Machine-interpretability

SELFIES Workshop - 13/08/2021

Questions

- Can models trained with SELFIES learn faster compared to SMILES? Can they achieve better accuracy in less time compared to SMILES?
- Can the machine pick chemically relevant structures?
- SELFIES are never wrong. How can we be sure that when the model says something, it was what the model was meant to say?
- How does it perform on different tasks compared to other representations?

Comparing representations

- Decrease model complexity - lowering the number of layers and neurons and increase regularization, making the model is more simple, and forcing models to become better at generalization.
- Train model on different string formats and decreasing the number of neurons, see which models perform best
- Being able to monitor how well the model is doing by some other metrics than valid structures, since selfies are always valid. Example: check if the generated molecules have weird functional groups or the similarity with the training set (ex: In drug discovery, you don't want the molecule to stray away from the training set, since they won't be drug-like).

Proposed experiments

- Substructure highlighting to see why the model is outputting that structure.
- Design a task that shows chemical intuition. Example: attention/attruibution mechanisms - human labeling for adding chemical intuition.
- Look at the intermediate layers of convolutional neural network.
- Benchmark for different tasks (to compare SMILES and SELFIES): time/number of epochs needed to extract the features, accuracy.
- Are there differences for different tasks? property prediction, generative models
- Compare selfies with 3D representations on tasks that involve 3D interactions.

Wishlist of properties for a machine interpretable representation

- Representation should be as unique as possible
- You shouldn't have to train 1000 epochs to get the machine to understand them
- Should work for big molecules
- Similar molecules should have similar representations (or devise a distance metric to show that similar molecules are close, even though they have different representations).