Fraunhofer IPA

Fraunhofer Institute for Manufacturing Engineering and Automation IPA

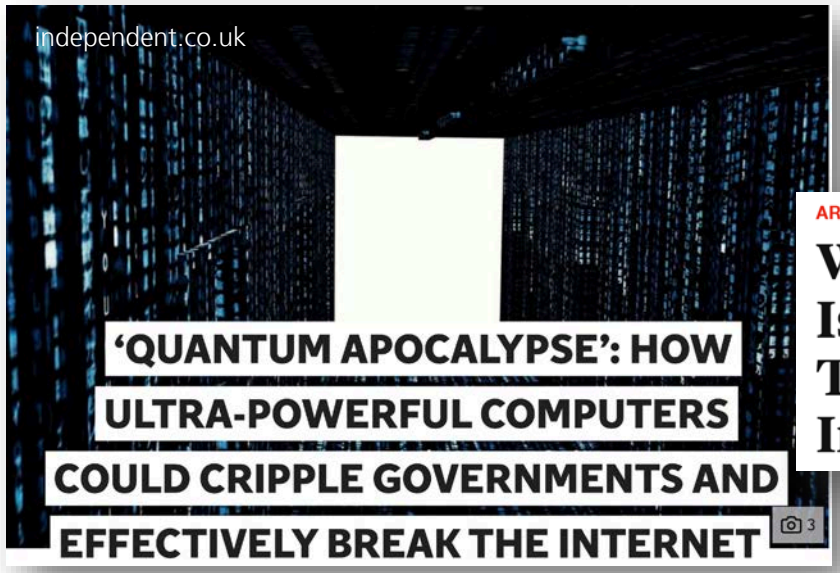
Quantum Machine Learning – What (not) to expect

30.11.2023 – Engineering Intelligence

Marco Roth

Quantum Computing in the Media

Could be more accurate



DEEP TECH

How quantum computers can save us from the coronavirus

https://thenextweb.com/

ARGUMENT *An expert's point of view on a current event.*

Why Quantum Computing Is Even More Dangerous Than Artificial Intelligence

https://https://foreignpolicy.com//

The Day When Computers Can Break All Encryption Is Coming

Quantum computers will be able to overpower current encryption within a decade. That has security experts scrambling to come up with new ways to protect our data before it is too late

https://www.wsj.com/articles/the-race-to-save-encryption-11559646737

CLIMATE CHANGE

How quantum computing could be one of the most innovative climate change solutions?

Dec 17, 2019

https://www.weforum.org/agenda/2019/12/quantum-computing-applications-climate-change/

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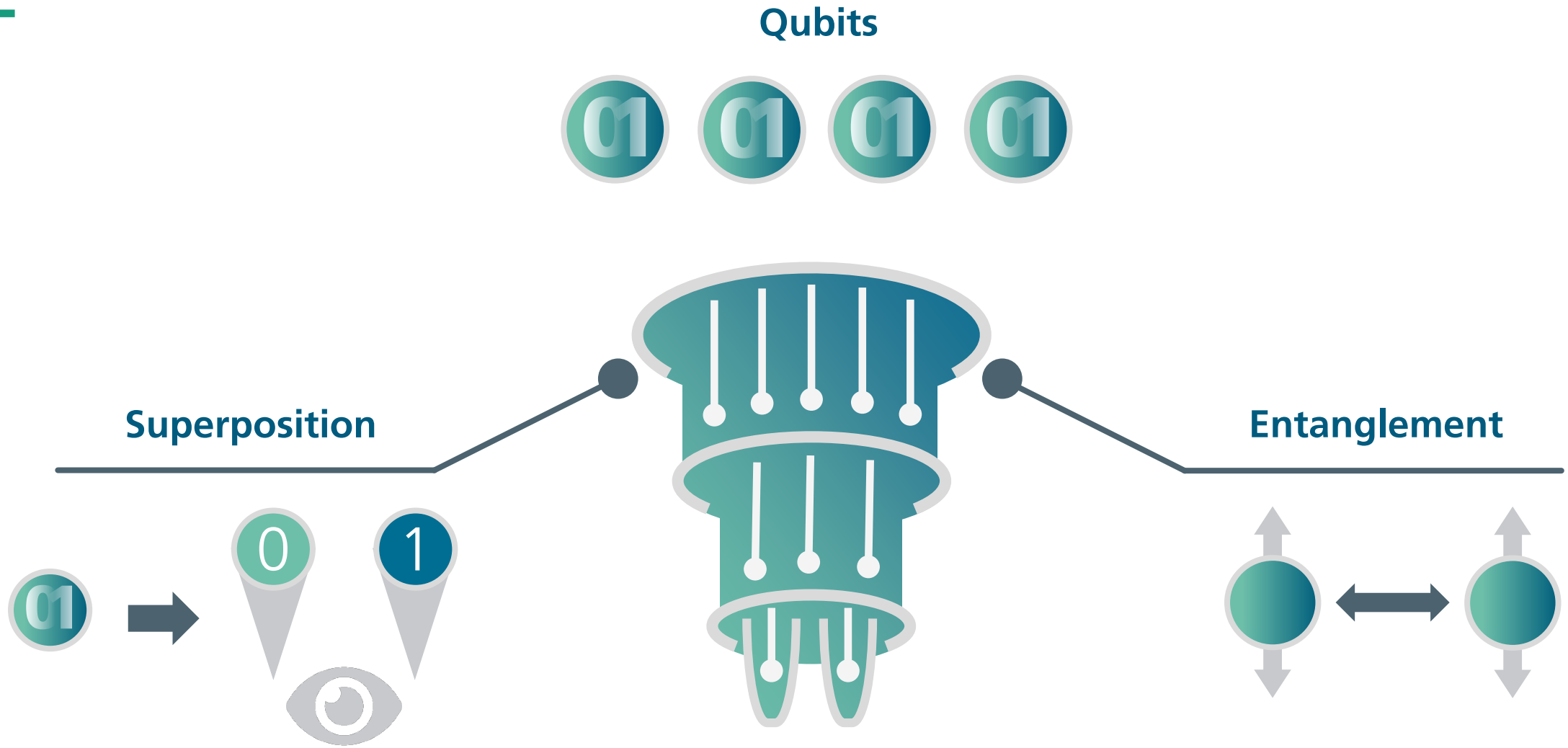
Focus Areas

- Since 2022: independent research group
- Part of the Fraunhofer Competence Network Quantum Computing
- Focus on method-driven research in the field of quantum machine learning, quantum simulations and quantum optimization
- Areas of application
  - Manufacturing
  - Hydrogen production
  - Automated machine learning

What is Quantum Computing?

Quantum Computing

In a nutshell



Quantum computing

Advantages and Impact

- Promise:
  - (Exponential) efficiency advantages compared to classical methods
  - Access to classically intractable problems
- Core applications
  - Machine learning
  - Optimization and search
  - Quantum simulations
  - Cryptography
- Application domains are determined by the core applications
- Quantum computing is not superior to conventional computing **in general**

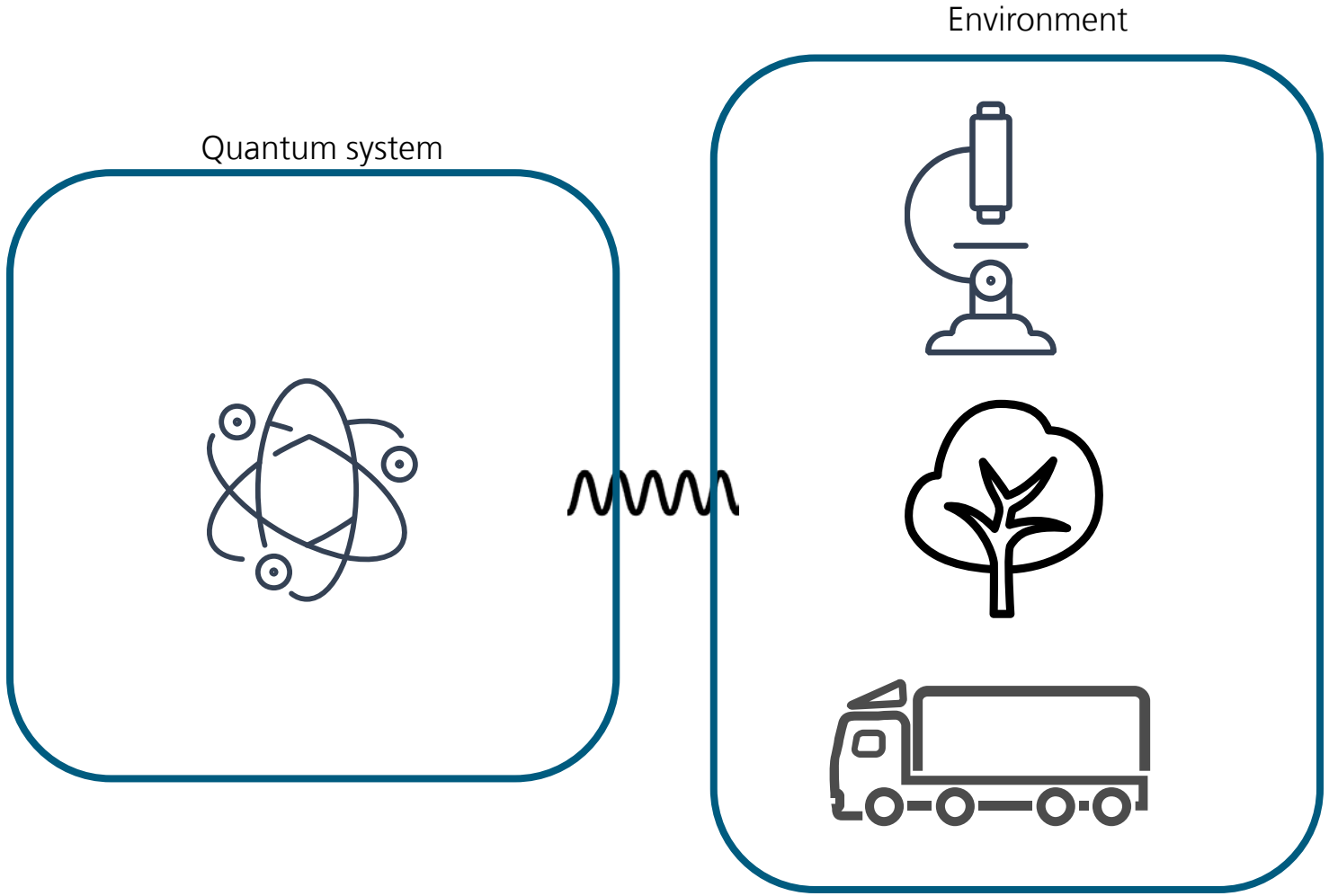
Economic value + Incremental ++ Significant +++ Disruptive

Industry	Key segment for QC	2025–30	2030–35
Global energy and materials	Oil and gas	+	++
	Sustainable energy	+	+++
	Chemicals	++	+++
Life sciences	Pharmaceuticals	++	+++
Advanced industries	Automotive	++	++
	Aerospace and defense	+	++
	Advanced electronics	+	++
	Semiconductors	+	++
Finance	Financial services	++	+++
Telecom, media, and technology	Telecom	+	++
	Media	+	+
Travel, transport, and logistics	Logistics	+	++
Insurance	Insurance	+	+

Source: Quantum Technology Monitor (McKinsey 2023)

Core Challenge

Quantum states are not stable



If Errors are not avoidable, how can we proceed?

Mitigation vs. Correction

Short-term perspective: Work with what we have

- Current regime: noisy intermediate-scale quantum devices (NISQ)
- Only use a few qubits with short circuits
- Workhorse: Variational circuits
- Advantage not proven

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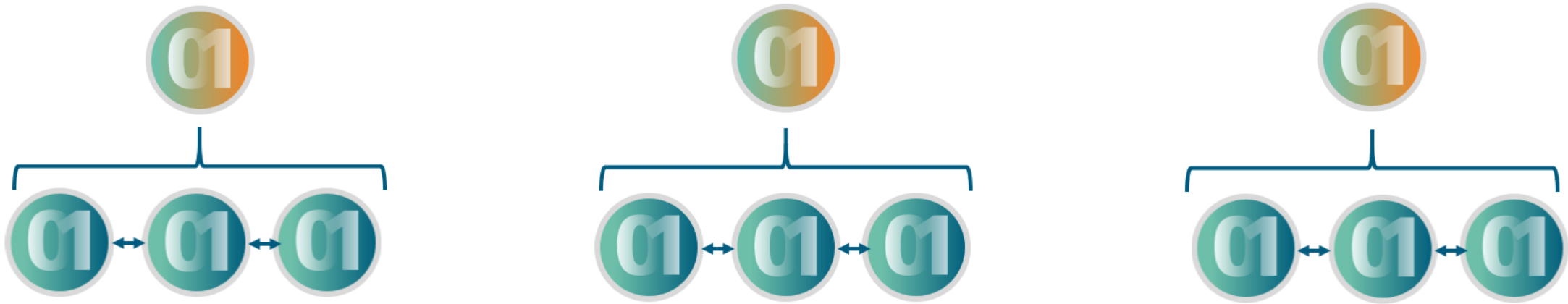

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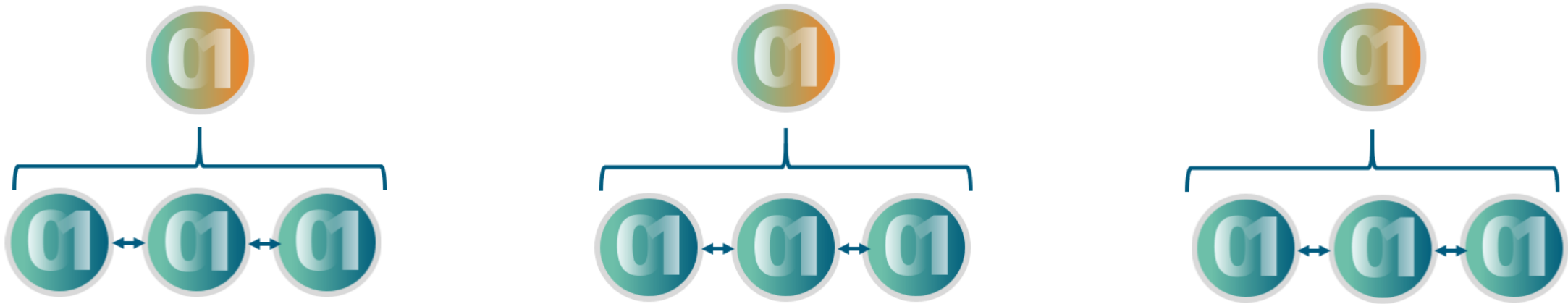
Long-term goal: Error correction

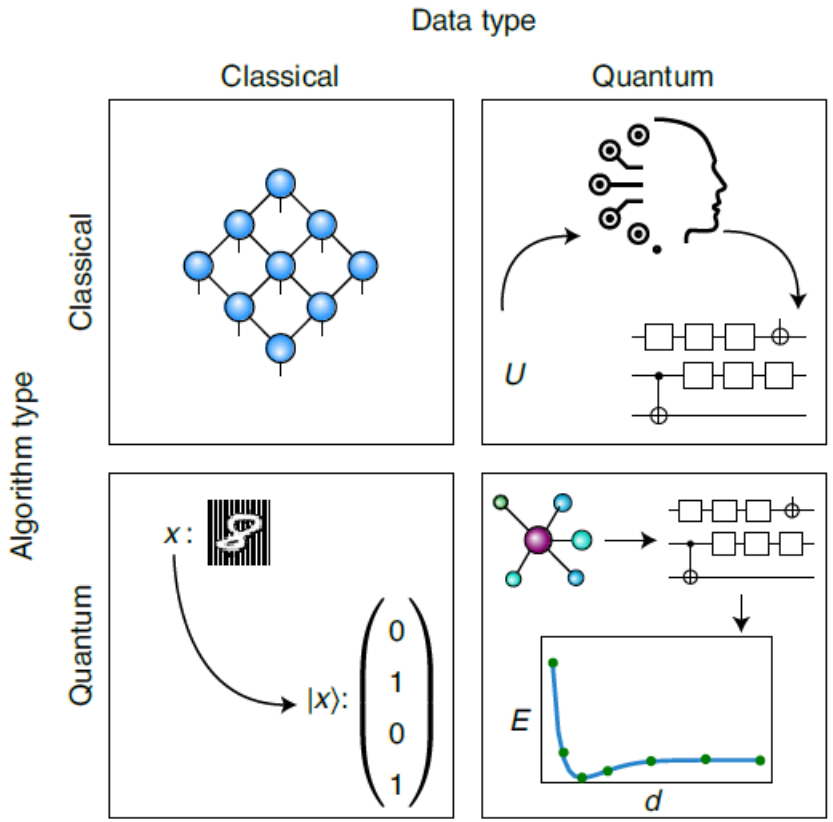
- Join multiple physical qubits to a fault-tolerant logical qubit
- Requires
  - Large number of qubits
  - Low error rates
- Proofable speed-ups (up to exponential) for some applications
- Time line: 10–20 years

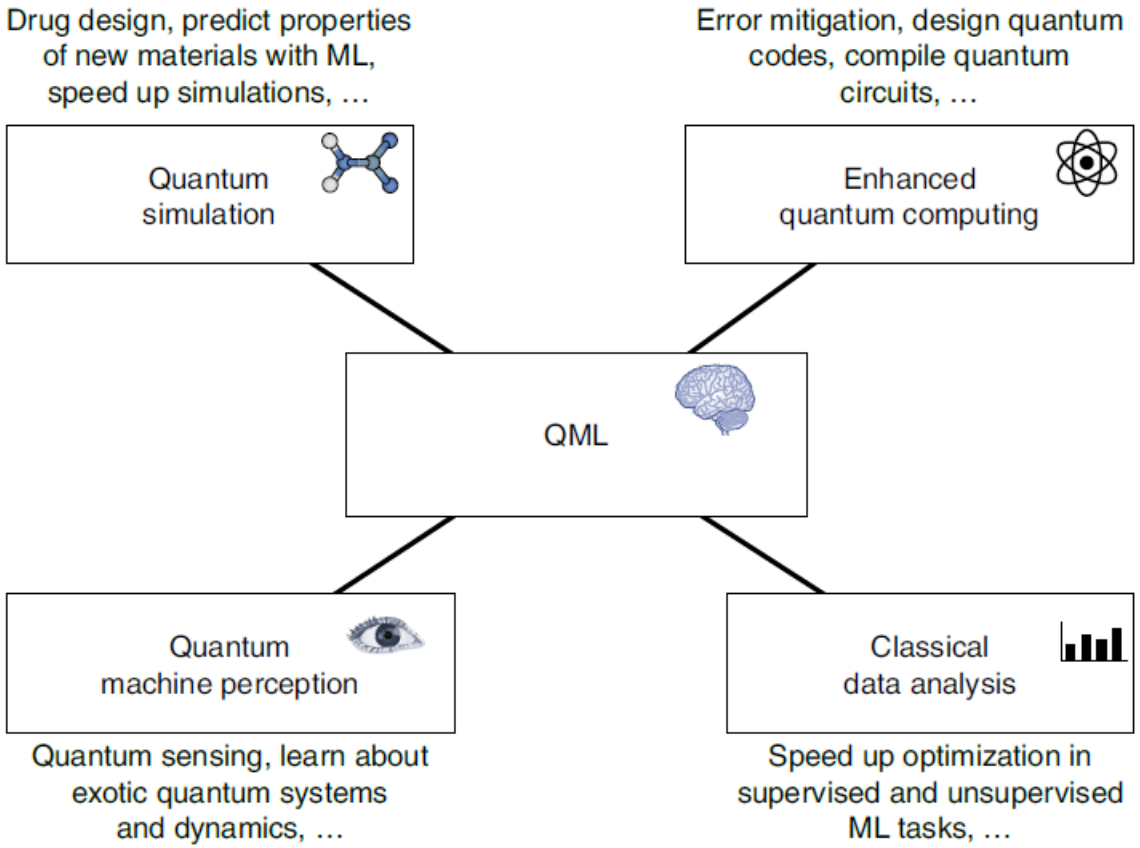


Quantum Machine Learning

Quantum Machine Learning

Applications



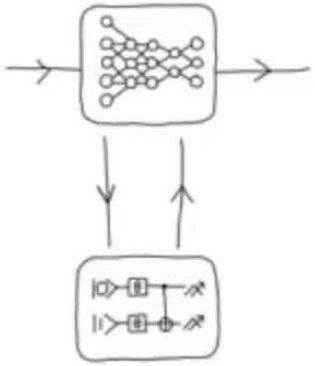


Source: Cerezo et al., Nature Computational Science, 2, 567–576 (2022)

How to incorporate QC into ML?

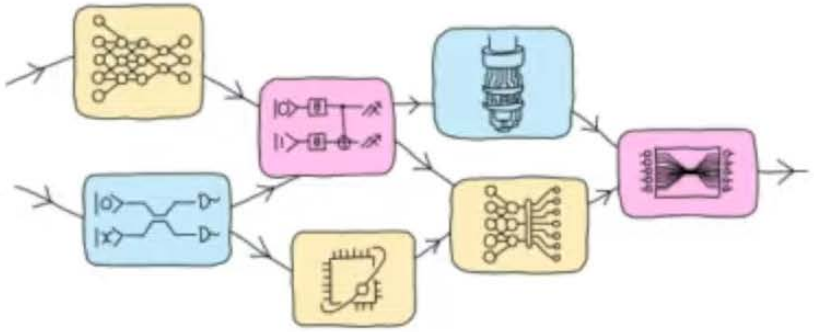
Short-term vs. long-term

Fault-tolerant



Outsource parts of the computation to a quantum computer

NISQ



Use a model that is intrinsically quantum

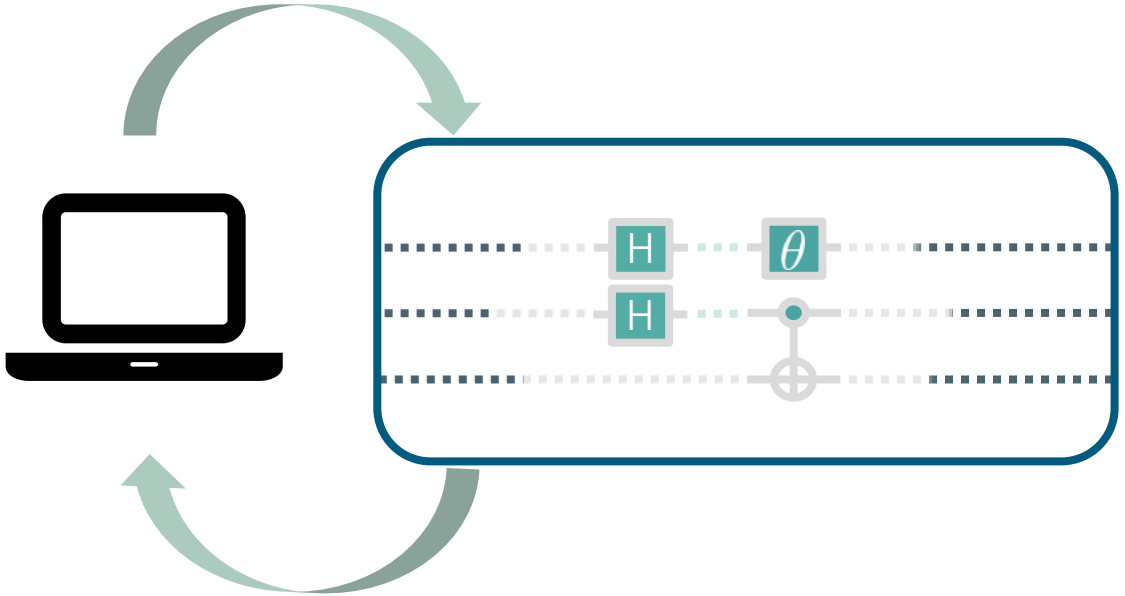
Source: Xanadu Quantum Technologies Inc. - QML: 2023 and Beyond!

NISQ Algorithms

Quantum algorithms in the NISQ era

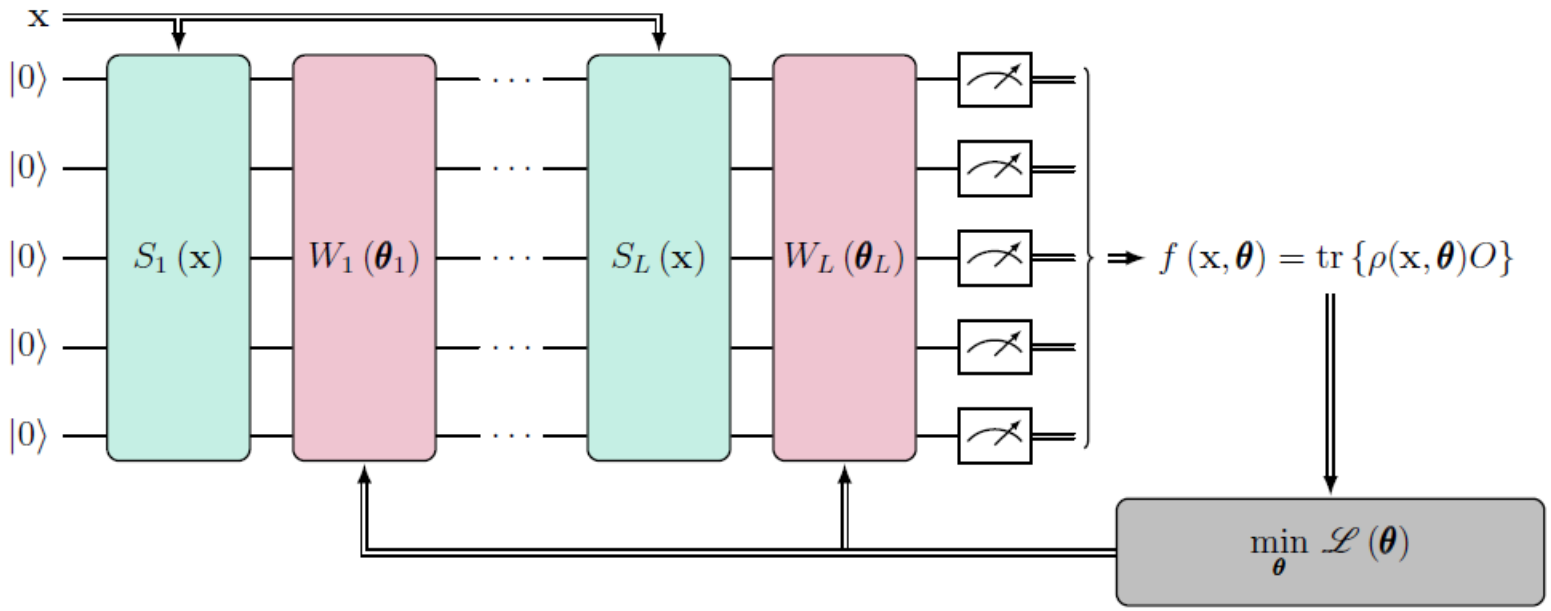
Variational Algorithms

- Maintaining coherent quantum states is difficult
- The technology is at an early stage of development
- Current quantum algorithms are generally hybrid. Calculations on the quantum computer are supported by classical optimization loops.



Quantum Neural Networks (QNNs)

A general function approximation



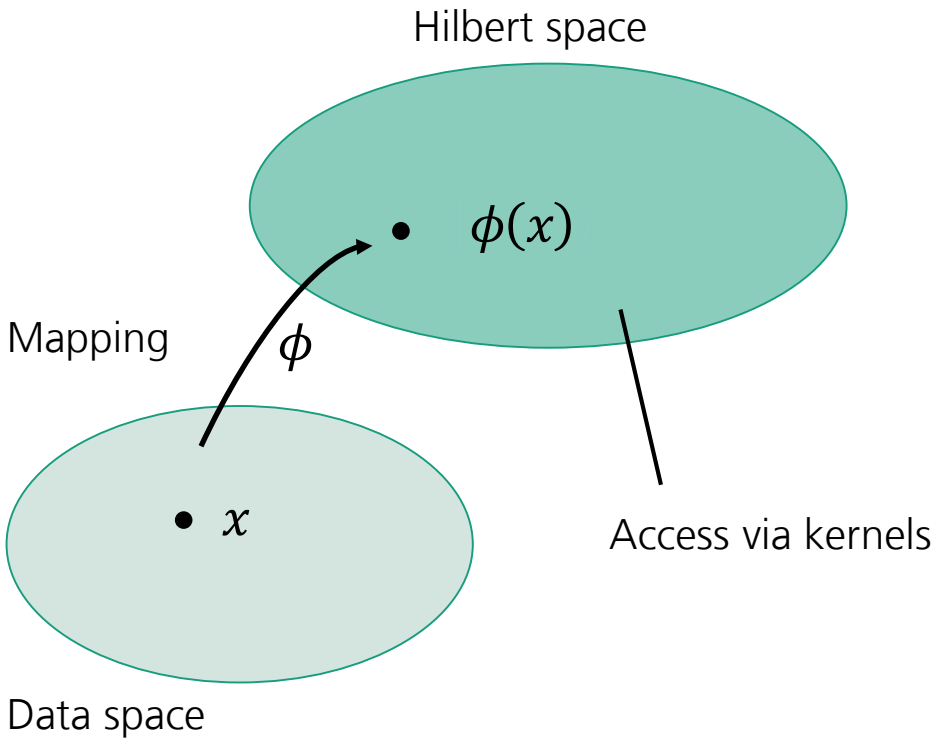
- Also known as Variational Quantum Regression (VQR)
- Same application domain as classical artificial neural networks
- Gradient based loss function optimization with the parameter-shift rule (for example SLSQP, ADAM)
- **Potential advantage:** complexity of the QNN can increase exponentially with the redundancy of the input data

Kreplin, Willmann, Schnabel, Rapp, Roth - sQUlearn – A Python Library for Quantum Machine Learning, arXiv:2311.08990 [quant-ph] .

Quantum Kernel Methods

Basic Principles

Kernel Methods

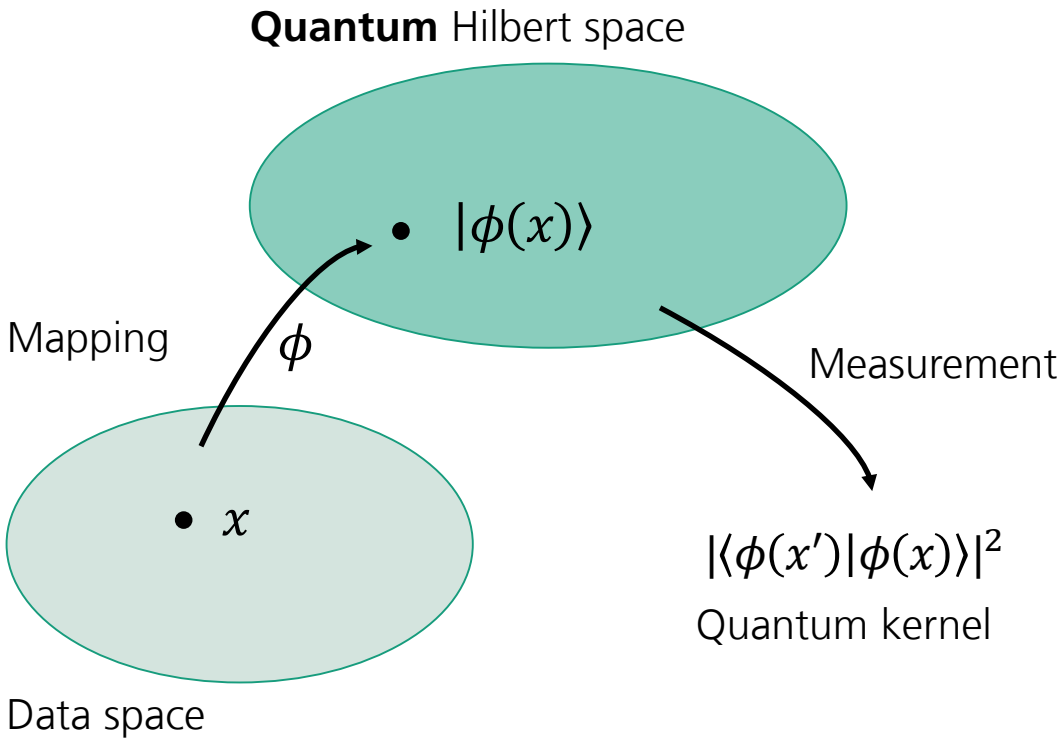


- Classical kernel methods are established methods

Quantum Kernel Methods

Basic Principles

Quantum Kernel Methods

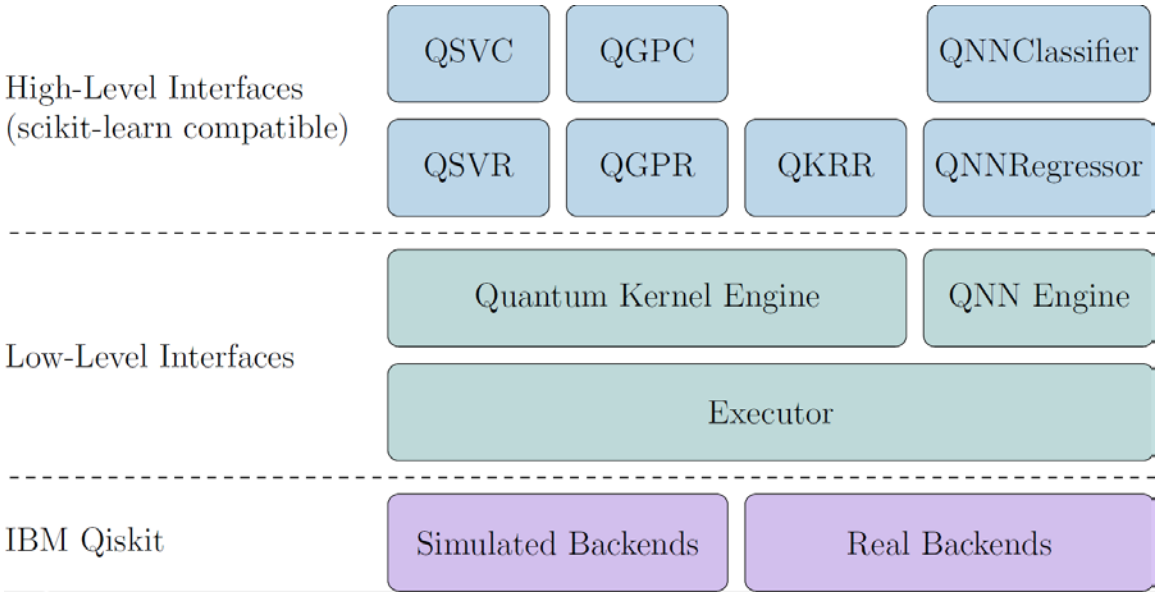


- Classical kernel methods are established methods
- Incorporating quantum computers promises
  - Efficiency and speed advantages
  - Solving problems that are classically inaccessible

sQUlearn

Open-Source Python Library for QML

- **High-level Algorithms:** Seamless integration into existing ML pipelines via sklearn interface
- **Low-level Algorithms:** Tools for the development of QML algorithms
- Quantum Kernel and Quantum Neuronal Networks



GitHub

```
pip install squlearn
```

[1] Kreplin, Willmann, Schnabel, Rapp, Roth - sQUlearn – A Python Library for Quantum Machine Learning, arXiv:2311.08990 [quant-ph] .

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Webinarreihe »Quantum Brunch«

ab 29. September 2023 jeden vierten Freitag
von 10:00 bis 10:30 Uhr, online

Quantum Brunch

Agenda und Termine

Anmeldung

- **29. September 2023** Was ist Quantencomputing? – Eine Einführung
- **27. Oktober 2023** Ein Einblick in die Funktionsweise verschiedener Quantencomputer
- ***1. Dezember 2023*** Eine Bestandsaufnahme und ein Blick in die Zukunft des Quantencomputings
- **26. Januar 2024** Optimierung von Fertigungsstraßen – Quantenoptimierung in der Praxis
- **23. Februar 2024** Einführung in Quantum Machine Learning
- **22. März 2024** Anwendung von Quantum Machine Learning zur Preisvorhersage von Industriemaschinen
- **26. April 2024** Quanten Neuronale Netze und deren Anwendungen

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Thank you for your attention!

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www.ipa.fraunhofer.de/quantum

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Fraunhofer-Institut für Produktions-technik und Automatisierung IPA

LinkedIn

Quantum machine learning

Quantum improvements of AutoML

Supported by:
Federal Ministry for Economic Affairs and Climate Action
on the basis of a decision by the German Bundestag

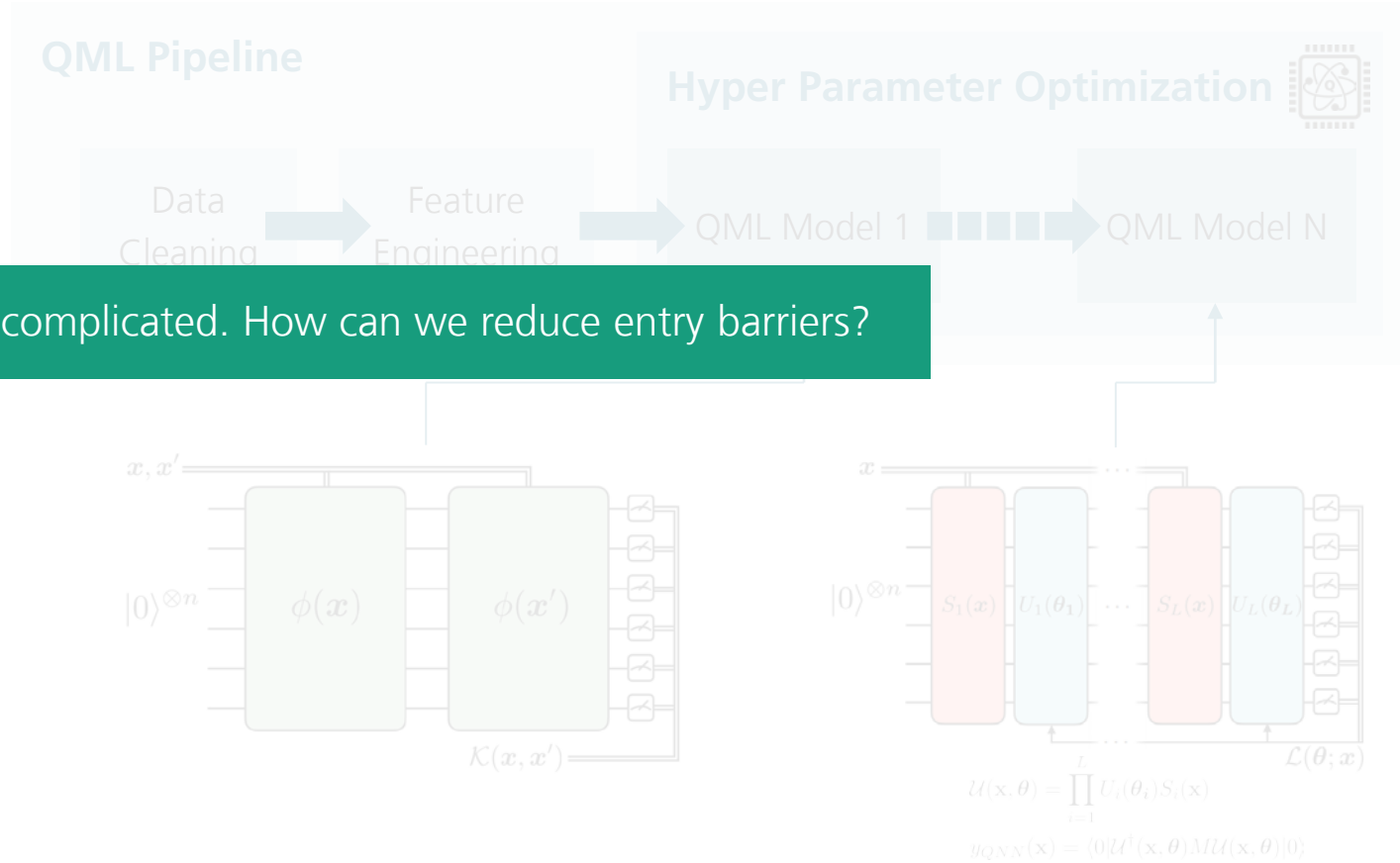
AutoQML

1) Integration of Quantum ML in AutoML

- State-of-the-art methods on NISQ hardware
- Implementation of various QML algorithms, e.g.
  - Quantum Kernel Meth
  - Quantum Neural Networks

2) Improvements of AutoML method

- Feature engineering
- Optimization of the ML pipeline
- Optimization of the hyper parameters



Motivation: QML is complicated. How can we reduce entry barriers?

Mangini et al (2021). Quantum computing models for artificial neural networks. *EPL 134*(1), 10002.

Quantum Neural Networks

Variance regularization against shot noise

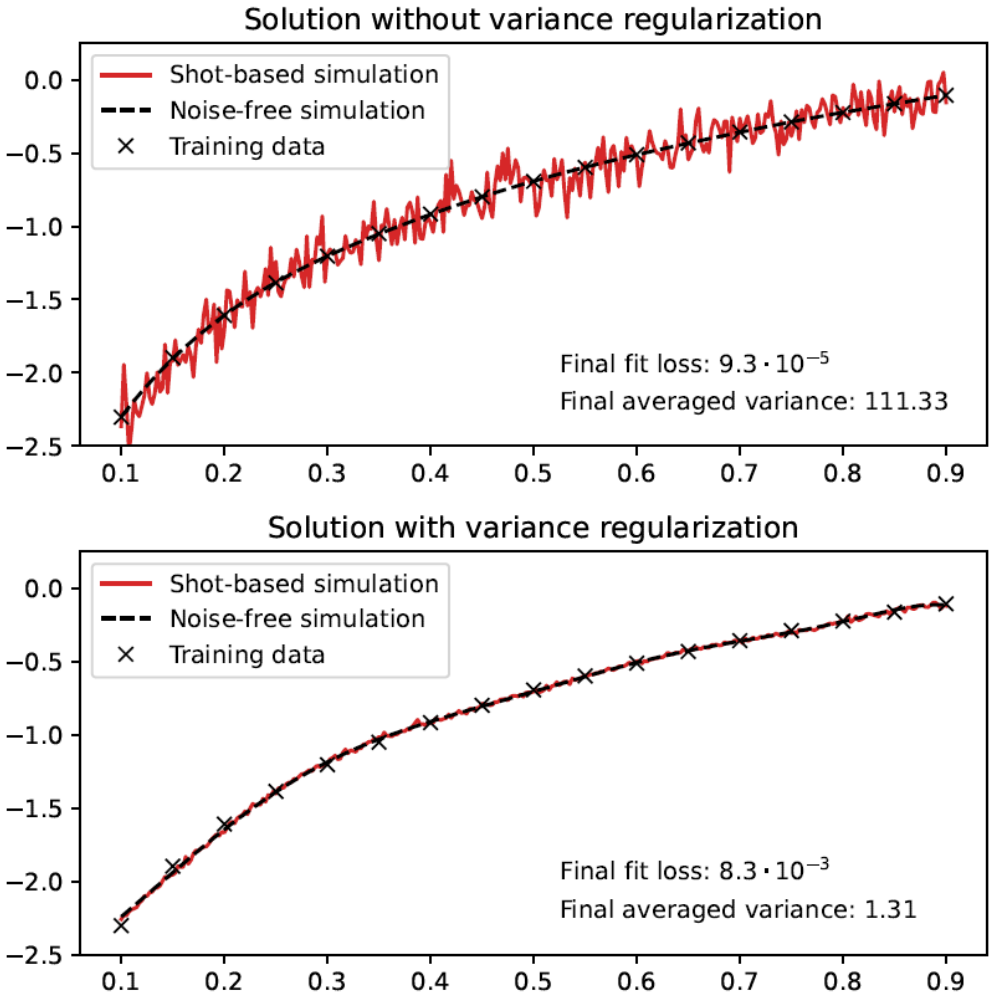
- Shot noise has a large impact on the trainability and quality of QNNs
- Idea: Use the large expressivity of a QNN to additionally reduce the variance of the QNN
- Add the variance as a regularization term to the loss function:

$$L(\theta) = \sum_i |f(x_i, \theta) - y_i|^2 + \alpha \sum_i \mathrm{var}(f(x_i, \theta))$$

with

$$f(x, \theta) = \langle \Psi(x, \theta) | \hat{C}(\theta) | \Psi(x, \theta) \rangle$$

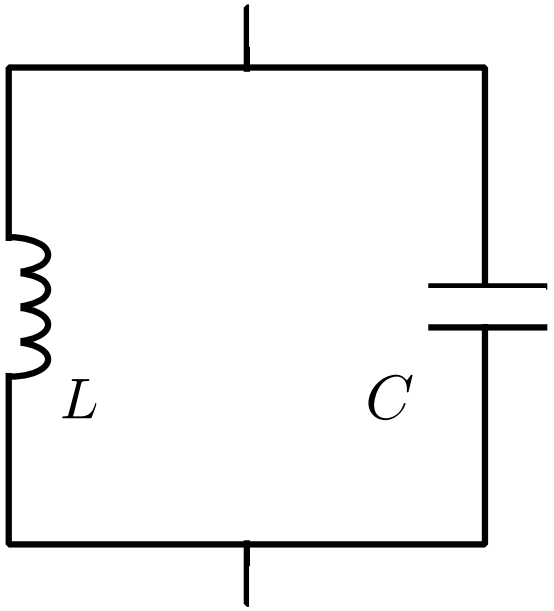
$$\mathrm{var}(f) = \langle \Psi | \hat{C}^2 | \Psi \rangle - \langle \Psi | \hat{C} | \Psi \rangle^2$$



D. Kreplin, M. Roth; Reduction of finite sampling noise in quantum neural networks; arXiv:2306.01639 (2023)

How to make a qubit

Superconducting qubits



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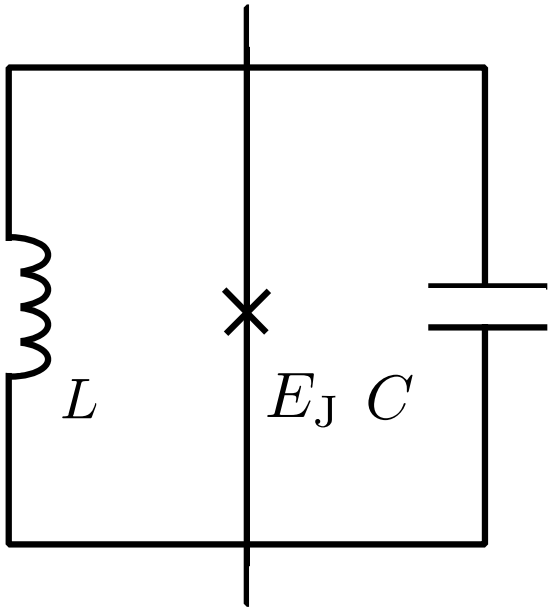

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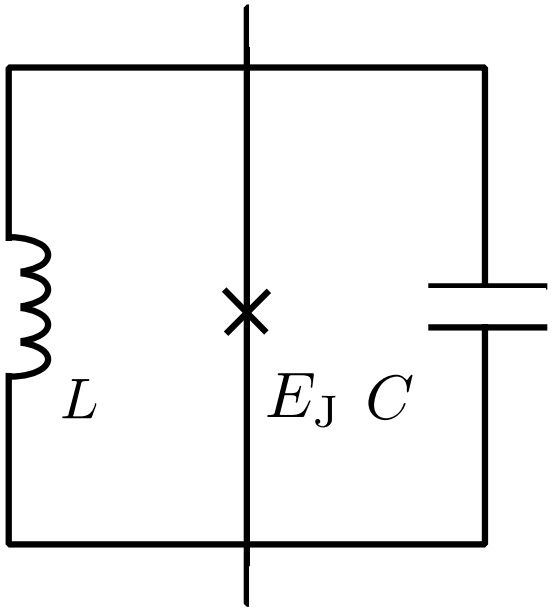

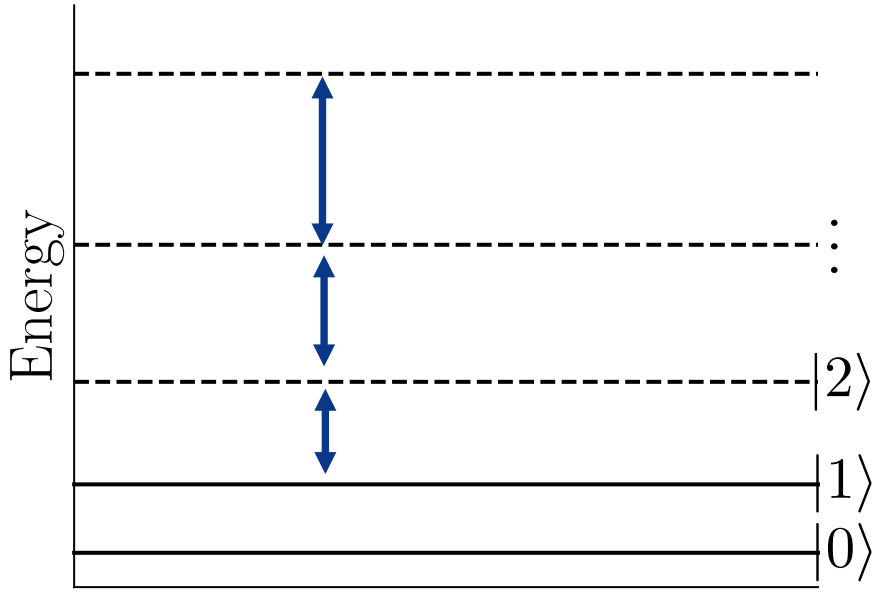

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