Robust Stochastic Graph Generator for Counterfactual Explanations

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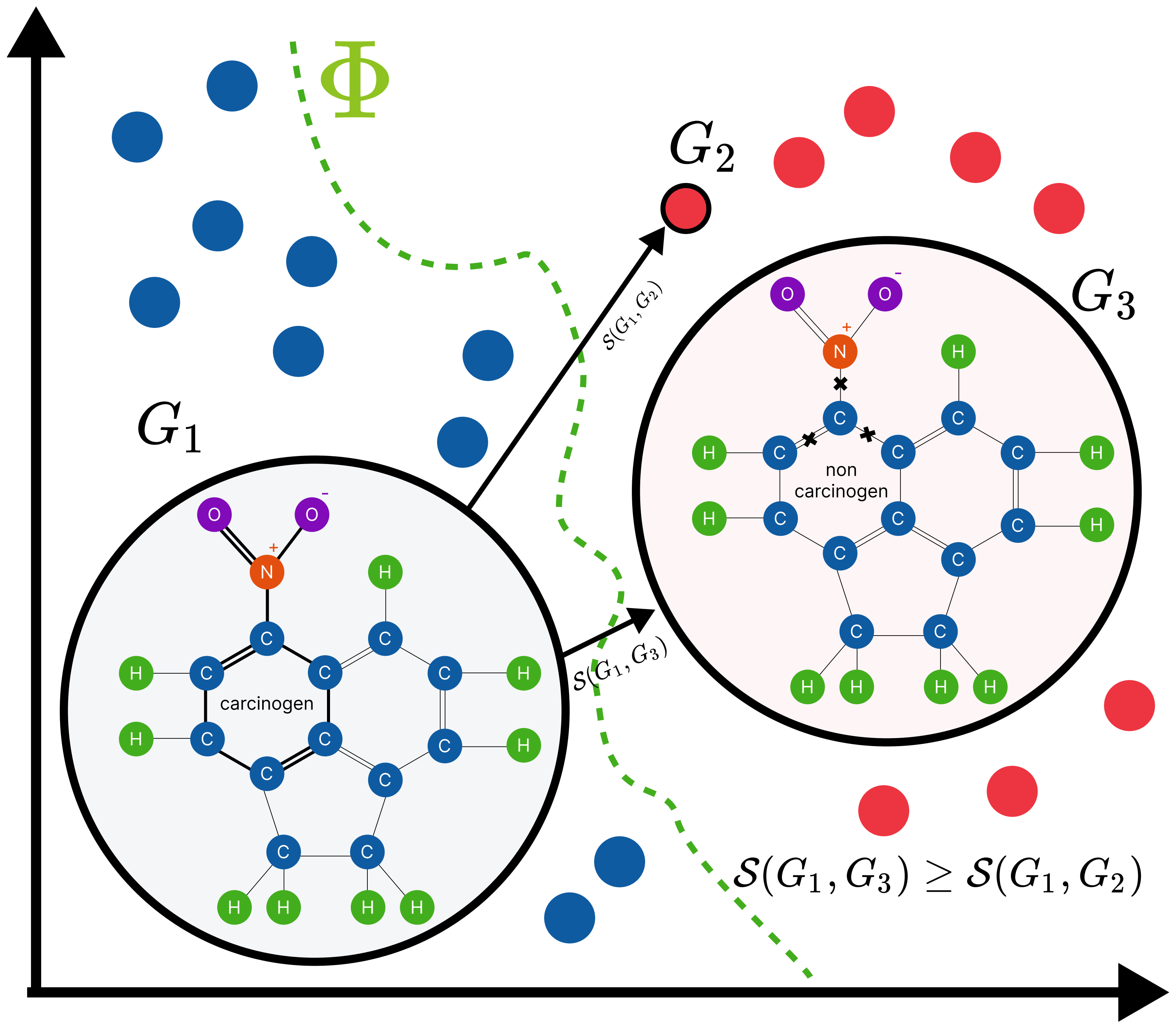
Graph Counterfactual Explainability (GCE)



$$\mathcal{E}_\Phi(G) = \underset{G' \in \mathcal{G}', G \neq G', \Phi(G) \neq \Phi(G')}{\arg\max} \mathcal{S}(G, G')$$

$$\equiv$$

$$\mathcal{E}_\Phi(G) = \underset{G' \in \mathcal{G}'}{\arg\max} P(G' \mid G, \Phi(G), \neg\Phi(G))$$

Problems with GCE

- SoA is generally **constrained** to the **input data** (search-based GCE) and relies on **learned perturbation masks** (learning-based GCE)
- Defaulting to factual-based explainers falters when dual classes clash (e.g., **acyclic vs cyclic graphs**)
- Crossing the decision boundary isn't enough; one must be **close to** the original instance

What’s been done until now…

- Learning-based GCE [1-5]:
  1) generate masks of relevant features given a graph G;
  2) combine this mask with G to derive G';
  3) feed G' to the oracle Φ and update the mask

- CLEAR [5] uses a VAE to encode graphs into a latent representation which, at inference, is used to generate complete stochastic graphs

- G-CounteRGAN [6,7] relies on 2D convolutions on the adjacency matrix of graphs

Intuition

- Using a generative approach possibly a GAN allows having brand new in-distribution counterfactuals examples;
- We'll exploit the generator to engender counterfactual candidates
- Use the discriminator to guide the generator in learning how to cross the decision boundary

Classic GANs vs GANs for counterfactuals

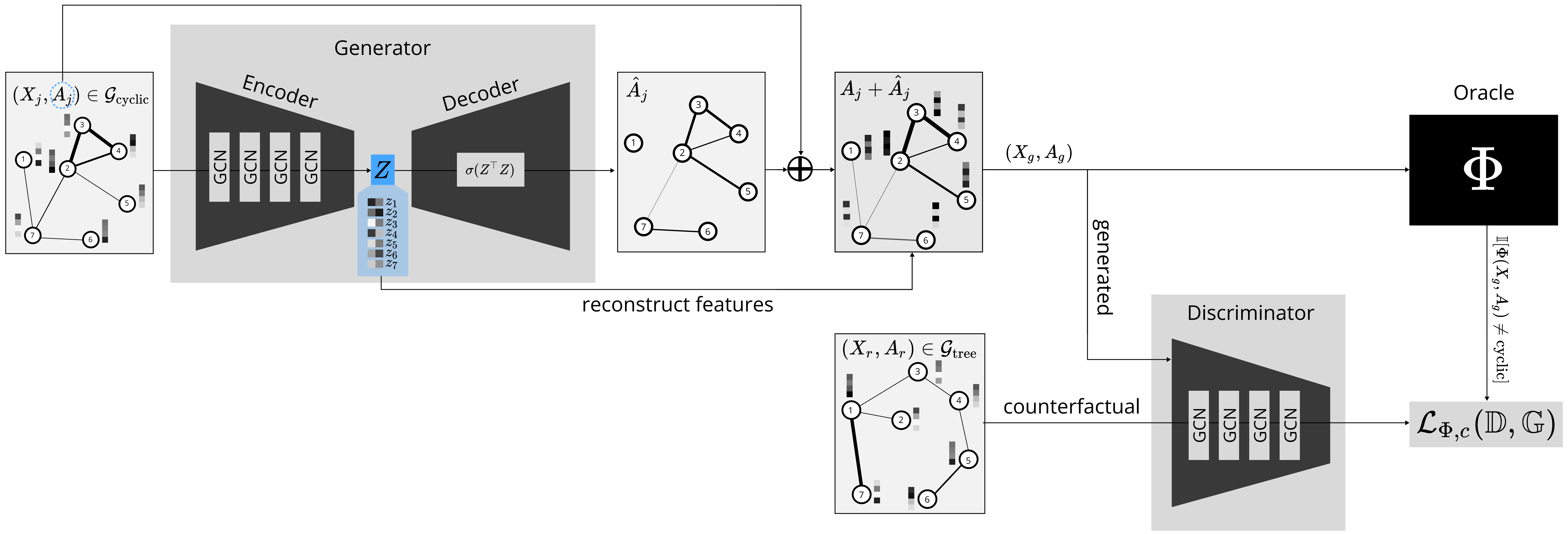
$$\mathcal{L}(\mathbb{D},\mathbb{G}) = \underset{(X_i,A_i)\in\mathcal{G}}{\mathbb{E}} \underbrace{\Big[\log \mathbb{D}(Y \mid X_i, A_i)\Big]}_{\text{discriminator optimisation}} + \underset{\substack{X_j\in P_z, A_j\in P_{z'},\\ \hat{X}_j, A_j+\hat{A}_j=\mathbb{G}(X_j,A_j)}}{\mathbb{E}} \underbrace{\Big[\log(1-\mathbb{D}(Y \mid \hat{X}_j, A_j+\hat{A}_j))\Big]}_{\text{generator optimisation}}$$

$$\mathcal{L}_{\Phi,c}(\mathbb{D},\mathbb{G}) = \sum_{(X_r,A_r)\in\mathcal{G}_{\neg c}} \underbrace{\Big(\log \mathbb{D}(Y \mid X_r, A_r)\Big)}_{\text{discriminator optimisation on real data}}$$

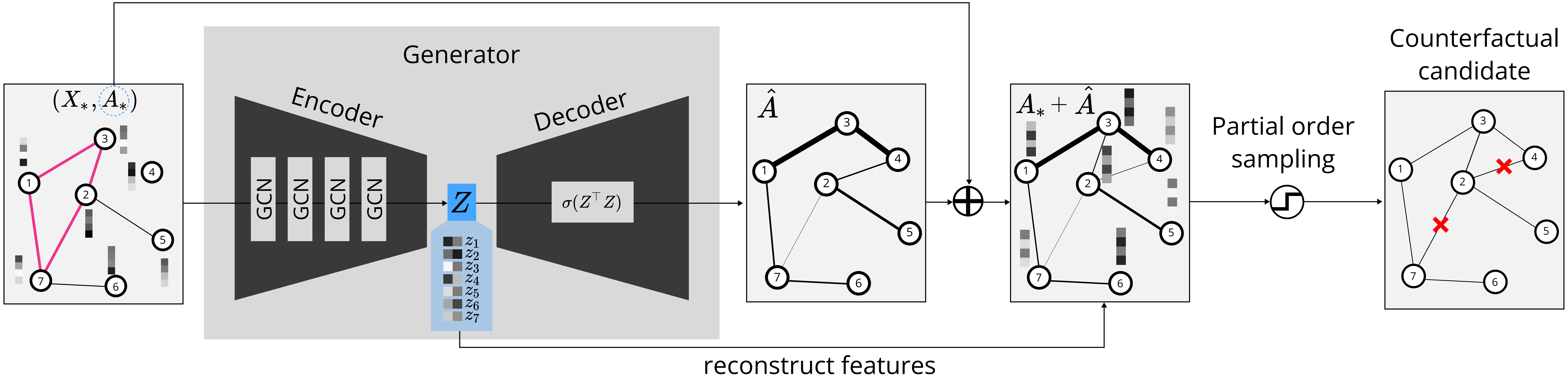
$$+ \sum_{(X_g,A_g)\in\mathbb{G}(\mathcal{G}_c)} \underbrace{\Big(\mathbb{I}[\Phi(X_g,A_g)\neq c] \log \mathbb{D}(Y \mid X_g, A_g)\Big)}_{\text{discriminator optimisation on generated data}}$$

$$+ \sum_{\substack{(X_j,A_j)\in\mathcal{G}_c,\\ \hat{X}_j, A_j+\hat{A}_j=\mathbb{G}(X_j,A_j)}} \underbrace{\log\Big(1-\mathbb{D}(Y \mid \hat{X}, A_j+\hat{A}_j)\Big)}_{\text{generator optimisation}}$$

A closer look at RSGG-CE



RSGG-CE (inference)



RSGG-CE (inference)

Algorithm 1: Partial order sampling to produce a counterfactual.

Require: $G_* = (X_*, A_*), \mathbb{G} : \mathcal{G} \rightarrow \mathcal{G}, \Phi,$

$\hat{X}_*, A_* + \hat{A}_* = \mathbb{G}(X_*, A_*)$
$X_g, A_g \leftarrow \hat{X}_*, A_* + \hat{A}_*$
$\mathcal{P} \leftarrow \texttt{partial\_order}(A_*)$
$A' \leftarrow 0^{n \times n}$
for $\mathbb{O} \in \mathcal{P}$ **do**
    for $e = (u, v) \in \mathbb{O}.\mathcal{E}$ **do**
        $A'[u, v] \leftarrow \texttt{sample}(e, A_g[u, v])$
        if $\mathbb{O}.o \wedge \Phi(X_g, A') \neq \Phi(X_*, A_*)$ **then**
            return (X_g, A')
        end if
    end for
end for
return (X_*, A_*)

Algorithm 2: Example of `partial_order`

Require: $A \in \mathbb{R}^{n \times n}$

$E \leftarrow \texttt{positive\_edges}(A)$ ▷ *Get the set of edges from the adjacency matrix A*
$\neg E \leftarrow \texttt{negative\_edges}(A)$ ▷ *Get the set of non-existing edges from the adjacency matrix A*
$\mathcal{P} \leftarrow \{(\mathcal{E}=E, o=0), (\mathcal{E}=\neg E, o=1)\}$ ▷ *Build the partial order of the existing and non-existing edges with group tuples consisting of edge set $\mathcal{E}$, and oracle verification guard o.*
return $\mathcal{P}$

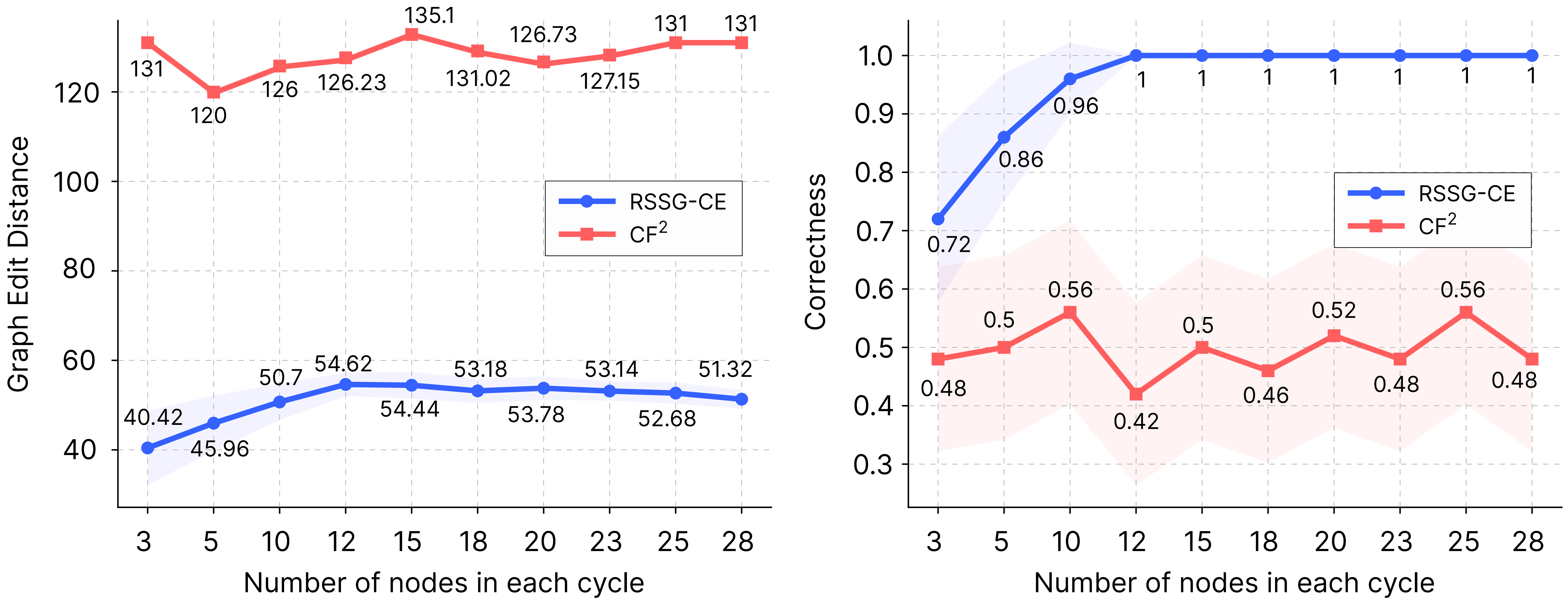
Pretty good actually when you have dual classes.

What we learned through RSGG-CE

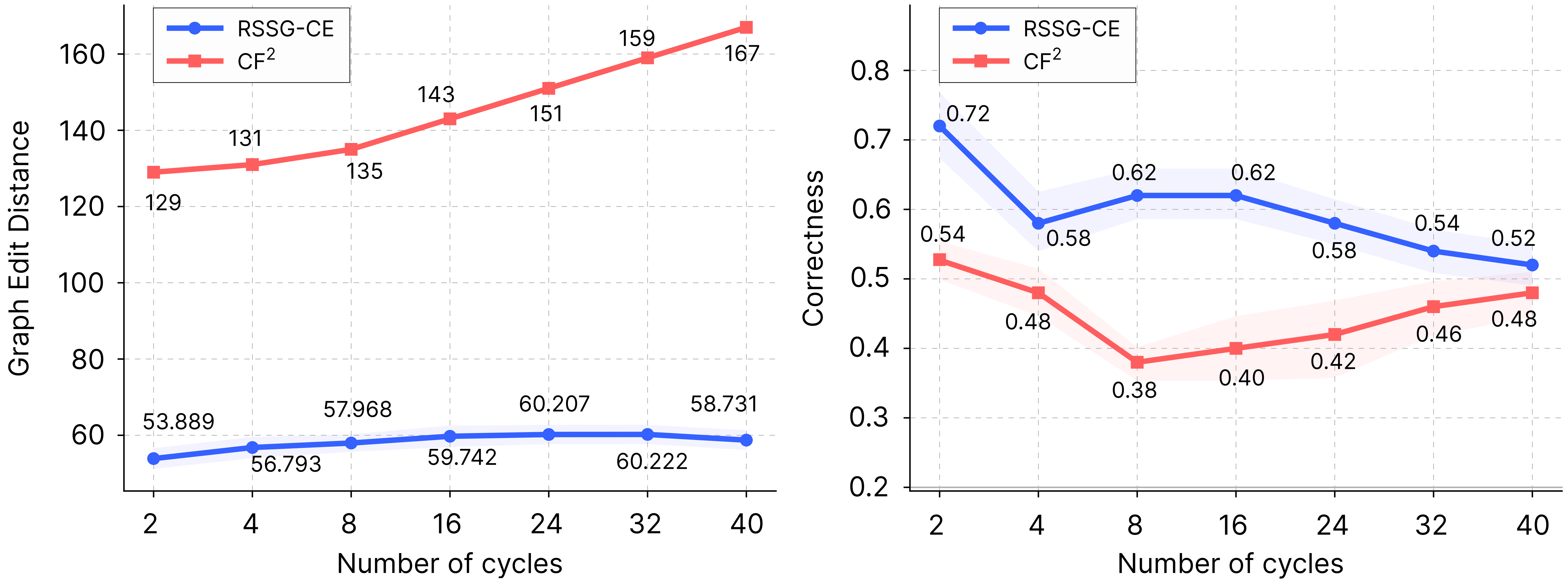
RSGG-CE has a gain of 66.98% and 19.65% in correctness.

		Methods				
		MEG †	CF^2 †	CLEAR ‡	G-CounteRGAN ‡	**RSGG-CE ‡**
TC	Runtime (s) ↓	272.110	4.811	25.151	632.542	**0.083**
	GED ↓	159.700	27.564	61.686	182.414	**11.000**
	Oracle Calls ↓	**0.000**	**0.000**	4341.600	1321.000	121.660
	Correctness ↑	0.530	0.496	0.504	0.504	**0.885**
	Sparsity ↓	2.510	0.496	1.110	3.283	**0.199**
	Fidelity ↑	0.530	0.496	0.504	0.504	**0.885**
	Oracle Acc. ↑	1.000	1.000	1.000	1.000	1.000
ASD	Runtime (s) ↓	×	**15.313**	275.884	969.255	80.000
	GED ↓	×	655.661	1479.114	3183.729	**234.853**
	Oracle Calls ↓	×	**0.000**	5339.455	1182.818	794.805
	Correctness ↑	×	0.463	0.554	0.529	**0.603**
	Sparsity ↓	×	0.850	1.917	4.125	**0.304**
	Fidelity ↑	×	**0.287**	0.319	0.265	**0.287**
	Oracle Acc. ↑	×	0.773	0.773	0.773	0.773

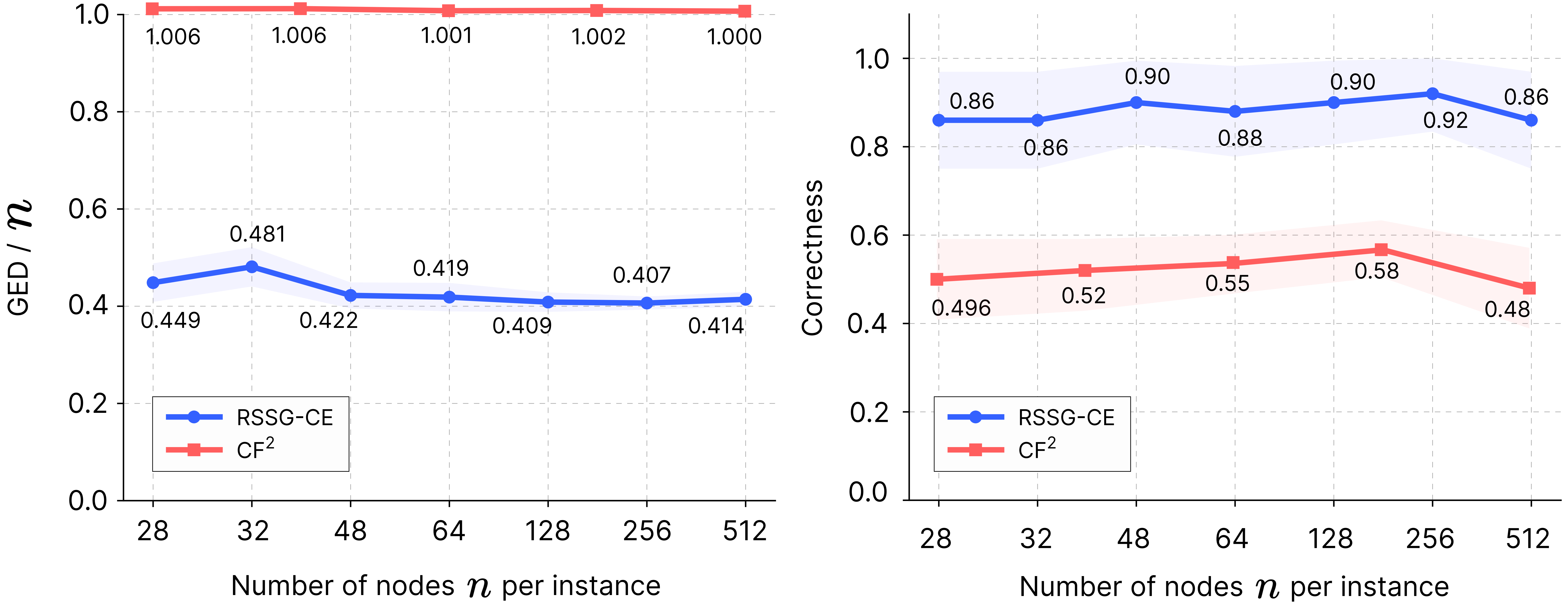
We scale perfectly when the number of nodes in a cycle increases (GED plateaus, and correctness is 1).



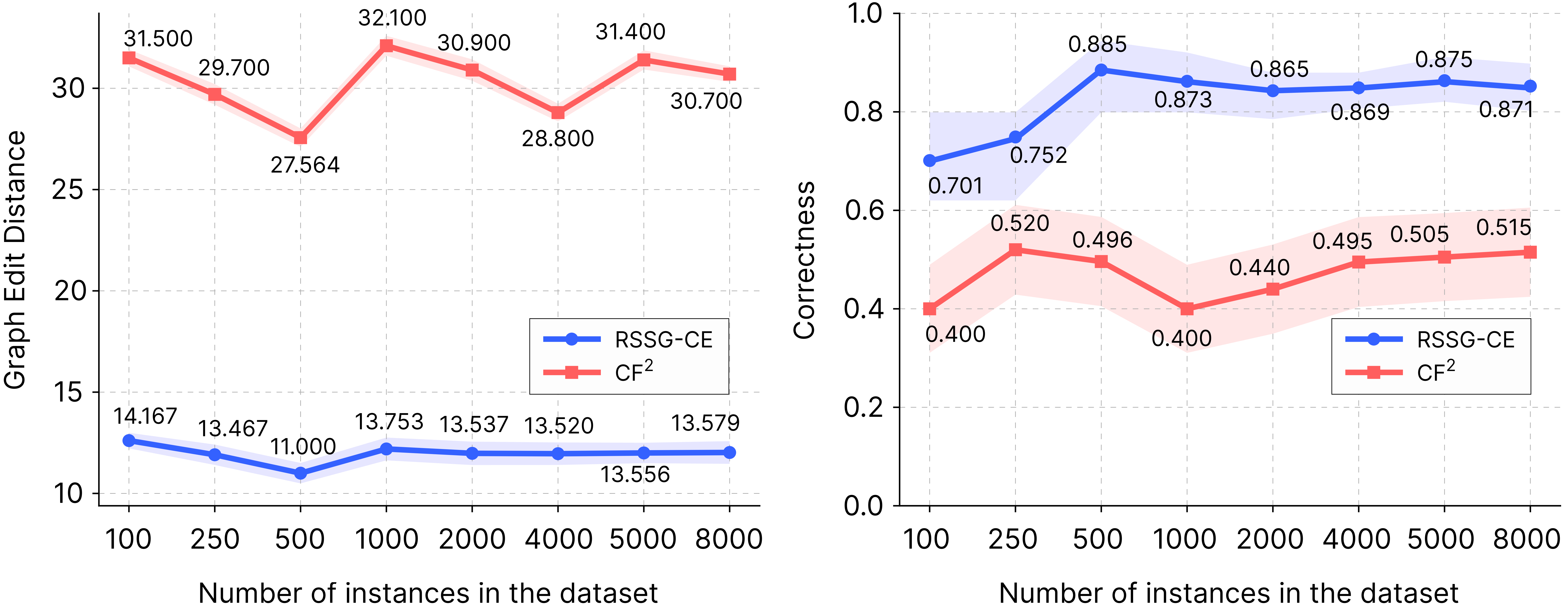
Even when the number of cycles increases, we don't need as many edge-cutting operations.



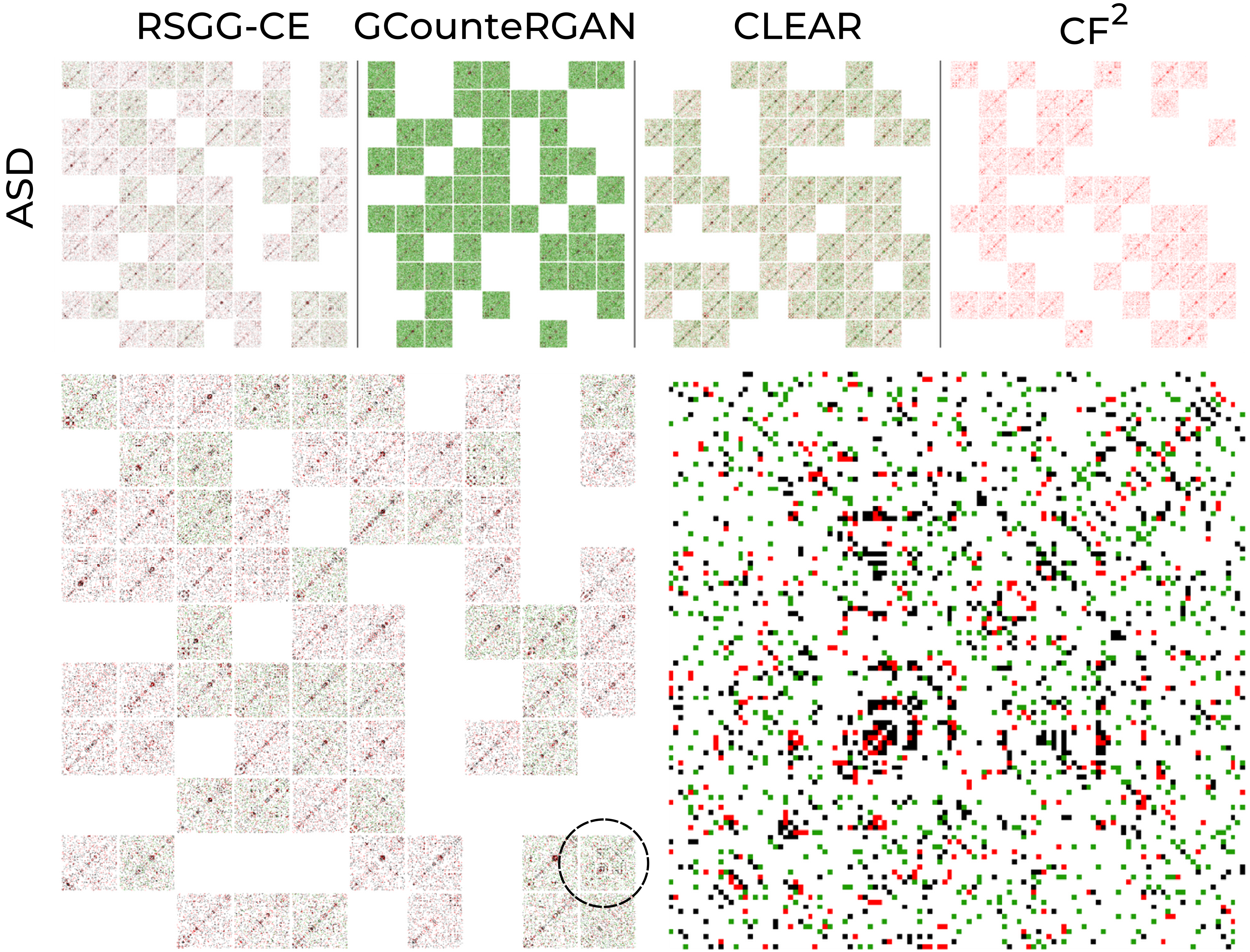
We don't care about larger graphs. Results depend only on dataset complexity.



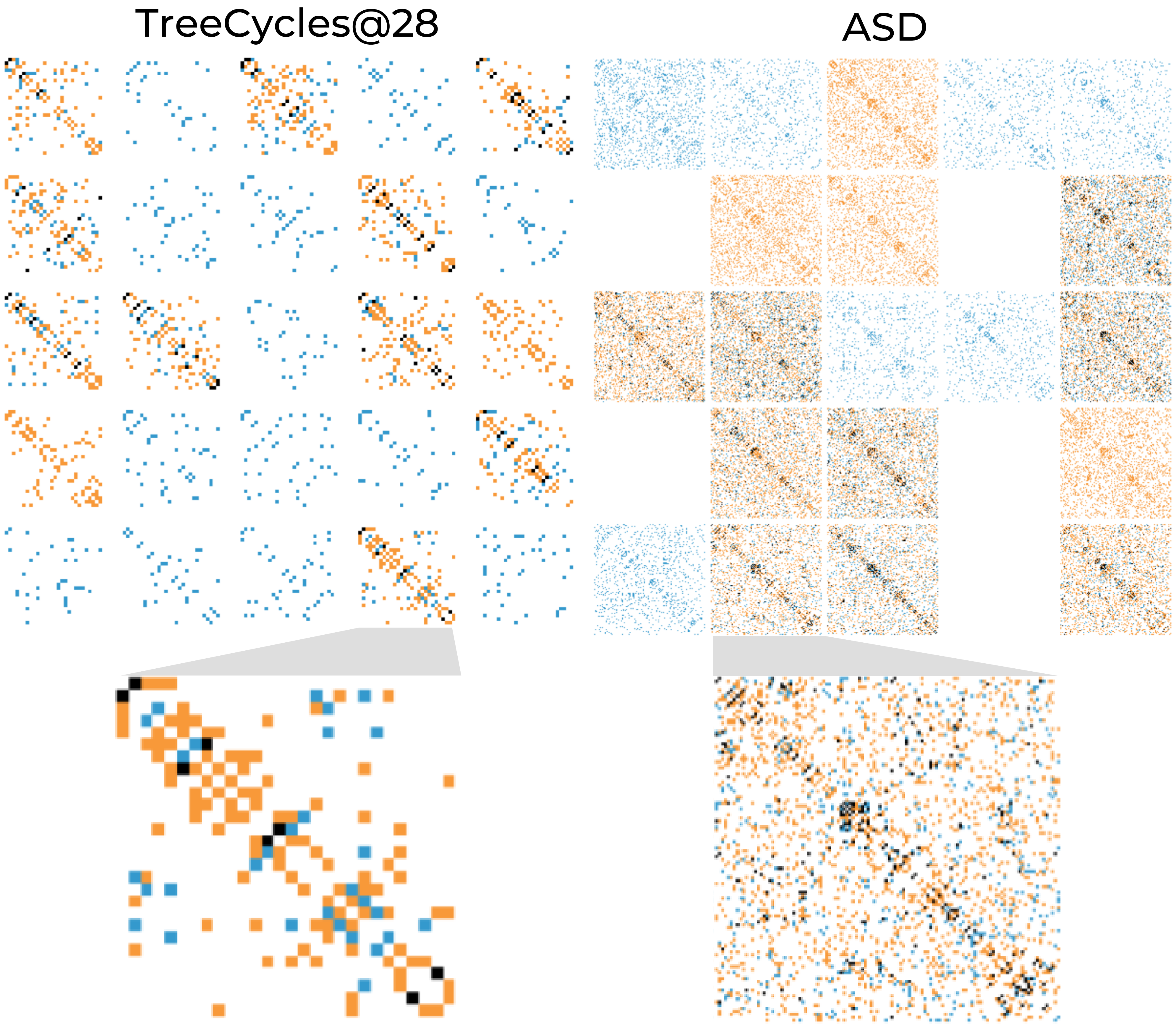
Performance **stabilizes** when the number of instances is greater than 250.



We can do **both** edge additions and removals



We perform **a lot less** perturbation on the graphs **vs CLEAR**



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Food for Thought

Finding counterfactuals is mathematically equivalent to adversarially attacking a predictor, but they have different social connotations

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