Deep Generative Models for Molecular Science - DTU Orbit (26/08/2019)

**Deep Generative Models for Molecular Science**

Generative deep machine learning models now rival traditional quantum-mechanical computations in predicting properties of new structures, and they come with a significantly lower computational cost, opening new avenues in computational molecular science. In the last few years, a variety of deep generative models have been proposed for modeling molecules, which differ in both their model structure and choice of input features. We review these recent advances within deep generative models for predicting molecular properties, with particular focus on models based on the probabilistic autoencoder (or variational autoencoder, VAE) approach in which the molecular structure is embedded in a latent vector space from which its properties can be predicted and its structure can be restored.

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