Finding density functionals with machine learning

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There has been a recent surge of interest in applying machine learning methods (developed in computer science and statistics) to chemical and materials problems. Such applications are mostly aimed at extracting a few descriptors from a species to predict some property of interest, e.g binding energy from information about equilibrium geometry of a molecule.

In collaboration with the group of Klaus Muller (computer science, TU Berlin), we have been exploring if this methodology can be applied to age-old questions of approximating density functionals. For simple model cases, including breaking a bond in a model, we have found that arbitrarily accurate energies can be obtained with sufficient training data. We have also developed a method for extracting accurate densities from such machine-learned functionals, despite their poor functional derivatives. I will summarize our present work and challenges for this field.

For references, see http://dft.uci.edu/ML.php.