Quantum-Assisted Machine Learning in Near-Term Quantum Devices

Alejandro Perdomo-Ortiz

Senior Quantum Scientist, Zapata Computing, Canada

Honorary Senior Research Associate, Computer Science Dept., UCL, UK

@aperdomoortiz, @ZapataComputing

ZAPATA

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Capabilities of Near-Term Quantum Devices

0. Simulation of quantum systems

1. As a discrete optimization solver:

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

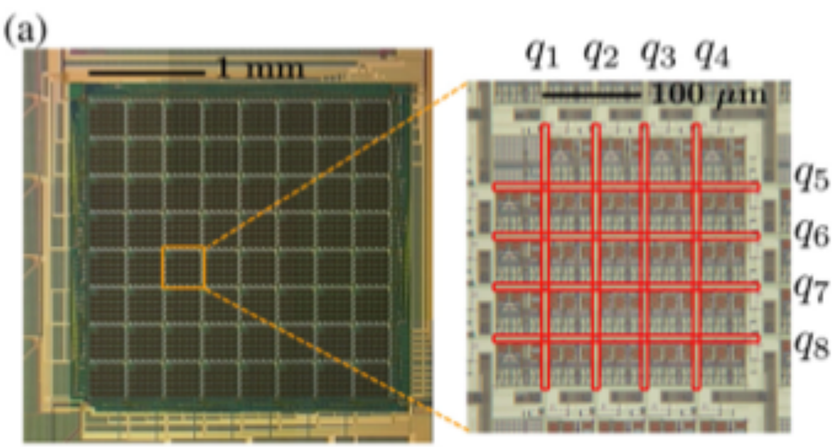
NP-hard problem

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

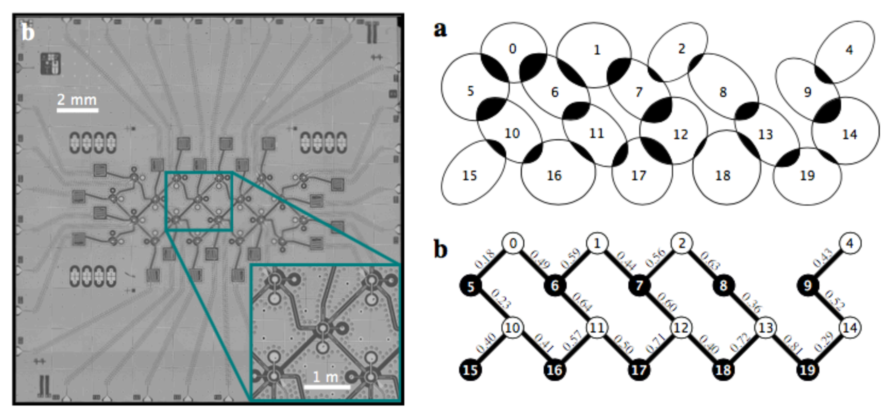
Potential applications:

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

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



Quantum annealing (D-wave)



Example QAOA (Rigetti)

Otterbach et al. **arXiv:1712.05771**.

Capabilities of Near-Term Quantum Devices

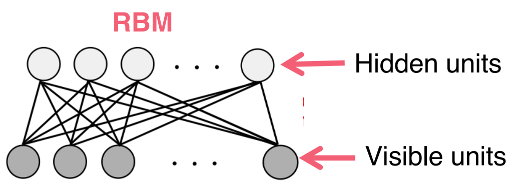
2a. As a physical device to sample from Boltzmann-like distributions:

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

Computationally bottleneck

Example: Quantum annealing

Widely used in **generative unsupervised** learning



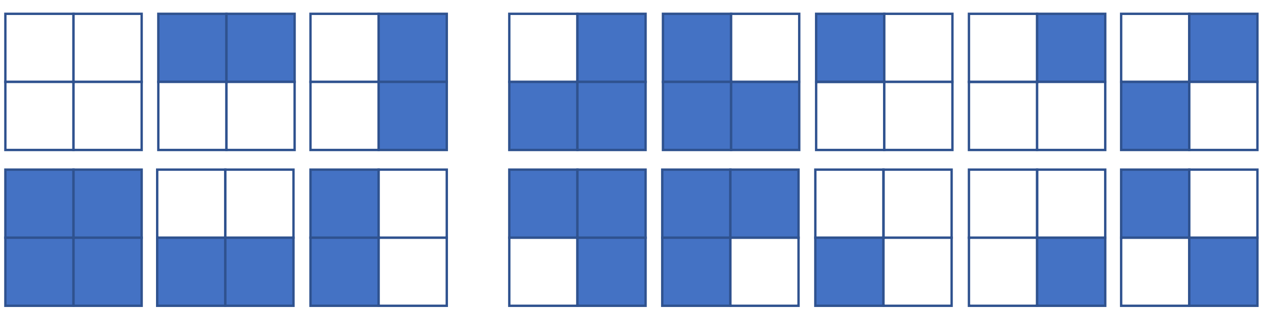
Potential applications:

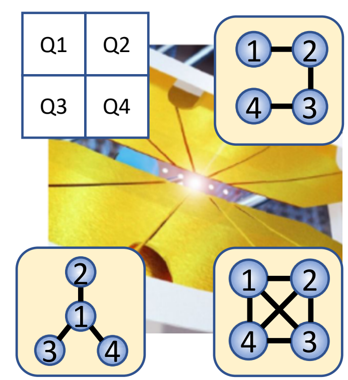
- *machine leaning (e.g., training of deep-learning networks)*

Examples for training probabilistic graphical models:
Benedetti, et al. **Phys. Rev. A 94, 022308** (2016); Benedetti, et al. **Phys. Rev. X 7, 041052 (2017).**

2b. Sampling from more broader quantum distributions

BAS patterns **Non-BAS pattern**





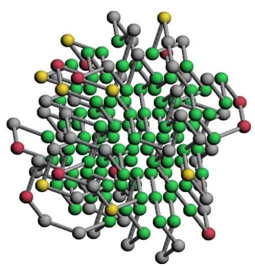
Benedetti et al. A generative modeling approach for benchmarking and training shallow quantum circuits. **npj QI, 5, 45 (2019).**

Motivation

- What are data sets and (non-obvious) real-world applications in need of quantum resources from NISQ devices?

    - **Combinatorial optimization?**

Protein Folding



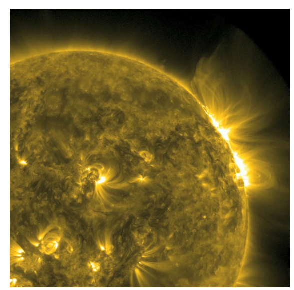
Lattice protein folding

- Perdomo-Ortiz et al. *Phys. Rev. A. 78(1):012320 (2008).*

- Perdomo-Ortiz et al. *Sci. Rep., 2, 571, (2012).*

- Kassal, et al. *Ann. Rev.Phys. Chem. 62, 185-207 (2011).*

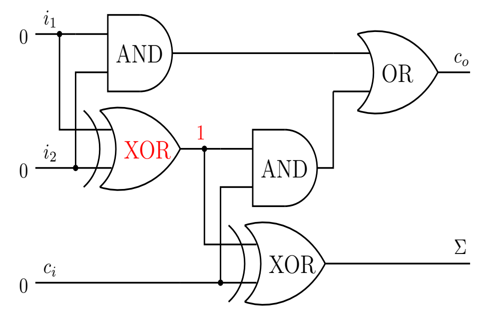
Bayesian networks



Solar Flare prediction

- O'Gorman, et al. *Eur. Phys. J. Spec. Topics. 224, 163- 188 (2015)*

Fault diagnosis Applications



- Perdomo-Ortiz et al. *arXiv:1503.01083 (2015)*

- Perdomo-Ortiz et al. *Eur. Phys. J. Spec. Topics. 224, 131-148 (2015).*

- Perdomo-Ortiz et al. *arXiv:1708.09780 (2017). Accepted in Phys. Rev. Applied.*

Motivation/Outline

- Are there data sets and (non-obvious) real-world applications in need of quantum resources from NISQ devices?
  - Combinatorial optimization? **Machine learning?**

Perspective: Perdomo-Ortiz, et al. Opportunities and Challenges in Quantum-Assisted Machine Learning in Near-term Quantum Computers. **Quantum Sci. Technol. 3, 030502 (2018).** Invited special issue on “What would you do with a 1000 qubit?”

Motivation/Outline

- Are there data sets and (non-obvious) real-world applications in need of quantum resources from NISQ devices?

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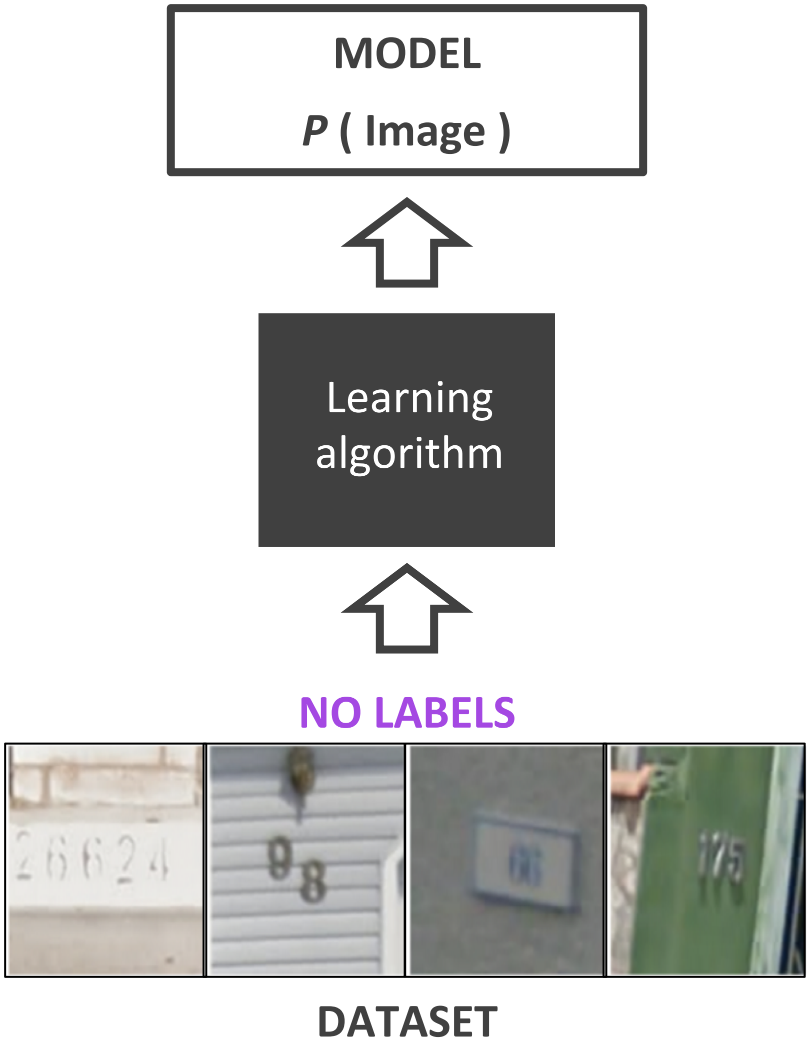
- Why and where to look for quantum advantage in quantum-assisted ML, with NISQ devices?

- Know your hybrid quantum-classical pipeline: classical optimizers, circuit ansatz, etc.

- NISQ quantum models in a real-world setting: an example from a financial application.

Unsupervised learning (generative models)

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



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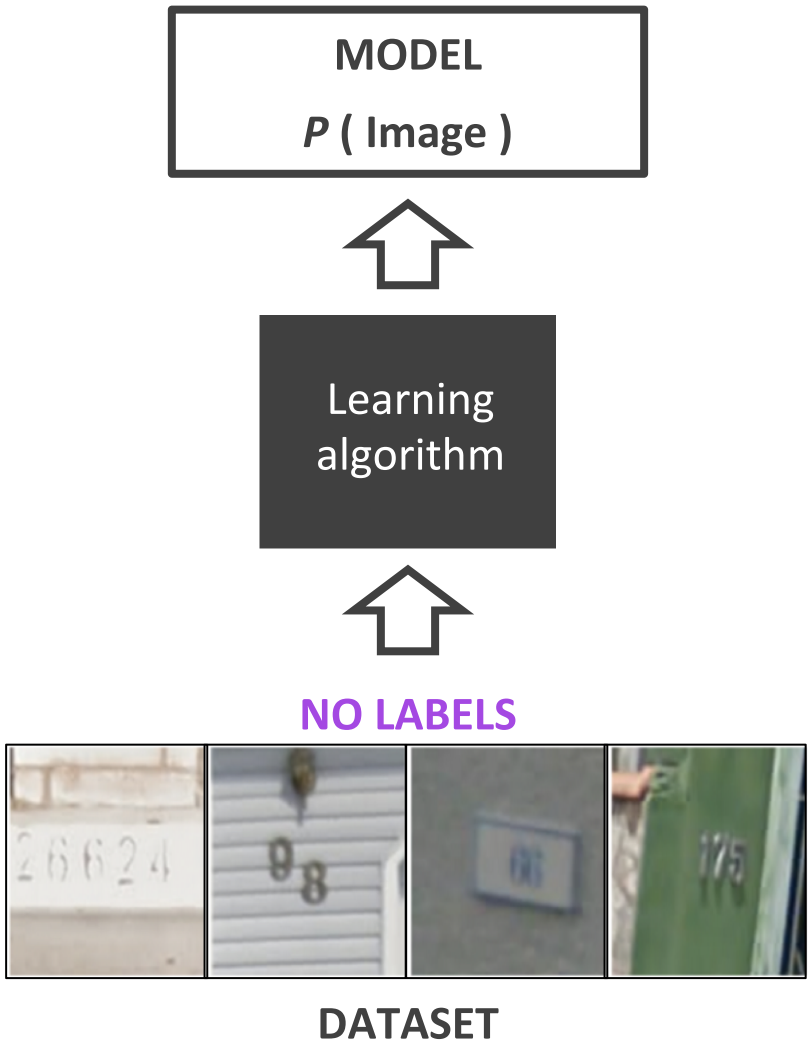
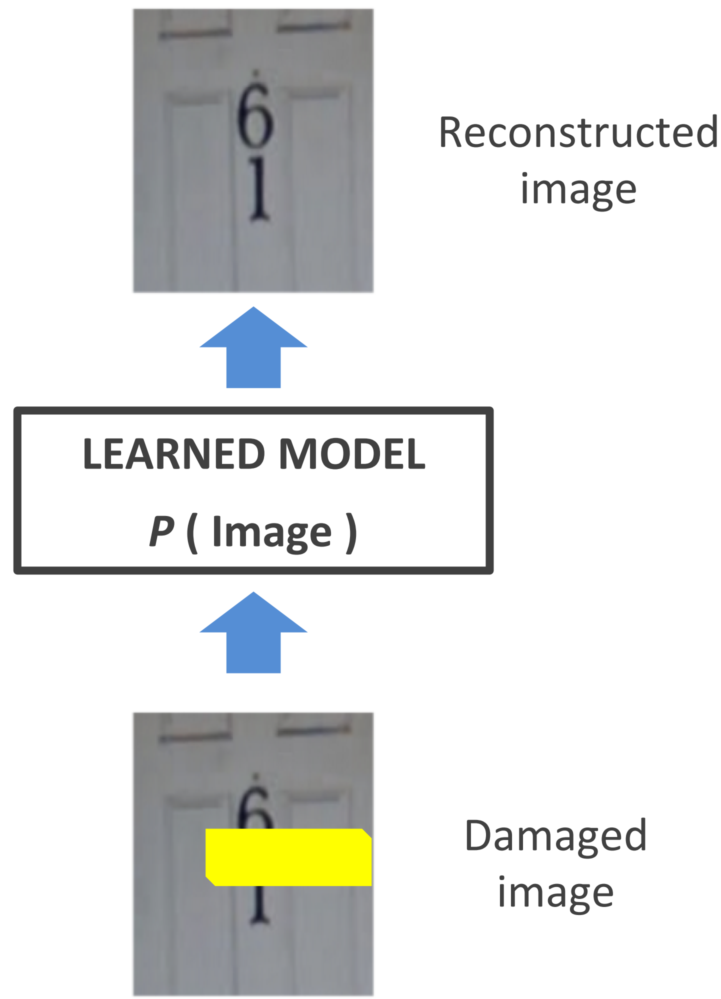
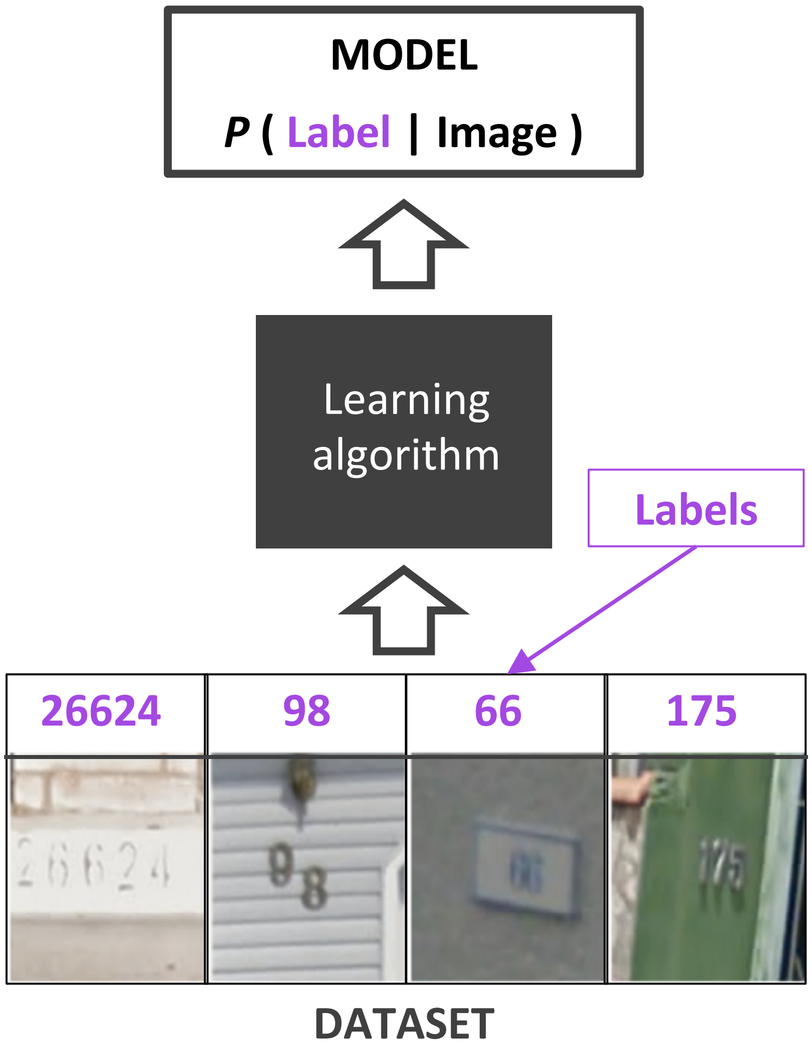


Example application:
Image reconstruction

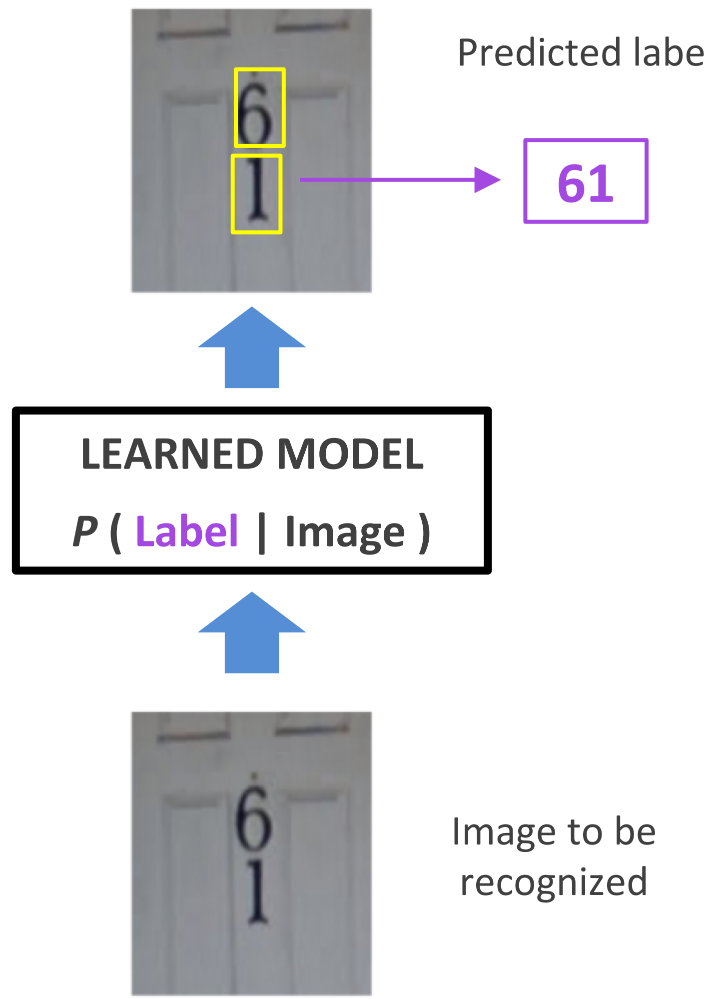


Supervised learning (discriminative models)

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



Example application:
Image recognition



A near-term approach for quantum-enhanced machine learning

Insight 1: Work on intractable problems of interest to ML experts (e.g., **generative models in unsupervised learning**). **Quantum advantage in near term.**

*"Unsupervised learning [... has] been overshadowed by the successes of purely supervised learning. [... We] expect **unsupervised learning to become far more important in the longer term**. Human and animal learning is largely unsupervised: we discover the structure of the world by observing it, not by being told the name of every object."*

LeCun, Bengio, Hinton, *Deep Learning*, **Nature 2015**

Perdomo-Ortiz, Benedetti, Realpe-Gomez, Biswas. **Quantum Sci. Technol. 3, 030502 (2018).**

A near-term approach for quantum-enhanced machine learning

Insight 1: Work on intractable problems of interest to ML experts (e.g., **generative models in unsupervised learning**). **Quantum advantage in near term.**

"In the context of the deep learning approach to undirected modeling, it is rare to use any approach other than Gibbs sampling. ***Improved sampling techniques are one possible research frontier.****"*

Goodfellow, Bengio, Courville, *Deep Learning*, book in preparation for MIT Press, **2016**

A near-term approach for quantum-enhanced machine learning

Insight 1: Work on intractable problems of interest to ML experts (e.g., **generative models in unsupervised learning**). **Quantum advantage in near term.**

*"Most of the previous work in **generative models** has focused on variants of **Boltzmann Machines** [...] While these models **are very powerful**, each iteration of **training requires a computationally costly step of MCMC** to approximate derivatives of an intractable partition function (normalization constant), making it **difficult to scale** them **to large datasets**."*

Mansimov, Parisotto, Ba, **Salakhutdinov**, ICLR **2016**

Perdomo-Ortiz, Benedetti, Realpe-Gomez, Biswas. **Quantum Sci. Technol. 3, 030502 (2018).**

A near-term approach for quantum-enhanced machine learning

Insight 2: Focus on hybrid quantum-classical approaches.
Cope with hardware constrains and available quantum resources

Perdomo-Ortiz, Benedetti, Realpe-Gomez, Biswas. **Quantum Sci. Technol. 3, 030502 (2018).**

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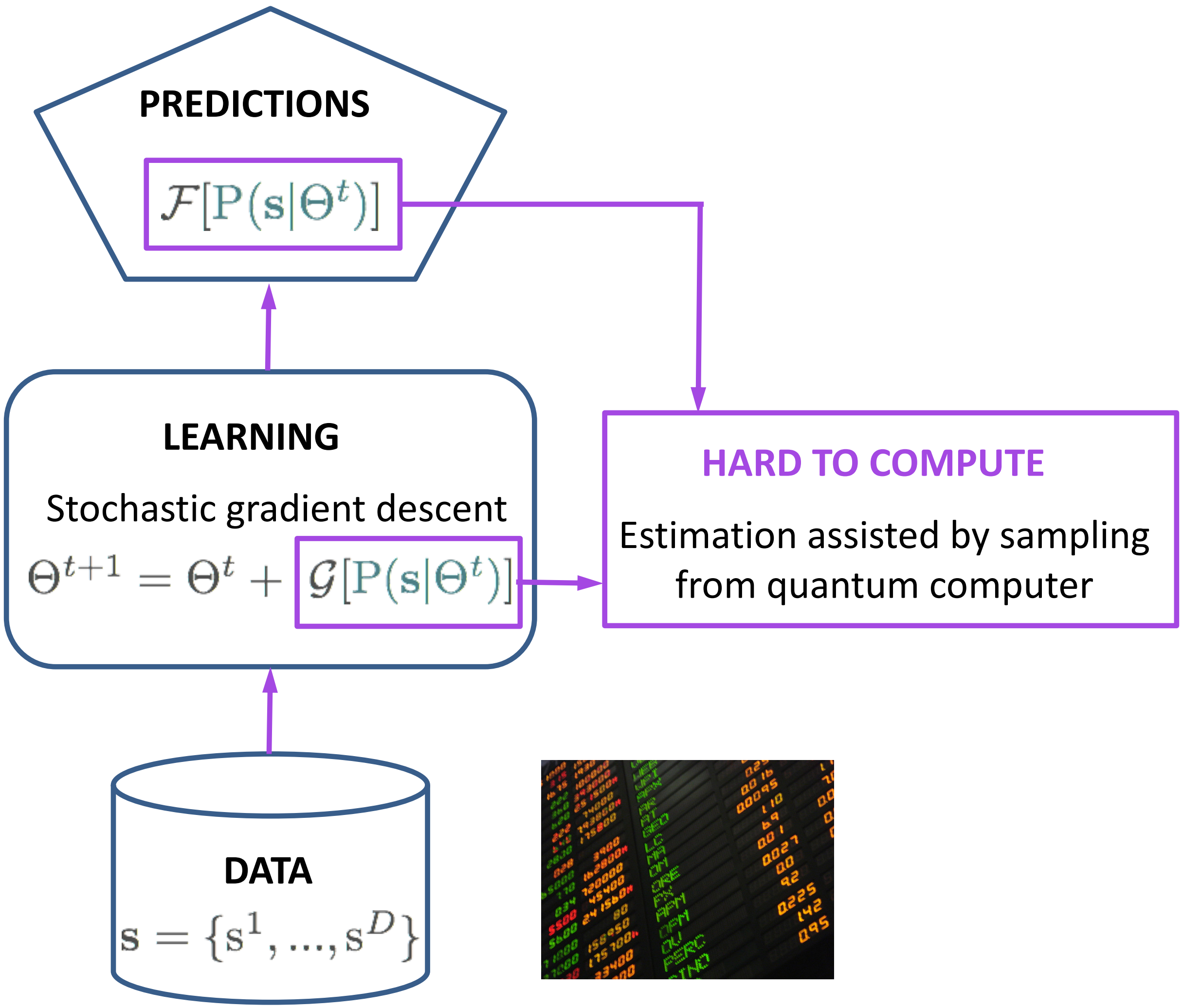

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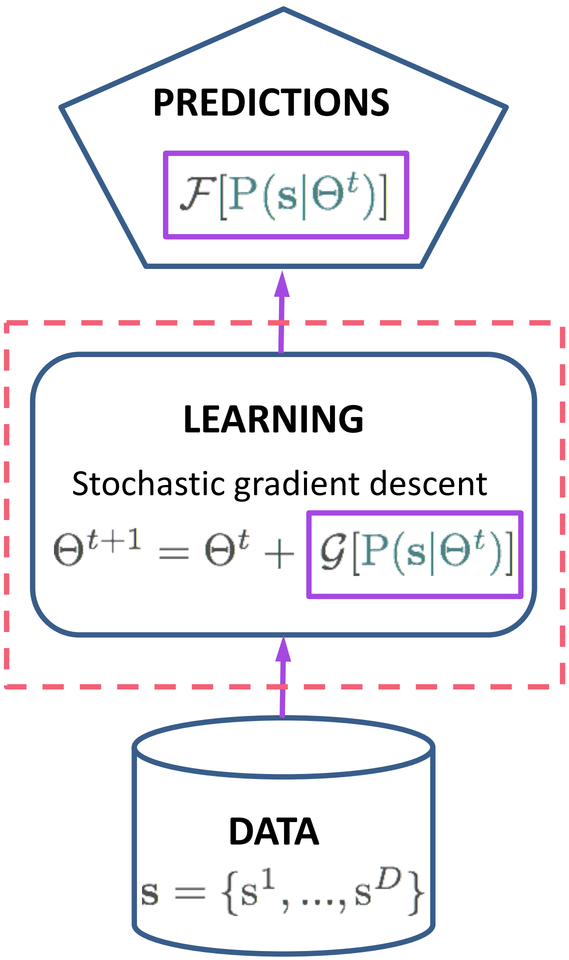

Challenges solved:

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

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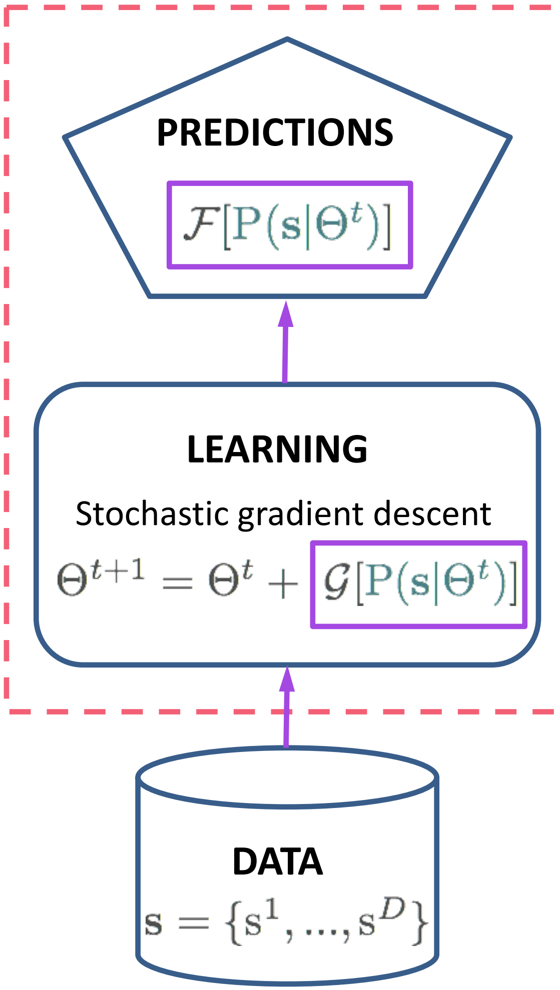

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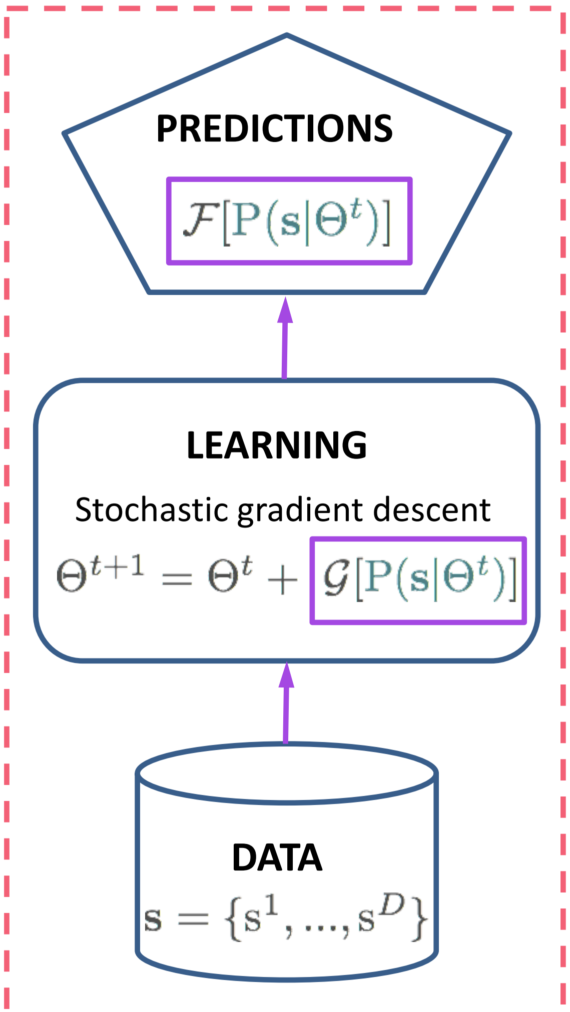

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4. Benedetti, et al. Quantum-assisted Helmholtz machines: A quantum-classical deep learning framework for **industrial datasets in near-term devices**. *<u>Quantum Sci. Technol</u>. 3, 034007 (2018).*

A near-term approach for quantum-enhanced machine learning

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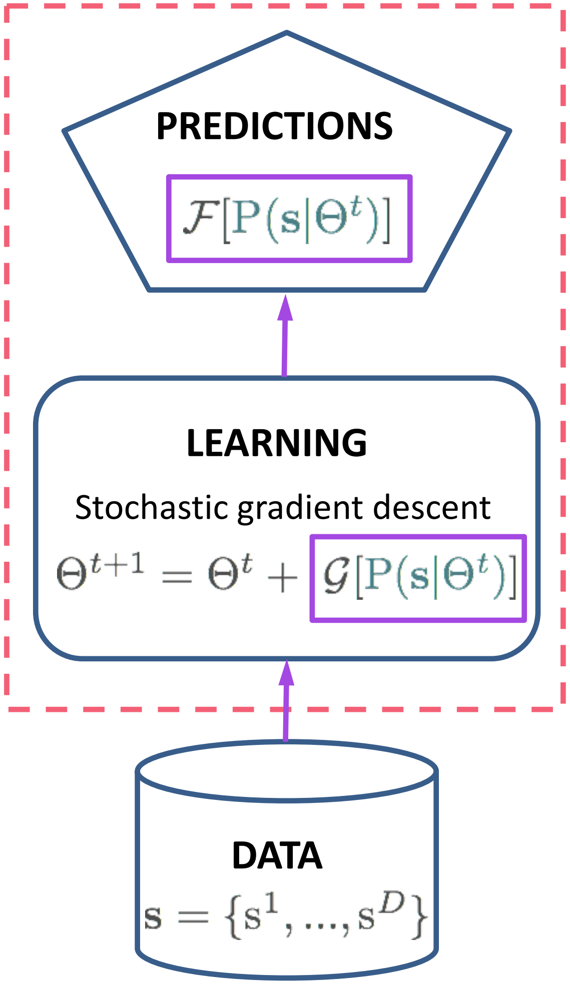

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5. Benedetti, et al. A generative modeling approach for **benchmarking and training shallow quantum circuits**. *npj QI, 5, 45 (2019)*.

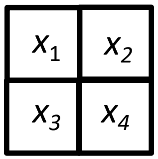
6. Zhu et al. **Training** of Quantum Circuits on a Hybrid Quantum Computing. *arXiv:1812.08862 (2018).*

7. Leyton-Ortega, et al. **Robust** Implementation of Generative Modeling with Parametrized Quantum Circuits. *arXiv:1901.08047 (2019).*

8. Leyton-Ortega, et al. **Benchmarking Optimizers** for Hybrid Quantum-Classical Algorithms. *To appear soon in arXiv.*

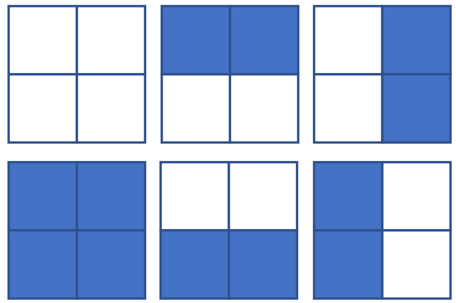
9. Alcazar et al. Classical **versus** Quantum Models in ML: Insights from a Finance Application. *arXiv:To appear soon in arXiv.*

Unsupervised generative modeling with NISQ devices



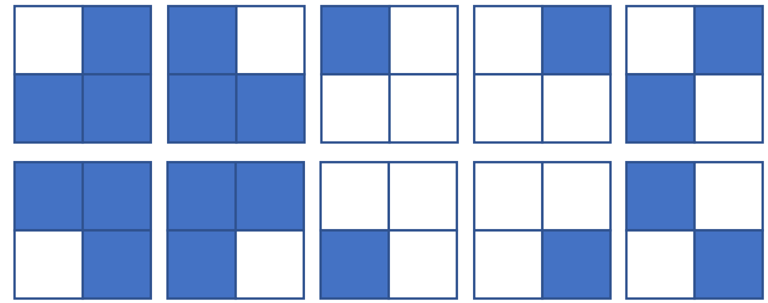
$x_1x_2x_3x_4$

BAS patterns



{0000,1100, 0101,
1111,0011,1010}

Non-BAS pattern



Ludwig Boltzmann (1844-1906)

Boltzmann machines

$$P_{Boltzman} \propto exp[-\xi(s_1, ..., s_N)/T_{eff}]$$

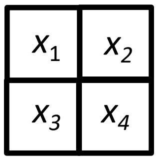
Max Born (1882-1970)

Quantum Circuit Born machines (QCBM) $P_{\boldsymbol{\theta}}(\mathbf{x}) = |\langle \mathbf{x} | \psi(\boldsymbol{\theta}) \rangle|^2.$

Generative modeling with NISQ devices, beyond Boltzmann

QCBMs: Benedetti, Garcia-Pintos, Perdomo, Leyton-Ortega, Nam, and Perdomo-Ortiz. A generative modeling approach for benchmarking and training shallow quantum circuits. **npj QI, 5, 45 (2019).**

Unsupervised generative modeling with NISQ devices



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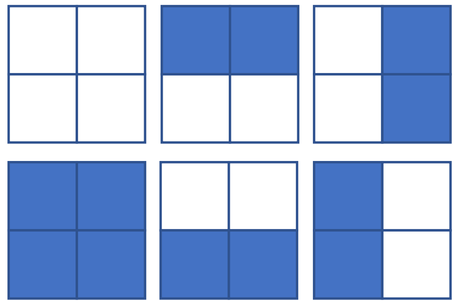

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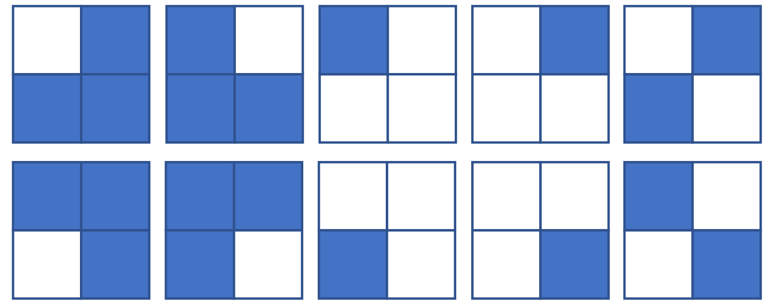

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Max Born (1882-1970)

Born machines $P_{\boldsymbol{\theta}}(\mathbf{x}) = |\langle \mathbf{x}|\psi(\boldsymbol{\theta})\rangle|^2.$

Tensor networks: Chen, Chen, Wang. **arXiv:1712.04144**.

Generative Modeling.

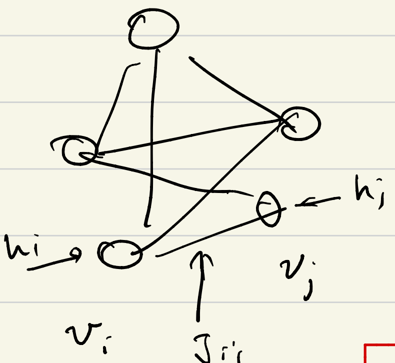
Dataset:

$\{\vec{v}^{(i)}\}_{i=1}^{D}$ D samples that are i.i.d. from $p(\vec{v})$
↳ data dist.

Find $\vec{\theta}$: $q(\vec{v}|\theta) \simeq p(\vec{v})$ → learning

Boltzmann Machines (BMs)

Energy PGM



$$\vec{v}^{(i)} = v_1^{(i)}\, v_2^{(i)} \ldots v_N^{(i)}$$

$\vec{v}$ = visible units

$$E(\vec{v}, \{\vec{h}, \vec{J}\}) = \sum_i h_i v_i + \sum_{ij} J_{ij} v_i v_j$$

↓

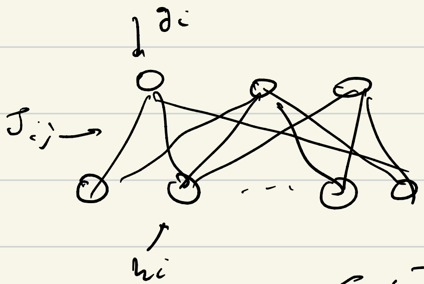
$$E(\vec{v}|\theta)$$

FVBM

$$q_\theta(\vec{v}) = \frac{e^{-E(\vec{v}|\theta)/T}}{Z(\theta)}$$

$$Z(\theta) = \sum_{\vec{v}} e^{-E(\vec{v}|\theta)/T}$$

Restricted Boltzmann Machine (RBM)



$\vec{u}$ = unseen or hidden variable

$\vec{v}$ = visible units

$$E(\vec{v},\vec{u}|\theta) = \sum_i h_i v_i + \sum_i g_i u_i + \sum_{ij} J_{ij} v_i u_j$$

$$\theta = \{\vec{h}, \vec{g}, \vec{J}\}$$

$$q_\theta(\vec{v},\vec{u}) = \frac{e^{-E(\vec{v},\vec{u}|\theta)/T}}{Z(\theta)}$$

$$\boxed{q_\theta(\vec{v}) = \sum_{\vec{u}} q_\theta(\vec{v},\vec{v})}$$

Likelihood and NLL(θ):

$$\mathcal{L}(\theta) = \prod_{i=1}^{D} q_\theta(v^{(i)})$$

$$NLL(\theta) = -\log \mathcal{L}(\theta) = -\sum_{i=1}^{D} \log q_\theta(\vec{v}^{(i)})$$

$$\approx -D \langle \log q_\theta(\vec{v}) \rangle_{p(\vec{v})}$$

Kullback-Leibler Divergence (KL)

(cross-entropy)

$$KL(p(\vec{v}) \| q(\vec{v})) = \sum_{\vec{v}} p(\vec{v}) \log \frac{p(\vec{v})}{q(\vec{v})}$$

$KL \geq 0$ $\quad$ $KL = 0$ iff $p = q$

$$KL(p \| q_\theta) = \sum_{\vec{v}} p(\vec{v}) \log p(\vec{v}) - \sum_{\vec{v}} p(\vec{v}) \log q_\theta(\vec{v})$$

(-entropy) → 0 when taking gradient

$$\nabla_\theta KL(p \| q_\theta) = -\sum_{\vec{v}} p(\vec{v}) \nabla_\theta \log q_\theta(\vec{v})$$

$$= -\nabla_\theta \langle \log q_\theta(\vec{v}) \rangle_{p(\vec{v})}$$

Averaging!

$$\langle A(x) \rangle_{p(x)} = \sum_x p(x) A(x) \simeq \frac{1}{N} \sum_{i=1} A(x^{(i)})$$

if $\vec{x}^{(i)}$ is iid from $p(x)$

Stochastic Gradient Descent (SGD)

$$\theta_i = \theta_i - \eta \frac{\partial NLL(\theta)}{\partial \theta_i}$$

Example for FVBM:

$$E(\vec{v}|\theta) = \sum h_i v_i + \sum_{ij} J_{ij} v_i v_j$$

$$q_\theta(\vec{v}) = \frac{e^{-E(\vec{v}|\theta)/T}}{Z(\theta)} \qquad Z(\theta) = \sum_{\vec{v}} e^{-E(\vec{v}|\theta)/T}$$

$$NLL(\theta) = -\sum_{i=1}^{D} \log q_\theta(\vec{v})$$

$$= -\sum_{i=1}^{D} \left(-\frac{E(\vec{v}|\theta)}{T} - \log Z(\theta) \right)$$

$\partial \log Z(\theta)$

$$\frac{\partial NLL(\theta)}{\partial h_j} = \sum_{i=1}^{D} \frac{v_j^{(i)}}{T} + \sum_{i=1}^{D} \frac{1}{Z(\theta)} \sum_{\vec{v}} \left(\frac{-v_j}{T}\right) e^{-E(\vec{v}|\theta)/T}$$

$$= \frac{D}{T} \left(\frac{1}{D} \sum_{i=1}^{D} v_j^{(i)} - \sum_{\vec{v}} v_j q_\theta(\vec{v}) \right)$$

$$= \frac{D}{T} \left(\langle v_j \rangle_{p(\vec{v})} - \langle v_j \rangle_{q_\theta(\vec{v})} \right)$$

$$\frac{\partial NLL(\theta)}{\partial h_j} = \frac{D}{T} \left(\langle v_j \rangle_{data} - \langle v_j \rangle_{model} \right)$$

$$\frac{\partial NLL(\theta)}{\partial J_{ij}} = \frac{D}{T}\left(\langle v_i v_j \rangle_{data} - \langle v_i v_j \rangle_{model} \right)$$

MCMC.