Machine learning density functionals

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Historically, density functional approximations have been created by humans, both for the elusive exchange-correlation energy and for the Kohn-Sham kinetic energy (in orbital-free) DFT. I will describe our ongoing work (with Klaus-Robert Mueller's group, and others) to hand this problem over to machines. Most importantly, unlike almost all human-made functionals, the machines have no biases toward local-type approximations. This allows them to break bonds and incorporate strong correlation effects without any particular difficulty.
I will discuss two new works in which (a) we do calculations on real (3D) molecules, bypassing the Kohn-Sham scheme, and (b) show that machines can find the exact functional for strongly correlated solids (but our demo is in 1D).

All papers/preprints are available at http://dft.uci.edu.

If time permits, I will discuss if this work is a breakthrough or an abomination.