Opportunities and challenges in quantum-enhanced machine learning in near-term quantum computers

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Funding:

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QUANTUM ENHANCED OPTIMIZATION

Perdomo-Ortiz, Benedetti, Realpe-Gomez, and Biswas. **arXiv:1708.09757** (2017). To appear in the Quantum Science and Technology (QST) invited special issue on “What would you do with a 1000 qubit device?”

QUBITS D-wave User Group 2017

National Harbor, MD, September 28, 2017

D-Wave System Capability

1) As a discrete optimization solver:

Given $\{h_j, J_{ij}\}$, find $\{s_k = \pm 1\}$ that minimizes

NP-hard problem

$$\xi(s_1, \ldots, s_N) = \sum_{j=1}^{N} h_j s_j + \sum_{i,j \in E}^{N} J_{ij} s_i s_j$$

Potential NASA applications:

- *planning*
- *scheduling*
- *fault diagnosis*
- *graph analysis*
- *communication networks, etc.*

QUBO: Quadratic Unconstrained Binary Optimization (Ising model in physics jargon).

2) As a physical device to sample from Boltzmann distribution:

$$P_{Boltzman} \propto exp[-\xi(s_1, \ldots, s_N)/T_{eff}] \longrightarrow \langle v_i h_j \rangle_{p(\mathbf{h},\mathbf{v})}$$

Computationally bottleneck

Early work:
Bian et al. 2010. The Ising model: teaching an old problem new tricks.

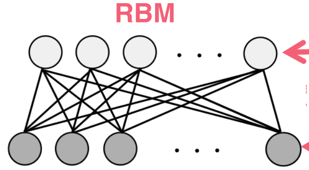
Follow-up work:
Raymond et al. Global warming: Temperature estimation in annealers. Frontiers in ICT, 3, 23 (2016).

Our work: Benedetti et al. PRA 94, 022308 (2016)

- We provide a robust algorithm to estimate the effective temperature of problem instances in quantum annealers.
- Algorithm uses the same samples that will be used for the estimation of the gradient

Widely used in **unsupervised** learning

RBM



Hidden units

Visible units

Potential NASA applications:

- *machine leaning (e.g., training of deep-learning networks)*

Unsupervised learning (generative models)

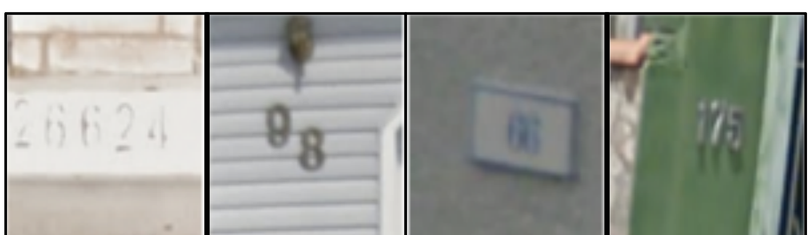
Learn the “best” model distribution that can generate the same kind of data

MODEL

P **(Image)**

Learning algorithm

NO LABELS



DATASET

Unsupervised learning (generative models)

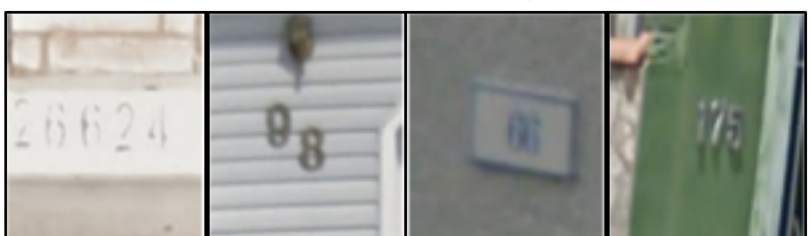
Learn the "best" model distribution that can generate the same kind of data

MODEL

***P* (Image)**

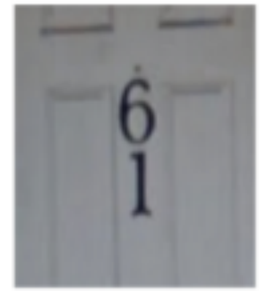
Learning algorithm

NO LABELS



DATASET

Example application:
Image reconstruction



Reconstructed image

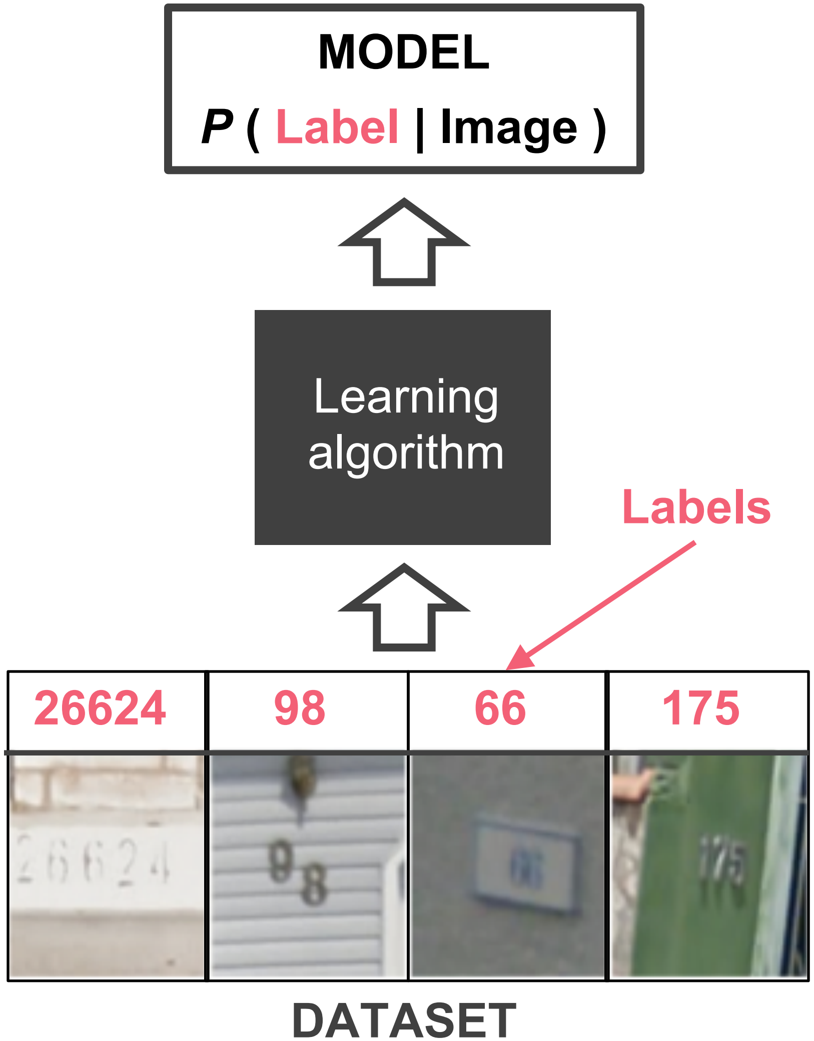
LEARNED MODEL

***P* (Image)**

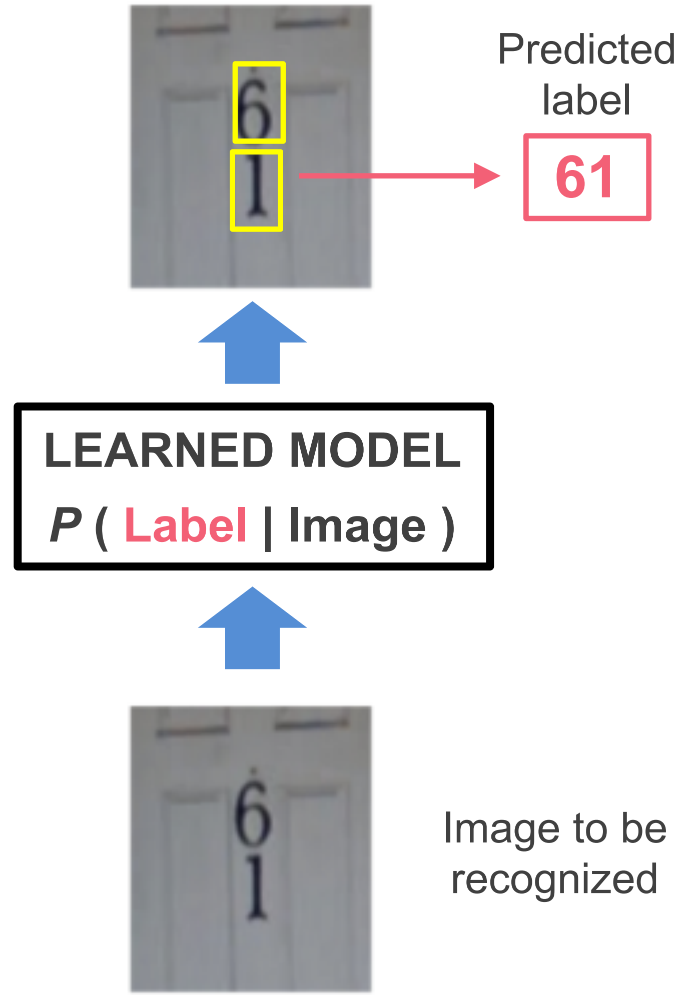
Damaged image

Supervised learning (discriminative models)

Learn the “best” model that can perform a specific task



Example application:
Image recognition

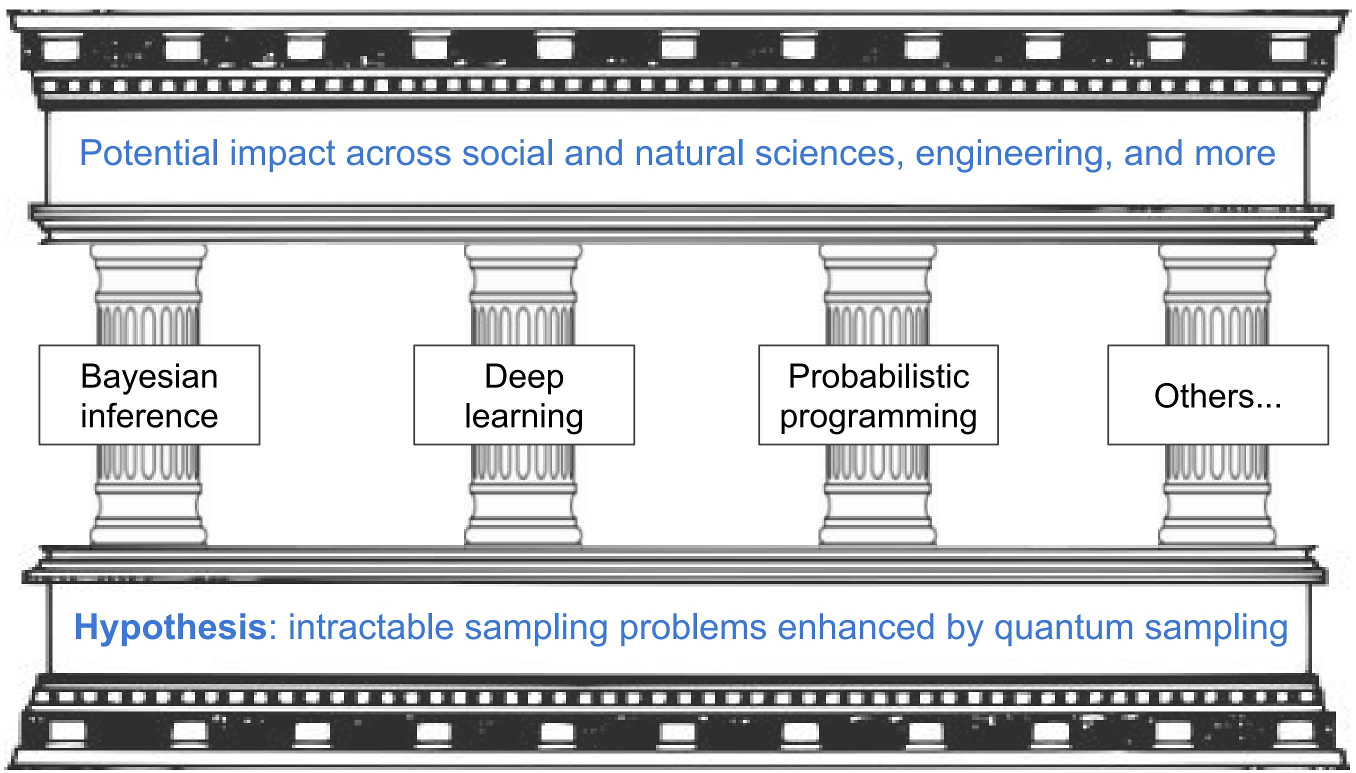


A near-term approach for quantum-enhanced machine learning

State-of-the-art QML

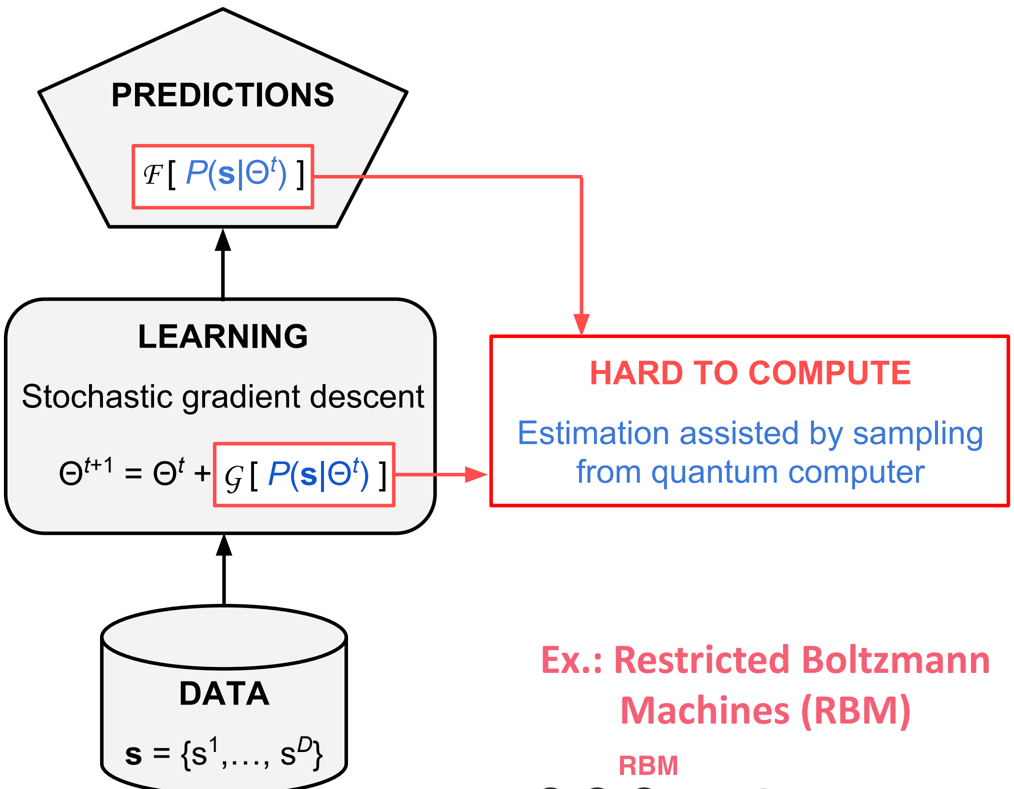
- **Most previous proposed work have highly optimized powerful classical counterparts** (e.g., on discriminative/classification tasks)
- **Need for qRAM** (case of most gate-based proposal).
- **Qubits represent visible units**; issue for case of large datasets

Lesson 1: Move to intractable problems of interest to ML experts (e.g., **generative models in unsupervised learning**).

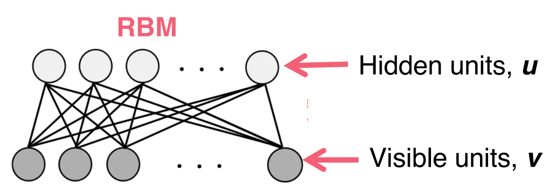


A near-term approach for quantum-enhanced machine learning

Lesson 2: Need for novel hybrid approaches.



Ex.: Restricted Boltzmann Machines (RBM)



Computationally bottleneck

$$\langle v_i u_j \rangle_{p(\mathbf{v},\mathbf{u})}$$

Where,

$$p(\mathbf{v},\mathbf{u}) = \frac{e^{-E(\mathbf{v},\mathbf{u}|\theta)/T_{\mathrm{eff}}}}{Z(\theta)}$$

Widely used in **unsupervised** learning

Challenges solved:

Benedetti, et al. **Estimation of effective temperatures** in quantum annealers for sampling applications: A case study with possible applications in deep learning. **PRA 94, 022308** (2016).

Benedetti, et al. Quantum-assisted learning of graphical models with **arbitrary pairwise connectivity**. **arXiv:1609.02542** (2016).

Benedetti, et al. Quantum-assisted Helmholtz machines: A quantum-classical deep learning framework for **industrial datasets in near-term devices**. **arXiv:1708.09784** (2017).

Perdomo-Ortiz, et al. **Opportunities and Challenges** in Quantum-Assisted Machine Learning in Near-term Quantum Computer. **arXiv:1708.09757**. (2017).

A near-term approach for quantum-enhanced machine learning

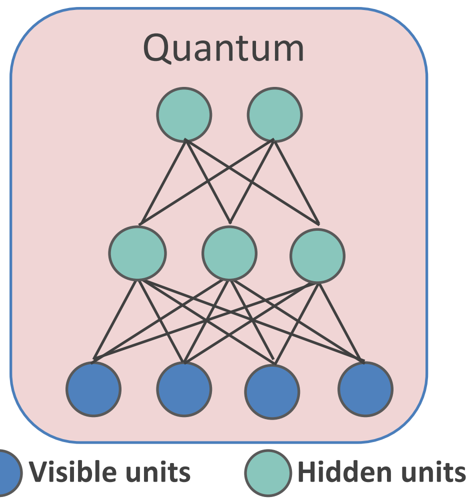
Challenges of the hybrid approach:

- Need to solve classical-quantum model mismatch

Training Method: Stochastic gradient ascent

$$\sum_{\mathbf{v}\in D} \frac{\partial \ln \mathcal{L}(\theta|\mathbf{v})}{\partial J_{ij}} \propto \boxed{\langle v_i u_j\rangle_{\mathrm{data}}} - \boxed{\langle v_i u_j\rangle_{\mathrm{model}}}$$

Classical - T_{eff}?

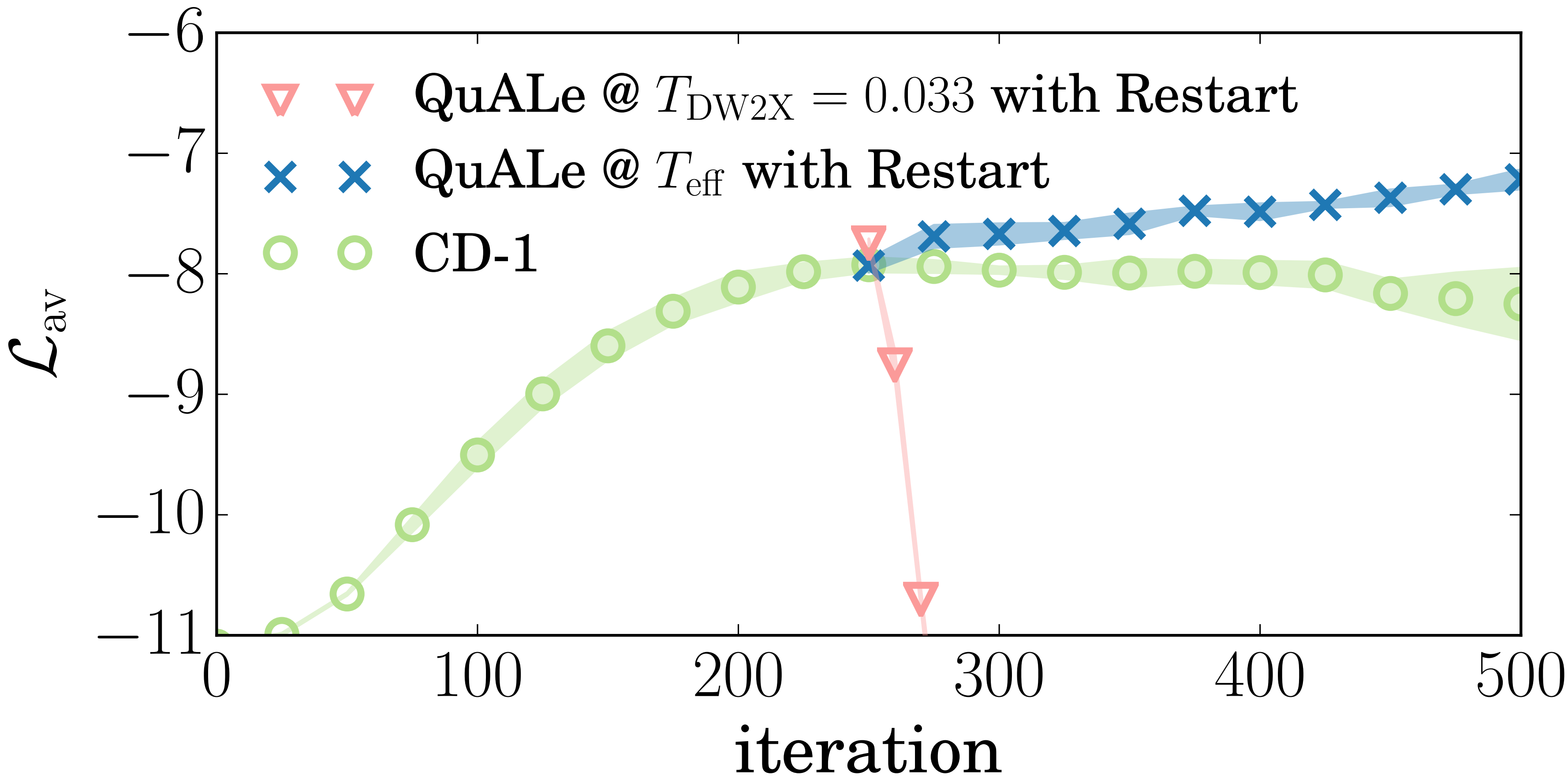


Benedetti et al . Phys. Rev. A 94, 022308 (2016)

No significant progress in 2010-2015 for generative modeling and QA sampling.

A near-term approach for quantum-enhanced machine learning

Resolving model mismatch allows for restarting from classical preprocessing



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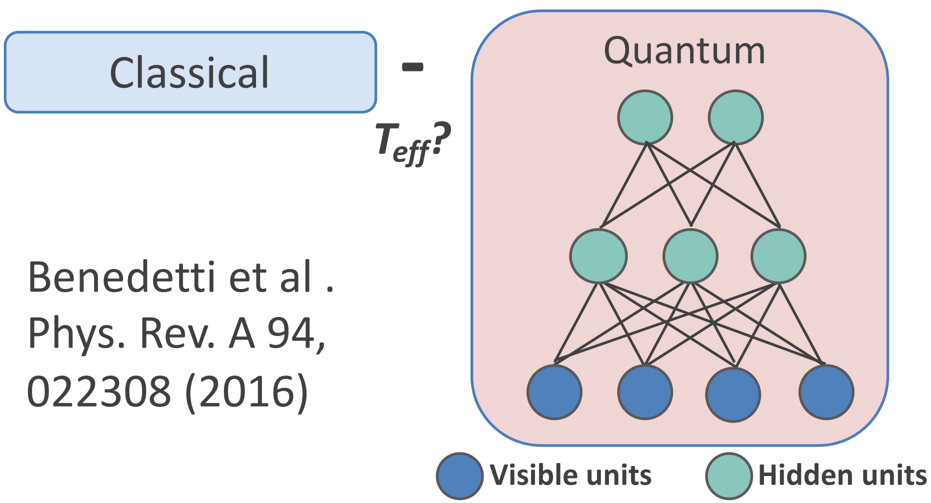

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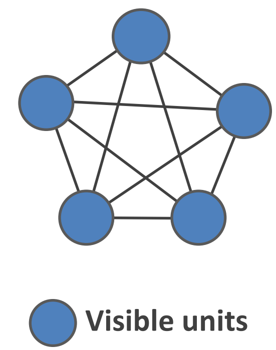
No significant progress in 2010-2015 for generative modeling and QA sampling.

- Robustness to noise, intrinsic control errors, and to deviations from sampling model (e.g., Boltzmann)

- *Curse of limited connectivity* – parameter setting

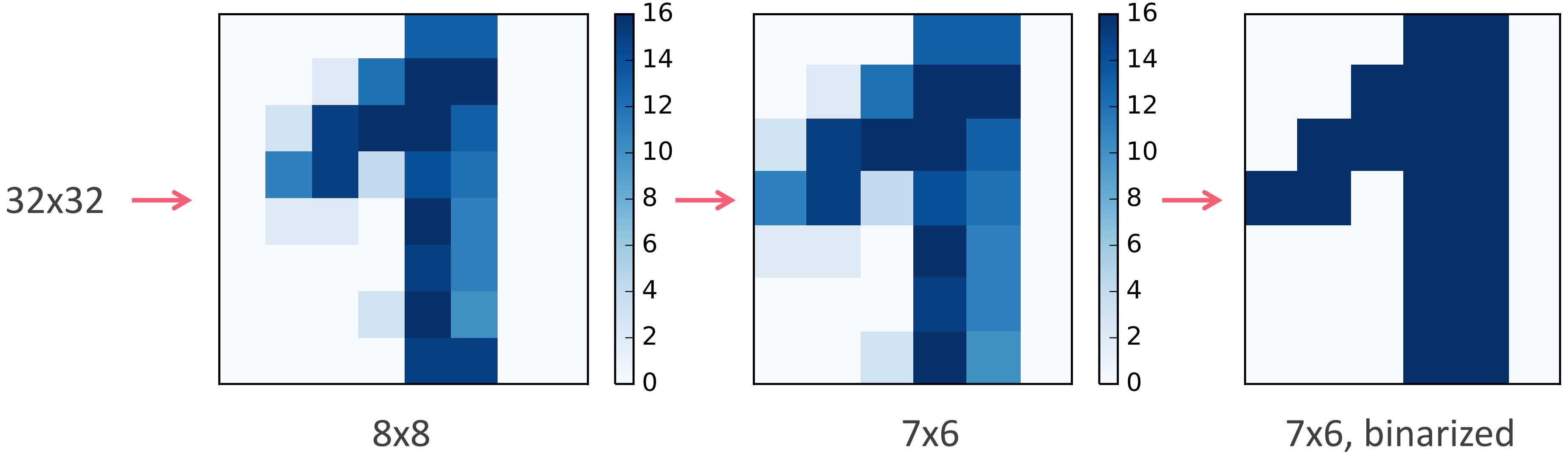
Fully visible models



Benedetti et al. arXiv:1609.02542

Quantum-assisted unsupervised learning on digits

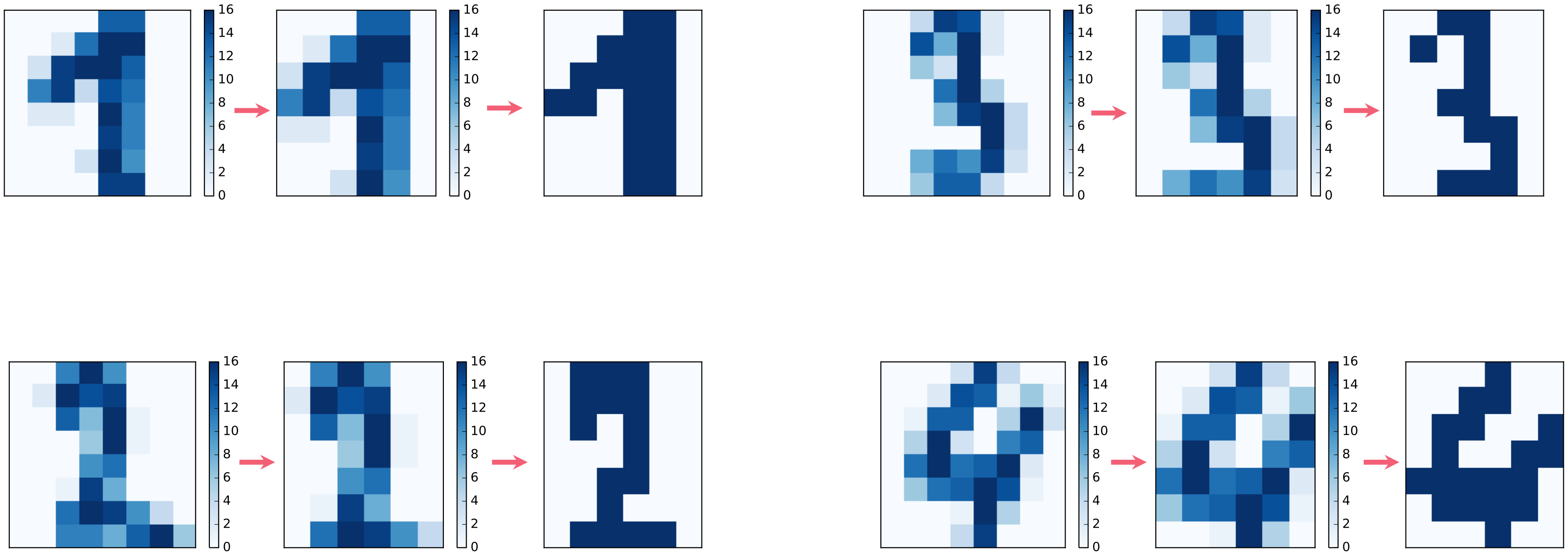
OptDigits Datasets



Dataset: Optical Recognition of Handwritten Digits (OptDigits)

Quantum-assisted unsupervised learning on digits

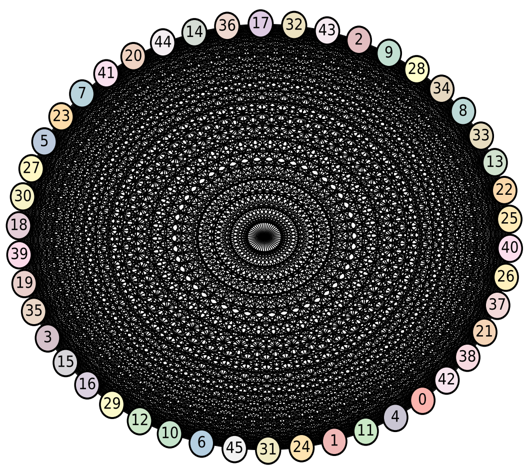
OptDigits Datasets



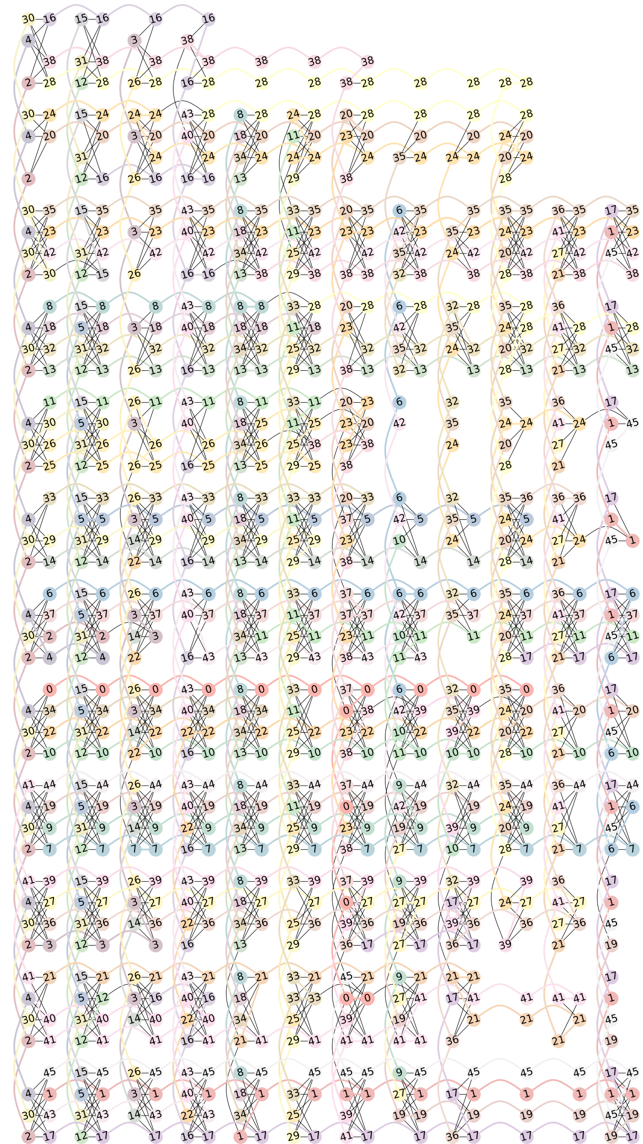
Dataset: Optical Recognition of Handwritten Digits (OptDigits)

Quantum-assisted unsupervised learning on digits

Overcoming the curse of limited connectivity in hardware.



46 fully-connected
logical (visible) variables



940 physical qubits

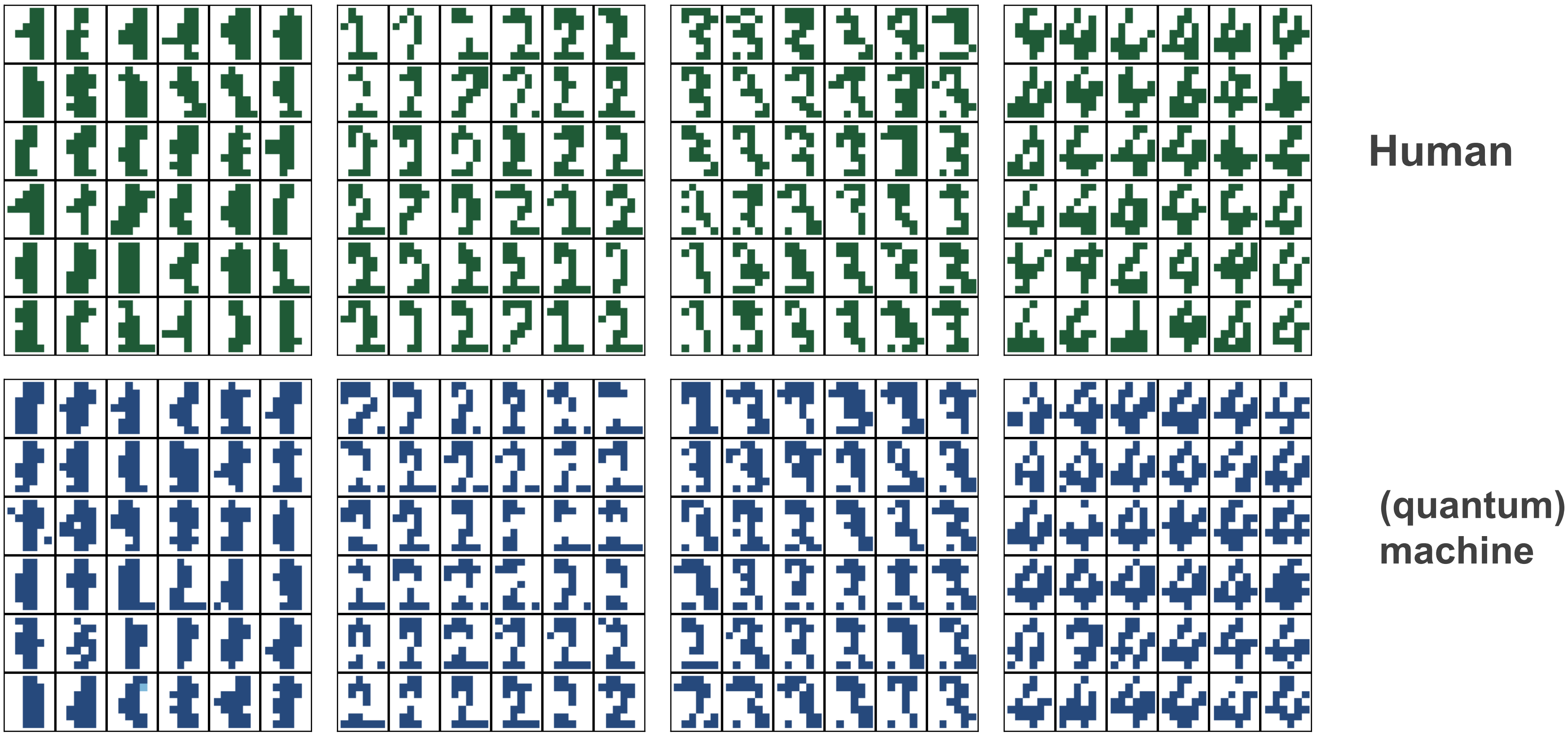
42 for pixels + 4 to one-hot encode the class (only digits 1-4)

- Are the results from this training on 940 qubit experiment meaningful?
- Is the model capable of generating digits?

Min. CL =12, Max. CL = 28

Quantum-assisted unsupervised learning on digits

Human or (quantum) machine? (Turing test)



Dataset: Optical Recognition of Handwritten Digits (OptDigits)

Results from experiments using 940 qubits, without post-processing.
The hardware-embedded model represents a 46 node fully connected graph.

A near-term approach for quantum-enhanced machine learning

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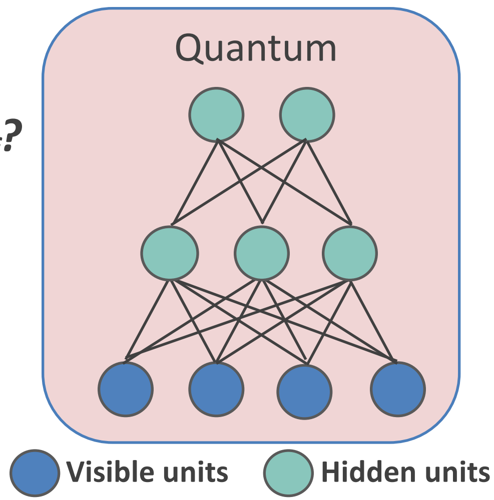
$$\sum_{\boldsymbol{v}\in S}\frac{\partial \ln \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{v})}{\partial w_{ij}} \propto \boxed{\langle v_i h_j\rangle_{\text{data}}} - \boxed{\langle v_i h_j\rangle_{\text{model}}}$$

Classical - T_{eff}?

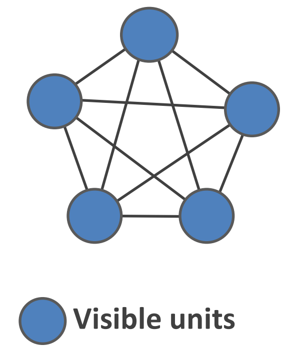


Benedetti et al . Phys. Rev. A 94, 022308 (2016)

No progress in five years since QA sampling was proposed as a promissing appplication.

- Robustness to noise, intrinsic control errors, and to deviations from sampling model (e.g., Boltzmann)
- *Curse of limited connectivity* – parameter setting

Fully visible models



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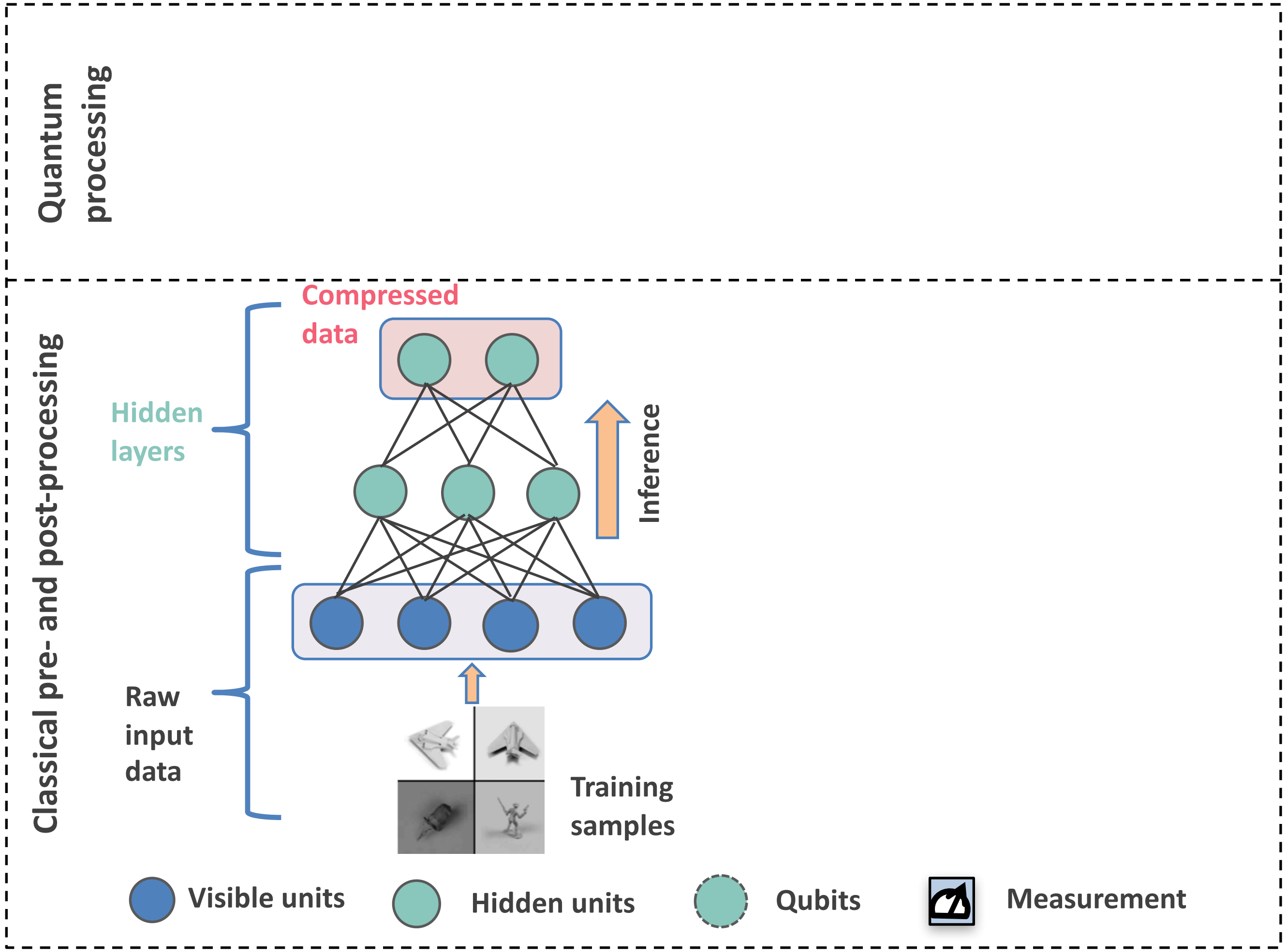
How about large complex datasets with continuous variables?
All previous fail to do that (fully quantum and hybrid here)

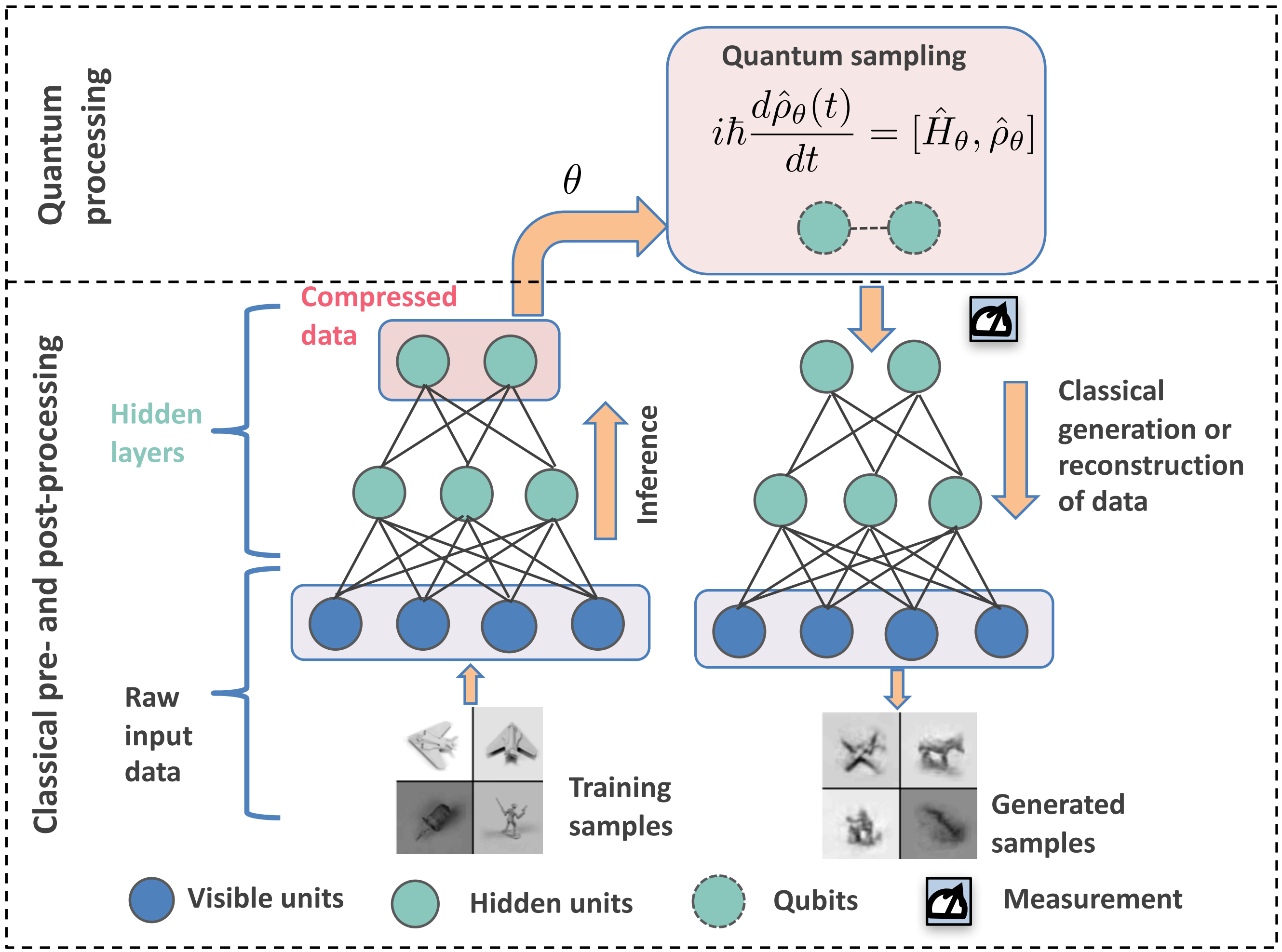
Perspective on quantum-enhanced machine learning

- **New hybrid proposal that works directly on a low-dimensional representation of the data.**



Perspective on quantum-enhanced machine learning

- **New hybrid proposal that works directly on a low-dimensional representation of the data.**



Perspective on quantum-enhanced machine learning

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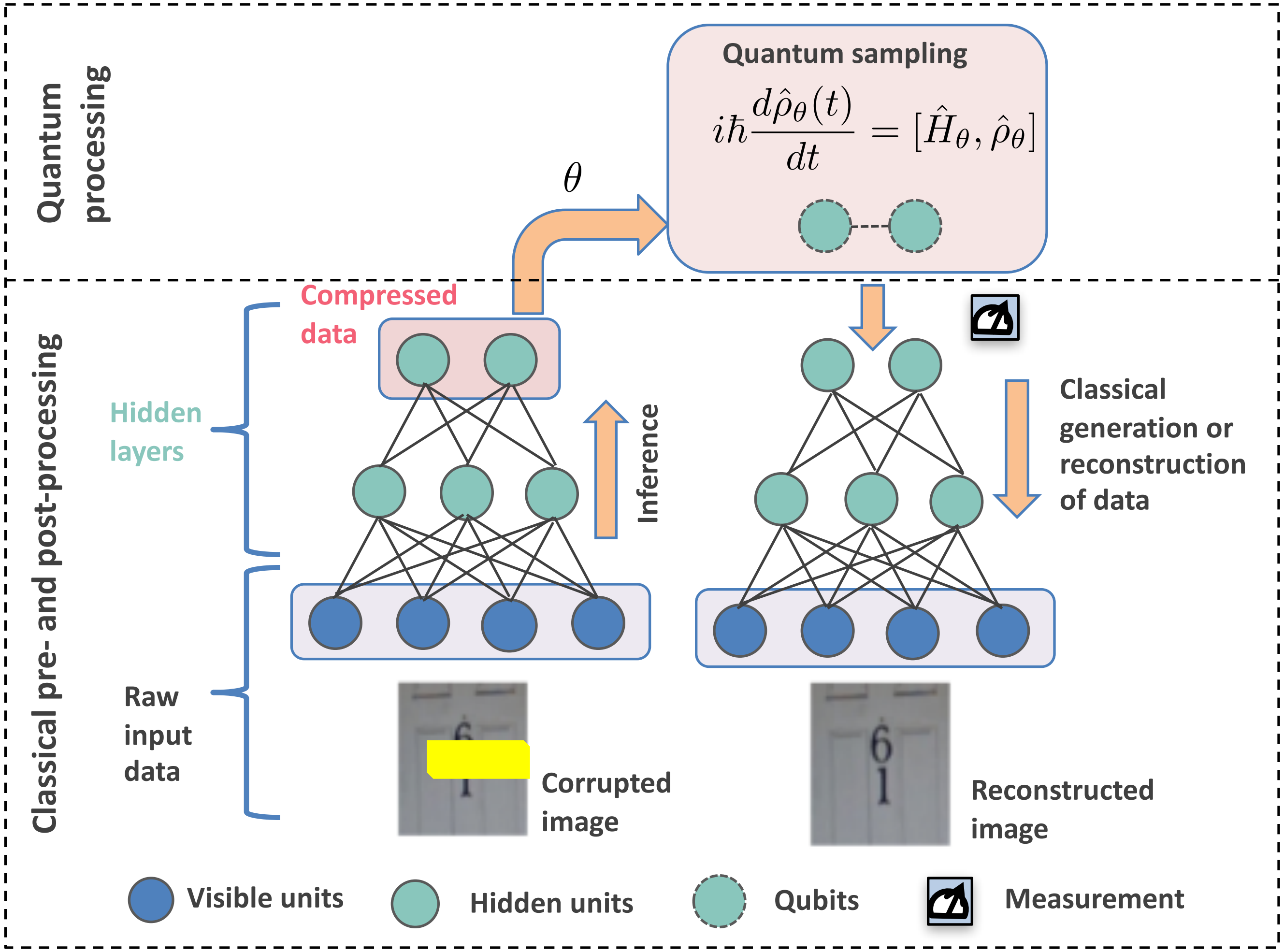
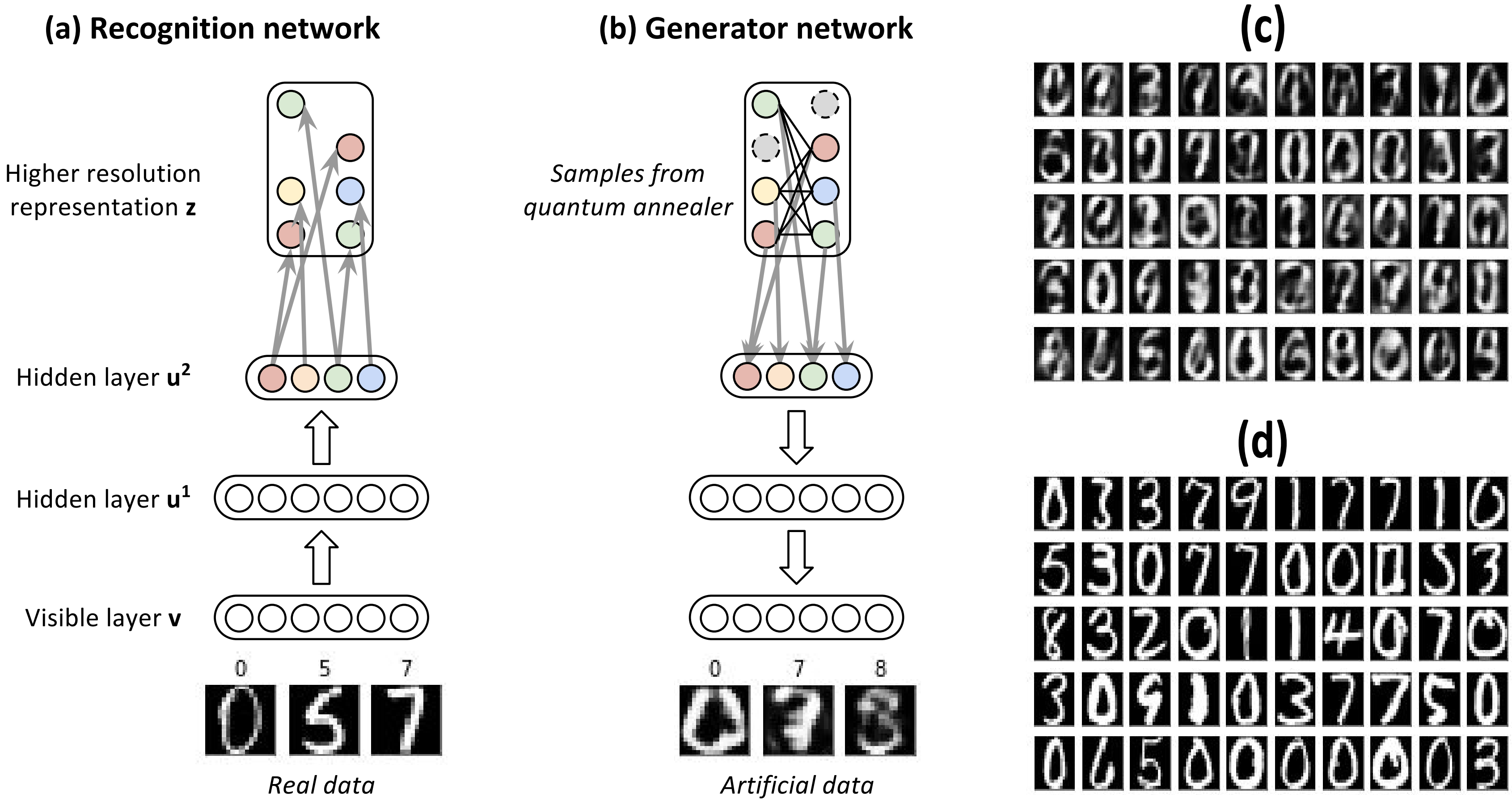


Benedetti, Realpe-Gomez, and Perdomo-Ortiz. Quantum-assisted Helmholtz machines: A quantum-classical deep learning framework for industrial datasets in near-term devices. **arXiv:1708.09784** (2017).

Experimental implementation of the QAHM



Experiments using 1644 qubits (no further postprocessing!)

Max. CL = 43

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Opportunities and challenges for quantum-assisted machine learning in near-term quantum computers

Alejandro Perdomo-Ortiz,[1,2,3,*] Marcello Benedetti,[1,3] John Realpe-Gómez,[1,4,5] and Rupak Biswas[6]

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- **Opportunities:** Emphasis in moving from popular ML to not-so-popular but still highly value ML applications. Example: From discriminative models to more powerful generative models. Also, classical datasets with intrinsic quantum correlations.

- **Challenges:** Limited qubit-qubit connectivity, limited precision, intrinsic control errors, digital representation, classical-quantum feedback (in case of hybrid).

- **Proposed directions:** Emphasis on hybrid quantum-classical algorithms. New approach capable of tackling large complex datasets in machine learning.

arXiv:1708.09757. (2017). To appear in the Quantum Science and Technology (QST) invited special issue on “What would you do with a 1000 qubit device?”

Job advertisement

Opportunities at NASA Quantum AI Lab. (NASA QuAIL) at different levels: internships, postdoc, or Research Scientist.

For details, please contact:
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Alejandro Perdomo-Ortiz: Quantum Machine Learning Lead.
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