Quantum machine learning with qudits

Sebastián Roca-Jerat

Juan Román-Roche, Fernando Luis, David Zueco

INMA - CSIC

31-05-23

Plan de Recuperación, Transformación y Resiliencia

Financiado por la Unión Europea NextGenerationEU

Outline

I. **Introduction of single qudit processors**

II. Learning with qudits

III. Results

IV. Conclusions

Introduction of single qudit processors

Quantum SPAIN

PHYSICAL REVIEW APPLIED **17**, 064030 (2022)

Dispersive Readout of Molecular Spin Qudits

Álvaro Gómez-León,[1,*] Fernando Luis,[2] and David Zueco[2]

PHYSICAL REVIEW APPLIED **17**, 064028 (2022)

Optimal Control of Molecular Spin Qudits

Alberto Castro,[1,2,*] Adrián García Carrizo,[2] Sebastián Roca,[3,4] David Zueco,[3,4] and Fernando Luis[3,4]

Chemical Science
ROYAL SOCIETY OF CHEMISTRY
EDGE ARTICLE
View Article Online
View Journal | View Issue
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Cite this: *Chem. Sci.*, 2021, 12, 5621
All publication charges for this article have been paid for by the Royal Society of Chemistry

Broad-band spectroscopy of a vanadyl porphyrin: a model electronuclear spin qudit†

Ignacio Gimeno,[a] Ainhoa Urtizberea,[ab] Juan Román-Roche,[a] David Zueco,[a] Agustín Camón,[a] Pablo J. Alonso,[a] Olivier Roubeau[*a] and Fernando Luis[*a]

communications physics
ARTICLE
https://doi.org/10.1038/s42005-022-01017-8 OPEN
Check for updates

High cooperativity coupling to nuclear spins on a circuit quantum electrodynamics architecture

Victor Rollano[1,2], Marina C. de Ory[3], Christian D. Buch[4], Marcos Rubín-Osanz[1,2], David Zueco[1,2], Carlos Sánchez-Azqueta[5], Alessandro Chiesa[6,7,8], Daniel Granados[9], Stefano Carretta[6,7,8], Alicia Gomez[3], Stergios Piligkos[4] & Fernando Luis[1,2✉]

Accepted Paper | Featured in Physics

Blueprint for a molecular-spin quantum processor

Phys. Rev. Applied

A. Chiesa, S. Roca, S. Chicco, M. C. de Ory, A. Gómez-León, A. Gomez, D. Zueco, F. Luis, and S. Carretta

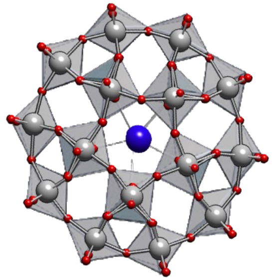
Accepted 24 April 2023

Quantum
Materials and Devices

Introduction of single qudit processors

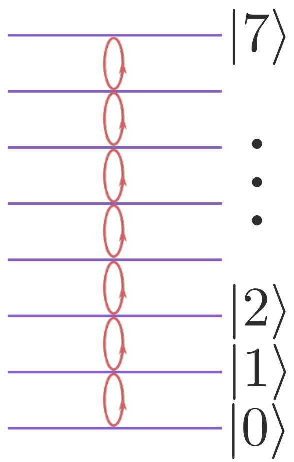
Quantum computing

d-level system → Qudit!

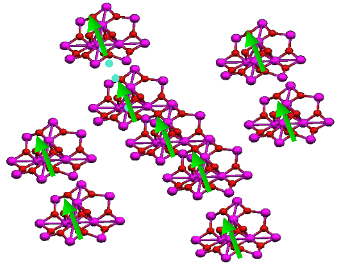


GdW_{30}

Phys. Rev. B. 95, 064423 (2017)



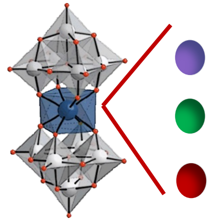
Reproducibility



Identical microscopic qudits

Nature chemistry 11 (4), 301-309 (2019)

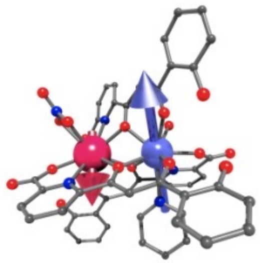
Tunability



Fine tuning of qudit properties

Phys. Rev. Lett. 108, 247213 (2012)

Scalability



Molecular NISQs

Appl. Phys. Lett. 118, 240501 (2021)

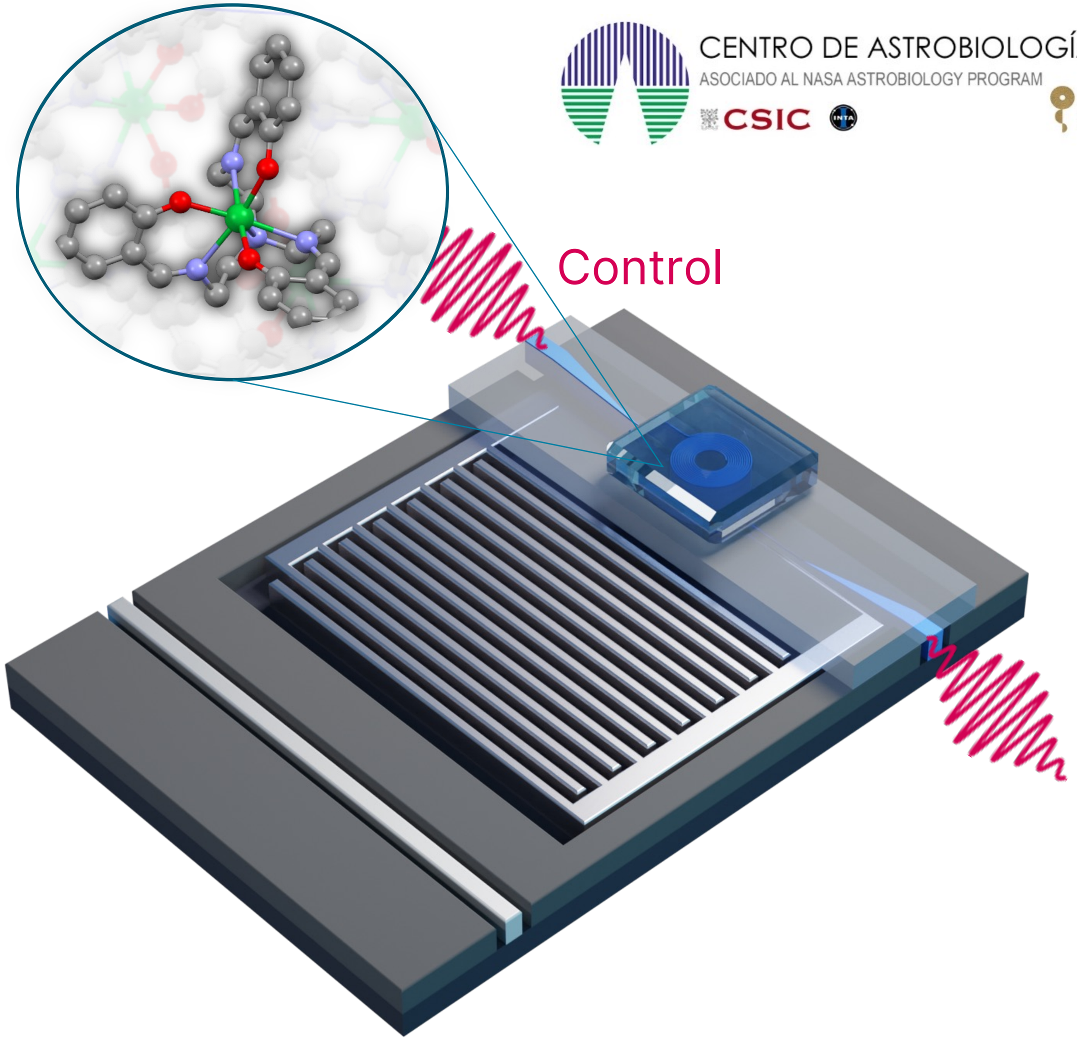
Introduction of single qudit processors

- Coupling molecules to superconducting circuits: Lumped Element Resonators

Tunable resonant frequency to match spin levels

$$\omega_r = \frac{1}{\sqrt{LC}}$$

- Coupling via microwave electromagnetic fields



M. Jenkins *et al. NJP 15, 095007 (2013)*

V. Rollano *et al. Comm. Phys. 5, 246 (2022)*

Outline

I. Introduction of single qudit processors

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Learning with qudits

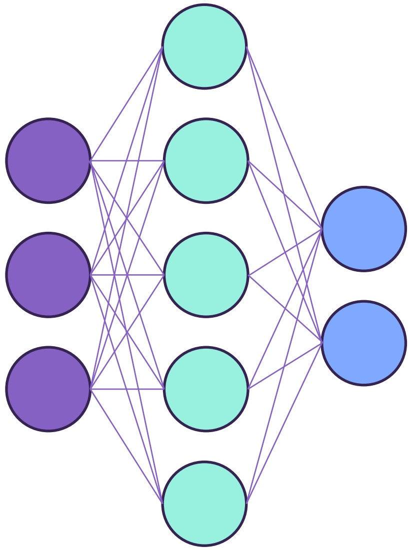
Motivation: supervised learning tasks

- Digital paradigm

  → Usual neural network models, random forests, Xgboost...

TensorFlow + Keras

PyTorch



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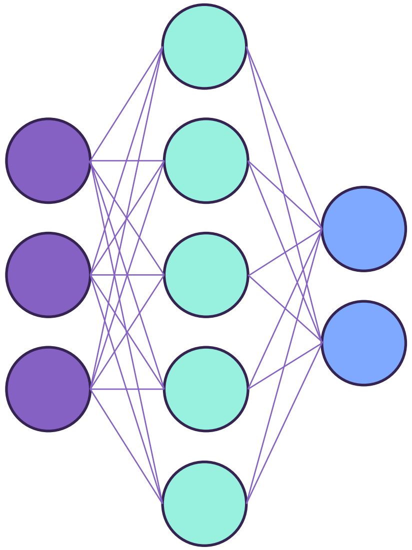
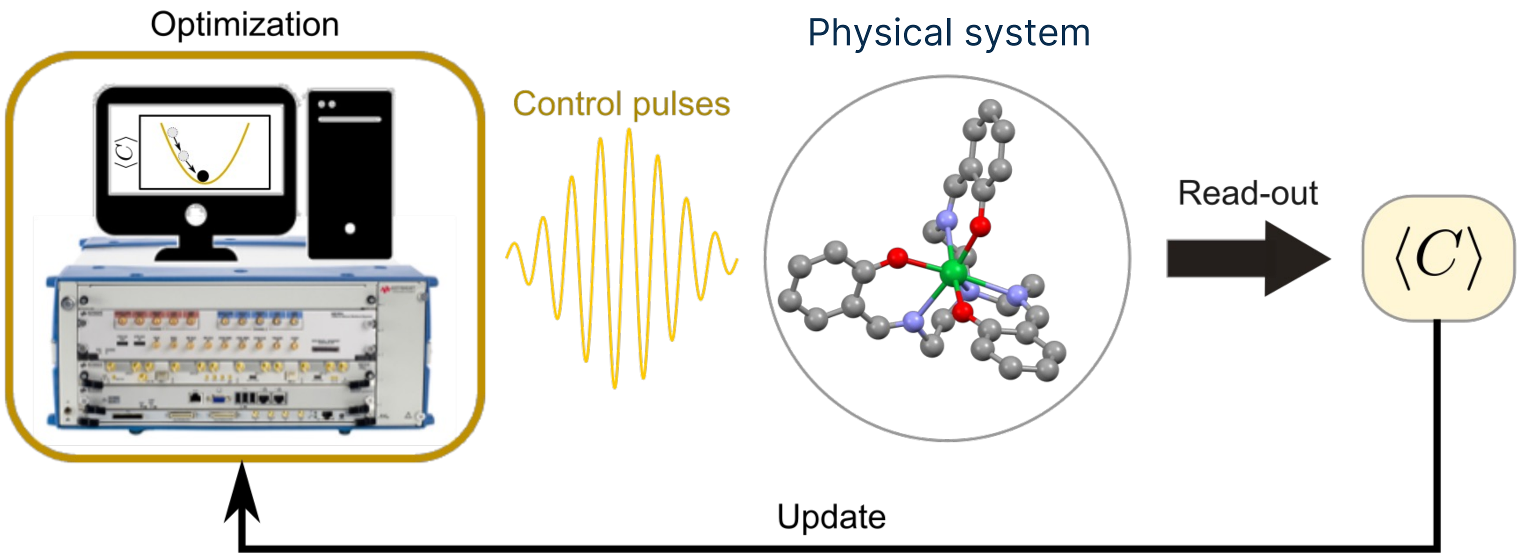


- Digital-analog perspective

  → Ising machines, reservoir computing, etc



L. G. Wright *et al. Nature 601, 549-555 (2022)*

Learning with qudits

Quantum SPAIN

Motivation: supervised learning tasks

Data re-uploading for a universal quantum classifier

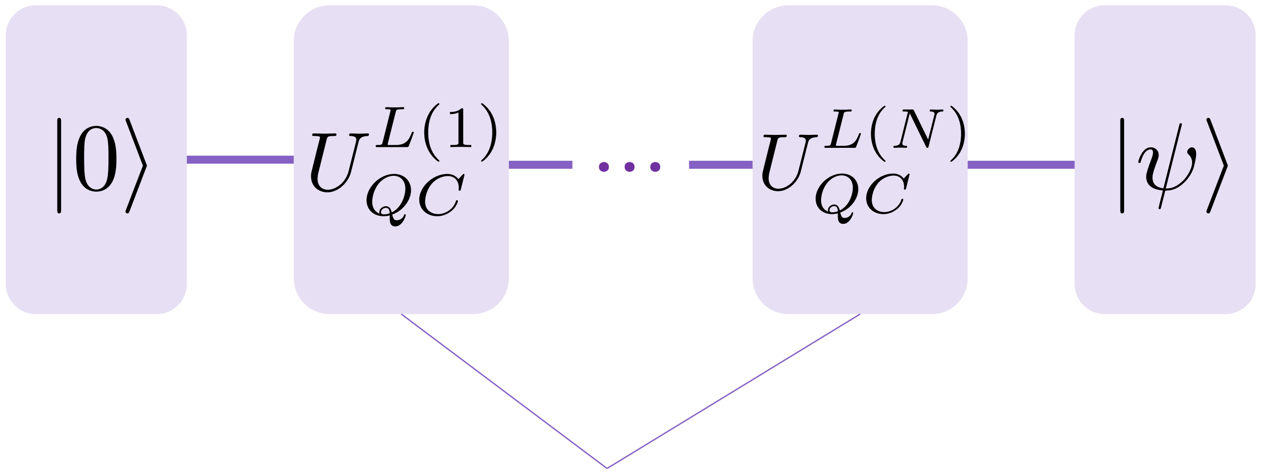
Adrián Pérez-Salinas[1,2], Alba Cervera-Lierta[1,2], Elies Gil-Fuster[3], and José I. Latorre[1,2,4,5]

[1]Barcelona Supercomputing Center
[2]Institut de Ciències del Cosmos, Universitat de Barcelona, Barcelona, Spain
[3]Dept. Física Quàntica i Astrofísica, Universitat de Barcelona, Barcelona, Spain.
[4]Nikhef Theory Group, Science Park 105, 1098 XG Amsterdam, The Netherlands.
[5]Center for Quantum Technologies, National University of Singapore, Singapore.

Quantum 4, 226 (2020)

$$\mathcal{L}(\vec{x};\vec{\varphi}) = \sum_{n=1}^{N} \left(1 - |\langle\psi(\vec{x}_n;\vec{\varphi}_n)|\psi_n^R\rangle|^2\right)$$

$$|\psi\rangle = \prod_{l=1}^{N} U_{QC}^{l}(\vec{x},\vec{\phi}_l)|\psi_0\rangle \quad \max\left\{|\langle\psi|\psi_{\mathrm{i}}^{\mathrm{R}}\rangle|\right\} \to \text{class}$$



Layers to increase non-linearity in the model

Learning with qudits

Motivation: supervised learning tasks

- Generalization to more than two levels? Any advantage? Any new paradigm?

Learning with qudits

Motivation: supervised learning tasks

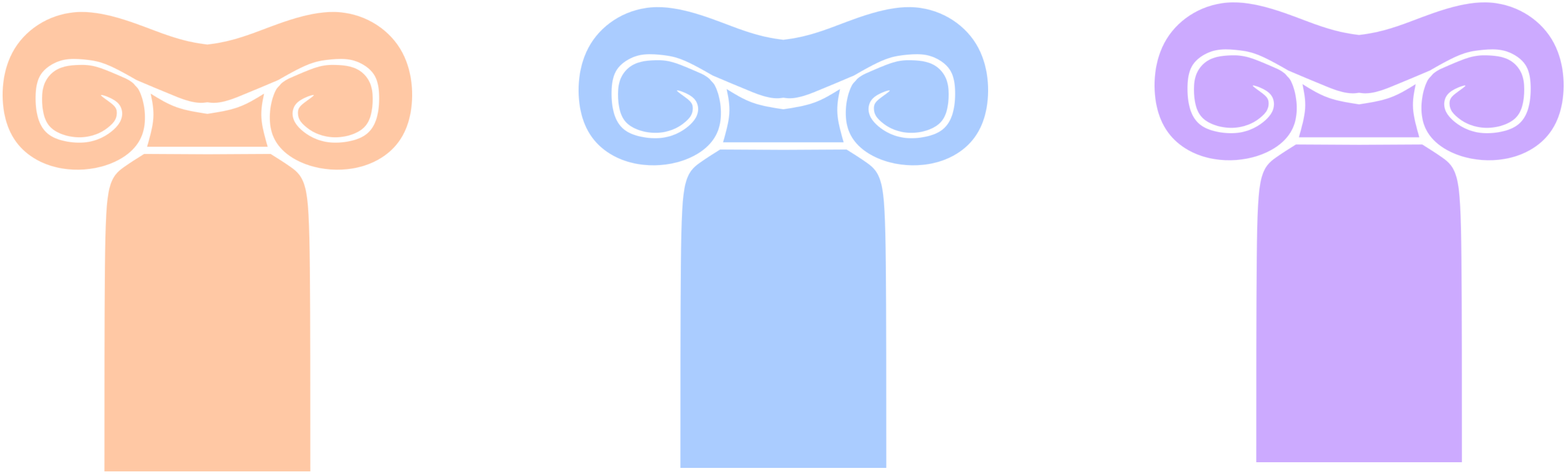
- Generalization to more than two levels? Any advantage? Any new paradigm?
- What is the model really “learning”?

Learning with qudits

Variational Algorithms

Encoding strategy

Metric Learning

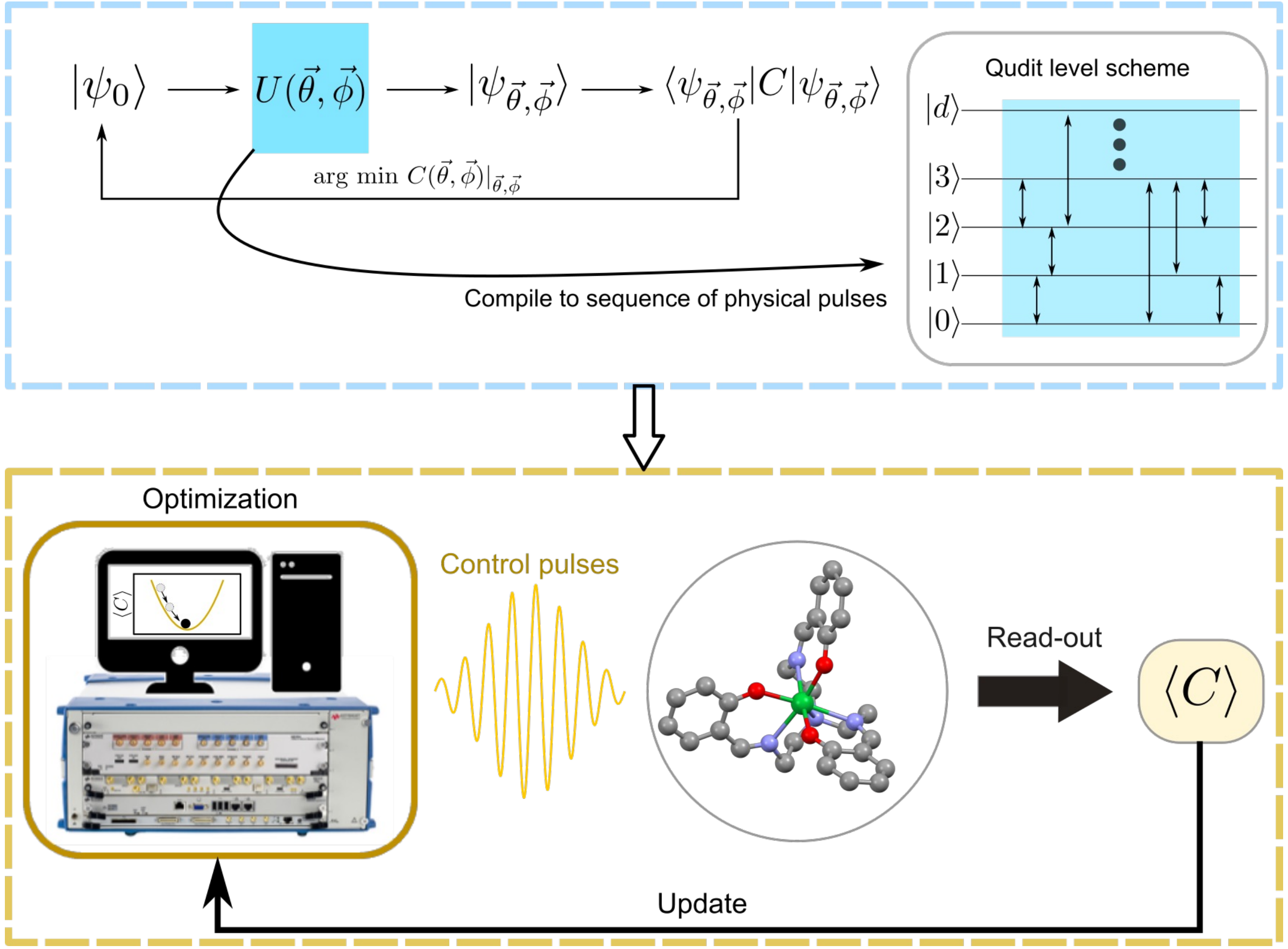


Learning with qudits

Variational algorithms

- Hybrid quantum-classical algorithm: classical optimizer + quantum processor

- Finding ground states, dynamical simulations, error correction, machine learning…



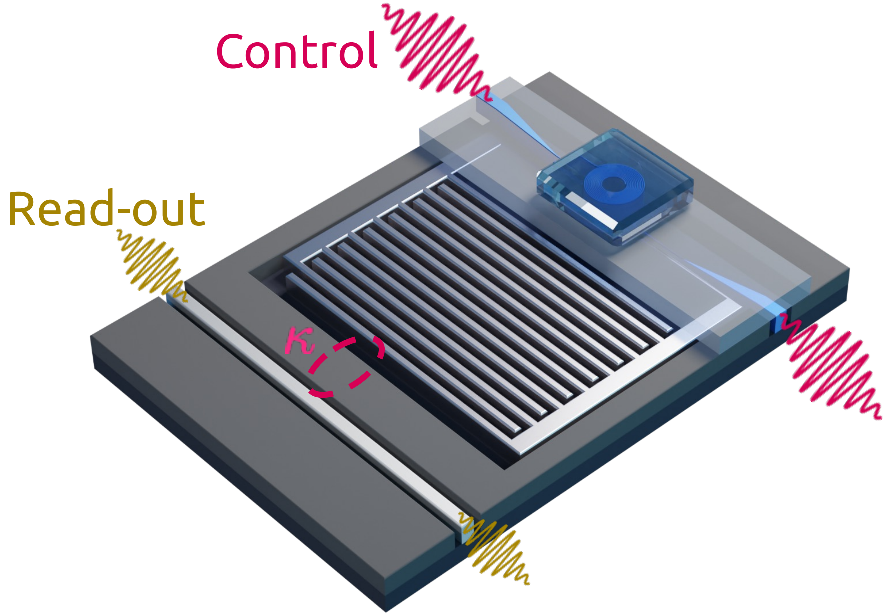
A. Peruzzo *et al. Nat Comm 5, 4213 (2014)*
A. Kandala *et al. Nature 549, 242-246 (2017)*
A. Chiesa *et al. Nat Phys 15, 455-459 (2019)*
M. Cerezo *et al. Nat. Rev. Phys. 3, 625-644 (2021)*

Learning with qudits

Variational algorithms: ansatz

Our ansatz: monochromatic RF pulses → Rotations in the XY-plane of the two levels involved

$$\mathcal{H}_{\rm d} = -g\mu_{\rm B}\cos(\omega t + \phi)\vec{b}_{\rm rf} \cdot \vec{S}$$



A. Castro *et al. Phys. Rev. Applied 17, 064028* (2022)

Learning with qudits

Variational algorithms: ansatz

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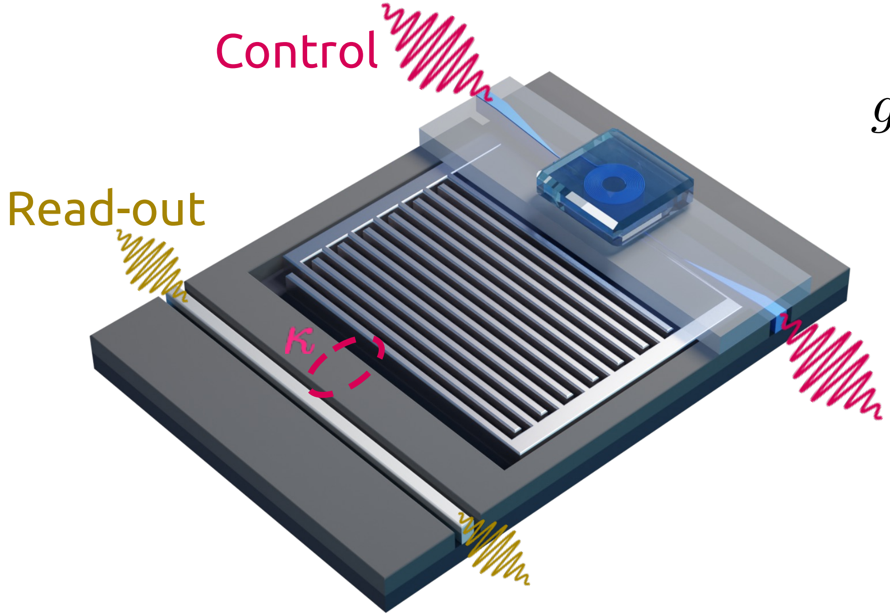
$$\mathcal{H}_{\rm d} = -g\mu_{\rm B}\cos(\omega t + \phi)\vec{b}_{\rm rf}\cdot\vec{S} \longrightarrow R_{j,k}(\theta,\varphi) = g_{j,k}(\theta,\varphi)\oplus\mathbb{I}_{\overline{jk}}$$



$$g_{j,k}(\theta,\varphi) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2)e^{i\varphi} \\ -i\sin(\theta/2)e^{-i\varphi} & \cos(\theta/2) \end{pmatrix}$$

$$\theta = g\mu_{\rm B}|M_{j,k}|t$$

$$\varphi = \arg M_{j,k} + \phi$$

$$M_{j,k} = \langle j|\vec{b}_{\rm rf}\cdot\vec{S}|k\rangle$$

A. Castro *et al. Phys. Rev. Applied 17, 064028 (2022)*

Learning with qudits

Encoding strategy

Our ansatz: monochromatic RF pulses → Rotations in the XY-plane of the two levels involved

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We have 2(d-1) parameters to tune in a qudit → data of dimension 2(d-1)

However, we can encode higher dimensional data by dividing each point into n vectors of dimension 2(d-1):

$$U_{QC}^{L(i)} = \prod_{j=1}^{n}\prod_{k=0}^{d-2} R_{k,k+1}(\theta_k^{(j)},\varphi_k^{(j)}) \qquad (\vec{\theta},\vec{\varphi}) = \vec{f}(\vec{x},\vec{\phi})$$

A. Pérez-Salinas *et al. Quantum 4, 226 (2020)*

Learning with qudits

Encoding strategy

$$\mathcal{E} : \mathbb{R}^{dim(\vec{x})} \to \mathcal{H}^d$$
$$\vec{x} \mapsto |\psi\rangle$$

$$g : \mathbb{R}^{D_x} \to \mathbb{R}^{D_{x'}}$$
$$\vec{x} \mapsto \vec{x}' = \bar{\omega}\vec{x} + \vec{b}$$

$$(\theta_i, \phi_i) = (x'_{2i}, x'_{2i+1})$$

$$|\psi(\vec{x};\vec{\varphi})\rangle = \hat{U}(\vec{x};\vec{\varphi})|\psi_0\rangle$$

Learning with qudits

Metric learning: implicit vs explicit

In supervised learning, one of the most powerful approaches is Metric Learning.

We want to map our data to a feature space where points belonging to the same class are near to each other while being as far as possible from points belonging to other classes: learning some metric.

Learning with qudits

Metric learning: implicit vs explicit

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We do so in QM! → Our data-points are mapped into the Hilbert space of our qudit.
We seek to map points belonging to the same class to a quantum state that is close to the reference state defined for that class and as far as possible (maximally orthogonal) to the other reference states.

V. Havlícek *et al. Nature 567, 209-212 (2019)*

M. Schuld & N. Killoran *Phys. Rev. Lett. 122, 040504 (2019)*

S. LLoyd *et al. Arxiv:2001.03622v2 (2022)*

Learning with qudits

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S. LLoyd *et al. Arxiv:2001.03622v2 (2022)*

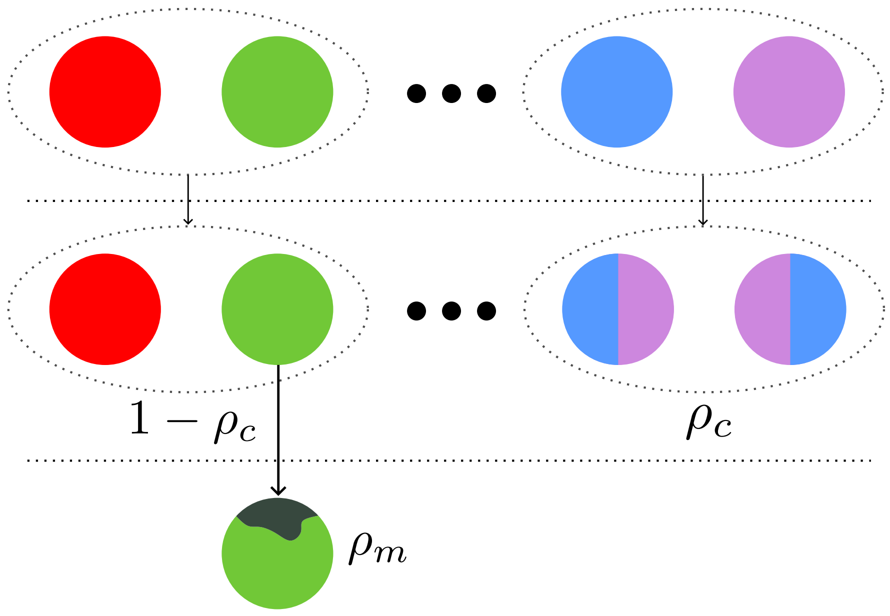
Implicit: you fix the reference states
Explicit: you include these states as parameters to be found in the optimization process

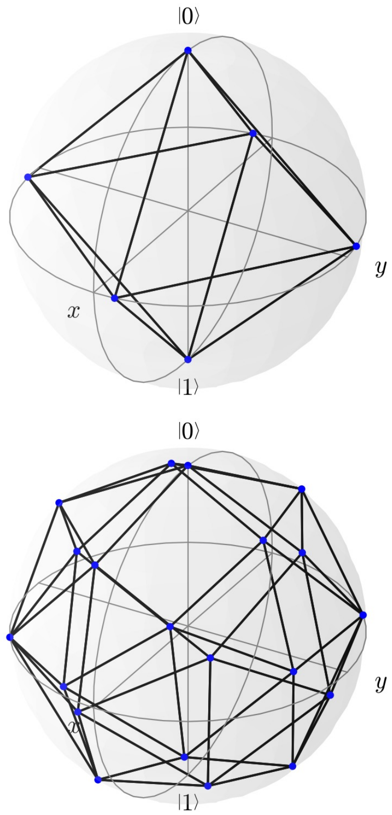
N. A. Nghiem *et al. Phys. Rev. Res. 3, 033056 (2021)*

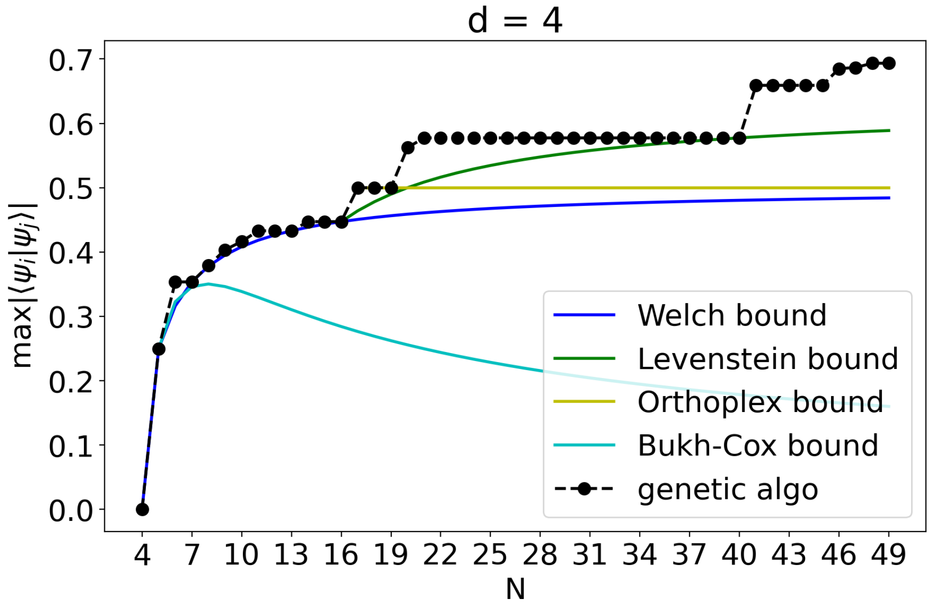
Learning with qudits

Maximally orthogonal states: More classes than levels?

Genetic algorithm for finding maximally orthogonal states for any configuration (d, N)







A. Pérez-Salinas *et al. Quantum 4, 226 (2020)*

S. Smale. *The mathematical intelligencer 20.2 pp. 7-15 (1998)*

J. R. Morris *et al. Phys. Rev. B 53, R1740(R) (1996)*

Learning with qudits

Metric learning: implicit vs explicit

$$\mathcal{L}' = 1 - \frac{T}{N}\sum_m \mathcal{F}(\sigma_m, \rho_m) \qquad \mathcal{F}(\sigma, \rho) = ||\sqrt{\sigma}\sqrt{\rho}||^2$$

$$\mathcal{F}(\sigma_m, \rho_m) \geq (1-\epsilon) \qquad ||\sigma_m - \rho_m|| \leq 2\sqrt{\epsilon}$$

$$||\rho_m - \rho_{m'}|| \leq ||\rho_m - \sigma_m|| + ||\rho_{m'} - \sigma_{m'}|| + ||\sigma_{m'} - \sigma_m||$$

$$\underline{||\rho_m - \rho_{m'}||} \leq 4\sqrt{\epsilon} + \underline{||\sigma_{m'} - \sigma_m||}$$

To maximize the distance between data-points ensembles we have to obtain the furthest possible centres:
Maximally orthogonal states!

M. M. Wilde. *Cambridge University Press (2013)*

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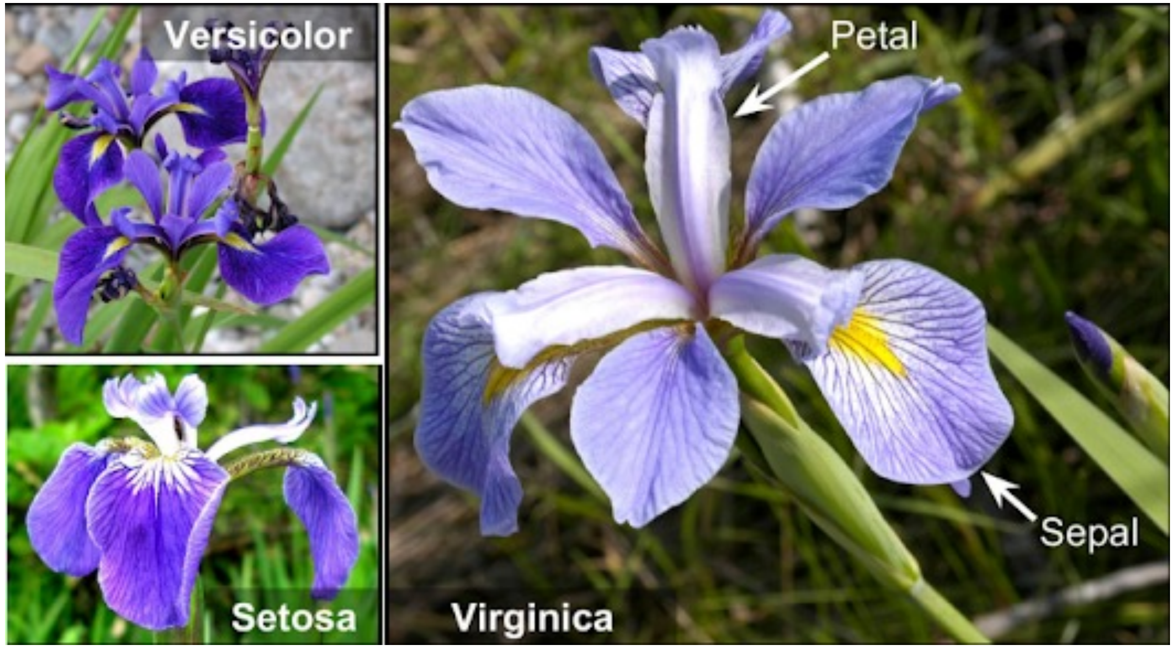
Results

Quantum SPAIN

- **Iris dataset**: 4 features & 3 classes

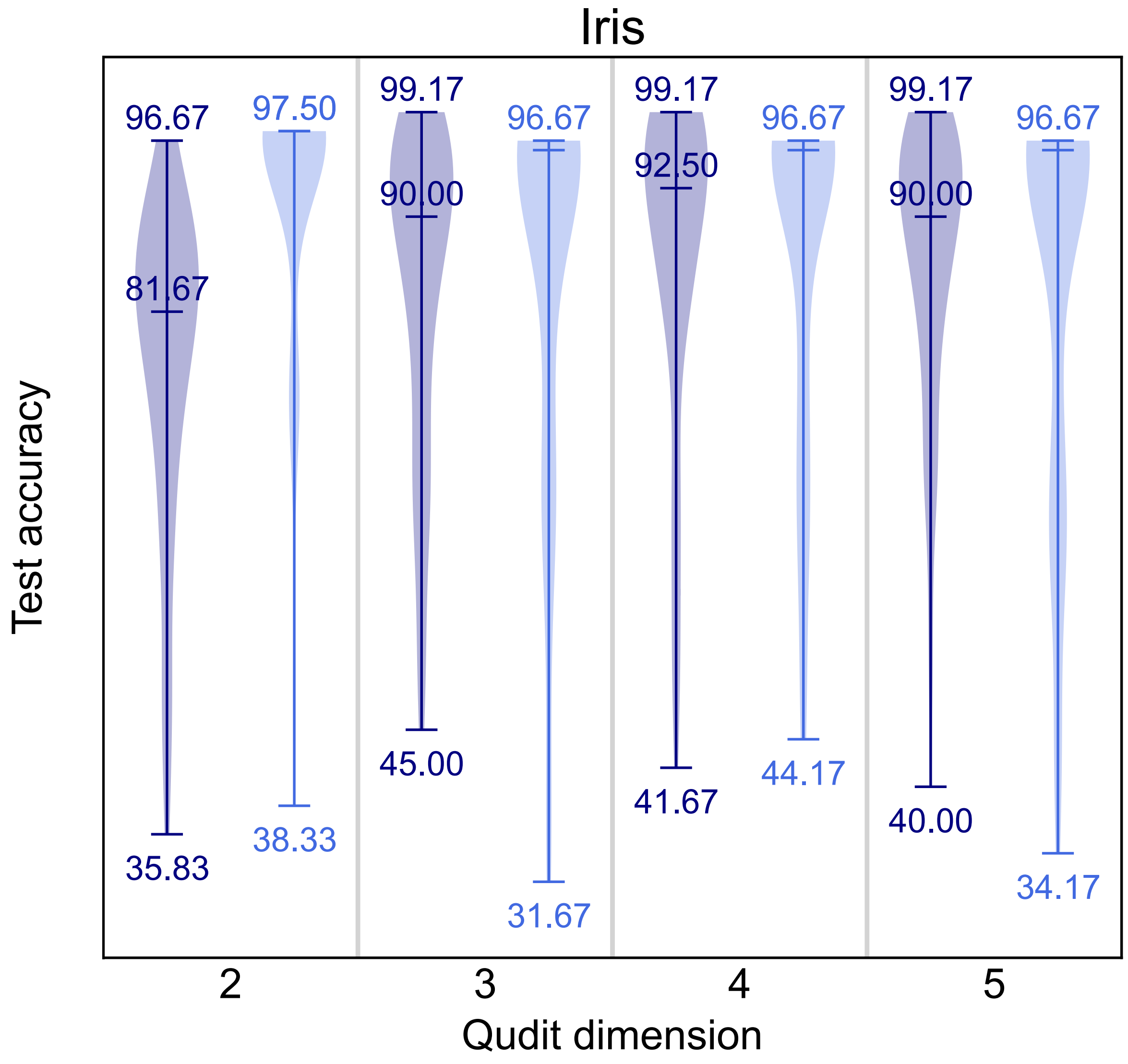


- One of the simplest datasets that we can use to benchmark our model
- Data dimension and number of classes low

https://www.pycodemates.com/2022/05/iris-dataset-classification-with-python.html

Results

- Implicit vs explicit in Iris dataset

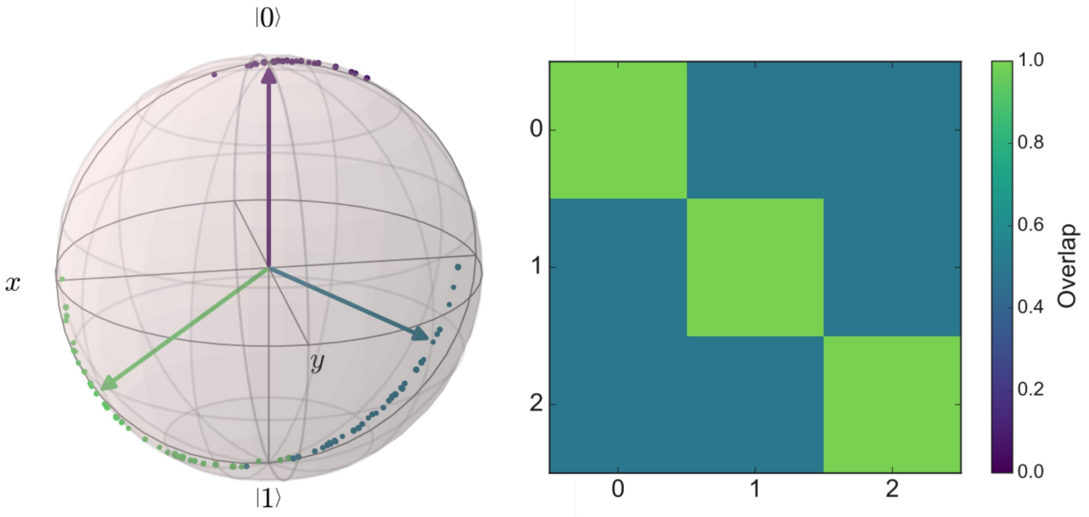


- ➢ The system is able to find better solutions by itself in some cases: higher accuracies for the implicit method
- ➢ Test accuracy saturates at d = 3

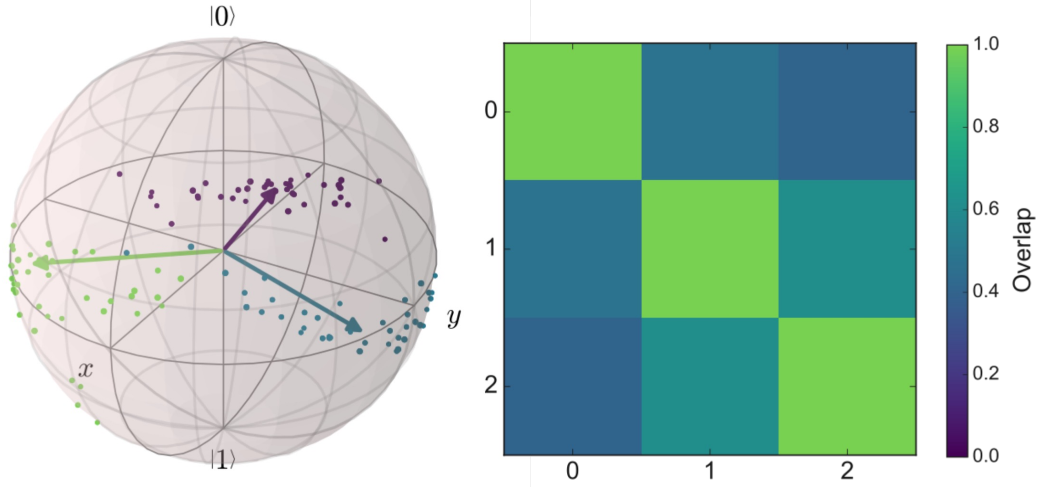
Results

- Implicit vs explicit in Iris dataset

$$\mathcal{L}_{\text{explicit}} = 1 - \frac{1}{K}\sum_k Tr(\rho_k \sigma_k)$$



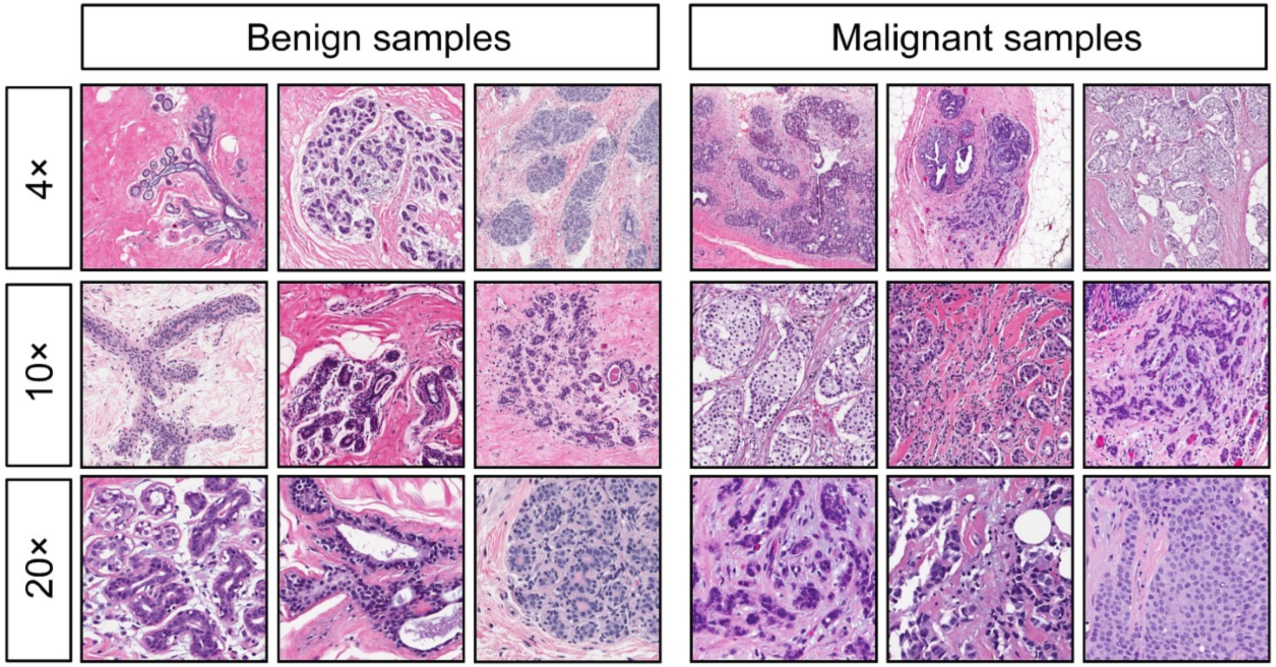
$$\mathcal{L}_{\text{implicit}} = 1 - \frac{1}{K}\sum_k Tr(\rho_k^2) + \frac{2}{K}\sum_{k<l} Tr(\rho_k \rho_l)$$



Results

Quantum SPAIN

- **Breastcancer Wisconsin dataset**: 10 features & 2 classes

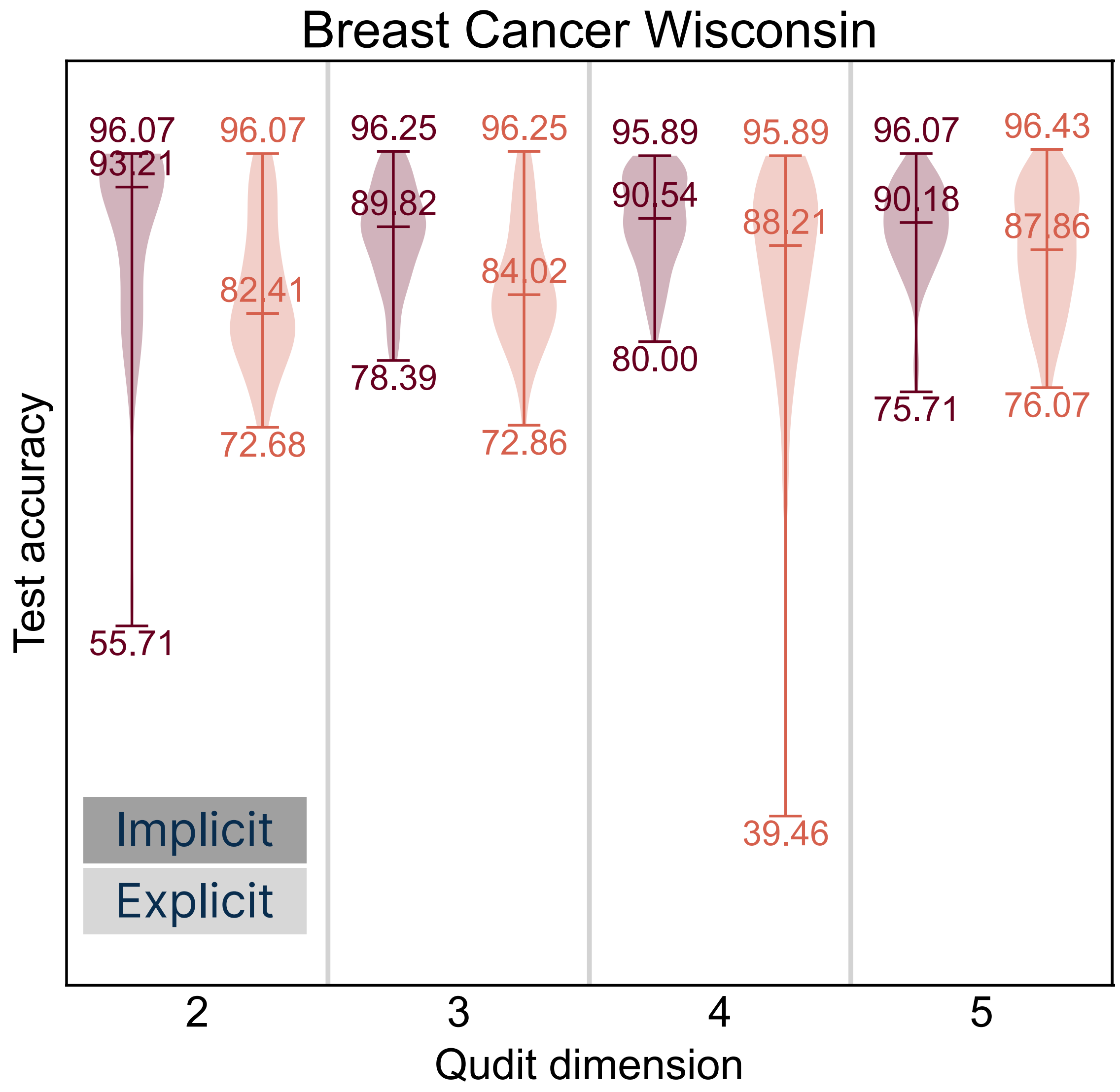


➢ More sophisticated problem in terms of number of points and features

https://medium.com/analytics-vidhya/breast-cancer-diagnostic-dataset-eda-fa0de80f15bd

Results

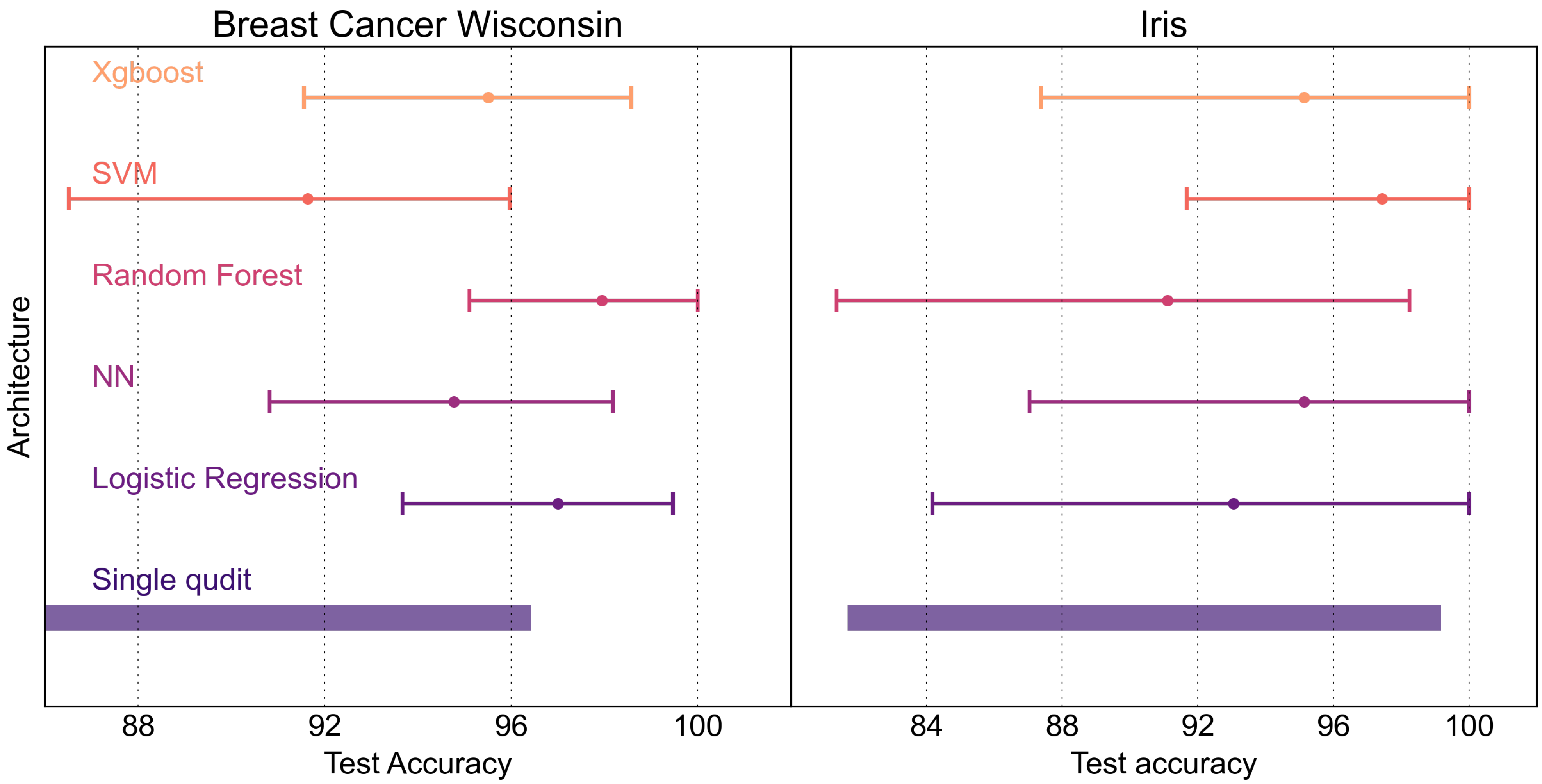
- Implicit vs explicit in Breast Cancer dataset



- Lower accuracies than for the Iris dataset
- Both methods offer similar performance
- Qudit dimension does not play a crucial role

Results

- Comparison with best classical models



https://archive-beta.ics.uci.edu/datasets

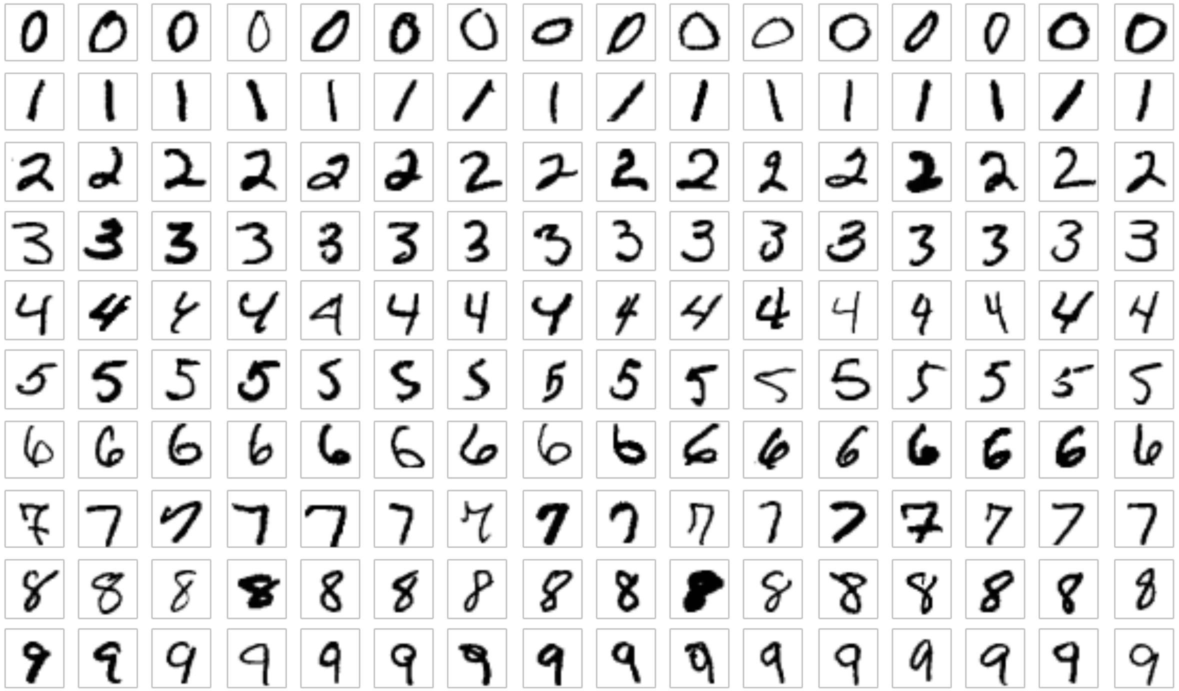
Results

- What happens when the data dimension is much higher than the qudit dimension?

$\text{Dim}(\vec{x}) >> d$

Results

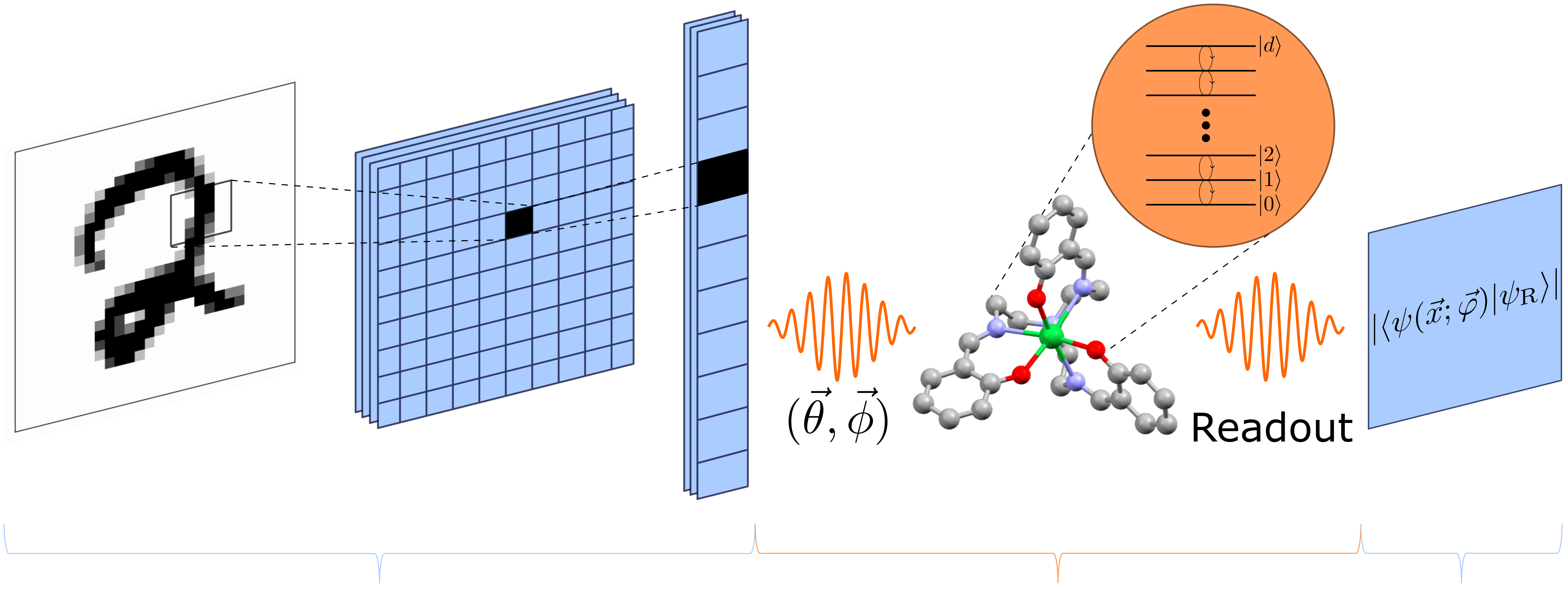
- $\text{Dim}(\vec{x}) >> d$
  - **Image classification**: MNIST digits 28x28 features and 10 classes



https://en.wikipedia.org/wiki/MNIST_database

Results

- Hybrid Convolutional Network



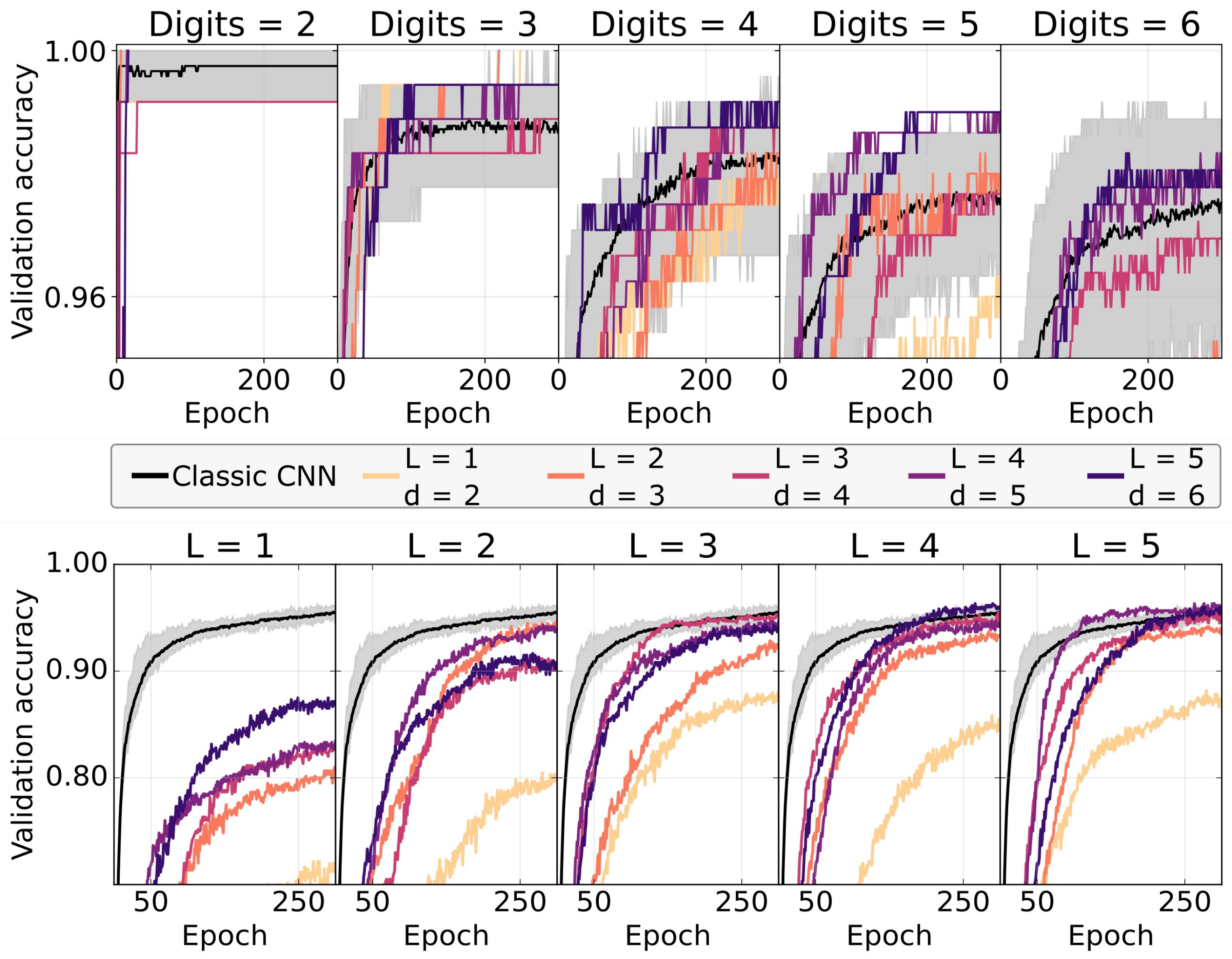
Classical convolutional network as dimension reducer (*PyTorch*)

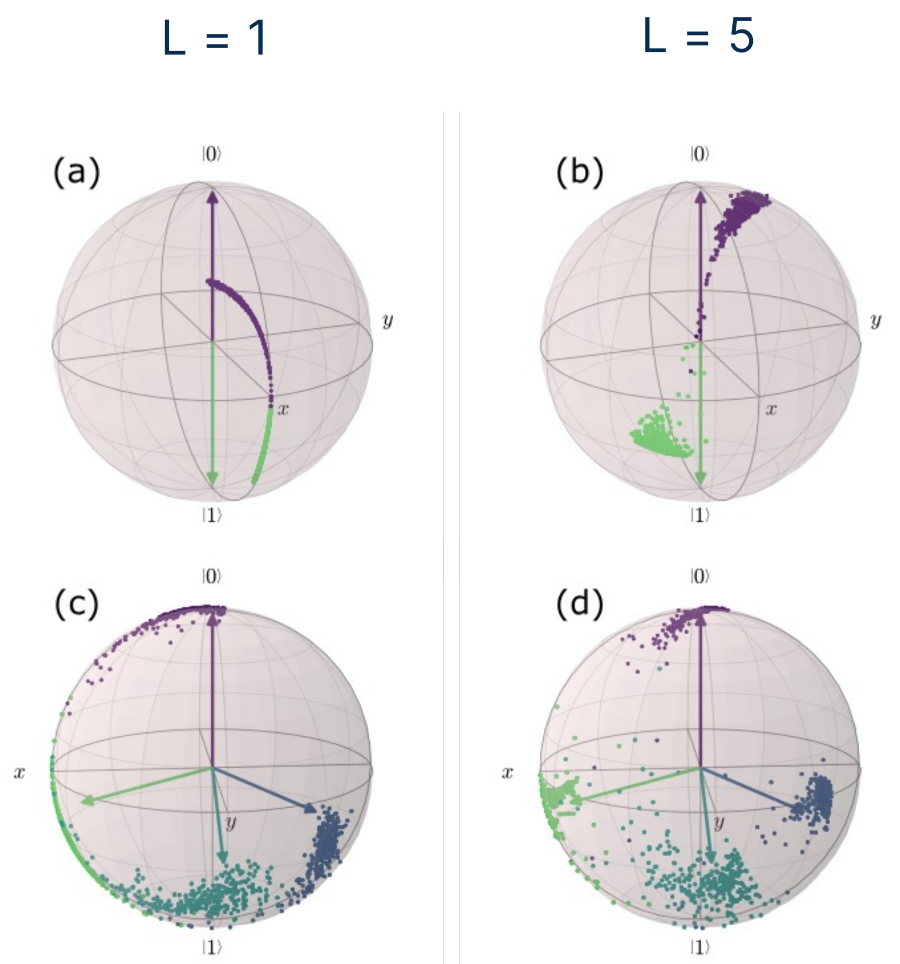
Quantum processor

Updating the classical optimizer with the read-out

Results

○ Hybrid Convolutional Network





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Conclusions

- Increasing the number of levels offers advantages in terms of information management and processing.

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- We have developed tools to deal with any kind of dataset (number of levels and data dimension) in supervised learning tasks with a single unit of information.

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Quantum SPAIN

- Increasing the number of levels offers advantages in terms of information management and processing.
- We have developed tools to deal with any kind of dataset (number of levels and data dimension) in supervised learning tasks with a single unit of information.
- These tools are hardware efficient: it can be easily implemented in any experimental architecture.

Conclusions

Quantum SPAIN

- Increasing the number of levels offers advantages in terms of information management and processing.
- We have developed tools to deal with any kind of dataset (number of levels and data dimension) in supervised learning tasks with a single unit of information.
- These tools are hardware efficient: it can be easily implemented in any experimental architecture.
- Moreover, we can extract a geometrical interpretation of what does it mean to learn for this particular kind of model and strategy.

Acknowledgments

Quantum SPAIN

Quantum Materials and Devices

qmad.es

Juan Román

David Zueco

Fernando Luis

INMA INSTITUTO DE NANOCIENCIA Y MATERIALES DE ARAGÓN

Universidad Zaragoza 1542

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RES RED ESPAÑOLA DE SUPERCOMPUTACIÓN

QUANTERA FATMOLS

QTEP

European Commission

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