Belief Propagation & Beyond

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Outline

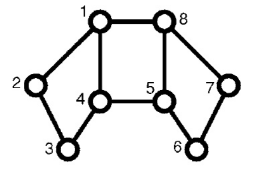
1. Introduction
   - Graphical Models
   - Message Passing/ Belief Propagation
   - Gauge Transformations & Loop Calculus
2. Planar Graphical Models
   - Dimer and Ising Models on Planar Graphs
   - Planar (and surface) graphical models which are det-easy
3. The Story of Permanent
   - BP for Permanent
   - Loop Calculus, Lower and Upper Bounds for Permanent

Binary Graphical Models

Forney style - variables on the edges

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

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



$$f_a \geq 0$$

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

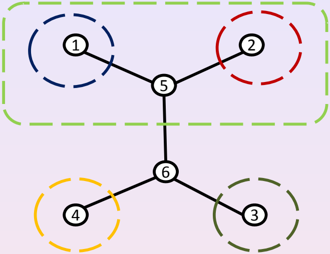
$$\vec{\sigma}_1 = (\sigma_{12}, \sigma_{14}, \sigma_{18})$$

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

- 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** – Our main object of interest

Examples

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



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

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

Belief Propagation Equations

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

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

Belief Propagation (BP) and Message Passing

- Apply what is exact on a tree (the equation) to other problems on graphs with loops [heuristics ... but a good one]
- To solve the system of N equations is EASIER then to count (or to choose one of) 2^N states.

Bethe Free Energy formulation of BP [Yedidia, Freeman, Weiss '01]

Minimize the Kubblack-Leibler functional

$$\mathcal{F}\{b(\{\sigma\})\} \equiv \sum_{\{\sigma\}} b(\{\sigma\}) \ln \frac{b(\{\sigma\})}{\mathcal{L}(\{\sigma\})}$$

Difficult/Exact

under the following "almost variational" substitution" for beliefs:

$$b(\{\sigma\}) \approx \frac{\prod_i b_i(\boldsymbol{\sigma}_i) \prod_j b^j(\boldsymbol{\sigma}^j)}{\prod_{(i,j)} b_i^j(\sigma_i^j)} \quad \text{[tracking]}$$

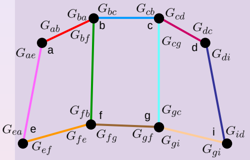
Easy/Approximate

- Message Passing is a (graph) Distributed Implementation of BP
- Graphical Models = the language

Gauge Transformations

Chertkov, Chernyak '06

Local Gauge, G, Transformations



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

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

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

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

The partition function is invariant under any G-gauge!

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

Belief Propagation as a Gauge Fixing

Chertkov, Chernyak '06

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

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

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

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

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

Belief Propagation as a Gauge Fixing (II)

$\underline{\forall a \;\&\; \forall b \in a:}$

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

Belief Propagation in terms of Messages

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

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

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

Loop Series:

Chertkov,Chernyak '06

Exact (!!) expression in terms of BP

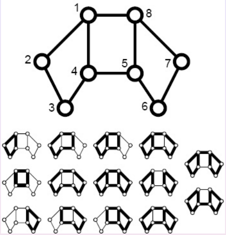
$$Z = \sum_{\vec{\sigma}_\sigma} \prod_a f_a(\vec{\sigma}_a) = Z_0 \left(1 + \sum_C r(C)\right)$$

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

$C \in$ 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.

BP (Loop Calculus) + results ('06-...)

... not discussed today ...

- Exact Algorithm & Efficient Truncation of Loops [V. Gómez, J.M. Mooij, H.J. Kappen '06]
- Improving LP/BP decoding with loops [MC '07]
- Loop Tower (general finite alphabet) [VC,MC '07]
- Low bound on partition function for some special (attractive) graphical models [Sudderth, Wainwright, Willsky '07]
- Fermions & Loops, e.g. monomer-dimer =series over dets [VC,MC '08]
- Counting Independent Sets Using the Bethe Approximation [V. Chandrasekaran, MC, D. Gamarnik, D. Shah, J. Shin '09]
- Beyond Gaussian BP (det=BP*det & orbit product) [J. Johnson, VC, MC '09-'10]
- ... also ... Particle Tracking (Learning with BP), Phase Transitions in Power Grids, Interdiction and OTHER APPLICATIONS

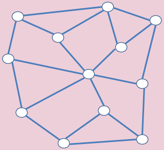
- BP+ and gauges on planar and surface graphs [VC, MC '09-'10]
- BP+ for Permanents (of non-negative matrices) [Y. Watanabe, MC '09]

Outline

Glassy Ising & Dimer Models on a Planar Graph

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

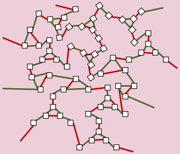
$$Z = \sum_{\vec{\sigma}} \exp\left(\frac{\sum_{(i,j)\in\Gamma} J_{ij}\sigma_i\sigma_j}{T}\right)$$



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

perfect matching

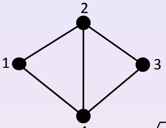
$$Z = \sum_{\vec{\pi}} \prod_{(i,j)\in\Gamma} (z_{ij})^{\pi_{ij}} \prod_{i\in\Gamma} \delta\left(\sum_{j\in i} \pi_{ij}, 1\right)$$



Ising & Dimer Classics

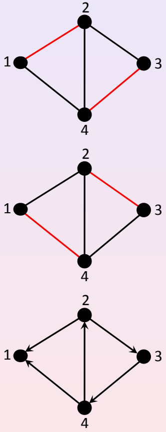
- L. Onsager, *Crystal Statistics*, Phys.Rev. **65**, 117 (1944)
- M. Kac, J.C. Ward, *A combinatorial solution of the Two-dimensional Ising Model*, Phys. Rev. **88**, 1332 (1952)
- C.A. Hurst and H.S. Green, *New Solution of the Ising Problem for a Rectangular Lattice*, J.of Chem.Phys. **33**, 1059 (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)

Pfaffian solution of the Matching problem



$$Z = z_{12}z_{34} + z_{14}z_{23} = \sqrt{\mathrm{Det}\hat{A}} = \mathrm{Pf}[\hat{A}]$$

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



Odd-face [Kasteleyn] rule (for signs)

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

Planar is generally difficult [Barahona '82]

- Planar spin-glass problem with magnetic field is difficult
- Dimer-monomer matching is difficult even in the planar case

Are there other (than Ising and dimer) planar graphical models which are det-easy?

Holographic Algorithms [Valiant '02-'08]

- reduction to dimers via
- "classical" one-to-one gadgets
  (e.g. Ising model to dimer model)
- "holographic" gadgets (e.g. ▸ Ice model to Dimer model)
- resulted in discovery of variety of new easy planar models

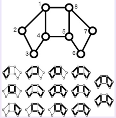
Gauge Transformations [Chertkov, Chernyak '06-'09]

- Equivalent to the holographic gadgets
  (different gauges = different transformations)
- Belief Propagation (BP) is a special choice of the gauge freedom ...
  other gauges may also be useful

BP+ for Planar [degree ≤ 3]

Loop Series (general)
[MC,Chernyak '06]

$$Z = Z_0 \cdot z,\ \ z \equiv 1 + \sum_C r_C$$



Summing 2-regular (closed curve) partition is det-easy!!
[MC,Chernyak,Teodorescu '08]

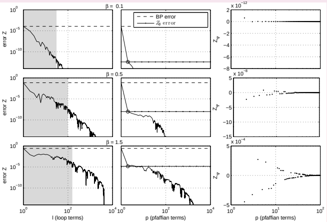
$$Z_s = Z_0 \cdot z_s, \quad z_s = 1 + \sum_{C \in \mathcal{G}}^{\forall a \in C,\ |\delta(a)|_C = 2} r_C$$

[JSTAT '08]

Efficient Approximate Scheme
[Gomez,MC,Kappen '09]

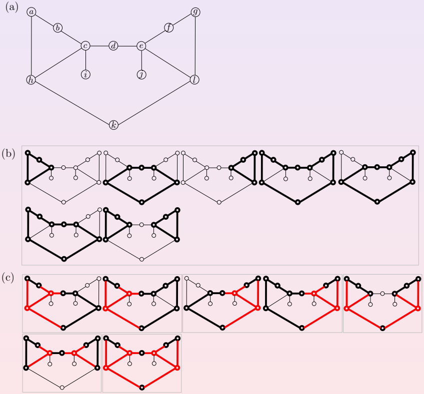
http://arXiv.org/abs/0901.0786

UAI, 2009 + to appear in JML '10



Easy Models of degree ≤ 3 [MC,Chernyak,Teodorescu '08]

Generic planar problem is difficult



"three-colorings" are shown in red

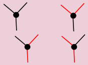
A planar problem is easy if

- All (!!) "three-colorings" are zero after a BP-transformation [BP gauge= all (!!) "one-colorings" are zero]

Easy Models of degree ≤ 3 (II)

To describe the family of easy edge-binary models of degree not larger than three (partition function is reducible to Pfaffian of a $|\mathcal{G}_1| \times |\mathcal{G}_1|$-dimensional skew-symmetric matrix) one needs to:

Item #1: Generate an arbitrary factor-function set which satisfies: $\forall a: \quad W^{(a)}(\vec{\sigma}_a) = 0 \quad \text{if} \quad \sum_{b\sim a} \sigma_{ab} \neq 0 (\text{mod } 2)$



Item #2: Apply an arbitrary skew-orthogonal Gauge-transformation:

$$W^{(a)}(\boldsymbol{\pi}_a) \to f_a(\boldsymbol{\pi}_a) = \sum_{\boldsymbol{\pi}'_a} \left(\prod_{b\sim a} G_{ab}(\pi_{ab}, \pi'_{ab}) \right) W^{(a)}(\boldsymbol{\pi}'_a)$$

$$\forall \{a, b\} \in \mathcal{G}_1 : \quad \sum_{\pi} G_{ab}(\pi, \pi') G_{ba}(\pi, \pi'') = \delta(\pi', \pi'')$$

$$Z = \sum_{\boldsymbol{\pi}} \prod_{a\in\mathcal{G}_0} f_a(\boldsymbol{\pi}_a) = \sum_{\boldsymbol{\pi}} \prod_{a\in\mathcal{G}_0} \left(\sum_{\boldsymbol{\pi}'_a} \left(\prod_{b\sim a} G_{ab}(\pi_{ab}, \pi'_{ab}) \right) W^{(a)}(\boldsymbol{\pi}_a) \right)$$

Next Step:

Generalize construction (Item #1) to degree> 3 [Item #2 is already generic]

Easy Planar and Surface Models of arbitrary degree [MC,VC '09-]

- We constructed the family of graphical models of a given planar graph which are det-easy arXiv:0902.0320
  Dirty Planar Details
- We generalized this construction to g-surface graphs (graphs embedded into a surface of genus g): Described a family of graphical models defined on a given g-surface graph which are surface-easy = partition function is a sum of 2^{2g} dets
  Dirty Surface Details

Selling:

Family of computationally tractable planar and surface graphical models

Buying:

Applications in IT (capacity, decoding) and CS (counting, inference)

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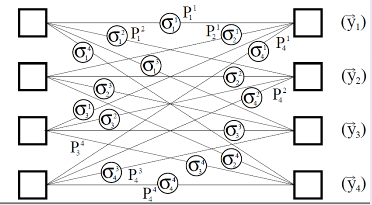
Tracking Particles = Motivational Example



$$\mathcal{L}(\{\sigma\}|\boldsymbol{\theta}) = C(\{\sigma\}) \prod_{(i,j)} \left[P_i^j \left(\mathbf{x}_i, \mathbf{y}^j | \boldsymbol{\theta} \right) \right]^{\sigma_i^j}$$

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

Surprising Exactness of BP for ML-assignement

- Exact Polynomial Algorithms (auction, Hungarian) are available for the problem
- Generally BP is exact only on a graph without loops [tree]
- In this [Perfect Matching on Bipartite Graph] case it is still exact in spite of many loops!! [Bayati, Shah, Sharma '08], also Linear Programming/TUM interpretation [MC '08]

Computing permanent of a positive matrix (weighted number of possible matchings) is an important subtask [MC, Kroc, Krzakala, Vergassola, Zdeborova '09]

BP for Permanent

The Graphical Model

$$\sigma = (\sigma_i^j = 0,1 | i,j = 1,\cdots,N \text{ s.t.} \forall i: \ \sum_j \sigma_i^j = 1 \ \& \ \forall j: \ \sum_i \sigma_i^j = 1)$$
$$\mathcal{P}(\sigma) = P(\sigma)/Z = (p_i^j)^{\sigma_i^j/T}/Z, \quad Z \equiv \sum_\sigma (p_i^j)^{\sigma_i^j/T}$$

Bethe Free Energy

$$\mathcal{F}_{BP} \equiv E - TS, \quad E\{\beta_i^j\} = -\sum_{(i,j)} \beta_i^j \log(p_i^j)$$
$$S\{\beta_i^j\} = \sum_{(i,j)} \left((1-\beta_i^j)\ln(1-\beta_i^j) - \beta_i^j \ln \beta_i^j\right)$$

conditions: $\forall i: \quad \sum_j \beta_i^j = 1; \qquad \forall j: \quad \sum_i \beta_i^j = 1$

BP equations

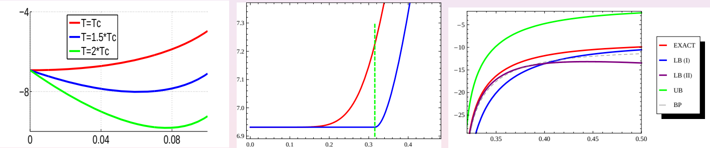
$$\forall (i,j): \quad \beta_i^j(1-\beta_i^j) = (p_i^j)^{1/T} \exp\left(\mu_i + \mu^j\right)$$
$$\forall i: \quad \sum_j \beta_i^j = 1; \qquad \forall j: \quad \sum_i \beta_i^j = 1$$

BP for Permanents (II)

[Y.Watanabe & MC '09]

Example: Homogeneous weight model biased towards a perfect solution

- $\Pi_*(i) = i$: $p_i^j = 1$ if $i \neq j$ and $p_i^i = W (W > 1)$
- Looking for solution in the form: $\beta_i^j(T) = \begin{cases} 1 - \epsilon(N-1) & \text{:if } i = j \\ \epsilon & \text{:otherwise,} \end{cases}$.
- A nontrivial BP solution, $\beta_i^j \neq 0, 1$ for all $(i,j) \in E$, is realized only at $T > T_c = \ln W / \ln(N-1)$.



(a) $\mathcal{F}_{BP}$ vs ϵ. (b) $T \ln Z$ vs T. (c) $\ln(Z/Z_{BP})$ vs T for different estimators.

Proposition: The threshold behavior is generic!

$\det(P_i^j - 2\delta_{\Pi_*(i),j} P_i^j) = 0$ is eq. for T_c, where Π_* is the ML solution.

Three faces of Loop Calculus for Permanent

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

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

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

Main Theorem of [arxiv:0911.1419 Y. Watanabe & MC '09]

$$Z = \text{perm}(P) = Z_{BP} * \text{perm}(\beta. * (1 - \beta)) \prod_{(i,j) \in E} (1 - \beta_i^j)^{-1}$$

where β is the double-stochastic BP-solution matrix for P

Upper and Lower Bounds for Permanent [Y. Watanabe & MC '09]

Gurvits (2008)-van der Waerden (1926) Theorem

For an arbitrary non-negative $N \times N$ matrix A, $\text{perm}(A) \geq \text{cap}(p_A)\frac{N^N}{N!}$, where $p_A(x) = \prod_i \sum_j a_{i,j} x_j$, $\quad \text{cap}(p_A) = \inf_{x \in \mathbb{R}^N_{>0}} \frac{p_A(x)}{\prod_j x_j}$

Application of the Gurvits-van der Waerden Theorem to the Loop Series yields

- The low bound is invariant wrt BP transformation
- $\text{perm}(\beta .* (1-\beta)) \geq \frac{N!}{N^N} \prod_{(i,j)\in E} (1-\beta_i^j)^{\beta_i^j}$

Another (dominating at high temperature) low bound on the Loop Series

$$\text{perm}(\beta .* (1-\beta)) \geq 2\prod_i \beta_i^{\Pi(i)}(1-\beta_i^{\Pi(i)})$$

Upper Bound following from the Godzil-Gutman representation for permanent

$$\text{perm}(\beta .* (1-\beta)) \leq \prod_j (1 - \sum_i (\beta_i^j)^2)$$

Summary of the Permanent Story

Selling: arxiv:0911.1419

- Threshold behavior of BP solution wrt temperature
- New low and upper bounds for permanent based on Loop Calculus

Buying:

- Improved Algorithm correcting permanent beyond BP
- New Applications for the technique

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, $N \to \infty$
- Phase Transitions

Binary Graphical Models

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

Probabilistic Reconstruction (Statistical Inference)

$\vec{\sigma}_{\text{orig}}$	$\Rightarrow$	$\vec{x}$	$\Rightarrow$	$\vec{\sigma}$
original *data* $\vec{\sigma}_{\text{orig}} \in \mathcal{C}$ codeword	noisy channel $\mathcal{P}(\vec{x}\|\vec{\sigma})$	corrupted data: log-likelihood magnetic field	statistical inference	possible preimage $\vec{\sigma} \in \mathcal{C}$

Maximum Likelihood [ground state]

Marginalization

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

Counting (Partition Function): $Z(\vec{x}) = \sum_{\vec{\sigma}} \mathcal{P}(\vec{x}|\vec{\sigma})$

Binary Graphical Models

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

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Binary Graphical Models

Grassmann (fermion, nilpotent) Calculus for Pfaffians

Grassman (nilpotent) 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

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

Pfaffian Formula

Ice Model [vertexes of max degree 3]

#PL-3-NAE-ICE [Valiant '02]

- Input: A planar graph G = (V;E) of maximum degree 3.
- Output: The number of orientations (arrows) such that no node has all the edges directed towards it or away from it.

From arrows to binary variables

- Edge $\{a, b\}$ is broken in two by insertion of $a - b$ vertex
- Introduce binary variables s.t. if
  $a \to b \Rightarrow \pi_{a,a-b} = 0, \pi_{b,a-b} = 1$
  $b \to a \Rightarrow \pi_{a,a-b} = 1, \pi_{b,a-b} = 0$

$$Z_{ice} = \sum_{\boldsymbol{\pi}'} \left(\prod_{a \in \mathcal{G}_0} f_a(\tilde{\boldsymbol{\pi}}_a) \right) \left(\prod_{\{a,b\} \in \mathcal{G}_1} g_{a-b}(\pi_{a,a-b}, \pi_{b,a-b}) \right)$$

$$f_a(\boldsymbol{\pi}'_a) = \begin{cases} 1, & \exists\ b, c \in \delta_{\mathcal{G}}(a), \quad \text{s.t.} \quad \pi_{a,a-b} \neq \pi_{a,a-c} \\ 0, & \text{otherwise} \end{cases}$$

$$g_{a-b}(\boldsymbol{\pi}'_a) = \begin{cases} 1 & \pi_{a,a-b} \neq \pi_{b,a-b} \\ 0, & \text{otherwise} \end{cases}$$

Holographic Gadgets & Gauges

Ice Model [vertexes of max degree 3] II

General Gauge Transformation

$$f_a(\boldsymbol{\pi}_a) \to \tilde{f}_a(\boldsymbol{\pi}_a) = \sum_{\boldsymbol{\pi}'_a} \left(\prod_{b\sim a} G_{ab}(\pi_{ab}, \pi'_{ab}) \right) f_a(\boldsymbol{\pi}'_a)$$

$$\forall \{a,b\} \in \mathcal{G}_1 : \quad \sum_{\pi} G_{ab}(\pi, \pi') G_{ba}(\pi, \pi'') = \delta(\pi', \pi'')$$

$$Z = \sum_{\boldsymbol{\pi}} \prod_{a\in\mathcal{G}_0} \tilde{f}_a(\boldsymbol{\pi}_a) = \sum_{\boldsymbol{\pi}} \prod_{a\in\mathcal{G}_0} \left(\sum_{\boldsymbol{\pi}'_a} \left(\prod_{b\sim a} G_{ab}(\pi_{ab}, \pi'_{ab}) \right) f_a(\boldsymbol{\pi}_a) \right)$$

Gauge Transformation for the Ice model

$$G^{(ice)}_{a,a-b} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad \tilde{g}_{a-b}(\boldsymbol{\pi}'_a) = \begin{cases} 1, & \pi_{a,a-b} = \pi_{b,a-b} = 0 \\ -1, & \pi_{a,a-b} = \pi_{b,a-b} = 1 \\ 0, & \text{otherwise} \end{cases}$$

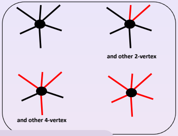
$$\tilde{f}_a(\pi_{a,a-1}, \pi_{a,a-2}, \pi_{a,a-3}) = \frac{3}{\sqrt{2}} * \begin{cases} 1, & \pi_{a,a-1} = \pi_{a,a-2} = \pi_{a,a-3} = 0 \\ -1/3, & \sum_i \pi_{a,a-i} = 2 \\ 0, & \text{otherwise} \end{cases}$$

Holographic Gadgets & Gauges

Edge Binary Wick (EBW) Models

[Chernyak, MC '09]

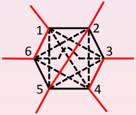
$$Z_{EBW}(W) = \sum_{\gamma=\{\gamma_{ab}\}\in\mathcal{Z}_1(\mathcal{G};\mathbb{Z}_2)} \prod_{b\in\mathcal{G}_0}^{\sum_{a\sim b}\gamma_{ab}\neq 0} W^{(b)}_{\{a_1,\cdots,a_{2k}\}\equiv\{a|a\sim b;\gamma_{ab}=1\}}$$



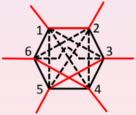
- All odd weights are zero
- Even $(d > 2)$ weights are expressed via pair-wise weights

$$W^{(b)}_{\{a_1,\cdots,a_{2k}\}} \equiv \sum_{\xi\in P([2k-1])} W^{(b)}_{\xi,a_1\cdots a_{2k}}, \quad W^{(b)}_{\xi,a_1\cdots a_{2k}} \equiv (-1)^{\overbrace{\sum_{p,p'\in\xi}^{p<p'} C_{\alpha(p)}\cdot C_{\alpha(p)'}}^{\text{number of crossings (mod 2)}}} \cdot \prod_{p\in\xi} W^{(b)}_{\alpha(p)}$$

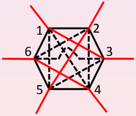
Examples of 6-colorings and extensions of a EBW-model 6 vertex



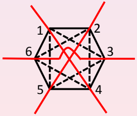
$W_{16}W_{25}W_{34}$ [zero crossing]



$-W_{12}W_{35}W_{46}$ [one crossing]



$W_{13}W_{25}W_{46}$ [two crossings]



$-W_{14}W_{25}W_{36}$ [three crossings]

Edge Binary Wick Models (II)

Known Easy Planar Graphical Models & EBW

$\exists$ a gauge transformation reducing any easy planar model to a EBW

- Dimer Model
- Ising Model
- Ice Model
- Possibly all models discussed in the "holographic" papers

Any EBW model on a planar graph is EASY

- Equivalent to Gaussian Grassman Models on the same graph
- Partition function is Pfaffian of a $|\mathcal{G}_1| \times |\mathcal{G}_1|$ matrix

Related Grassmann/Fermion Models

Vertex Gaussian Grassmann Graphical (VG^3) Models

$$Z_{VG^3}(\varsigma,\boldsymbol{\sigma};\mathbf{W}) = \frac{\int \exp\left(\frac{1}{2}\sum\limits_{(b\to a\to c)\in\mathcal{G}_1}\varphi_{ab}\varsigma^{(a)}_{bc}W^{(a)}_{bc}\varphi_{ac}\right)\exp\left(\frac{1}{2}\sum_{(a,b)\in\mathcal{G}_1}\varphi_{ab}\sigma_{ab}\varphi_{ba}\right)\prod\limits_{(a,b)}d\varphi_{ab}}{\int \exp\left(\frac{1}{2}\sum_{(a,b)\in\mathcal{G}_1}\varphi_{ab}\sigma_{ab}\varphi_{ba}\right)\prod\limits_{(a,b)}d\varphi_{ab}}$$

$$= \frac{\mathrm{Pf}(H(\varsigma,\boldsymbol{\sigma};\mathbf{W}))}{\mathrm{Pf}(H(\varsigma,\boldsymbol{\sigma};\mathbf{0}))}, \qquad H_{ij} = \begin{cases} \varsigma^{(a)}_{bc}W^{(a)}_{bc}, & i=(a,b)\ \&\ j=(a,c),\ \text{where } b\neq c\sim a,\\ \sigma_{ab}, & i=(a,b),\ \&\ j=(b,a).\end{cases}$$

Grassmann (anti-commuting) variables: $\forall (a,b),(c,d)\in\mathcal{G}_1 \quad \varphi_{ab}\varphi_{cd} = -\varphi_{cd}\varphi_{ab}$
Berezin (formal) integration rules: $\forall (a,b)\in\mathcal{G}_1: \quad \int d\varphi_{ab} = 0, \quad \int \varphi_{ab}d\varphi_{ab} = 1$

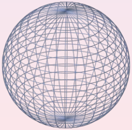
Main Theorem of [Chernyak,MC '09/planar]

- $\exists \sigma,\varsigma = \pm 1:$ s.t. $Z_{VG^3}(\varsigma,\boldsymbol{\sigma};\mathbf{W}) = Z_{EBW}(\mathbf{W})$
- The special configuration of σ,ς corresponds to Kastelyan (spinor) orientation on the extended planar graph

Dimer Model on Surface Graphs (I)

Partition function of dimer model on a surface graph of genus g is expressed in terms of a (± 1)-weighted sum over 2^{2g} determinants $=$ surface-easy

- Kasteleyn '63;'67 - non-constructive (??) conjecture
- Gallucio, Loebl '99 - first [combinatorial] proof
- Cimasoni, Reshetikhin '07 - topological proof and relation to gauge fermion models



genus $g = 0$

genus $g = 1$

genus $g = 2$

Dimer Model on Surface Graphs (II)

Partition Function of Dimer Model, $\pi_{ij} = 0, 1$, on a surface graph $\mathcal{G}$

$$Z(\mathcal{G}; \mathbf{z}) = \sum_{\vec{\pi}}^{\text{dimers}} \prod_{(i,j)\in\Gamma} (z_{ij})^{\pi_{ij}}$$

Theorem: (formulation of Cimasoni, Reshetikhin)

$$Z(\mathcal{G}; \mathbf{z}) = \frac{1}{2^g} \sum_{[\mathbf{s}]} \underbrace{\mathrm{Arf}(q^{\mathbf{s}}_{\boldsymbol{\pi}_0})\varepsilon^{\mathbf{s}}(\boldsymbol{\pi}_0)}_{=\pm 1;\ \boldsymbol{\pi}_0-\text{independent};\ \text{depends only on } [\mathbf{s}]} \mathrm{Pf}(A^{\mathbf{s}}(z))$$

- $\boldsymbol{\pi}_0$ is a reference dimer configuration
- $\mathbf{s}$ is a Kasteleyn orientation; $[\mathbf{s}]$ equivalence classes of the Kasteleyn orientations, 2^{2g} of them
- $\varepsilon^{\mathbf{s}}(\boldsymbol{\pi}) = \pm 1$ defines total signature of the dimer configuration π wrt the Kasteleyn orientation $\mathbf{s}$
- $q^{\mathbf{s}}_{\boldsymbol{\pi}_0}(\alpha)$ is a well-defined quadratic form associated with $\mathbf{s}$, $\boldsymbol{\pi}_0$ and α is a closed curve on $\mathcal{G}$; $\mathrm{Arf}(q^{\mathbf{s}}_{\boldsymbol{\pi}_0})$ is the Arf-invariant of the quadratic form.

Dimer Model on Surface Graphs (III)

[Cimasoni, Reshetikhin]

$$Z(\mathcal{G};\mathbf{z}) = \frac{1}{2^g}\sum_{[\mathbf{s}]} \mathrm{Arf}(q^{\mathbf{s}}_{\boldsymbol{\pi}_0})\varepsilon^{\mathbf{s}}(\boldsymbol{\pi}_0)\mathrm{Pf}(A^{\mathbf{s}}(z))$$

- the sum over determinants can be transformed into the sum over partition functions of Kasteleyn-fermion models
- Kasteleyn orientation is a discrete version of spin(or) structures [from topological field theories]
- Powerful derivation techniques from topology [homology and immersion theories]

Generic graphical model on a surface graph is SURFACE-DIFFICULT

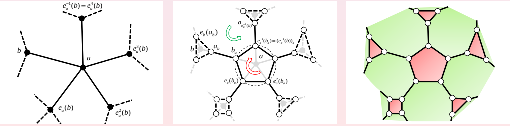
Our next task is:
To classify graphical models which are SURFACE-EASY

Edge-Binary-Wick (EBW) Models and Vertex Gaussian Grassman Graphical (VG^3) models on Surface Graphs

Main Theorem of [Chernyak,MC '09/surface]

$Z_{EBW}(\mathbf{W})Z_{EBW}(\mathbf{1}) = \sum_{[\mathbf{s}]} Z_{VG^3}([\mathbf{s}];\mathbf{1})Z_{VG^3}([\mathbf{s}];\mathbf{W})$ where

- $\mathbf{s} = (\boldsymbol{\sigma};\varsigma)$ corresponds to a Kastelyan/spinor orientation defined on extended graph
- $[\mathbf{s}]$ are equivalence classes (2^{2g} of them) of the Kastelyan/spinor $\mathbf{s}$ orientations



(d) Original graph (e) Extended graph (f) Surface graph

EBW and VG^3 models on Surface Graphs (II)

$$Z_{EBW}(\mathbf{W})Z_{EBW}(\mathbf{1}) = \sum_{[\mathbf{s}]} Z_{VG^3}([\mathbf{s}];\mathbf{1})Z_{VG^3}([\mathbf{s}];\mathbf{W})$$

The multi-step proof of the main surface theorem includes

- Extended/fat graph construction and partitioning ξ of the even generalized loop γ configurations into closed curves [Wick structure]
- Analysis and relation between invariant objects (quadratic forms) for the generalized loops, $[\gamma]$, and spinors, $[s]$, defined on fat graphs and respective Riemann surfaces.
- Term by term comparison of the relation between the partial $\tilde{Z}_{EBW}([\gamma];\mathbf{W})$ and $\tilde{Z}_{VG^3}([\gamma],[\mathbf{s}];\mathbf{W})$, where $Z_{EBW}(\mathbf{W}) = \sum_{[\gamma]} \tilde{Z}_{EBW}([\gamma];\mathbf{W})$ and $Z_{VG^3}([\mathbf{s}];\mathbf{W}) = \sum_{[\gamma]} \tilde{Z}_{VG^3}([\gamma],[\mathbf{s}];\mathbf{W})$. This results in the system of 2^{2g} linear equations for 2^{2g} unknowns $\tilde{Z}_{EBW}([\gamma];\mathbf{W})$.
- Solving the linear equations we recover the main statement of the theorem.
- $2^g Z_{VG^3}([\mathbf{s}];\mathbf{1}) = \mathrm{Arf}(q([s]))Z_{EBW}(\mathbf{1})$, where $q(s)(\gamma) = q([s])([\gamma])$ is a well-defined quadratic form.

Main "take home" message

Q:

Describe the family of surface-easy edge-binary models on an arbitrary surface graph $\mathcal{G}$ (partition function is reducible to a sum of 2^{2g} Pfaffians)

A: [constructive]

- Generate an arbitrary Vertex Gaussian Grassmann binary-Gauge (VG^3) Model on the graph
- Fix the binary-gauge according to the Kasteleyn (spinor) rule on the extended graph
- Construct respective Edge-Binary Wick model on the original graph
- Apply an arbitrary skew-orthogonal (holographic) gauge/transformation

The partition function of the resulting model is the sum of 2^{2g} $\pm$-weighted Pfaffians. [All terms in the sum are explicitly known.]

Where do we go from here?

Future work

- Use the described hierarchy of easy planar models as a basis for efficient variational approximation of generic (difficult) planar problems. (The approach may also be useful for building efficient variational matrix-product state wave functions for quantum models. Dynamical Bayesian Networks: 1+1, tree+1, ...)
- Study Wick Gaussian models on non-planar but Pfaffian orientable or k-Pfaffian orientable graphs (where any dimer model on surface graph of genus g is 2^{2g}-Pfaffian orientable).
- Almost Planar = Geographical Graphical Models, Renormalization Group, Generalized BP
- Analogs of all of the above for Surface-Difficult Problems