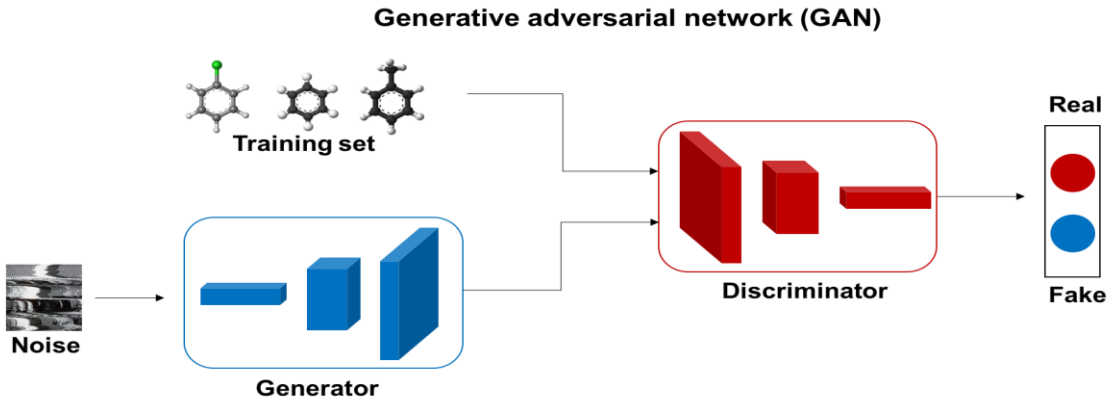
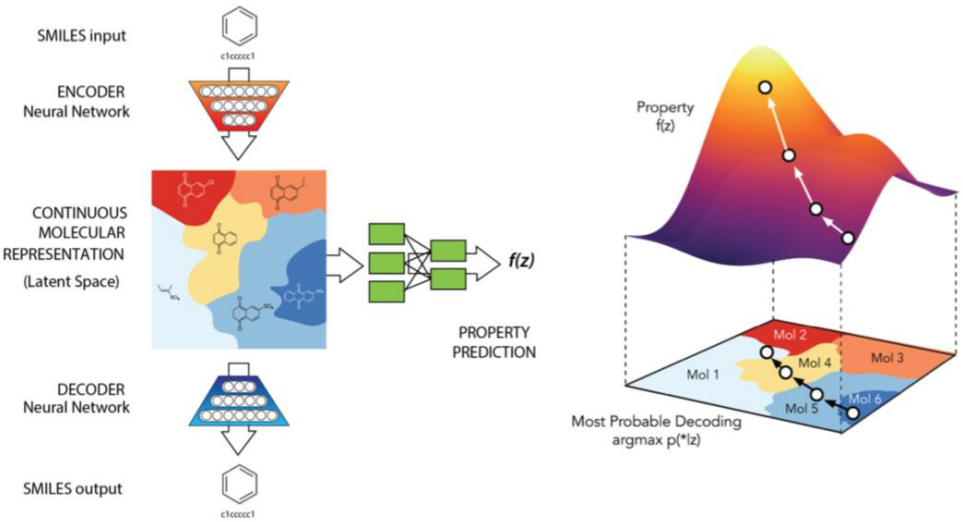
Machine Learning for de novo Molecular Design

The introduction of a new drug or a new material to the commercial market follows a complex and long process that typically spans over several years and entails large monetary costs due to a high attrition rate. Because of this, there is an urgent need to improve this process using innovative technologies such as machine learning.

Within the discovery process, a key first step is to generate an initial pool of candidate molecules which potentially optimize a property of interest (such as binding affinity to a biological target). However, the chemical space is huge, and exploring it in an efficient manner is extremely challenging. Generative models aim at solving this challenge by automatically proposing molecules with desired properties. In this talk, I provided a critical review of the main generative models used for molecular design, and highlighted relevant future work directions.





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