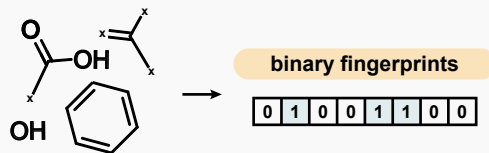


a Molecular descriptors

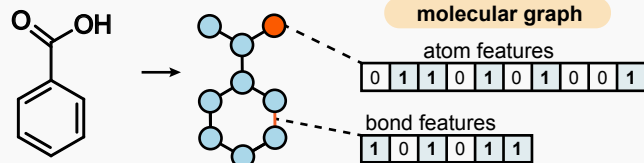


- molecular weight
- logP
- n rings
- n atoms
- etc.

classical descriptors

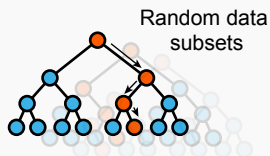
0.2	0.6	0.3	0.2	0.9	0.1
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b Molecular representations

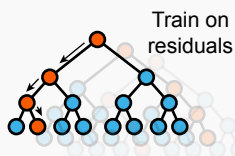


d Classical machine learning

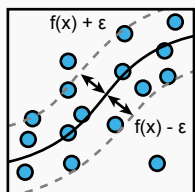
RF



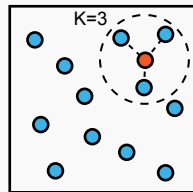
GBM



SVM

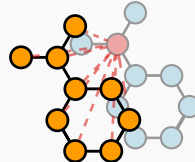


KNN

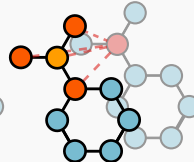


e Deep learning

MPNN



GCN



GAT



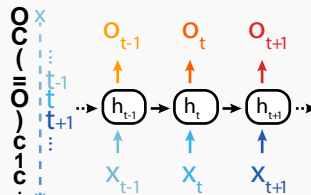
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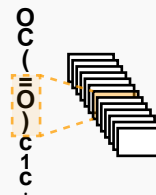
node impact

f

LSTM



CNN



Transformer

