MaxEnt 22 Institut Henri Poincaré

Local Max-Entropy and Free Energy Principles Solved by Belief Propagation

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Introduction

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Belief Propagation (BP) is an old algorithm with many applications [Gallager 64, Pearl 82]
(low-density decoding, bayesian inference, AI, stereovision, condesed matter simulation ...)

[Yedidia 05]
Generalized Belief Propagation (GBP) works with hypergraphs (i.e. coverings) instead of graphs

This talk is not about GBP, [Kikuchi 51, Morita 57, Yedidia 05]
It is about the geometric and statistical problems solved by GBP stationary states

GBP can be viewed a soft constraint satisfaction solver trying to reach consistent
local probability distributions under energy conservation constraints.

Continuous-time diffusion equations generalise GBP with improved stability [P 20, 21]

Introduction

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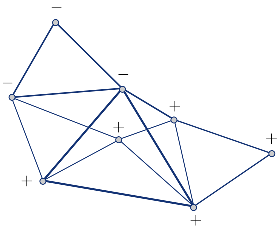
Example: Spin Glasses



K random graph on a set of vertices $\Omega = \{1, \dots, N\}$

$(x_i) \in \{\pm 1\}^N$ random microstate of the system

$(w_{ij}) \in \mathbb{R}^{K_1}$ random couplings on the edges of K

$(b_i) \in \mathbb{R}^N$ random magnetic fields (or $b_i = B$)

Hamiltonian = Total Energy

$$H(x) = \sum_{ij \in K_1} w_{ij} x_i x_j + \sum_{i \in K_0} b_i x_i$$

Gibbs state = Graphical Model

$$p(x) = \frac{\mathrm{e}^{-\beta H(x)}}{\sum_x \mathrm{e}^{-\beta H(x)}}$$

Introduction

In thermodynamics, it is common to work with the following functionals:

- $S(\mathcal{U})$ *Boltzmann entropy* : defined as log-number of microstates having energy $\mathcal{U}$
- $\mathcal{F}(\beta,\mathcal{U})$ *variational free energy* : defined by $\mathcal{U} - \frac{1}{\beta} S(\mathcal{U})$
- $F(\beta)$ *free energy* : defined as $\min_{\mathcal{U}} \mathcal{F}(\beta,\mathcal{U})$, or from the partition function by $-\frac{1}{\beta} \ln Z(\beta)$

The Legendre transform relates these functionals, defining an energy-temperature relationship $\mathcal{U}(\beta)$

Thermodynamic equilibrium with different constraints: on $\mathcal{U}$ and β respectively

not tractable in practice

Short range interactions $\Rightarrow$ local approximations efficiently computed by GBP

Bethe-Kikuchi approximations

Cluster Variation Method

Outline

I.1. Microstates and Total Energy

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We consider a free sheaf $E : \mathcal{P}^{op}(\Omega) \to \mathbf{Set}$ of microstates, given by:

$$E_{\mathrm{a}} = \prod_{i \in \mathrm{a}} E_i \qquad \text{for all} \quad \mathrm{a} \subseteq \Omega$$

The restriction maps $\pi^{\mathrm{a} \to \mathrm{b}} : E_{\mathrm{a}} \to E_{\mathrm{b}}$ for every $\mathrm{b} \subseteq \mathrm{a}$ simply forget the state of atoms outside of b
We will write:

$$x_{\mathrm{a}|\mathrm{b}} = \pi^{\mathrm{a} \to \mathrm{b}}(x_{\mathrm{a}})$$

A statistical system on E_Ω is classically defined by a hamiltonian or energy function $H_\Omega : E_\Omega \to \mathbb{R}$
One can always define a finest covering $K \subseteq \mathcal{P}(\Omega)$ such that H_Ω decomposes as a sum of local interactions:

$$H_\Omega(x_\Omega) = \sum_{\mathrm{a} \in K} h_{\mathrm{a}}(x_{\Omega|\mathrm{a}})$$

I.2. Observables

Local observables form a cosheaf $\mathbb{R}^E : \mathcal{P}(\Omega) \to \mathbf{Alg}_c$ of commutative algebras

The extension maps $\pi^{\mathrm{a}\to\mathrm{b}\,*} : \mathbb{R}^{E_\mathrm{b}} \to \mathbb{R}^{E_\mathrm{a}}$ for all $\mathrm{b} \subseteq \mathrm{a}$ can be viewed as inclusions $\mathbb{R}^{E_\mathrm{b}} \subseteq \mathbb{R}^{E_\mathrm{a}}$

Def.

Observable fields on $K \subseteq \mathcal{P}(\Omega)$ form a chain complex $\big(C_\bullet(K, \mathbb{R}^E), \delta\big)$ where:

- $C_0 = \oplus_\mathrm{a} \mathbb{R}^{E_\mathrm{a}}$ consists of potentials $[h_\mathrm{a} : E_\mathrm{a} \to \mathbb{R} \mid \mathrm{a} \in K]$
- $C_1 = \oplus_{\mathrm{b}\subset\mathrm{a}} \mathbb{R}^{E_\mathrm{b}}$ consists of heat fluxes $[\varphi_{\mathrm{a}\to\mathrm{b}} : E_\mathrm{b} \to \mathbb{R} \mid \mathrm{a}, \mathrm{b} \in K \text{ and } \mathrm{b} \subseteq \mathrm{a}]$

and the codifferential $\delta : C_1 \to C_0$ acts by:

$$\delta\varphi_\mathrm{b}(x_\mathrm{b}) = \sum_{\mathrm{b}\subseteq\mathrm{a}} \varphi_{\mathrm{a}\to\mathrm{b}}(x_\mathrm{b}) - \sum_{\mathrm{c}\subseteq\mathrm{b}} \varphi_{\mathrm{b}\to\mathrm{c}}(x_{\mathrm{b}|\mathrm{c}})$$

Gauss thm. = Total energy conservation P 20

Two potentials h and h' are homologous, i.e. $h' = h + \delta\varphi$ if and only if:

$$\sum_{\mathrm{a}\in K} h_\mathrm{a}(x_{\Omega|\mathrm{a}}) = \sum_{\mathrm{a}\in K} h'_\mathrm{a}(x_{\Omega|\mathrm{a}})$$

I.3. Densities and Beliefs

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Local densities define a functor $\mathbb{R}^{E\,*} : \mathcal{P}(\Omega)^{op} \to \mathbf{Vect}$ of vector spaces

The pushforwards $\pi_*^{\mathrm{a}\to\mathrm{b}} : \mathbb{R}^{E_\mathrm{a}*} \to \mathbb{R}^{E_\mathrm{b}*}$ for all $\mathrm{b} \subseteq \mathrm{a}$ denote partial integration on fibers $\{x_{\mathrm{a}|\mathrm{b}} = x_\mathrm{b}\}$

Def. (Prop.)

Density fields on $K \subseteq \mathcal{P}(\Omega)$ form a cochain complex $\big(C_\bullet(K, \mathbb{R}^E)^*, d\big)$ where the differential $d : C_0^* \to C_1^*$ acts by:

$$dp_{\mathrm{a}\to\mathrm{b}}(x_\mathrm{b}) \;=\; p_\mathrm{b}(x_\mathrm{b}) \;-\; \sum_{x_{\mathrm{a}|\mathrm{b}} = x_\mathrm{b}} p_\mathrm{a}(x_\mathrm{a})$$

A density field $p \in C_0^*$ is said consistent if $dp = 0$

Def.

Beliefs lie in the convex subspace $\Delta_0 \subseteq C_0^*$ of positive local probability measures

Consistent beliefs lie in the convex polytope $\Gamma_0 \subseteq \Delta_0$ intersecting $\mathrm{Ker}(d)$

Consistent beliefs $p \in \Gamma_0$ act as local substitutes for global probabilities $p_\Omega \in \mathrm{Prob}(E_\Omega)$

(although positivity of the linear extension $p_\Omega \in \mathbb{R}^{E_\Omega *}$ is generally not guaranteed)

I.4. Local Gibbs Correspondence

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GBP tries to solve 2 different kinds of constraints simultaneously:

- Energy conservation on $h \in C_0$: potentials lie in $[h] = h + \delta C_1$ during evolution
- Marginal consistency on $p \in \Delta_0$: beliefs lie in $\Gamma_0 \subseteq \mathrm{Ker}(d)$ at equilibrium

A local correspondence $C_0 \to \Delta_0$ is therefore essential to the dynamic of GBP:

$$C_0 \xrightarrow[\text{linear}]{\zeta} C_0 \xrightarrow[\text{softmin}]{\rho^\beta} \Delta_0$$

Def.

The Gibbs correspondence for $\beta > 0$ is written $p = \rho^\beta(H)$ with $H = \zeta h$ as:

$$p_{\mathrm{a}}(x_{\mathrm{a}}) = \frac{1}{Z^\beta_{\mathrm{a}}} \mathrm{e}^{-\beta H_{\mathrm{a}}(x_{\mathrm{a}})} \qquad \text{with} \qquad H_{\mathrm{a}}(x_{\mathrm{a}}) = \sum_{\mathrm{b} \subseteq \mathrm{a}} h_{\mathrm{b}}(x_{\mathrm{a|b}})$$

- $\zeta : C_0 \to C_0$ is the zeta transform, combinatorial automorphism of C_0
- $\rho^\beta : C_0 \to \Delta_0$ is a softmin yielding local Gibbs states at inverse temperature $\beta = \frac{1}{T}$

I.5. Möbius inversion and Bethe numbers

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Thm. (Möbius inversion) (Dirichlet, Rota 64, P 20)

The Möbius transform $\mu : C_0 \to C_0$ inverting ζ acts by Dirichlet convolution as:

$$\mu(H)_{\mathrm{a}}(x_{\mathrm{a}}) = \sum_{\mathrm{b} \subseteq \mathrm{a}} \mu_{\mathrm{a} \to \mathrm{b}} \cdot H_{\mathrm{b}}(x_{\mathrm{a}|\mathrm{b}}) \qquad = \quad h_{\mathrm{a}}(x_{\mathrm{a}})$$

Coefficients $\mu_{\mathrm{a} \to \mathrm{b}} \in \mathbb{Z}$ can be recursively computed by N sparse matrix products,
denoting by N the maximal degree of $C_\bullet$ (= maximal length of a strict chain in K)

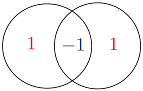
The reciprocal pair (ζ, μ) can moreover be extended to full automorphisms $C_\bullet \to C_\bullet$

Def. (Prop.)

Bethe-Kikuchi numbers $(c_{\mathrm{a}})_{\mathrm{a} \in K}$ are defined by the following equivalent formulas:

(i) $\forall \mathrm{b} \in K \qquad \sum_{\mathrm{a} \supseteq \mathrm{b}} c_{\mathrm{a}} = 1$

(ii) $\forall \mathrm{b} \in K \qquad c_{\mathrm{b}} = \sum_{\mathrm{a} \supseteq \mathrm{b}} \mu_{\mathrm{a} \to \mathrm{b}}$



Outline

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I. Local statistics : topology and combinatorics

II. Cluster variational principles solved by GBP

III. Example of diffusion with singularities

II.2 Regionwise Information Functionals

Def.

For all $\mathrm{a} \subseteq \Omega$ and $\beta > 0$ consider the following functionals:

- Shannon entropy given by: $S_\mathrm{a} : \mathrm{Prob}(E_\mathrm{a}) \to \mathbb{R}$

$$S_\mathrm{a}(p_\mathrm{a}) = -\sum_{E_\mathrm{a}} p_\mathrm{a} \ln(p_\mathrm{a})$$

- Variational free energy given by: $\mathcal{F}^\beta_\mathrm{a} : \mathrm{Prob}(E_\mathrm{a}) \times \mathbb{R}^{E_\mathrm{a}} \to \mathbb{R}$

$$\mathcal{F}^\beta_\mathrm{a}(p_\mathrm{a}, H_\mathrm{a}) = \mathbb{E}_{p_\mathrm{a}}[H_\mathrm{a}] - \frac{1}{\beta} S_\mathrm{a}(p_\mathrm{a})$$

- Free energy given by: $F^\beta_\mathrm{a} : \mathbb{R}^{E_\mathrm{a}} \to \mathbb{R}$

$$F^\beta_\mathrm{a}(H_\mathrm{a}) = -\frac{1}{\beta} \ln \sum_{E_\mathrm{a}} \mathrm{e}^{-H_\mathrm{a}}$$

Then:

(i) $F^\beta_\mathrm{a}(H_\mathrm{a}) = \min \mathcal{F}^\beta_\mathrm{a}(-, H_\mathrm{a})$ for all $H_\mathrm{a} \in \mathbb{R}^{E_\mathrm{a}}$

(ii) the differential $F^\beta_{\mathrm{a}*} : H_\mathrm{a} \mapsto \rho^\beta_\mathrm{a}(H_\mathrm{a})$ of F^β_a coïncides with the Gibbs state map

(iii) $\rho^\beta_\mathrm{a}(H_\mathrm{a})$ maximises S_a under the constraint $\mathbb{E}_{p_\mathrm{a}}[H_\mathrm{a}] = \mathcal{U}_\mathrm{a}$ for some $\mathcal{U}_\mathrm{a} \in \mathbb{R}$

II.1 Faithful Diffusions

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We consider continuous-time diffusion equations in C_0 defined by a flux functional $\Phi : C_0 \to C_1$

$$\frac{dv}{dt} = \delta\Phi(v) \qquad \text{with} \qquad v_{|t=0} = h$$

Energy conservation $\boxed{v \in [h] = h + \delta C_1}$ is therefore naturally enforced by any discrete integrator.

homology class

(GBP equivalent but with $\Delta t = 1$!)

Def.

Given $\beta > 0$, we call consistent manifold the subspace $\mathrm{Fix}^\beta \subseteq C_0$ defined by ;

$$\mathrm{Fix}^\beta = \{v \in C_0 \mid \; p = \rho^\beta(\zeta v) \in \Gamma_0\}$$

Given a flux functional $\Phi : C_0 \to C_1$, we say that:

- Φ is consistent if $\Phi_{|\mathrm{Fix}^\beta} = 0$
- Φ is faithful if $\delta\Phi(v) = 0 \;\Rightarrow\; v \in \mathrm{Fix}^\beta$ and Φ is consistent.

Consistent diffusions are stationary for $v \in [h] \cap \mathrm{Fix}^\beta$

Faithful diffusions are stationary only for $v \in [h] \cap \mathrm{Fix}^\beta$

II.3 Variational Free Energy Principle

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Problem 1.

Chose an inverse temperature $\beta > 0$ and local energies $H = \zeta h \in C_0$

Find $p \in \Gamma_0$ critical for the Bethe-Kikuchi variational free energy $\check{\mathcal{F}} : \Delta_0 \times C_0 \to \mathbb{R}$:

$$\check{\mathcal{F}}(p, H) = \sum_{\mathrm{a} \in K} c_{\mathrm{a}} \mathcal{F}_{\mathrm{a}}(p_{\mathrm{a}}, H_{\mathrm{a}})$$

Thm 1. [Yedidia 05, P 19]

Let $\beta > 0$ and $H = \zeta h \in C_0$

Solutions of problem 1 are given by $p = \rho^\beta(\zeta v)$ for all $v \in C_0$ such that:

$$v \in [h] \cap \mathrm{Fix}^\beta$$

II.4 Max-Entropy Principle

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Problem 2.

Chose a mean energy $\mathcal{U} \in \mathbb{R}$ and local energies $H = \zeta h \in C_0$

Find $p \in \Gamma_0$ constrained to $\langle p, h \rangle = \mathcal{U}$ for the Bethe-Kikuchi entropy $\check{S} : \Delta_0 \to \mathbb{R}$:

$$\check{S}(p) = \sum_{\mathrm{a} \in K} c_{\mathrm{a}} S_{\mathrm{a}}(p_{\mathrm{a}})$$

Where $\langle p, h \rangle = \sum_{\mathrm{a} \in K} \mathbb{E}_{p_{\mathrm{a}}}[h_{\mathrm{a}}] = \sum_{\mathrm{a} \in K} c_{\mathrm{a}} \, \mathbb{E}_{p_{\mathrm{a}}}[H_{\mathrm{a}}] = \mathcal{U}$ $\quad \Leftarrow \quad$ Bethe mean energy is exact by $\sum_{\mathrm{a}} h_{\mathrm{a}} = \sum_{\mathrm{a}} c_{\mathrm{a}} H_{\mathrm{a}}$ and linearity of expectations

Thm 2.

Let $\mathcal{U} \in \mathbb{R}$ and $H = \zeta h \in C_0$

Solutions of problem 2 are given by $p = \rho^1(\zeta \bar{v})$ for all $\bar{v} \in C_0$ such that:

$$\exists \beta > 0 \qquad \bar{v} \in [\beta h] \cap \mathrm{Fix}^1$$

N.B. Letting $v = \beta \bar{v}$ one then recovers $v \in [h] \cap \mathrm{Fix}^\beta$

II.5 Free Energy Principle

Problem 3.

Chose an inverse temperature $\beta > 0$ and local energies $H = \zeta h \in C_0$

Find $V = \zeta v \in C_0$ constrained to $v \in [h]$ critical for the Bethe-Kikuchi free energy $\check{F} : C_0 \to \mathbb{R}$:

$$\check{F}(V) = \sum_{\mathrm{a} \in K} c_{\mathrm{a}} F_{\mathrm{a}}(V_{\mathrm{a}})$$

Let us call weakly consistent manifold $\mathrm{Fix}^{\beta}_{+} = \{v + \epsilon \,|\, v \in \mathrm{Fix}^{\beta}, \epsilon \in \mathrm{Ker}(c\zeta)\}$

(retracts linearly on Fix^{β}, coïncides with Fix^{β} when $c_{\mathrm{a}} \neq 0$ for all $\mathrm{a} \in K$)

Thm 3.

Let $\beta > 0$ and $H = \zeta h \in C_0$

Solutions of problem 1 are given by $V = \zeta v$ for all $v \in C_0$ such that:

$$v \in [h] \cap \mathrm{Fix}^{\beta}_{+}$$

Outline

III.1 Energy-Temperature Relationship(s)

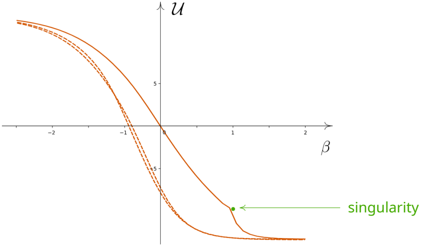
Problems 1, 2 and 3 all imply finding some $v \in [h] \cap \mathrm{Fix}^\beta$ (i.e. conservative and consistent), however with different constraints:

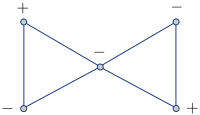
- Free energy principles (1,3) with temperature constraints on $\beta = \frac{1}{T}$
- The max-entropy principle (2) with mean energy constraints on $\mathcal{U} = \langle p, h \rangle$

Therefore solutions of (2) might not coïncide with solutions of (1) and (3).

There may exist multiple stationnary energies fore one given temperature constraint, and reciprocally.

Energy-Temperature Diagrams:





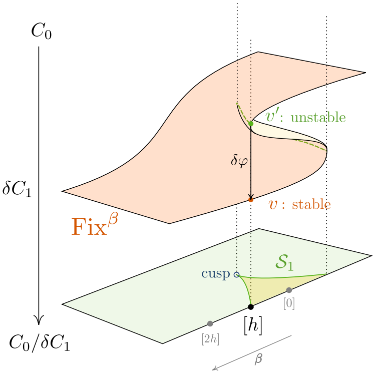
K graph with two loops

$$E_i = \{\pm\}$$
$$E_{ij} = \{\pm\}^2$$

III.2 Singularities on cyclic graphs

Singularities of the projection $\Pi : C_0 \to C_0/\delta C_1$ restricted to Fix^β are ranked by dimension

$$\mathcal{S}_k = \{ v \in \mathrm{Fix}^\beta \mid \mathrm{Ker}(\Pi_*) \cap \delta C_1 \text{ of dimension } k \}$$



This makes $\mathrm{Fix}^\beta = \sqcup_{k \geq 0} \mathcal{S}_k$ a stratified space

On simple graphs with 2+ loops one can parameterise the singular surface $\mathcal{S}_1$

(smooth in C_0)

Linearised diffusion does not restrict to an isomorphism of δC_1 on singularities

Continuous-time diffusion improves over GBP by yielding smooth trajectories, even nearby singularities

III.3 GBP and Bethe Diffusions

Let us define the conditional free energy functional $F_{\mathrm{a}\to\mathrm{b}} : \mathbb{R}^{E_\mathrm{a}} \to \mathbb{R}^{E_\mathrm{b}}$ by:

$$F_{\mathrm{a}\to\mathrm{b}}[V_\mathrm{a}|x_\mathrm{b}] = -\ln \sum_{x_{\mathrm{a}|\mathrm{b}}=x_\mathrm{b}} \mathrm{e}^{-V_\mathrm{a}(x_\mathrm{a})} \qquad \Rightarrow F_{\mathrm{a}\to\mathrm{b}}[V_\mathrm{b}|x_\mathrm{b}] = V_\mathrm{b}(x_\mathrm{b})$$

And the free energy gradient $\mathcal{D} : C_0 \to C_1$ by:

$$\mathcal{D}(V)_{\mathrm{a}\to\mathrm{b}}(x_\mathrm{b}) = V_\mathrm{b}(x_\mathrm{b}) - F_{\mathrm{a}\to\mathrm{b}}[V_\mathrm{a}|x_\mathrm{b}] \qquad = F_{\mathrm{a}\to\mathrm{b}}[V_\mathrm{b} - V_\mathrm{a} \,|\, x_\mathrm{b}]$$

We may then define the diffusion fluxes $\Phi_{\mathrm{GBP}} = -\delta\mathcal{D}\zeta$ and $\Phi_{\mathrm{Bethe}} = -\delta\mu\mathcal{D}\zeta$:

$$\begin{tikzcd} C_0 \arrow[r, "\zeta"] & C_0 \arrow[d, "\mathcal{D}"] \\ & C_1 \arrow[ul, "\delta"] \end{tikzcd}$$

$$\frac{dV_\mathrm{b}}{dt} = \sum_{\mathrm{a}\not\subseteq\mathrm{b}} \sum_{\mathrm{c}\subseteq\mathrm{b}} F_{\mathrm{a}\to\mathrm{c}}\big(V_\mathrm{a} - V_\mathrm{c}\big)$$

FAITHFUL

$$\begin{tikzcd} C_0 \arrow[r, "\zeta"] & C_0 \arrow[d, "\mathcal{D}"] \\ C_1 \arrow[u, "\delta"] & C_1 \arrow[l, "\mu"] \end{tikzcd}$$

$$\frac{dV_\mathrm{b}}{dt} = \sum_{\mathrm{a}\not\subseteq\mathrm{b}} c_\mathrm{a}\, F_{\mathrm{a}\to\mathrm{a}\cap\mathrm{b}}\big(V_\mathrm{a} - V_{\mathrm{a}\cap\mathrm{b}}\big)$$

LOCALLY FAITHFUL

Thm
(P 20)

Thank you!

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Repository:
github.com/opeltre/topos

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