Structured representations in learning and action

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Structure and space I

Relate : Structured input $\longleftrightarrow$ Space

- Input :
  1. samples for inference $\rightarrow$ output estimator
  2. dataset for learning $\rightarrow$ network
  3. observations for decision/choice of policy (POMDP)$\rightarrow$ actions
  4. optimization over parameters (output) conditionned by input

Structure and space II

- Structured input $\to$ Space
  - $*$ Space in which one represents structured input
- Structure $\leftarrow$ Space
  - $*$ Space of (representation of) inputs itself has additional structure

- Combinatorics and optimization
  - $**$ Combinatorics : structure represented as space.
  - $**$ Optimisation : optimization over spaces representing combinatorial structures.

Equivariance I

- Symmetries (structure) act on the space of inputs.
  - Input $\leftarrow$ Images
  - Symmetries/group $\leftarrow$ Translations, rotations
- Learn invariant features
- How ?
  - Equivariant neural networks : output space is structured by symmetries.
  - Average pooling $\rightarrow$ invariant features

Equivariance II

- Invariant representations in self-supervised learning
  - Symmetries $\rightsquigarrow$ Augmentations, different view on data
  - Adapt loss to account for this structure: Barlow-Twins [ZJM+21], VICReg [BPL22]
  - Medical images: CT volumes segmentation/classification (**data scientist** at Median Technologies)

- Go beyond translations, rotations?
  - Finite groups : permutations
  - Infinite dimension group
- Infinite dimension group
  - Why? $\rightarrow$ Input with uncountable degrees of freedom
  - e.g. Shapes, fluids
  - Biggest possible group : diffeomorphisms *Diff*

Equivariance III

- Infinite dimension groups
  - Characterization of networks equivariant to *Diff*,
  - *On Non-Linear operators for Geometric Deep Learning*, Neurips 2022 [tMBO22] with J.Maier, J. Bruna, **E. Oyallon**

Example of Structure: dependencies between variables I

Example of structure:

- Dependencies between variables $\rightarrow$ Graphical Model
  - $*$ Graph $G = (V, E)$, V vertices, E edges
  - $*$ $V \leftarrow$ variables $(X_i, i = 1...n)$
  - $*$ $E \leftarrow$ modeled dependencies between variables
- Example : Markov Chains (**M**DP: Markov Decision Process)

$$V = (X_1, X_2, X_3)$$
$$E = \{(X_1, X_2), (X_2, X_3)\}$$

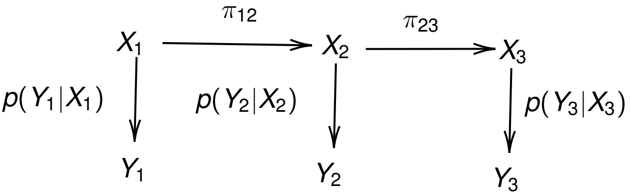
$$X_1 \longrightarrow X_2 \longrightarrow X_3$$

Hammersley–Clifford theorem (e.g. see [19])

$$\mathbb{P}_{X_1,X_2,X_3} = f_{12}(X_1, X_2) f_{23}(X_2, X_3)$$

Example of Structure: dependencies between variables II

- Graphical Model
  - ∗ HMM for Partially Observable Markov Decision Process (POMDP):



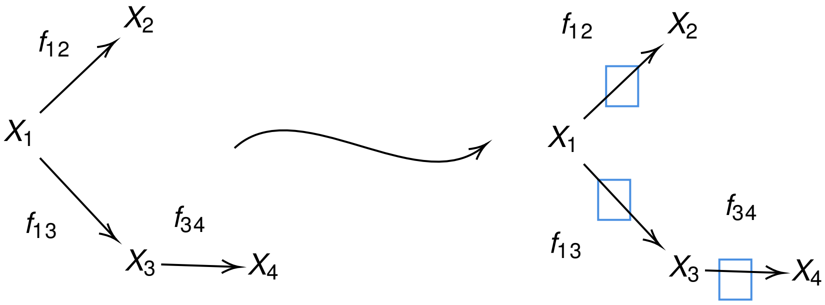
- Inference on graphical models? $\rightarrow$ Bioinformatics [TtB21][Tt21]
  - ∗ Viterbi algorithm
  - ∗ Em algorithm for HMM: Baum-Welch algorithm
  - ∗ Forward-Backward algorithm $\rightsquigarrow$ Message Passing algorithms.
  - ∗ Computing marginals efficiently $\rightarrow$ **Belief Propagation**

Example of Structure: dependencies between variables III

Interpretation of Belief Propagation

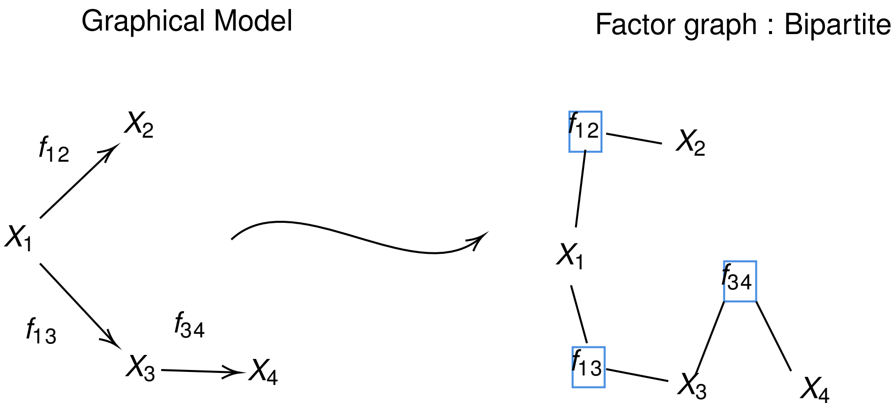
- Belief propagation (BP) is an **optimization method of entropy** for Graphical Models
  - ∗ Fix points of BP $\leftrightarrow$ critical points of entropy over a Graphical Model.
- restate as Belief propagation (BP) is a **variational inference method** for Graphical Models
- Why? Key argument: a Graphical model can be represented a a constrained space (see for example introduction in [22]).

Representing the Structure of Graphical Models



Transformation of graphical model to factor graph

Representation of graphical model II

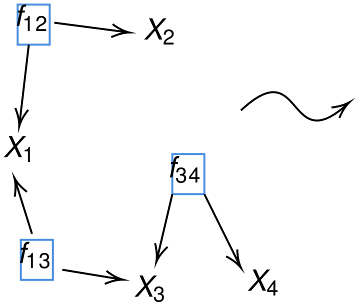


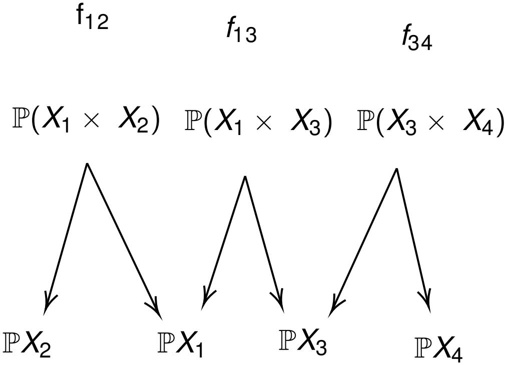
Transformation of Graphical Model to factor graph

Representation of graphical model III

Factor graph : choice of a direction

Enriched nodes

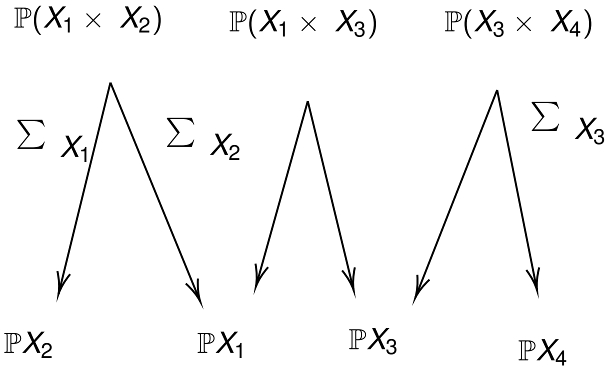




Transformation of factor graph to enriched graph

Representation of graphical model IV

Enriched edges

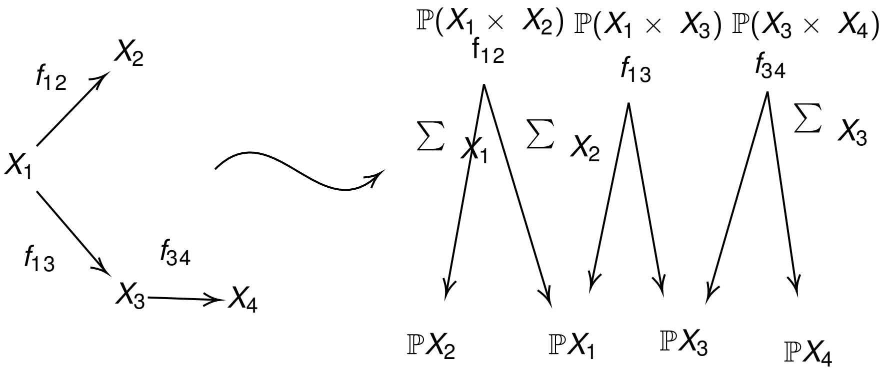


Enriched graph

Representation of graphical model V

Graphical Model

Enriched graph



Transformation of Graphical Model to enriched graph

Representation of graphical model Last

From enriched graph to a constrained space

- Each arrow is a constraint on 'q':

$$\sum_{X_2} : \mathbb{P}(X_1 \times X_2) \to \mathbb{P}(X_1) \quad \longleftrightarrow \quad \sum_{y_2} q_{X_1,X_2}(x_1, y_2) = q_{X_1}(x_1)$$

Other Structure: higher order of structure on input

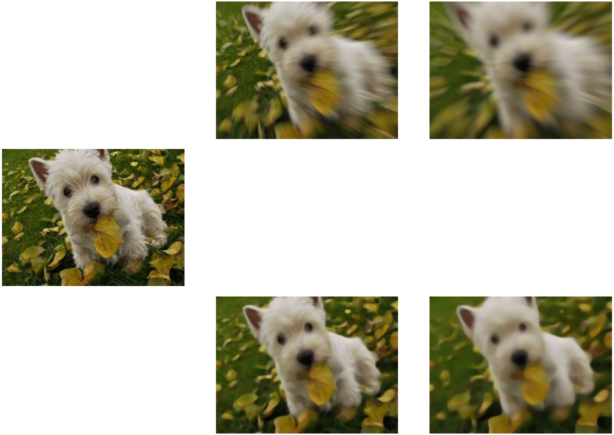
Higher structures than graphs (hypergraphs, sheafs)

- When ?
  - ∗ graph dependencies are not rich enough
  - ∗ dependencies other than independence between variables.
- Example: General Belief Propagation [YFW05], Message passing on Sheaf Neural Networks [BDGC+22]

BP is a particular case of a correspondence that holds for Higher structured dependencies [22]

Higher order correspondence: Example of Motivation I [22]

Data with multiple point of view on it: for example images of Dog with two **types of blurs at different intensity of blurring**



Motivation II [22]

Cat with two **types of blur at different intensity of blurring**:

How to classify dogs and cats taking into account the extra data given by the different point of views?

Key ingredients

- In this example dependencies are given by the blurring applied to go from one image to an other; more generally : several (local) views on parameters with compatibility conditions
- There is a loss on each view (local loss)
- Problem? solve the global optimization problem (made up of local ones) over the compatible local views.

What to learn from Structure $\leftrightarrow$ Space?

- With these two examples, we want to stress that more generally:
  - $\ast$ looking for structured representations can guide the design of algorithms for learning (translation $\to$ CNN, Barlow-Twins loss)
  - $\ast$ but also help understand what it does (correspondence BP $\leftrightarrow$ Entropy over some constraint)
- A geometric interpretation of an algorithm allows for easier generalization and better transfer to other problems (Higher order of structure correspondence)

Structured latent spaces for social agents I

- Setting : exploration and exploitation (POMDP)
- Multi-agent
  - ∗ Standard framework: agent have internal models of their environment and of other agents + beliefs.
  - ∗ They make observations to update their beliefs.

- **How to account for perspective taking on the environment?**
  - ∗ the agent changes its perspective, can take perspective of others.

Structured latent spaces for social agents II

In [RtB+22][RtT+21] we propose,

- Homogeneous treatment of integrated information in the latent space
- the extra information of a frame (collection of coordinates) in this space
- action through changes of frames

Structured latent spaces for social agents III

- Geometry offers many properties that allow for intertwining representation of information and integration of information (selection of information) in a way compatible with perception

Allow to model in a uniform way :

- ∗ Attention
- ∗ Emotional reward
- ∗ Epistemic drive : acting in order to reduce uncertainty
- ∗ Taking perspective of others.

- Interestingly: perspective taking changes exploration behaviour.

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