

Moving beyond I.I.D.

Causal de Finetti and OOV Generalization

Siyuan Guo

Max Planck Institute for Intelligent Systems
University of Cambridge

April 18th, 2023

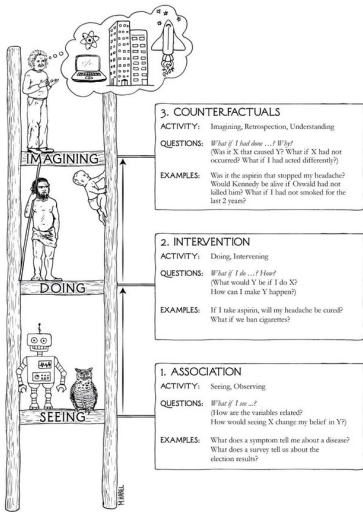
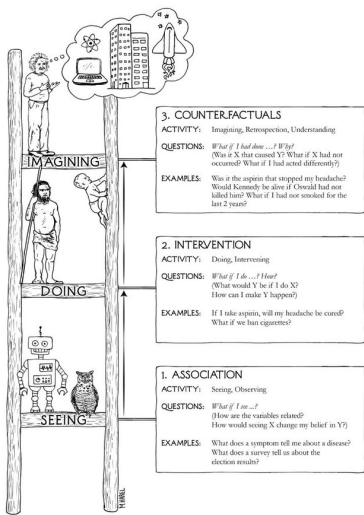


Figure 1: Pearl's Ladder of Causality



I.I.D.

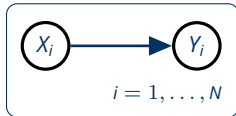


Figure 2: Pearl's Ladder of Causality

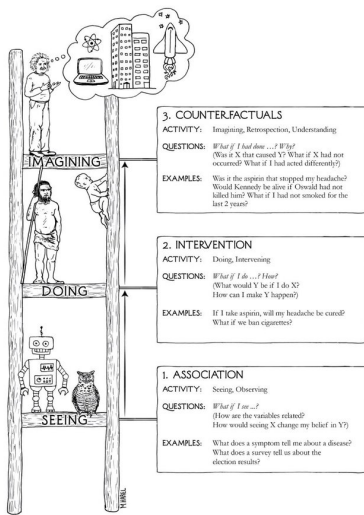
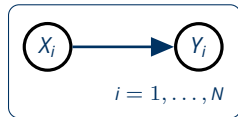


Figure 3: Pearl's Ladder of Causality

I.I.D.



Exchangeable

Let X_1, X_2, \dots, X_n be a finite sequence of random variables. For any permutation π of $\{1, \dots, n\}$, it satisfies:

$$\mathbb{P}(X_{\pi(1)}, \dots, X_{\pi(n)}) = \mathbb{P}(X_1, \dots, X_n) \quad (1)$$

Then the finite sequence is **exchangeable**.
Infinite exchangeable sequence if above holds for any $N \in \mathbb{N}$.

De Finetti

Let $(X_n)_{n \in \mathbb{N}}$ be an infinite sequence of binary¹ random variables. The sequence is **exchangeable** *if and only if* there **exists** a latent variable θ such that X_1, X_2, \dots are conditionally i. i. d. given θ .

$$\mathbb{P}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \int \prod_{i=1}^n p(\mathbf{x}_i | \theta) d\mu(\theta) \quad (2)$$

¹De Finetti holds for categorical and continuous random variables.

De Finetti

Let $(X_n)_{n \in \mathbb{N}}$ be an infinite sequence of binary random variables. The sequence is **exchangeable** if and only if there **exists** a latent variable θ such that X_1, X_2, \dots are conditionally i. i. d. given θ .

$$\mathbb{P}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \int \prod_{i=1}^n p(\mathbf{x}_i | \theta) d\mu(\theta) \quad (3)$$

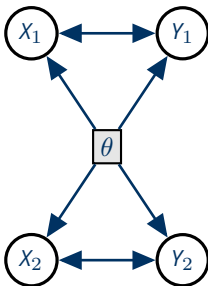
Bayesian Model

- $\mathcal{D} = \{x_1, \dots, x_n\}$
- Statistical Model $\mathcal{M} = \{P(\cdot | \theta) | \theta \in \mathcal{T}\}$
- Prior $\theta \sim \pi$

De Finetti Applications

Let $(X_n, Y_n)_{n \in \mathbb{N}}$ be an infinite exchangeable sequence of binary random variables. De Finetti representation theorem states that

$$\mathbb{P}(\mathbf{x}_1, \mathbf{y}_1, \dots, \mathbf{x}_n, \mathbf{y}_n) = \int \prod_{i=1}^n p(\mathbf{x}_i, \mathbf{y}_i | \theta) d\mu(\theta) \quad (4)$$



Independent Causal Mechanism

The causal generative process of a system's variables is composed of autonomous modules that do **not inform** and do **not influence** each other.

$$\mathbb{P}(X_1, \dots, X_n) = \prod_i \underbrace{\mathbb{P}(X_i \mid \mathbf{PA}_i)}_{\text{causal conditional}} \quad (5)$$

Example



Causal De Finetti

Let $\{X_n, Y_n\}_{n \in \mathbb{N}^2}$ be an infinite sequence of binary random variables.

The sequence is

- exchangeable, and
- $\forall n \in \mathbb{N} : Y_{[n]} \perp\!\!\!\perp X_{n+1} \mid X_{[n]}$ ³ \rightarrow “ $P(Y \mid X) \perp\!\!\!\perp P(X)$ ”

if and only if there exists two independent latent variables θ, ψ such that X_1, X_2, \dots are conditionally i. i. d. given θ and Y_1, Y_2, \dots are conditional i. i. d. given ψ and its corresponding X_i .

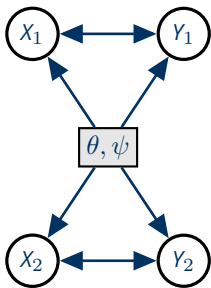
$$\mathbb{P}(\mathbf{x}_1, \mathbf{y}_1, \dots, \mathbf{x}_n, \mathbf{y}_n) = \int \prod_{i=1}^n p(\mathbf{y}_i \mid \mathbf{x}_i, \psi) p(\mathbf{x}_i \mid \theta) d\mu(\theta) d\nu(\psi) \quad (6)$$

²Can extend to multivariate version

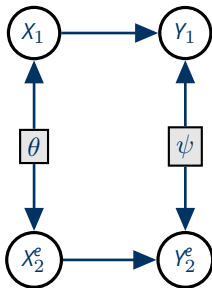
³ $[n] := \{1, \dots, n\}$

Disentangle the Latents

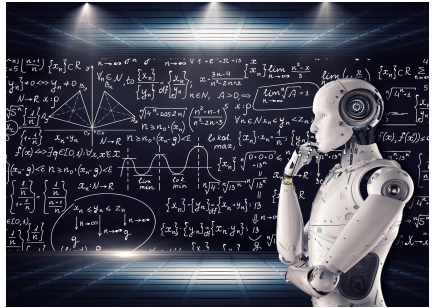
De Finetti:



Causal De Finetti:



Generalization

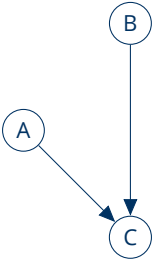


Out-of-Variable Generalization

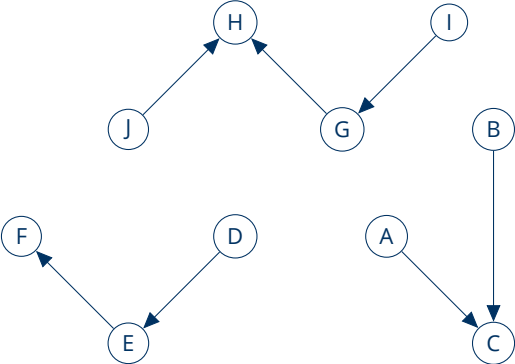
Out-of-Variable Generalization



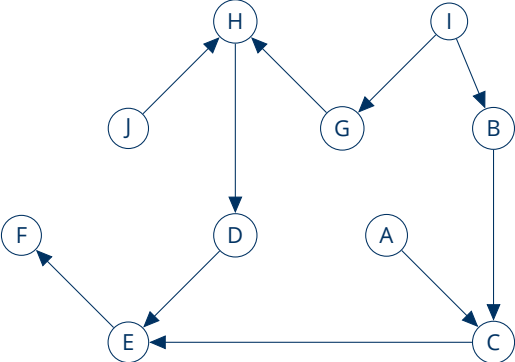
Out-of-Variable Generalization



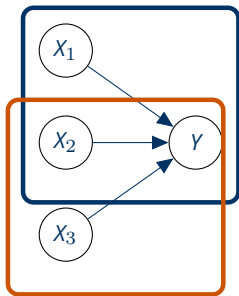
Out-of-Variable Generalization



Out-of-Variable Generalization



Out-of-Variable Generalization



$$\mathcal{D} := (X_1, X_2, Y), (X_2, X_3)$$

$$f_S(x_1, x_2) = \mathbb{E}[Y \mid X_1, X_2]$$

$$f_T(x_2, x_3) = \mathbb{E}[Y \mid X_2, X_3]$$

Figure 4: **Toy example:** (a) the blue box includes variables observed in the source environment, and the orange box those in the target environment. A directed edge represents a causal relationship between two variables. The goal is to improve the zero-shot (i.e., without additional data) prediction of Y in the target environment using the source environment.

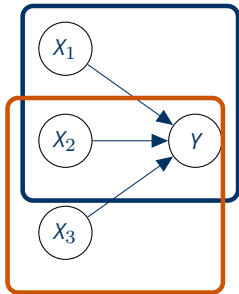
Out-of-Variable Generalization

- Consider $Y = \phi(X_1, X_2, X_3) + \epsilon$
- Residual Distribution: $Y - f_S(X_1, X_2)$
- Moments of the residual distribution:

$$\mathbb{E}[(Y - f_S(x_1, x_2))^n \mid x_1, x_2]$$

- Entangled interaction between noise ϵ and $\left. \frac{\partial \phi}{\partial X_3} \right|_{x_1, x_2, \mu_3}$

$$\mathbb{E}[(Y - f_S(x_1, x_2))^n \mid x_1, x_2] = \sum_{k=0}^n \binom{n}{k} \mathbb{E}[\epsilon^k] \left(\left. \frac{\partial \phi}{\partial X_3} \right|_{x_1, x_2, \mu_3} \right)^{n-k} \mathbb{E}[(X_3 - \mu_3)^{n-k}]$$

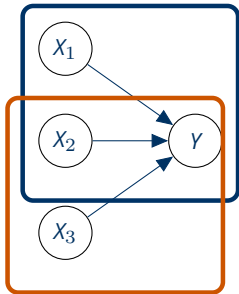


Out-of-Variable Generalization

- Consider $Y = \phi(X_1, X_2, X_3) + \epsilon$
- Residual Distribution: $Y - f_S(X_1, X_2)$
- Moments of the residual distribution:

$$\mathbb{E}[(Y - f_S(x_1, x_2))^n \mid x_1, x_2]$$

- Entangled interaction between noise ϵ and $\left. \frac{\partial \phi}{\partial X_3} \right|_{x_1, x_2, \mu_3}$

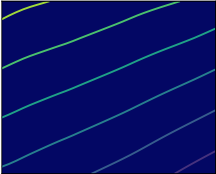


When $n = 3$:

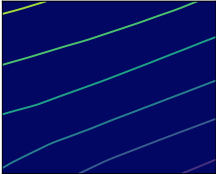
$$\mathbb{E}[(Y - f_S(x_1, x_2))^3 \mid x_1, x_2] = \left(\left. \frac{\partial \phi}{\partial X_3} \right|_{x_1, x_2, \mu_3} \right)^3 \mathbb{E}[(X_3 - \mu_3)^3] + \mathbb{E}[\epsilon^3]$$

Experiments

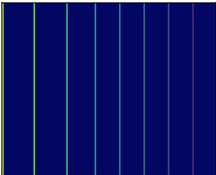
Proposed



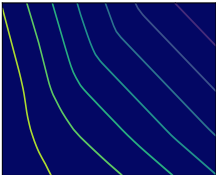
Optimal



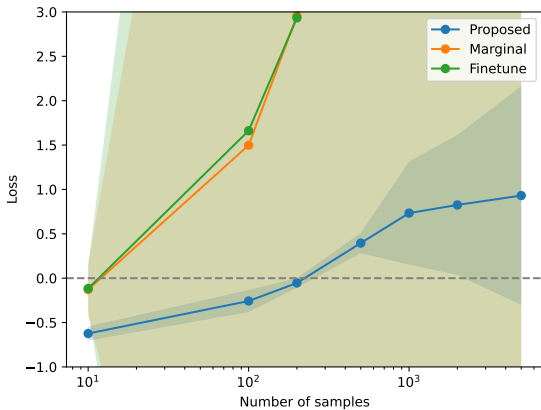
Marginal



FineTune



Experiments



Conclusions

Causal de Finetti: On the Identification of Invariant Causal Structure in Exchangeable Data

Siyuan Guo^{a,b,1}, Viktor Tóth^{a,1}, Bernhard Schölkopf^a, and Ferenc Huszár^a

^aUniversity of Cambridge; ^bMax Planck Institute for Intelligent Systems

Out-of-Variable Generalization

Siyuan Guo ^{a†‡}

Jonas Wildberger [†]

Bernhard Schölkopf [†]