At iteration k=1
$U^{(0)} = 1$
State preparation
$|\psi^{(k-1)}\rangle = U^{k-1}(\theta_{k-1})|\psi_{HF}\rangle$
START
Gradients measurement
$\frac{\partial E^{(k-1)}}{\partial \vec{\theta}_m} = \langle \psi(\vec{\theta}_{k-1})|[H, A_m]|\psi(\vec{\theta}_{k-1})\rangle$
Excitation pool operators
$A_m = \{A_m(p,q), A_m(p,q,r,s)\}$
θ_{k-1}
Is from previous VQE iteration
Terminate Condition
$k-1=k$
END
Yes
$\|\vec{g}^{(k-1)}\| = \sqrt{\left(\frac{\partial E^{(k-1)}}{\partial \theta_1}\right)^2 + \cdots + \left(\frac{\partial E^{(m)}}{\partial \theta_m}\right)^2} \leq \varepsilon$
The convergence criterion
No
VQE: Re-optimize all parameters
$E^{(k)} = \min_{\vec{\theta}_k} \langle \psi_{\mathrm{HF}}|e^{-\theta_1 A_1} \ldots e^{-\theta_k A_k} H e^{\theta_k A_k} \ldots e^{\theta_1 A_1}|\psi_{\mathrm{HF}}\rangle$
Select operator with largest gradient
$\vec{\theta}_m \rightarrow \vec{\theta}_k$
& expand the ansatz
$|\psi^{(k)}\rangle = e^{\theta_k A_k}|\psi^{(k-1)}\rangle = e^{\theta_k A_k} \ldots e^{\theta_3 A_3} e^{\theta_2 A_2} e^{\theta_1 A_1}|\psi_{\mathrm{HF}}\rangle$