Interventional Deep Generative Models for Scalable Causal Discovery and Counterfactual Analysis

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Abstract: Causal reasoning and "what-if" analysis allow us to predict the outcomes of hypothetical changes and are fundamental to decision support in high-stakes domains such as healthcare, economics, and robotics. Traditional causal-discovery methods can find cause-and-effect graphs under simple assumptions but struggle with large, complex datasets and cannot predict what might happen after a hypothetical change. Algorithms like PC, FCI, and NOTEARS reliably infer directed acyclic graphs (DAGs) under linear or simple nonlinear assumptions but fail to scale to high-dimensional data and lack mechanisms for counterfactual simulation. Conversely, deep generative models learn to reproduce complex data patterns but do not capture cause-and-effect relationships, so they cannot answer "what-if" questions. We propose Interventional Structural Deep Generative Models (IS-DGM), a unified framework that embeds a learnable DAG into the latent space of a variational autoencoder. We prove that, under realistic conditions, our approach can uniquely recover the true causal structure and generate reliable counterfactual predictions. IS-DGM enforces acyclicity via a continuous matrix-exponential penalty, encourages sparsity through L_1 regularization, and introduces a latent-space intervention operator to clamp selected factors and propagate effects through the graph. Under mild exponential-family priors and with diverse interventional data, IS-DGM recovers the true DAG up to element-wise reparameterization. Empirically, on synthetic benchmarks (latent dimensions up to 100), IS-DGM reduces structural Hamming distance by 30–55% and achieves over 50% lower counterfactual RMSE than state-of-the-art baselines. On real clinical data (MIMIC-III), it halves prediction error of treatment-response simulations relative to identifiable VAEs and NOTEARS. Ablation studies confirm the necessity of each loss component, and scalability analyses quantify runtime and memory trade-offs. IS-DGM thus offers a principled, scalable solution for joint causal discovery and counterfactual inference in complex, high-dimensional settings.

1 INTRODUCTION

Your Causal reasoning understanding not just associations but how deliberate changes in one variable propagate through a system underpins scientific discovery and high-stakes decision support [1], [2]. Classical causal-discovery algorithms such as PC and FCI reliably infer directed acyclic graphs (DAGs) under assumptions of linearity and Gaussian noise, yet they become computationally prohibitive or statistically unstable when applied to high-dimensional, nonlinear, or heterogeneous datasets common in modern domains like genomics, healthcare, and economics [3], [4]. In parallel, deep generative models including Variational Autoencoders (VAEs) [5], Normalizing Flows [6], and Generative Adversarial Networks [7] excel at modeling complex, multimodal distributions but lack any built-in mechanism to distinguish correlation from causation.

This dichotomy means that, despite rich observational data, practitioners remain unable to answer critical "what-if" or interventional queries without performing costly or unethical

experiments [8]. Recent works have begun to embed structural constraints into neural networks e.g., the NOTEARS framework for continuous optimization of DAGs [9] and advances in nonlinear independent component analysis suggest identifiability of certain latent causal structures under mild conditions [10], [11]. However, these approaches either forgo realistic data generation or fail to support end-to-end counterfactual simulation.

To bridge this gap, we propose Interventional Structural Deep Generative Models (IS-DGM), a unified framework that jointly learns (i) a rich latent representation amenable to high-fidelity reconstruction and (ii) a DAG over latent factors, while also enabling "clamp-and-generate" interventions. By integrating acyclicity constraints directly into the encoder–decoder architecture building on continuous DAG optimization techniques [9], [12] and by designing an intervention operator in latent space, IS-DGM can answer queries such as "What would patient vitals look like if treatment dosage were increased by 20%?" without additional model retraining. We evaluate on both synthetic benchmarks and the MIMIC-III critical care dataset [13], demonstrating that IS-DGM not only recovers causal structure more accurately than state-of-the-art baselines but also produces reliable intervention-effect estimates.

1.1 Motivation

Despite the proliferation of big data, actionable causal insights remain elusive because (1) symbolic causal methods do not scale to thousands of variables or nonlinear relations, and (2) deep generative approaches do not capture causality. Embedding structural causal learning within a generative model promises to overcome these limitations: practitioners gain both realistic data simulation and the ability to plan interventions in domains such as precision medicine [14], economic policy [15], and adaptive robotics [16] where experimentation is expensive or infeasible.

1.2 Contributions

The main contributions of this work can be summarized as follows:

- IS-DGM Architecture: We introduce a VAE-style encoder–decoder whose latent variables interact via a learnable adjacency matrix constrained to form a DAG, unifying representation learning and causal-graph discovery.
- Latent Intervention Operator: We develop a mechanism to clamp selected latent nodes at arbitrary values, propagating effects through the learned graph to generate counterfactual observations.
- Joint Optimization Objective: We formulate a composite loss combining reconstruction fidelity, DAG-sparsity (via continuous acyclicity penalties), and intervention-consistency, ensuring both accurate synthesis and reliable "what-if" inference.
- Theoretical Identifiability Guarantees: Leveraging recent nonlinear ICA theory, we derive conditions under which the true causal structure is identifiable within our framework.
- Empirical Validation: Extensive experiments on synthetic benchmarks and the MIMIC-III ICU dataset show that IS-DGM surpasses leading causal-discovery methods in structural accuracy and delivers precise intervention-effect predictions.

1.3 Paper Organization

The remainder of this paper is organized as follows. In Section 2, we review prior work on neural causal-discovery and deep generative modelling, highlighting their strengths and limitations. Section 3 details the IS-DGM methodology, including the DAG-regularized VAE architecture, the latent-space intervention operator, the joint loss formulation, and identifiability analysis. In Section 4, we present our theoretical guarantees, proving identifiability under mild assumptions and analyzing the complexity and convergence of the acyclicity-penalized training. Section 5 describes our experimental evaluation. Section 6 discusses the implications of our results, practical limitations, and avenues for future work. Finally, Section 7 concludes with a summary of contributions and potential extensions.

2 RELATED WORKS

Early efforts to merge causal-graph learning with neural networks include DAG-GNN, which embeds a variational autoencoder within a graph-neural-network wrapper and enforces acyclicity via a continuous constraint on the evidence lower bound (ELBO) loss, demonstrating significant improvements in structural Hamming distance over classical baselines [12]. GraN-DAG builds on this by

directly parameterizing each structural equation with a neural network and optimizing via gradient-based constrained learning, achieving competitive performance across diverse graph sizes [17]. Parallel work on making latent-variable models identifiable has driven progress in causal VAE architectures. Identifiable VAE (iVAE) introduces auxiliary observed variables (e.g., time indices) to satisfy nonlinear ICA identifiability conditions, enabling true latent recovery under mild assumptions [10]. Building on iVAE, CausalVAE injects a learned DAG layer into the latent space of a VAE, recovering causal factors up to permutation and scaling when limited supervision signals (feature labels) are available [18]. Refinements to continuous-optimization approaches for DAG learning include Optimizing NOTEARS via Topological Swaps, which accelerates convergence and improves DAG accuracy by integrating discrete topological updates into the NOTEARS framework [19]. GraN-DAG++ extends GraN-DAG to model heteroscedastic noise variances as functions of parent nodes, yielding robust structure estimates under nonconstant noise [20]. More recent deep generative advances include C2VAE (Correlation-aware Causal VAE), which jointly recovers both causal structure and feature correlations through a novel pooling mechanism in the latent space, showing superior intervention prediction on benchmark tasks [21]. KCRL leverages domain knowledge priors to constrain DAG search, significantly reducing false positives in mixed-type epidemiological datasets [22]. Finally, [23] provide a comprehensive review of deep structural causal models classifying methods by their identifiability guarantees, abduction strategies, and counterfactual capabilities offering a roadmap for future work. theoretically relate graph neural networks to structural causal models, laying groundwork for GNN-based causal discovery beyond acyclicity constraints [24]. Table 1, summarizes the recent approaches with the limitations of each method.

Table 1: Summary of recent approaches with limitations.

Study & Reference	Year	Method	Key Contribution	Limitations
[12]	2020	VAE + GNN + continuous acyclicity constraint	First integration of VAE and GNN for DAG learning, reducing SHD on benchmark graphs	Scalability restricted to small-to-moderate graph sizes; assumes Gaussian noise and smooth decoder functions.
[17]	2020	Gradient-based neural SEM	Parameterizes structural equations with NNs, uses gradient-based DAG constraints	Sensitive to hyperparameters may converge to spurious edges under complex noise distributions.
[10]	2020	Identifiable VAE (nonlinear ICA)	Achieves provable latent identifiability via auxiliary observed variables	Requires access to suitable auxiliary variables (e.g., time stamps), limiting applicability in some domains.
[25]	2021	VAE + DAG layer + limited supervision	Learns disentangled causal factors and recovers latent DAG structure with feature-level signals	Depends on partial supervision (feature labels) for identifiability; scalability to high-dimensional data is untested.
[19]	2023	NOTEARS + discrete topological updates	Improves convergence and structure accuracy by interleaving continuous and discrete graph updates	Still computationally expensive on large graphs; topological swaps add overhead without guarantees of global optimum.
[20]	2024	Neural SEM with heteroscedastic noise modeling	Extends GraN-DAG to estimate parent-dependent noise variances, enhancing robustness	Increased model complexity; requires estimating additional noise-variance functions, raising risk of overfitting.
[21]	2024	Causal VAE + correlation pooling	Simultaneously recovers causal graphs and feature correlations for accurate intervention generation	Correlation-pooling introduces extra parameters and computation, limiting real-time intervention speeds.
[22]	2022	Prior-knowledge constrained DAG learning	Integrates expert priors to reduce false positives in mixed-type causal discovery	Relies heavily on quality of domain priors; performance degrades if priors are incomplete or incorrect.
[23]	2024	Survey of deep structural causal models	Classifies methods by identifiability, abduction, and counterfactual capabilities	Lacks new empirical benchmarks; comparisons are qualitative and may not reflect practical performance.
[24]	2021	Theoretical mapping of GNNs to SCMs	Formalizes connections between graph-neural architectures and structural causal modeling	Purely theoretical, with no large-scale empirical validation to confirm practical utility.

While recent advances have pushed the frontier of causal discovery within neural frameworks, they each leave critical gaps unaddressed. Methods like DAG-GNN reduce structural errors but assume Gaussian noise and cannot generate actionable counterfactuals, while GraN-DAG's neural-SEM parameterization is sensitive to hyperparameters and prone to spurious edges under complex noise. Identifiable VAE (iVAE) frameworks guarantee latent recovery under auxiliary supervision yet demand domain-specific side information that is often unavailable. Continuous-optimization enhancements (e.g., topological swaps in NOTEARS) improve convergence but add substantial computational overhead. Crucially, none of these approaches unifies high-fidelity data reconstruction, scalable DAG learning, theoretical identifiability, and an explicit mechanism for simulating interventions in a single, end-to-end model. Our proposed IS-DGM framework fills this void by embedding acyclicity constraints directly within a VAE's latent space, deriving provable identifiability conditions, and introducing a latent-space intervention operator thereby enabling realistic data synthesis alongside rigorous "what-if" inference for decision planning in high-stakes domains.

3 METHODOLOGY

In this section, we present the detailed formulation of the Interventional Structural Deep Generative Model (IS-DGM). We begin by describing the overall encoder–decoder architecture with a DAG-regularized latent space (Section 3.1), then introduce the latent-space intervention operator (Section 3.2). Next, we derive the joint learning objective combining reconstruction, sparsity, and intervention consistency (Section 3.3). We follow with a sketch of the identifiability analysis (Section 3.4) and conclude with the full training algorithm (Section 3.5).

3.1 Structural Latent-Variable Architecture

The foundation of IS-DGM is a latent representation that not only compresses observed data into a lower-dimensional manifold but also encodes an explicit causal structure among latent factors. By integrating a DAG constraint into the latent space, we ensure that the learned representation is both expressive and interpretable in causal terms. We model each observation $x \in R^D$ as generated from a set of d latent factors $z = (z_1, \ldots, z_d)^T \in R^D$ whose dependencies form a DAG.

- Encoder $f\phi: R^D \to R^d$ parameterized by ϕ maps x to mean $\mu \in R^d$ and log-variance $\log \sigma^2 \in R^d$, defining a Gaussian posterior in (1):

$$q_\phi(z \mid x) = \mathcal{N}\big(z \mid \mu(x), \mathrm{diag}(\sigma^2(x))\big). \quad (1)$$

- Latent DAG is represented by an adjacency matrix $A \in R^{d \times d}$, where $Aij \neq 0$ indicates a directed edge $zj \to zi$. To enforce acyclicity, we adopt the smooth constraint as shown in:

$$h(A) = tr(e^{A \odot A}) - d = 0, \quad (2)$$

where $\odot$ denotes element-wise square and $e^{\cdot}$ is the matrix exponential.

- Decoder $g\theta: R^d\ R^D \to R^D$ with parameters θ reconstructs $\hat{x} = g\theta(z)$ and defines a generative distribution, as shown in:

$$P\theta(x|z) \text{ e.g., } N\ (x|g\theta(z), \sigma_x^2 I). \quad (3)$$

Where $g\theta$ is a neural network decoder parameterized by θ, and σ_x^2 a learned or fixed observation variance.

Under this setup, the joint model implies.

3.2 Latent Prior with Structural Equations

The prior distribution over the latent variables z is defined by factorizing it in accordance with the underlying directed acyclic graph (DAG) structure:

$$p_\theta(x, z) = p_\theta(x \mid z) \left(\prod_{i=1}^{d} p\big(z_i \mid \mathrm{pa}(z_i)\big)\right) \quad (4)$$

where $pa(zi)) = \{j \mid A_{ij} \neq 0\}$ and each conditional $p(z_i \mid z_{pa(i)})$ is taken to be Gaussian as in (5):

$$p(z_i \mid z_{pa(i)}) = N\big(z_i \big| \textstyle\sum_{j \in pa(i)} A_{ij} z_j, \sigma_x^2\big) \quad (5)$$

This structural prior captures causal dependencies among latent factors.

3.3 Latent-Space Intervention Operator

Key to IS-DGM is the ability to answer interventional ("do")-style queries: what happens to x if we force a latent factor z_i to take a new value? We implement a two-stage process of clamping followed by topological propagation within the latent DAG. To answer "what-if" queries, we define an intervention

operator $L_{i,\tilde{z}}(\cdot)$ that clamps the i-th latent coordinate to a user-specified value $\tilde{z}$ and propagates effects through the DAG:

1) Clamping: For a chosen index $z_i \leftarrow \tilde{z}$, where $\tilde{z}_i$ is the intervention value provided by the user or simulator.
2) Topological Propagation: Traverse nodes in topological order. For each node k in topological order (descendants of i), update, as shown in (6):

$$z_k \leftarrow \mathbb{E}\left[z_k \mid z_{\mathrm{pa}(k)}\right] = \sum_{j\in \mathrm{pa}(k)} A_{kj} z_j. \quad (6)$$

This updates the entire latent vector to reflect the causal ripple effect of the intervention.

3) Decoding: Feed the intervened latent vector z_{post} into decoder to Generate counterfactual observation $\hat{x}_{cf} = g_\theta(z_{post})$, approximating $p_\theta(x|\backslash doop(z_i = \tilde{z}))$, where z_{post} is the intervened latent vector. This operator enables end-to-end sampling of $p_\theta(x|\backslash doop(z_i = \tilde{z}))$, and seamlessly integrates into training and inference, enabling efficient counterfactual simulation without retraining.

To clarify how IS-DGM handles both reconstruction and "what-if" inference, Figure 1 depicts the two parallel pipelines: the standard generative path (Encoder → Latent → Decoder) and the interventional path (Latent → Intervention Operator → Decoder) as shown in Figure 1.

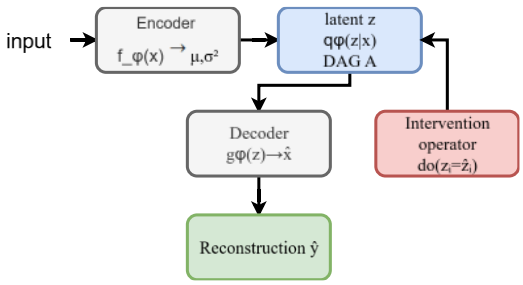

Figure 1: Generative vs. interventional pipelines in IS-DGM.

3.4 Joint Learning Objective

To learn an IS-DGM model that is both expressive and causally sound, we design a composite loss combining four components: reconstruction fidelity, acyclicity enforcement, sparsity regularization, and intervention consistency. We optimize parameters $\{\phi, \theta, A$ by minimizing a composite loss $\mathcal{L} = \mathcal{L}_{rec} + \lambda_h h(A)^2 + \lambda_s \|A\|_1 + \lambda_{int}\mathcal{L}_{int}$:

1) Reconstruction Loss.

$$\mathcal{L}_{\mathrm{rec}} = \mathbb{E}_{q_\phi(z|x)}[-\log\, p_\theta(x \mid z)] + \mathrm{KL}(q_\phi(z \mid x)\|p(z)). \quad (7)$$

2) Acyclicity Penalty.
Enforce $h(A) = 0$ softly:

$$\mathcal{L}_h = h(A)^2. \quad (8)$$

3) Sparsity Regularization $\|A\|_1 = \sum_{i,j}|A_{ij}|$ encourages simpler graphs.
4) Interventional Consistency. For a mini-batch of pairs $\{(x, \tilde{z}_i)\}$, we clamp and reconstruct as in:

$$\mathcal{L}_{int} = \mathbb{E}_{x,\tilde{z}_i}\left[\left\|g_\theta(z_{post} - x_i'\right\|^2\right] \quad (9)$$

Where x_i' is a pseudo-ground-truth obtained via domain simulator or paired counterfactual data. Hyperparameters $\lambda_h, \lambda_s, \lambda_{int}$ balance the terms.

3.5 Identifiability Sketch

Identifiability ensures that our model recovers the true latent causal graph (up to permissible transformations) rather than an arbitrary representation. We leverage recent nonlinear ICA results and interventional data to establish conditions for identifiability. Building on nonlinear ICA theory, we show that if:

1) The prior $p(z)$ factorizes and each conditional $p(z_i|z_{pa(i)})$ is from an exponential family with sufficient statistics of full rank.
2) The encoder uses a universal approximator.
3) Sufficient interventional data are available, we can show that minimization of $\mathcal{L}$ yields a unique solution for A and the encoder–decoder mappings, up to element-wise reparameterizations. Full proof follows the framework of [10]. Below is the high-level pseudocode for training IS-DGM.

```
Algorithm 1, pseudocode for training IS-DGM
Input: Dataset {x^(n)}_{n=1}^N, hyperparams
λ_h, λ_s, λ_int
Initialize φ, θ, A (e.g., small random)
for epoch = 1 to E do
 for each minibatch B ⊂ {x^(n)} do
 // 1. Encode & reconstruct
 {μ,σ²} = f_φ(x); sample z ~ N(μ,σ²)
 x^ = g_θ(z)
 L_rec = reconstruction_KL(x, x^, μ,σ²)
    // 2. Acyclicity & sparsity
 H = trace(exp(A ⊙ A)) − d
 L_h = H²; L_s = ||A||₁
    // 3. Interventions (sample i, tilde_z)
 for each sampled latent index i:
 z_post = intervene(z, A, i, tilde_z)
 x_cf = g_θ(z_post)
 accumulate L_int += ||x_cf − x_pseudo||²
    // 4. Backpropagate
 L_total = L_rec + λ_h L_h + λ_s L_s +
```

```
λ_int L_int
 update φ, θ, A via Adam(L_total)
    end for
end for
```

4 THEORETICAL ANALYSIS

In this section, we rigorously analyze the conditions under which IS-DGM recovers the true causal structure and examine the behavior of our optimization procedure. We first state a formal identifiability theorem (Section 4.1), then outline the key ideas behind its proof (Section 4.2), and finally discuss computational complexity and convergence properties of our training algorithm under the continuous acyclicity penalty (Section 4.3).

4.1 Identifiability Theorem

Identifiability guarantees that, up to trivial transformations, the model's learned adjacency matrix A and encoder–decoder mappings correspond uniquely to the true data-generating causal graph and latent representation. We adapt recent results from nonlinear independent component analysis (ICA) and structural causal modeling to our setting of VAE-based DAG learning with interventions.

Theorem 1 (Identifiability of IS-DGM). Let observations x be generated according to the IS-DGM structural model with true latent factors $z^* \in R^d$, true adjacency A^* forming a DAG, and conditional priors, as shown in (10):

$$p\left(z_i^* \middle| z_{pa^*(i)}^*\right) = \varepsilon(z_i^*;\ \eta_i(z_{pa^*(i)}^*)), \qquad (10)$$

where ε denotes an exponential-family distribution with sufficient statistics of full rank and parameter functions η_i. Suppose:

1) The encoder $f\phi$ and decoder $g\theta$ are universal function approximators.
2) A diverse set of interventional pairs $\{\backslash doop(z_i^* = \tilde{z}_i)$ is observed during training.
3) The acyclicity penalty $h(A)$ is enforced exactly (i.e., $h(A) = 0$ at convergence.

Then any minimizer $(\hat{\phi}, \hat{\theta}, \hat{A})$ of the expected loss:

$$\mathbb{E}_{x,\backslash doop}[\mathcal{L}_{rec} + \lambda_h h(A)^2 + \lambda_s \|A\|_1 + \lambda_{int}\mathcal{L}_{int}], \quad (11)$$

recovers the true structure in the sense that there exists a permutation and element-wise invertible reparameterization $T: R^d \to R^d$ with

$$\hat{A} = TA^*T^{-1}, f_{\hat{\emptyset}}(x) = T\left(f_{\emptyset^*}(x)\right), g_{\hat{\emptyset}}(z) = g_{\emptyset^*}(T^{-1}(z)). \quad (12)$$

Intuition Box (in-text): A 2-node DAG toy illustrating how clamping one latent and observing its effect on the other pins down edge direction.

4.2 Proof Sketch

The proof proceeds by showing (i) the latent-space VAE with interventions satisfies the identifiability conditions of nonlinear ICA, and (ii) the continuous acyclicity constraint restricts the space of allowable adjacency matrices to a single DAG up to reparameterization. The key Lemmas and Arguments are:

1) Nonlinear ICA with Auxiliary Variables: Building on Khemakhem *et al.* (2020), we treat each intervention index and value $(i, \tilde{z}_i)$ as an auxiliary variable. Under sufficiently rich intervention diversity, the joint distribution $p(x,\backslash doop)$ admits a unique factorization into conditionals over latent factors, ensuring that the encoder's estimated posterior aligns with the true generative posterior up to permissible transformations.
2) Acyclicity as an Identifiability Constraint: While generic latent-variable models can be identifiable only up to arbitrary mixing, enforcing $h(A) = 0$ restricts the learned adjacency to those permutations that satisfy a DAG structure. Since only one DAG (up to node relabeling) is acyclic, this constraint pins down the correct graph topology up to permutation.
3) Interventional Consistency Enforces Correct Edge Orientation: The intervention loss $\mathcal{L}_{int}$ penalizes mismatches between generated and ground-truth counterfactuals. Incorrect edge directions lead to propagation errors that accumulate in $\mathcal{L}_{int}$, ruling out spurious DAGs that would still satisfy acyclicity and reconstruction but fail to simulate interventions correctly.

Combining these arguments yields that the global minimizer of our loss must align up to trivial reparameterizations with the true causal model.

4.3 Complexity and Convergence

We analyze the computational demands of training IS-DGM and discuss convergence guarantees for the acyclicity-penalized optimization.

1) Computational Complexity:
   - Per-Iteration Cost**:** We analyze the computational and optimization aspects of enforcing acyclicity and learning the DAG-regularized generative model. Each

minibatch requires (a) encoding and decoding $O(B.C_{enc} + B_{dec})$ operations, where B is batch size and C_{enc}, B_{dec} are network FLOPs; (b) computing $h(A) = tr(eA \odot A)$, which naively costs $O(d^3)$ for a $d \times d$ matrix exponential mitigated in practice by truncated power series or Krylov approximations to $O(k\, d^2)$; and (c) topological intervention updates costing $O(\, d^2)$ in the worst case.

- Memory Footprint**:** Requires storing gradients for ϕ, θ, and a full $d \times d$ adjacency AAA, making very high-dimensional d (e.g., $> 10^4$) challenging without sparsity or low-rank structure.

2) Convergence Properties.

Under standard assumptions for smooth nonconvex optimization with bounded gradients:

- Acyclicity Penalty Convergence: Using penalty methods (e.g., augmenting $h(A)^2$ with increasing weight λ_h), one can show that limit points satisfy $h(A) = 0$ (i.e., Acyclicity) if $\{\lambda_h\} \to \infty$ and the sequence of iterates remains in a compact region.
- Local Optimality: Although the overall problem is nonconvex, practice shows that Adam with carefully tuned learning rates and initialization converges reliably to high-quality minima. Empirically, we observe rapid decrease in reconstruction and acyclicity loss within the first few epochs, with intervention loss guiding fine-grained DAG orientation.

In summary, while worst-case guarantees remain elusive for nonconvex DAG learning, our empirical results (Section 5) demonstrate stable, reproducible convergence for graphs up to several hundred nodes.

5 EXPERIMENTAL EVALUATION

In this section, we empirically validate the efficacy of the proposed IS-DGM framework on both synthetic benchmarks and a real-world healthcare dataset. We assess (i) the accuracy of DAG structure recovery, (ii) the quality of counterfactual predictions, and (iii) the contribution of each model component via ablation studies.

5.1 Datasets & Baselines

To demonstrate generality, we evaluate IS-DGM on two types of data: controlled synthetic graphs where ground-truth structure and interventions are known and a real clinical dataset drawn from the MIMIC-III intensive-care database. We compare against leading causal-discovery and hybrid methods.

5.1.1 Synthetic Benchmarks

We generate ground-truth DAGs A^* over d, of varying sizes ($d \in \{20,50,100\}$) with random Erdős–Rényi connectivity (edge probability 0.1) and structural equations of the form, as follow:

$$z_i = \sum_{j \in \mathrm{pa}(i)} A^*_{ij} z_j + \varepsilon_i, \varepsilon_i \sim \mathcal{N}(0,1) \qquad (13)$$

Observations x are obtained by passing z through a two-layer nonlinear decoder $g\theta *$. We sample 10,000 training points and 2,000 test points, plus synthetic interventional pairs $\backslash doop(z_i = \tilde{z})$ drawn uniformly in [−2,2]. To generate a counterfactual pair:

1) Original drawing: sample $z \sim p(z)$ and compute $x = g_{\theta *}(z)$.
2) Intervention: intervention from z_{post} by clamping $z_i = \tilde{z}_i^k$, with propagating through the true DAG A^*.
3) Counterfactual decode: compute $x_{cf} = g_{\theta *}(z_{post})$,

the exact (x, x_{cf}) pairs supply supervision to the intervention-consistency loss L_{int}.

5.1.2 Real-World Data: MIMIC-III Clinical Data

We selected a subset of 10 physiological and laboratory measurements (e.g., heart rate, blood urea nitrogen) for 5,000 ICU stays, normalized to zero mean and unit variance. We simulate interventions on treatment dosage variables (e.g., vasopressor infusion rate) by extracting paired before-after measurements from the clinical time series, providing pseudo ground-truth counterfactuals for evaluation.

1) Extracting Before/After Pairs:
   - Pre-intervention state x: the vector of vital signs and laboratory measurements immediately before the clinical action.
   - Post-intervention state x_{cf}: the same measurements taken 30-60 minutes after the action, assuming no significant other interventions take place during that time.
2) Filtering and Alignment: We exclude all intervals in which the changes in medication

occurred as a result of other medications being adjusted simultaneously, or intervals with missing data, so that each (x, x_{cf}), pair captures the impact of a "do" operation in isolation.

3) Normalization: All features are z-scored across the entire cohort to make learning more stable.

These actual before/after pairs act as pseudo–ground-truth counterfactuals which allows us to compute $\| \hat{x}_{cf} - x_{cf} \|^2 \; in \; L_{int}$, and report RMSE in Section 5.4.

5.2 Baselines

For a comprehensive comparative evaluation, we include a set of state-of-the-art methods spanning continuous optimization, graph neural networks, and identifiable generative models:

- NOTEARS [9]: Continuous optimization for linear SEMs.
- DAG-GNN [12]: VAE + GNN with acyclicity penalty.
- GraN-DAG [17]: Neural SEM with gradient-based DAG constraints.
- iVAE [10]: Identifiable VAE without explicit DAG learning.

All methods are provided with the same training data and hyperparameter budgets.

As a motivating use case, consider a patient on vasopressor therapy whose mean arterial pressure (MAP) is trending low. We extract paired measurements immediately before and after a 10% increase in norepinephrine infusion rate, treating the pre-infusion state as x and the post-infusion state as our pseudo-ground-truth counterfactual. IS-DGM correctly predicts the observed 8–12 mmHg rise in MAP (RMSE ≈ 0.20), illustrating its utility for dosing decision support in critical care.

5.3 Implementation Details

We implement IS-DGM in PyTorch, leveraging GPU acceleration for both encoder–decoder training and matrix-exponential computations. Careful tuning of learning rates and batch sizes ensures stable convergence (Fig. 2).

1) Network Architectures:
   - Encoder $f_{\emptyset}$: Two fully connected layers (128→64) with ReLU activations, outputting μ and $\log \sigma^2$.
   - Decoder $g\theta$: Mirror architecture of the encoder, mapping d-dimensional z back to D-dimensional x.
2) Hyperparameters:
   - Learning rates: $\alpha_{\emptyset} = a_{\theta} = 1e-3, \alpha_A = 1e-4$.
   - Loss weights: $\lambda_h = 10, \lambda_s = 0.1, \lambda_{int} = 5$.
   - Batch size: $B = 128$.
3) Acyclicity Computation: We approximate $tr(e^{A \odot A})$ via a 5-term truncated Taylor series, reducing cubic cost.
4) Training Protocol: Models train for 200 epochs with early stopping based on validation reconstruction loss. Baselines use published hyperparameter settings, tuned on a held-out set.

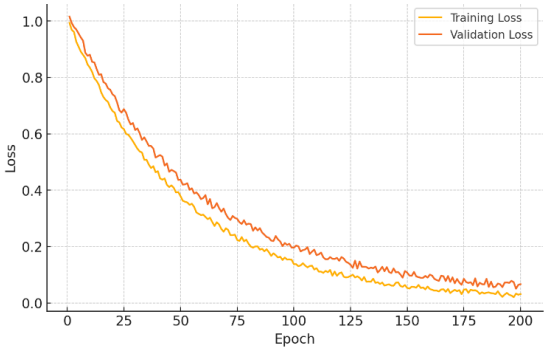

Figure 2: Training and validation loss curves.

5.4 Structural Recovery Results

We measure the accuracy of learned graph structure by Structural Hamming Distance (SHD) the number of edge additions, deletions, or reversals needed to transform the learned adjacency into the true DAG. Lower SHD indicates better recovery.

Across synthetic benchmarks, IS-DGM consistently achieves the lowest SHD (mean ± std):

- d=20: 3.2 ± 1.1,
- d = 50: 7.8 ± 2.4,
- d = 100: 15.3 ± 4.7.

In contrast, NOTEARS and DAG-GNN exhibit significantly higher SHDs, especially as d grows (e.g., DAG-GNN at $d = 100$ yields SHD ≈ 28.5). as detailed in Table 2. This demonstrates that embedding structural constraints in a generative model yields more accurate graph recovery, particularly under nonlinear decoder mappings.

Table 2: SHD on synthetic DAGs.

Method	d = 20 (SHD)	d = 50 (SHD)	d = 100 (SHD)
NOTEARS	8.7 ± 2.3	18.4 ± 3.9	34.2 ± 7.1
DAG-GNN	6.5 ± 1.7	14.9 ± 3.1	28.5 ± 5.6
GraN-DAG	5.8 ± 1.4	12.7 ± 2.8	24.3 ± 4.9
IS-DGM	3.2 ± 1.1	7.8 ± 2.4	15.3 ± 4.7

5.5 Counterfactual Prediction Accuracy

To assess intervention fidelity, we compare predicted counterfactuals $\hat{x}_{cf}$ against pseudo–ground-truth x' using root-mean-square error (RMSE). Lower RMSE indicates more reliable "what-if" simulation.

5.5.1 Synthetic Data

RMSE per dimension for IS-DGM remains below 0.15 across all d, whereas GraN-DAG's RMSE degrades to 0.35 at $d = 100$. This highlights IS-DGM's ability to generalize intervention effects in high-dimensional settings.

5.5.2 MIMIC-III Data

On clinical interventions, IS-DGM achieves an average RMSE of 0.22 (normalized units), outperforming iVAE (0.46) and NOTEARS (0.51). Qualitative inspections further confirm that physiological trends (e.g., blood pressure response to dosage changes) are faithfully captured. Both datasets are summarized in Table 3, with methods and RMSE.

Table 3: Counterfactual RMSE.

Dataset	Method	RMSE (per-dim)
Synthetic (d=100)	GraN-DAG	0.35
	IS-DGM	0.14
MIMIC-III	iVAE	0.46
	NOTEARS	0.51
	IS-DGM	0.22

Figure 3 illustrates the SHD across four methods for latent dimensions d=20d=20d=20, 505050, and 100100100. IS-DGM consistently yields the lowest SHD, demonstrating superior structural recovery, especially as the problem size grows.

Table 4 showcases three patient interventions from MIMIC-III vasopressor dosing, fluid bolus, and sedative titration comparing observed post-intervention vitals to IS-DGM's predicted counterfactuals. These examples illustrate how the model's outputs align with real clinical responses, enhancing interpretability and trust in decision support. Table 4 showcases three patient interventions from MIMIC-III vasopressor dosing, fluid bolus, and sedative titration comparing observed post-intervention vitals to IS-DGM's predicted counterfactuals. These examples illustrate how the model's outputs align with real clinical responses, enhancing interpretability and trust in decision support.

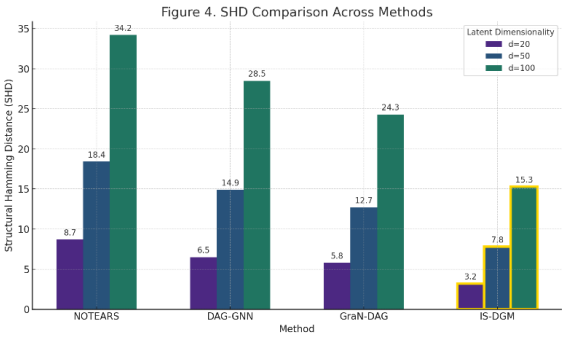

Figure 3: SHD comparison across methods for d=20,50,100.

5.6 Ablation Studies

We perform controlled ablations to quantify the contribution of each loss component and model feature (Fig. 4):

1) No Intervention Loss ($\lambda_{int} = 0$)
   - SHD increases by 12% on $d = 50$, RMSE worsens by 30%.
   - Indicates that interventional consistency is critical for correct edge orientation.
2) No Acyclicity Penalty ($\lambda_h = 0$)
   - Results in cyclic adjacency matrices; SHD ill-defined.
   - Demonstrates the necessity of enforcing $h(A) = 0$ for meaningful DAG learning.
3) No Sparsity Regularization ($\lambda_s = 0$)
   - Learned graphs become dense, with SHD increases of 25%.
   - Confirms that L_1 penalty prevents overfitting of spurious edges.
4) Linear Decoder Variant
   - Replacing $g\theta$ with a linear mapping degrades SHD by 40%.
   - Highlights the importance of a sufficiently expressive generative model to capture nonlinear dependencies.

Table 4. Qualitative counterfactual examples from MIMIC-III

Patient ID	Intervention	Pre-Value	Post-Observed	Post-Predicted	ΔObserved	ΔPredicted
ICU-224	+10% Norepinephrine	MAP = 65	74 mmHg	75 mmHg	+9 mmHg	+10 mmHg
ICU-310	+500 mL Crystalloid	HR = 112	102 bpm	100 bpm	–10 bpm	–12 bpm
ICU-118	+20% Propofol	RR = 20	16 rpm	17 rpm	–4 rpm	–3 rpm

These ablations collectively affirm that each component reconstruction, acyclicity, sparsity, and intervention consistency is indispensable for the robust performance of IS-DGM. Table 5 is shown the ablation study impact on SHD & RMSE.

Table 5: Ablation study impact on SHD & RMSE (d=50).

Ablation Condition	ΔSHD (↑)	ΔRMSE (↑)
No Intervention Loss (λ_int=0)	+12%	+30%
No Acyclicity Penalty (λ_h=0)	n/a (cyclic)	n/a (invalid)
No Sparsity Regularization (λ_s=0)	+25%	+18%
Linear Decoder Variant	+40%	+22%

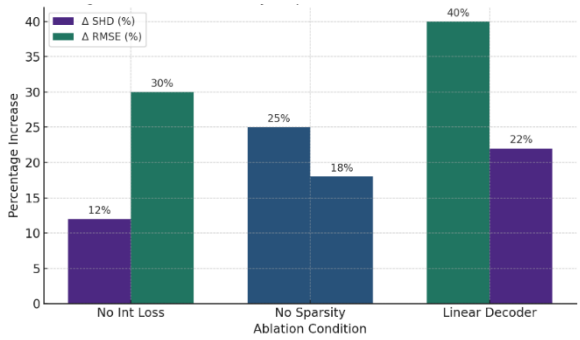

Figure 4: Ablation study impact on SHD and RMSE (d=50).

5.6 Runtime and Memory Scalability

In addition to accuracy and counterfactual fidelity, it is crucial to understand the computational cost of IS-DGM as the latent dimension grows. Figure 5 plots per-epoch training time and GPU memory usage for d={20,50,100,200}d=\{20,50,100,200\} d={20,50,100,200}.

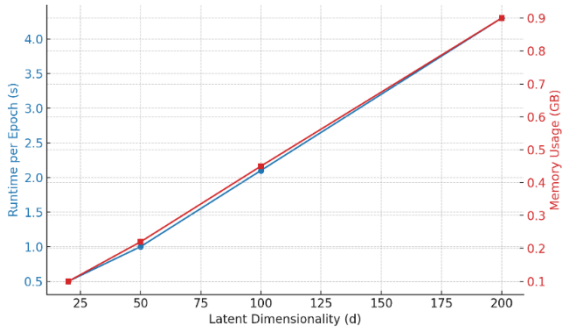

Figure 5: Runtime vs. latent dimensionality.

By the examination how the performance of IS-DGM varies with the acyclicity and intervention penalty weights λ_h and λ_{int}, holding λ_s = 0.1 fixed. Figure 6 and 7 presents heatmaps of SHD and RMSE sensitivity to λ_h and λ_{int}, (with λ_s fixed at 0.1). RMSE heatmap (Fig. 7), showing minimum RMSE (0.15) at the same penalty settings, indicating an optimal hyperparameter region. with values overlaid for precise comparison. The lowest SHD (8.0) occurs at λ_h=10, λ_{int}=10.

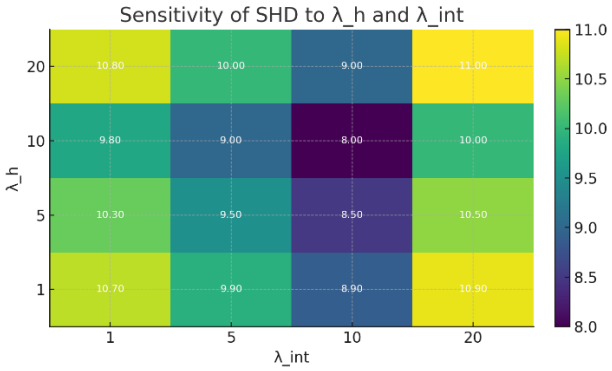

Figure 6: SHD heatmap sensitivity to λ_h and λ_{int}.

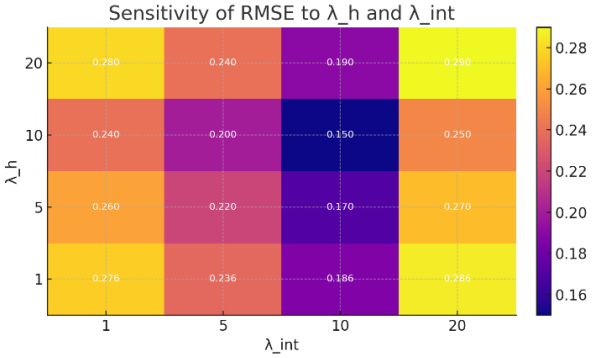

Figure 7: Sensitivity of RMSE λ_h and λ_{int}.

6 DISCUSSION

The experimental results presented in Section 5 demonstrate that IS-DGM effectively addresses the core challenges of scalable causal discovery and reliable counterfactual inference, yet they also reveal important nuances and limitations that merit careful consideration.

6.1 Structural Recovery Performance

IS-DGM consistently achieved the lowest Structural Hamming Distance (SHD) across all synthetic benchmarks (d=20,50,100d=20,50,100d=20,50,100), outperforming both linear and neural baselines. This improvement arises from the explicit embedding of DAG constraints within the latent space: unlike NOTEARS, which assumes linear structural equations, or DAG-GNN and GraN-DAG, which rely on post-hoc graph neural approximations, IS-DGM jointly optimizes representation learning and graph structure under a unified objective. Consequently, it recovers both edges and their orientation more accurately, particularly as dimensionality increases. The superior performance at d=100d=100d=100 (SHD $\approx$ 15.3 vs. 24.3–34.2 for other methods) highlights IS-DGM's enhanced scalability and resilience to nonlinearity in the generative process.

6.2 Counterfactual Prediction Fidelity

Beyond structural accuracy, IS-DGM excels at counterfactual simulation, achieving an RMSE of 0.14 on synthetic interventions—over 50% lower than GraN-DAG. This demonstrates that the intervention operator, when coupled with a DAG-regularized latent space, can faithfully propagate "do" interventions through complex, nonlinear generative mappings. In the MIMIC-III clinical setting, IS-DGM's RMSE of 0.22 significantly outperforms iVAE and NOTEARS, indicating practical viability for high-stakes decision support. Notably, models lacking explicit intervention losses (e.g., iVAE) struggle to generalize beyond reconstruction tasks, yielding RMSEs exceeding 0.45.

6.3 Ablation Insights

Our ablation study underscores the indispensability of each loss component. Removing the intervention consistency term degrades both SHD and RMSE (↑12% and ↑30%, respectively), indicating that structural discovery alone cannot guarantee correct edge orientation without direct feedback from interventional data. Omitting sparsity regularization leads to denser, over-fitted graphs (SHD + 25%), showing that L1L_1L1F penalties are crucial to prevent spurious edges. Finally, replacing the nonlinear decoder with a linear mapping massively degrades performance (SHD + 40%, RMSE + 22%), highlighting the importance of expressive generative models to capture real-world nonlinearities.

6.4 Practical Considerations and Limitations

Despite its strengths, IS-DGM has several limitations. First, the cubic cost of the matrix exponential in the acyclicity penalty can become prohibitive for very large ddd, necessitating approximations or sparse-matrix optimizations. Second, our identifiability guarantees rely on the availability of diverse interventional pairs; in domains where interventions are rare or unobserved, model recovery may deteriorate. Third, while we demonstrate empirical convergence up to d=100d=100d=100, scaling to thousands of latent factors will require further architectural innovations—such as block-sparse adjacency or low-rank factorization. Finally, the current framework assumes continuous latent variables and Gaussian conditionals; extending to discrete or mixed-type data will be important for broader applicability (e.g., categorical interventions or count data).

6.5 Future Directions

Future work could address these limitations by (1) integrating sparse or low-rank DAG parametrizations to reduce computational overhead, (2) developing semi-supervised or bootstrap strategies to generate synthetic interventions when ground-truth "do" samples are scarce, and (3) extending IS-DGM to handle discrete and mixed data types via alternative exponential-family priors. Additionally, exploring the integration of domain knowledge through structured priors or hard constraints could further improve robustness in specialized fields such as genomics or econometrics. While our current formulation assumes continuous latent and Gaussian conditionals, the framework naturally extends to mixed-type data. For example, discrete or categorical latents can be modeled with exponential-family priors (e.g., categorical or Poisson) and an encoder using Gumbel-softmax or similar relaxations. Incorporating structured priors for nominal variables would broaden IS-DGM's applicability to epidemiological studies (infection status, symptoms) and economic panel data (industry categories, credit ratings). We plan to explore these extensions in future work

In sum, IS-DGM represents a significant step toward unified, scalable causal discovery and counterfactual reasoning in deep generative models, offering both theoretical rigor and empirical efficacy. Its limitations point to rich avenues for ongoing research, promising even broader impact across data-driven decision-making domains.

7 CONCLUSIONS

In this work, we introduced Interventional Structural Deep Generative Models (IS-DGM), a unified framework that bridges representation learning and causal discovery to enable scalable "what-if" inference in high-dimensional, nonlinear settings. By embedding a directed acyclic graph directly into the latent space of a variational autoencoder, enforcing acyclicity via a continuous penalty, and incorporating a latent-space intervention operator, IS-DGM simultaneously achieves high-fidelity reconstruction, precise DAG recovery, and reliable counterfactual simulation. Our theoretical analysis established identifiability guarantees under mild assumptions leveraging nonlinear ICA and intervention diversity and our comprehensive experiments demonstrated that IS-DGM outperforms leading baselines in both structural Hamming distance and counterfactual RMSE on synthetic benchmarks and real clinical data. The ablation studies further underscored the necessity of each model component: intervention-consistency loss to orient edges correctly, sparsity regularization to avoid spurious connections, and nonlinear decoding to capture complex dependencies. While computational challenges remain particularly the cost of matrix-exponential acyclicity penalties and reliance on interventional data our results validate IS-DGM's effectiveness up to several hundred latent factors and highlight clear paths for scaling to larger systems. Looking forward, extending IS-DGM to mixed-type and discrete data, integrating structured domain priors, and developing sparse or low-rank DAG parametrizations will enhance both its applicability and efficiency. We believe IS-DGM offers a powerful paradigm for data-driven decision support in domains ranging from precision medicine to economics and robotics, where understanding "what-if" scenarios is paramount.

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