Learning Density Functionals from Noisy Quantum Data

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Density Functional Theory

$$H = \overbrace{T}^{\text{kinetic}} + \overbrace{V}^{\text{potential}} + \overbrace{U}^{\text{interaction}}$$

Wavefunction Theory ⟶ Density Functional Theory

$|\psi_{\text{GS}}\rangle \in \mathbb{C}^{2^n}$ $\quad \mathcal{F}[\rho_{\text{GS}}] := \langle \psi_{\text{GS}} | T + U | \psi_{\text{GS}} \rangle \quad$ $\rho_{\text{GS}} \in \mathbb{R}^n$

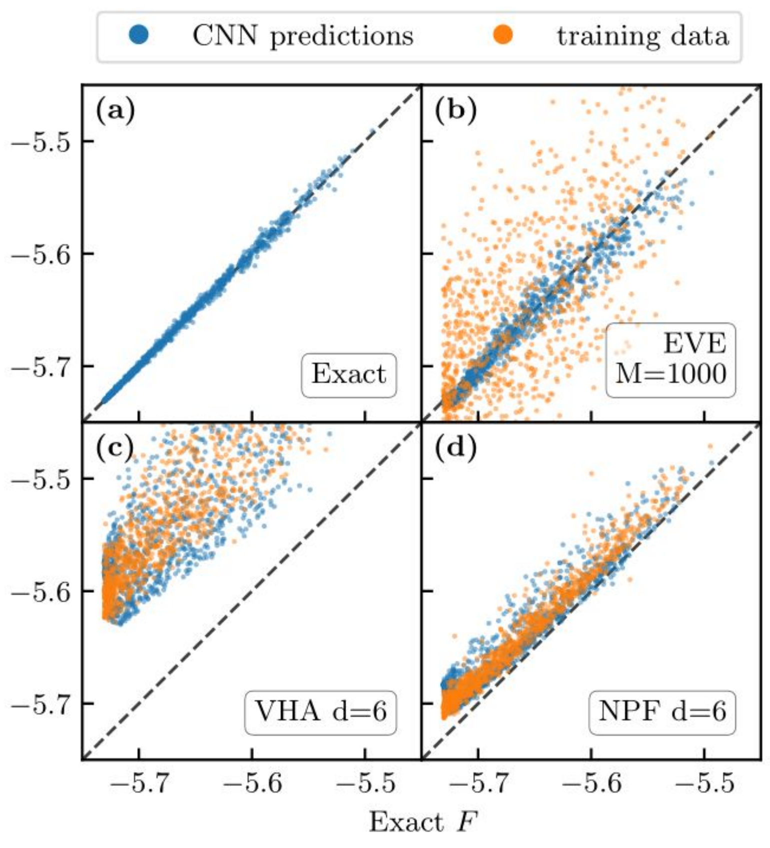
$$E_{\text{GS}} = \langle \psi_{\text{GS}} | H | \psi_{\text{GS}} \rangle = \min_{|\psi\rangle} \langle \psi | H | \psi \rangle$$

$$E_{\text{GS}} = \mathcal{F}[\rho_{\text{GS}}] + \rho_{\text{GS}} \cdot V = \min_{\rho} \mathcal{F}[\rho] + \rho \cdot V$$

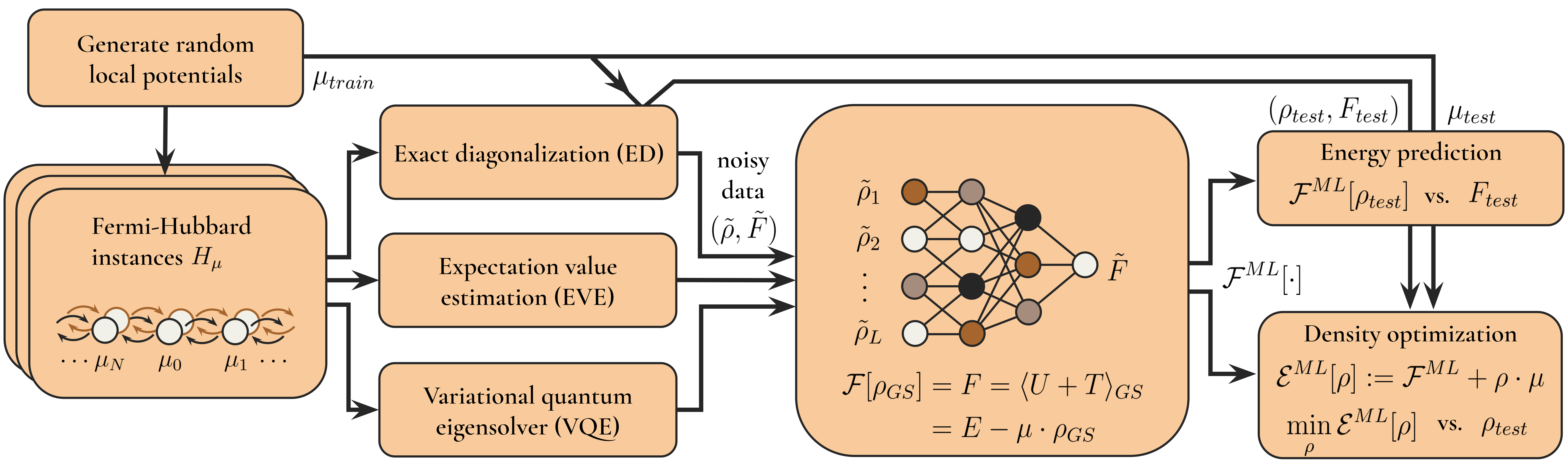
Machine Learned Functionals

Approximate functional with neural network regression
$\mathcal{F}^{ML} : \rho_{GS}(\mu) \to F_{GS}(\mu)$

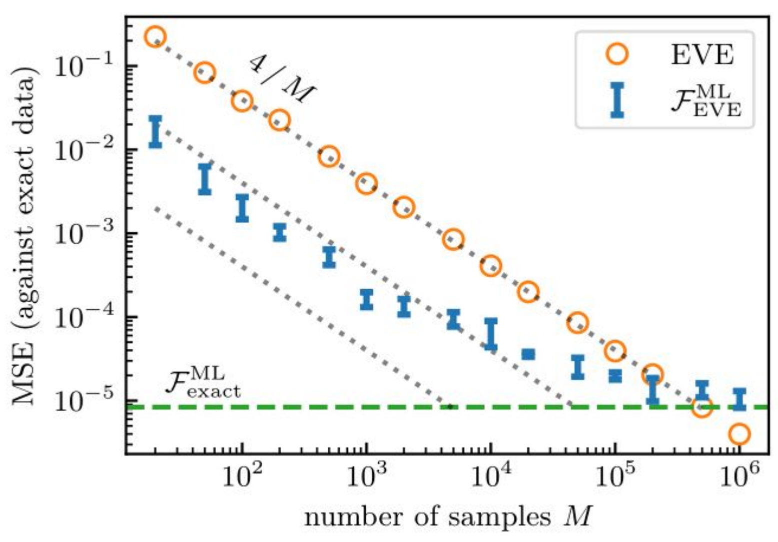
Could NISQ devices be useful training data generators despite their inherent noise?

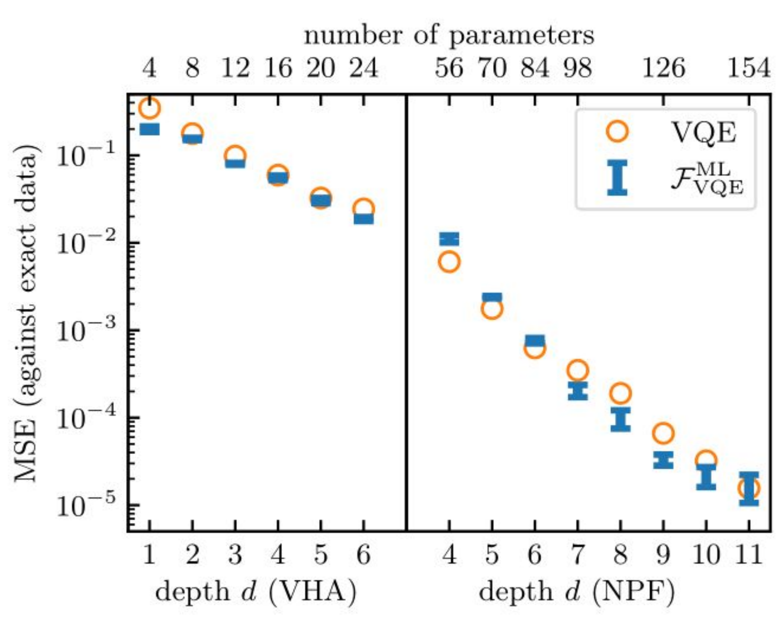


Generate instances — Solve — Learn — Benchmark



Energy Prediction



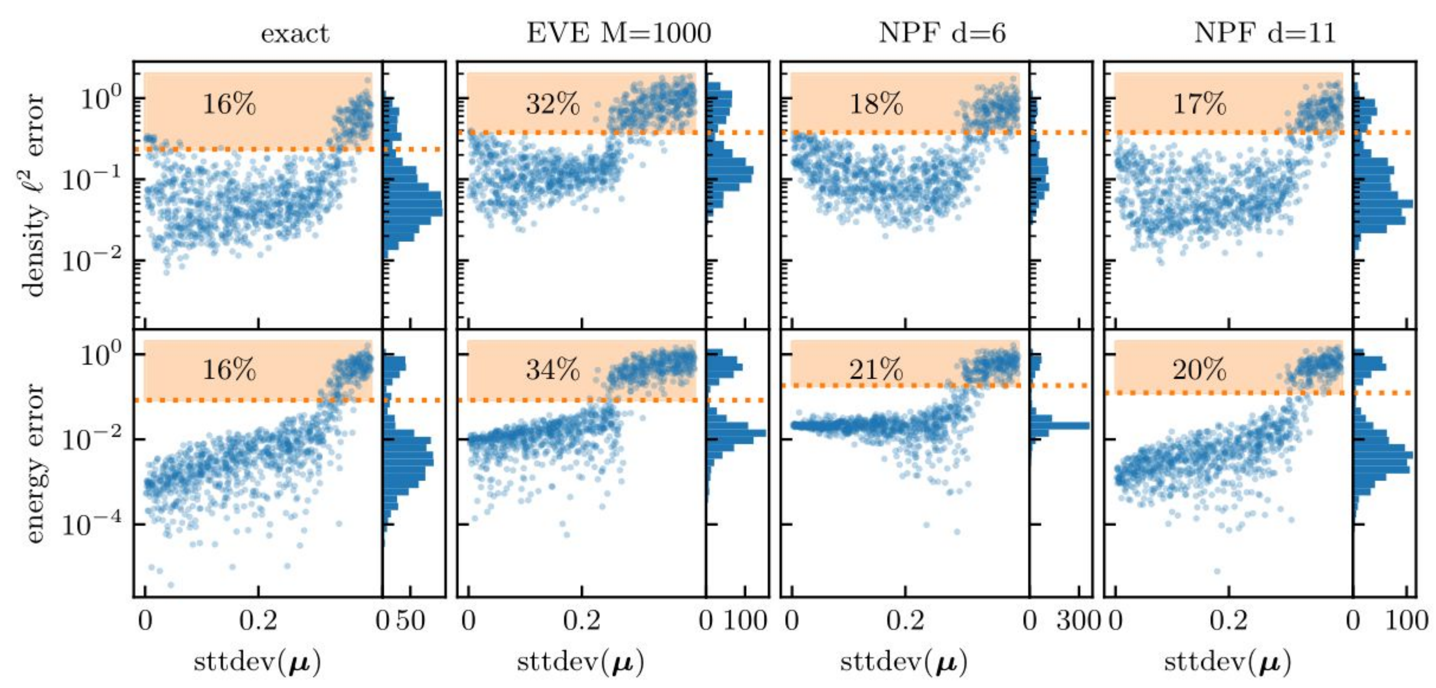


Learn approximate functional from 1k density-energy pairs: small for machine learning, large for quantum computing

Expectation Value Estimation:
Unbiased Sampling noise is mitigated well

Variational Quantum Eigensolver:
Model learns biased expressibility and optimization noise, limiting generalization to slight improvements

Density Optimization



Kohn-Sham-like optimization scheme of new instances:
Use model's automatic differentiability to minimize total energy functional with respect to density, achieving reasonably accurate solutions across instances

Outlook:
Experiment - Additional DFT targets - Mixed Datasets

J. Kirkpatrick *et al.* Science 374 (2021)
J. Nelson *et al.* Phys. Rev. B 99 (2019)

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