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GRACED: A Plug-and-Play Solution for Certifiable Graph Classification

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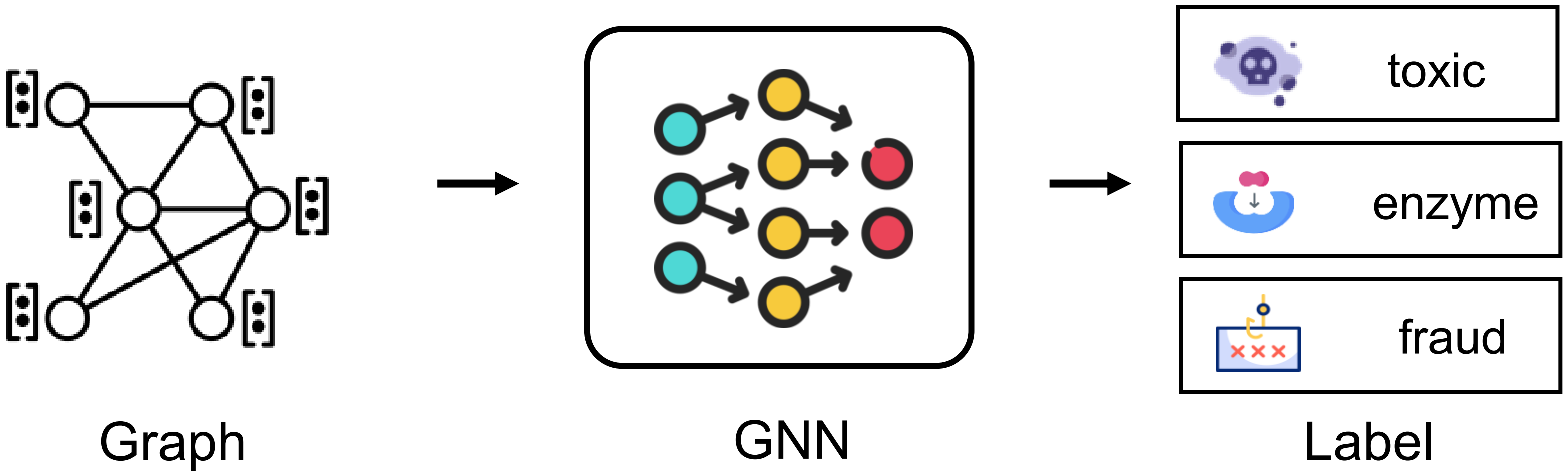
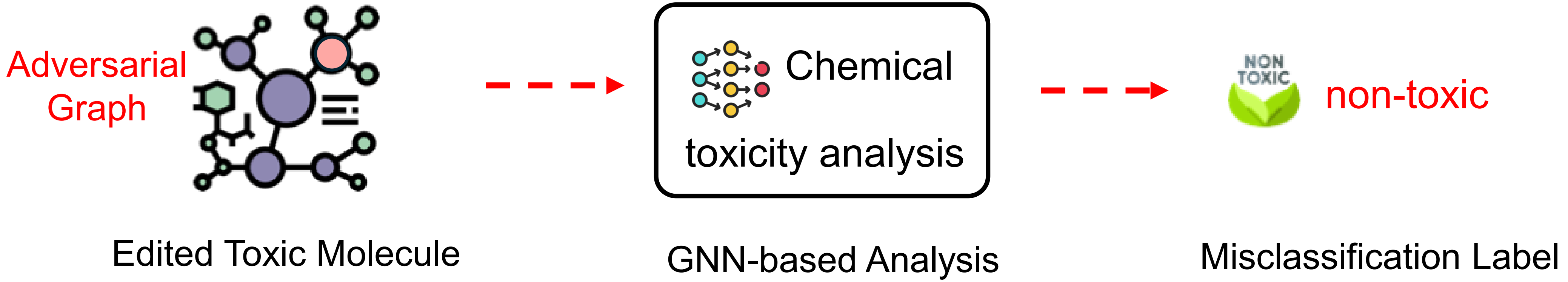
Background: GNN for Graph Classification

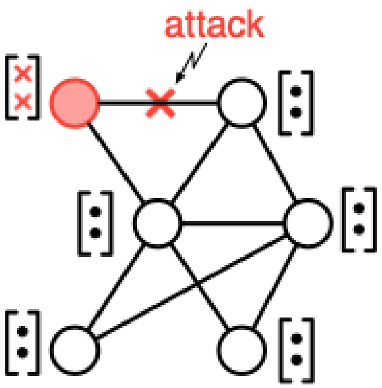


Real-world relationships are often abstracted into **graphs.**

Graph neural networks (**GNN**) is used for **graph classification** in tasks like toxicity prediction, protein function prediction, and fraud detection.

Background: Adversarial Attack on GNN

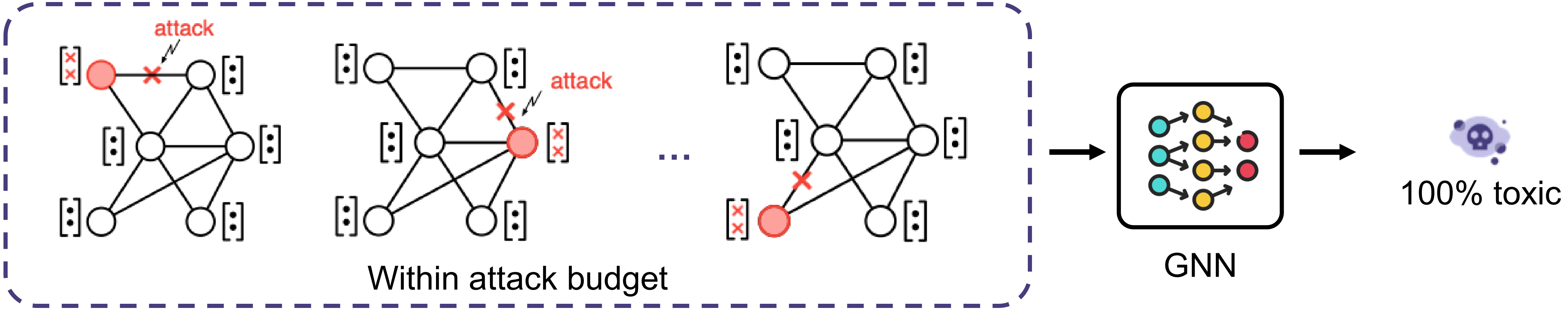




- **Adversarial Attack**

Unnoticeable perturbations on **graph structure** and **node attributes** could lead to misclassification of graph by high-accuracy GNN.

Background: Robustness Certificate



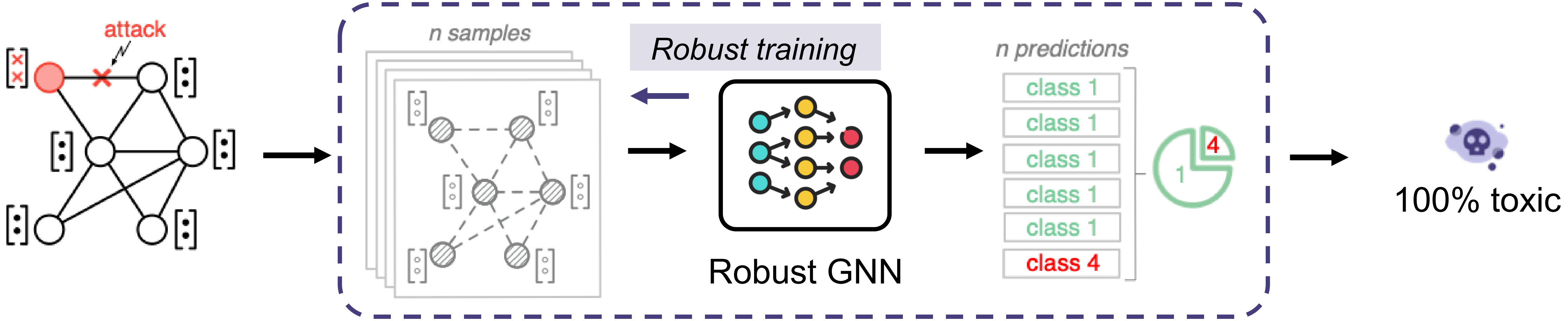
- **Certification**

Given the input graph $G = (X, A)$, base classifier f_θ and attack budget (magnitude of perturbation) Δ: guarantee that for all $\delta \in \Delta$, $f_\theta(G + \delta) = f_\theta(G)$.

- **Threat Model**

$\Delta = (\Delta_X, \Delta_A)$ specifies a ℓ_0-ball around input G, which is to limit the magnitude of changes in X and A.

Background: Randomized Smoothing



- **Randomized Smoothing** (Cohen 2019, Bojchevski 2020)

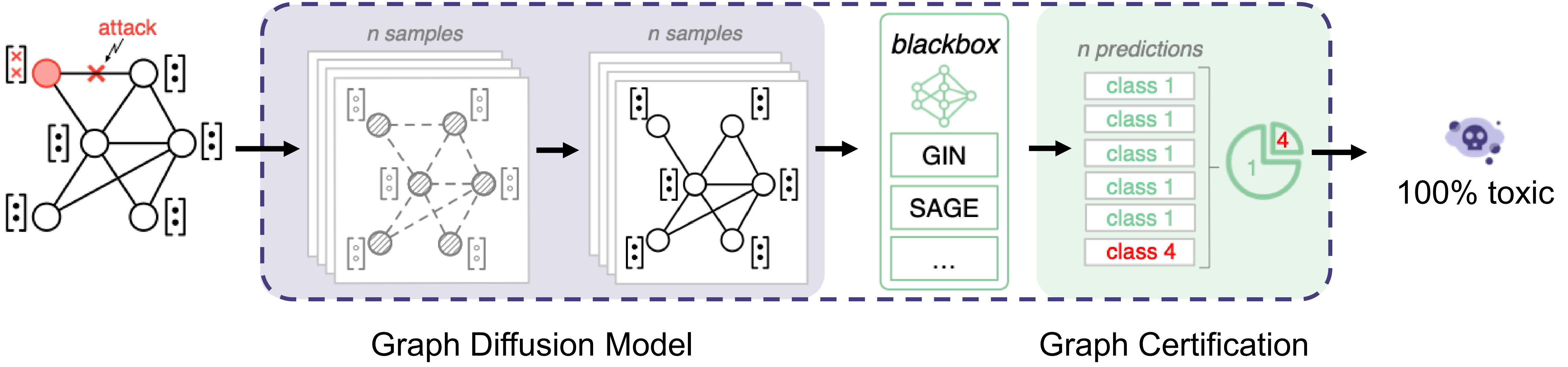
RS-based method predicts the label with a smoothed base classifier, noted as $g_\theta(G)$:

$$g_\theta(G) := \arg_y\max \Pr_{\boxed{\tilde{G}\sim\phi(G)}}[f_{\theta^*}(\tilde{G}) = y],$$ where $\phi(G)$ is randomization scheme

RS methods require retraining or fine-tuning as f cannot handle noisy samples

i) Retraining for diverse adversaries; ii) accuracy drop on clean samples.

How to provide plug-and-play certified defense for GNN?



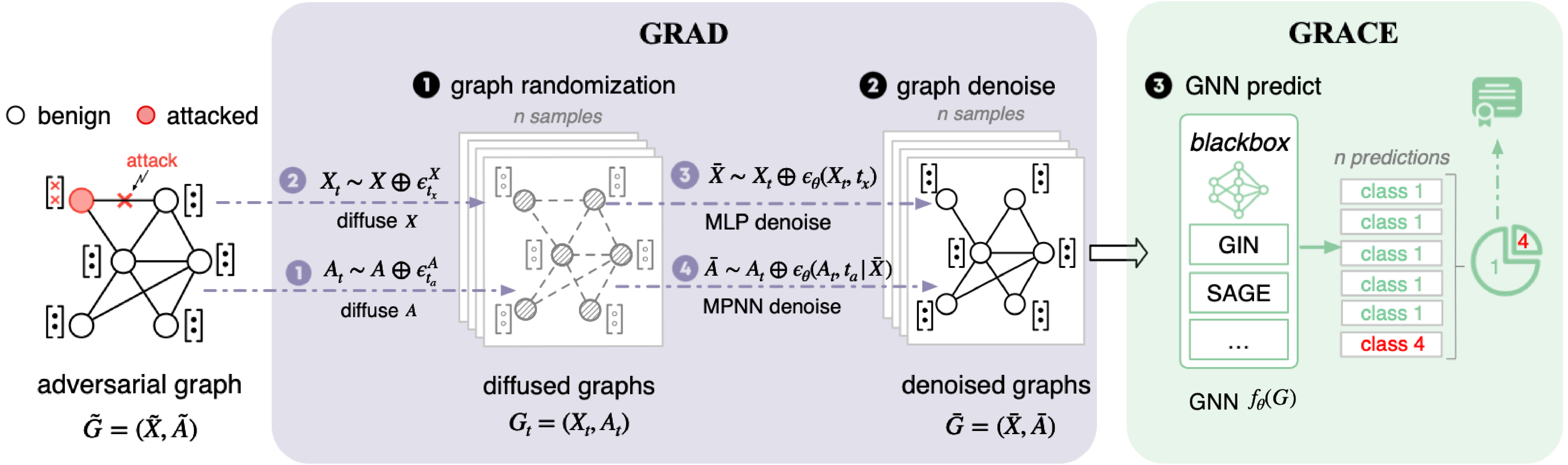
Diffusion Models

- **GRACED: Denoised Smoothing**

$$f_{\theta^*}(\tilde{G}) := f_\theta(\boxed{\mathcal{D}}(\tilde{G}))$$

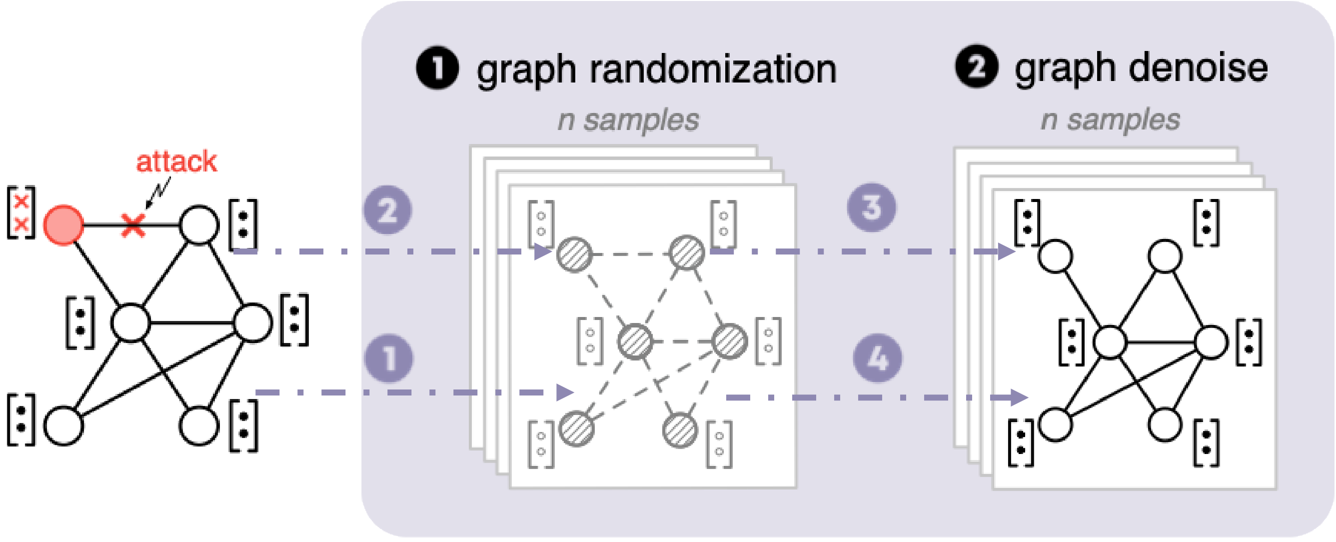
$\mathcal{D}$ is a diffusion-based denoiser, which purify the adversarial graph before obtain certified classification with black-box GNN.

GRACED Framework



GRACED - a plug-and-play solution to guarantee **GRA**ph classification with **CE**rtifiable robustness via a Diffusion model

GRAD: A Graph Diffusion Model



1. $X_t \sim X \oplus \epsilon^{X}_{t_x}$
2. $A_t \sim A \oplus \epsilon^{A}_{t_a}$
3. $\bar{X} \sim X_t \oplus \epsilon_\theta(X_t, t_x)$
4. $\bar{A} \sim A_t \oplus \epsilon_\theta(A_t, t_a \,|\, \bar{X})$

- **Step 1: graph randomization**

Forward process of diffusion model adds data-dependent Bernoulli noise on X and A.

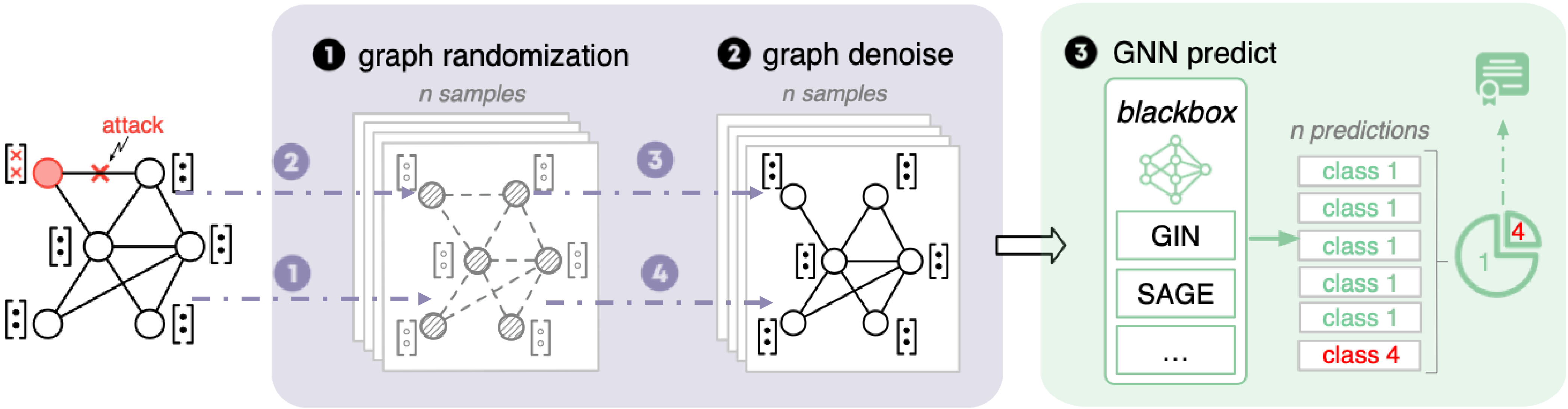
diffusion = randomization

- **Step 2: graph denoise**

Reverse process of diffusion model removes noise from X and A to reconstruct data.

reverse = purification

GRACE: A Graph Certification



- **Step 3: GNN predict**

Use black-box standard trained GNN to classify denoised graphs, providing robustness certificate with randomized smoothing method.

diffusion timestep = randomization parameter

Evaluation

- **Clean accuracy**

✓ Outperforming sparse smoothing (Bojchevski *et al*. 2020) on joint and singular perturbation.

✓ Outperforming hierarchical smoothing (Scholten *et al*. 2024) on singular perturbation on X.

✓ Outperforming Bernoulli smoothing (Wang *et al*. 2021) on singular perturbation on A.

TABLE I
CLEAN ACCURACY UNDER DIFFERENT PERTURBATION

Type		MUTAG	NCI1	PROTEINS	IMDB
Attr.& Adj.	Naïve$^{\phi}$	0.58	0.49	0.54	0.52
	Sparse	0.68	0.60	0.55	0.49
	Hier.^{A}	0.52	**0.64**	0.63	0.48
	Ber.^{X}	0.74	0.55	**0.67**	0.51
	GRACED	**0.79**	**0.64**	**0.67**	**0.63**
Attr.	Naïve$^{\phi}$	0.53	0.48	0.53	0.51
	Sparse	0.68	0.32	**0.49**	0.66
	Hier.	0.73	0.51	0.41	0.57
	GRACED	**0.78**	**0.59**	**0.61**	**0.63**
Adj.	Naïve$^{\phi}$	0.53	0.46	0.53	0.54
	Sparse	0.63	0.43	**0.61**	0.66
	Ber.	0.63	0.55	0.51	0.53
	GRACED	**0.78**	**0.62**	**0.61**	**0.75**

Note: The randomization parameters are set as the noise scale when diffusion timestamp $t = 300$. Hier.^{A} denotes adaptation of hierarchical smoothing with ϵ^{Z} set the same as sparse method and corruption ratio $p = 0.8$. Ber.^{X} is the adaptation of Bernoulli smoothing with $\epsilon^{Z} = \text{Ber}(p = \frac{1}{2}(p^{+} + p^{-}))$.

Evaluation

- **Clean accuracy**

✓ Outperforming sparse smoothing (Bojchevski *et al*. 2020) under different randomization setting on bioinformatics graph dataset MUTAG and social network dataset IMDB-BINARY.

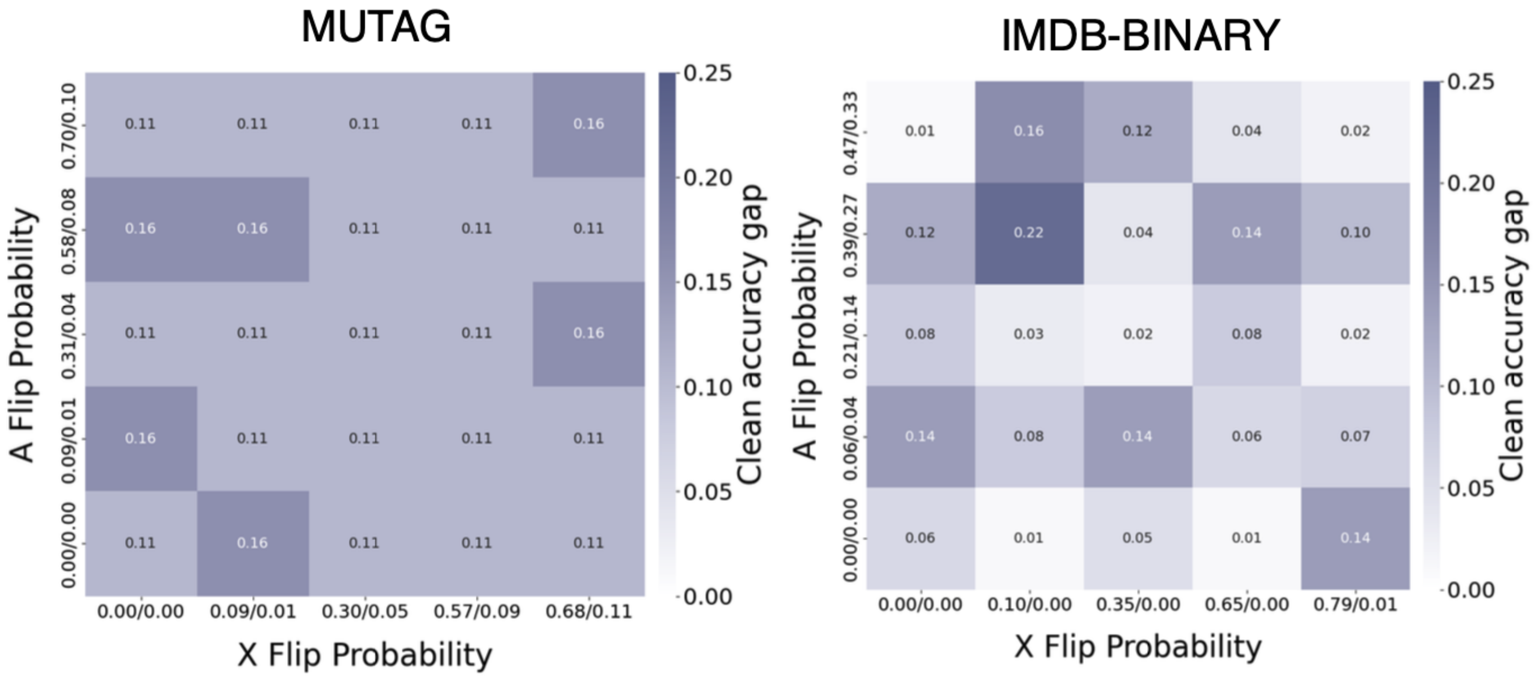


Fig. 3. **Clean accuracy gap**: Each heatmap shows the clean accuracy gap between GRACED and Sparse Smoothing per dataset, with noise scales for attributes and adjacent matrices on the horizontal and vertical axes.

Evaluation

- **Certified accuracy**

Achieving high certified accuracy on large attack budget, for both singular and joint perturbation scenario.

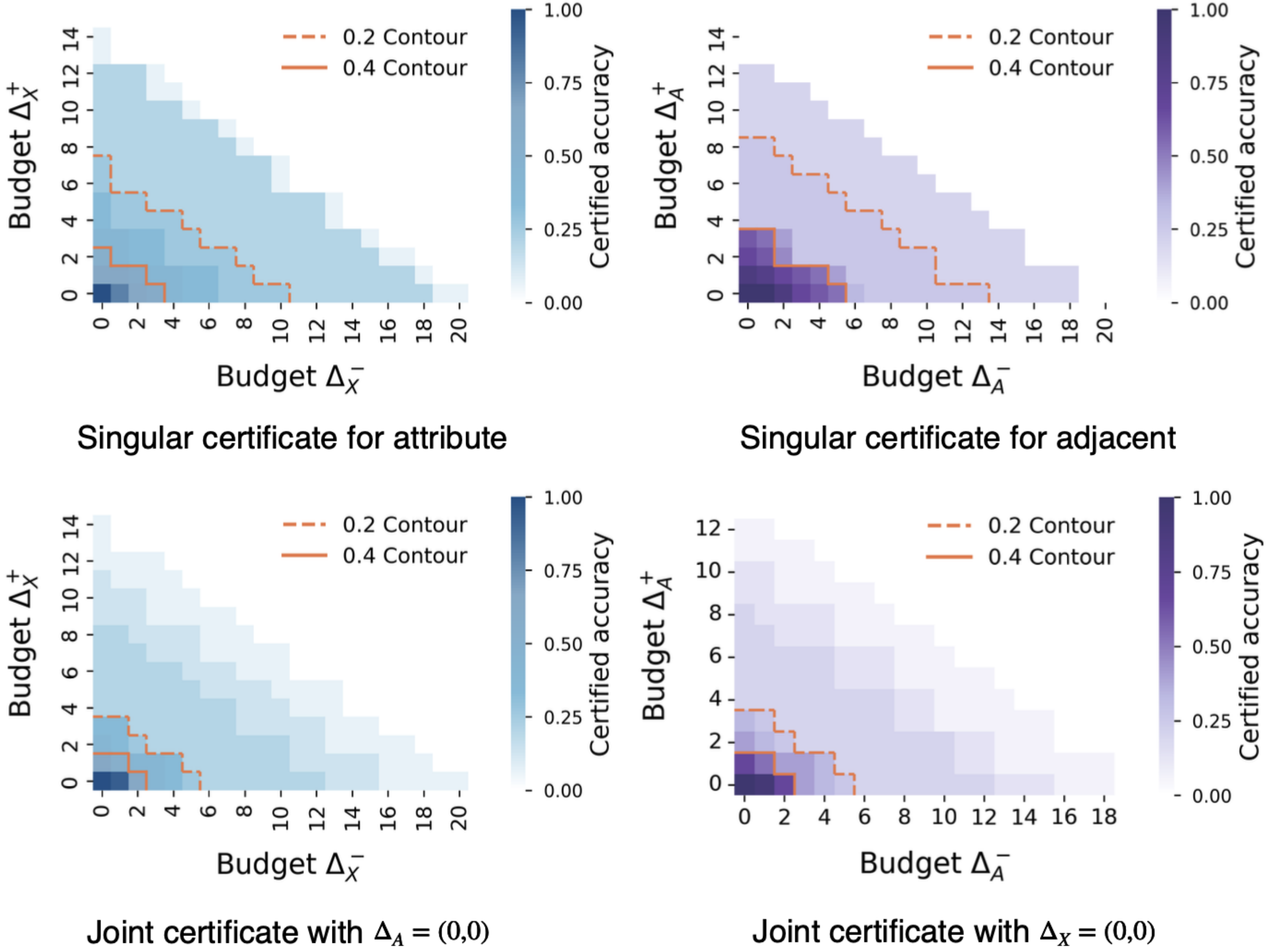


Fig. 4. **Certificate**: The top row depicts singular certificates, and the bottom shows joint perturbation defense. Blue and purple heatmaps represent certificates for node attributes and sctructure, respectively.

Summary

- **Plug-and-play Certification**

We present GRACED to effectively tackling the verifiable robustness of black-box graph classification models in a plug-and-play style.

- **Graph Diffusion Model**

We design GRAD, a graph diffusion based on D3PM (Austin *et al*. 2021) to purify the adversarial graph into a benign graph, preserving the structure stability of the graph in the process.

- **High Accuracy**

We have validated the efficacy of our approach through comprehensive testing on real-world datasets, showing accuracy improvement of approximate 10% over randomized smoothing.

Thank you for your attention.

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