// Nathan Killoran

XANADU

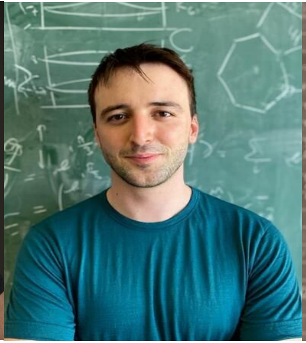
Better than classical?
The subtle art of benchmarking quantum ML models

QTML, November 2023

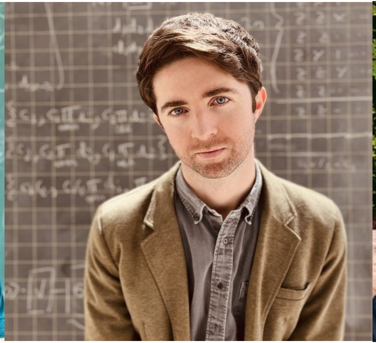
// Credits

Xanadu’s quantum machine learning team

Dr Maria Schuld
QML Team lead



Dr Richard East
Researcher



Dr Joseph Bowles
Researcher

Dr David Wakeham
Researcher

Dr Shahnawaz Ahmed
Researcher

Dr Nathan Killoran
CTO Software

Dr Chae-Yeun Park
Researcher

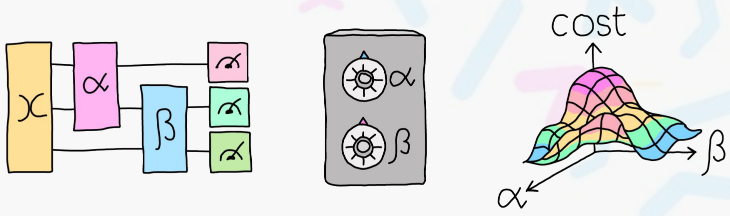
Dr David Wierichs
Researcher

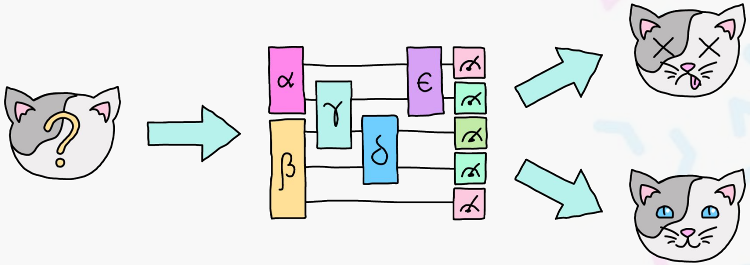
Dr Korbinian Kottmann
Researcher

We’re hiring!

// The QML team objective

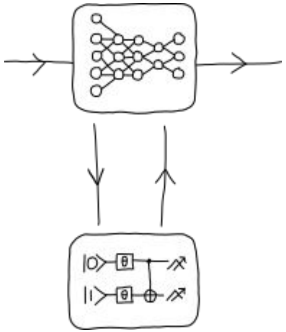
Make quantum computers useful for machine learning





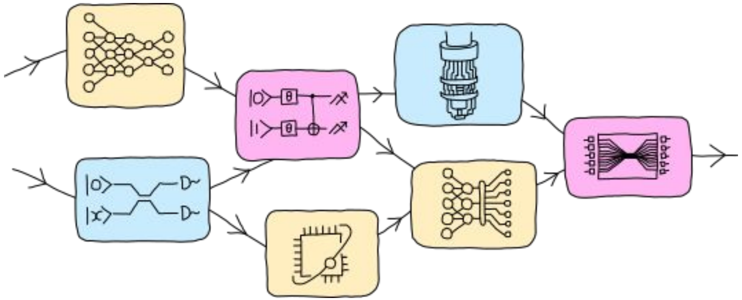
Progress in quantum machine learning

Pre-NISQ: Fault-tol. subroutines



Outsource parts of the computation to a quantum computer

NISQ era: Variational circuits

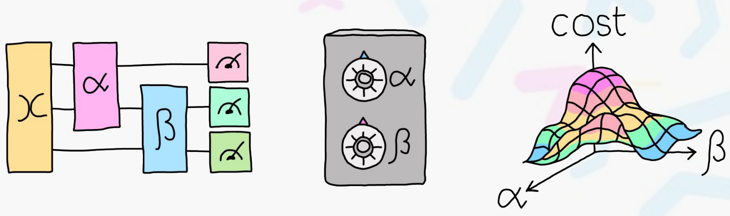


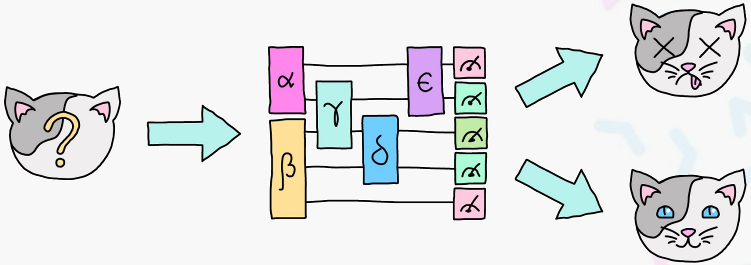
Use a model that is intrinsically quantum

// The QML team objective

Make quantum computers useful for machine learning

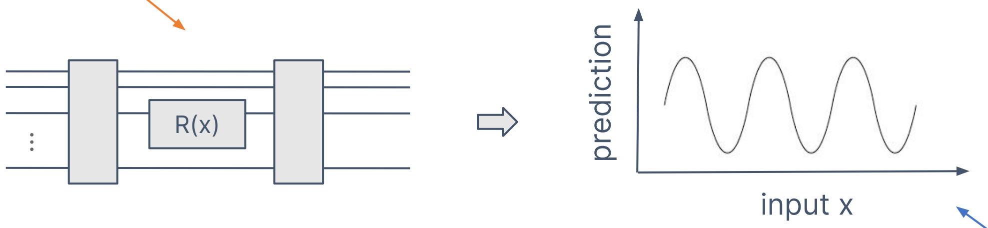
For this to happen we need to change some things in our approach to research





"We use an ansatz of Pauli gates and entanglers…"

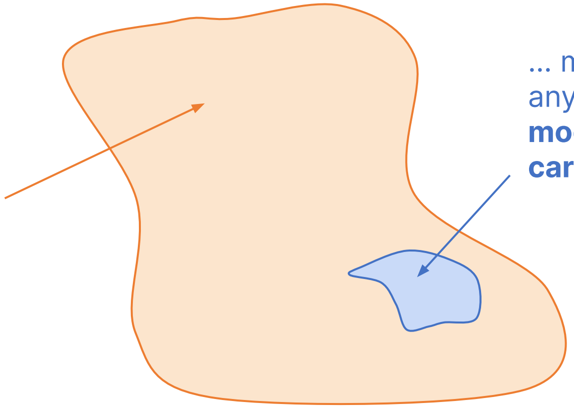
An impressive quantum circuit
(of 10,000 qubits and 1 billion parameters with universal, classically intractable unitary evolutions imitating a deep learning technique)…



…can be a **useless ML model.**

Our circuit designs should be motivated better.

"Quantum models generalise/train better/worse…"

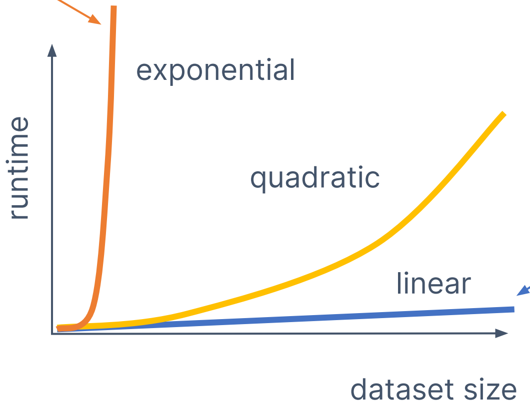


We don't know if our theory targets relevant questions.

// Checking the compass: Performance

“We prove an exponential speedup for QML…”

The problem that neural networks solve is **exponentially hard in theory…**

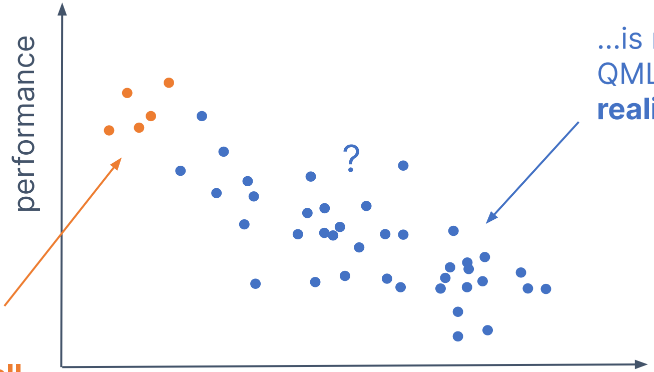


…but in practice neural nets run in **linear time.**

Our performance measures are not meaningful for (mainstream) ML.

// Checking the compass: Performance

“Our quantum model does better on MNIST…”



Our experiments do not probe the right regimes yet.

The subtle art of benchmarking

[Note: work in progress!]

What is the best benchmark design we can come up with?

Model selection

- Arxiv papers >2018 with keywords “classif”, “learn”, “supervised”, “MNIST” [3500 papers]
- >=30 Google Scholar citations [561 papers]
- New NISQ quantum model for classification on conventional classical data [29 papers]
- In random subset of 15 papers
- Found implementable [11 papers]

→ Coded up 12 models

QNN

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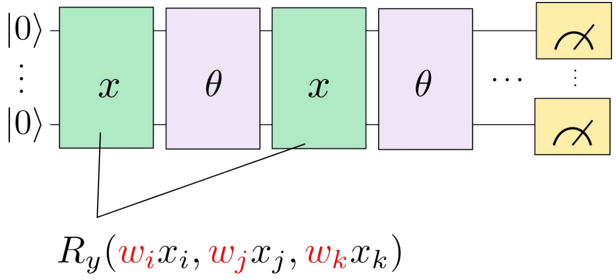

DataReuploadingClassifier

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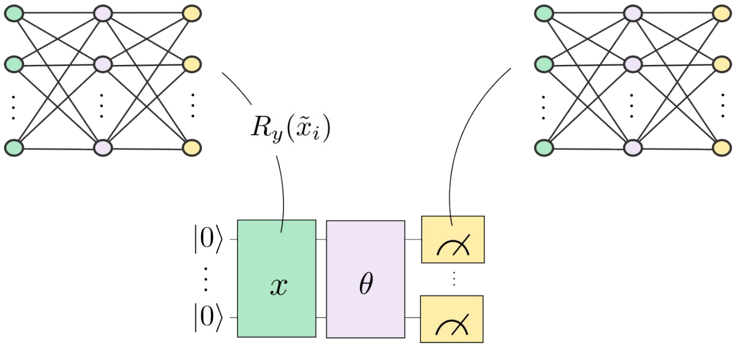

DressedQuantumCircuitClassifier

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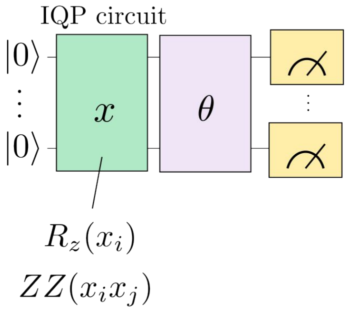

IQPVariationalClassifier

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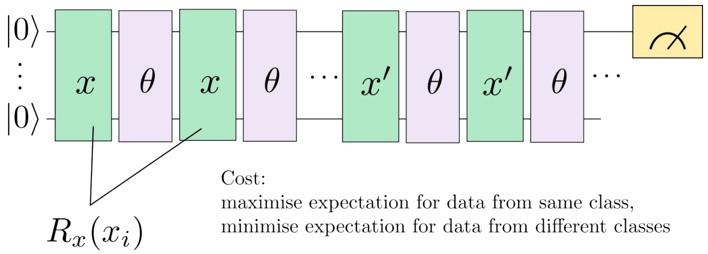

QuantumMetricLearner

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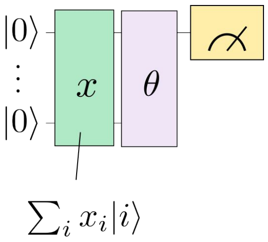

CircuitCentricClassifier

QNN

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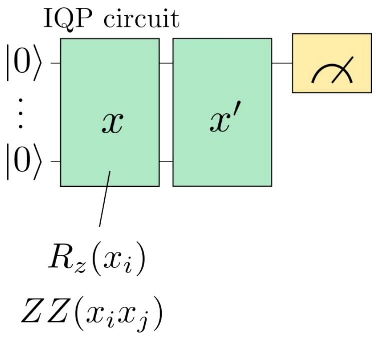

IQPKernelClassifier

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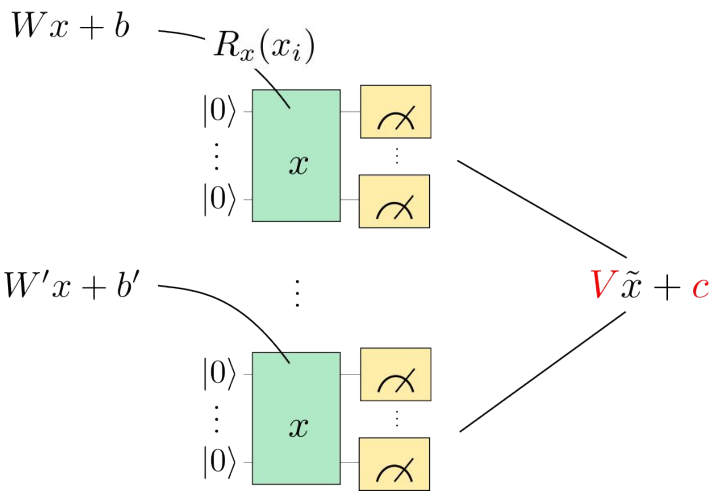

QuantumKitchenSinks

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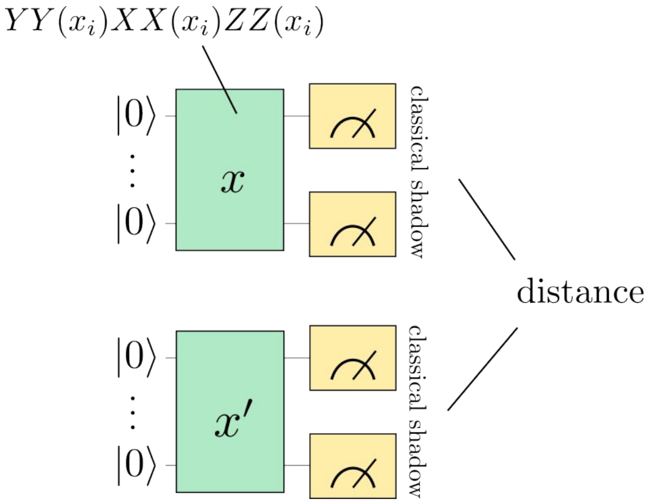

ProjectedQuantumKernel

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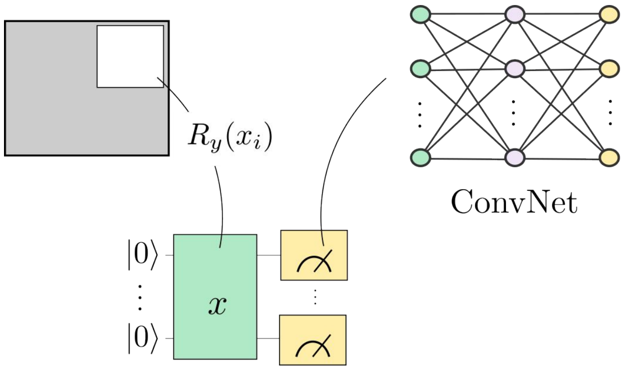

QuanvolutionalNeuralNetwork

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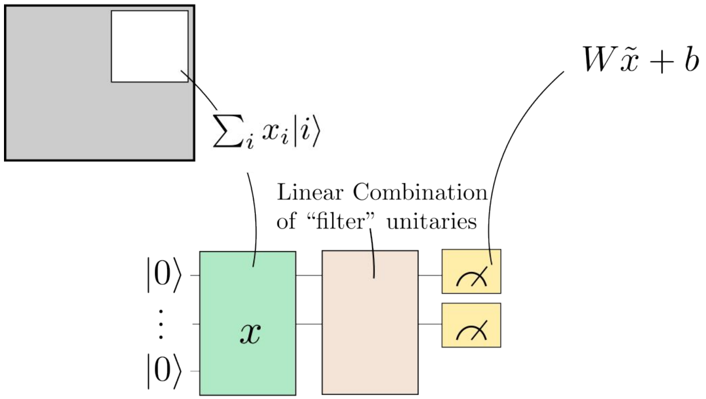

WeiNet

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// Assess how good quantum models really are

What is the best benchmark design we can come up with?

Tasks

- Binary classification
- Figure of merit: accuracy
- 4 datasets of variable dimension:

// Assess how good quantum models really are

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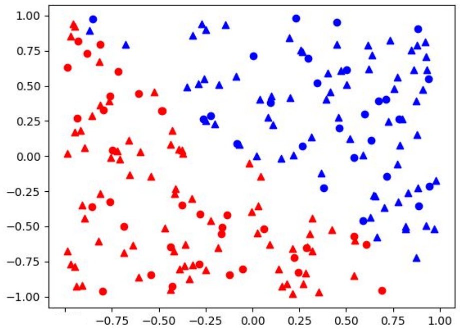
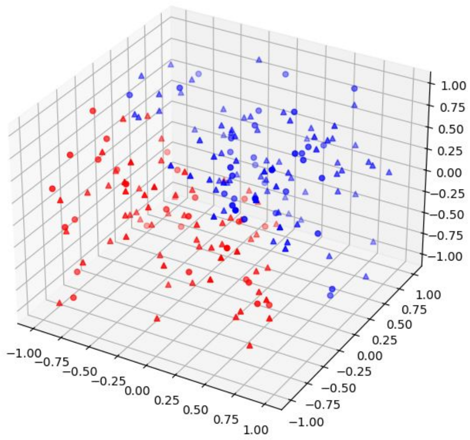


Tasks

- Binary classification
- Figure of merit: accuracy
- 4 datasets of variable dimension:
    - **SIMPLE:** Linearly separated points in hypercube



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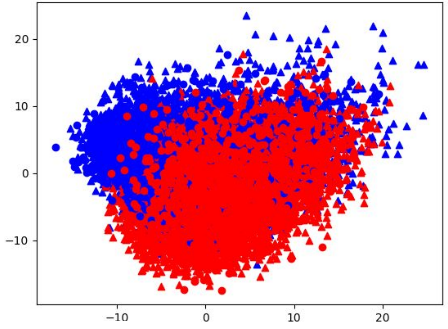
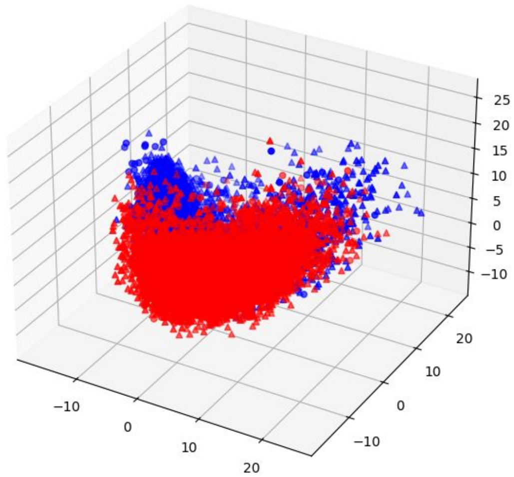


Tasks

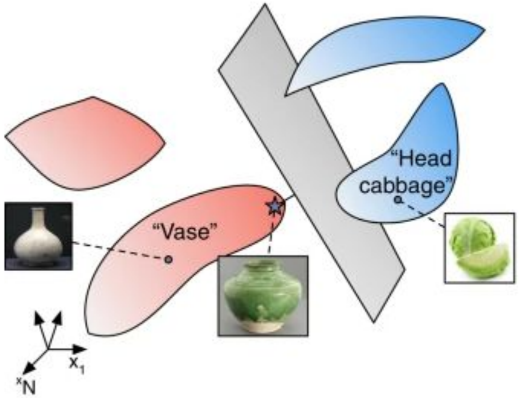
- Binary classification
- Figure of merit: accuracy
- 4 datasets of variable dimension:
    - **SIMPLE:** Linearly separated points in hypercube
    - **WIDELY USED:** Pre-processed MNIST



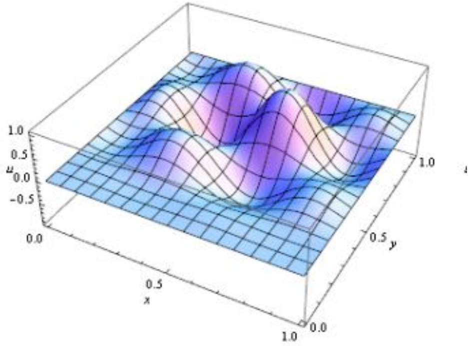
What is the best benchmark design we can come up with?

Tasks

- Binary classification
- Figure of merit: accuracy
- 4 datasets of variable dimension:
  - **SIMPLE:** Linearly separated points in hypercube
  - **WIDELY USED:** Pre-processed MNIST
  - [**REALISTIC:** Low-dimensional manifolds (Goldt 2019, Buchanan 2020)]
  - [**TAILORMADE:** Multi-dimensional Fourier series]



https://www.nature.com/articles/s41467-020-14578-5



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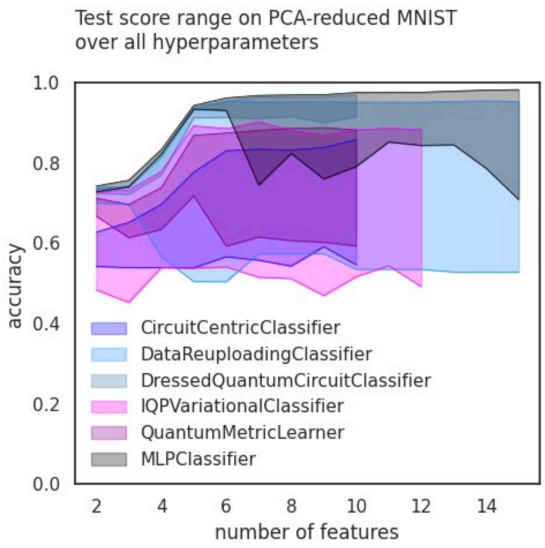
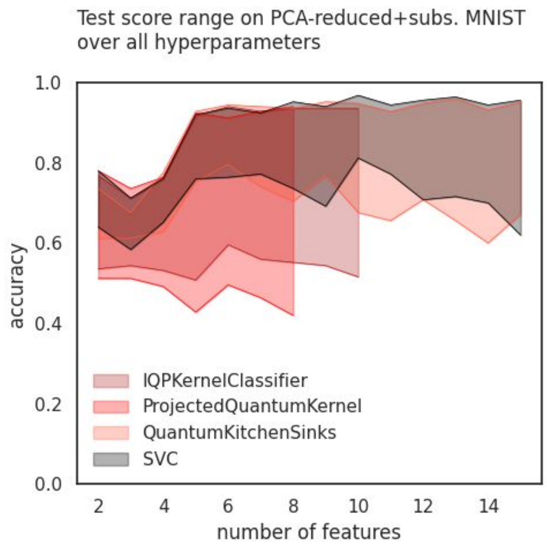
What is the best benchmark design we can come up with?

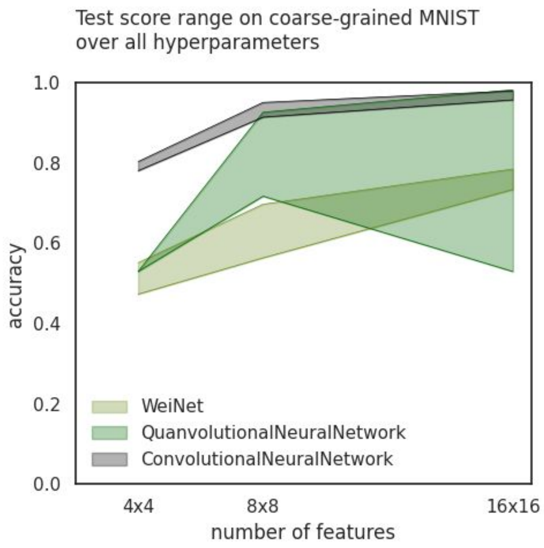
Crucial decisions

- Faithful implementation
  We carefully deduced the model design and training procedure from the paper
- Convergence criteria
  We compare averages over 2 loss intervals
- Batches in SGD
  We didn’t optimize this hyperparameter, but adapted it to runtime needs
- Data preprocessing
  We always prescaled data to a meaningful interval (like [0, 2pi])
- Hyperparameter optimisation grid
  We balanced choices from paper, common sense and runtime considerations
- Classical comparison
  We pick matching box classical models with typical sizes: NN, SVM, CNN

Hyperparameters matter

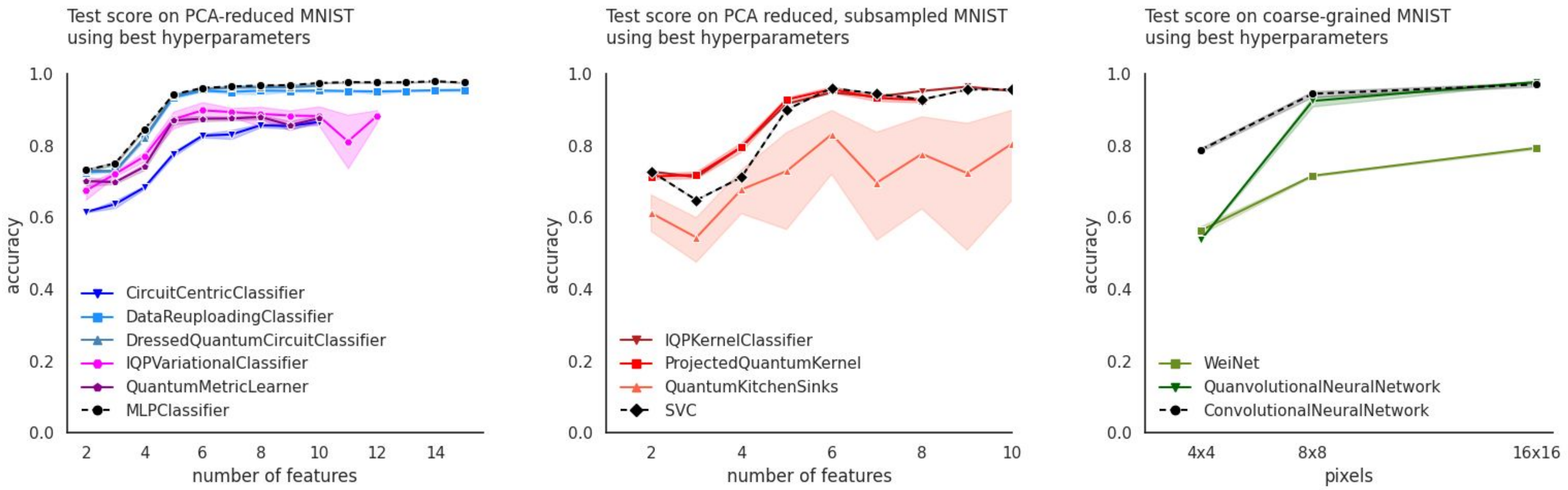






// Preliminary results

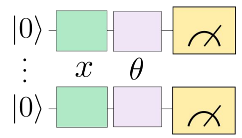
Out-of-the box classical models are not easily beaten

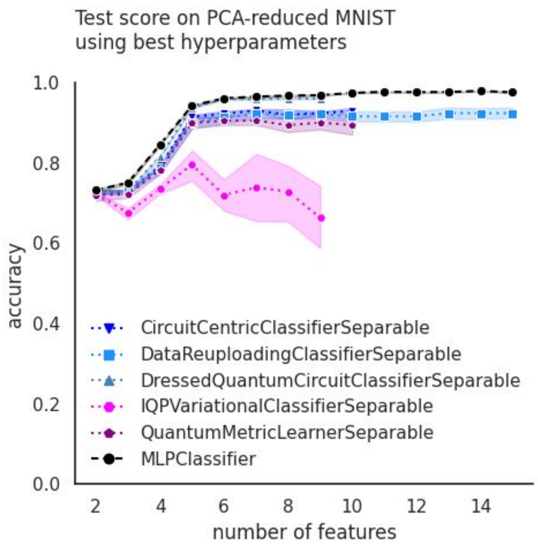


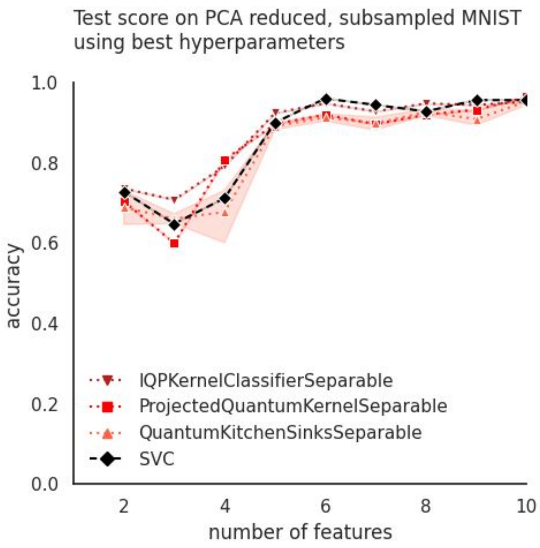
// Preliminary results

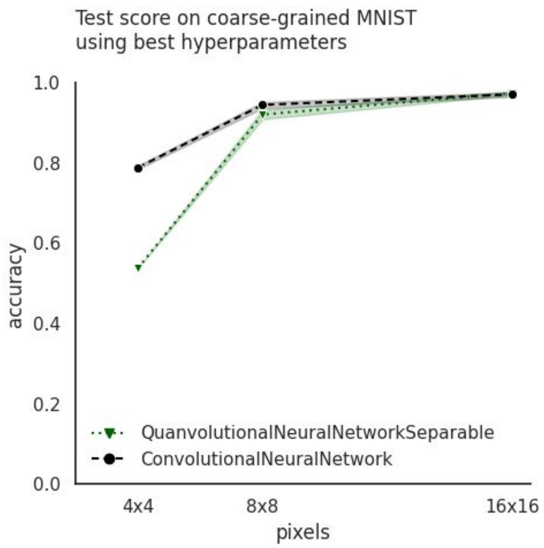
Separable circuits perform the same

This is (more or less) the basic circuit we replace all quantum circuits with!









// A possible explanation

What “features” do our quantum models create?

Example for input $x = [x_1, x_2]$

trigonometric

$\sin(x_1)\sin(x_2)$
$\sin(x_1)\cos(x_2)$
$\cos(x_1)\sin(x_2)$
$\cos(x_1)\cos(x_2)$

QNN

Pérez-Salinas et al. "Data re-uploading for a universal quantum classifier." 1907.02085v3

Mari et al. "Transfer learning in hybrid classical-quantum neural networks." 1912.08278v2

*Havlíček et al. "Supervised learning with quantum-enhanced feature spaces." 1804.11326v2

Lloyd et al. "Quantum embeddings for machine learning." 2001.03622

Schuld et al. "Circuit-centric quantum classifiers." 1804.00633v1

[Zhang et al. "Toward trainability of quantum neural networks." 2011.06258v2]

[Zoufal et al. "Variational quantum Boltzmann machines." 2006.06004v1]

QKernel

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QConv

Henderson et al. "Quanvolutional neural networks: powering image recognition.." 1904.04767v1

Wei "A quantum convolutional neural network on NISQ devices." 2104.06918v3

Schuld, Sweke, Meyer (2020) arXiv 2008.08605

// A possible explanation

What “features” do our quantum models create?

Example for input $x = [x_1, x_2]$

scaling + trigonometric

$\sin(w_1 x_1)\sin(w_2 x_2)$
$\sin(w_1 x_1)\cos(w_2 x_2)$
$\cos(w_1 x_1)\sin(w_2 x_2)$
$\cos(w_1 x_1)\cos(w_2 x_2)$

QNN

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// A possible explanation

What “features” do our quantum models create?

Example for input $x = [x_1, x_2]$

linear + trigonometric

```
sin(vx+b1)sin(wx+b2)
sin(vx+b1)cos(wx+b2)
cos(vx+b1)sin(wx+b2)
cos(vx+b1)cos(wx+b2)
```

QNN

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// A possible explanation

What “features” do our quantum models create?

Example for input $x = [x_1, x_2]$

NN + trigonometric

```
sin(φ(vx))sin(φ(wx))
sin(φ(vx))cos(φ(wx))
cos(φ(vx))sin(φ(wx))
cos(φ(vx))cos(φ(wx))
```

QNN

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// A possible explanation

What "features" do our quantum models create?

Example for input $x = [x_1, x_2]$

poly + trigonometric

```
sin(x1)sin(x2)sin(x1x2)
sin(x1)sin(x2)cos(x1x2)
…
cos(x1)cos(x2)cos(x1x2)
```

QNN

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// A possible explanation

What “features” do our quantum models create?

Example for input $x = [x_1, x_2]$

polynomial

$c \ldots cc$
$c \ldots cx_1$
$\ldots$
$x_2 \ldots x_2 x_2$

QNN

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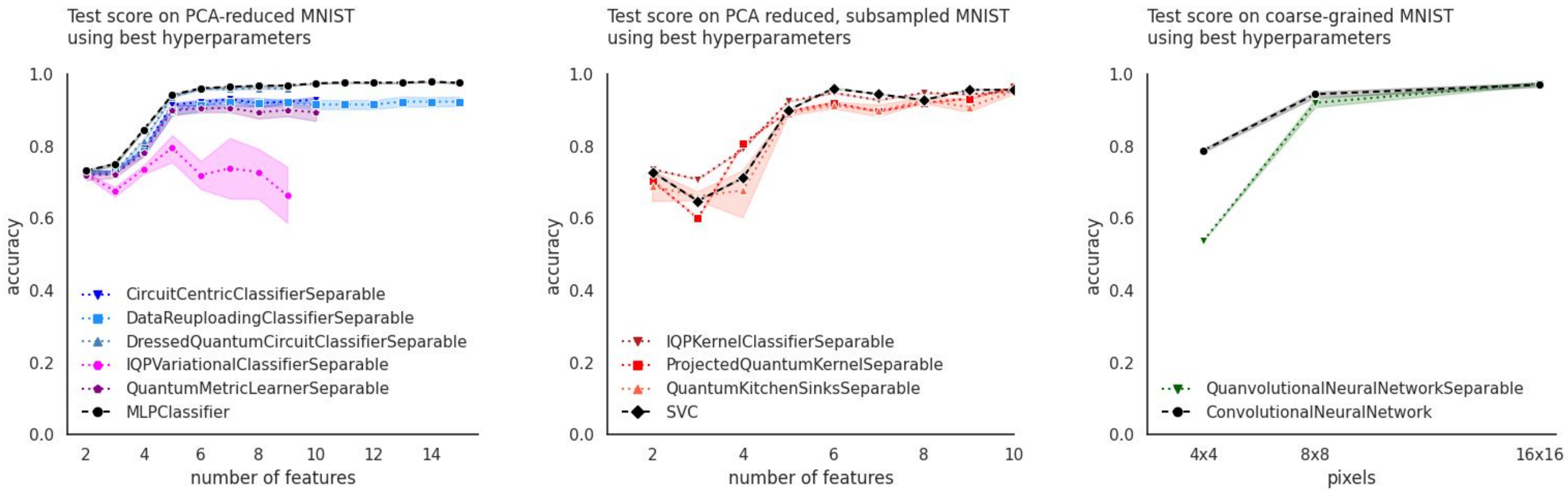
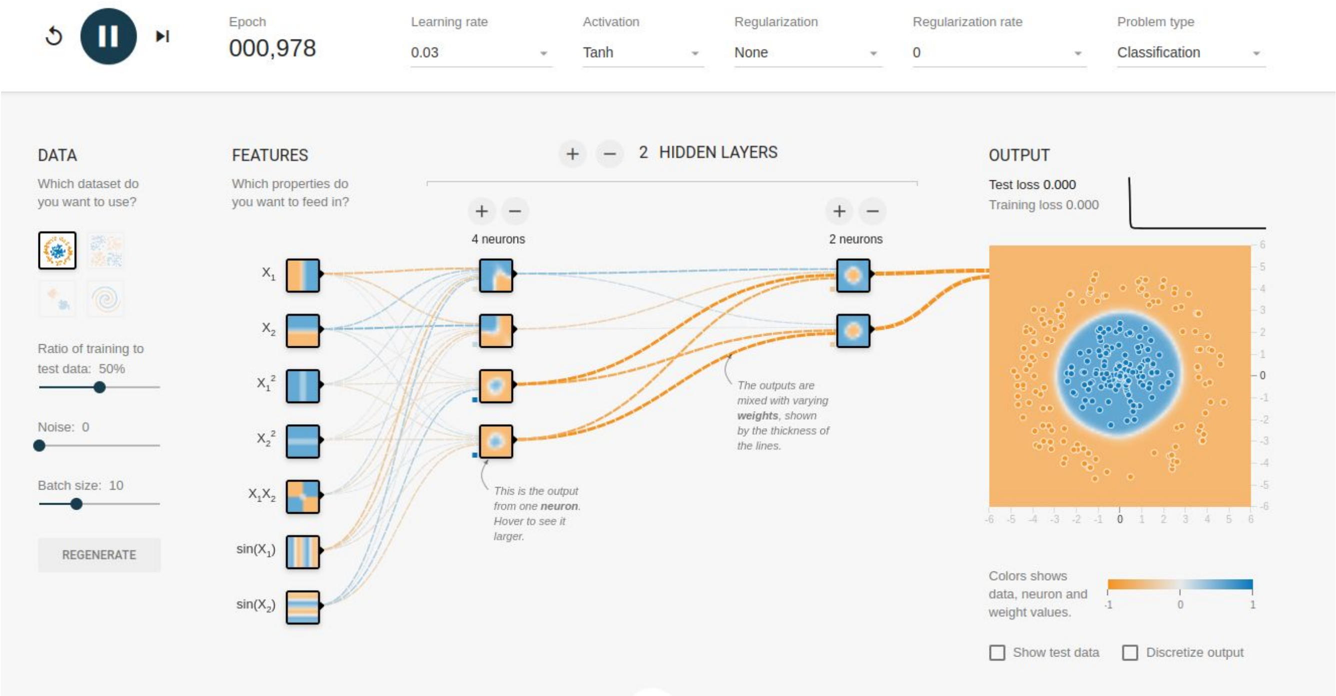
// Preliminary results

Separable circuits perform the same



// A possible explanation

Are we “just” building trigonometric/polynomial feature extractors?

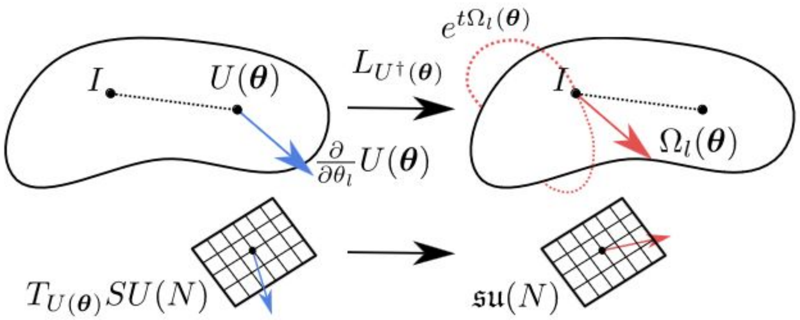


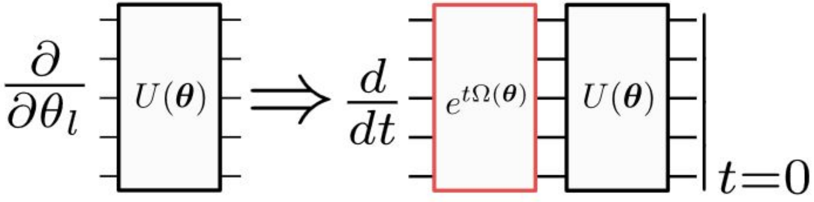
https://playground.tensorflow.org/

Here comes the SU(N): multivariate quantum gates and gradients

Roeland Wiersema,[1,2] Dylan Lewis,[3] David Wierichs,[4] Juan Carrasquilla,[1,2] and Nathan Killoran[4]

[1] Vector Institute, MaRS Centre, Toronto, Ontario, M5G 1M1, Canada
[2] Department of Physics and Astronomy, University of Waterloo, Ontario, N2L 3G1, Canada
[3] Department of Physics and Astronomy, University College London, London WC1E 6BT, United Kingdom
[4] Xanadu, Toronto, ON, M5G 2C8, Canada





Tomorrow!

21 Nov 2023, 16:45

Thank you

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