Equivariant Denoisers Cannot Copy Graphs: Align Your Graph Diffusion Models

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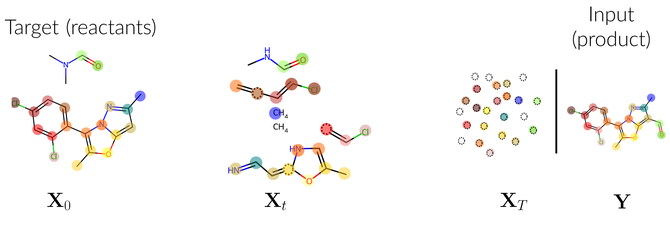
TL;DR

- Standard permutation-equivariant graph diffusion models struggle with graph-to-graph translation due to symmetry.
- We propose aligned denoisers, which break symmetry where needed, preserving equivariance elsewhere.
- Our approach achieves SOTA results in retrosynthesis (e.g., 54.7% top-1 vs. 4.1% for unaligned models).

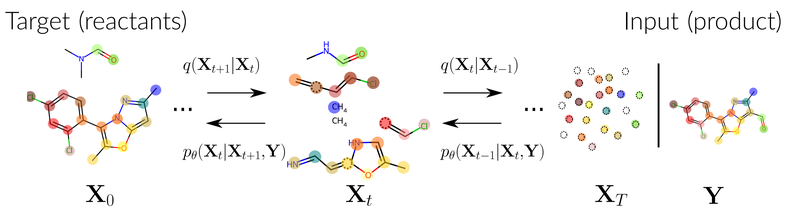
Motivation

Graph-to-graph translation underpins molecule editing, dynamic graph prediction, and **retrosynthesis**, etc. Following the success of graph diffusion in a number of graph-based tasks, we investigate its adaption to graph-to-graph translation.



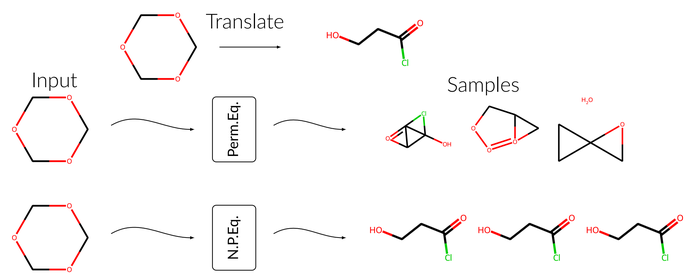
Background

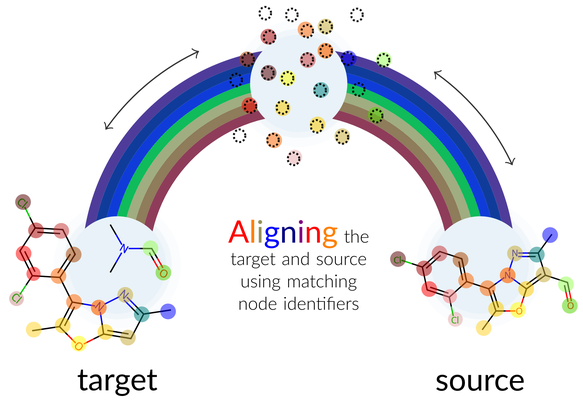
Graph diffusion models consist of a forward process, a reverse process, and a denoiser architecture.



$$= \sum_{\mathbf{X}_0} q(\mathbf{X}_0|\mathbf{X}_T,\mathbf{X}_0)p_\theta(\mathbf{X}_0|\mathbf{X}_T,\mathbf{Y},\mathbf{P}^{\mathbf{Y}\to\mathbf{X}})$$

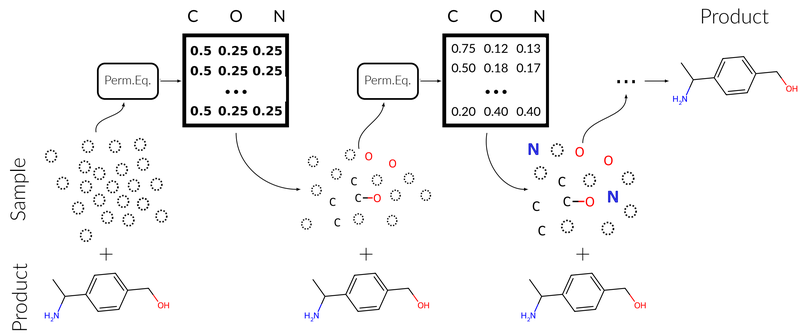
Equivariant functions struggle to map symmetrical inputs to less symmetrical outputs. We observe this in an experiment contrasting a permutation-equivariant (PE) and a non-permutation equivariant (NPE) GNNs.





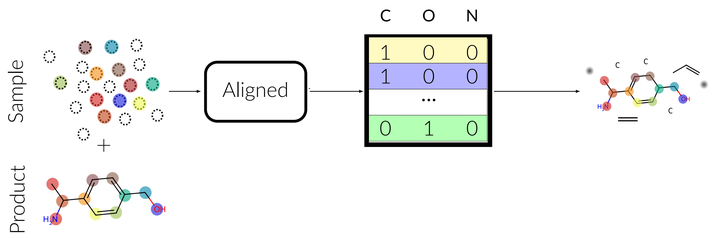
Equivariant denoisers cannot copy graphs

When asked to maintain equivariance while assigning different labels to similar input, equivariant denoisers learn the marginal distribution of node and edge labels of the training dataset. We prove this result formally in Theorem 1 of the paper. This effect is mitigated (inefficiently) through iterative denoising until we obtain a plausible sample.



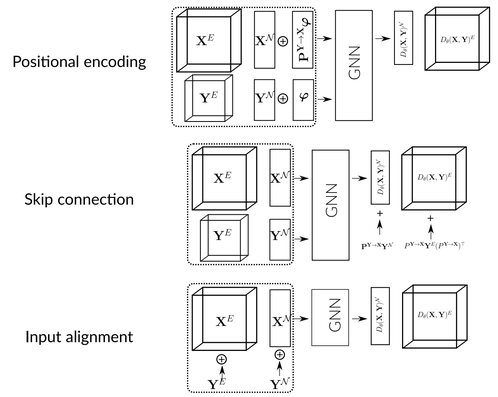
Solution: Aligned Equivariance

We can use indentifiers (e.g. atom-mapping numbers in a chemical reaction) to match source and target graph components. This *aligned equivariance* breaks the self-symmetries in the input while maintaining equivariance in the non-matched parts.



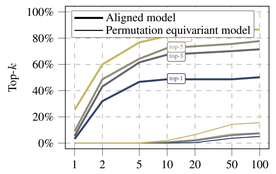
How to ensure alignment?

We explore three methods and their combinations.



Results

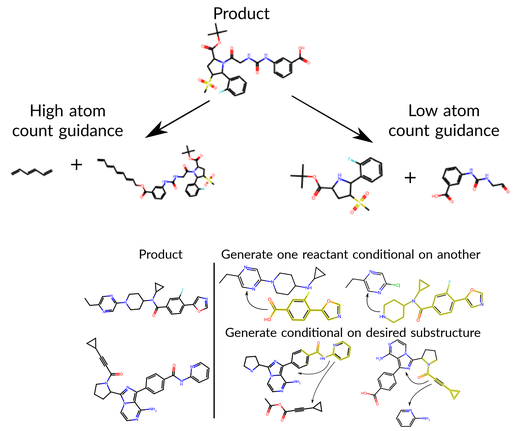
Our PE+skip model matches SOTA in retrosynthesis, and maintains high performance with few sampling steps.



Method	$k=1\uparrow$	$k=3\uparrow$	$k=5\uparrow$	$k=10\uparrow$	MRR $\uparrow$
Unaligned	4.1	6.5	7.8	9.8	0.056
DiffAlign-input	44.1	65.9	72.2	78.7	0.554
DiffAlign-PE	49.0	70.7	76.6	**81.8**	0.601
DiffAlign-PE+skip	**54.7**	**73.3**	**77.8**	81.1	**0.639**

Downstream applications

Diffusion unlocks interesting features in retrosynthesis, including inpainting and inference-guidance.



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