Discrete Object Generation with Reversible Inductive Construction

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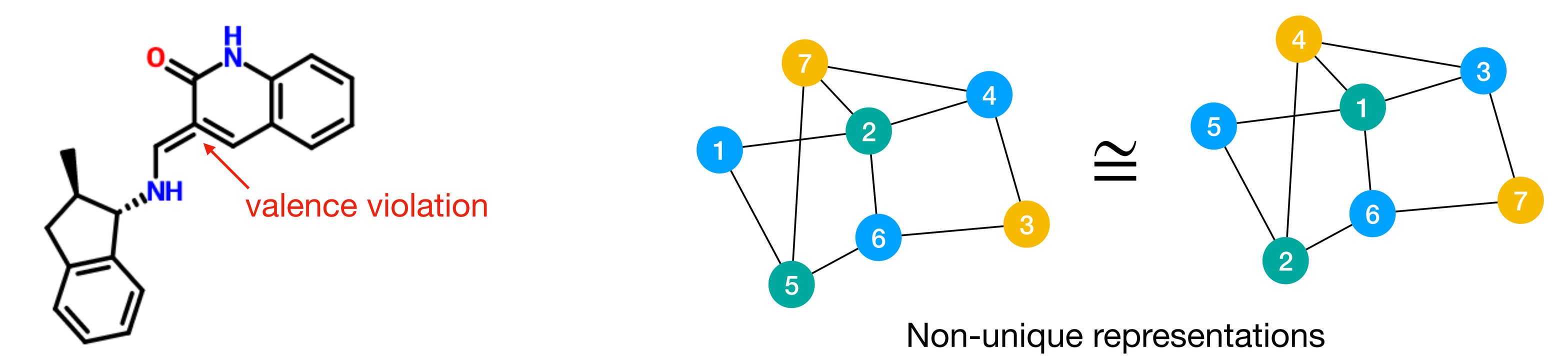
Generative Modeling and Structured Domains

- Generative modeling may serve as a first step in many applied domains: e.g., generating libraries of candidate drug compounds.
- Target domain is often discrete (e.g., a graph), structured (e.g., a molecule is not simply a set of atoms but is defined by the specific connectivity), and subject to strict validity requirements and a large space of possible construction histories.



- Building generative models that perform well on discrete domains under these constraints is challenging.

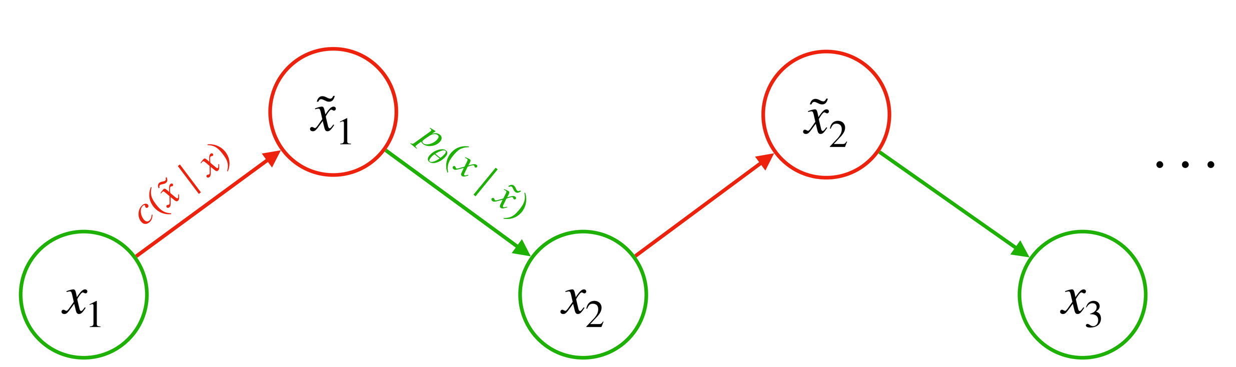
Generation from Denoising

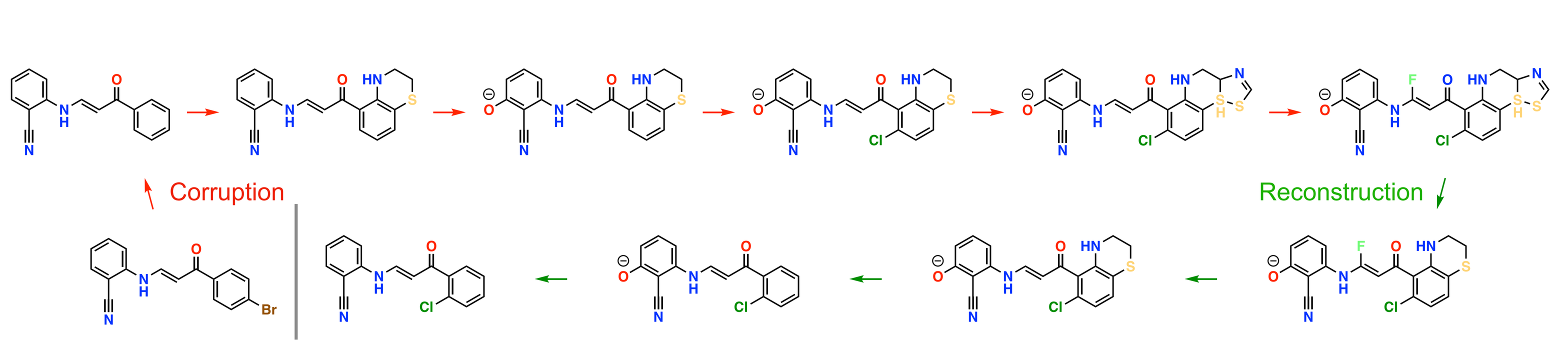
Construct a Markov chain whose equilibrium distribution matches the data distribution. The Markov chain is specified through two components: an arbitrary corrupter and a learned reconstructor.

Corrupter $\mathbf{c}(\tilde{\mathbf{x}} \mid \mathbf{x})$ We specify an arbitrary corrupter on the domain of interest $\mathcal{X}$.

Reconstructor $\mathbf{p}_\theta(\mathbf{x} \mid \tilde{\mathbf{x}})$ We specify a learned reconstructor, which attempts to reverse the corrupter's moves.

These two components are asymptotically sufficient to construct a Markov chain with the correct equilibrium distribution (see Bengio et al. (2013)).





Reversible Inductive Construction

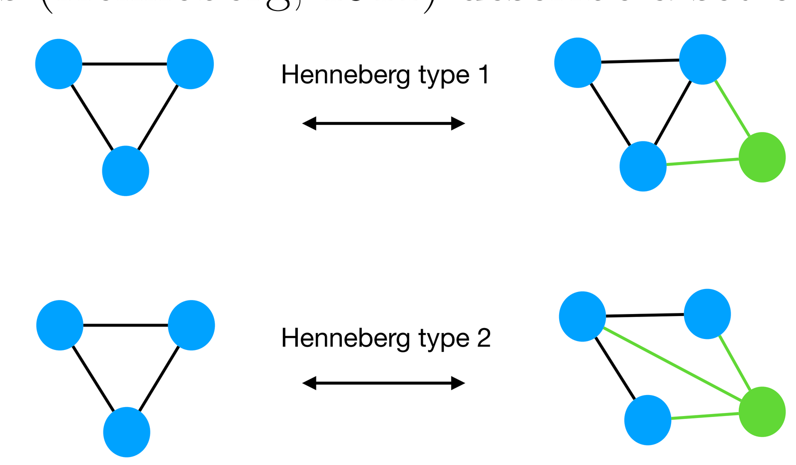
This framework gives us a powerful tool to work with strong constraints: we define a set of *inductive* moves that enforce the validity rules.

Tree decomposition of molecules

Jin et al. (2018) propose a tree-decomposition of molecular graphs and a reduced number of "vocabulary" elements, which we leverage here to define legal insertions and deletions.

Henneberg construction of Laman graphs

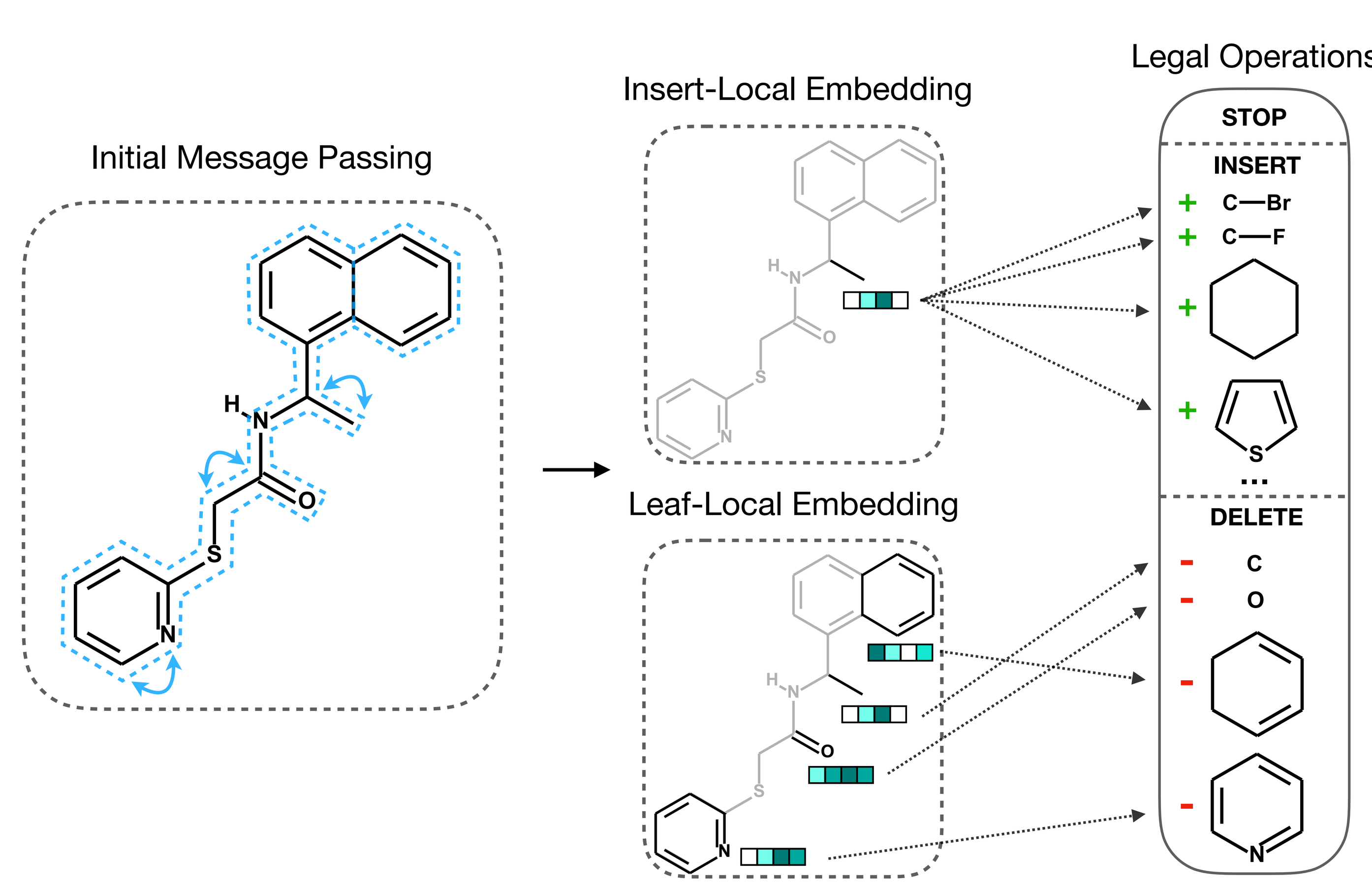
Laman graphs describe minimally rigid structures in the plane and are useful in modeling and solving geometric constraint systems. The Henneberg moves (Henneberg, 1911) describe a set of inductive moves.



The corrupter and reconstructor are restricted to operate using the inductive moves, which automatically enforces validity.

In addition, by restricting the corruption sequences to be short (sequence length is sampled from a geometric distribution), we only require the reconstructor to discover *local* modifications to the objects, avoiding direct reasoning over full construction histories.

Reconstruction Model



Our reconstruction model couples location-specific embeddings computed via message passing with a vocabulary of legal move types in order to sample actions.

Reconstruction Model Cont'd.

Message-Passing Network

A message-passing network (Gilmer et al., 2017; Duvenaud et al., 2015) aggregates location-specific information across the topology of the graph in a learned fashion.

Vocabulary of Legal Operations

The action space is a large discrete set. To enable representation sharing and efficient computation, we factorize actions into two components:

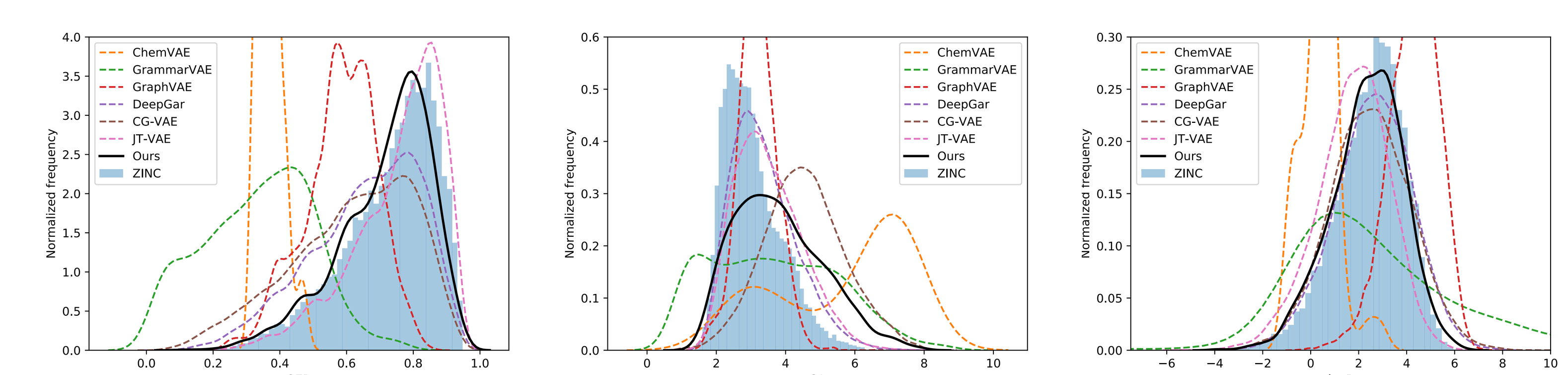
- the type of action (e.g. delete a leaf, insert an atom, etc.),
- the location of the action (an atom, a bond, a ring, etc.).

Reconstruction is a *supervised* problem: we may train the reconstructor in a standard fashion by generating samples $(x, s, \tilde{x})$ where s is a sequence of corrupting operations.

$$\theta^* = \underset{\theta}{\operatorname{argmin}}\, \mathbb{E}_{p(x,s,\tilde{x})} \left[D_{\mathrm{KL}}(p(s, x \mid \tilde{x}) \,\|\, p_\theta(s, x \mid \tilde{x})) \right]$$

Experimental Results

For molecular generation, we compare the distributional characteristics for logP (log octanol-water partition coefficient), SA (synthetic accessibility) and QED (quantitative estimate of drug-likeness).



For Laman graphs, we compare the distribution over degree of decomposability (DoD) (Moussaoui, 2016).

Method	DoD KS	% valid
Erdős–Rényi (Erdös and Rényi, 1959)	0.95 (0.03)	0.08 (0.02)
GraphRNN (You et al., 2018)	0.96 (0.00)	0.15 (0.03)
Ours	0.33 (0.01)	100 (0.00)

Code and Paper

github.com/PrincetonLIPS/reversible-inductive-construction
arxiv.org/abs/1907.08268