

Quantum Neural Network Simulation

Project Proposal

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Overview

Classical Neural Networks
have shown to be effective in
a wide variety of uses.

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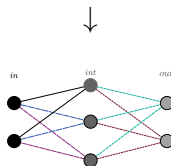
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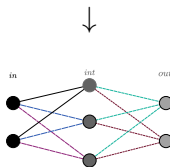
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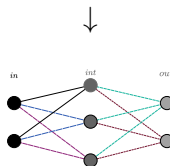
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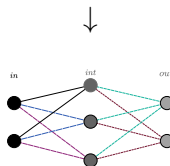
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Training Data Structure

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Data will be provided for the training of the network via a set of arbitrary states (inputs), and the set of these same states after having some common unitary action act upon them (outputs). Hence, we will assume some given data set of the following form:

$$\text{Training Data: } \{(|\psi_i\rangle, V|\psi_i\rangle) \mid 1 \leq i \leq N\}$$

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This is a reasonable set of data since the most general quantum network will apply an arbitrary unitary gate, and hence the most general circuit should be able to approximate such actions.

Architecture

The overall action of the network is composed of layer-by-layer composition of the transition map ϵ^ℓ for each layer ℓ s.t. $in \leq \ell \leq out$.

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Each layer may have a different number of qubits M_ℓ .

Explicitly, the ℓ -th layer's transition map takes the form:

$$\begin{aligned}\epsilon^\ell(\rho_{\ell-1}) &= \\ \text{Tr}_{\ell-1} \left[\left(\prod_{m=1}^{M_\ell} U_\ell^{m-M_\ell} \right) ((|0\rangle^{\otimes M_\ell} \langle 0|^{\otimes M_\ell})_\ell \otimes \rho_{\ell-1}) \left(\prod_{m=1}^{M_\ell} U_\ell^{m\dagger} \right) \right] \\ &= \rho_\ell\end{aligned}$$

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And, hence, a total circuit of L layers returns ρ_{out} , defined below, for given some input state ρ_{in} .

$$\rho_{out} = \epsilon^{out} \left(\epsilon^L \left(\epsilon^{L-1} \left(\dots \epsilon^1 (\rho_{in}) \dots \right) \right) \right)$$

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Architecture: Step-by-step

For each layer ℓ ,

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Architecture: Step-by-step

For each layer ℓ ,

1. The next layer's M qubits are prepared in the initial state $|0\rangle^{\otimes M} \langle 0|_l^{\otimes M}$ and tensor producted with the previous layer's output $\rho_{\ell-1}$.

$$\rho'_\ell = \left(|0\rangle^{\otimes M} \langle 0|_l^{\otimes M} \right)_\ell \otimes \rho_{\ell-1}$$

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2. The ℓ -th layer's M associated unitary matrices U_ℓ^m are applied to this tensor product state (from top to bottom).

$$\rho''_\ell = \left(\prod_{m=0}^{M-1} U_\ell^{M-m} \right) (\rho'_\ell) \left(\prod_{m=1}^M U_\ell^{m\dagger} \right)$$

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3. The partial trace over the $(\ell - 1)$ th layer's Hilbert space is taken, resulting in the output state ρ_{ℓ} of the ℓ -th layer.

$$\rho_{\ell} = \text{Tr}_{\ell-1}[\rho''_{\ell}]$$

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Simple Example: $2 \times 3 \times 2$

As a simple example, consider a QNN with one hidden layer of three qubits, and a two qubit input and output.

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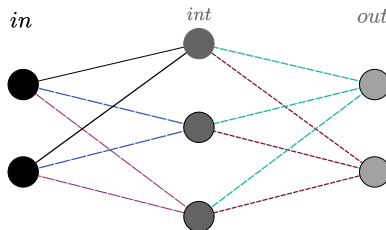
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Simple Example: $2 \times 3 \times 2$

As a simple example, consider a QNN with one hidden layer of three qubits, and a two qubit input and output.



$$\text{Tr}_{int} \left[U_2^{out} U_1^{out} \left(\text{Tr}_{in} \left[U_3^{int} U_2^{int} U_1^{int} (\rho_{in} \otimes |000\rangle\langle 000|_{int}) U_1^{int\dagger} U_2^{int\dagger} U_3^{int\dagger} \right] \right) U_1^{out\dagger} U_2^{out\dagger} \right] = \rho_{out}$$

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The metric by which we will judge the performance of the network on the training data is the cost, here taken as the average fidelity between the networks output state and the corresponding state given in training and explicitly defined as:

$$C = \frac{1}{N} \sum_{i=1}^N \langle \psi_i^{out} | \rho_{out} | \psi_i^{out} \rangle$$

Note that this cost function is only applicable for training data based on pure states, for which the fidelity takes an especially nice form.

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Note that this cost function is only applicable for training data based on pure states, for which the fidelity takes an especially nice form.

For input mixed states, we may replace the above with an averaged fidelity between output and target states of the form:

$$C = \frac{1}{N} \sum_{i=1}^N \left(\text{Tr} \left[\sqrt{\sqrt{\rho_i} \rho_i^{out} \sqrt{\rho_i}} \right] \right)^2$$

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We now wish to maximize the previously defined cost function (which has a maximum value of 1). This may be accomplished through training.

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We now wish to maximize the previously defined cost function (which has a maximum value of 1). This may be accomplished through training.

Training may be performed by evolving each unitary via the following map:

$$U_m^\ell \rightarrow e^{i\varepsilon K_m^\ell} U_m^\ell$$

which is parameterized by the step size ε , and where K_ℓ^m is derived from the derivative of the cost function and takes the following form:

$$K_m^\ell = \eta \frac{2^{m_\ell-1}}{N} \sum_{i=1}^N \text{Tr}_{-\ell} \left[\left(\prod_{n=0}^{m-1} U_{m-n}^\ell \right) \left((|0\rangle^{\otimes m_\ell} \langle 0|^{\otimes m_\ell})_\ell \otimes \rho_i^{\ell-1} \right) \left(\prod_{n=1}^m U_m^{\ell\dagger} \right), \right. \\ \left. \left(\prod_{n=m+1}^{m_\ell} U_n^{\ell\dagger} \right) (\sigma_i^\ell \otimes \mathbb{I}_{\ell-1}) \left(\prod_{n=1}^{m_\ell-(m+1)} U_{m_\ell-n}^\ell \right) \right]$$

where the square brackets denote a commutator and $\sigma_i^\ell = \mathcal{F}^{\ell+1}(\dots \mathcal{F}^{\text{out}}(\rho_i^{\text{out}})\dots)$ is the adjoint channel to the layer-to-layer transition map ϵ^ℓ for layer ℓ .

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Implementation: Software Choice

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The project's task will be to implement this general structure in a quantum computational SDK.

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The most likely candidate (as of now) is IBM's Qiskit, which may be developed in python.

Implementation: Software Choice

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The project's task will be to implement this general structure in a quantum computational SDK.

The most likely candidate (as of now) is IBM's Qiskit, which may be developed in python. Other options include: Google's Cirq, the open source Qutip, Pennylane, etc.

Implementation: Goals

Goals will include the following:

- 1 Define auxiliary functions in an appropriate manner (partial trace, concatenated unitary actions, etc.)
- 2 Define layer-to-layer transition maps of arbitrary qubit size
- 3 Define arbitrary depth layer composition (network of arbitrary depth)
- 4 Define appropriate cost function
- 5 Implement corresponding training scheme
- 6 Test on set(s) of data
 - (a) Compare performance on different underlying unitaries
 - (b) Compare performance for data set size used in training
 - (c) (*time permitting*) Compare performance on noisy data

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