TDVP

Alessandro Sinibaldi

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0.1 Introduction

0.2 Time dependent variational principle

In the time dependent variational principle (TDVP) method we consider a linearization in δt of the exact evolution:

$$|\phi(t+\delta t)\rangle = |\phi(t)\rangle - i\delta t\hat{H}\,|\phi(t)\rangle + O(\delta t^2). \tag{1}$$

Similarly, we perform an expansion for the evolved variational state in the first order for δt:

$$|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle = |\psi[\boldsymbol{\theta}(t)]\rangle + \delta t\sum_k \dot{\theta}_k(t)\hat{O}_k(t)\,|\psi[\boldsymbol{\theta}(t)]\rangle + O(\delta t^2), \tag{2}$$

where the operators $\hat{O}_k(t)$ are diagonal and they have the following matrix elements on a system's configuration $\mathbf{x}$:

$$O_k(\mathbf{x},t) = \frac{\partial_{\theta_k}\psi(\mathbf{x};\boldsymbol{\theta}(t))}{\psi(\mathbf{x};\boldsymbol{\theta}(t))}. \tag{3}$$

where $\psi(\mathbf{x};\boldsymbol{\theta}(t)) = \langle\mathbf{x}|\psi[\boldsymbol{\theta}(t)]\rangle$. Therefore, the operators $\hat{O}_k(t)$ perform the derivatives of the variational state with respect to the parameters, namely $\hat{O}_k(t)\,|\psi[\boldsymbol{\theta}(t)]\rangle = \partial_{\theta_k}|\psi[\boldsymbol{\theta}(t)]\rangle$.

The TDVP employs the fidelity as distance among states and maximize it with respect to the $\boldsymbol{\theta}(t)$, according to the McLachlan's variational principle. Actually, the McLachlan's variational principle is valid only if $\boldsymbol{\theta}(t)$ are real, thus when the $\boldsymbol{\theta}(t)$ are complex they can be splitted in real and imaginary parts. In the special case of complex $\boldsymbol{\theta}(t)$ and holomorphic *ansätz* the Dirac-Frenkel variational principle can be used simplifying the problem.

Therefore,the fidelity among $|\phi(t+\delta t)\rangle$ and $|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle$ is given by:

$$\mathcal{F}(\dot{\boldsymbol{\theta}}(t)) = \frac{|\,\langle\phi(t+\delta t)|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle\,|^2}{\langle\phi(t+\delta t)|\phi(t+\delta t)\rangle\,\langle\psi[\boldsymbol{\theta}(t+\delta t)]|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle}. \tag{4}$$

The denominator is present because $|\phi(t+\delta t)]\rangle$ and $|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle$ are not normalized in general. Moreover, we observe that the fidelity depends on the time derivatives of the parameters $\dot{\boldsymbol{\theta}}(t)$, which becomes the variational parameters to optimize. On the contrary, $\boldsymbol{\theta}(t)$ only fix the starting state and are not changed during the optimization. Imposing the maximum condition:

$$\frac{\partial\mathcal{F}(\dot{\boldsymbol{\theta}}(t))}{\partial\dot{\theta}_k} = 0 \tag{5}$$

while keeping the first non trivial order in δt, which is $O(\delta t^2)$, yields to a linear system with unknowns: $\dot{\boldsymbol{\theta}}(t)$:

$$\sum_{k'} S^R_{kk'}\dot{\theta}_{k'}(t) = C^I_k, \tag{6}$$

where $S^R_{kk'}$ and C^I_k are respectively the real and imaginary parts of the quantities:

$$\begin{aligned} S_{kk'} &= \frac{\langle\partial_{\theta_k}\psi\mid\partial_{\theta_{k'}}\psi\rangle}{\langle\psi\mid\psi\rangle} - \frac{\langle\partial_{\theta_k}\psi\mid\psi\rangle\,\langle\psi\mid\partial_{\theta_{k'}}\psi\rangle}{\langle\psi\mid\psi\rangle^2}, \\ C_k &= \frac{\langle\partial_{\theta_k}\psi|\,\hat{H}\,|\psi\rangle}{\langle\psi\mid\psi\rangle} - \frac{\langle\partial_{\theta_k}\psi\mid\psi\rangle}{\langle\psi\mid\psi\rangle}\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi\mid\psi\rangle}, \end{aligned} \tag{7}$$

with $|\psi\rangle \equiv |\psi[\boldsymbol{\theta}(t)]\rangle$. The detailed calculation to obtain (6) from (5) is reported in the repository [?]. From the solution $\dot{\boldsymbol{\theta}}(t)$ of (6) we can update the parameters $\boldsymbol{\theta}(t) \longrightarrow \boldsymbol{\theta}(t+\delta t)$ using an integration scheme. The matrix $S_{kk'}$ and the vector C_k are stochastically computed using variational Monte Carlo (VMC), thus the overall algorithm based on the TDVP is called time-dependent variational Monte Carlo.