Statistical Systems and Local Structures

Cluster Variational Methods, Message-Passing Algorithms and Homology

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IMJ-PRG

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Global system Ω

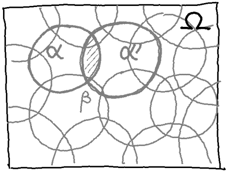
Covering $X \subseteq \mathcal{P}(\Omega)$ by subregions

$\leftarrow$ $\rightarrow$

Local approximation of free energy:

$$\mathcal{F}_\Omega \simeq \sum_{\alpha \in X} c_\alpha \mathcal{F}_\alpha$$

[Bethe 35, Kikuchi 51...]



Diffusion equation on interaction potentials:

$$\dot{u}_\alpha = \delta_\alpha \Phi(u)$$

[Gallagher 63, Pearl 82...]

Hamiltonian $H_\Omega = \sum_{\alpha \in X} u_\alpha$

Outline

Statistical Systems

Local Statistics

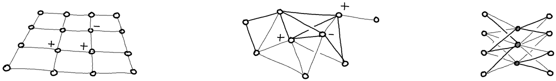
Cluster Variational Method

Statistical Diffusion

Statistical Systems

– Set $\Omega = \{i, j, k, \dots\}$ of atoms/neurons/bits/...

– Covering $X \subseteq \mathcal{P}(\Omega)$ of Ω by subregions: *hypergraph*



Crystal | Spin glass | Deep NN

– Variable $x_i \in E_i$ on each vertex

– Global configuration space $E_\Omega = \prod_{i \in \Omega} E_i$

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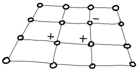

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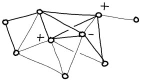
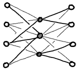


Spin glass



Deep NN

- Variable $x_i \in E_i$ on each vertex

local joint var. $x_\alpha = (x_i)_{i \in \alpha}$

- Global configuration space $E_\Omega = \prod_{i \in \Omega} E_i$

local conf. space $E_\alpha = \prod_{i \in \alpha} E_i$

$X \subseteq \mathcal{P}(\Omega)$ can describe an **interaction graph** (or hypergraph)

– The global hamiltonian $H_\Omega \in \mathbb{R}^{E_\Omega}$ is given as a **sum of interaction potentials**:

$$H_\Omega(x_\Omega) = \sum_{\alpha \in X} h_\alpha(x_\alpha)$$

e.g. $H_\Omega(x_\Omega) = \sum_i h_i(x_i) + \sum_{ij} h_{ij}(x_i, x_j)$

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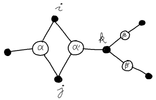
Problem: The dimension of $\mathbb{R}^{E_\Omega}$ grows exponentially with $|\Omega|$.

$\to$ $H_\Omega \in \mathbb{R}^{E_\Omega}$ actually lives in a much lower dimensional subspace

$\to$ The summing operation $\prod_\alpha \mathbb{R}^{E_\alpha} \to \mathbb{R}^{E_\Omega}$ **has a kernel**

The Gibbs distribution $p_\Omega = \frac{1}{Z_\Omega}\, \mathrm{e}^{-H_\Omega}$ is a **probabilistic graphical model**:

$$p_\Omega(x_\Omega) = \frac{1}{Z_\Omega} \prod_{\alpha \in X} f_\alpha(x_\alpha)$$



$X \leftrightarrow$ factor graph

In particular p_Ω is a **Markov random field**.

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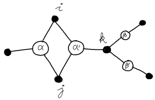


$X \leftrightarrow$ factor graph

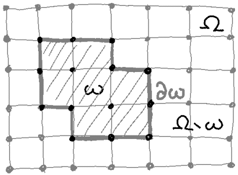
In particular p_Ω is a **Markov random field**.

→ **Conditional independence relations:**

$$p(x_\Omega | x_{\partial\omega}) = p(x_\omega | x_{\partial\omega}) \cdot p(x_{\Omega\setminus\omega} | x_{\partial\omega})$$

for every $\omega \subseteq \Omega$ union of maximal cells in X

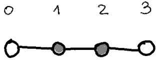
and $\partial\omega = \bigcup\{\alpha \in X | \omega \cap \alpha \neq \varnothing\}$



Gibbs and Markov random fields

Example: Markov chain when X is a linear graph.

$$p(x_0, \ldots, x_n) = p(x_0) \cdot \prod_{i=0}^{n-1} p(x_{i+1}|x_i)$$



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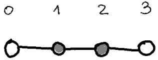
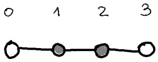


Example: Markov chain when X is a linear graph.

$$p(x_0, \dots, x_n) = \frac{\prod_{i=0}^{n-1} p(x_i, x_{i+1})}{\prod_{i=1}^{n-1} p(x_i)}$$



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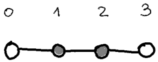

The **Hammersley-Clifford theorem** establishes a correspondence between Markov random fields and Gibbs random fields:

Markov properties $\Leftrightarrow$ Factorisability w.r.t. coarser covering

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Example: Markov chain when X is a linear graph.

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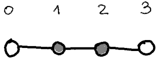

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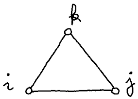
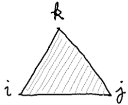


$p_{ijk} = f_{ij}\, f_{jk}\, f_{ki}$



$p_{ijk} = f_{ijk}$

X is not fully described by Markov properties (only its cliques are)

Partition function

Local factors: $p_\Omega = \frac{1}{Z_\Omega} \prod_\alpha f_\alpha = \frac{1}{Z_\Omega} \exp\left(- \sum_\alpha h_\alpha \right)$

Problem: computing $Z_\Omega = \sum_{x_\Omega \in E_\Omega} \mathrm{e}^{-H_\Omega(x_\Omega)}$ is intractable!

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Problem: computing $Z_\Omega = \displaystyle\sum_{x_\Omega \in E_\Omega} \mathrm{e}^{-H_\Omega(x_\Omega)}$ is intractable!

$\rightarrow$ Algorithms exist to compute Z_Ω in **linear time** when X is an acyclic graph, or when X is a *retractable* hypergraph.

$\rightarrow$ When X is not retractable, these algorithms yield **good estimates** of Z_Ω.

Local Observations

No **global** observations

Only **local** observations

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$\rightarrow$ *Find a good formalism to make locality explicit.*

Local Microstates

For all $\alpha \subseteq \Omega$:

- $E_\alpha = \prod_{i \in \alpha} E_i$ local configuration space, $x_\alpha \in E_\alpha$ local microstate

For all $\alpha \supseteq \beta$:

- restriction map $x_\alpha \in E_\alpha \mapsto x_\beta \in E_\beta$ forgetting the state of $\alpha \setminus \beta$

$$\begin{tikzcd}
\cdots \arrow[dr] & & E_\alpha \arrow[dl] \arrow[dr] & & \cdots \arrow[dl] \\
& E_\beta \arrow[dl] \arrow[dr] & & E_{\beta'} \arrow[dl] \arrow[dr] & \\
\cdots & & E_\gamma & & \cdots
\end{tikzcd}$$

$\rightarrow$ **projective system of sets**

sheaf: $E_\Omega = \lim_{\alpha \in X} E_\alpha$

Local Observables

For all $\alpha \subseteq \Omega$:

- $A_\alpha = \mathbb{R}^{E_i}$ algebra of local observables e.g. potential $u_\alpha(x_\alpha)$

For all $\alpha \supseteq \beta$:

- $A_\beta \subseteq A_\alpha$ is a subalgebra: $u_\beta(x_\beta)$ extends to a function of $x_\alpha \in E_\alpha$.

$$
\begin{tikzcd}
\cdots & & A_\alpha & & \cdots \\
& A_\beta \arrow[ul] \arrow[ur] & & A_{\beta'} \arrow[ul] \arrow[ur] & \\
\cdots \arrow[ur] & & A_\gamma \arrow[ul] \arrow[ur] & & \cdots \arrow[ul]
\end{tikzcd}
$$

$\rightarrow$ **inductive system of algebras**

H_Ω lies in $\operatorname*{colim}_{\alpha \in X} A_\alpha \subseteq A_\Omega$

$\mathrm{colim}_\alpha A_\alpha \simeq \sum_\alpha A_\alpha$

Local Measures and Probabilities

For all $\alpha \subseteq \Omega$:

– $\Delta_\alpha \subseteq A^*_\alpha$ space of local probabilities e.g. $p_\alpha(x_\alpha)$ marginal of the Gibbs state

For all $\alpha \supseteq \beta$:

– partial integration map $\Sigma^{\beta\alpha} : A^*_\alpha \to A^*_\beta$ integrating over the state of $\alpha \setminus \beta$:

$$\Sigma^{\beta\alpha}(p_\alpha)(x_\beta) = \sum_{x' \in E_{\alpha\setminus\beta}} p_\alpha(x_\beta, x')$$

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$\to$ **projective system of top. spaces**

Gibbs state marginals $(p_\alpha)_{\alpha \in X}$ lie in

$$\Gamma = \lim_{\alpha \in X} \Delta_\alpha$$

space of **consistent** local probabilities.

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space of **consistent** local probabilities.

substitute for a global probability p_Ω

In many applications, only the marginals (p_α) are necessary to compute the gradient of a loss function and perform gradient descent optimisation.

Energy and Entropy

Thermal equilibrium:

The Gibbs state $p_\Omega = \frac{1}{Z_\Omega}\,\mathrm{e}^{-H_\Omega}$ is characterised by **variational principles**.

– Free energy: $\mathbb{F}^\Omega(H_\Omega) = -\ln \sum \mathrm{e}^{-H_\Omega}$

– Shannon entropy: $S_\Omega(p_\Omega) = -\sum p_\Omega \, \ln p_\Omega$

– Variational free energy: $\mathcal{F}_\Omega(p_\Omega, H_\Omega) = \langle\, p_\Omega \,|\, H_\Omega \,\rangle - S_\Omega(p_\Omega)$

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Legendre: $S_\Omega \longleftrightarrow \mathbb{F}^\Omega$

– Free energy: $\mathbb{F}^\Omega(H_\Omega) = -\ln \sum \mathrm{e}^{-H_\Omega}$

$\rightarrow$ $p_\Omega = d\mathbb{F}^\Omega(H_\Omega)$

– Shannon entropy: $S_\Omega(p_\Omega) = -\sum p_\Omega \, \ln p_\Omega$

$\rightarrow$ $H_\Omega = dS_\Omega(p_\Omega) \mod \mathbb{R}$

– Variational free energy: $\mathcal{F}_\Omega(p_\Omega, H_\Omega) = \langle\, p_\Omega \,|\, H_\Omega \,\rangle - S_\Omega(p_\Omega)$

$\rightarrow$ p_Ω is extremal for $\mathcal{F}_\Omega(\,-\,, H_\Omega)$

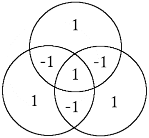
Combinatorics and Extensivity

Möbius inversion and inclusion-exclusion principles:

$$H_\alpha = \sum_{\alpha \supseteq \beta} h_\beta$$

$$\updownarrow$$

$$h_\alpha = \sum_{\alpha \supseteq \beta} \mu_{\alpha\beta} H_\beta$$



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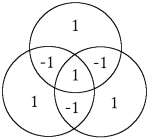

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Extensivity of internal energy: $\langle\, p_\Omega \mid H_\Omega \,\rangle = \sum_{\alpha \in X} \langle\, p_\alpha \mid h_\alpha \,\rangle = \sum_{\beta \in X} c_\beta \langle\, p_\beta \mid H_\beta \,\rangle$

linearity of internal energy $\rightarrow$ **exact** decomposition as a sum of local functionals

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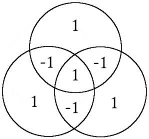

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linearity of internal energy $\to$ **exact** decomposition as a sum of local functionals

Extensivity of entropy: $S_\Omega(p_\Omega) \simeq \sum_{\beta \in X} c_\beta S_\beta(p_\beta)$

coarser covering X $\to$ more precise approximation

[Bethe 1935, Kikuchi 1951, Schlijper 1983]

Cluster Variational Method

Given a hamiltonian $H_\Omega = \sum_\beta c_\beta H_\beta$,

$\to$ Approximate the global functional $\mathcal{F}_\Omega(p_\Omega, H_\Omega)$ by the **local functional**:

$$\check{\mathcal{F}}(q, H) = \sum_{\beta \in X} c_\beta \Big[\langle\, q_\beta \mid H_\beta \,\rangle - S_\beta(q_\beta) \Big]$$

$\to$ Extremise $\check{\mathcal{F}}(\,-\,, H)$ w.r.t. the **consistency constraints**:

$$q \in \Gamma(X) \quad \Leftrightarrow \quad q_\beta \text{ marginal of } q_\alpha \text{ for all } \beta \subseteq \alpha$$

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N.B. consistent beliefs are not always the marginals of a global probability!

$\to$ depends on the geometry of X

$\to$ liar circles, (quantum) contextuality, ... [Abramsky 2011]

Theorem: When X is an **acyclic graph** *(retractable hypergraph)*,

the unique extremum q of $\check{\mathcal{F}}(\,-\,, H)$ coincides with the Gibbs state marginals:

$$q_\alpha(x_\alpha) = \frac{1}{Z_\Omega} \sum_{x' \in E_{\Omega \setminus \alpha}} \mathrm{e}^{-H_\Omega(x_\alpha, x')}$$

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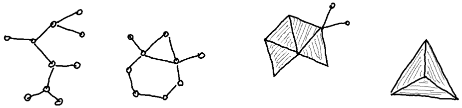

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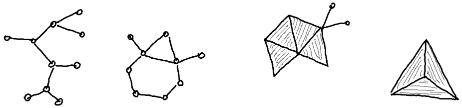


+ X + X

Corollary: When X is an **acyclic graph** *(retractable hypergraph)*,

the global Gibbs state factorises by its marginals:

$$p_\Omega = \prod_{\beta \in X} (p_\beta)^{c_\beta} \quad \Leftarrow \quad p_\Omega = \frac{\prod_{ij} p_{ij}}{\prod_i p_i^{d_i - 1}}$$

In general: Solutions (q_α) of the CVM are multiple.

They yield good approximations of the true Gibbs state marginals (p_α).

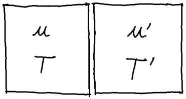
$\rightarrow$ What kind of algorithms solve the CVM?

synonyms: belief propagation, sum-product algorithm, message-passing algorithm...

Message-Passing Algorithms are equivalent to discrete integrators of

continuous-time diffusion equations.

Thermodynamics and Heat

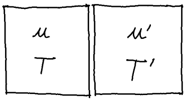


Thermodynamics:

Conservation: $u_{eq} + u'_{eq} = u_0 + u'_0$

Heat flux: $\vec{\varphi} = u_{eq} - u_0 = u'_0 - u_{eq}$

Equilibrium: $T_{eq} = T'_{eq}$



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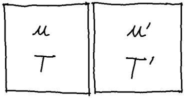
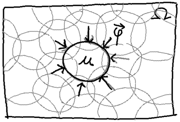
$\rightarrow$ else **non-linear** relationship between u and T





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Heat:

Conservation: $\dot{u} = -\mathrm{div}(\vec{\varphi})$

Heat flux: $\vec{\varphi} = -\lambda\, \vec{\mathrm{grad}}(T)$

Equilibrium: $\vec{\mathrm{grad}}(T) = 0$

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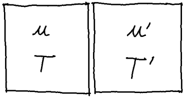
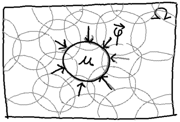
Thermodynamics and Heat





Thermodynamics:

Conservation: $u_{eq} + u'_{eq} = u_0 + u'_0$

Heat flux: $\vec{\varphi} = u_{eq} - u_0 = u'_0 - u_{eq}$

Equilibrium: $T_{eq} = T'_{eq}$

$\rightarrow$ if $u = cT$ then $T_{eq} = \frac{cT_0 + c'T'_0}{c + c'}$

$\rightarrow$ else **non-linear** relationship between u and T

Heat:

Conservation: $\dot{u} = -\mathrm{div}(\vec{\varphi})$

Heat flux: $\vec{\varphi} = -\lambda\, \vec{\mathrm{grad}}(T)$

Equilibrium: $\vec{\mathrm{grad}}(T) = 0$

$\rightarrow$ Laplace equation $\dot{u} = -\frac{\lambda}{c}\,\Delta u$

$\rightarrow$ or $\dot{u} = -\lambda \Delta T$ and non-linear $u \leftrightarrow T$.

Heat and Homology

Energy conservation: $\mathcal{U} = \int_{\mathbb{R}^3} u_{eq} = \int_{\mathbb{R}^3} u_0$

$\rightarrow$ u_0 and u_{eq} are said **homologous**: $\exists \vec{\psi}$ s.t. $u_{eq} = u_0 + \mathrm{div}(\vec{\psi})$

Thermal equilibrium: $\vec{\mathrm{grad}}(T) = 0$

$\rightarrow$ $T \in \mathrm{Ker}(\vec{\mathrm{grad}})$ is called a **cocycle**.

Homology is a central concept of modern mathematics [Noether, Poincaré]

Concepts actually stem from **physics** and **electromagnetism** [Gauss, Maxwell]

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Gauss theorem: $\quad u = h + \delta\varphi \quad \Leftrightarrow \quad \sum_\alpha u_\alpha = \sum_\alpha h_\alpha \qquad$ [O.P.]

The global hamiltonian is a **homology class** of interaction potentials.

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Consistent belief: $q \in \Gamma(X) = \mathrm{Ker}(d)$ i.e. q_β marginal of q_α for all $\alpha \supseteq \beta$.

Consistent beliefs are **cohomology classes** of local probability densities.

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(review)

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$$\to \dot{u} = \delta\Phi$$

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Fix a reference hamiltonian $H_\Omega = \sum_\alpha h_\alpha$.

Correspondence Theorem: [Yedidia et al 2005, O.P. 2019]

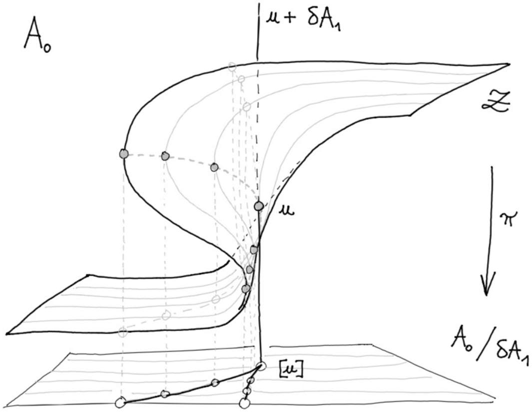
Assume $q \in \Gamma(X)$ is consistent and let $U = -\ln(q)$ with $U_\alpha = \sum_{\alpha \supseteq \beta} u_\beta$.

The following are equivalent:

– $q \in \Gamma(X)$ is **extremal** for the constrained free energy $\check{\mathcal{F}}(-, H)$

– There exists $\varphi \in A_1(X)$ such that $u = h + \delta\varphi$ is **stationary** under diffusion.

Singularities



The intersection is not transverse: there are **singularities**.

Thank you for your attention

Slides should be available at:

http://opeltre.github.io/assets/bib/msc.pdf