Applied Quantum Algorithms - Lecture 8 - Quantum Neural Networks

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Contents

Supervised learning

Aim: Given some data and their **labels**, predict the function[1] that assigns **unseen** data to the correct label.

[1] A different formulation may be to predict the distributions $p(x, y)$ or $p\left(y|x\right)$.

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\text{Given} & D = \{(x_i, y_i) \mid x_i \in S;\ y_i = f(x_i)\}, \\
\text{where} & S \subseteq \mathbb{R}^n, \\
\text{predict} & f : S \to \mathit{labels}
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- *Classification*: discrete labels
- *Regression*: continuous labels

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Supervised learning

function family and training

Instead of searching among all possible $f\colon S \to \mathit{labels}$, we choose a *function family* or *ansatz*, characterized by *free parameters*.

$$\{ f_\theta | \, f_\theta : S, \Theta \to \mathit{labels} \}$$
$$\Theta \subseteq \mathbb{R}^p$$

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Training a supervised learning model - practical definition

Find θ s.t. f_θ best approximizes f w.r.t. a metric of error or *loss*.

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Mean squared error	$\sum_{i=1}^{N} \left(y_i - f_\theta\left(x_i\right)\right)^2$	Regression
Hinge loss	$\sum_{i=1}^{N} \max\left(0, 1 - y_i f(x_i)\right)$	Classification

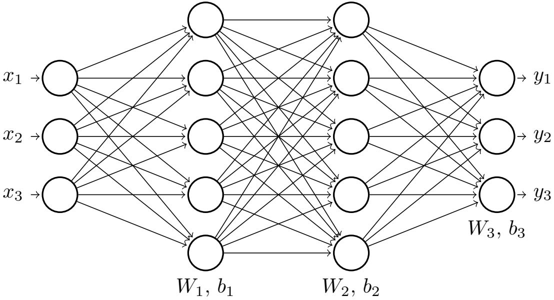
Supervised learning algorithms

- Neural networks (this lecture)
- Support vector machines (next lecture)

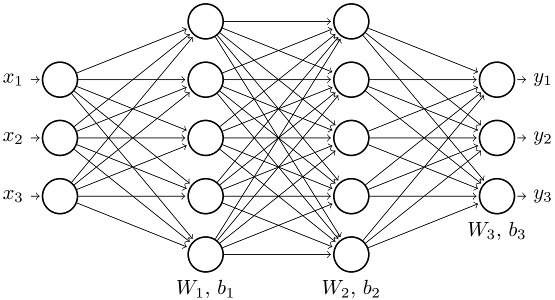
Supervised learning algorithms

- Neural networks (this lecture)
- Support vector machines (next lecture)
- Naive Bayes
- Linear regression
- Logistic regression
- k-nearest neighbours
- Random forest
- ...

Classical neural networks



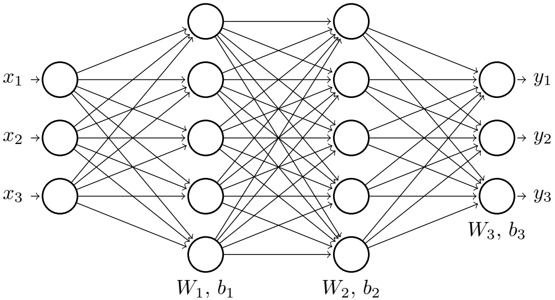
Classical neural networks



- $f_\theta = f\Big(\mathbf{x}, W^{(1)}, \mathbf{b}^{(1)} W^{(2)}, \mathbf{b}^{(2)}, \ldots, W^{(l)}, \mathbf{b}^{(l)}\Big)$
- Layered structure: $\mathbf{x}^{(l+1)} = \sigma\left(W^{(l)}\mathbf{x}^{(l)} + \mathbf{b}^{(l)}\right)$

[2] M. A. Nielsen (2018). *Neural Networks and Deep Learning*. misc

Classical neural networks



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Furthermore, NNs are universal function approximators[2].

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Classical neural networks

Training - backpropagation

Training neural networks uses gradient-based algorithms

$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla_{\theta^{(t)}} L$$

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2. model
3. loss function

we can build the so-called *computation graph*.

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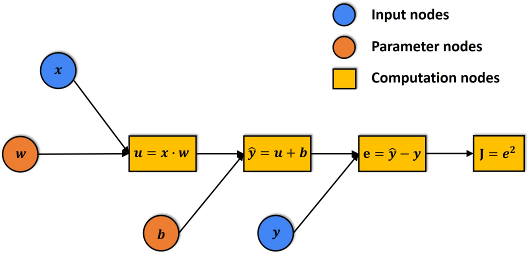

Classical neural networks

Training - backpropagation

To build the gradient at time (epoch) t, we need 2 steps

1. *forward* direction - get the loss value and evaluate local gradients
2. *backward* direction: multiplications (chain rule)

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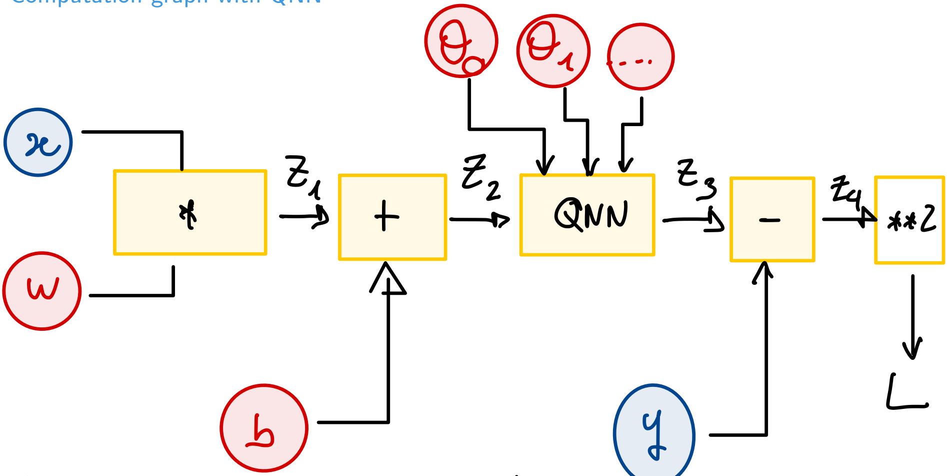
It works differently in QNNs, since *we cannot store intermediate gradients*, due to the no-cloning theorem. More later...

Intermezzo

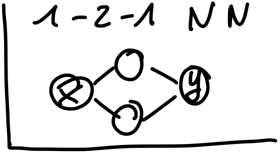
Computation graph with QNN

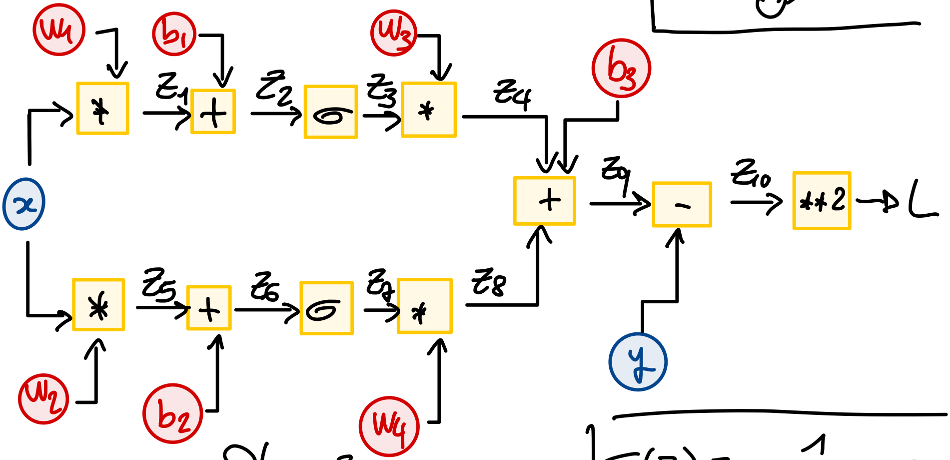


- Backprop @ graph level
- No backprop for $\frac{\partial QNN}{\partial \theta_i}$

Classical neural networks

Backpropagation example





$$\frac{\partial L}{\partial w_1} = ?$$

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

Quantum machine learning

Some informal definitions

Quantum-enhanced machine learning

Quantum computation to speed-up classical machine learning operations.

Example: SVM with quantum linear systems solver algorithm

Quantum machine learning

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Quantum-enhanced machine learning

Quantum computation to speed-up classical machine learning operations.

Example: SVM with quantum linear systems solver algorithm

Limitations

- Input/output problem (QRAM?)
- De-quantization argument: for a fair comparison, *both classical and quantum* algorithm must have access to a QRAM → classical algorithm also runs in $O(\log(N))$

Quantum machine learning

Some informal definitions

Machine learning in quantum feature spaces

Information is *encoded* into quantum states and classical algorithms find the optimal model.

[3] J. Biamonte, P. Wittek, N. Pancotti, P. Rebentrost, N. Wiebe, and S. Lloyd (Sept. 2017). "Quantum machine learning". In: *Nature* 549.7671, pp. 195–202. DOI: 10.1038/nature23474

Quantum machine learning

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Information is *encoded* into quantum states and classical algorithms find the optimal model.

Note: From here on, we will be focusing on ML in quantum feature spaces. For a review of quantum-enhanced ML, see [3]

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Why QML?

The advantage POV

As with all quantum algorithms, we ask ourselves: *how is QML better than ML?*

[4] Y. Liu, S. Arunachalam, and K. Temme (July 2021). "A rigorous and robust quantum speed-up in supervised machine learning". In: *Nature Physics* 17.9, pp. 1013–1017. DOI: 10.1038/s41567-021-01287-z

[5] the key idea of kernel theory, more in the next lecture

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Quantum advantage can be proved by

- Mapping data to certain states
- These states are hard to produce classically, but easy to produce (BQP) via a quantum algorithm
  - e.g. by solving the discrete log problem [4]
- We can compute inner products efficiently[5]

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However...

- Are there any *practically interesting* dataset in which QML can achieve advantage?

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The advantage POV

However...

- Are there any *practically interesting* dataset in which QML can achieve advantage?
- Is advantage even the right thing to look for?

Why QML?

Is quantum advantage the right goal for quantum machine learning? [6]

Advantage is just one of the possible points of view and maybe not the most useful one.

[6] M. Schuld and N. Killoran (July 2022). "Is Quantum Advantage the Right Goal for Quantum Machine Learning?" In: *PRX Quantum* 3.3. DOI: 10.1103/prxquantum.3.030101

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2. Can classical learning theory give us guarantees on the learning performance of QML models?
   - Yes, and the link is kernel theory.

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2. Can classical learning theory give us guarantees on the learning performance of QML models?
   - Yes, and the link is kernel theory.
3. Can we automate the learning process of (certain) QML models?
   - In particular, automatic differentiation.

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The quantum neural network model

3 ingredients

- A data encoding unitary: $U(\mathbf{x})$
- A variational unitary (anzatz): $W(\theta)$
- An observable (measurement operator): $\mathcal{M}$

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$$f(\mathbf{x}, \theta) = \langle \psi(\mathbf{x}, \theta) | \mathcal{M} | \psi(\mathbf{x}, \theta) \rangle ,$$

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$$f(\mathbf{x}, \theta) = \langle \psi(\mathbf{x}, \theta) | \mathcal{M} | \psi(\mathbf{x}, \theta) \rangle,$$

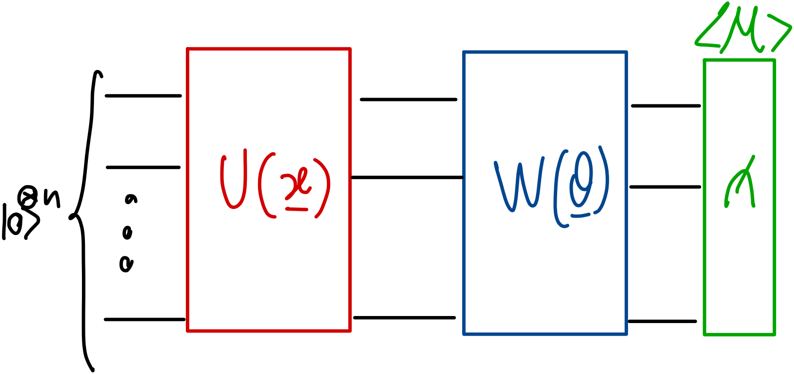
where

$$|\psi(\mathbf{x}, \theta)\rangle = W(\theta)\, U(\mathbf{x})\, |0\rangle$$

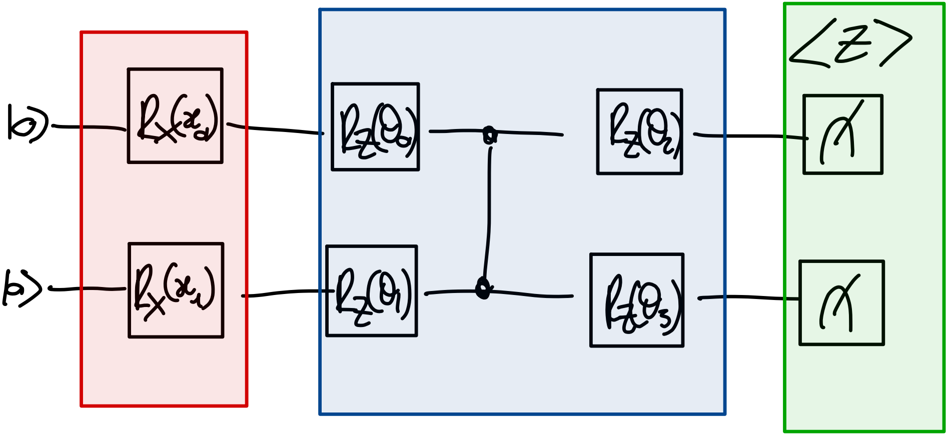
and

$$\mathbf{x} \in \mathbb{R}^m,\ \theta \in \mathbb{R}^p$$

The quantum neural network model



A simple QNN example



QNN model evaluation

The model $f = \langle \mathcal{M} \rangle_{\mathbf{x},\theta}$ is the expectation value of the observable $\mathcal{M}$ of the state $\psi(\mathbf{x}, \theta)$

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- In practice, we can compute $\left\langle \mathcal{M}_{\mathbf{x},\theta} \right\rangle$ if we know how to measure in $\mathcal{M}$ basis
- See previous slide where we measured in the X basis.

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- See previous slide where we measured in the X basis.
- Alternatively, we use Hadamard[7] or SWAP[8] tests
- Finite sampling: $O(1/\varepsilon^2)$ measurement to estimate $\langle M \rangle$ up to precision ε
    - Due to Chebyshev's inequality
    - In practice, a convergence study is necessary

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QNN model training

Training is hybrid, as for all variational algorithms. At each epoch

QNN model training

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1. (Quantum step) *Evaluate* the model $f = \langle \mathcal{M} \rangle_{\mathbf{x},\theta^{(t)}}$ and maybe $\nabla_\theta f$.
   - More on gradients later on...
2. (Classical step 1) *Forward step* in the computation graph.
   - i.e. we evaluate a loss function $L\left(\theta^{(t)}\right)$ and the local gradients.
3. (Classical step 2) *Backward step* in the computational graph.
4. (Classical step 3) *Parameter update*.

$$\mathrm{GD}: \qquad \theta^{(t+1)} = \theta^{(t)} - \eta \nabla_{\theta^{(t)}} L$$

QNN model training

Do you think it is a good idea to evaluate $\nabla_\theta f$ with finite differences?
Why? Why not?

Encoding classical data in quantum states

[9] even better, with high *margin*

Encoding classical data in quantum states

A good choice of data embedding can make the difference in terms of

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Encoding classical data in quantum states

- Runtime of the QML routine
  - how does the number of operations scale in the number of features N and dataset dimension M

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Encoding classical data in quantum states

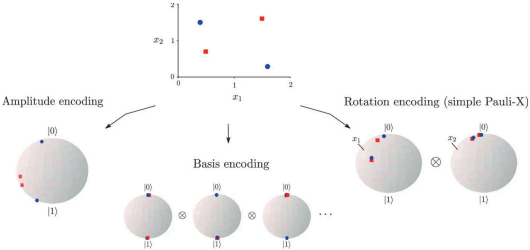
- Runtime of the QML routine
  - how does the number of operations scale in the number of features N and dataset dimension M
- Learning performance
  - Encoding data means to *map them to a high-dimensional Hilbert space*
  - E.g., in classification, we can linearly separate the data of different classes[9], but also completely shuffle them!

[9] even better, with high *margin*

Encoding classical data in quantum states

Data encoding as a feature map

$$\phi(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{F} \subseteq \mathcal{H}^{2^n}$$



Encoding classical data in quantum states

Amplitude encoding

Encoding classical data in quantum states

Amplitude encoding

We have $\mathbf{x} \in \mathbb{R}^N$. To make it a valid quantum state:

1. Normalize: $\frac{\mathbf{x}}{\|x\|_2}$
2. Pad until the closest power of 2: $x_N, \ldots, x_{2^n-1} = 0$

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Amplitude encoding (AE) is the identity transformation of this preprocessed state

$$\phi(\mathbf{x}) = |x\rangle = \sum_{i=0}^{N-1} x_i |i\rangle$$

[10] M. Mottonen, J. J. Vartiainen, V. Bergholm, and M. M. Salomaa (2004). *Transformation of quantum states using uniformly controlled rotations*. arXiv: quant-ph/0407010 [quant-ph]

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- AE is a linear transformation: if data is not linearly separable in the (normalized and padded) original space, then it won't be in the mapped space.
- num. qubits: $\log(N)$
- runtime: $O(N)$[10] *in general*

[10] M. Mottonen, J. J. Vartiainen, V. Bergholm, and M. M. Salomaa (2004). *Transformation of quantum states using uniformly controlled rotations*. arXiv: quant-ph/0407010 [quant-ph]

Encoding classical data in quantum states

Amplitude encoding

By adding an additional $\log(M)$ qubits, we can also encode data in superposition

$$|\psi_{\mathbf{x}}\rangle = \frac{1}{\sqrt{M}} \sum_{m=0}^{M-1} \sum_{i=0}^{N-1} x_i |i\rangle |m\rangle = \frac{1}{\sqrt{M}} \sum_{m=0}^{M-1} |\psi_{\mathbf{x}_m}\rangle |m\rangle$$

- num. qubits: $\log(NM)$
- runtime: $O(NM)$

Encoding classical data in quantum states

Basis encoding

Encoding classical data in quantum states

Basis encoding

For basis encoding, we first need to choose a binary representation of the features x_i. E.g., in floating point

$$b_i = b_{i,s} b_{i,n_e-1} \dots b_{i,0} b_{i,n_m-1} \dots b_{i,0}$$

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With $\tau = 1 + n_e + n_m$ we can encode *each feature of each datapoint* into a different basis state. If we concatenate the features:

$$\phi(\mathbf{x}) = |b_0 \ldots b_{N-1}\rangle$$

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Of course, we can also create superpositions

$$|\psi_{\mathbf{x}}\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} \left|\mathbf{x}^{(i)}\right\rangle$$

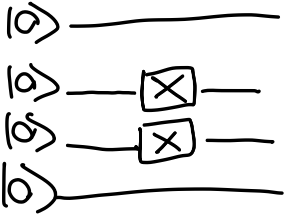
Encoding classical data in quantum states

Basis encoding

	Single sample	Dataset
num. qubits	$N\tau$	$N\tau$
runtime	$O(N\tau)$	$O(Mn\tau)$[11]

$$x = [01, 10]_b \xrightarrow{\Phi} |0110\rangle$$

$N = 2$,
$\tau = 2$



[11] D. Ventura and T. Martinez (1998). *Quantum Associative Memory*. arXiv: quant-ph/9807053 [quant-ph]

Encoding classical data in quantum states

Basis encoding

If basis encoding achieves perfect orthogonality between datapoints, why shouldn't we always use it for classification?

Encoding classical data in quantum states

Time-evolution encoding

Encoding classical data in quantum states

Time-evolution encoding

We're not constrained to *exactly* representing features. For instance, each feature can be the *evolution time of a certain Hamiltonian*

$$\phi(\mathbf{x}) = e^{-iH\mathbf{x}} |0\rangle$$

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Time-evolution encoding

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Typically, we do *angle encoding*, i.e. each feature is encoded as a Pauli rotation.

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$$\phi(\mathbf{x}) = e^{-iH\mathbf{x}} |0\rangle$$

Typically, we do *angle encoding*, i.e. each feature is encoded as a Pauli rotation.

Example: one feature, per rotation, per qubit, using Pauli X

$$\phi(\mathbf{x}) = e^{-iXx_{N-1}} \otimes e^{-iXx_{N-2}} \otimes \cdots \otimes e^{-iXx_0} |0\rangle$$

Encoding classical data in quantum states

Time-evolution encoding

For angle encoding:

	Single sample	Dataset
num. qubits	N	$N\lceil\log(M)\rceil$
runtime	$O(N)$	$O(MN)$

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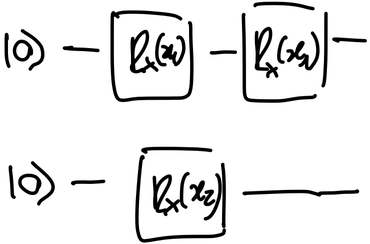

Encoding classical data in quantum states

Hamiltonian encoding of a dataset

[12] S. Lloyd (1996). "Universal Quantum Simulators". In: *Science* 273.5278, pp. 1073–1078. DOI: 10.1126/science.273.5278.1073. eprint: https://www.science.org/doi/pdf/10.1126/science.273.5278.1073

Encoding classical data in quantum states

Hamiltonian encoding of a dataset

If we keep the original data matrix $\mathbf{X} \in \mathbb{R}^{M \times N}$ and we can rewrite it as an Hermitian matrix $H_{\mathbf{X}}$, then we can encode the entire dataset as a Hamiltonian simulation

$$\phi : |0\rangle \to e^{-iH_{\mathbf{X}} t}$$

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- The general way to simulate $H_{\mathbf{X}}$ is to use *Trotterization*[12]

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Encoding classical data in quantum states

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If we keep the original data matrix $\mathbf{X} \in \mathbb{R}^{M \times N}$ and we can rewrite it as an Hermitian matrix $H_{\mathbf{X}}$, then we can encode the entire dataset as a Hamiltonian simulation

$$\phi : |0\rangle \to e^{-iH_{\mathbf{X}} t}$$

- The general way to simulate $H_{\mathbf{X}}$ is to use *Trotterization*[12]
  - *Requirement*: we need to know how to decompose $H_{\mathbf{X}}$ in terms that are *easy to simulate*.
  - We can always decompose an Hermitian matrix in $O(MN)$ Pauli strings.

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- More efficient algorithms exist for *sparse* Hamiltonians, but they require an *oracle*
    - Row i, jth non-zero element

$$|i, j, 0\rangle \rightarrow |i, j, H_{ij}\rangle$$

    - Likely need to hard-code it and full of multi-controlled gates

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Encoding classical data in quantum states

Hamiltonian encoding of a dataset

- Num. qubits: $\log(N)$
- Runtime: $O(MN)$ or $O(\log(MN))$
  - $O(\log(MN))$ only for sparse $\mathbf{X}$ and a few other cases.

Encoding classical data in quantum states

Quantum models as sums of periodic functions

Encoding classical data in quantum states

Quantum models as sums of periodic functions

1. time-evolution embedding: $S(x_i) = e^{iHx_i}$ for feature i.
2. *layered* model circuit

$$U(\mathbf{x}, \theta) = W_{N-1}(\theta_{N-1}) \prod_{i=N-2}^{0} S_i(x_i) W_i(\theta_i)$$

3. $H = \mathrm{diag}\left(\lambda_0^{\mathrm{i}}, \ldots \lambda_{\mathrm{d}-1}^{\mathrm{i}}\right)$

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$$f(\mathbf{x}, \theta) = \sum_{\omega_0 \in \Omega_0} \cdots \sum_{\omega_{N-1} \in \Omega_{N-1}} c_{\omega_0 \ldots \omega_{N-1}}\left(\theta\right) e^{i\omega_0 x_0} \ldots e^{i\omega_{N-1} x_{N-1}},$$

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where **the frequencies are completely determined by the eigenvalues of the data-encoding Hamiltonian**

$$\Omega_i = \left\{ \lambda_s^i - \lambda_t^i | s, t \in \{1, \ldots d\} \right\}$$

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Encoding classical data in quantum states

Quantum models as sums of periodic functions

Furthermore, if λ_s^i, λ_t^i are integer (s.a. for Pauli gates), $f(\mathbf{x}, \theta)$ becomes a *Fourier series*

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In particular, by repeating the encoding of a feature, we can obtain multiple of the period.

For instance, if two of the features are the same, then $x_i = x_j = x$

$$e^{i n_i x_i} e^{i n_j x_j} = e^{i\left(n_i + n_j\right) x}$$

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From this observation and the universality of Fourier series follows the *universality of quantum models with time evolution encoding*.

Practical matters

Access to Fourier coefficients in time evolution encoding

What about the coefficients $c_{n_0,\dots n_{N-1}}(\theta)$?

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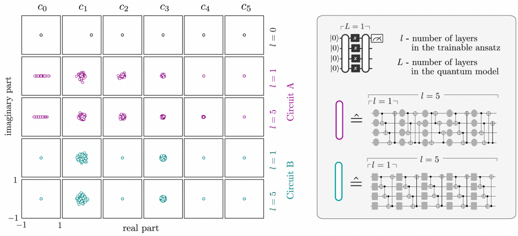
- All the elements of the circuit model determine them (data encoding, ansatz, measurement).
- No matter the frequency that we encode for x_i, if some $c_{n_i} = 0$, then we cannot *access* those frequencies.
- How each element affects each coefficient is a matter of active research.



Practical matters

Gradients

Computing gradients is done with the *parameter shift rule* (PSR). E.g. for Pauli gates:

$$\frac{\partial f}{\partial \theta_i} = \frac{f(\theta_i + s) - f(\theta_i - s)}{2}$$

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How many *model evaluations* we need to compute the *full gradient*?

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How many *model evaluations* we need to compute the *full gradient*?

backpropagation	2
PSR	$2 n_{\text{params}} n_{\text{shots}}$

Practical matters

Gradients

Is this a fair comparison?

Practical matters

Gradients

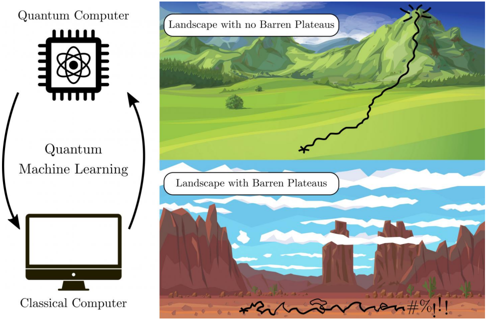
Is this a fair comparison?

Not really...

	n. steps	$O(N)$ linear algebra	parallelization	optimized libraries
Classical	$+$	-	$++$	$++$
Quantum	$-$	$+$	$+$	$+$

Practical matters

Barren plateaus



Practical matters

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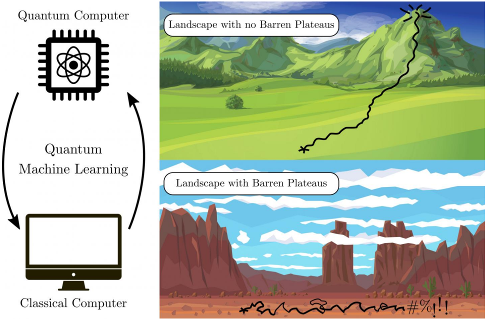

$$\mathrm{Var}\left[\partial_{\theta_i} C(\theta)\right] \leq F(n),$$

$$F(n) \in O\left(\frac{1}{b^n}\right), \; b > 1$$

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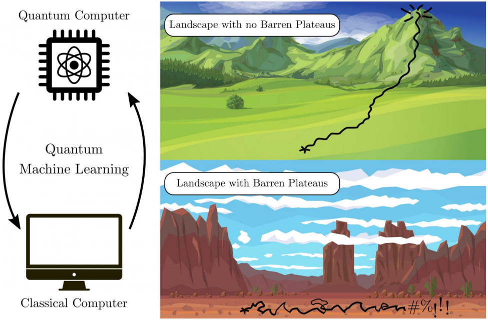

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- Different reasons, the main one is the ansatz $W(\theta)$
- *Problem-agnostic* ansatze suffer from BPs with high n and high depths[14]

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Links for demos

https://colab.research.google.com/github/debrevitatevitae/LabSessionQML/blob/main/variational-classifier-parity.ipynb

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