Learning to Optimimize: Solving the time dependent Schrödinger equation faster

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The scientific problem

- The time-dependent Schrödinger equation in atomic units:

$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \tag{1}$$

- Rothe's method reformulates time evolution as an optimization problem, the wave function at the next time step is obtained by solving:

$$\Psi(t_{i+1}) = \arg\min_{\chi} \| \left(I + i\frac{\Delta t}{2}H\right)\chi - \left(I + i\frac{\Delta t}{2}H\right)^{\dagger}\Psi(t_i)\|^2, \tag{2}$$

- Goal: Find parameters $\boldsymbol{c}, \boldsymbol{\alpha}$ that represent wave function optimally:

$$\Psi(t) = \sum_{m=1}^{N} c_m(t) g_m(\alpha_m(t)), \tag{3}$$

where $g_m(\alpha_m)$ are Gaussian basis functions with nonlinear parameters α_m and coefficients c_m.

Learning to Optimize

- Problem: The optimization on the previous slide is hard – hundreds of iterations - per time step. However, each optimization is "similar" to the one at the previous time step.
- "Learning to Optimize" (L2O) uses machine learning to improve optimization processes by learning an optimizer.[1,2,3,4]
- Recurrent Neural Networks (RNNs) with LTSM are commonly used for learning iterative updates:
  - RNNs can model sequential dependencies, making them well-suited for optimization processes that involve iterative updates.
- Other architectures: Autoencoders for dimensionality reduction, GNNs as an alternative for serial data?
- Goal: Develop an ML model that converges with fewer iterations than BFGS.

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[1] Li & Malik, arXiv (2016), 1606.01885
[2] Andrychowicz et al., NeurIPS (2016), 29
[3] Chen et al., arXiv (2021), 2103.12828
[4] Tang & Yao, Natl. Sci. Rev. (2024), 11(8), nwae132

Project Layout

- Step 0: Do a thorough literary review and pick a reasonable architecture, loss functions etc. - check for existing packages.
- Step 1: Train RNNs (and possibly autoencoders/GNNs) on hard synthetic optimization problems (with known solutions, i.e. Rastrigin function) and benchmark against BFGS: Reproduce the literature
- Step 2: Re-train models to Rothe's method for Hydrogen atom in strong fields and vibrational dynamics.[5,6]
- Goal: Achieve faster and more robust optimization in quantum dynamics. See if we can reproduce Rothe-papers quicker or even improve upon them?

[5] Schrader et al., J. Chem. Phys. (2024), 161, 044105
[6] Schrader et al., J. Chem. Phys. (2025), 162, 024109