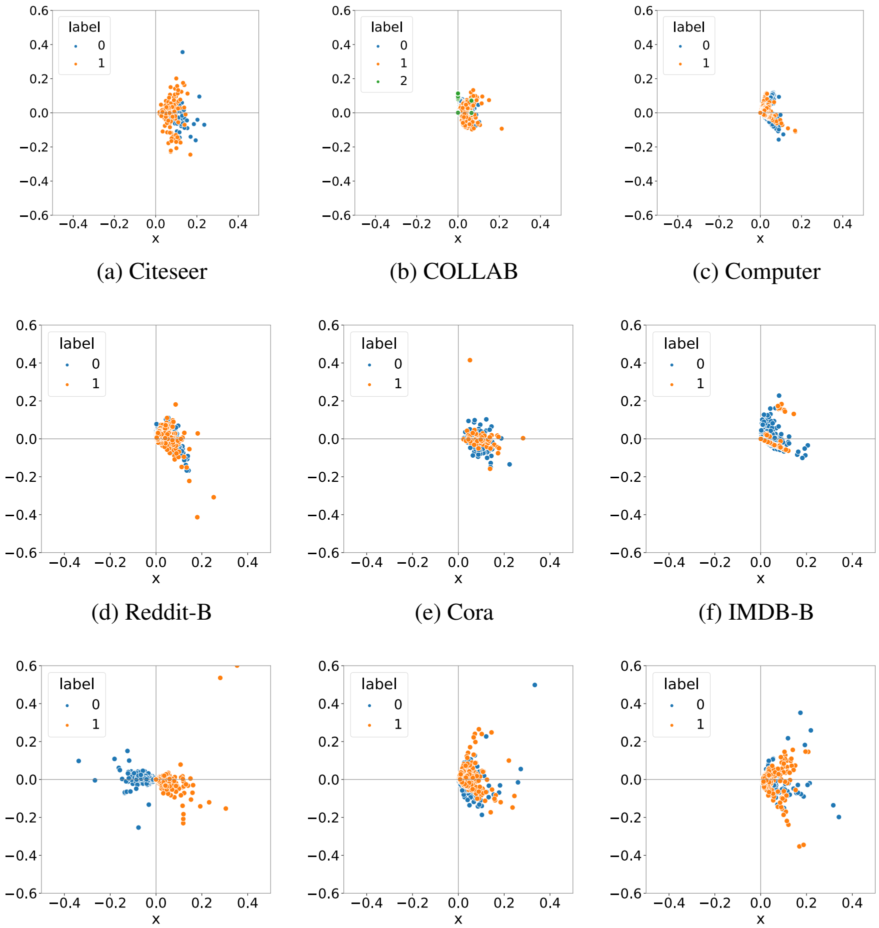
Supplementary Material

A Visualizing all other graph datasets

We visualize 9 graph datasets using their SVD decomposition, as shown in Figure 6. All the existing graph data exhibits strong anisotropic data structures.



(a) Citeseer (b) COLLAB (c) Computer

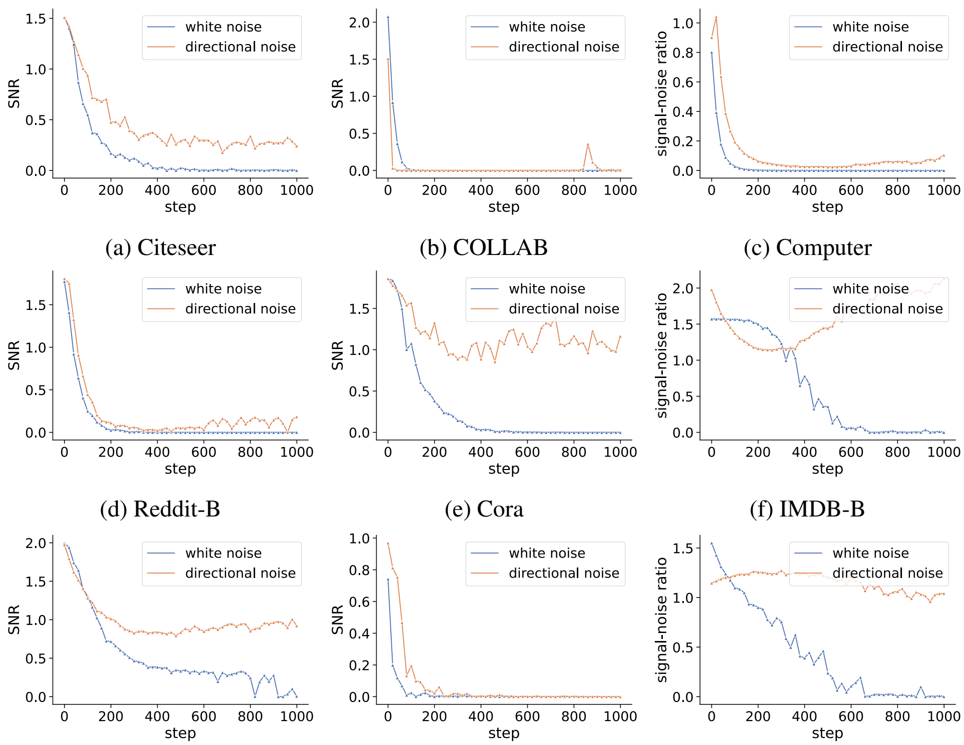
(d) Reddit-B (e) Cora (f) IMDB-B

(g) OGBN-arxiv (h) Proteins (i) Pubmed

Figure 6: 2D visualization of the data using SVD decomposition.

B Signal-to-noise ratios analysis

In this section, we examine the signal-to-noise ratios at various diffusion steps in various graph datasets, as shown in Fig 7.



(a) Citeseer (b) COLLAB (c) Computer

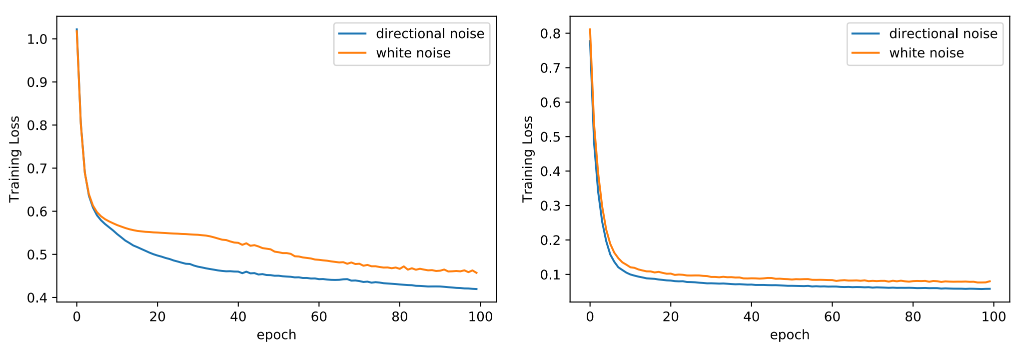
(d) Reddit-B (e) Cora (f) IMDB-B

(g) OGBN-arxiv (h) Proteins (i) Pubmed

Figure 7: Signal-to-noise ratio changes with diffusion steps.

C Training loss curve

In this section, we analyze the training losses of our directional diffusion model and the vanilla diffusion approach, as shown in Figure 8. Apparently, our model converges faster.



(a) Amazon-Photo (b) IMDB-M

Figure 8: The training loss curve.

D Ablation studies

Table 5 collects the network structures of the baselines used in the comparison experiments below. Specifically, existing approaches, including contrastive learning, GraphMAE, and our proposed method, utilize similar foundational architectures and have comparable number of parameters.

Table 5: Comparing architectures.

Method	GCN	MLP	Number of GCN Layers
GraphMAE	✓	✓	2-4
MVGRL	✓	✓	4
Our (DDM)	✓	✓	4

We also perform additional ablation experiments to evaluate the impact of our specific denoising architecture designs, such as symmetric skip-connections and symmetric network structures. Table 6 collects the results (classification accuracy), which validate our choice to incorporate U-net-inspired ideas and demonstrate the effectiveness of these detailed design choices.

Table 6: An ablation study on the architectured design.

	Citeseer	PubMed	MUTAG
wo-head	73.1±0.2	80.2±0.2	87.8±1.4
wo-encoder	73.4±0.1	81.4±0.3	88.9±1.3
wo-skip_connection	73.5±0.2	81.3±0.5	86.7±1.1
Baseline	74.3±0.3	81.7±0.8	91.51±1.4

E The complete algorithm

In this section, we present the complete algorithm for our proposed directional diffusion models.

Algorithm 1 The training algorithm.

Input: A batch of graphs $\mathcal{G} = \{G_1, \cdots G_B\}$
Output: The denoising network f_θ

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Initialize: the denoising network f_θ
Compute μ, the mean of node features across batch 𝒢
Compute σ, the standard deviation of node features across batch 𝒢
while not convergence do
    for G_i in 𝒢 do
        for t = 1, ..., T do
            Sample directional noise ε′ using equation (2)
            Take gradient descent step on
            ∇_θ ‖X_0 − f_θ(√(ᾱ_t) X_i + √(1 − ᾱ_t) ε′, A, t)‖
        end for
    end for
end while
```

$$\nabla_\theta \left\| \mathbf{X}_0 - f_\theta(\sqrt{\bar{\alpha}_t}\mathbf{X_i} + \sqrt{1-\bar{\alpha}_t}\epsilon', \mathbf{A}, t) \right\|$$

Algorithm 2 Extracting representations.

Input: $G = (\mathbf{A}, \mathbf{X})$, forward step set $\{T_0, T_1, \ldots, T_K\}$, pre-trained denoising network f_θ
Output: $\mathbf{H}$, the representation of G

1: **Compute** μ the mean of node features
2: **Compute** σ the standard deviation of node features
3: **for** k in $\{T_0, T_1, \ldots, T_K\}$ **do**
4: **Sample** directional noise ϵ' using equation (2)
5: $\mathbf{X_k} \leftarrow \sqrt{\bar{\alpha}_k}\mathbf{X_0} + \sqrt{1 - \bar{\alpha}_k}\epsilon'$
6: $\mathbf{H}_k \leftarrow f_\theta(\mathbf{X_k}, \mathbf{A}, k)$
7: **end for**
8: **Concatenate** $\mathbf{H} = [\mathbf{H}_{T_0}, \mathbf{H}_{T_1}, \ldots, \mathbf{H}_{T_K}]$
9: **return** $\mathbf{H}$

F Statistics and hyper-parameters

In this section, we provide the statistics and hyperparameters in the main experiments in Table 7 and Table 8. The description of each hyperparameter is collected in Table 9.

Table 7: Statistics and hyper-parameters for node classification datasets. "s" indicates multi-class classification, and "m" indicates multi-label classification.

	Dataset	Cora	Citeseer	PubMed	Ogbn-arxiv	Computer	Photo
Statistics	# nodes	2708	3327	19717	169343	13752	7650
	# edges	5429	4732	44338	1166243	245861	119081
	# classes	7(s)	6(s)	3(s)	40(s)	10	8
Hyper-para.	feat_drop	0.1	0.2	0.2	0.2	0.4	0.2
	attn_drop	0.3	0.4	0.4	0.2	0.2	0.3
	num_head	4	4	4	4	4	4
	num_hidden	1024	1024	1024	512	512	1024
	learning_rate	6e-5	2e-4	2e-4	2e-4	2e-4	1e-4
	norm	LayerNorm	LayerNorm	LayerNorm	LayerNorm	BatchNorm	BatchNorm
	beta_schedule	Sigmoid	Linear	Const	Linear	Quad	Sigmoid

Table 8: Statistics and hyper-parameters for graph classification datasets.

	Dataset	IMDB-B	IMDB-M	COLLAB	REDDIT-B	PROTEINS	MUTAG
Statistics	# graphs	1000	1500	5000	2000	1113	188
	# classes	2	3	3	2	3	2
	Avg. # nodes	19.8	13.0	74.5	429.7	13.0	17.9
Hyper-para.	feat_drop	0.4	0.4	0.4	0.2	0.2	0.2
	attn_drop	0.4	0.4	0.4	0.4	0.2	0.1
	num_head	2	4	4	8	4	4
	num_hidden	128	512	512	512	512	512
	learning_rate	1e-5	1e-5	1e-5	3e-4	3e-4	3e-4
	norm	LayerNorm	LayerNorm	LayerNorm	LayerNorm	LayerNorm	LayerNorm
	beta_schedule	Sigmoid	Linear	Const	Linear	Linear	Sigmoid

Table 9: Hyper-parameter description.

Hyper-parameter	**Interpretation**
feat_drop	the drop-out rate of hidden layers
attn_drop	the drop-out rate of attention modules
num_head	the number of heads
num_hidden	the number of hidden layers
learning_rate	the learning rate in training stage
norm	the method of normalization
beta_schedule	the schedule of β_t