



Statistical Physics of Algorithms or Belief Propagation & Beyond (subjective mini-course, 6 lectures)

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MIT/LIDS

Outline

- 1 Preamble
 - Graphical Models
 - Examples (Physics, IT, CS)
 - Complexity & Algorithms
 - Easy & Difficult
- 2 Bethe Free Energy & Belief Propagation (approx)
 - BP is Exact on a Tree
 - Variational Method in Statistical Mechanics
 - Bethe Free Energy
 - Linear Programming and BP
- 3 Exact Inference with BP
 - Loops ... Questions
 - Gauge Transformations and BP
 - Loop Series
 - Self-avoiding Tree Approach
- 4 Spin Glasses, Particle Tracking and Planar Models
 - Spin Glass & Min-Cut/Max-Flow
 - BP is exact on some problems with Loops
 - Learning the Flow: Particle Tracking & Loop Calculus
 - Dimers & Planar algorithm
 - BP and Loop Series on Planar Graphs
- 5 q -ary Model, Determinants, Fermions & Loops
 - Loop Tower
 - Intro (again): Gaussian, Fermions & Monomer-Dimers
 - Determinants, Belief Propagation & Loop Series
 - Monomer-Dimer Model, Cycles and Determinants

Books, Reviews, Papers

No **perfect** book on the subject, yet

Good books on related subjects

- David J. C. MacKay, *Information Theory, Inference and Learning Algorithms*, Cambridge University Press, 2003
- Marc Mezard & Anrea Montanari, *Information, Physics and Computation*, in progress see Mezard's webpage
- Tom Richardson, Rüdiger Urbanke, *Modern Coding Theory* Cambridge University Press, 2005
- Alexander K. Hartmann, Heiko Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, 2002

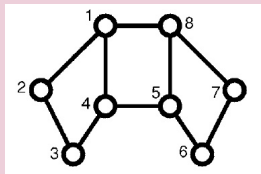
Many recent **research** papers, and few **reviews** scattered over Physics, Computer Science and Information Theory journals

Boolean Graphical Models = The Language

Forney style - variables on the edges

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

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



$$f_a \geq 0$$

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

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

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

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

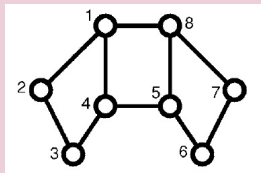
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Example (1): Statistical Physics

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)

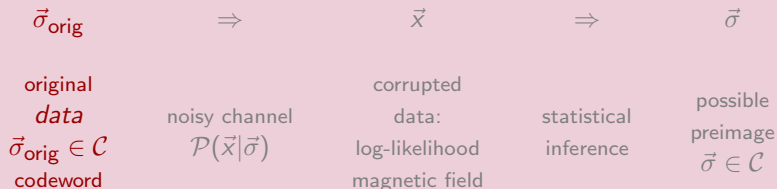
Graphical Representation

Variables are usually associated with vertexes ... but transformation to the Forney graph (variables on the edges) is straightforward

- Ferromagnetic ($J_{ij} < 0$), Anti-ferromagnetic ($J_{ij} > 0$) and 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. forward error correction

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

Probabilistic Reconstruction (Statistical Inference)

$\vec{\sigma}_{\text{orig}}$

\Rightarrow

\vec{x}

\Rightarrow

$\vec{\sigma}$

original
 data

noisy channel

corrupted

statistical
 inference

possible
 preimage
 $\vec{\sigma} \in \mathcal{C}$

$\vec{\sigma}_{\text{orig}} \in \mathcal{C}$
 codeword

$\mathcal{P}(\vec{x}|\vec{\sigma})$

data:
 log-likelihood
 magnetic field

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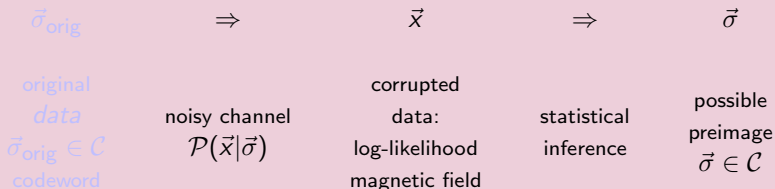
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e.g. forward error correction

Example (3): Combinatorial Optimization, K-SAT

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

$1, 2, \dots, N$ – variables

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

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

\bar{x}_i is negation of x_i

$\vee = \text{OR}$ $\wedge = \text{AND}$

\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 $\alpha = M/N$, $M, N \rightarrow \infty$

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 Algebraic) in N is **EASY**, Exponential is **DIFFICULT**

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Easy & Difficult Boolean Problems

EASY

- Any graphical problems **on a tree** (Bethe-Peierls, Dynamical Programming, BP, TAP 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**

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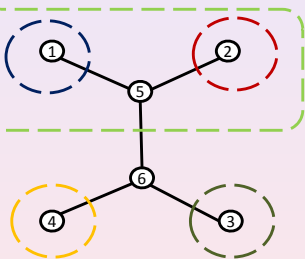
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BP is Exact on a Tree

Bethe '35, Peierls '36



$$Z_{51}(\sigma_{51}) = f_1(\sigma_{51}), \quad Z_{52}(\sigma_{52}) = f_2(\sigma_{52}),$$

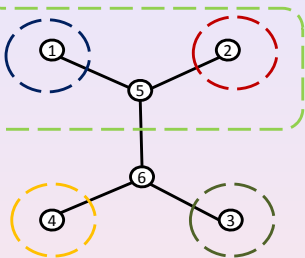
$$Z_{63}(\sigma_{63}) = f_3(\sigma_{63}), \quad Z_{64}(\sigma_{64}) = f_4(\sigma_{64})$$

$$Z_{65}(\sigma_{56}) = \sum_{\vec{\sigma}_5 \setminus \sigma_{56}} f_5(\vec{\sigma}_5) Z_{51}(\sigma_{51}) Z_{52}(\sigma_{52})$$

$$Z = \sum_{\vec{\sigma}_6} f_6(\vec{\sigma}_6) Z_{63}(\sigma_{63}) Z_{64}(\sigma_{64}) Z_{65}(\sigma_{65})$$

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

Belief Propagation Equations

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

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

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

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

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

Variational Ansatz

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

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

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

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Bethe Free Energy: variational approach

(Yedidia, Freeman, Weiss '01 -

inspired by Bethe '35, Peierls '36)

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

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

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

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

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Linear Programming version of Belief Propagation

In the limit of large SNR, $\ln f_a \rightarrow \pm\infty$: **BP \rightarrow LP**

Minimize $F \approx E = - \sum_a \sum_{\vec{\sigma}_a} b_a(\vec{\sigma}_a) \ln f_a(\vec{\sigma}_a) = \text{self energy}$
under set of linear constraints

LP decoding of LDPC codes

Feldman, Wainwright, Karger '03

- ML can be restated as an LP over a codeword polytope
- LP decoding is a “local codewords” relaxation of LP-ML
- Codeword convergence certificate
- Discrete and Nice for Analysis
- Large polytope $\{b_\alpha, b_i\} \Rightarrow$ Small polytope $\{b_i\}$

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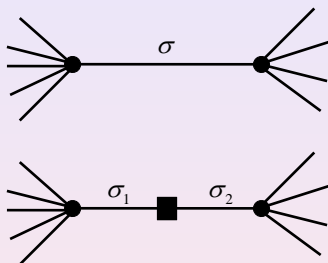
BP does not account for Loops

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]



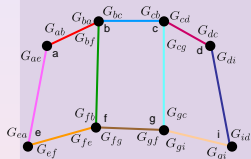
$$\forall \sigma_1, \sigma_2 = \pm 1, \quad \forall \eta_1, \eta_2 \in \mathcal{C}$$

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

Gauge Transformations

Chertkov, Chernyak '06

Local Gauge, G , Transformations



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

$$\sigma_{ab} = \sigma_{ba} = \pm 1; \quad q\text{-ary case will be discussed later}$$

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

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

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

The partition function is invariant under any G -gauge!

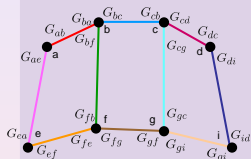
$$Z = \sum_{\vec{\sigma}} \prod_a f_a(\vec{\sigma}_a) = \sum_{\vec{\sigma}} \prod_a \left(\sum_{\vec{\sigma}'_a} f_a(\vec{\sigma}'_a) \prod_{b \in a} G_{ab}(\sigma_{ab}, \sigma'_{ab}) \right)$$



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

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

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Belief Propagation Gauge

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

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

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

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Belief Propagation as a Gauge Fixing (II)

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

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Belief Propagation in terms of Messages

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

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

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

Variational Principle and Gauge Fixing

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

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 directly related to the **Bethe Free Energy**
of *Yedidia, Freeman, Weiss '01* Bethe Free Energy

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

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Loop Series:

Chertkov, Chernyak '06

Exact (!!) expression in terms of BP

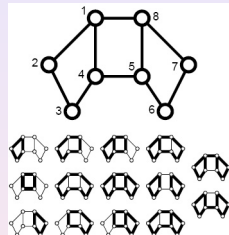
$$Z = \sum_{\vec{\sigma}} \prod_a f_a(\vec{\sigma}_a) = Z_0 \left(1 + \sum_C r(C) \right)$$

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

$C \in$ **Generalized Loops** = 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
- BP is a **Gauge fixing** condition. Other choices of Gauges would lead to different representation.

Summary (Loop Calculus)

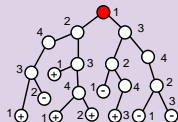
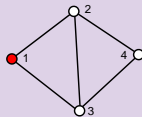
- BP eqs. solve **Gauge fixing** conditions
- BP eqs also explains **no-loose-end coloring** constraints
- BP **minimizes gauge dependence** in the ground state
- Loop series expresses partition function in terms of a sum of terms, each associated with a **generalized loop** of the graph
- Each term in the Loop Series **depends** explicitly on the **BP** solution

Self-avoiding Tree

Weitz '06

Bipartite. Binary.

$$\left. \begin{aligned} \mathcal{P}(\vec{\sigma}) &= Z^{-1} \prod_{(i,j)} f(\sigma_i, \sigma_j) \\ p_i(\sigma_i) &= \sum_{\vec{\sigma} \setminus \sigma_i} \mathcal{P}(\vec{\sigma}) \\ \frac{p_i(+)}{p_i(-)} &= \frac{\sum_{\vec{\sigma} \setminus \sigma_i} \left(\prod_{(k,j)} f(\sigma_k, \sigma_j) \right) \Big|_{\sigma_i=+}}{\sum_{\vec{\sigma} \setminus \sigma_i} \left(\prod_{(k,j)} f(\sigma_k, \sigma_j) \right) \Big|_{\sigma_i=-}} \end{aligned} \right\} \Rightarrow$$



Self-avoiding Tree

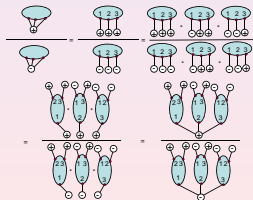
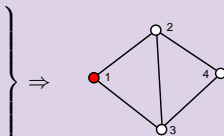
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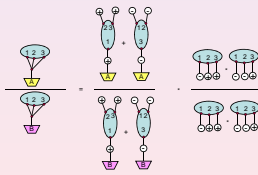
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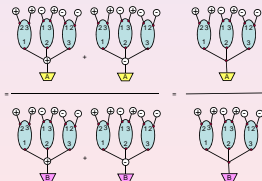
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▶ Magnify



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Complementarity of Loop Calculus & Graphical Transformations

Speculations

- Loop Calculus is built on Gauge Transformations. Gauge Transformations do not change the graph but reparametrize factor functions.
- Graphical Transformations keep factor functions but modify the graph.
- Loop Calculus & Graphical Transformations are complementary.
- It may be advantageous to build efficient optimality achieving algorithms on the combination of the two: the Loop Calculus and the Graphical Transformations.

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Outline

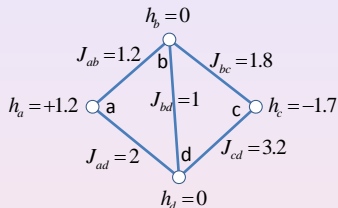
- 1 Preamble
 - Graphical Models
 - Examples (Physics, IT, CS)
 - Complexity & Algorithms
 - Easy & Difficult
- 2 Bethe Free Energy & Belief Propagation (approx)
 - BP is Exact on a Tree
 - Variational Method in Statistical Mechanics
 - Bethe Free Energy
 - Linear Programming and BP
- 3 Exact Inference with BP
 - Loops ... Questions
 - Gauge Transformations and BP
 - Loop Series
 - Self-avoiding Tree Approach
- 4 **Spin Glasses, Particle Tracking and Planar Models**
 - Spin Glass & Min-Cut/Max-Flow**
 - BP is exact on some problems with Loops**
 - Learning the Flow: Particle Tracking & Loop Calculus**
 - Dimers & Planar algorithm**
 - BP and Loop Series on Planar Graphs**
- 5 q -ary Model, Determinants, Fermions & Loops
 - Loop Tower
 - Intro (again): Gaussian, Fermions & Monomer-Dimers
 - Determinants, Belief Propagation & Loop Series
 - Monomer-Dimer Model, Cycles and Determinants

Ferromagnetic Random-Field Ising Model

$$p(\vec{\sigma}) = Z^{-1} \exp \left(\frac{1}{2T} \sum_{(i,j)} J_{ij} \sigma_i \sigma_j + \frac{1}{T} \sum_i h_i \sigma_i \right)$$

$$J_{ij} \geq 0, \quad h_i \geq 0$$

(i,j) are edges on an undirected graph \mathcal{G}



Ground State, $T \rightarrow 0$

$$\min_{\sigma} \left(-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}} J_{ij} \sigma_i \sigma_j - \sum_{i \in \mathcal{G}} h_i \sigma_i \right) \Big|_{\forall i \in \mathcal{G}: \sigma_i = \pm 1}$$

► FRFI → Min-cut, Max-flow

FRFI/Min-Cut/Max-Flow is EASY

- Many network algorithms. See e.g. T.H. Cormen, et al, *Introduction to Algorithms*, MIT-Press (2001)
- Reduction to **Linear Programming**. See e.g. H. Papadimitriou, I. Steiglitz, *Combinatorial Optimization: Alg. and Complexity*, Dover (1998)

Relaxation of Min-Cut **Integer LP** to respective **LP** is exact

$$-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'_d} J_{ij} + \min_{\{\eta, p\}} \sum_{(ij) \in \mathcal{G}'_d} J_{ij} \eta_{ij} \quad \begin{array}{l} p_s = 0, \quad p_t = 1; \quad \forall i \in \mathcal{G}', p_i = 0, 1 \\ \forall (i, j) \in \mathcal{G}' : p_i - p_j + \eta_{ij} = 0, 1 \end{array}$$

- Matrix of LP constraints is **Totally Uni-Modular** (TUM)
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How about using BP for FRFI?

First Impression:

Should not work for arbitrary graph because of Loops

On Second Thought:

May be the $T \rightarrow 0$ limit is not that hopeless? After all we know that the problem is easy!

Tree reweighted BP of Kolmogorov & Wainwright '05

At $T \rightarrow 0$ BP solves the FRFI model exactly on any graph!

Another Easy Example with Loops: Bayati, Shah and Sharma '06

Maximum Weight Matching of a Bi-partite graph

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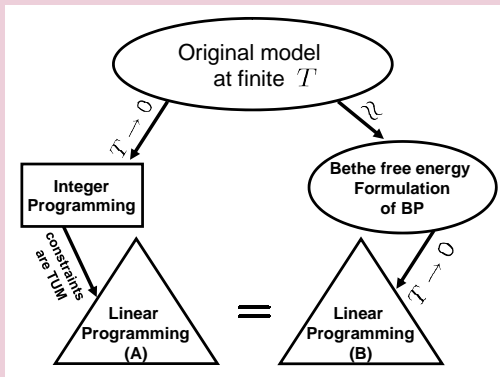
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Easy Problems with Loops and Bethe Free energy

Proof of the BP-exactness via the Bethe Free energy approach



Chertkov '08

Bethe Free Energy for FRFI

At any Temperature

Minimize the Free Energy :

$$\mathcal{F} = E - TS, \quad E = - \sum_{(i,j)} \sum_{\sigma_i, \sigma_j} b_{ij}(\sigma_i, \sigma_j) \frac{J_{ij}}{2} \sigma_i \sigma_j - \sum_i \sum_{\sigma_i} b_i(\sigma_i) h_i \sigma_i$$

$$S = \sum_{(i,j)} \sum_{\sigma_i, \sigma_j} b_{ij}(\sigma_i, \sigma_j) \ln b_{(i,j)}(\sigma_i, \sigma_j) - \sum_i \sum_{\sigma_i} b_i(\sigma_i) \ln b_i(\sigma_i)$$

$$\forall i \text{ \& \ } \forall j \in i: \quad b_i(\sigma_i) = \sum_{\sigma_j} b_{ij}(\sigma_i, \sigma_j), \quad \forall i: \quad \sum_{\sigma_i} b_i(\sigma_i) = 1$$

$T \rightarrow 0 \Rightarrow$ Linear Programming

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Linear Programming (B) for FRFI

$$\text{(s-t) modification: } \begin{cases} J_{si} = 2h_i & b_{si}(\sigma_s, \sigma_i) = b_i(\sigma_i)\delta(\sigma_s, +1) & h_i > 0 \\ J_{it} = 2|h_i| & b_{it}(\sigma_i, \sigma_t) = b_i(\sigma_i)\delta(\sigma_t, -1) & h_i < 0 \end{cases}$$

$$\min_{\{b_i; b_{ij}\}} \left(- \sum_{(i,j) \in \mathcal{G}'} \sum_{\sigma_i, \sigma_j} b_{ij}(\sigma_i, \sigma_j) \frac{J_{ij}}{2} \sigma_i \sigma_j \right) \left| \begin{array}{l} \forall i \in \mathcal{G}' \quad \& \quad \forall j \in i: \quad b_i(\sigma_i) = \sum_{\sigma_j} b_{ij}(\sigma_i, \sigma_j) \\ \forall i \in \mathcal{G}': \quad \sum_{\sigma_i} b_i(\sigma_i) = 1 \\ b_s(+)=1 \quad \& \quad b_d(-)=1 \end{array} \right.$$

$$-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'} J_{ij} + \min_{\{\mu, \pi\}} \sum_{(i,j) \in \mathcal{G}'} J_{ij} \mu_{ij} \quad \left| \begin{array}{l} \forall (i,j) \in \mathcal{G}': \quad \pi_i - \pi_j + \mu_{ij} \geq 0 \\ \forall (i,j) \in \mathcal{G}': \quad 1 \geq \pi_i, \mu_{ij} \geq 0 \\ \pi_s = 0, \quad \pi_t = 1 \end{array} \right.$$

Linear Programming (B) for FRFI

$$\text{(s-t) modification: } \begin{cases} J_{si} = 2h_i & b_{si}(\sigma_s, \sigma_i) = b_i(\sigma_i)\delta(\sigma_s, +1) & h_i > 0 \\ J_{it} = 2|h_i| & b_{it}(\sigma_i, \sigma_t) = b_i(\sigma_i)\delta(\sigma_t, -1) & h_i < 0 \end{cases}$$

$$\min_{\{b_i; b_{ij}\}} \left(- \sum_{(i,j) \in \mathcal{G}'} \sum_{\sigma_i, \sigma_j} b_{ij}(\sigma_i, \sigma_j) \frac{J_{ij}}{2} \sigma_i \sigma_j \right) \left| \begin{array}{l} \forall i \in \mathcal{G}' \quad \& \quad \forall j \in i: \quad b_i(\sigma_i) = \sum_{\sigma_j} b_{ij}(\sigma_i, \sigma_j) \\ \forall i \in \mathcal{G}': \quad \sum_{\sigma_i} b_i(\sigma_i) = 1 \\ b_s(+)=1 \quad \& \quad b_d(-)=1 \end{array} \right.$$

$$\{b\} \rightarrow \{\mu, \pi\} : \begin{cases} \mu_{ij} \equiv b_{ij}(+, -) + b_{ij}(-, +) = 1 - b_{ij}(+, +) - b_{ij}(-, -), & \forall (i, j) \in \mathcal{G}' \\ \pi_i = b_i(-) = b_{ij}(-, +) + b_{ij}(-, -), & \forall i \in \mathcal{G}' \end{cases}$$

$$-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'} J_{ij} + \min_{\{\mu, \pi\}} \sum_{(i,j) \in \mathcal{G}'} J_{ij} \mu_{ij} \quad \left| \begin{array}{l} \forall (i, j) \in \mathcal{G}': \quad \pi_i - \pi_j + \mu_{ij} \geq 0 \\ \forall (i, j) \in \mathcal{G}': \quad 1 \geq \pi_i, \mu_{ij} \geq 0 \\ \pi_s = 0, \quad \pi_t = 1 \end{array} \right.$$

Linear Programming (B) for FRFI

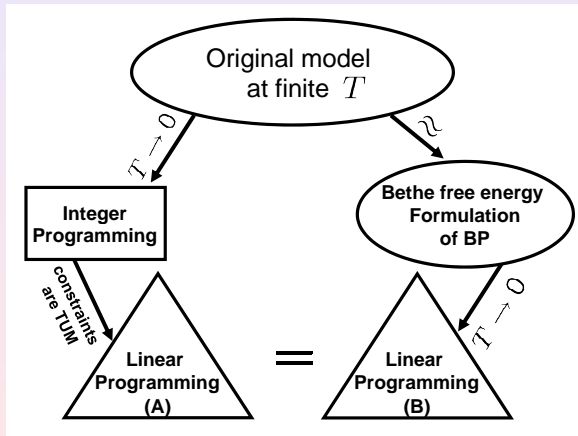
$$\text{(s-t) modification: } \begin{cases} J_{si} = 2h_i & b_{si}(\sigma_s, \sigma_i) = b_i(\sigma_i)\delta(\sigma_s, +1) & h_i > 0 \\ J_{it} = 2|h_i| & b_{it}(\sigma_i, \sigma_t) = b_i(\sigma_i)\delta(\sigma_t, -1) & h_i < 0 \end{cases}$$

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FRFI at $T = 0$ is solved exactly by BP



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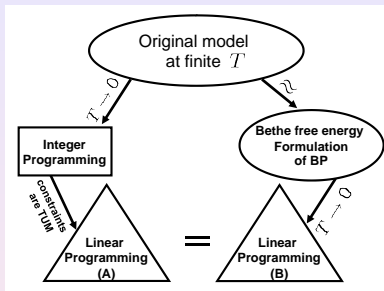
LP(A)

$$-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'} J_{ij} + \min_{\{\eta, \rho\}} \sum_{(ij) \in \mathcal{G}'_d} J_{ij} \eta_{ij} \quad \left| \quad \begin{array}{l} p_s = 0, \quad p_t = 1; \quad \forall i \in \mathcal{G}', p_i = [0, 1] \\ \forall (i, j) \in \mathcal{G}' : p_i - p_j + \eta_{ij} = [0, 1] \end{array} \right.$$

LP(B)

$$-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'} J_{ij} + \min_{\{\mu, \pi\}} \sum_{(i,j) \in \mathcal{G}'_d} J_{ij} \mu_{ij} \quad \left| \quad \begin{array}{l} \forall (i, j) \in \mathcal{G}' : \pi_i - \pi_j + \mu_{ij} \geq 0 \\ \forall (i, j) \in \mathcal{G}' : 1 \geq \pi_i, \mu_{ij} \geq 0 \\ \pi_s = 0, \quad \pi_t = 1 \end{array} \right.$$

LP(A)=LP(B)



The scheme also works for $T \rightarrow 0$ of

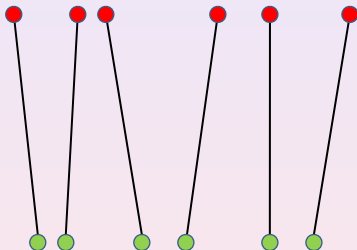
$$p(\sigma) = Z^{-1} \exp \left(-T^{-1} \sum_i h_i \sigma_i \right) \prod_{\alpha} \delta \left(\sum_i J_{\alpha i} \sigma_i, m_{\alpha} \right).$$

where \hat{J} is a Totally Uni-Modular matrix

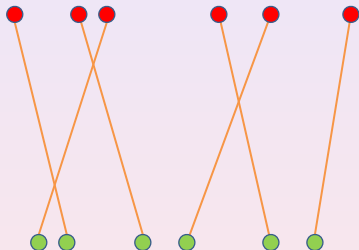
Particle Tracking in Fluid Mechanics



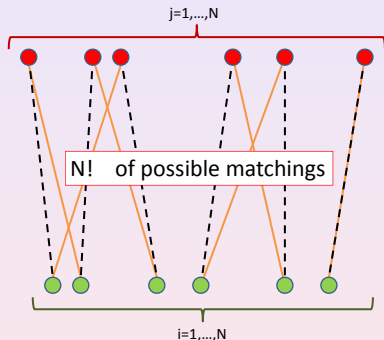
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Particle Tracking in Fluid Mechanics



Particle Tracking in Fluid Mechanics



$d = 1$ advection and diffusion [example]

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

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

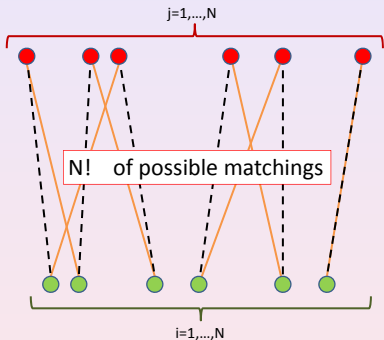
$$F(\hat{\sigma}) \equiv \prod_i \delta\left(\sum_j \sigma_i^j, 1\right) \prod_j \delta\left(\sum_i \sigma_i^j, 1\right)$$

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

- 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]

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

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

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

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

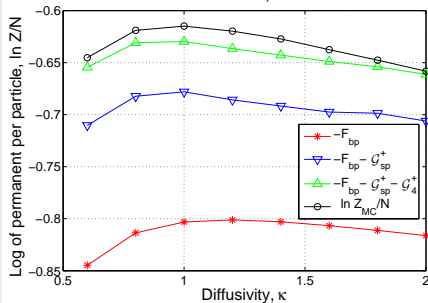
$$\mathcal{Z}(\vec{\rho}) \equiv \exp \left(\sum_i \rho_i + \sum_j \rho^j \right) \prod_{(i,j)} \left(1 + \frac{\beta_i^j}{(1 - \beta_i^j)} \exp(-\rho_i - \rho^j) \right)$$

Cauchy Integral

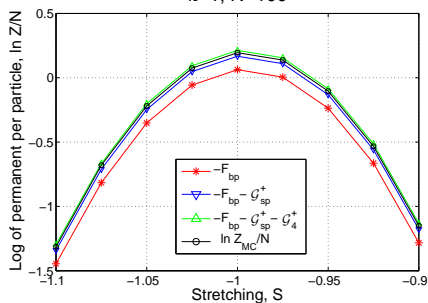
$$z = \oint_{\Gamma_\rho} \exp(-\mathcal{G}(\vec{\rho})) \frac{\prod_i d\rho_i \prod_j d\rho^j}{(2\pi i)^{2N}}, \quad \mathcal{G}(\vec{\rho}) \equiv \sum_i 2 \ln \rho_i + \sum_j 2 \ln \rho^j - \ln \mathcal{Z}$$

"Learning": Cauchy-based heuristics vs FPRAS

no advection, $N=100$



$\kappa=1, N=100$



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

Fully Polynomial Randomized Algorithmic Scheme (Monte Carlo)

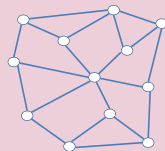
Shopping List for Matching & Learning +

- 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)

Glassy Ising & Dimer Models on a Planar Graph

Partition Function of $J_{ij} \geq 0$ Ising Model, $\sigma_i = \pm 1$

$$Z = \sum_{\vec{\sigma}} \exp \left(\frac{\sum_{(i,j) \in \Gamma} J_{ij} \sigma_i \sigma_j}{T} \right)$$



Partition Function of Dimer Model, $\pi_{ij} = 0, 1$

$$Z = \sum_{\vec{\pi}} \prod_{(i,j) \in \Gamma} (z_{ij})^{\pi_{ij}} \prod_{i \in \Gamma} \delta \left(\sum_{j \in i} \pi_{ij}, 1 \right)$$

perfect matching

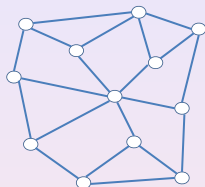


Ising & Dimer Classics

- L. Onsager, *Crystal Statistics*, Phys.Rev. **65**, 117 (1944)
- M. Kac, J.C. Ward, *A combinatorial solution of the Two-dimensional Ising Model*, Phys. Rev. **88**, 1332 (1952)
- C.A. Hurst and H.S. Green, *New Solution of the Ising Problem for a Rectangular Lattice*, J.of Chem.Phys. **33**, 1059 (1960)
- M.E. Fisher, *Statistical Mechanics on a Plane Lattice*, Phys.Rev **124**, 1664 (1961)
- P.W. Kasteleyn, *The statistics of dimers on a lattice*, Physics **27**, 1209 (1961)
- P.W. Kasteleyn, *Dimer Statistics and Phase Transitions*, J. Math. Phys. **4**, 287 (1963)
- M.E. Fisher, *On the dimer solution of planar Ising models*, J. Math. Phys. **7**, 1776 (1966)
- F. Barahona, *On the computational complexity of Ising spin glass models*, J.Phys. A **15**, 3241 (1982)

From Ising to Dimer (I)

$$Z = \sum_{\vec{\sigma}} \exp \left(\frac{\sum_{(i,j) \in \Gamma} J_{ij} \sigma_i \sigma_j}{T} \right)$$

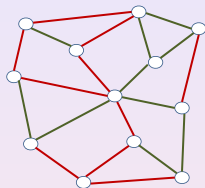


- For a given $\vec{\sigma}$ an edge is **sat**:
if $J_{ij} > 0$ & $\sigma_i \sigma_j = 1$ or $J_{ij} < 0$ & $\sigma_i \sigma_j = -1$
- Cycle (e.g. face/cell) is **frustrated** if the number of **negative** edges is odd. (N.B. Frustration of a cycle is invariant wrt $\vec{\sigma}$.)
- Equivalent configurations, $\vec{\sigma}$ and $-\vec{\sigma}$, have the same weight
- Introduce dual graph, Γ^* . A vertex of Γ^* correspondent to a **frustrated** (**unfrustrated**) face is odd (even).

$$E = - \sum_{(ij)} J_{ij} \sigma_i \sigma_j = - \sum_{(ij)} |J_{ij}| + 2 \sum_{\text{unsat edges}} |J_{ij}|$$

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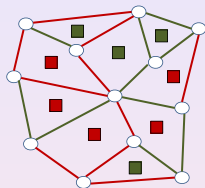


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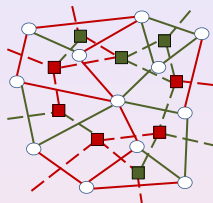


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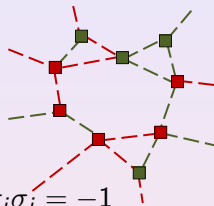
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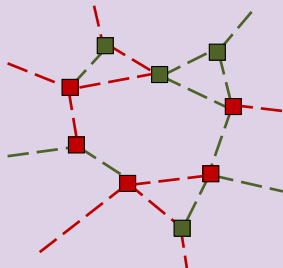
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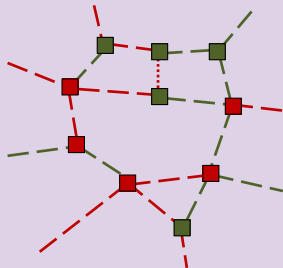
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From Ising to Dimer (II)



- The graphical transformations are **invariant**, i.e. they do not depend on the original configuration of $\vec{\sigma}$ (colors of vertexes/edges of the dual lattice stay/change)
- Spin glass Ising model on a planar graph is reduced to the Dimer Matching model on an auxiliary planar graph with all nodes of the connectivity three or smaller (graph. transformations in two steps)

From Ising to Dimer (II)

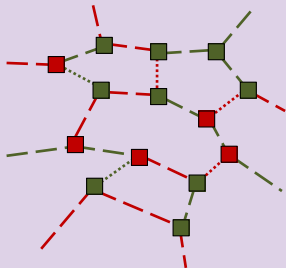


- New edges (dotted) have zero energy
- Color of a new edge is fixed by colors of the vertexes it neighbors

- All copies of an **even** vertex are **even**, one copy of an **odd** vertex is **odd** and the others are **even**
- Infinite node should also be 3-plicated (not shown)

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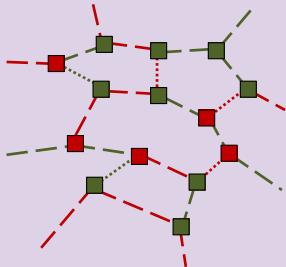


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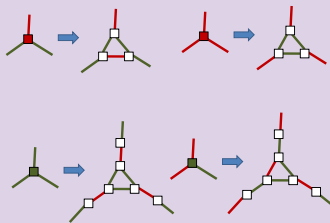
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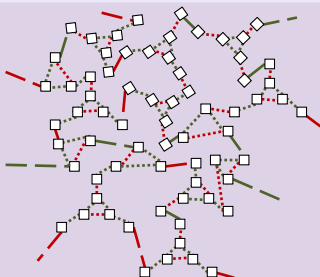
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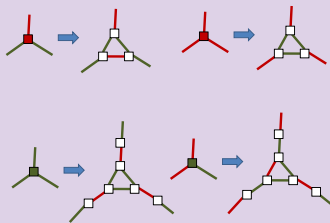
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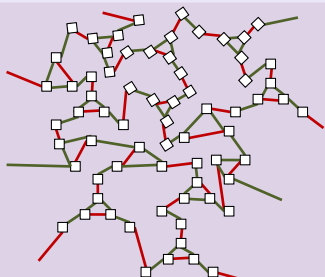
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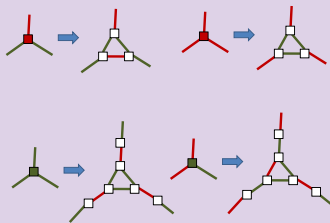
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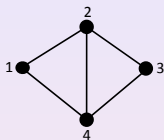
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Pfaffian solution of the Matching problem

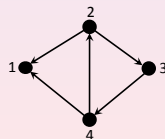
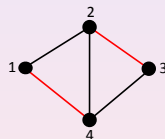
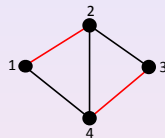


$$Z = z_{12}z_{34} + z_{14}z_{23} = (\text{if } z > 0) = \sqrt{\text{Det} \hat{A}} = \text{Pf}[\hat{A}]$$

$$\hat{A} = \begin{pmatrix} 0 & -z_{12} & 0 & -z_{14} \\ z_{12} & 0 & z_{23} & -z_{24} \\ 0 & -z_{23} & 0 & z_{34} \\ z_{14} & z_{24} & -z_{34} & 0 \end{pmatrix}$$

Odd-face [Kastelyan orientation] rule

Direct edges of the graph such that for every internal face the number of edges oriented clockwise is odd



► Fermion/Grassman Representation

Planar Spin Glass and Dimer Matching Problems

The Pfaffian formula with the “odd-face” orientation rule extends to any planar graph thus proving **constructively** that

- Counting weighted number of **dimer matchings on a planar graph is easy**
- Calculating partition function of the **spin glass Ising model on a planar graph is easy**

N.B.

- Adding magnetic field to planar, non-planar geometry, or non-binary alphabet makes the spin-glass problem difficult
- Dimer-monomer matching is difficult even in the planar case
- Planar-Graph Decomposition [*Globerson, Jaakola '06*] is an example of an approximate algorithm that could be constructed for “nearly” planar problems

Loop Series for Planar

Chertkov, Chernyak, Teodorescu '08

- Functions are on vertexes; variables (binary) are on edges
- Vertexes are of degree three (not restrictive)

Loop Series = BP + sum over generalized loops

$$Z = Z_0 \cdot z, \quad z \equiv \left(1 + \sum_C \prod_{a \in C} \mu_{a, \bar{a}_C} \right), \quad \mu_{a, \bar{a}_C} \equiv \frac{\tilde{\mu}_{a, \bar{a}_C}}{\prod_{b \in C} \sqrt{1 - m_{ab}(C)}}$$

$$m_{ab} = \sum_{\sigma_{ab}} \sigma_{ab} b_{ab}(\sigma_{ab}), \quad \tilde{\mu}_{a, \bar{a}_C} = \sum_{\vec{\sigma}_a} \prod_{b \in \bar{a}_C} (\sigma_{ab} - m_{ab}) b_a(\vec{\sigma}_a),$$

Disjoint-Cycle Partition

$$Z_s = Z_0 \cdot z_s, \quad z_s = 1 + \sum_{C \in \mathcal{G}}^{\forall a \in C, |\delta(a)|_C = 2} r_C,$$

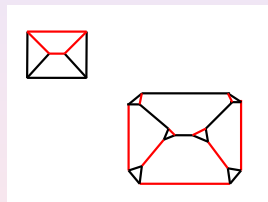
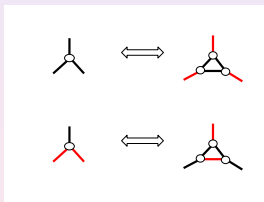
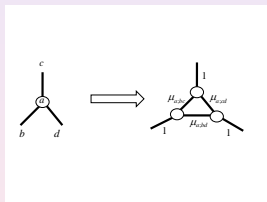
Is the Disjoint-Cycle Partition on a planar graph summable (easy)?

Disjoint-Cycle Partition (II)

Chertkov, Chernyak, Teodorescu '08

Reduction to the dimer-matching model on an auxiliary graph

- reminiscent of the Fisher's transformation



$$Z_S = \sum_{\vec{\pi}} \prod_{(a,b) \in \mathcal{G}_e} (\mu_{ab})^{\pi_{ab}} \prod_a \delta \left(\sum_b \pi_{ab}, 1 \right)$$

- z_S is a Pfaffian on a planar graph [Kasteleyn] \rightarrow EASY !

Problems Reducible to Disjoint-Cycle Partition

Generic planar problem is difficult

A planar problem is easy if

the factor functions (in a model with degree three nodes) satisfy

$$\forall a \in \mathcal{G} : \sum_{\vec{\sigma}_a} f_a(\vec{\sigma}_a) \prod_{(a,b) \in \mathcal{E}} \prod_b (\exp(\eta_{ab} \sigma_{ab}) (\sigma_{ab} - \tanh(\eta_{ab} + \eta_{ba}))) = 0.$$

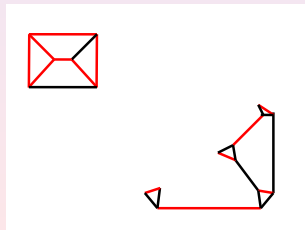
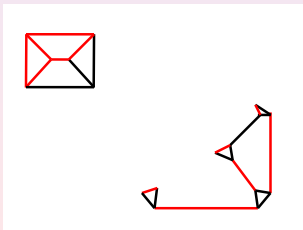
where η are messages from a BP solution for the model

Loop Series as a Pfaffian Series

$$z = \sum_{\Psi} z_{\Psi} \prod_{a \in \Psi}^{|a|=3} \mu_{a;\bar{a}}, \quad z_{\Psi} = \text{Pf}(\hat{A}_{\Psi}) = \sqrt{\text{Det}(\hat{A}_{\Psi})}$$

All z_{Ψ} are computationally tractable (Pfaffians)

- “Exclude” the fully connected part (vertexes of degree three within the generalized loop and adjusted edges)
- “Extend” the remaining graph (part of the generalized loop)



- N.B. \hat{A}_{Ψ} is not simply a minor of \hat{A} (exclusion changes signs)

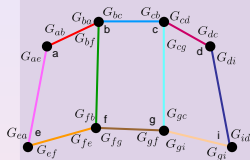
Some Future Challenges (Planar+)

- Search for new approximate schemes for intractable planar problems
- Perturbative exploration of a larger set of intractable non-planar problems which are close, in some sense, to planar problems (e.g. in the spirit of Globerson, Jaakkola '06)
- Extension to models on Surface Graphs, sum over 2^{2g} (=number of irreducible Kastelyan orientations) partitions
- Extension to q -ary case. Potts model, etc.
- Possible Relation to Integrable Hierarchies and Quantum Computations
- Disorder-averaged planar problems
- Homogeneous Planar Problems tractable in thermodynamic limit (only)

Outline

- 1 Preamble
 - Graphical Models
 - Examples (Physics, IT, CS)
 - Complexity & Algorithms
 - Easy & Difficult
- 2 Bethe Free Energy & Belief Propagation (approx)
 - BP is Exact on a Tree
 - Variational Method in Statistical Mechanics
 - Bethe Free Energy
 - Linear Programming and BP
- 3 Exact Inference with BP
 - Loops ... Questions
 - Gauge Transformations and BP
 - Loop Series
 - Self-avoiding Tree Approach
- 4 Spin Glasses, Particle Tracking and Planar Models
 - Spin Glass & Min-Cut/Max-Flow
 - BP is exact on some problems with Loops
 - Learning the Flow: Particle Tracking & Loop Calculus
 - Dimers & Planar algorithm
 - BP and Loop Series on Planar Graphs
- 5 **q -ary Model, Determinants, Fermions & Loops**
 - Loop Tower
 - Intro (again): Gaussian, Fermions & Monomer-Dimers
 - Determinants, Belief Propagation & Loop Series
 - Monomer-Dimer Model, Cycles and Determinants

Local Gauge G -Transformations e.g. for q -ary



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

$$\sigma_{ab} = \sigma_{ba} = 0, \dots, q-1$$

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

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

The partition function is invariant under any G -gauge!

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

σ'_a – unconstrained = independent for different “a”

BP as a Gauge Fixing Condition e.g. for q -ary

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

$$Z = \underbrace{Z_0(G)}_{\substack{\text{"ground" state} \\ \sigma = 0}} + \underbrace{\sum_{\sigma \neq 0} Z_c(G)}_{\text{all other = "excited" states}}$$

Belief Propagation Gauge

$$\underline{\forall a \ \& \ \forall b \in a} : \sum_{\sigma'_a} f_a(\sigma'_a) G_{ab}^{(bp)}(\sigma_{ab} \neq 0, \sigma'_{ab}) \prod_{\substack{c \neq b \\ c \in a}} G_{ac}^{(bp)}(0, \sigma'_{ac}) = 0$$

No loose "excited" edges at any vertex of the graph!

BP Eqs. for "ground" sector e.g. for q -ary

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

Belief Propagation in terms of Messages

$$\epsilon_{ab}(\sigma) = G_{ab}(0, \sigma) = \frac{\exp(\eta_{ab}(\sigma))}{\sqrt{\sum_{\sigma} \exp(\eta_{ab}(\sigma) + \eta_{ba}(\sigma))}}$$

$$\frac{\exp(\eta_{ab}^{(bp)}(\sigma_{ab}))}{\sum_{\sigma_{ab}} \exp(\eta_{ab}^{(bp)}(\sigma_{ab}) + \eta_{ba}^{(bp)}(\sigma_{ab}))} = \frac{\sum_{\sigma_a \setminus \sigma_{ab}} f_a(\sigma_a) \exp(\sum_{b \in a} \eta_{ab}^{(bp)}(\sigma_{ab}))}{\sum_{\sigma_a} f_a(\sigma_a) \exp(\sum_{b \in a} \eta_{ab}^{(bp)}(\sigma_{ab}))}$$

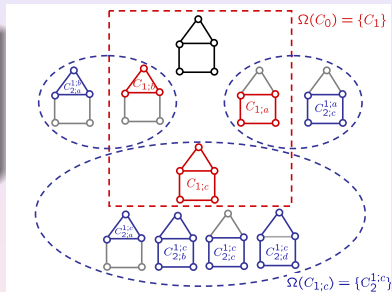
- Ground state BP gauges, $G(0, \sigma')$, are fixed by BP equations
- There exists a freedom in selecting excited BP gauges, $G(\sigma \neq 0, \sigma')$, at $q > 2$

Loop Tower for q -ary alphabet

$$Z_{C_0} = \sum_{\sigma_{C_0}} \bar{p}(G | \sigma_{C_0}) = Z_{0;C_0} + \sum_{C_1 \in \Omega(C_0)} Z_{C_1}$$

$$Z_{C_1} = \sum_{\sigma_{C_1}} \bar{p}(G^{(bp)} | \sigma_{C_1})$$

- Freedom in selecting "excited" gauges at $q > 2$;
 $\{G_{ab;C_0}^{(bp)}(\sigma_{ab} \neq 0, \sigma'_{ab}); (ab) \in C_0\}$
- $\sigma_{ab;C_1} = 1, \dots, q-1$ are not fixed at $q > 2 \Rightarrow$
 Z_{C_1} is a partition function over **reduced alphabet**



Loop Tower =

Embedded set of Loop Series over sequentially reduced alphabets

$$j = 1, \dots, q-2 : Z_{C_j} = Z_{0;C_j} + \sum_{C_{j+1} \in \Omega(C_j)} Z_{C_{j+1}}$$

Gaussian Belief Propagation

Gaussian Graphical Model

$$p(x|J; h) = \frac{\exp\left(-\frac{1}{2}x^+ Jx + h^+ x\right)}{Z(J)}$$

- Gaussian Belief Propagation (GBP) is exact for marginals – Weiss, Freeman (2001); Rusmevichientong, Roy (2001)
- Walk-Sum approach – Johnson (2002); Malioutov, Johnson, Willsky (2007)
- Walk-Sum for determinant and ζ -functions – Johnson (2007)

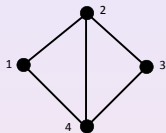
Beyond BP

- $q = \infty$ -ary ... the series is infinite
- finite series ... via fermions \Rightarrow

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)

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

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

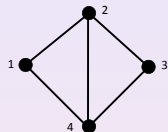
$$w_{ab} \equiv -H_{ab}H_{ba} \quad \text{and} \quad w_a \equiv H_{aa}$$

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

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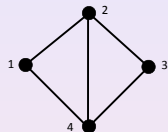
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$$\pi \equiv \pi_v \cup \pi_e, \quad \pi_v \equiv (\pi_a = 0, 1; a \in \mathcal{G}_0), \quad \text{and} \quad \pi_e \equiv (\pi_{ab} = 0, 1; \{a, b\} \in \mathcal{G}_1)$$

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

Highlights (of the last two lectures)

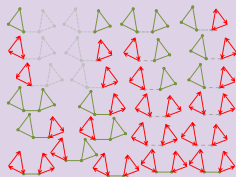
[Chernyak, Chertkov '08]

Loop Series for Determinant

[BP gauge]

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

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

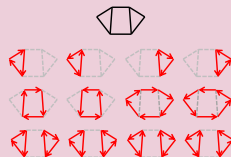


MD as Series of Determinants

[non-BP gauge]

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

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



Berezin/Grassman (super) Calculus

Berezin/Grassman (anti-commuting) Variables, Integrals

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

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

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 Grassmans on vertexes

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

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

via Grassmans on edges

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

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

$$\alpha = \{a, b\}, \quad \chi_\alpha = \{\chi_{ab}, \chi_{ba}\}, \quad \bar{\chi}_\alpha = \{\bar{\chi}_{ab}, \bar{\chi}_{ba}\}$$

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

$$\chi_a = \{\chi_{ba}\}_{b \in \mathcal{G}_0, b \sim a}, \quad \bar{\chi}_a = \{\bar{\chi}_{ba}\}_{b \in \mathcal{G}_0, b \sim a}$$

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 $\forall \alpha = \{a, b\}$:

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

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

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

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

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

- Variational constraints:

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

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 $\{a, c\} \in \mathcal{G}_1$:

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

- Variational constraints:

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

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”: $Z_{BP;fermi} Z_{BP;bose} = 1$

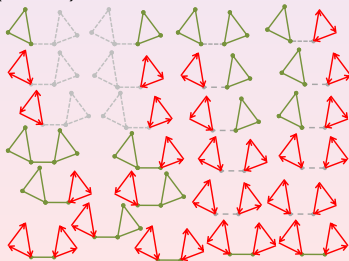
Loop Series for Determinant

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

$GL(\mathcal{G})$ - 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



Gauge Theory

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

\equiv

Monomer-Dimer

\equiv

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

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

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

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

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

From Gauge Theory to Determinants

From Graphical Gauge Model

$$\begin{aligned} Z &= \int_{\mathcal{G}_1} \mathcal{D}\sigma \int \mathcal{D}\theta \mathcal{D}\bar{\theta} \exp(S_0(\bar{\theta}, \theta; \sigma)) \\ &= \int \mathcal{D}\theta \mathcal{D}\bar{\theta} \prod_{a \in \mathcal{G}_0} e^{w_a \bar{\theta}_a \theta_a} \prod_{\{a,b\} \in \mathcal{G}_1} \left(e^{H_{ab} \bar{\theta}_a \theta_b + H_{ba} \bar{\theta}_b \theta_a} - [H_{ab} \bar{\theta}_a \theta_b + H_{ba} \bar{\theta}_b \theta_a] \right) \end{aligned}$$

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-monomers

Monomer-Dimer Models and Determinants [Cycle Series]

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

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

Series over “odd” states

▶ Det as Series over non-BP gauges :

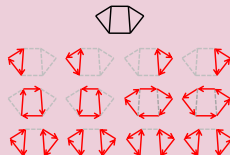
$$\det(H) = \sum_{C \in ODC(\mathcal{G})} r(C), \quad r(C) = (-1)^{|C|} \prod_{(a,b) \in C} H_{ab} Z_{\text{MD}}(\mathcal{G} \setminus C)$$

MD as Series of Determinants

[non-BP gauge]

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

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



Future Challenges (Loops +)

- Efficient Approximate Algorithms
- Relation, Complementarity to MCMC, Mixed Schemes
- Graphical Transformations as Gauges
- Mixed (continuous/discrete) constructions
- Disorder Average (ensembles, density evolution), Relation to Cavity, Replica Calculations
- Phase Transitions in Glasses (Physics) and SAT (CS, IT)
- Dynamical Graphical Models (non-equilibrium)

Fermion-Gauge Approach

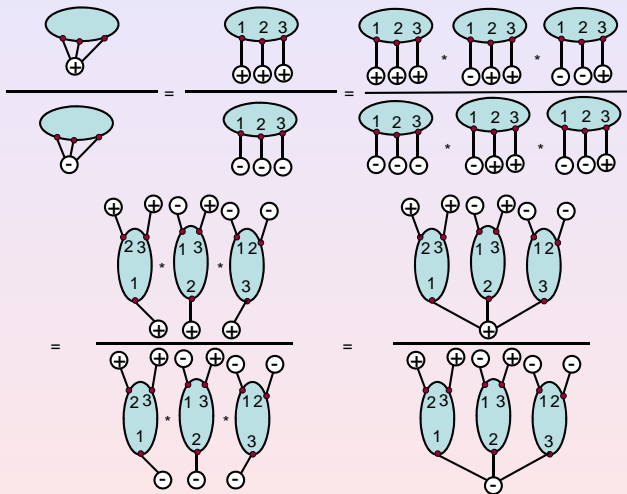
- Extension to Surface Graphs (embedded into surfaces with nonzero genus)
- Easy and almost-easy planar and surface models
- From loops, cycles to walks/paths (e.g. in relation with Walk-Sum and ζ -functions). From sums to products (sums for log-partitions)
- Super-Symmetric (fermions and bosons) Graphical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

Thank You!

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

▶ Bibliography List (A)

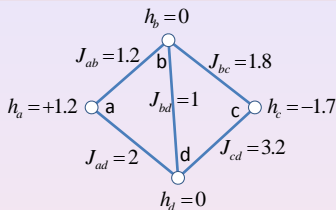
▶ Bibliography List (B)



◀ Self Avoiding Tree

Undirected \Rightarrow Directed \Rightarrow (s-t)-Extended

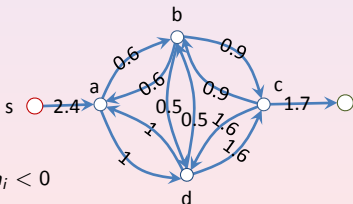
$$\min_{\sigma} \left(-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}} J_{ij} \sigma_i \sigma_j - \sum_{i \in \mathcal{G}} h_i \sigma_i \right) \Big|_{\forall i \in \mathcal{G}: \sigma_i = \pm 1}$$



$$\min_{\sigma} \left(-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'_d} J_{i \rightarrow j} \sigma_i \sigma_j \right) \Big|_{\forall i \in \mathcal{G}'_d: \sigma_i = \pm 1; \sigma_s = +1; \sigma_t = -1}$$

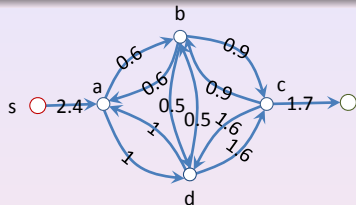
directed: $J_{i \rightarrow j} = J_{j \rightarrow i} = J_{ij}/2$

(s-t) extended: $J_{s \rightarrow i} = 2h_i$, if $h_i > 0$ $J_{i \rightarrow t} = 2|h_i|$, if $h_i < 0$



From Vertexes to Edges

$$\min_{\sigma} \left(-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'_d} J_{i \rightarrow j} \sigma_i \sigma_j \right) \left| \begin{array}{l} \forall i \in \mathcal{G}'_d: \sigma_i = \pm 1; \sigma_s = +1; \sigma_t = -1 \end{array} \right.$$



Integer Linear Programming

$$\eta_{i \rightarrow j} = \begin{cases} 1, & \sigma_i = 1, \sigma_j = -1 \\ 0, & \text{otherwise} \end{cases} \quad p_i = (1 - \sigma_i)/2 = 0, 1$$

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2 - 4(\eta_{i \rightarrow j} + \eta_{j \rightarrow i}), \quad \sigma_s \sigma_i = 1 - 2\eta_{s \rightarrow i}, \quad \sigma_i \sigma_t = 1 - 2\eta_{i \rightarrow t}$$

$$-\frac{1}{2} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} + \min_{\{\eta, p\}} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} \eta_{i \rightarrow j} \left| \begin{array}{l} \forall i \in \mathcal{G}'_d, p_i = 0, 1; \quad p_s = 0, \quad p_t = 1 \\ \forall (i \rightarrow j) \in \mathcal{G}'_d: \\ p_i - p_j + \eta_{i \rightarrow j} = 0, 1 \end{array} \right.$$

FRFI=Min-Cut=Max-Flow

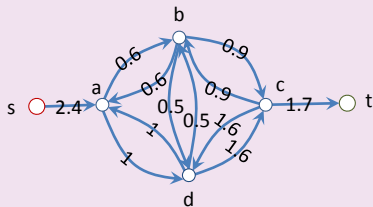
$$-\frac{1}{2} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} + \min_{\{\eta, p\}} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} \eta_{i \rightarrow j}$$

$$\forall i \in \mathcal{G}'_d, p_i = 0, 1; p_s = 0, p_t = 1$$

$$\forall (i \rightarrow j) \in \mathcal{G}'_d:$$

$$p_i - p_j + \eta_{i \rightarrow j} = 0, 1$$

Min-Cut



Max-Flow

A.K. Hartman & H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, 2002,
 and references therein

FRFI=Min-Cut=Max-Flow

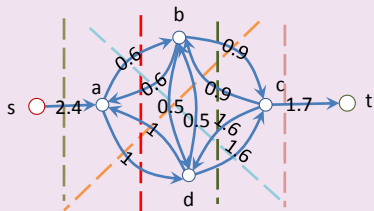
$$-\frac{1}{2} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} + \min_{\{\eta, p\}} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} \eta_{i \rightarrow j}$$

$$\forall i \in \mathcal{G}'_d, p_i = 0, 1; p_s = 0, p_t = 1$$

$$\forall (i \rightarrow j) \in \mathcal{G}'_d:$$

$$p_i - p_j + \eta_{i \rightarrow j} = 0, 1$$

Min-Cut



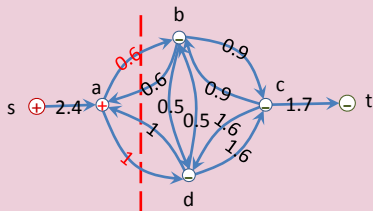
Max-Flow

A.K. Hartman & H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, 2002,
 and references therein

FRFI=Min-Cut=Max-Flow

$$-\frac{1}{2} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} + \min_{\{\eta, p\}} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} \eta_{i \rightarrow j} \quad \left| \quad \begin{aligned} \forall i \in \mathcal{G}'_d, p_i = 0, 1; p_s = 0, p_t = 1 \\ \forall (i \rightarrow j) \in \mathcal{G}'_d: \\ p_i - p_j + \eta_{i \rightarrow j} = 0, 1 \end{aligned} \right.$$

Min-Cut



Max-Flow

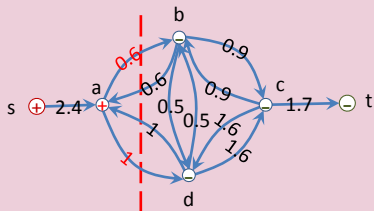
A.K. Hartman & H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, 2002,
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FRFI=Min-Cut=Max-Flow

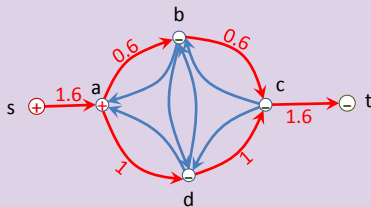
$$-\frac{1}{2} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} + \min_{\{\eta, p\}} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} \eta_{i \rightarrow j} \quad \forall i \in \mathcal{G}'_d, p_i = 0, 1; p_s = 0, p_t = 1$$

$$\forall (i \rightarrow j) \in \mathcal{G}'_d: p_i - p_j + \eta_{i \rightarrow j} = 0, 1$$

Min-Cut



Max-Flow



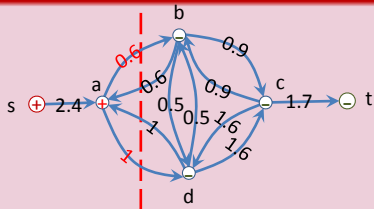
A.K. Hartman & H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, 2002,
 and references therein

Back to Undirected Graph

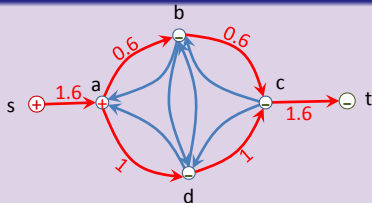
$$-\frac{1}{2} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} + \min_{\{\eta, p\}} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} \eta_{i \rightarrow j} \quad \forall i \in \mathcal{G}'_d, p_i = 0, 1; p_s = 0, p_t = 1$$

$$\forall (i \rightarrow j) \in \mathcal{G}'_d : p_i - p_j + \eta_{i \rightarrow j} = 0, 1$$

Min-Cut



Max-Flow



$$-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'} J_{ij} + \min_{\{\eta, p\}} \sum_{(ij) \in \mathcal{G}'_d} J_{ij} \eta_{ij} \quad \forall i \in \mathcal{G}', p_i = 0, 1; p_s = 0, p_t = 1$$

$$\forall (i, j) \in \mathcal{G}' : p_i - p_j + \eta_{ij} = 0, 1$$

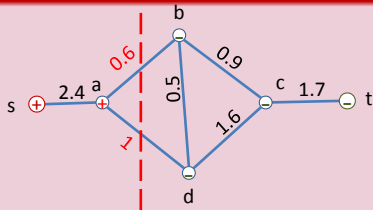
$$J_{si} = 2h_i, \quad \text{if } h_i > 0 \quad J_{it} = 2|h_i|, \quad \text{if } h_i < 0$$

Back to Undirected Graph

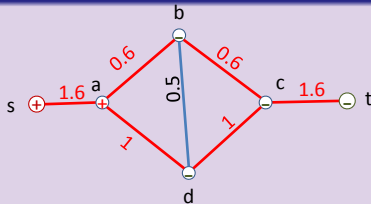
$$-\frac{1}{2} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} + \min_{\{\eta, p\}} \sum_{(i \rightarrow j) \in \mathcal{G}'_d} J_{i \rightarrow j} \eta_{i \rightarrow j} \quad \forall i \in \mathcal{G}'_d, p_i = 0, 1; p_s = 0, p_t = 1$$

$$\forall (i \rightarrow j) \in \mathcal{G}'_d : p_i - p_j + \eta_{i \rightarrow j} = 0, 1$$

Min-Cut



Max-Flow



$$-\frac{1}{2} \sum_{(i,j) \in \mathcal{G}'} J_{ij} + \min_{\{\eta, p\}} \sum_{(ij) \in \mathcal{G}'_d} J_{ij} \eta_{ij} \quad \forall i \in \mathcal{G}', p_i = 0, 1; p_s = 0, p_t = 1$$

$$\forall (i,j) \in \mathcal{G}' : p_i - p_j + \eta_{ij} = 0, 1$$

$$J_{si} = 2h_i, \quad \text{if } h_i > 0 \quad J_{it} = 2|h_i|, \quad \text{if } h_i < 0$$

Grassmann (fermion) Calculus for Pfaffians

Grassman Variables on Vertexes

$$\forall (a, b) \in \mathcal{G}_e : \quad \theta_a \theta_b + \theta_b \theta_a = 0 \quad \int d\theta = 0, \quad \int \theta d\theta = 1$$

Pfaffian as a Gaussian Berezin Integral over the Fermions

$$\int \exp\left(-\frac{1}{2} \vec{\theta}^t \hat{A} \vec{\theta}\right) d\vec{\theta} = \text{Pf}(\hat{A}) = \sqrt{\det(\hat{A})}$$

◀ Pfaffian Formula

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

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

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

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

My papers on ... (A)

Loop Calculus, Loop Series, Loop 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](http://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](http://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](http://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](http://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](http://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](http://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](http://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.

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