Linear Method as Used in VQE's

Ronja Johanna Zijderveld

September 2021

1 Linearizing

This derivation is based on the Linear Method described by Frank Thorben in 2021. The relevant paper can be found https://arxiv.org/abs/2104.11011 here. This derivation was written up as a part of an internship that sought to use the linear method as an optimization algorithm in variational quantum eigensolver. The first step is to linearize the wavefunction:

$$|\psi_{lin}\rangle = |\psi_0\rangle + \sum_{i=1}^{N} \Delta\theta_i \, |\psi_i\rangle \,, \tag{1}$$

where

$$|\psi_i\rangle = \frac{\partial|\psi_i\rangle}{\partial\theta_i} \tag{2}$$

Then the linearlized energy is

$$E = \frac{\langle\psi_{lin}| \hat{H} |\psi_{lin}\rangle}{\langle\psi_{lin}|\psi_{lin}|\psi_{lin}|\psi_{lin}\rangle}. \tag{3}$$

Filling (1) into this then gives for the numerator

$$\langle\psi_0| \hat{H} |\psi_0\rangle + \sum_{i=1}^{N} \Delta\theta_i \langle\psi_i| \hat{H} |\psi_0\rangle + \langle\psi_0| \hat{H} \sum_{i=1}^{N} \Delta\theta_i \, |\psi_i\rangle + \sum_{i=1}^{N}\sum_{j=1}^{N} \Delta\theta_i\Delta\theta_j \langle\psi_i| \hat{H} |\psi_j\rangle \,. \tag{4}$$

Defining the first term as:

$$E(\theta_0) = \langle\psi_0| \hat{H} |\psi_0\rangle \,. \tag{5}$$

Manipulating the second term and third term together to get:

$$\sum_{i=1}^{N} \Delta\theta_i \langle\psi_i| \hat{H} |\psi_0\rangle + \langle\psi_0| \hat{H} \sum_{i=1}^{N} \Delta\theta_i \, |\psi_i\rangle = \sum_{i=1}^{N} \Delta\theta_i\partial_i\langle\psi_0| \hat{H} |\psi_0\rangle = \boldsymbol{\Delta\theta} \cdot \boldsymbol{\nabla} E(\theta_0) \tag{6}$$

And turning the last term into:

$$\sum_{i,j=1}^{N} \Delta\theta_i\Delta\theta_j \langle\psi_i| \hat{H} |\psi_j\rangle = \boldsymbol{\Delta\theta} \cdot \underline{\boldsymbol{H}} \cdot \boldsymbol{\Delta\theta} \tag{7}$$

Now expanding equation (3) in a similar manner by filling in (1) the denominator becomes:

$$\langle\psi_0|\psi_0|\psi_0|\psi_0\rangle + \sum_{i=1}^{N}\Delta\theta_i\,\langle\psi_i|\psi_0|\psi_i|\psi_0\rangle + \left\langle \psi_i|\sum_{i=1}^{N}\Delta\theta_i\psi_0\middle|\psi_i|\sum_{i=1}^{N}\Delta\theta_i\psi_0\right\rangle + \sum_{i,j=1}^{N}\Delta\theta_i\Delta\theta_j\,\langle\psi_i|\psi_j|\psi_i|\psi_j\rangle \tag{8}$$

The first term is equal to one and the second and third term together become:

$$\sum_{i=1}^{N}\Delta\theta_i\,\langle\psi_i|\psi_0|\psi_i|\psi_0\rangle + \left\langle \psi_i|\sum_{i=1}^{N}\Delta\theta_i\psi_0\middle|\psi_i|\sum_{i=1}^{N}\Delta\theta_i\psi_0\right\rangle = \boldsymbol{\Delta\theta}\cdot\boldsymbol{\nabla}\,\langle\psi_0|\psi_0|\psi_0|\psi_0\rangle = 0 \tag{9}$$

and similarly the last term becomes:

$$\sum_{i,j=1}^{N}\Delta\theta_i\Delta\theta_j\,\langle\psi_i|\psi_j|\psi_i|\psi_j\rangle = \boldsymbol{\Delta\theta}\cdot\underline{\boldsymbol{S}}\cdot\boldsymbol{\Delta\theta} \tag{10}$$

Then all together using equations (4) until (10) we can transform (3) into:

$$E = \frac{E(\theta_0) + \boldsymbol{\Delta\theta}\cdot\boldsymbol{\nabla}E(\theta_0) + \boldsymbol{\Delta\theta}\cdot\underline{\boldsymbol{H}}\cdot\boldsymbol{\Delta\theta}}{1 + \boldsymbol{\Delta\theta}\cdot\underline{\boldsymbol{S}}\cdot\boldsymbol{\Delta\theta}} \tag{11}$$

This can be turned into matrices then giving:

$$E = \frac{\boldsymbol{v^T}\underline{\tilde{\boldsymbol{H}}}\boldsymbol{v}}{\boldsymbol{v^T}\underline{\tilde{\boldsymbol{S}}}\boldsymbol{v}}, \tag{12}$$

where the H-Tilde matrix is:

$$\underline{\tilde{\boldsymbol{H}}} = \begin{pmatrix} E(\theta_0) & \frac{1}{2}\boldsymbol{\nabla}E(\theta_0) \\ \frac{1}{2}\boldsymbol{\nabla}E(\theta_0) & \underline{\boldsymbol{H}} \end{pmatrix} \tag{13}$$

and the S-Tilde matrix is:

$$\underline{\tilde{\boldsymbol{S}}} = \begin{pmatrix} 1 & \boldsymbol{0} \\ \boldsymbol{0} & \underline{\boldsymbol{S}} \end{pmatrix} \tag{14}$$

and lastly the vector is:

$$\boldsymbol{v} = \begin{pmatrix} 1 \\ \boldsymbol{\Delta\theta} \end{pmatrix} \tag{15}$$

Equation 12 can then be turned into a generalized eigenvalue equation

$$\underline{\tilde{\boldsymbol{H}}}\boldsymbol{v} = \epsilon\underline{\tilde{\boldsymbol{S}}}\boldsymbol{v} \tag{16}$$

which can be solved for vector $\boldsymbol{v}$ to obtain the updatestep $\boldsymbol{\Delta\theta}$