Amortized Inference of Causal Models via Conditional Fixed-Point

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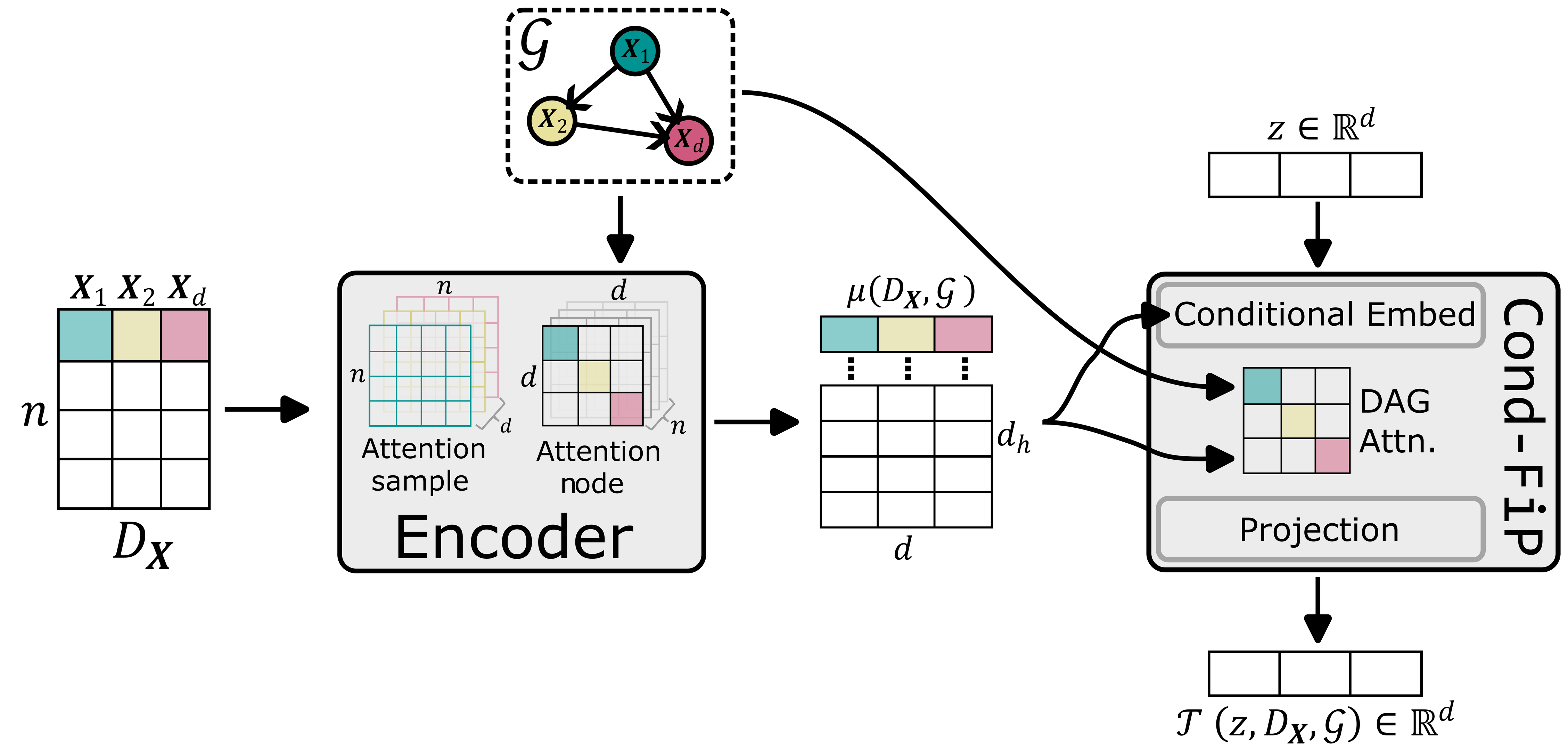
Contributions

- **Amortized SCM Learning**:
  - Learn a shared inference mechanism (single model) for SCMs sampled from a synthetic data simulator
  - Zero-shot generation of observation and interventional samples from novel SCMs at test time
- **Proposed Approach:**
  - *Encoder:* In-context learning of dataset embeddings
  - *Decoder*: Conditional fixed-point iteration for recovering causal mechanisms
- **Empirical Results:**
  - *OOD Generalization*: SCMs with larger graphs, unknown causal graphs, and real-world datasets
  - *Fast Adaptation:* Competitive with baselines trained from scratch for each test task, and outperforms them in scare data regimes

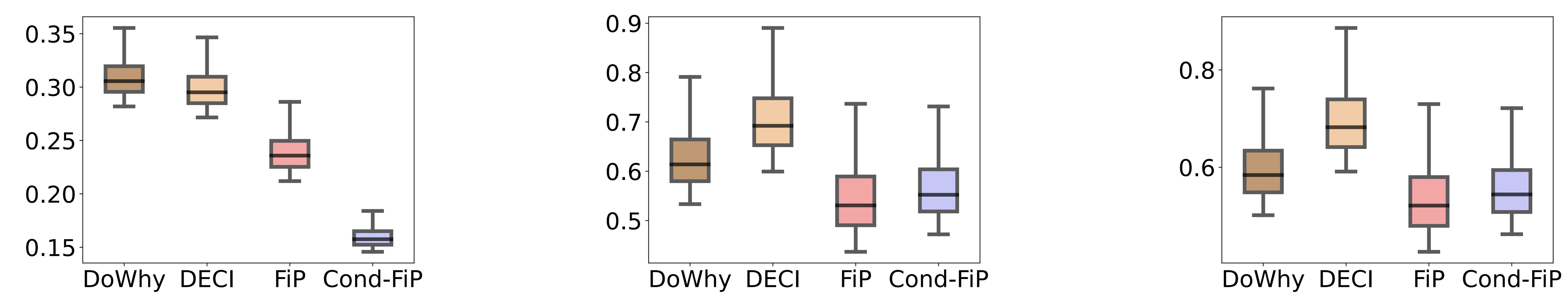


Problem Setup

- **Assumptions:**
  - Markovian & Additive Noise SCM: $S(\mathbb{P}_{\mathbf{N}}, \mathbf{G}, \mathbf{F})$: $X_i = F_i(PA(X_i)) + N_i$
- **Amortized Learning of SCMs:**
  - Learn model T_θ to predict $\mathbf{F}$ from observational dataset $D_{\mathbf{X}}$ and causal graph $\mathbf{G}$:

$$argmin_\theta\ \mathbb{E}_{S\sim \mathbf{P}_S}\ \mathbb{E}_{z\sim \mathbf{P}_X}\ L\Big(F(z), T_\theta(z, D_{\mathbf{X}}, \mathbf{G})\Big)$$

Results: OOD ($d = 100$)



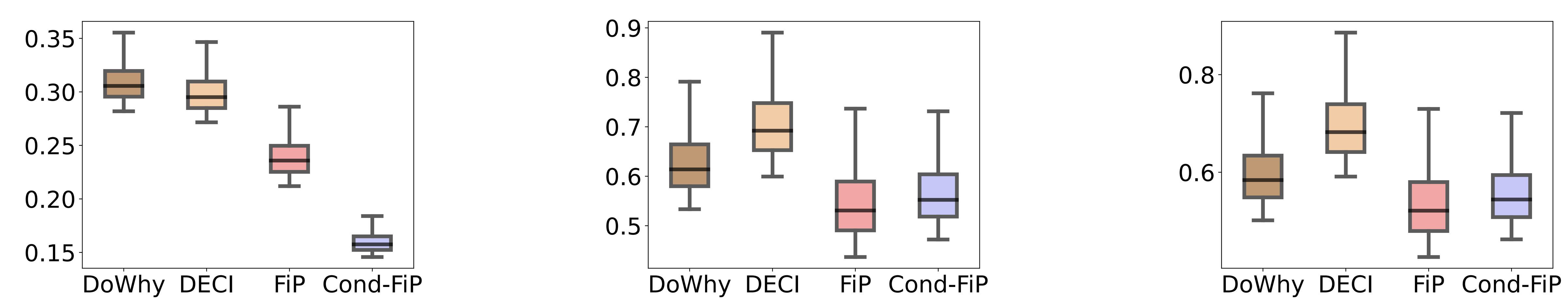
(a) Noise Prediction (b) Sample Generation (c) Interventional Generation

Encoder

- **Objective:** Generate dataset representations $\mu(D_{\mathbf{X}}, \mathbf{G})$
- **Training:** $\mathbb{E}_{S\sim \mathbf{P}_S}\ ||\ \mathbf{F}(D_{\mathbf{X}}) - H \circ E(D_{\mathbf{X}}, \mathbf{G})\ ||_2^2$

  Projection Layer Attention Layer
- **Assumption:** Encoder requires the assumption of additive noise SCM as we need an invertible map between the observations and noise variables!

Results: OOD ($d = 100$) (Unknown Causal Graph)



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Decoder

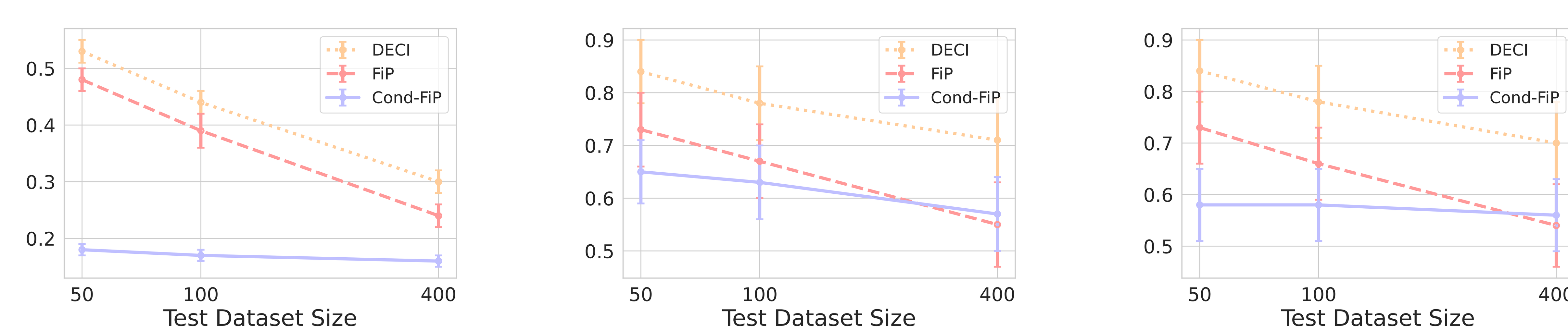
- **Objective:** Infer causal mechanisms conditioned on dataset representations
- **Training:** $\mathbb{E}_{S\sim \mathbf{P}_S}\ \mathbb{E}_{z\sim \mathbf{P}_X}\ ||\ \mathbf{F}(z) - T(z \mid \mu(D_{\mathbf{X}}, \mathbf{G}))\ ||_2^2$
  - $T(z \mid \mu)$ transform n_0 into z_{emb} via fixed-point iteration modeled by DAG attention

$$n_{l+1} = h\big(DA(n_l, z_{emb})\ z_{emb} + n_l\big)$$

- **Inference**: Sample $z \sim \mathbb{P}_{\mathbf{N}}$ and generate novel samples via fixed-point iterations:

$$z_{l+1} = T(z_l \mid \mu(D_{\mathbf{X}}, \mathbf{G})) + z$$

Results: Scarce Data Regime ($d = 100$)



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