Compositional statistical mechanics, entropy and variational inference

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Statistical mechanics: motivation and problems

Statistical mechanics: motivation

- What for? $\rightsquigarrow$ modelling interaction between random variables, e.g. $X = X_1 ... X_N \in \{-1, 1\}$.
- How? $\rightsquigarrow$ Energy-based modeling
  - energy function (Hamiltonian), e.g.

$$H = X_1 \cdot X_2 + X_2 \cdot X_3 + X_3 \cdot X_4 \dots$$

  - Probability distribution: Boltzmann distribution

$$p_X \propto e^{-\beta H} \propto e^{\beta X_1 \cdot X_2} \cdot e^{\beta X_2 \cdot X_3} \cdot e^{\beta X_3 \cdot X_4} \dots \qquad \text{(Markov chain)}$$

- Relation to computer science [MM09], (key words):
  - Markov chain, Hidden Markov model (HMM)
  - Graphical models, factor graphs ...
  - Inference (maximum likelihood), Bayesian inference $\rightsquigarrow$ machine learning ($\neq$ deep learning)

Statistical mechanics: problems of interest

When there are a (countable) infinity of random variables $(X_1, \dots X_n, \dots)$ then:

- one Hamiltonian $H \to$ how to make sense of $p_X \propto e^{-\beta H}$
  - $\rightsquigarrow$ several possible distribution p (Dobrushin-Lanford-Ruelle condition)
  - $\to$ Phases, pure phases, e.g "solid, gaz, liquid"
- Characterizing the phases is a hard problem
- "Manipulating" (transforming) the phases is difficult
- For translation invariant potential:
  - $\to$ Correspondance: phases $\leftrightarrow$ tangent of a convex functional ("Helmholtz free energy") at H.
  - $\Lsh$ relates to variational principle

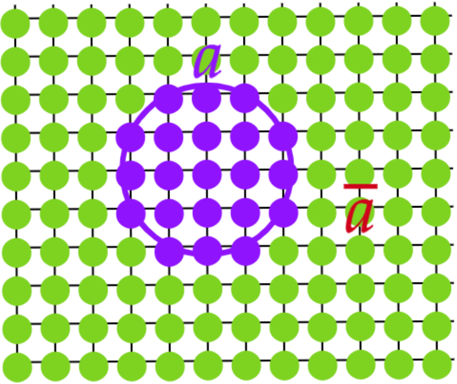
Statistical mechanics: formal definitions

Setting

- I index of (finite) random variables: $(X_i \in E_i, i \in I)$
- Global state space $\Omega = \prod_{i \in I} E_i$ denoted as E with $\sigma-$algebra $\mathscr{E}$,
- $\mathbb{P}(E)$ space of measures

- $a \subseteq I$ finite subset of I, $\mathscr{P}_f(I)$ the set of finite subsets
- $X_a \in E_a = \prod_{i \in a} E_i$ or $(E, \mathscr{E}_a)$ when seen in $(E, \mathscr{E})$
- for $b \subseteq a$, $i^a_b : E_a \to E_b$ in $\mathbf{Mes}(E_a, E_b)$

- Statistical system: collection of border conditions



- Probability kernel $p : E_{\overline{a}} \to E$,
- $p \in \mathbf{Kern}(E_{\overline{a}}, E)$
- $\forall \omega_{\overline{a}} \in E_{\overline{a}}, p_{\omega_{\overline{a}}} \in \mathbb{P}(E)$
- For $A \in \mathscr{E}$, $p(A|\omega_{\overline{a}})$ "$\cong$" $\mathbb{E}[A|\mathscr{E}_{\overline{a}}]$

Proper kernel

Definition: Proper Kernel [Geo11]

Let $\mathscr{E}_1 \subseteq \mathscr{E}$ be two σ-algebras of a set E, a kernel $p \in \mathbf{Kern}((E, \mathscr{E}_1), (E, \mathscr{E}))$ is proper if and only if, for any $A \in \mathscr{E}$, any $B \in \mathscr{E}_1$ and any $\omega \in E$,

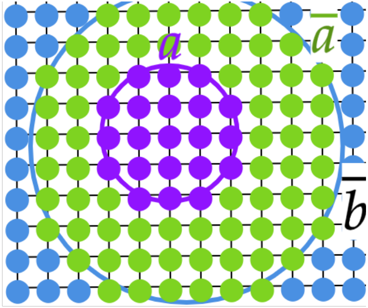
$$p(A \cap B|\omega) = p(A|\omega)1[\omega \in B]$$

For f a $\mathscr{E}_1-$measurable function,

$$p(f|\omega) = \int f(x)p(dx|\omega) = f(\omega)$$

Let $i : (E, \mathscr{E}) \to (E, \mathscr{E}_1)$ the set identity map. $p : (E, \mathscr{E}_1) \to (E, \mathscr{E})$ proper if and only if, $i \circ p = \mathrm{id}$.

Tower rule



- Tower rule: for $A \in \mathscr{E}$,

$$\mathbb{E}\left[\mathbb{E}[A|\mathscr{F}_{\overline{a}}]|\mathscr{F}_{\overline{b}}\right] = \mathbb{E}[A|\mathscr{F}_{\overline{b}}]$$

- For $\omega \in E$,

$$p_{\overline{a}} \circ p_{\overline{b}}(A|\omega_{\overline{b}}) = \int p(A|x_{\omega_{\overline{a}}})p(dx|\omega_{\overline{b}})$$

$$p_{\overline{b}}\left(p_{\overline{a}}(A|.)|\omega_{\overline{b}}\right) = p_{\overline{b}}(A|\omega_{\overline{b}})$$

Specification

Definition: Specification [Geo11]

A specification with parameter set I and state spaces $(E, \mathscr{E})$ is a collection $(\gamma_a, a \in \mathscr{P}_f(I))$ of proper kernels such that for any $a \in \mathscr{P}_f(I)$, $\gamma_a \in \mathbf{Kern}\,((E, \mathscr{E}_{\overline{a}}), (E, \mathscr{E}))$ and which satisfies that for any $a \subseteq b$, i.e $\overline{b} \subseteq \overline{a}$, any $A \in \mathscr{E}$ and $\omega \in E$,

$$\gamma_a \gamma_b(A|\omega) = \gamma_b(A|\omega)$$

Gibbs measures

Definition: Gibbs measures

Let γ be a specification with state space E, the set of probability measures,

$$\mathscr{G}(\gamma) = \{\mu \in \mathbb{P}(E) \quad : \quad \mathbb{E}_\mu(A|\mathscr{E}_{\overline{a}}) = \gamma_a(A|.)\ \mu \text{ a.s.}\}$$

is called the set of Gibbs measures of γ.

Contribution: Proposed categorical formulation

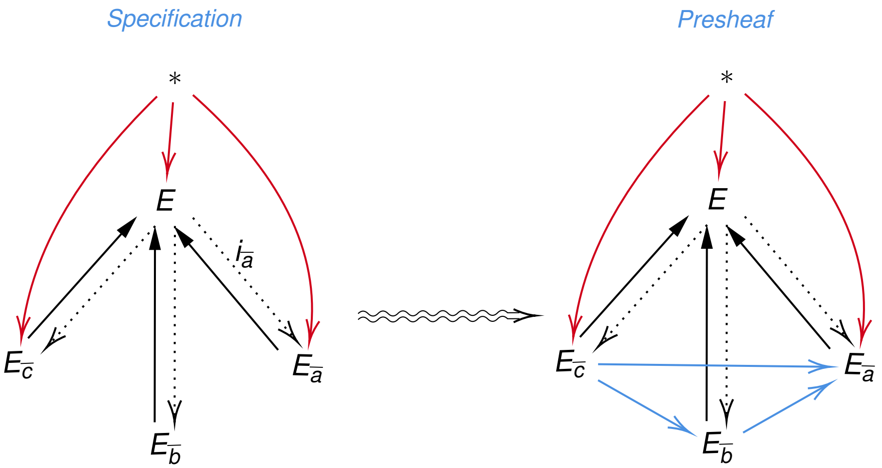
Problem:

- reference to ‘global’ $E \leftrightarrow$ difficult to “transform phases”, in fact:
  - $\rightarrow$ Hamiltonian don’t behave well with respect to maps $E \rightarrow E_1$
  - $\rightarrow$ local operation on H $(+\phi)$ are not compositional for $\mu \in \mathscr{G}(\gamma)$

What we would like:

- *“to build complex statistical systems from simple ones in a way that allows controlling and computing the phases of the associated statistical systems from the phases of the simpler one.”*
- other motivation:
  - $\rightarrow$ model statistical systems with incomplete/incompatible information on variables $+$ heterogeneity
    (related to use of sheaves in data science [SP22, Cur13, BGC$^+$22])

From classical description to categorical description



- The collection $(i_{\overline{a}}, a \in \mathscr{P}(I))$ encodes the functor of observables

Link with functors

Proposition (SP '21)

Let γ be a specification with the state space E. For any $a, b \in \mathscr{P}_f(I)$ such that $b \subseteq a$, there is a unique Markov kernel $F^a_b : E_{\overline{a}} \to E_{\overline{b}}$ such that the following diagram commutes,

$$\begin{array}{ccc} E_{\overline{a}} & \xrightarrow{\gamma_a} & E \\ {\scriptstyle F^a_b}\downarrow & \nearrow{\scriptstyle \gamma_b} & \\ E_{\overline{b}} & & \end{array} \tag{0.1}$$

i.e. such that $\gamma_b \circ F^a_b = \gamma_a$. Furthermore for any collection $a, b, c \in \mathscr{P}_f(I)$ with $a \subseteq b \subseteq c$,

$$F^b_c \circ F^a_b = F^a_c \tag{0.2}$$

Categories of measurable spaces and probability kernels

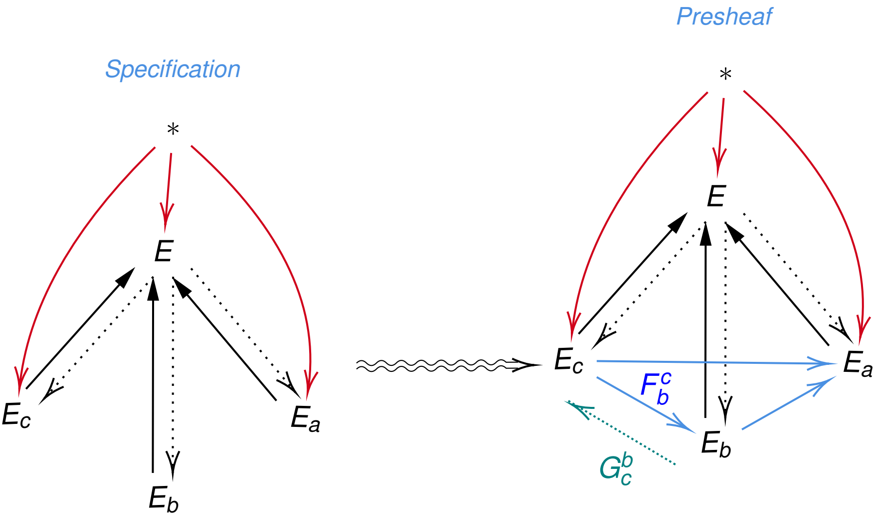
- **Mes**: Objects are measurable space, Morphisms are measurable applications
- **Kern**: Objects are measurable spaces, Morphisms are probability kernel

Proposed categorical formulation: specifications

Definition (Generalized Specification, $\mathscr{A}$-Specifications)

Let $\mathscr{A}$ be a poset, a generalized specification over $\mathscr{A}$, or simply $\mathscr{A}$-specification, is a couple (G, F) of a presheaf and a functor where $G : \mathscr{A}^{op} \to \mathbf{Mes}$ and $F : \mathscr{A} \to \mathbf{Kern}$ are such that for any $a, b \in \mathscr{A}$ with $b \leq a$,

$$G^a_b F^b_a = \text{id} \tag{0.3}$$



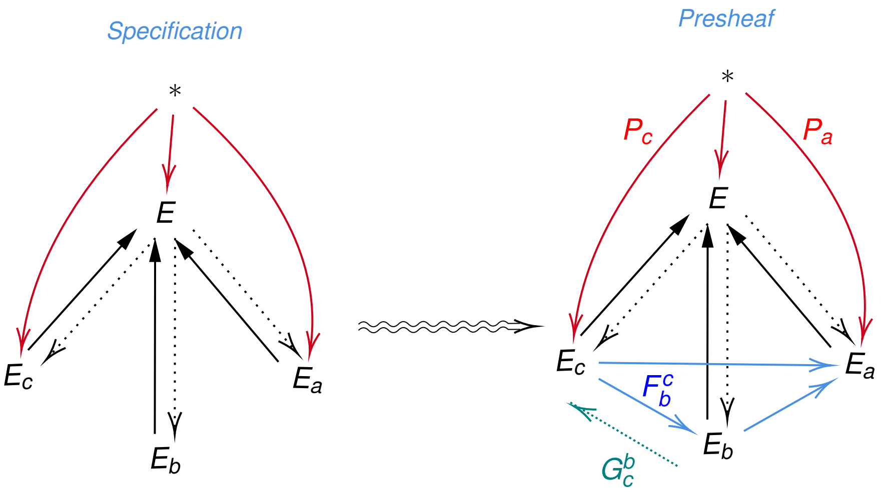
$$G_c^b F_b^c = \mathrm{id}$$

Proposed categorical formulation: Gibbs measures of a specification

Definition 8.3.7: Gibbs measures for specifications

Let $\gamma = (G, F)$ be a specification over $\mathscr{A}$, we shall call the Gibbs measures of γ the sections of F,

$$\mathscr{G}_g(\gamma) = \{P_a \in \mathbb{P}(F(a)), a \in \mathscr{A} | \quad \forall b \leq a, F_a^b P_b = P_a\}$$


Specification
Presheaf
*
E
E_c
E_b
E_a
P_c
P_a
F_b^c
G_c^b

Use homological algebra to compute phases.

- Phases are invariants: H^0
- Use resolutions to compute H^0.
- Projective and injective objects characterized in previous work (next slides)

$\implies$ Projectives extend independent random variables
Corollary 3.2 [SP20] (necessary condition harder)

Projective presheaves

Definition (Projective presheaf)

$F : \mathscr{A}^{op} \to \textbf{Vect}$ is projective if there is a collection S_a, $a \in \mathscr{A}$ such that,

$$F(a) \cong \bigoplus_{c \leq a} S_c \tag{0.4}$$

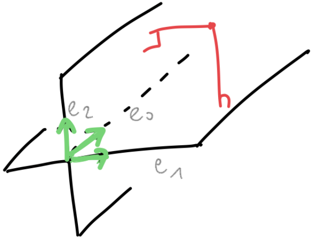
and,

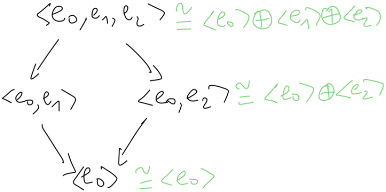
$$F_b^a \cong pr_b^a : \bigoplus_{c \leq a} S_c \to \bigoplus_{c \leq b} S_c \tag{0.5}$$

$\to$ Characterized in [SP20]: "$F_b^a \circ F_c^a = F_{b \wedge c}^a$"

Projective presheaves: example

- $V := \mathbb{R}^3$, $V_1 := \langle e_0, e_1 \rangle$, $V_2 := \langle e_0, e_2 \rangle$, $V_3 := \langle e_0 \rangle$
- Projections: orthogonal with respect to scalar product
- Collection of projections defines a projective presheaf





- Change scalar product $\rightsquigarrow$ not projective anymore.

Projective specifications

- $L^\infty(E)$, the set of bounded, real-valued, measurable functions over E
- L^∞: presheaf from **Mes** and **Kern** to the category of vector spaces **Vect**
- Consider $L^\infty \circ F : \mathscr{A}^{op} \to \textbf{Vect}$

Definition (Projective $\mathscr{A}$-specifications)

An $\mathscr{A}$-specification (G, F) is called projective when $L^\infty \circ F$ is a projective presheaf (in **Vect**).

Phases of projective presheaves

- poset $\mathscr{A}$, equivalence relation by symmetrizing the order:

$$\forall a, b \in \mathscr{A}, \; a \sim b \iff a \leq b \text{ or } b \leq a \tag{0.6}$$

- equivalence classes are connected components
- denote $\mathscr{C}(a)$ the connected component of $a \in \mathscr{A}$
- if each connected component has a minimum element, denote $\mathscr{C}_*(\mathscr{A})$ the set of these minimas. If not $\mathscr{C}_*(\mathscr{A}) := \emptyset$

Phases of projective presheaves

Theorem (SP '21)

Let $\gamma = (G, F)$ be a projective $\mathscr{A}$-specification. If at least one of the connected components of $\mathscr{A}$ does not have a minimum element, i.e. when,

$$\mathscr{C}_*(\mathscr{A}) = \emptyset \tag{0.7}$$

then,

$$\mathscr{G}_g(\gamma) = \emptyset \tag{0.8}$$

if not,

$$\mathscr{G}_g(\gamma) = \prod_{a \in \mathscr{C}_*(\mathscr{A})} \mathbb{P}(\gamma(a)) \tag{0.9}$$

Characterizing extreme Gibbs measures of $\mathscr{A}$ -specifications

$\hookrightarrow$ ~~towards~~ a $0-1$ law for extreme Gibbs measures of $\mathscr{A}$ -specifications

Classical setting

For simplicity of presentation: $I = \mathbb{N}$,

- $E = \prod_{i \in \mathbb{N}} E_i$
- $\mathscr{E}_{\geq k}$, σ-algebra generated by the cylinders: $i_{\geq k}^{-1}(A)$ where $A \subseteq \prod_{n \geq k} E_n$.
- tail σ-algebra: $\mathscr{E}_\infty := \bigcap_{k \in \mathbb{N}} \mathscr{E}_{\geq k}$.
- Set of Gibbs measures $\mathscr{G}(\gamma)$ is convex.

From [Geo11]):

→ Gibbs measures are fully characterized by their restriction to the tail σ-algebra $\mathscr{E}_\infty$.

→ Extreme Gibbs measures, $\mu \in \text{ext}\, \mathscr{G}_g(\gamma)$, are 'trivial' on $\mathscr{E}_\infty$, i.e. for any $A \in \mathscr{E}_\infty$,

$$\mu(A) = 0 \text{ or } 1$$

Assumptions

- Recall $\gamma = (G, F)$, $G : \mathscr{A}^{op} \to \mathbf{Mes}$, $F : \mathscr{A} \to \mathbf{Kern}$
- Assumptions: $G(a)$ are finite ($\mathscr{A}$ does not need to be finite) and a "positivity condition" on F.
  - ↼ Assumption (probably) not required for weaker version of $0-1$ law.

Tail σ-algebra for $\mathscr{A}$-specifications

Definition (Tail σ-algebra for $\mathscr{A}$-specifications)

Let $\gamma = (G, F)$ be a $\mathscr{A}$-specification. Pose $\sigma(G)^b_a A_b := G^{a^{-1}}_b A_b$,for $b \leq a$. The tail σ-algebra of $\mathscr{A}$-specification is defined as:

$$\lim \sigma(G) := \{(A_a \in \sigma(G(a)), a \in \mathscr{A}) | \forall a, b \in \mathscr{A}, \quad A_a = G^{a^{-1}}_b A_b\}$$

$0 - 1$ law for $\mathscr{A}$-specifications

Theorem (SP '24, Section 7 [SP24])

Let $\gamma = (G, F)$ be a specification, let $G(a)$ be finite sets for any $a \in \mathscr{A}$, let $F > 0$. $\mathscr{G}_g(\gamma)$ is a convex set. Each $\mu \in \mathscr{G}_g(\gamma)$ is uniquely determined by it's restriction to $\lim \sigma(G)$. Furthermore μ is extreme in $\mathscr{G}_g(\gamma)$ if and only if for any $A \in \lim \sigma(G)$, $\forall a \in \mathscr{A}$, $\mu_a(A_a) = 0$ or 1.

$\rightarrow$ Echoes with $0-1$ laws in a categorical setting for i.i.d sequences and Markov chains [FGP21, MP23].

$\hookrightarrow$ Full relation to be explored in future work.

Toward an entropy and variational principle for $\mathscr{A}$-specifications
$\rightsquigarrow$ Section 8 Paper arXiv:2403.16104

Thank you for your attention

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