Functoriality of inference on diagrams in the category of Markov kernels.

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Introduction to geometric deep learning [BBCV21]:

- Deep learning $\leftarrow$ curse of dimensionality
- Accounting for symmetry
  - $\rightarrow$ Translation $\rightsquigarrow$ CNN
  - $\rightarrow$ Other groups [SPMBO22]
- Geometry $\rightsquigarrow$ discretize
  - $\rightarrow$ Graph NN [BBCV21]
  - $\rightarrow$ Nodes share same features
  - $\rightarrow$ Limitations: heterogeneous data
- Heterogeneity
  - $\rightarrow$ Cellular sheaves [Cur13]
  - $\rightarrow$ Cell complex, faces $\rightsquigarrow$ feature space, inclusions $\rightsquigarrow$ linear maps
  - $\rightarrow$ Functor from a poset to **Vect** [SP22, SP24a, SPR24, SP24b]
  - $\rightarrow$ Sheaf Neural Networks [BGC+22]

- Our focus:
  - $\rightarrow$ Bayesian inference, graphical models, Markov random fields, factor graphs

Context:

Let X be a random variable taking values in a finite measurable space E_X, and $\theta \in \Theta \subseteq \mathbb{R}^d$ that parametrizes a collection of probability measures $P(x|\theta)$, where $x \in E_X$.
Assume that one is given a prior $Q \in \mathbb{P}(\Theta)$, where $\mathbb{P}(\Theta)$ denotes the space of probability measures on Θ. For any observation $x_0 \in E_X$, one computes the posterior using Bayes' rule:

$$P(\theta|x) = \frac{P(x|\theta)Q(\theta)}{\int P(x|\theta)Q(\theta)\,d\theta}$$

- Problem: When $\theta = (\theta_i, i \in [0, N])$ is a collection of variables, where each $\theta_i \in E$.
- $\sum_\theta P(x|\theta)Q(\theta) = \sum_{\theta_0} \cdots \sum_{\theta_N} P(x|\theta_0, \ldots, \theta_N)Q(\theta_0, \ldots, \theta_N)$

  $\rightarrow$ Number of operations: $\mathscr{O}(|E|^N)$
- Notation: For a set of indices I and a subset $a \subseteq I$, $\theta_a := (\theta_i \in E_i, i \in a)$.
- In what follows, all the sets in which variables take values will be finite: E_i are finite sets.

- One relation to statistical mechanics:

Let $\theta = (Y_i \in E_i, i \in I)$ be the unobserved variables, and $X = (X_j \in F_j, j \in J)$ the observed variables. Both I and J are finite sets, and E_j for $j \in J$ and F_i for $i \in I$ are finite sets.

$$\ln P(\theta, X) = -\beta \sum_{a \subseteq I \sqcup J} H_a(X_{a \cap J}, Y_{a \cap I})$$

Given an observation $x = (x_i, i \in I)$, computing $\ln P(\theta|x)$ is equivalent to computing:

$$\ln \sum_{(y_i, i \in I)} e^{-\beta \sum_{a \subseteq I \sqcup J} H_a(x_{a \cap J}, y_{a \cap I})}$$

This is the same as:

$$\ln Z(x) := \ln \sum_{\theta \in \prod_i E_i} e^{-\beta \tilde{H}_x(\theta)}$$

- Similar frameworks but different names: Bayesian networks, graphical models, factor graphs, Markov random fields.

Definition (Factorisation Space)

Let I be a finite set, and let $\mathscr{A} \subseteq \mathscr{P}(I)$, where $\mathscr{P}(I)$ is the power set of I. Let $(E_i, i \in I)$ be a collection of sets, and let $E_a = \prod_{i \in a} E_i$ for any $a \in \mathscr{P}(I)$. For $x \in \Omega$, we denote by x_a its projection onto E_a. The factorisation space over $\mathscr{A}$ is defined as follows:

$$\mathrm{Fac}_{\mathscr{A}} = \{P \in \mathbb{P}(\Omega) : \exists (f_a \in \mathbb{R}_{>0}^{E_a}, a \in \mathscr{A}) \text{ s.t. } \forall x \in \Omega,\ P = \prod_{a \in \mathscr{A}} f_a(x_a)\}$$

Consider an undirected graph $G = (I, A)$ that is **acyclic.** Denote $\mathscr{A}(G)$ as the *partially ordered set* (poset) with elements $V = I \sqcup A$ and the following relations:

- $\forall i \in I,\ i \leq i$, and $\forall e \in A,\ e \leq e$
- $\forall i \in I,\ \forall e \in A,\ i \leq e \iff i \in e$

Proposition (Factorization on Acyclic Graphs)

Let I be a finite set, and let $\Omega = \prod_{i \in I} E_i$ be a product of finite sets, and $X_i, i \in I$, a collection of random variables taking values respectively in E_i. Let $G = (I, A)$ be a finite acyclic graph. $P_X \in \mathbb{P}_{>0}(E)$ factors according to $\mathscr{A}(G)$, i.e., $P_X \in \mathrm{Fac}_{\mathscr{A}(G)}$, if and only if for any $\omega \in \Omega$,

$$P_X(\omega) = \frac{\prod_{e \in A} P_{X_e}(\omega_e)}{\prod_{i \in I} P_{X_i}^{d(i)-1}(\omega_i)},$$

where $d(i)$ is the degree of node $i \in I$.

- Bayesian inference is maximizing (relative) entropy.
- **Entropy:**

$$S(Q) = -\sum_{\omega \in E} Q(\omega) \ln Q(\omega) \tag{0.1}$$

- Recall that minimizing Gibbs free energy gives Helmholtz free energy:

$$\beta \frac{-\ln Z}{\beta} = \inf_{Q \in \mathbb{P}(E)} (\mathbb{E}_Q[\beta H] - S(Q))$$

- Set $\beta = 1$.

- But entropy:

$$S(P_X) = \sum_{e \in A} S(P_{X_e}) - \sum_{i \in I} (d(i) - 1) S(P_{X_i})$$

- Inclusion-exclusion formula: $c(e) = 1$, $c(i) = -(d(i) - 1)$
- Remarkably, Bayesian inference is the same as minimizing [YFW05, YFW03]:

$$F_{\text{Bethe}}(Q) = \sum_{a \in V} c(a) \left(\mathbb{E}_{Q_a}[H_a] - S(Q_a)\right)$$

where $Q := (Q_a \in \mathbb{P}(X_a), a \in V)$ with compatibility by marginalization:

→ If a is an edge and i a vertex in a
→ $\pi^e_i : E_e \to E_i$
→ We ask that ${\pi^e_i}_*(Q_e) = Q_i$

- Bayesian inference corresponds to computing $\ln Z$ for a Hamiltonian $H : \prod_{i \in I} E_i \to \mathbb{R}$, with $Z = \sum_x e^{-\beta H(x)}$.
- From now on, set $\beta = 1$; notation $E = \prod_{i \in I} E_i$.
- It is computationally costly to compute directly, but note that

$$-\ln Z = \inf_{Q \in \mathbb{P}(E)} (\mathbb{E}_Q[H] - S(Q))$$

- The previous problem can be reformulated as minimizing:

$$F_{\text{Bethe}}(Q_a, a \in \mathscr{A}(G)) = \sum_{a \in \mathscr{A}(G)} c(a) \, (\mathbb{E}_{Q_a}[H_a] - S(Q_a))$$

  with $Q_i(x_i) = \sum_{y \in X_{i'}} Q_e(x_i, y)$ when $e = \{i, i'\}$.
- Belief propagation is an algorithm of complexity $\mathscr{O}(|A||E_i|^2)$ to solve this optimization problem, when $E_i = E_j$ for all $i, j \in I$.

$\rightarrow$ Extension to higher-order interactions: not just graphs.

$\rightarrow$ I did not invent it [Pel20, YFW05]... but no name?

Definition (Graphical Presheaves)

Let I be a finite set and $\mathscr{A} \subseteq \mathscr{P}(I)$ be a sub-poset of the powerset of I. Let $E_i, i \in I$ be finite sets. For $a \in \mathscr{A}$, define $E_a := \prod_{i \in a} E_i$. Let $F(a) := E_a$, and for $b \subseteq a$, let $F_b^a : E_a \to E_b$ be the projection map from $\prod_{i \in a} E_i$ to $\prod_{i \in b} E_i$. We call F a graphical presheaf from $\mathscr{A}$ to $\mathbf{Mes}^f$.

- Only projections.
- Only products of variables, and subcollections of variables.

- Consider any map, not just projections:
  - $\rightarrow$ Any measurable maps for $b \rightarrow a$ and even Markov kernels, i.e., stochastic matrices when the source and target are finite sets.
- Account for possible heterogeneity, incompleteness, and incompatibility in the description of variables:
  - $\rightarrow$ Agents with different world models that communicate their beliefs.
  - $\rightarrow$ Broader class of effective potentials in computational chemistry.

Extension done in previous work [SP22, SPR24, SP24a]

- **Kern**^{f}: objects are finite measurable spaces, morphisms are Markov kernels (stochastic matrices).
- F is a contravariant functor from $\mathscr{A}$ to **Kern**^{f}; $F_b^a : F(a) \to F(b)$ is denoted element-wise as $F_b^a(\omega_b \mid \omega_a)$, with $\omega_b \in F(b)$, $\omega_a \in F(a)$.
  - $\rightarrow$ F encodes all the ways our data can interact.
  - $\rightarrow$ $\mathscr{A}$ is any poset, not just a collection of subsets.
  - $\rightarrow$ Maps are not just projections.
- $Q = (Q_a \in \mathbb{P}(F(a)), a \in \mathscr{A})$
- $F_{Bethe}(Q) = \sum_{a \in \mathscr{A}} c(a) \, (\mathbb{E}_{Q_a}[H_a] - S(Q_a))$; $c(a) = \sum_{b \geq a} \mu(b, a)$ is the generalization of the inclusion-exclusion formula associated with $\mathscr{A}$.

For a finite poset $\mathscr{A}$,

- the 'zeta-operator' of $\mathscr{A}$, denoted ζ, from $\bigoplus_{a\in\mathscr{A}}\mathbb{R}$ to $\bigoplus_{a\in\mathscr{A}}\mathbb{R}$ is defined as, for any $\lambda\in\bigoplus_{a\in\mathscr{A}}\mathbb{R}$ and any $a\in\mathscr{A}$, $\zeta(\lambda)(a)=\sum\limits_{b\leq a}\lambda_b$
- its inverse is denoted as μ; $(\mu(a,b), b\leq a)$ Möbius function of $\mathscr{A}$.

We want to do Bayesian inference on these diagram.

- Constraint: the Q_a must be compatible under the actions of the F^a_b, i.e. $F^a_b\circ Q_a=Q_b$
- Problem: find an algorithm to 'solve' the optimization problem.
  - $\rightarrow$ New message passing algorithm!

F induces several actions: on probabilities, on probabilites seen as vectors, on their dual...

- $\tilde{F}^a_b : \mathbb{P}(F(a)) \to \mathbb{P}(F(b))$ is linear map that sends probability distributions $p \in \mathbb{P}(F(a))$ to $F^a_b \circ p$, we still note $\tilde{F}$ the linear map from $\mathbb{R}^{F(a)}$ to $\mathbb{R}^{F(b)}$.
- $\tilde{F}^*$ is the functor obtained by dualizing the morphisms $\tilde{F}^a_b$, i.e. $\tilde{F}^{*b}_a : \tilde{F}(b)^* \to \tilde{F}(a)^*$ sends linear maps $l_b : \tilde{F}(b) \to \mathbb{R}$ to $l_b \circ \tilde{F}^a_b : \tilde{F}(a) \to \mathbb{R}$.

μ can be extended to account for $\tilde{F}$ through $\tilde{F}^*$:

- for a functor G from $\mathscr{A}$ to $\mathbb{R}$-vector spaces, we define μ_G as, for any $a \in \mathscr{A}$ and $v \in \bigoplus_{a \in \mathscr{A}} G(a)$, $\mu_G(v)(a) = \sum_{b \leq a} \mu(a, b) G^b_a(v_b)$.
- ζ_G is it's inverse, $\zeta_G(v)(a) = \sum_{b \leq a} G^b_a(v_b)$.

Recall we want to solve $\inf F_{\text{Bethe}} = \sum_a c(a)F(Q_a)$ under

- Constraint: the Q_a must be compatible under the actions of the F^a_b, i.e., $F^a_b \circ Q_a = Q_b$
  - i.e., $Q \in \lim \tilde{F}$
  - In fact, no... need to add the condition that the distribution sums to one.
  - But it's okay!

Algorithm 1: Message passage algorithm for presheaves from $\mathscr{A}$ to $\mathbf{Kern}^f$

Data: Initialization: $(m^0_{a\to b} \in \mathbb{R}^{F(b)}, b, a \in \mathscr{A}$ s.t. $b \leq a)$, a poset $\mathscr{A}$, a presheaf $F : \mathscr{A} \to \mathbf{Kern}^f$;

for $t \leq T$ **do**

  for $a \in \mathscr{A}, b \in \mathscr{A}$ *such that* $b \leq a$ **do**

    $\forall \omega_a \in F(a), \quad n_{b\to a}(\omega_a) \leftarrow \prod_{\substack{c : b \leq c \\ c \nleq a}} \sum_{\omega_b' \in F(b)} m_{c\to b}(\omega_b') \cdot F^a_b(\omega_b' | \omega_a)$

  end

  for $a \in \mathscr{A}, b \in \mathscr{A}$ *such that* $b \leq a$ **do**

    $b_a = e^{-H_a} \prod_{\substack{b \in \mathscr{A} : \\ b \leq a}} n_{b\to a}$

    $p_a = \frac{b_a}{\sum_{\omega_a} b_a(\omega_a)}$

    $m_{a\to b} \leftarrow m_{a\to b} \cdot \frac{\tilde{F}^a_b(p_a)}{p_b}$

  end

end

- Fix point of this message passing algorithm are critical point of F_{Bethe}

- $FE : \prod_{a\in\mathscr{A}} \mathbb{P}(E_a) \to \prod_{a\in\mathscr{A}} \mathbb{R}$ defined as $FE(Q) = (\mathbb{E}_{Q_a}[H_a] - S_a(Q_a),\ a \in \mathscr{A})$, which sends a collection of probability measures over $\mathscr{A}$ to their Gibbs free energies.
- $\mathrm{d}_Q FE$ denotes the differential of FE at the point Q.

Proposition

Let $\mathscr{A}$ be a finite poset, and let F be a contravariant functor from $\mathscr{A}$ to $\mathbf{Kern}^f$. Let $H_a : F(a) \to \mathbb{R}$ be a collection of (measurable) functions. The critical points of F_{Bethe} are the $Q \in \lim \tilde{F}$ such that:

$$\mu_{\tilde{F}*} d_Q FE|_{T \lim \tilde{F}} = 0$$

$T \lim \tilde{F}$ is the underlying vector space of the affine space $\lim \tilde{F}$

Pose $I_a(Q_a) = \mathbb{E}_{Q_a}[H_a] - S(Q_a)$

Theorem (GSP)

F a functor from $\mathscr{A}^{op}$ to vector spaces. An element $u \in \lim \tilde{F}$ is a critical point of the F_{Bethe} if and only if there is $(m_{a\to b} \in \bigoplus_{\substack{a,b:\\ b\leq a}} \tilde{F}(b)^*)$ such that for any $a \in \mathscr{A}$,

$$d_u I_a = \sum_{b\leq a} \tilde{F}_b^{a*} \left(\sum_{c\leq b} \tilde{F}_c^{b*} m_{b\to c} - \sum_{c\geq b} m_{c\to b} \right) \tag{CP}$$

- To understand in greater detail these propositions and the previous algorithm, we need to extend the setting of the optimization problem.
- Change the loss:
  - $\rightarrow$ Replace entropy with a ”local loss.”
  - $\rightarrow$ $S(Q_a) \rightsquigarrow l_a(v_a)$
- Change the functor:
  - $\rightarrow$ Replace F with a contravariant functor from a poset $\mathscr{A}$ to **Vect**.
- Result: we can extend the message passing algorithm to solve:

$$\min_v \sum_{a \in \mathscr{A}} c(a) l_a(v_a)$$

  with $v := (v_a, a \in \mathscr{A})$ under the constraint $v \in \lim F$.
- This approach is different and on some points more general than decentralized optimization on cellular sheaves [HG19].

For F a functor from $\mathscr{A}^{op}$ to vector spaces, critical points u of $\sum_{a\in\mathscr{A}} c(a) l_a(v_a)$ are $u \in \bigoplus_{a\in\mathscr{A}} F(a)$ such that:

$$[\mu_{F^*} d_u l]|_{\lim F} = 0$$

where, $l(v) = (l_a(v_a), a \in \mathscr{A})$, $d_u l(a) = d_{u_a} l_a$ and,

$$[\mu_{F^*} d_u l](a) = \sum_{b\leq a} \mu(a,b) d_{u_b} l_b \circ F^a_b$$

$$0 \to \lim F \to \bigoplus_{a \in \mathscr{A}} F(a) \xrightarrow{\delta_F} \bigoplus_{\substack{a,b \in \mathscr{A} \\ a \geq b}} F(b)$$

where for any $v \in \bigoplus_{\substack{a,b \in \mathscr{A} \\ a \geq b}} F(b)$ and $a, b \in \mathscr{A}$ such that $b \leq a$,

$$\delta_F(v)(a, b) = F_b^a(v_a) - v_b$$

This is simply stating that $\ker \delta = \lim F$.

Understanding expression of critical points:

$$0 \leftarrow (\lim F)^* \leftarrow \bigoplus_{a \in \mathscr{A}} F(a)^* \overset{\mathrm{d}_F}{\leftarrow} \bigoplus_{\substack{a,b \in \mathscr{A} \\ a \geq b}} F(b)^*$$

Pose $\mathrm{d} = \delta^*$. For any $l_{a \to b} \in \bigoplus_{\substack{a,b \in \mathscr{A} \\ a \geq b}} F(b)^*$ and $a \in \mathscr{A}$,

$$\mathrm{d}m(a) = \sum_{a \geq b} F_b^{a*}(m_{a \to b}) - \sum_{b \geq a} m_{b \to a}$$

$$\mu_F^* d_u l \in \operatorname{im} \mathrm{d}$$

is the same as the fact that there is $(m_{a \to b} \in F(b)^* | a, b \in \mathscr{A}, b \leq a)$ such that,

$$d_u l = \zeta_{F^*} \mathrm{d} m$$

Assume that the local losses $l_a, a \in \mathscr{A}$ are such that there is a collection of functions $g_a, a \in \mathscr{A}$ that inverses the relation induced by differentiating the local losses, i.e.

$$d_{u_a} l_a = y_a \iff u_a = g_a(y_a)$$

It is the case for the free energy $\mathbb{E}_{Q_a}[H_a] - S(Q_a)$.
Messages:

$$m(t) \in \bigoplus_{\substack{a,b:\\ b\leq a}} F(b)^*\colon m_{a\to b} \text{ for } b \leq a$$

Understanding this choice of message passing algorithm:

g sends Lagrange multipliers m to $u \in \bigoplus_{a\in\mathscr{A}} F(a)$. $\delta_F(u) = 0$ defines the constraints on u.
$\delta_F g \zeta_{F^*} \mathrm{d}_F$ sends a Lagrange multiplier $m \in \bigoplus_{\substack{a,b\in\mathscr{A}\\ a\geq b}} F(b)^*$ to a constraint $c \in \bigoplus_{\substack{a,b\in\mathscr{A}\\ a\geq b}} F(b)$ defined as, for $a, b \in \mathscr{A}$ such that $b \leq a$,

$$c(a,b) = \delta_F g \zeta_{F^*} \mathrm{d}_F m(a,b) = F^a_b g_a(\zeta_{F^*}\mathrm{d}_F m(a)) - g_b(\zeta_{F^*}\mathrm{d}_F m(b))) \tag{0.2}$$

We are interested in $c = 0$, i.e.

$$\delta_F g \zeta_{F^*} \mathrm{d}_F m = 0$$

Understanding this choice of message passing algorithm:

Choice of algorithm on the Lagrange multipliers so that $\delta_F g \zeta_{F^*} \mathrm{d}_F m = 0$,

$$m(t+1) - m(t) = \delta_F g \zeta_{F^*} \mathrm{d}_F m(t)$$

Any other choice would also be a good candidate!

The message passing algorithm is defined as:

$$\delta m := \delta_{\tilde{F}} g \zeta_{\tilde{F}*} d_{\tilde{F}} m$$

Define $BP_{F,H} := \delta_{\tilde{F}} g \zeta_{\tilde{F}*} d_{\tilde{F}}$.
When differentiating the free energy:

$$y_a = H_a + \ln q_a + 1$$

Therefore, $g_a(y_a) = e^{y_a - H_a - 1}$.

- Joint work with Toby St Clere Smithe, in progress.
- Consider a natural transformation $\phi : F \to F_1$ where ϕ_a is a deterministic map, not a Markov kernel.
- The map ϕ extends into maps between $\tilde{F} \to \tilde{F}_1$ and $\tilde{F}^* \to \tilde{F}_1^*$.
- ϕ induces maps between $\bigoplus_b \tilde{F}(b) \to \bigoplus_b \tilde{F}_1(b)$ and $\bigoplus_{b\leq a} \tilde{F}(b) \to \bigoplus_{b\leq a} \tilde{F}_1(b)$. It also induces a map $\phi^* : \bigoplus_b \tilde{F}_1^*(b) \to \bigoplus_b \tilde{F}^*(b)$ and $\phi^* : \bigoplus_{b\leq a} \tilde{F}_1^*(b) \to \bigoplus_{b\leq a} \tilde{F}^*(b)$.

Pose:

$$\tilde{H}_a = \ln \sum_{\omega' : \phi_a(\omega') = \omega} e^{-H_a(\omega')}$$

Then we showed that:

$$BP_{F_1,\tilde{H}} = \phi \circ BP_{F,H} \circ \phi^*$$

- $\rightarrow$ Few results on characterizing critical points of the Bethe free energy.
- $\rightarrow$ Use transformations on the underlying functor to reduce to simpler cases (Hamiltonians, posets).

What about base change? $\phi : \mathscr{A} \to \mathscr{A}_1$

- $\rightarrow$ When a right adjoint to the pullback exists, results on natural transformations can be reused.
- $\rightarrow$ When $\mathscr{A}$ is isomorphic to a full subposet of $\mathscr{A}_1$, similar result holds.

Thank you for your attention!

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