
- Super-Symmetric (fermions and bosons) Graphical Models

My papers on ... (A)

Loop Calculus, Series, Tower

- M. CHERTKOV, *Exactness of Belief Propagation for Some Graphical Models with Loops*, JSTAT to appear, arxiv.org/abs/0801.0341
- V. CHERNYAK and M. CHERTKOV, "Loop Calculus and Belief Propagation for q -ary Alphabet: Loop Tower," *Proceedings of IEEE ISIT 2007*, June 2007, Nice, [arXiv:cs.IT/0701086](https://arxiv.org/abs/cs.IT/0701086).
- M. CHERTKOV and V. CHERNYAK, "Loop series for discrete statistical models on graphs," JSTAT/2006/P06009, [arXiv:cond-mat/0603189](https://arxiv.org/abs/cond-mat/0603189).
- M. CHERTKOV and V. CHERNYAK, "Loop Calculus in Statistical Physics and Information Science," *Phys. Rev. E*, **73**, 065102(R) (2006), [arXiv:cond-mat/0601487](https://arxiv.org/abs/cond-mat/0601487).

Loop Calculus for Graphical Codes

- M. CHERTKOV, "Reducing the Error Floor", invited talk at the *Information Theory Workshop '07 on "Frontiers in Coding"*, September 2-6, 2007.
- M. CHERTKOV and V. CHERNYAK, "Loop Calculus Helps to Improve Belief Propagation and Linear Programming Decodings of Low-Density-Parity-Check Codes," invited talk at *44th Allerton Conference*, September 27-29, 2006, Allerton, IL, [arXiv:cs.IT/0609154](https://arxiv.org/abs/cs.IT/0609154).

All papers are available at <http://cnls.lanl.gov/~chertkov/pub.htm>

My papers on ... (B)

Particle Tracking, BP and Loops

- M. CHERTKOV, L. KROC, M. VERGASSOLA, "Belief Propagation and Beyond for Particle Tracking", arXiv.org/abs/0806.1199.

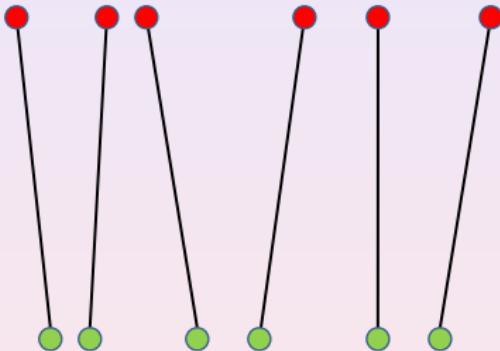
Fermions, Loops & Gauges, Planar & Surface Graphs

- V. CHERNYAK, M. CHERTKOV, "Fermions and Loops on Graphs. II. Monomer-Dimer Model as Series of Determinants", submitted to JSTAT, arXiv.org/abs/0809.3481.
- V. CHERNYAK, M. CHERTKOV, "Fermions and Loops on Graphs. I. Loop Calculus for Determinant", submitted to JSTAT, arXiv.org/abs/0809.3479.
- M. CHERTKOV, V. CHERNYAK, R. TEODORESCU, "Belief Propagation and Loop Series on Planar Graphs", JSTAT/2008/P05003, arxiv.org/abs/0802.3950.

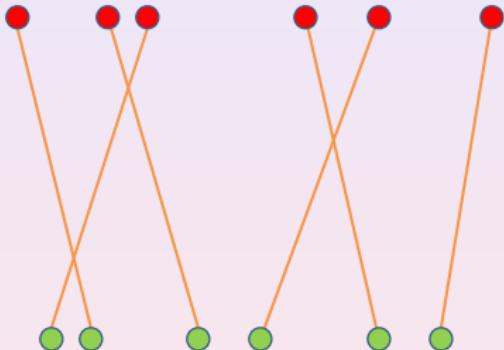
Particle Tracking in Fluid Mechanics



Particle Tracking in Fluid Mechanics

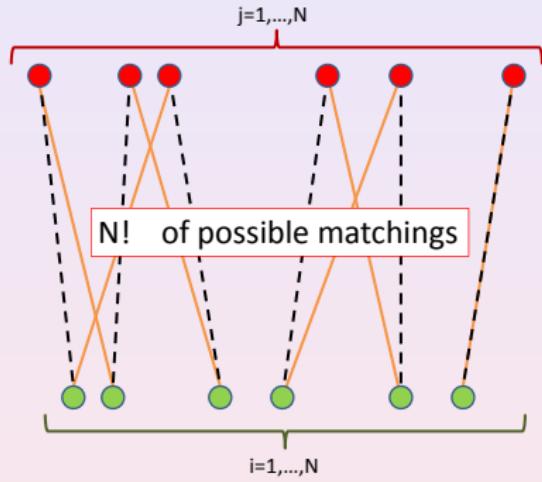


Particle Tracking in Fluid Mechanics



Particle Tracking in Fluid Mechanics

$d = 1$ advection and diffusion [example]



$$p_i^j = p(y^j | x_i) = \frac{\exp(-(y^j - e^S x_i)^2 / (\kappa(e^{2S} - 1)))}{\sqrt{\pi \kappa(e^{2S} - 1)}}$$

probability of the i-j matching

$$p(\hat{\sigma} | \vec{x}; \vec{y}) = Z^{-1} \prod_{(i,j)} \left(p_i^j \right)^{\sigma_i^j} F(\hat{\sigma})$$

$$F(\hat{\sigma}) \equiv \prod_i \delta \left(\sum_j \sigma_i^j, 1 \right) \prod_j \delta \left(\sum_i \sigma_i^j, 1 \right)$$

$$Z(\kappa, S) \equiv \sum_{\hat{\sigma} \in \{0,1\}^{N^2}} \prod_{(i,j)} \left(p_i^j \right)^{\sigma_i^j} F(\hat{\sigma})$$

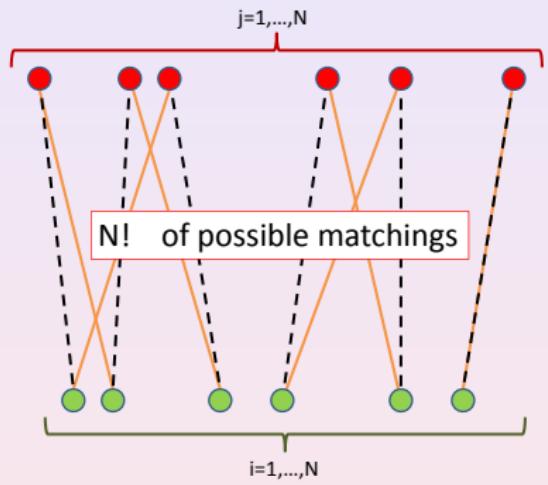
- Matching: $\operatorname{argmax}_{\hat{\sigma}} p(\hat{\sigma} | \vec{x}; \vec{y})$ – [EASY, e.g. Bayati, Shah and Sharma '06]
- “Learning”: $\operatorname{argmax}_{\kappa, S} Z(\kappa, S)$ – [DIFFICULT]



"Learning" the environment

[MC, Kroc, Vergassola '08]

$d = 1$ advection and diffusion [example]



$$p_i^j = p(y^j | x_i) = \underbrace{\frac{\exp(-(y^j - e^S x_i)^2 / (\kappa(e^{2S} - 1)))}{\sqrt{\pi \kappa(e^{2S} - 1)}}}_{\text{probability of the } i-j \text{ matching}}$$

$$p(\hat{\sigma} | \vec{x}; \vec{y}) = Z^{-1} \prod_{(i,j)} \left(p_i^j \right)^{\sigma_i^j} F(\hat{\sigma})$$

$$F(\hat{\sigma}) \equiv \prod_i \delta \left(\sum_j \sigma_i^j, 1 \right) \prod_j \delta \left(\sum_i \sigma_i^j, 1 \right)$$

$$Z(\kappa, S) \equiv \sum_{\hat{\sigma} \in \{0,1\}^{N^2}} \prod_{(i,j)} \left(p_i^j \right)^{\sigma_i^j} F(\hat{\sigma})$$

$$\operatorname{argmax}_{\kappa, S} Z(\kappa, S)$$

BP = bare approximation (heuristics)+ Loop Series



Loop Calculus for Matching

$$Z = Z_{BP} * z, \quad z \equiv 1 + \sum_C r_C, \quad r_C = \left(\prod_{i \in C} (1 - q_i) \right) \left(\prod_{j \in C} (1 - q^j) \right) \prod_{(i,j) \in C} \frac{\beta_i^j}{1 - \beta_i^j}$$

- $\forall C : |r_C| \leq 1$

Mixed Derivative

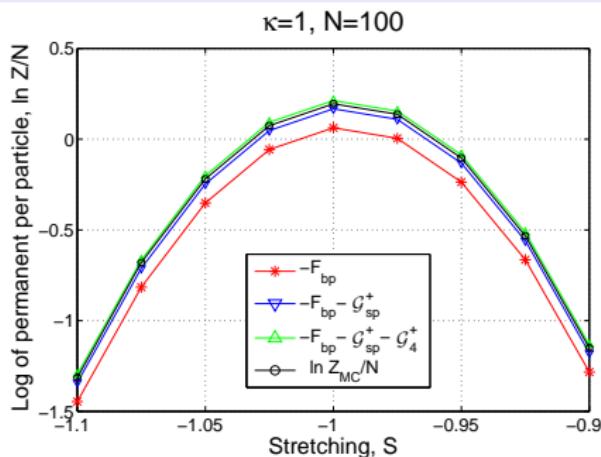
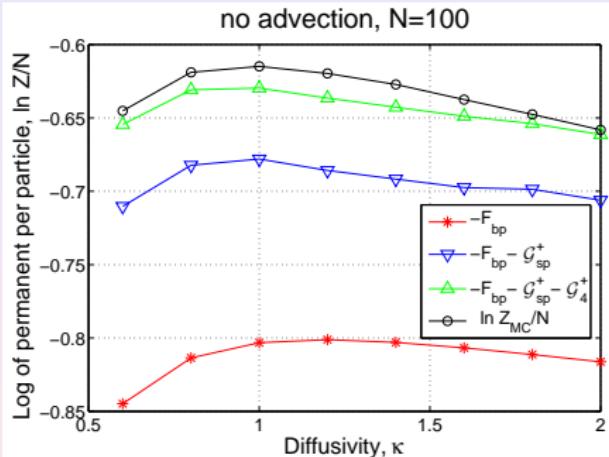
$$z = \left. \frac{\partial^{2N} \mathcal{Z}(\rho_1, \dots, \rho_N, \rho^1, \dots, \rho^N)}{\partial \rho_1 \cdots \partial \rho_N \partial \rho^1 \cdots \partial \rho^N} \right|_{\rho_1 = \dots = \rho_N = \rho^1 = \dots = \rho^N = 0}$$

$$\mathcal{Z}(\vec{\rho}) \equiv \exp \left(\sum_i \rho_i + \sum_j \rho^j \right) \prod_{(i,j)} \left(1 + \frac{\beta_i^j}{(1 - \beta_i^j)} \exp(-\rho_i - \rho^j) \right)$$

Cauchy Integral

$$z = \oint_{\Gamma_\rho} \exp(-\mathcal{G}(\vec{\rho})) \frac{\prod_i d\rho_i \prod_j d\rho^j}{(2\pi i)^{2N}}, \quad \mathcal{G}(\vec{\rho}) \equiv \sum_i 2 \ln \rho_i + \sum_j 2 \ln \rho^j - \ln \mathcal{Z}$$

"Learning": Cauchy-based heuristics vs FPRAS



BP, Loop Series = Mixed Derivatives = Cauchy Integral
 ≈ Saddle Point (heuristics) + Determinant + 4th order corr.

Fully Polynomial Randomized Algorithmic Scheme (Monte Carlo)

Shopping List for Matching & Learning +

- Analytical control of the saddle approximation quality
- Matching-Reconstruction as a Phase Transition
- $d = 2, 3$, realistic flows (multi scale)
- Multiple snapshots (a movie)
- ... technology for other reconstr. problems (e.g. phylogeny)

◀ Loop Calculus +

Details for BP-fermi Loop Series

$$Z_{BP;fermi} = \prod_{\{a,b\} \in \mathcal{G}_1} \frac{H_{ab} H_{ba} \gamma_{ab}^{(bp)} \gamma_{ba}^{(bp)}}{1 - H_{ab} H_{ba} \gamma_{ab}^{(bp)} \gamma_{ba}^{(bp)}} \prod_{c \in \mathcal{G}_0} \left(H_{cc} - \sum_{a' \sim c} (\gamma_{a'c}^{(bp)})^{-1} \right)$$

$$r(C, C') = (-1)^{\deg(C')} \prod_{a \in C_0} r_a(C, C') \prod_{\alpha \in C_1} r_\alpha(C, C')$$

$$a \in C_0 \setminus C'_0 : \quad r_a(C, C') = \frac{H_{aa} - \sum_{a' \sim a}^{a' \in C_0} H_{a'a} H_{aa'} \gamma_{aa'}^{(bp)} - \sum_{a' \sim a}^{a' \in C_0 \setminus C'_0} (\gamma_{a'a}^{(bp)})^{-1}}{H_{aa} - \sum_{a' \sim a} (\gamma_{a'a}^{(bp)})^{-1}}$$

$$a \in C'_0 : \quad r_a(C, C') = \frac{1}{H_{aa} - \sum_{a' \sim a} (\gamma_{a'a}^{(bp)})^{-1}},$$

$$\alpha \in C_1 \setminus C'_1, \quad c = \partial_0 \alpha, \quad d = \partial_1 \alpha : \quad r_\alpha(C, C') = - \frac{1}{H_{cd} H_{dc} \gamma_{cd}^{(bp)} \gamma_{dc}^{(bp)}},$$

$$\alpha \in C'_1, \quad c = \partial_0 \alpha, \quad d = \partial_1 \alpha : \quad r_\alpha(C, C') = \frac{1 - H_{cd} H_{dc} \gamma_{cd}^{(bp)} \gamma_{dc}^{(bp)}}{H_{cd} \gamma_{cd}^{(bp)} \gamma_{dc}^{(bp)}}$$

Cycle Series for Determinant

$$\det H = \left(\prod_{(a,b) \in \mathcal{G}_1} (H_{ab} H_{ba}) \right) \left(\prod_{a \in \mathcal{G}_0} H_{aa} \right) \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \prod_{a \in \mathcal{G}_0} f_a(\bar{\chi}_a, \chi_a) \prod_{\alpha \in \mathcal{G}_1} g_\alpha(\bar{\chi}_\alpha, \chi_\alpha)$$

$$g_\alpha(\bar{\chi}_\alpha, \chi_\alpha) = \exp \left(\frac{\bar{\chi}_{ab} \chi_{ba}}{H_{ab}} + \frac{\bar{\chi}_{ba} \chi_{ab}}{H_{ba}} \right)$$

Simple [non-BP] choice of the γ -Gauge

$$g_\alpha = \underbrace{1 - \frac{\bar{\chi}_{ab}\chi_{ab}\bar{\chi}_{ba}\chi_{ba}}{H_{ab}H_{ba}}}_{\text{even [ground] state} = g_\alpha^{(0)}} + \underbrace{\frac{\bar{\chi}_{ab}\chi_{ba}}{H_{ab}} + \frac{\bar{\chi}_{ba}\chi_{ab}}{H_{ba}}}_{\text{odd [excited] state} = g_\alpha^{(1)}}$$

Determinant as a series

$$\det H = \sum_{\sigma} Z_{\sigma}, \quad \sigma = (\sigma_{ab} = 0, 1 | \{a, b\} \in \mathcal{G}_1), \quad Z(\sigma) \equiv \\ \left(\prod_{(a,b) \in \mathcal{G}_1} (H_{ab} H_{ba}) \right) \left(\prod_{a \in \mathcal{G}_0} H_{aa} \right) \int D\chi D\bar{\chi} \prod_{a \in \mathcal{G}_0} f_a(\bar{\chi}_a, \chi_a) \prod_{\alpha \in \mathcal{G}_1} g_{\alpha}^{(\sigma_{ab}; \gamma)}(\bar{\chi}_{\alpha}, \chi_{\alpha})$$

Only Oriented Disjoint Cycles survive [give non-zero contribution]