Towards Quantum Machine Learning with Tensor Networks

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Tensor networks have been a useful tool for physicists for many years, but more recently they have been applied to a wide spread of problems in machine learning:

- Classification
- Analyzing Represenational Power of Neural Networks
- Generative Models
- Data Completion
- Model Compression

Motivation

Tensor networks have been a useful tool for physicists for many years, but more recently they have been applied to a wide spread of problems in machine learning:

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Tensor network approaches to machine learning also demonstrate variety in their connection to existing machine learning paradigms:

- Probabilistic Graphical Models
- Convolutional Neural Networks
- Kernel Learning

Goal: Given some pieces of data $\vec{x} \in \mathbb{R}^n$ and their associated labels $\ell \in \{1, ..., k\}$, learn a function that maps from the data to the labels.

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We could use a linear classifier.

$$f(\vec{x}) := argmax_\ell(\vec{w}_\ell \cdot \vec{x})$$

However, this might not be flexible enough.

Working in a Higher Dimensional Space

A more powerful option is to first 'lift' $\vec{x}$ into a higher dimensional space before performing linear classification.

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We will construct $g(\vec{x})$ by taking the tensor product of short feature vectors built from the entries of $\vec{x}$. For example:

$$g(\vec{x}) := \begin{bmatrix} sin(\frac{\pi}{2}x_0) \\ cos(\frac{\pi}{2}x_0) \\ 1 \end{bmatrix} \otimes \begin{bmatrix} sin(\frac{\pi}{2}x_1) \\ cos(\frac{\pi}{2}x_1) \\ 1 \end{bmatrix} \otimes ... \otimes \begin{bmatrix} sin(\frac{\pi}{2}x_{n-1}) \\ cos(\frac{\pi}{2}x_{n-1}) \\ 1 \end{bmatrix}$$

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We parameterize $\vec{w}_\ell$ using a tensor network to allow for efficient evaluation and optimization.

Graphical Notation for Tensor Networks

Tensor Networks allow us to approximate a high order tensor using a collection of lower order tensors and a prescription for contracting them together.

Rather than writing out a summation over a collection of different variables and indices, we use a graphical notation.

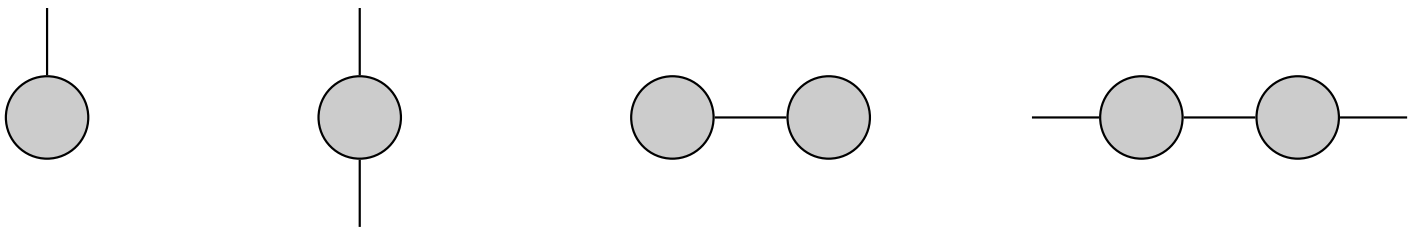
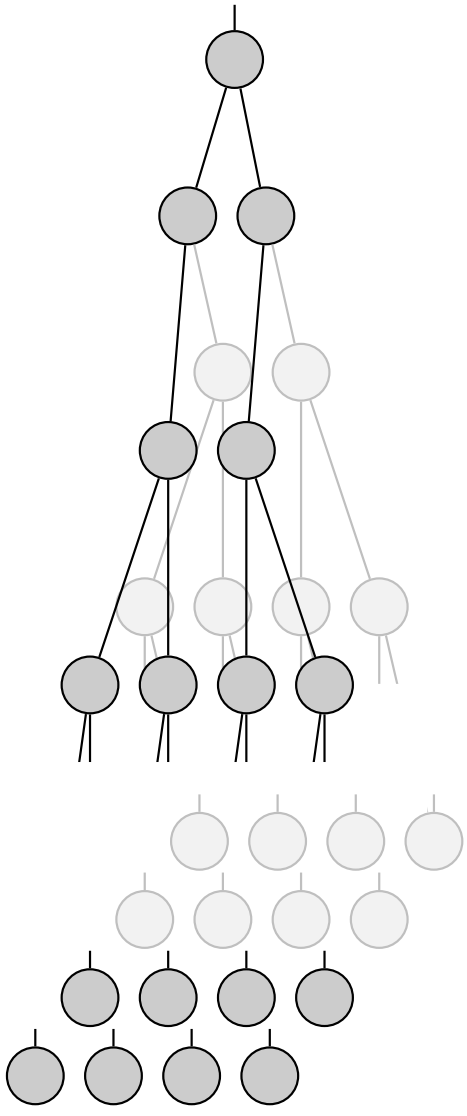


Figure 1: Left to right: A vector, $\vec{x}_i$; A matrix, $A_{i,j}$; The dot product of two vectors, $\sum_i \vec{x}_i \vec{y}_i$; The product of two matrices, $\sum_j A_{i,j} B_{j,k}$

Tree Tensor Networks

To the right is a Tree Tensor Network shown above sixteen feature vectors.



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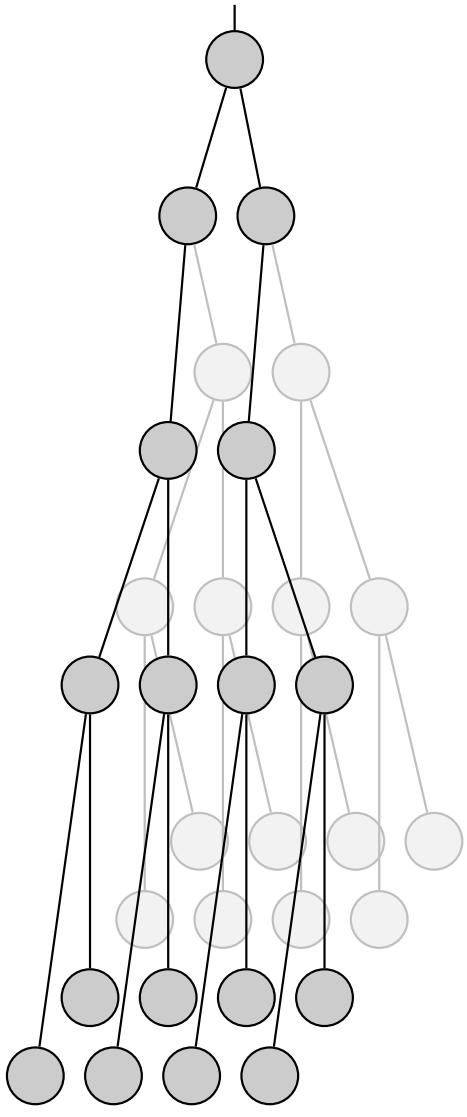
Its structure allows for tractable inference, optimization, and marginalization.



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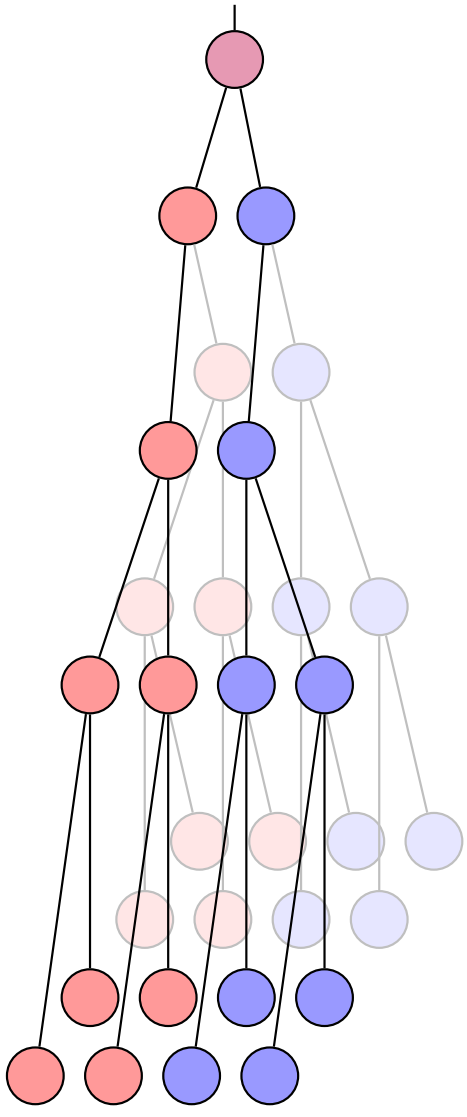
Unfortunately, this same structure limits its ability to capture long range correlations.



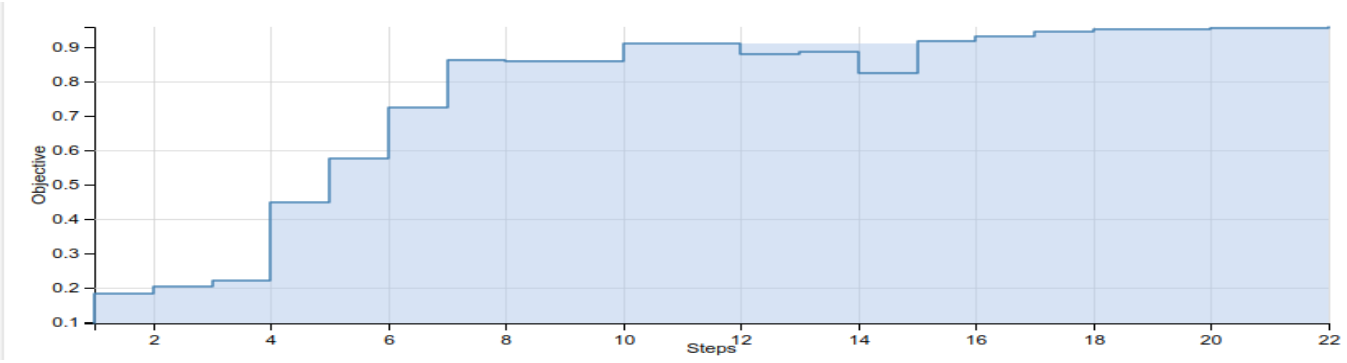


Figure 2: Training a Tree Tensor Network on the full MNIST data set.

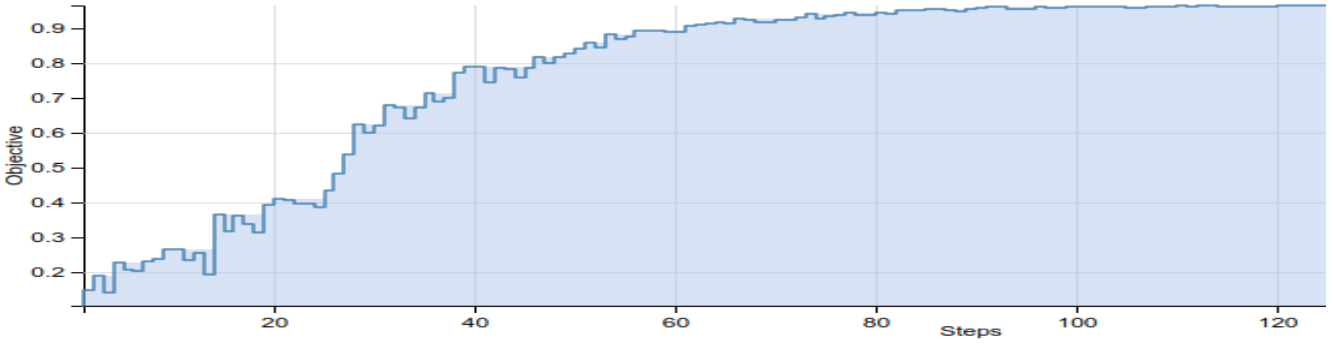


Figure 3: Using Stochastic Gradient Descent.

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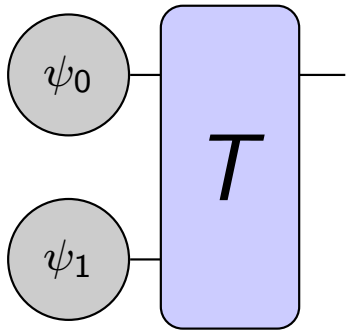
However, our approach is not immediately suitable for implementation on a quantum computer.

Let's zoom in on a single node, choosing the top of the network for convenience.



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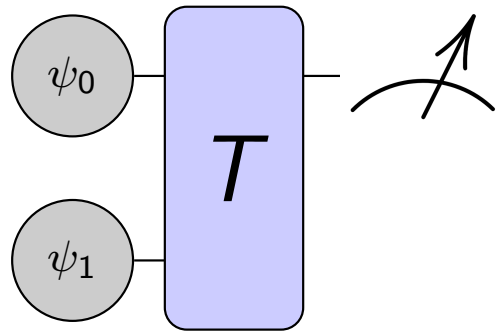
We aim to prepare a state which we can characterize with repeated measurement.



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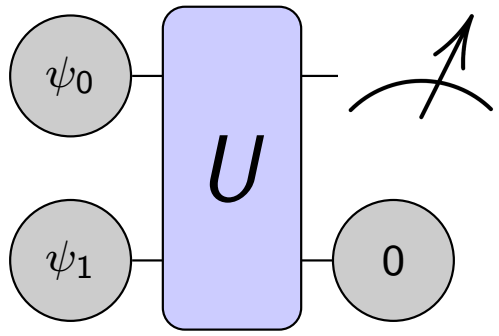
Our operations can be interpreted as unitary rotations followed by projections.

Unfortunately, implementing these projections on a quantum computer requires post-selection.



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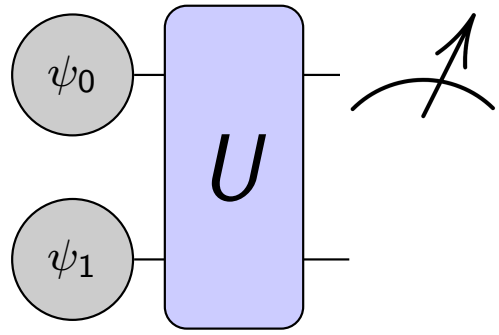
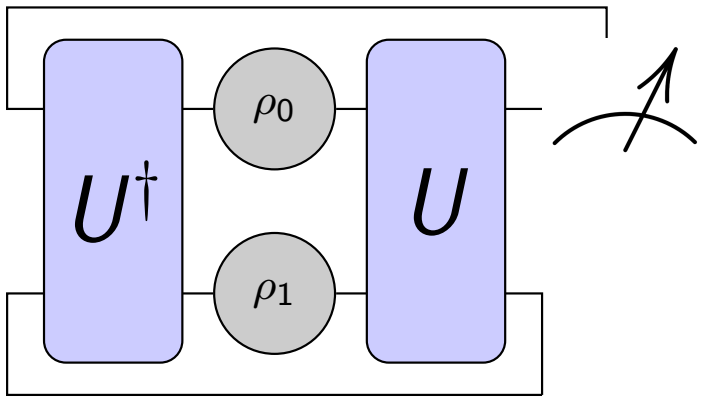
What happens if we just ignore this other qubit instead?



We must use density matrices to describe the states of the qubits, and our operations become CPTP maps.



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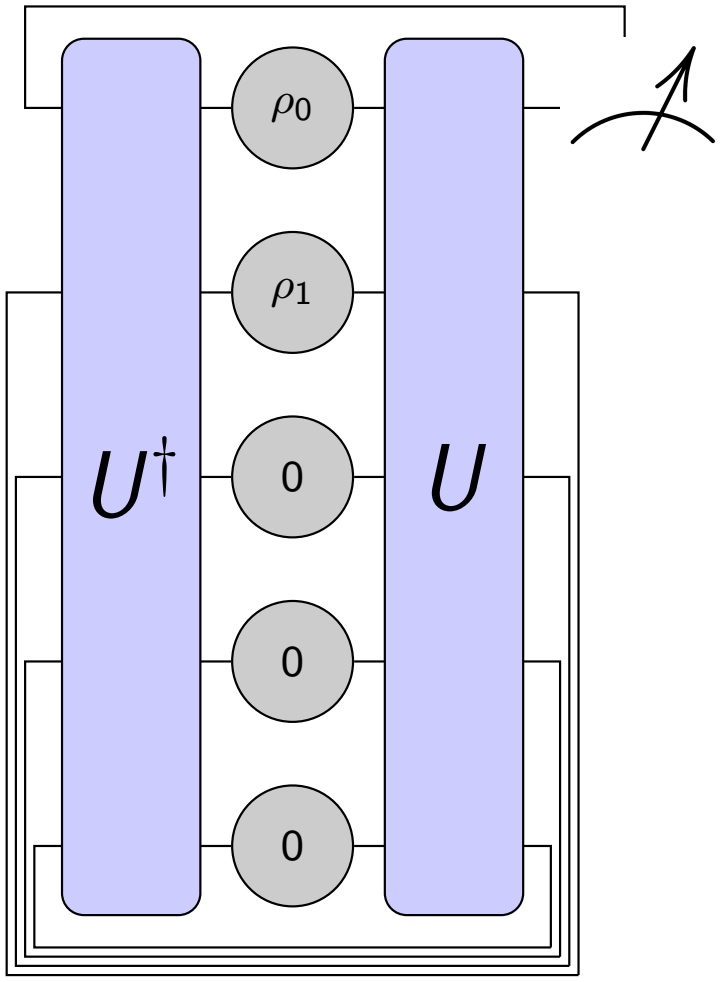

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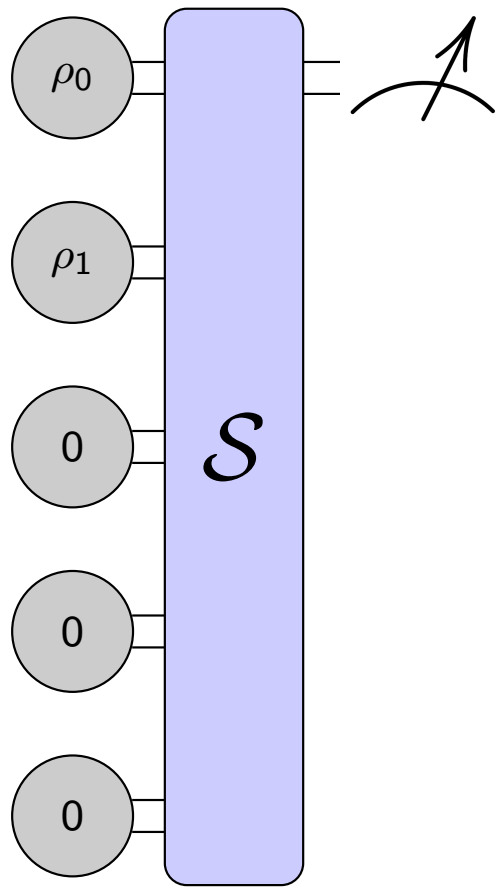

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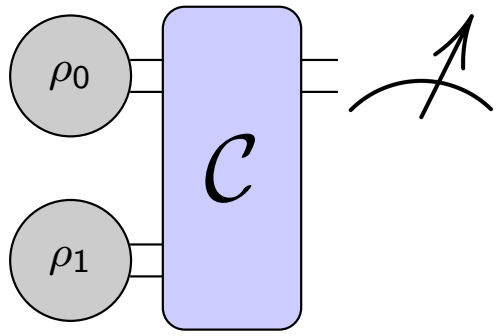
Simplifying even further, we can represent the operation at this node as the CPTP map $\mathcal{C}$ with nearly the same network geometry as before.



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We act on this initial state with a superoperator $\mathcal{S}$, producing a reduced state of one (or a few) qubits which we can tractably characterize.

$$\rho_{label} = \mathcal{S}|g(\vec{x})\rangle\langle g(\vec{x})|$$

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Is there a nice geometric interpretation of this procedure, akin to the arbitrary hyperplane separation of our original model?

More Intuition

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For example, we could construct the following POVM (for class labels a and b with an N dimensional feature space):

$$F_a = \begin{bmatrix} p(a|0) & 0 & \cdots & 0 \\ 0 & p(a|1) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & p(a|N-1) \end{bmatrix} \quad F_b = \begin{bmatrix} p(b|0) & 0 & \cdots & 0 \\ 0 & p(b|1) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & p(b|N-1) \end{bmatrix}$$

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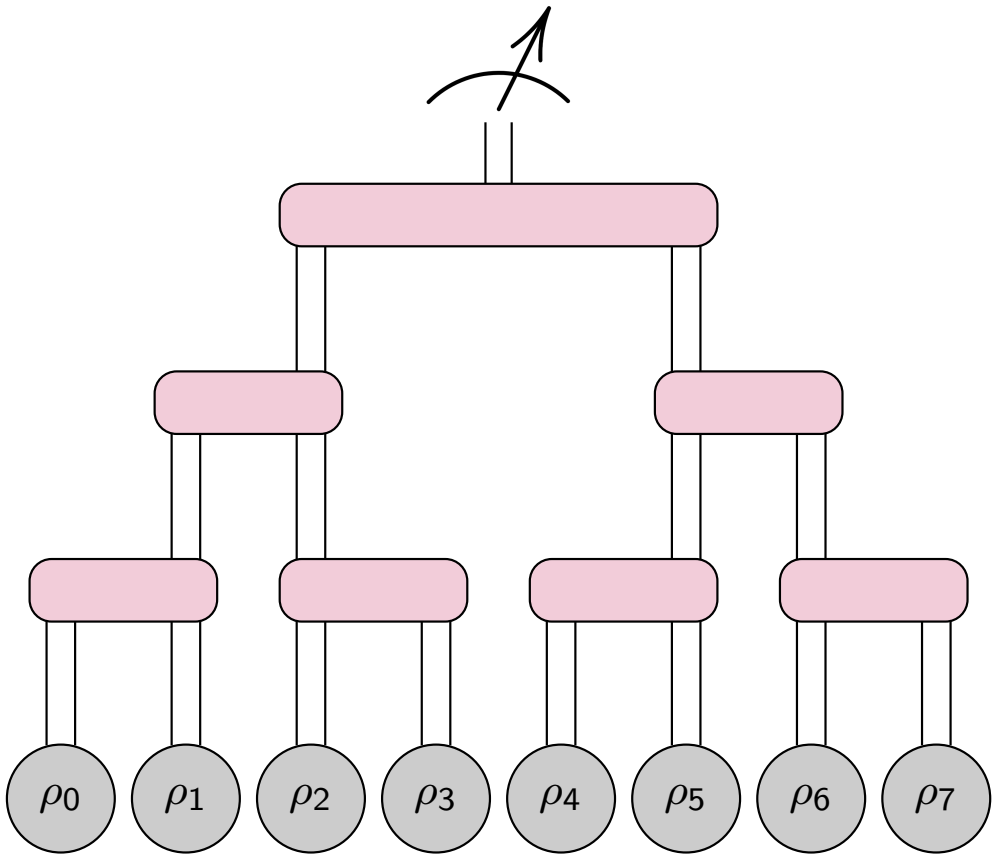
These measurement operators allow us to assign a probability distribution over class labels to each basis state in our feature map.

A tree-shaped classifier circuit can be efficiently simulated and optimized classically.



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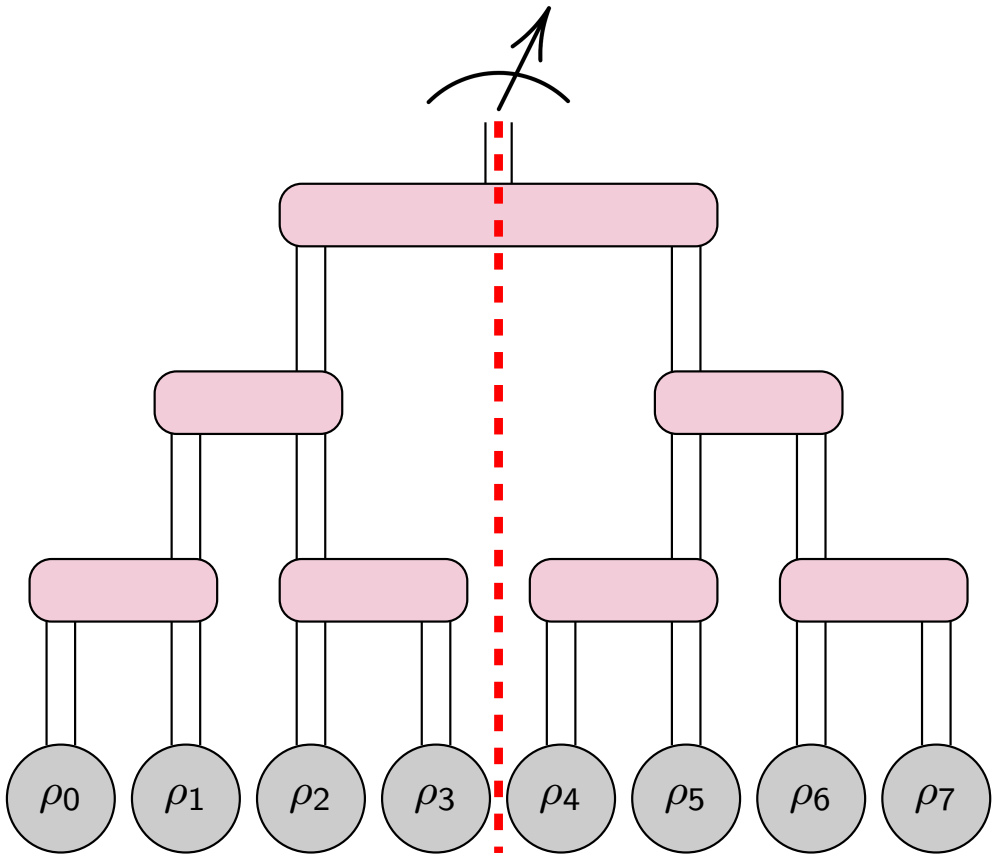

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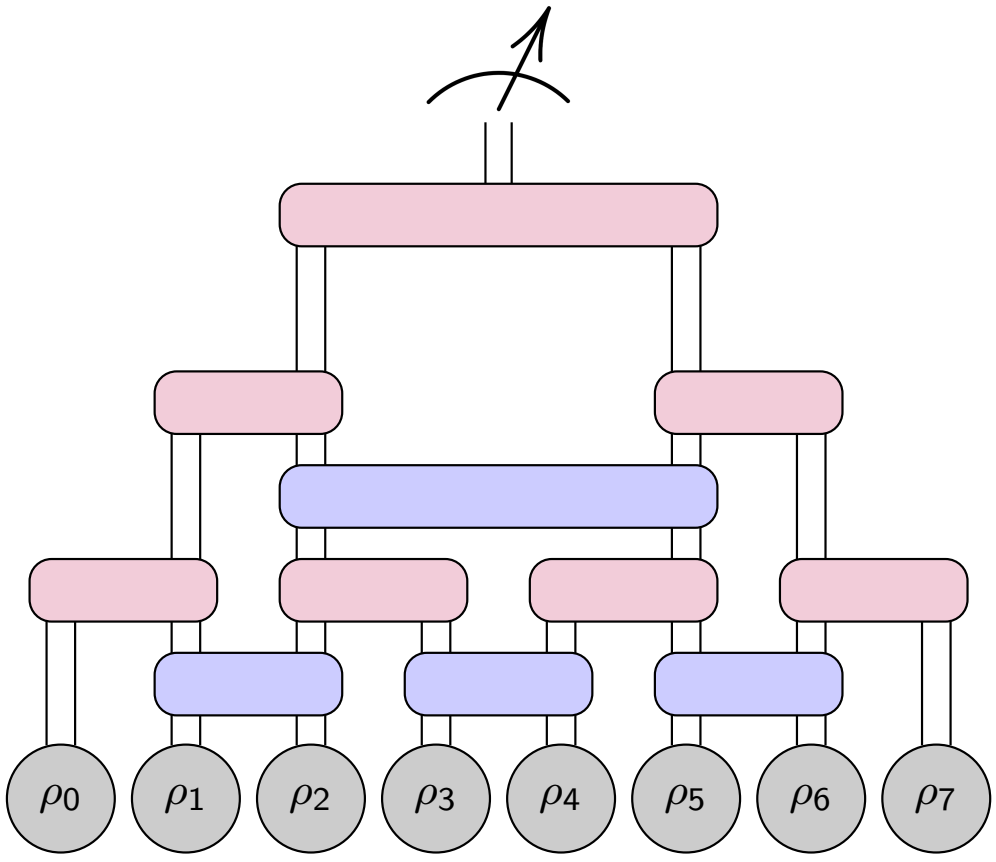
Using a quantum computer, we could add additional unitary elements to the circuit which address this shortcoming.



Future Directions and Questions

How resilient is this approach to noise? Can noise improve classifier robustness?

What is the right way to parameterize these circuits?

What is the best way to optimize them on a quantum computer?

How do they compare to classical implementations with non-linear copy operations?

Are there other useful feature maps for particular applications? Or network geometries?

Bibliography

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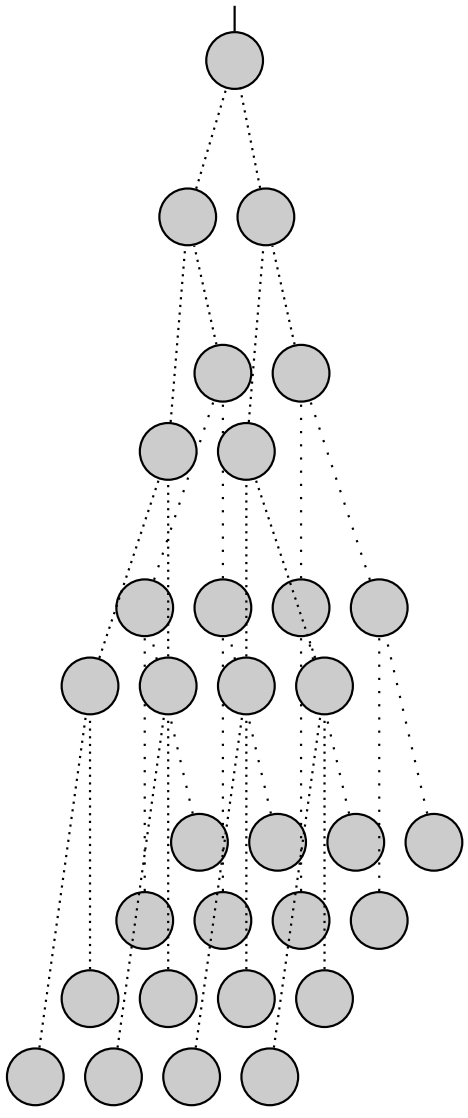
The standard approach to training a machine learning model is to use a global gradient descent procedure.

Given the raw outputs of the model for some piece of data, $\vec{w}_\ell \cdot g(\vec{x})$, and the true label, ℓ_{true}, we can define a loss function $L(\vec{w}_\ell \cdot g(\vec{x}), \ell_{true})$ that captures the distance between our model outputs and the ideal outputs.

We then take the gradient of L with respect to the parameters that define our model and update each parameter:

$$a_{n+1} = a_n - \epsilon \nabla L$$



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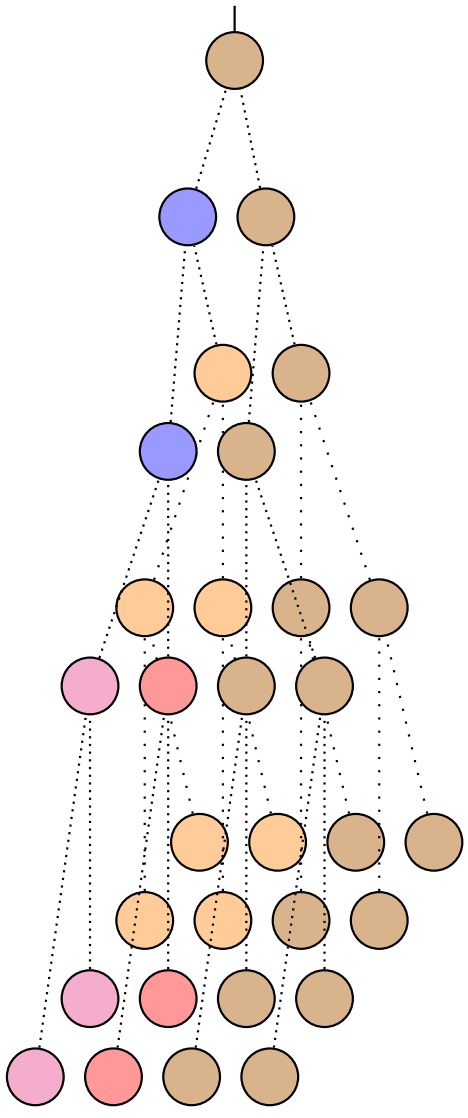

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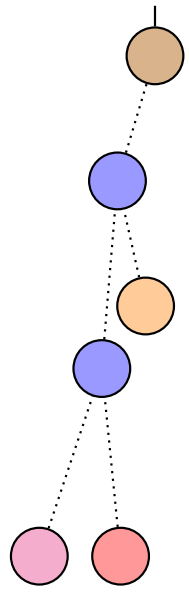

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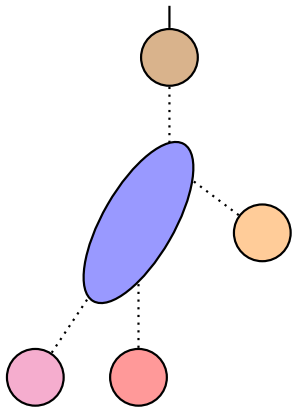

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Regularizing with Entanglement Entropy

Each of the tensors is a linear map from a larger space to a smaller space. One way to regularize the model would be to penalize these maps based on their rank, but matrix rank is integer valued.

$$T = USV^T \qquad or \qquad T_{i,j} = \sum_k U_{i,k} S_k V^T_{k,j}$$

However, we can define a related quantity, motivated by the notion of entanglement entropy from quantum mechanics:

$$exp(\sum_k |\tilde{S}_k|^2 log(|\tilde{S}_k|^2))$$

Where the $\tilde{S}_k$s are the original singular values normalized so that the sum of their squares is one.

Recall that, after mapping to our expanded space, our feature vector was something like:

$$g(\vec{x}) := \begin{bmatrix} x_0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} x_1 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} x_2 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} x_3 \\ 1 \end{bmatrix} \otimes \ldots \otimes \begin{bmatrix} x_{n-1} \\ 1 \end{bmatrix}$$

We can perform a dropout procedure on the model inputs in a straightforward way, yielding, for example:

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