Loop Calculus: Exact Inference in terms of Belief Propagation (Message Passing)

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Outline

Statistical Inference

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

Maximum Likelihood | symbol Maximum-a-Posteriori

$$\text{ML} = \arg\max_{\boldsymbol{\sigma}} \mathcal{P}(\mathbf{x}|\boldsymbol{\sigma}) \qquad \text{MAP}_i = \arg\max_{\sigma_i} \sum_{\boldsymbol{\sigma}\setminus\sigma_i} \mathcal{P}(\mathbf{x}|\boldsymbol{\sigma})$$

Exhaustive search is generally expensive: complexity $\sim 2^N$

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$$\boldsymbol{\sigma} = (\sigma_1, \cdots, \sigma_N), \quad N \text{ finite}, \quad \sigma_i = \pm 1 \text{ (example)}$$

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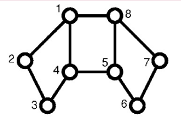
Graphical models of Statistical Inference

Factorization (Forney '01, Loeliger '01)

$$\mathcal{P}(\boldsymbol{\sigma}) = Z^{-1} \prod_{a \in X} f_a(\boldsymbol{\sigma}_a)$$

$$\underbrace{Z = \sum_{\boldsymbol{\sigma}} \mathcal{P}(\boldsymbol{\sigma})}_{\text{partition function}}$$

X = edges

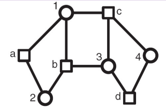


$$f_a \geq 0$$
$$\sigma_{ab} = \sigma_{ba} = \pm 1$$
$$\boldsymbol{\sigma}_1 = (\sigma_{12}, \sigma_{14}, \sigma_{18})$$
$$\boldsymbol{\sigma}_2 = (\sigma_{12}, \sigma_{13})$$

Example: Error-Correction (linear code, bipartite Tanner graph)

$$f_i(\boldsymbol{\sigma}_i) = \begin{cases} 1, & \sigma_{i\alpha} = \sigma_{i\beta} \\ 0, & \text{otherwise} \end{cases}$$

$$f_\alpha(\boldsymbol{\sigma}_\alpha) = \delta\left(\prod_{i \in \alpha} \sigma_i, +1\right) \exp\left(\sum_{i \in \alpha} \sigma_i h_i / q_i\right)$$



h_i - log-likelihoods
q_i-connectivity degrees

Variational Method in Statistical Mechanics

Gibbs measure: $P(\boldsymbol{\sigma}) = \frac{\exp(-E(\boldsymbol{\sigma}))}{Z}, \quad Z \equiv \sum_{\boldsymbol{\sigma}} \exp\left(-E(\boldsymbol{\sigma})\right)$

Exact Variational Principle — Kullback-Leibler '51

$$F\{b(\boldsymbol{\sigma})\} = \sum_{\boldsymbol{\sigma}} b(\boldsymbol{\sigma}) E(\boldsymbol{\sigma}) - \sum_{\boldsymbol{\sigma}} b(\boldsymbol{\sigma}) \ln b(\boldsymbol{\sigma})$$

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

Variational Ansatz

- Mean-Field: $p(\boldsymbol{\sigma}) \approx b(\boldsymbol{\sigma}) = \prod_i b_i(\sigma_i)$
- Belief Propagation:

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

$$b_a(\boldsymbol{\sigma}_a) = \sum_{\boldsymbol{\sigma} \setminus \boldsymbol{\sigma}_a} b(\boldsymbol{\sigma}), \quad b_{ab}(\sigma_{ab}) = \sum_{\boldsymbol{\sigma} \setminus \sigma_{ab}} b(\boldsymbol{\sigma})$$

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

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

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

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

MAP≈BP=Belief-Propagation (Bethe-Peirls): iterative ⇒ Gallager '61; MacKay '98

- Exact on a tree ▸ Derivation Sketch
- Trading optimality for reduction in complexity: $\sim 2^L \to \sim L$
- BP = solving equations on the graph:

$$\eta_{\alpha j} = h_j + \sum_{\beta \neq \alpha}^{j \in \beta} \tanh^{-1}\left(\prod_{i \neq j}^{i \in \beta} \tanh \eta_{\beta i}\right) \quad \Leftarrow \text{LDPC representation}$$

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Linear Programming version of Belief Propagation

In the limit of large SNR, $f_a \to \pm\infty$: BP→LP

Minimize $F \approx E = -\sum_a \sum_{\boldsymbol{\sigma}_a} b_a(\boldsymbol{\sigma}_a) \ln f_a(\boldsymbol{\sigma}_a) =$ 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?

Previous Considerations:

- Rizzo, Montanari '05 - Corrections to BP approximation
- Parisi, Slanina '05 - BP as a saddle-point + corrections

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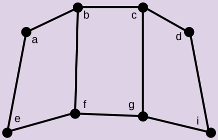
Local Gauge, G, Transformations



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

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

The partition function is invariant under any G-gauge!

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

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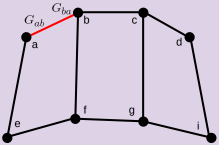

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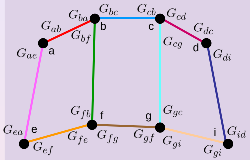

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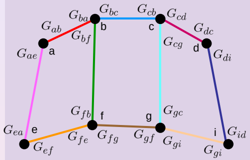

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Gauge Transformation: Binary Representation

$$Z=\sum_{\boldsymbol\sigma}\prod_a f_a(\boldsymbol\sigma_a)=\sum_{\boldsymbol\sigma'}\prod_a f_a(\boldsymbol\sigma_a)\prod_{bc}\frac{1+\sigma_{bc}\sigma_{cb}}{2},\quad \sigma_{bc}\neq\sigma_{cb}$$

The binary trick

$$1+\pi\sigma=\frac{\exp(\sigma\eta+\pi\chi)}{\cosh(\eta+\chi)}\left(1+(\tanh(\eta+\chi)-\sigma)(\tanh(\eta+\chi)-\pi)\cosh^2(\eta+\chi)\right)$$

$$\tilde f_a(\boldsymbol\sigma_a)=f_a(\boldsymbol\sigma_a)\prod_{b\in a}\exp(\eta_{ab}\sigma_{ab})$$

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$$Z=\Big(\prod_{bc}2\cosh(\eta_{bc}+\eta_{cb})\Big)^{-1}\sum_{\boldsymbol\sigma'}\prod_a\tilde f_a(\boldsymbol\sigma_a)\cdot\prod_{bc}V_{bc}$$

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$$Z=\underbrace{Z_0(\eta)}_{\text{ground state}}+\underbrace{\sum_{\text{all possible colorings of the graph}}\cdots}_{\text{excited states}}$$

Gauges and BP

Partition function in the colored representation

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Fixing the gauges ⇒ BP equations!!

$$\sum_{\boldsymbol{\sigma}_a}\left(\tanh(\eta_{ab}^{(bp)}+\eta_{ba}^{(bp)})-\sigma_{ab}\right)\tilde{f}_a(\boldsymbol{\sigma}_a;\boldsymbol{\eta}_a)=0\quad\Rightarrow\quad\underbrace{\eta_{\alpha j}^{bp}=h_j+\sum_{\beta\neq\alpha}^{j\in\beta}\tanh^{-1}\left(\prod_{i\neq j}^{i\in\beta}\tanh\eta_{\beta i}^{bp}\right)}_{\text{LDPC case}}$$

Color Principe: no loose ends

$$\prod_{(bc)}V_{bc}=1+\sum_{\text{colored edges}}*\cdots*\cdots*\cdots$$

Variational Principe:

$$\prod_{(bc)}V_{bc}\to 1,\quad Z\to Z_0,\quad \left.\frac{\delta Z_0}{\delta\eta_{ab}}\right|_{\eta^{(bp)}}=0$$

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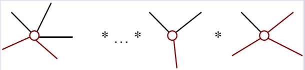
$$\sum_{\boldsymbol{\sigma}_a}\left(\tanh(\eta^{(bp)}_{ab}+\eta^{(bp)}_{ba})-\sigma_{ab}\right)\tilde{f}_a(\boldsymbol{\sigma}_a;\boldsymbol{\eta}_a)=0\quad\Rightarrow\quad\underbrace{\eta^{bp}_{\alpha j}=h_j+\sum_{\beta\neq\alpha}^{j\in\beta}\tanh^{-1}\Big(\prod_{i\neq j}^{i\in\beta}\tanh\eta^{bp}_{\beta i}\Big)}_{\text{LDPC case}}$$

Color Principe: no loose ends

$$\prod_{(bc)}V_{bc}=1+\sum_{\text{colored edges}}*\cdots*\cdots*\cdots$$



Variational Principe:

$$\prod_{(bc)}V_{bc}\to 1,\quad Z\to Z_0,\quad \left.\frac{\delta Z_0}{\delta\eta_{ab}}\right|_{\eta^{(bp)}}=0$$

$$Z_0=\Big(\prod_{bc}2\cosh(\eta_{bc}+\eta_{cb})\Big)^{-1}\sum_{\boldsymbol{\sigma}}\prod_a\tilde{f}_a(\boldsymbol{\sigma}_a)$$

Gauges and BP

Partition function in the colored representation

$$Z=\Big(\prod_{bc}2\cosh(\eta_{bc}+\eta_{cb})\Big)^{-1}\sum_{\boldsymbol{\sigma}'}\prod_a\tilde f_a\prod_{bc}V_{bc},\quad \tilde f_a(\boldsymbol{\sigma}_a;\boldsymbol{\eta}_a)=f_a(\boldsymbol{\sigma}_a)\prod_{b\in a}\exp(\eta_{ab}\sigma_{ab})$$

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Loop Series:

Chertkov,Chernyak '06

Exact (!!) expression in terms of BP

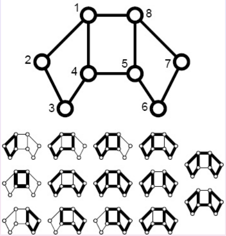
$$Z=\sum_{\boldsymbol{\sigma}_\sigma}\prod_a f_a(\boldsymbol{\sigma}_a)=Z_0\left(1+\sum_C r(C)\right)$$

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

$C\in$ Generalized Loops $=$ Loops without loose ends

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

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



- The Loop Series is finite
- All terms in the series are calculated within BP
- BP is exact on a tree
- BP is a Gauge fixing condition. Other choices of Gauges would lead to different representation.

Features of the Loop Calculus

$Z = Z_0(1 + r_C),\ r_C = \prod_{a \in C} \tilde{\mu}_a$

- Bethe Free Energy is related to the "ground state" term in the partition function: $F(b^*(\eta)) = -\ln Z_0(\eta)$, where
  $b_a^*(\boldsymbol{\sigma}_a) = \frac{f_a(\boldsymbol{\sigma}_a)\exp(\sum_{b \in a} \eta_{ab}\sigma_{ab})}{\sum_{\boldsymbol{\sigma}_a} f_a(\boldsymbol{\sigma}_a)\exp(\sum_{b \in a} \eta_{ab}\sigma_{ab})}, \quad b_{ab}^*(\sigma_{ab}) = \frac{\exp((\eta_{ab}+\eta_{ba})\sigma_{ab})}{2\cosh(\eta_{ab}+\eta_{ba})}$
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- Loop series can be built around any extremum (minimum, maximum or saddle-point) of the Bethe Free energy.
- $-1 \leq r_C, \tilde{\mu}_a \leq 1$. The tasks of finding all $\tilde{\mu}_a$ (over the graph) and r_C for a given loop are (computationally) not difficult. All that suggests simple heuristic for finding loops with large r_C.
- Linear Programming limit of the Loop Calculus is well defined.
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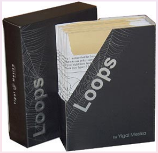
1. Introduction
   - Statistical Inference
   - Graphical Models
   - Bethe Free Energy and Belief Propagation (BP)

2. Loop Calculus
   - Gauge Transformations and BP
   - Loop Series in terms of BP



3. Applications
   - Analysis and Improvement of LDPC-BP/LP Decoding
   - Long Correlations and Loops in Statistical Mechanics

Error-floor Analysis

Truncation as an Approximation

$$Z = Z_0(1 + \sum_C r_C) \approx Z_0(1 + r(\Gamma))$$

Synthesis of Pseudo-Codeword Search Algorithm (Chertkov, Stepanov '06) & Loop Calculus

- Consider pseudo-codewords one after other
- For an individual pseudo-codeword/instanton identify a critical loop, Γ, giving major contribution to the loop series.
- Hint: look for single connected loops and use local "triad" contributions as a tester: $r(\Gamma) = \prod_{\alpha\in\Gamma} \tilde{\mu}_\alpha^{(bp)}$

Proof-of-Concept test [(155, 64, 20) code over AWGN]

- $\forall$ pseudo-codewords with $16.4037 < d < 20$ (~ 200 found) there always exists a simple single-connected critical loop(s) with $r(\Gamma) \sim 1$.
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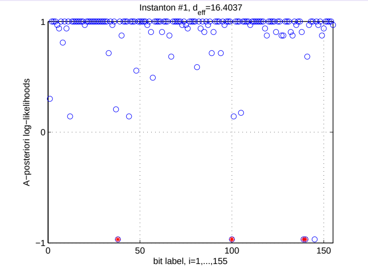
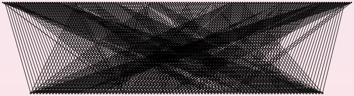


Bigger Set



Extended Variational Principe & Loop-Corrected BP

Bare BP Variational Principle:

$$\left.\frac{\delta Z_0}{\delta \eta_{ab}}\right|_{\eta^{(bp)}} = 0, \qquad Z_0 = \left(\prod_{bc} 2\cosh(\eta_{bc}+\eta_{cb})\right)^{-1} \sum_{\boldsymbol{\sigma}} \prod_a P_a(\boldsymbol{\sigma}_a)\Big|_{\eta^{(bp)}}$$

New choice of Gauges guided by the knowledge of the critical loop Γ

$$\left.\frac{\delta \exp(-\mathcal{F})}{\delta \eta_{ab}}\right|_{\eta_{\rm eff}} = 0, \quad \mathcal{F} \equiv -\ln(Z_0 + Z_\Gamma)$$

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- **1.** Run bare BP algorithm. Terminate if BP succeeds (i.e. a valid code word is found).
- **2.** If BP fails find the most relevant loop Γ that corresponds to the maximal $|r_\Gamma|$. Triad search is helping.
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$(155, 64, 20)$ Test

- **IT WORKS!**
  All troublemakers ($\sim$ 200 of them) previously found by LP-based Pseudo-Codeword-Search Algorithm method were successfully corrected by the LP-erasure algorithm.
- Method is invariant with respect the choice of the codeword (used to generate pseudo-codewords).

General Conjecture:

- Loop-erasure algorithm is capable of reducing the error-floor
- Bottleneck is in finding the critical loop
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Dilute Gas of Loops: $Z = Z_0\left(1+\sum_C r_C\right) \approx Z_0 \cdot \prod_{C_{sc}=\text{single connected}} (1+r_{sc})$

Applies to

- Lattice problems in high spatial dimensions
- Large Erdös-Renyi problems (random graphs with controlled connectivity degree)

- The approximation allows an easy multi-scale re-summation
- In the para-magnetic phase and $\mathbf{h}=0$: the only solution of BP is a trivial one $\boldsymbol{\eta}=0$, $Z_0 \to 1$, and the Loop Series is reduced to the high-temperature expansion [Domb, Fisher, et al '58-'90]

Ising model in the factor graph terms

$$Z = \sum_{\boldsymbol{\sigma}} \prod_{\alpha=(i,j)\in X} \exp\left(J_{ij}\sigma_i\sigma_j\right) = \sum_{\boldsymbol{\sigma}} \prod_{a\in\{i\}\cup\{\alpha\}} f_a(\boldsymbol{\sigma}_a)$$

$$f_i(\boldsymbol{\sigma}_i) = \begin{cases} \exp(h_i\sigma_i), & \sigma_{i\alpha}=\sigma_{i\beta}=\sigma_i \quad \forall\alpha,\beta \ni i \\ 0, & \text{otherwise;} \end{cases}$$

$$f_\alpha\left(\boldsymbol{\sigma}_\alpha = (\sigma_{\alpha i},\sigma_{\alpha j})\right) = \exp\left(J_{ij}\sigma_{\alpha i}\sigma_{\alpha j}\right)$$

Loop Series trivially passes common "loop" tests (from Rizzo, Montanari '05)

- Evaluation of the critical temperature in the constant exchange, zero field Ising model
- Leading $1/N$ corrections to the Free Energy of the Viana-Bray model in the vicinity of the critical point (glass transition)

Results

- BP is better then just a heuristic in the loopy case ... BP is the special Gauge condition eliminating all contributions but loops.
- Exact Marginal probability allows explicit Loop Series expression in terms of a solution of the Belief Propagation equations.
- Truncation and/or Re-summation of the Loop Series provide hierarchy of systematically improvable approximations/algorithms. Standard BP/LP is a first member in the hierarchy.
- Local example (truncation). Finding a critical loop, or a small number of critical loops, can be algorithmically sufficient for drastic improvement of BP decoding in the error-floor domain.
- Multi-scale example of stat-mech problems with long correlations. Re-summation is needed to improve upon BP.

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Future Challenges

- Better Algorithms: Loop Series Truncation/Resummation
- Generalizations. q-ary and continuous alphabets. Quantum spins, Quantum error-correction.
- Loop calculus based analysis of graph ensembles, e.g. understanding and improving the cavity method [Mézard, Parisi '85-'03]
- Extending the list of Loop Calculus Applications, e.g. SAT and cryptography
- Non-BP gauges, e.g. for stat problems on regular and irregular lattices
- Relation to graph ζ-functions [Koetter, Li, Vontobel, Walker '05]

Other complementary developments, e.g. wrt Algorithms:

- Improving BP [Survey Propagation = Mézard et.al '02; Generalized BP = Yedidia et.al '01]
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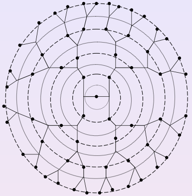
All papers are available at http://cnls.lanl.gov/∼chertkov/pub.htm



$$Z(\mathbf{h}) = \sum_{\boldsymbol{\sigma}} \prod_{\alpha=1}^{M} \delta\left(\prod_{i\in\alpha}\sigma_i, 1\right) \exp\left(\sum_{i=1}^{N} h_i\sigma_i\right)$$

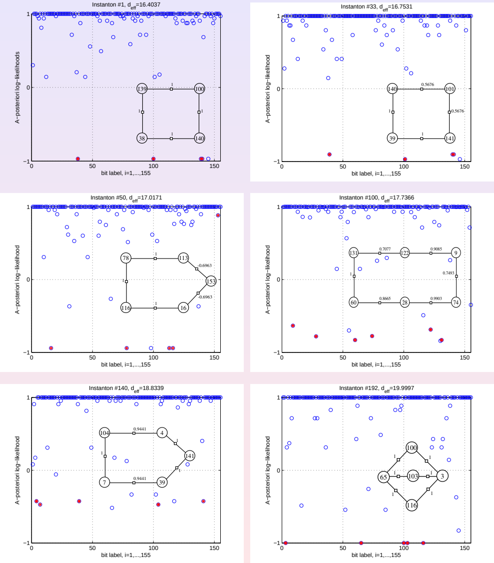
h_i is a log-likelihood at a bit (outcome of the channel)

$$Z_{j\alpha}^{\pm}(\mathbf{h}^{>}) \equiv \sum_{\boldsymbol{\sigma}^{>}}^{\sigma_j=\pm 1} \prod_{\beta>} \delta\left(\prod_{i\in\beta}\sigma_i, 1\right) \exp\left(\sum_{i>} h_i\sigma_i\right)$$

$$Z_{j\alpha}^{\pm} = \exp(\pm h_j) \prod_{\beta\neq\alpha}^{j\in\beta} \frac{1}{2}\left(\prod_{i\neq j}^{i\in\beta}(Z_{i\beta}^{+} + Z_{i\beta}^{-}) \pm \prod_{i\neq j}^{i\in\beta}(Z_{i\beta}^{+} - Z_{i\beta}^{-})\right)$$

$$\eta_{j\alpha} \equiv \frac{1}{2}\ln\left(\frac{Z_{j\alpha}^{+}}{Z_{j\alpha}^{-}}\right), \quad \eta_{j\alpha} = h_j + \sum_{\beta\neq\alpha}^{j\in\beta} \tanh^{-1}\left(\prod_{i\neq j}^{i\in\beta} \tanh\eta_{i\beta}\right)$$

◂ Bethe Free Energy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A−posteriori log−likelihood
bit label, i=1,...,155

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