Expressibility of Circuits - Report

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December 20, 2023

Introduction

The paper revolves around exploring certain kind of quantum circuits that can be tweaked based on some external parameters.

Definition. Parametrised Quantum Circuit(PQC): A PQC is a family of quantum circuits Q_θ where $\theta = (\theta_1, \theta_2, \ldots, \theta_n)$ is a vector with polynomially many entries.

This translates to the fact that the gates in the circuit rely on the input parameters, examples of such gates are the R_α or rotation by α gates and so on. We fix an initial state vector, usually $|0\rangle^{\otimes m}$ and the states that the circuit in question can explore are given by $|v_\theta\rangle = Q_\theta |0\rangle$.

Then we can loosely talk about expressibility of a circuit as how many different states it is able to create, in other words how varied are the $|v_\theta\rangle$ it can produce. The more varied the more is the circuits expressibility.

Expressibility

Before we can formally define expressibility, first consider the unitary group of operators acting on the Hilbert space, any element U can be written as e^{iH} where H is self adjoint and the self adjoint operators form a locally compact abelian group under addition and can hence be given a unique(upto constant) Haar measure. This in some sense corresponds to the uniform distribution over self adjoint operators, now we can define the uniform distribution or the Haar measure for the multiplicative group of unitaries by using the fact that if H is self adjoint then e^{iH} is unitary, so $d\mu(e^{iH}) = d\tilde{\mu}(H)$, where $\tilde{\mu}$ is the Haar measure over the self adjoint elements.

Now we fix a state $|\psi_0\rangle$ and a Haar random state is given by $U|\psi_0\rangle$ where U is picked according to the previously discussed uniform distribution. Further we can define the fidelity between two states as a heuristic to measure how similar they are, define

$$F(|\psi_1\rangle, |\psi_2\rangle) = |\langle\psi_1, \psi_2\rangle|^2$$

This way, once we fix a state $|\psi_0\rangle$ we can define a positive valued observable on a state distribution by $F(|\psi_0\rangle, \cdot)$. Lastly we define a frame $\mathcal{F}$ to be any spanning set of vectors $\mathcal{F} = \{f_i\}_I$ such that for all $|x\rangle$ we have the following where $A \leq B$ are constants and ν is a measure on I and in the case where I is finite or discrete, it is just the counting measure

$$A\|x\|^2 \leq \int_I |\langle f_i, x\rangle|^2 d\nu(i) \leq B\|x\|^2$$

Further we can speak about a frame potential which corresponds to the euclidean norm given to operators by considering the sum of squares of the matrix elements, similarly we define the frame potential as

$$\Phi_p(\mathcal{F}) = \int_I \int_I |\langle f_i, f_j\rangle|^2 d\nu(i) d\nu(j)$$

Now we can begin to define expressibility.

We want the expressibility to in some sense capture how different the current distribution is from the "standard"

Haar distribution. This can be done by considering the operator

$$A = \int_{\text{Haar}} |\psi\rangle \langle\psi| \, d\psi - \int_{\Theta} |\phi\rangle \langle\phi| \, d\phi$$

Where Θ is the state space of the parameters. Then we can quantify the difference by the Hillbert Schmidt norm or L^2 norm so that

$$\|A\|^2 = \text{Tr}(A^\dagger A) = \text{Tr}\left(\left[\frac{\Pi}{d} - \mu\right]^\dagger \left[\frac{\Pi}{d} - \mu\right]\right) = -\frac{1}{d} + \text{Tr}(\mu^2)$$

Where the Haar integral is rewritten as the normalized projector onto the symmetric subspace, and d is the corresponding dimension of the subspace. Note that

$$\text{Tr}(\mu^2) = \int_{\Theta}\int_{\Theta} |\langle \psi_\theta, \psi_\gamma \rangle|^2 d\theta d\gamma$$

This can be rewritten in terms of frame potentials as

$$\|A\|^2 = \Phi_p(\mathcal{F}_\Theta) - \Phi_p(\mathcal{F}_{\text{Haar}})$$

Hence the goal of expressibility should be to capture the difference between the frame potentials, notice that the frame potential is just the expected value of the fidelity over the joint distribution of $\Theta \times \Theta$ and similarly for the Haar case as well, hence we can measure their similarity using KL divergence.

Definition. Expressibility(Of a PQC Q_θ): It is defined as the Kullback-Leibler divergence between the distributions given by the observable $F(Q_\alpha |\psi_0\rangle, Q_\gamma |\psi_0\rangle)$ and $F(\tilde{U}_{\text{Haar}} |\psi_0\rangle, U_{\text{Haar}} |\psi_0\rangle)$. Where the distribution on α, γ is uniform over Θ. This can be expressed as

$$\text{Expr} = D_{\text{KL}}(P_{\text{PQC}}(F;\Theta) \;||\; P_{\text{Haar}}(F))$$

As it is in the normal case, a lower KL divergence implies that the distributions are similar hence the lower the divergence, the more it resembles the uniform distribution which means it has higher expressibility.

The expressibility of various circuits is calculated as well in the notebook.