

Table 3. Dataset statistics.

Dataset	#Nodes	#Edges	#Features	#Classes
Cora	2,485	5,429	1,433	7
Citeseer	2,110	3,757	3,703	6
BlogCataLog	5,196	343,486	8,189	6

Algorithm 1 Certified robustness inspired PGD (CR-PGD) graph evasion attack to GNNs

Input: Node classifier f , graph $G(\mathbf{A})$, testing nodes \mathcal{V}_{Te} , perturbation budget Δ , total iterations T , #samples N , noise parameter β , confidence level $1 - \alpha$, a , interval INT .

Output: Adversarial graph perturbation $\delta^{(T)}$.

Initialize: $t = 0$; graph perturbation $\delta^{(0)} = 0$;

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while  $t < T$  do
  // Stage 1: Obtaining the CR inspired loss
  if  $t \bmod INT \neq 0$  then
    Reuse the node weights:  $w^{(t)}(v) = w^{(t-1)}(v)$ ;
  else
    Define the perturbed graph:  $\mathbf{A}^{(t)} = \mathbf{A} \oplus \delta^{(t)}$ ;
    Sample  $N$  noise matrices  $\{\epsilon^j\}_{j=1}^N$  from the noise distribution Equation 7 with parameter  $\beta$ ;
    for each node  $v \in \mathcal{V}_{Te}$  do
      Compute the frequency  $N_{y_v}$  for label  $y_v$ :  $N_{y_v} = \sum_{j=1}^N \mathbb{I}(f(\mathbf{A}^{(t)} \oplus \epsilon^j; v) = y_v)$ ;
      Estimate the low bound probability  $\underline{p}_{y_v}$  with confidence  $1 - \alpha$ :  $\underline{p}_{y_v} = B(\alpha; N_{y_v}, N - N_{y_v} + 1)$ ;
      Calculate the certified perturbation size  $K(\underline{p}_{y_v})$  using  $\underline{p}_{y_v}$  and algorithm in [35];
      Assign a weight  $w(v)$  to each node  $v$ :  $w^{(t)}(v) = \frac{1}{1 + \exp(a \cdot K(\underline{p}_{y_v}))}$ ;
    end
  end
  Define the certified robustness inspired test loss:
   $\mathcal{L}_{CR}(f, \mathbf{A}^{(t)}, \mathcal{V}_{Te}) = \sum_{v \in \mathcal{V}_{Te}} w^{(t)}(v) \ell(f(\mathbf{A}^{(t)}; v), y_v)$ ;
  // Stage 2: Running the PGD attack with CR loss
   $\delta^{(t+1)} = \text{Proj}_{\mathbb{B}}(\delta^{(t)} + \eta \cdot \nabla_{\delta^{(t)}} \mathcal{L}_{CR}(f, \mathbf{A}^{(t)}, \mathcal{V}_{Te})$ ;
  Update  $t = t + 1$ .
end
return  $\delta^{(T)}$ 

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Algorithm 2 Certified robustness inspired Minmax (CR-Minmax) graph poisoning attack to GNNs

Input: GNN algorithm \mathcal{A} , Graph $G(\mathbf{A})$, training nodes \mathcal{V}_{Tr} , perturbation budget Δ , number of samples N , noise parameter β , confidence level $1 - \alpha$, a , interval INT .

Output: Adversarial graph perturbation $\delta^{(T)}$.

Initialize: $t = 0$; $\delta^{(0)} = 0$; random/pretrained GNN model $\theta^{(0)}$;

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while  $t < T$  do
  // Stage 1: Obtaining the CR inspired loss
  if  $t \bmod INT \neq 0$  then
    Reuse the node weights:  $w^{(t)}(v) = w^{(t-1)}(v)$ ;
  else
    Define the perturbed graph:  $\mathbf{A}^{(t)} = \mathbf{A} \oplus \delta^{(t)}$ ;
    Sample  $N$  noise matrices  $\{\epsilon^j\}_{j=1}^N$  from the noise distribution Equation 7 with parameter  $\beta$ ;
    Train  $N$  node classifiers  $\{\tilde{f}^n\}$  with current perturbed graph  $\mathbf{A}^{(t)}$  with the  $N$  sampled noisy matrices  $\{\epsilon^n\}$ :
     $\tilde{f}^1 = \mathcal{A}(\mathbf{A}^{(t)} \oplus \epsilon^1, \mathcal{V}_{Tr}), \dots, \tilde{f}^N = \mathcal{A}(\mathbf{A}^{(t)} \oplus \epsilon^N, \mathcal{V}_{Tr})$ 
    for each node  $v \in \mathcal{V}_{Tr}$  do
      Compute the frequency  $N_{y_v}$  for label  $y_v$ :  $N_{y_v} = \sum_{j=1}^N \mathbb{I}(\tilde{f}^j(\mathbf{A}^{(t)} \oplus \epsilon^j; v) = y_v)$ ;
      Estimate the low bound probability  $\underline{p}_{y_v}$  with confidence  $1 - \alpha$ :  $\underline{p}_{y_v} = B(\alpha; N_{y_v}, N - N_{y_v} + 1)$ ;
      Calculate the certified perturbation size  $K(\underline{p}_{y_v})$  using  $\underline{p}_{y_v}$  and algorithm in [35];
      Assign a weight  $w(v)$  to each node  $v$ :  $w^{(t)}(v) = \frac{1}{1 + \exp(a \cdot K(\underline{p}_{y_v}))}$ ;
    end
  end
  Define the certified robustness inspired training loss:
   $\mathcal{L}_{CR}(f, \mathbf{A}^{(t)}, \mathcal{V}_{Tr}) = \sum_{v \in \mathcal{V}_{Tr}} w^{(t)}(v) \cdot \ell(f(\mathbf{A}^{(t)}; v), y_v)$ ;
  // Stage 2: Running the Minmax attack with CR loss
  Step 1: Inner minimization over model parameter  $\theta$ :  $\theta^{(t+1)} = \theta^{(t)} - \eta_1 \nabla_{\theta} \mathcal{L}_{CR}(f_{\theta^{(t)}}, \mathbf{A}^{(t)}, \mathcal{V}_{Tr})$ ;
  Step 2: Outer maximization over graph perturbation  $\delta$ :
   $\delta^{(t+1)} = \text{Proj}_{\mathbb{B}}(\delta^{(t)} + \eta_2 \nabla_{\delta} \mathcal{L}_{CR}(f_{\theta^{(t+1)}}, \mathbf{A}^{(t)}, \mathcal{V}_{Tr})$ ;
  Update  $t = t + 1$ .
end
return  $\delta^{(T)}$ 

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