Exchange-Correlation Functionals from Machine Learning

Direct Learning: ML models to predict xc energy or potential from $\rho(\mathbf{r})$
Delta Learning: ML models to correct/augment existing functionals
Direct prediction of properties

Neural Networks
Gaussian Process Regression
Kernel Ridge Regression

Requirements:

- Need for a lot of high-level data: CC calculations, QMC, exact models
- Representation of $\rho(\mathbf{r})$

Examples:

- DM21, SchNet for xc, NICE functionals, GradDFT etc..

Challenges:

- Accuracy, amount and diversity of training data
- Transferability across chemical space
- Physical constraints
- Computational efficiency

Literature:

Kalita et al. *Acc. Chem. Res*. 54, 818 (2021); Kirkpatrick et al. *Science* 374, 1385 (2021); Wang et al. *JACS AU* 8, 3205 (2024)