Linear Method as Used in VQE's

Ronja Johanna Zijderveld

September 2021

1 Quantum Circuit proof S matrix

This is one of the derivations written up as part of an internship that sought to use the linear method as an optimization algorithm in variational quantum eigensolver. The derivation showing why the S matrix is a relevant quality which needs to be calculated can be found under the name 'LinearizingLinearMethod.pdf' on the same Github. The goal for matrix S is to obtain:

$$\langle \psi_i | \psi_j \rangle , \tag{1}$$

where ψ_i is given by:

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

The wavefunction is parameterized by a variational circuit consisting of gates. Each U_i is a rotation or a controlled rotation gate, it's derivative can be expressed by:

$$\frac{\partial U_i(\theta_i)}{\partial \theta_i} = \sum_k f_{k,i} U_i(\theta_i) \sigma_{k,i} \tag{3}$$

The derivative of the trial state is:

$$\frac{\partial |\psi\rangle}{\partial \theta_i} = \sum_k f_{k,i} \tilde{V}_{k,i} |0\rangle \tag{4}$$

where:

$$\tilde{V}_{k,i} = U_N(\theta_N) ..._{i+1}(\theta_{i+1}) U_i(\theta_i) \sigma_{k,i} ... U_2(\theta_2) U_1(\theta_1) \tag{5}$$

Thus the real part of matrix S is:

$$R\left(\sum_{k,l} f^*_{k,i} f_{l,j} \langle 0| \tilde{V}^\dagger_{k,i} \tilde{V}_{l,j} |0\rangle \right) \tag{6}$$

We then absorb the two scalars together as such:

$$f^*_{k,i} f_{l,j} = a e^{i\theta} \tag{7}$$

then we are left to evaluate:

$$\langle 0| \tilde{V}^\dagger_{k,i} \tilde{V}_{l,j} |0\rangle = \langle 0| U_1^\dagger ... U_{i-1}^\dagger \sigma^\dagger_{k,i} U_i^\dagger ... U_N^\dagger U_N ... U_j \sigma_{l,j} U_{j-1} ... U_1 |0\rangle \tag{8}$$

then combining the middle gates into identity matrices gives that:

$$\langle 0| \tilde{V}^\dagger_{k,i} \tilde{V}_{l,j} |0\rangle = \langle 0| U_1^\dagger ... U_{i-1}^\dagger \sigma^\dagger_{k,i} U_i^\dagger ... U_{j-1}^\dagger \sigma_{l,j} U_{j-1} ... U_i ... U_1 |0\rangle \tag{9}$$

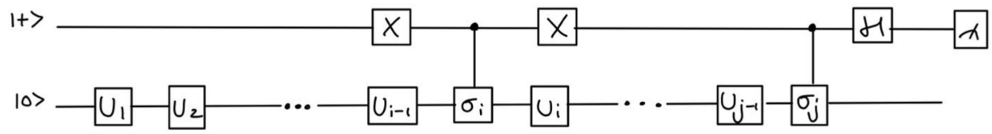

Figure 1: The quantum circuit needed to calculate element i,j of the S matrix. Derivation of why it works follows below.

Now drawing the circuit for this explicitly and working out how it results in this:

$$(I\otimes U_1)...(X\otimes U_{1-i})(|0\rangle\langle 0|\otimes I+|1\rangle\langle 1|\otimes G_i)(X\otimes U_i)(I\otimes U_{i+1})...(I\otimes U_{j-1})(|0\rangle\langle 0|\otimes I+|1\rangle\langle 1|\otimes G_j)(H\otimes I) \tag{10}$$

Now working from left to right resolving first the final two brackets and continuing on that way for a few lines:

$$(I\otimes U_1)...(X\otimes U_{1-i})(|0\rangle\langle 0|\otimes I+|1\rangle\langle 1|\otimes G_i)(X\otimes U_i)(I\otimes U_{i+1})...(I\otimes U_{j-1})(|0\rangle\langle 0|\, H\otimes I+|1\rangle\langle 1|\, H\otimes G_j) \tag{11}$$

$$(I\otimes U_1)...(X\otimes U_{1-i})(|0\rangle\langle 0|\otimes I+|1\rangle\langle 1|\otimes G_i)(X\otimes U_i)(|0\rangle\langle 0|\, H\otimes U_{i+1}...U_{j-1}+|1\rangle\langle 1|\, H\otimes U_{i+1}...U_{j-1}G_j) \tag{12}$$

$$(I\otimes U_1)...(X\otimes U_{1-i})(|0\rangle\langle 0|\otimes I+|1\rangle\langle 1|\otimes G_i)(X\,|0\rangle\langle 0|\, H\otimes U_iU_{i+1}...U_{j-1}+X\,|1\rangle\langle 1|\, H\otimes U_iU_{i+1}...U_{j-1}G_j) \tag{13}$$

now writing only the elements which will survive the following:

$$\begin{aligned}(I\otimes U_1)...(X\otimes U_{1-i})(&|0\rangle\langle 0|\, X\,|0\rangle\langle 0|\, H\otimes U_iU_{i+1}...U_{j-1}+|0\rangle\langle 0|\, X\,|1\rangle\langle 1|\, H\otimes U_iU_{i+1}...U_{j-1}G_j+\\ &|1\rangle\langle 1|\, X\,|0\rangle\langle 0|\, H\otimes G_iU_iU_{i+1}...U_{j-1}+|1\rangle\langle 1|\, X\,|1\rangle\langle 1|\, H\otimes G_iU_iU_{i+1}...U_{j-1}G_j)\end{aligned} \tag{14}$$

thus:

$$(I\otimes U_1)...(X\otimes U_{1-i})(|0\rangle\,\langle 1|\, H\otimes U_iU_{i+1}...U_{j-1}G_j+|1\rangle\,\langle 0|\, H\otimes G_iU_iU_{i+1}...U_{j-1}) \tag{15}$$

$$(I\otimes U_1)(X\,|0\rangle\langle 1|\, H\otimes U_{1-i}U_iU_{i+1}...U_{j-1}G_j+X\,|1\rangle\langle 0|\, H\otimes U_{1-i}G_iU_iU_{i+1}...U_{j-1}) \tag{16}$$

$$X\,|0\rangle\langle 1|\, H\otimes U_1...U_{1-i}U_iU_{i+1}...U_{j-1}G_j+X\,|1\rangle\langle 0|\, H\otimes U_1...U_{1-i}G_iU_iU_{i+1}...U_{j-1} \tag{17}$$

where we choose to denote, as follows:

$$A\equiv U_1...U_{1-i}G_iU_iU_{i+1}...U_{j-1} \tag{18}$$

$$B\equiv U_1...U_{1-i}U_iU_{i+1}...U_{j-1}G_j \tag{19}$$

Our initial state is $1/\sqrt{2}(|0\rangle+|1\rangle)\otimes|0\rangle$ thus then the total state of which we then get the expectation value is:

$$|\psi\rangle=\frac{1}{\sqrt{2}}H\,|0\rangle\otimes A\,|0\rangle+\frac{1}{\sqrt{2}}H\,|1\rangle\otimes B\,|0\rangle \tag{20}$$

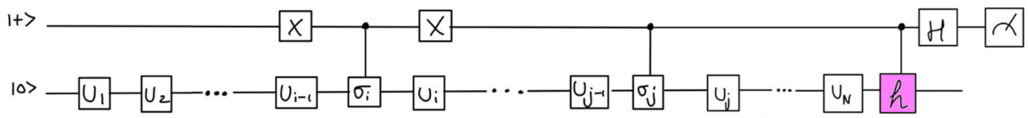

Figure 2: Quantum circuit needed to calculate the H-matrix. Very similar to Figure 1, except for the quantum gate which is highlighted in pink. This quantum gate represents all the terms of the Hamiltonian being entangled to the auxiliary qubit.

Now we aim to calculate the state $\langle\psi| Z |\psi\rangle$ thus:

$$(\frac{1}{\sqrt{2}}\langle 0| H \otimes \langle 0| A^{\dagger} + \frac{1}{\sqrt{2}}1H \otimes \langle 0| B^{\dagger})(Z \otimes I)(\frac{1}{\sqrt{2}}H|0\rangle \otimes A|0\rangle + \frac{1}{\sqrt{2}}H|1\rangle \otimes B|0\rangle) \tag{21}$$

$$\frac{1}{2}\langle 0| HZH |0\rangle \otimes \langle 0| A^{\dagger}A|0\rangle + \frac{1}{2}\langle 1| HZH |0\rangle \otimes \langle 0| B^{\dagger}A|0\rangle + \frac{1}{2}\langle 0| HZH |1\rangle \otimes \langle 0| A^{\dagger}B|0\rangle + \frac{1}{2}\langle 1| HZH |1\rangle \otimes \langle 0| B^{\dagger}B|0\rangle \tag{22}$$

using that $HZH = X$ we then finally get:

$$\frac{1}{2}I \otimes (\langle 0| B^{\dagger}A|0\rangle + \langle 0| A^{\dagger}B|0\rangle) \tag{23}$$

which are complex conjugates of each other, therefore leaving us with twice the real part of this. And then using our definitions for A and B gives:

$$I/2 \otimes Re(\langle 0| A^{\dagger}B|0\rangle) \tag{24}$$

$$I/2 \otimes Re(\langle 0| U_1^{\dagger}...U_{1-i}^{\dagger}G_i^{\dagger}U_i^{\dagger}U_{i+1}^{\dagger}...U_{j-1}^{\dagger}G_jU_{j-1}...U_{i+1}U_i...U_1|0\rangle) \tag{25}$$

To obtain the imaginary part all the steps are the same except for the fact that instead of making a z-measurement you make a y-measurement. It is then possible to combine the real and the imaginary part and you will get the S-matrix as set out to obtain.

2 Quantum Circuit proof H matrix

The calculation of the H matrix follows very similar steps to the ones above, therefore certain steps will be skipped and referenced above. This time our goal is to create the following element:

$$\langle\psi_i| \hat{H} |\psi_j\rangle , \tag{26}$$

To achieve this the same steps of derivation done in the S matrix above can be done until formula 7. Formula 7 will look like:

$$\langle 0| \tilde{V}_{k,i}^{\dagger}\tilde{V}_{l,j}|0\rangle = \langle 0| U_1^{\dagger}...U_{i-1}^{\dagger}\sigma_{k,i}^{\dagger}U_i^{\dagger}...U_N^{\dagger}\hat{H}U_N...U_j\sigma_{l,j}U_{j-1}...U_1|0\rangle \tag{27}$$

where previously we were able to cancel the $U_N^{\dagger}$ and U_N, this is no longer possible, because of the Hamiltonian which is now in between. The change that this gives to the circuit can be seen higlighted in Figure 2.

Because of the fact that the derivation is the exact same, except for a Hamiltonian which simply appears on the right hand side, the derivation will not be repeated here. Please do contact me (using the contact information given in the READMe if there are any issues at all).