DE LA RECHERCHE À L'INDUSTRIE

Quantum Deep Learning for Materials Science

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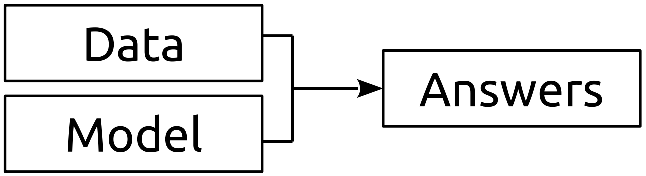
Overview

- Brief Introduction to Machine Learning
- A Material Science Problem
- Graph Neural Networks
- Why Quantum Deep Learning?
- Continuous Variable Information
- Continuous Variable Quantum Neural Networks
- Ending Thoughts

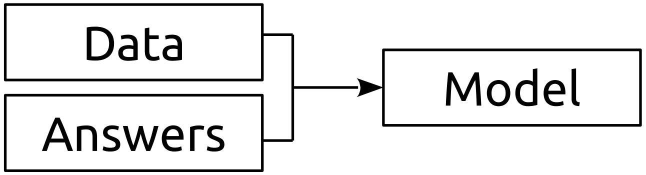
Brief Introduction to Machine Learning

- Machine learning = fancy word for fitting a curve.

- We are looking for a function that maps a feature vector to a target label. Two ways:
  - Using a physical model: Schrödinger's, Sternheimer's, Newton's equation, etc.
    - <u>Advantage :</u> Large domain of validity. Extrapolation possible.
    - <u>Drawback:</u> Impossible to solve analytically or numerically without approximations.



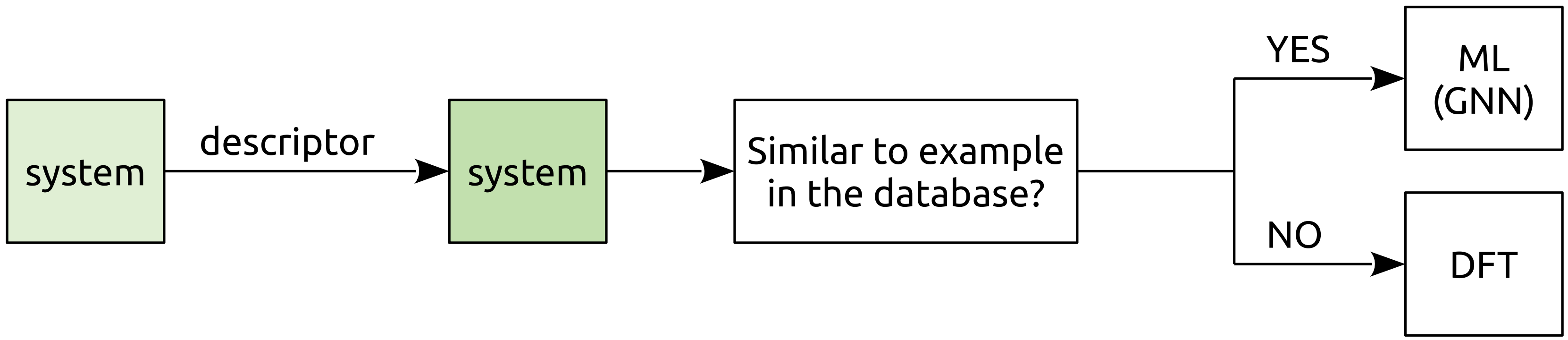
  - Using machine learning. The model learns from examples.
    - <u>Advantage :</u> Numerical solving is in principle exact. No approximation beside the form of the function (linear, polynomial, mix of linear and nonlinear, etc.).
    - <u>Drawback:</u> Interpretability is difficult or impossible. No extrapolation.



A Material Science Problem

- Some DFT calculations of materials properties are difficult or currently impossible.
- In particular, properties derived from successive derivatives of the total energy:
  - Phonons, magnetic couplings, IR spectra (2nd derivatives).
  - Thermal conductivity, Raman signals height (3rd derivative)
  - Etc.

- Idea: Acceleration by calculating these properties with ML rather than DFT.



- Already used extensively for global (system-level) properties but scarse for local (atom-level) properties.

Graph Neural Networks

- For global properties, lots of models are available and work just fine.

- For local properties, best model (following a Kaggle competition) is a Graph Neural Network (GNN).

- How it works :
  - The system is featurized into a graph: atoms = nodes, bonds = edges.
  - The graph goes through an interaction bloc, which updates every atoms with information about their environment → Message Passing (or Information Diffusion) step.
  - The message passing step is repeated until the states of all atoms reach convergence.
  - Once convergence is reached, the graph goes through a regression bloc, which calculates the desired property.

Graph Neural Networks

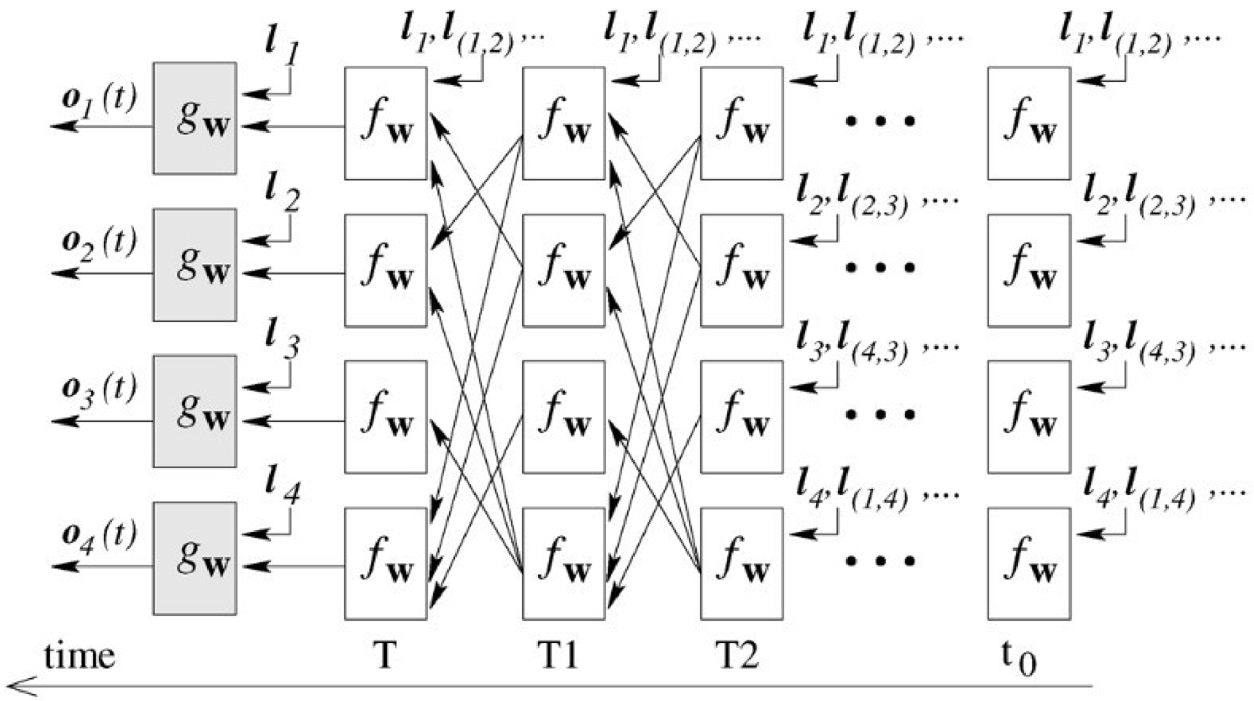
- Unfolding a GNN → Dense recurring neural network (RNN).

  $\mathbf{l}_i$: state of atom *i* $\mathbf{l}_{(i,j)}$: state of bond between atom *i* and *j*

  w : weight matrix. Contains information from environment (aka labels $\mathbf{l}_i$ and $\mathbf{l}_{(i,j)}$).

  f_w : local transition function, parameterized by **w.** Updates states of atoms.

  g_w : local output function, parameterized by **w**. Calculates the desired property.



So What?

- Timings:
  - Training of the GNN: 3-4 days.
  - Inference: < 1 ms.

  → Training time is incompatible with active learning.

- In principle, QC could provide exponential speedups for the following ML methods and models:
  - Principle component analysis (PCA): exploratory data method that reduces feature dimensions.
  - Bayesian inference: inference based on Bayes conditional probabilities.
  - Support Vector Machine (SVM): ML method based on the projection of features in lower or higher dimensional vector spaces. Extensively used in materials science.
  - Recommendation systems: systems that suggest which movie you should see next.
  - And more…

So What?

- Solution 1: hybrid approach. Classical GNN with quantum optimizations.
- Solution 2: quantum GNN → quantum RNN → quantum ANN (q-NN).

- Problem with current realizations for q-NN: based on qubits, which are a discrete unit of information → measurement output is discrete.
  - OK for discrete variables (e.g. binary or multi-class/multi-label classification).
  - NOT OK for continuous variables (e.g. regression on forces on atoms, vibrational frequencies, etc.).
  - No easy extension to convolutional NN (images) or recurrent NN (times series).

- One solution: the continuous variable q-NN, based on continuous variable information [1,2].
  - « Easy » extension to CNN and advanced RNN.
  - Though a different paradigm, circuits can be implemented in the qubits approach.
  - Can be used for discrete variables.

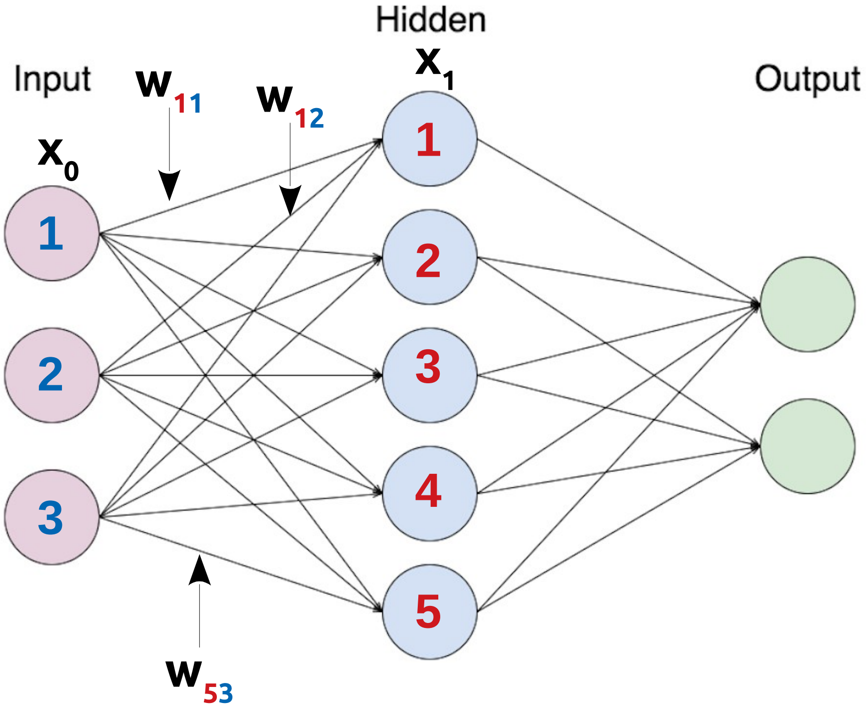
[1] Weedbrook *et al.*, *Rev. Mod. Phys.* **84**, 621 (2012)
[2] Killoran *et al.*, *arXiv e-print* **arXiv:1806.06871v1** (2018)

Continuous Variable information

- Quantum information comes in two forms :
  - Discrete, aka the qubit. Examples: spin 1/2 particles, energy states of quantum dots, quantized superconducting circuits.
  - Continuous. Example: quantum harmonic oscillator. Representative systems: quantization of electromagnetic field (photons) and vibrational modes of solids (phonons).
- Primary tools: Gaussian states and Gaussian transformations.
  - Gaussian states: represented by Gaussian functions.
  - Gaussian transformations: map Gaussian states to Gaussian states.
- Gaussian formalism extensively used by quantum optics (QO) community.
- Mapping between discrete/continuous approach :
  - Number of modes in a Gaussian state (qumodes) ↔ Number of qubits.
  - Gaussian unitaries ↔ quantum gates.
- All Gaussian unitaries have experimental counterparts in quantum optics.

Continuous Variable q-NN

- Feedforward neural network = a big pile of linear algebra = matrix multiplication.



- When units are activated, two things happen: matrix multiplication and nonlinear transformation.
- Therefore, one layer of a quantum NN needs to perform the following classical operation:

$$\varphi(\boldsymbol{W}\cdot\boldsymbol{X}+\boldsymbol{b}) \quad \left| \begin{array}{l} \boldsymbol{W}\in M_{n\times m}(\mathbb{R}) \\ \boldsymbol{X}\in M_{m\times 1}(\mathbb{R}) \\ \boldsymbol{b}\in M_{n\times 1}(\mathbb{R}) \end{array} \right.$$

Continuous Variable q-NN

- Affine transformation $\boldsymbol{W}\cdot\boldsymbol{X}+\boldsymbol{b}$:
  - Singular value decomposition: break linear operator **W** into simpler parts.

$$\boldsymbol{W}=\boldsymbol{O}_2\cdot\boldsymbol{D}\cdot\boldsymbol{O}_1 \quad \left|\begin{array}{l} \boldsymbol{O}_1\in O_{n\times k}(\mathbb{R}) \\ \boldsymbol{D}\in D_{k\times k}(\mathbb{R}) \\ \boldsymbol{O}_2\in O_{k\times m}(\mathbb{R}) \end{array}\right.$$

  - This can be achieved with the following quantum operations:

$$D\circ U_2\circ S\circ U_1$$

Continuous Variable q-NN

- Affine transformation $W \cdot X + b$:
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  This can be achieved with the following quantum operations:

$$D \circ \boxed{U_2} \circ S \circ \boxed{U_1}$$

  - N-mode Interferometers:
    - ✗ QO: device to measure small phase shifts.
    - ✗ QC: combination of 2-mode beamsplitters and single-mode phase shifters.

  Applying an interferometer is equivalent to multiplying by an orthogonal matrix.

Continuous Variable q-NN

- Affine transformation $W \cdot X + b$:
  - Singular value decomposition: break linear operator **W** into simpler parts.

$$W = O_2 \cdot D \cdot O_1 \quad \left| \begin{array}{l} O_1 \in O_{n\times k}(\mathbb{R}) \\ D \in D_{k\times k}(\mathbb{R}) \\ O_2 \in O_{k\times m}(\mathbb{R}) \end{array} \right.$$

This can be achieved with the following quantum operations:

$$D \circ U_2 \boxed{\circ S \circ} U_1$$

  - Single-mode Squeezing:
    - ✗ QO: photons splitting in a nonlinear crystal. More photons → squeezed.
    - ✗ QC: apply a positive or negative scaling to a mode.

Applying a squeezing gate is equivalent to multiplying by a diagonal matrix.

- Affine transformation $\boldsymbol{W}\cdot\boldsymbol{X}+\boldsymbol{b}$:
  - Singular value decomposition: break linear operator **W** into simpler parts.

$$\boldsymbol{W}=\boldsymbol{O}_2\cdot\boldsymbol{D}\cdot\boldsymbol{O}_1 \quad \left| \begin{array}{l} \boldsymbol{O}_1 \in O_{n\times k}(\mathbb{R}) \\ \boldsymbol{D} \in D_{k\times k}(\mathbb{R}) \\ \boldsymbol{O}_2 \in O_{k\times m}(\mathbb{R}) \end{array} \right.$$

This can be achieved with the following quantum operations:

$$\boxed{D} \circ U_2 \circ S \circ U_1$$

  - Single-mode Displacement :
    - ✗ QO: displacement of a state.
    - ✗ QC: displacement of a state.

Applying the displacement operator is equivalent to adding a vector.

Continuous Variable q-NN

- Affine transformation $\boldsymbol{W} \cdot \boldsymbol{X} + \boldsymbol{b}$:
  - Singular value decomposition: break linear operator **W** into simpler parts.

$$\boldsymbol{W} = \boldsymbol{O}_2 \cdot \boldsymbol{D} \cdot \boldsymbol{O}_1 \quad \left| \begin{array}{l} \boldsymbol{O}_1 \in O_{n \times k}(\mathbb{R}) \\ \boldsymbol{D} \in D_{k \times k}(\mathbb{R}) \\ \boldsymbol{O}_2 \in O_{k \times m}(\mathbb{R}) \end{array} \right.$$

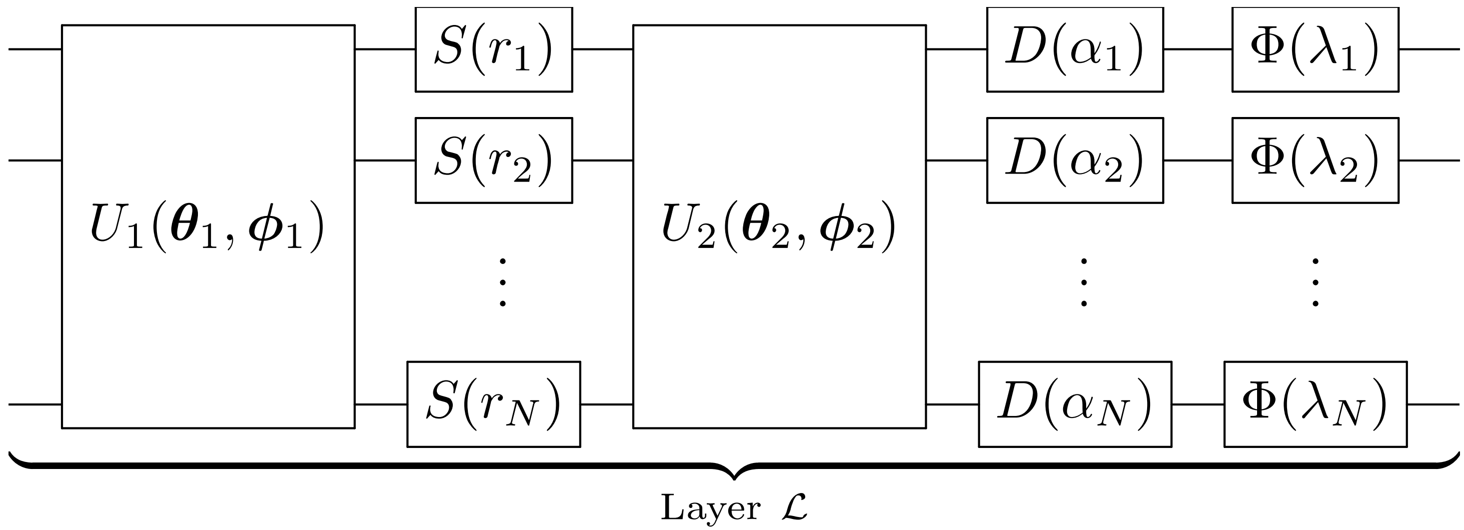
  - This can be achieved with the following quantum operations:

$$\boxed{D \circ U_2 \circ S \circ U_1 |x\rangle = |\boldsymbol{W} \cdot \boldsymbol{X} + \boldsymbol{d}\rangle}$$

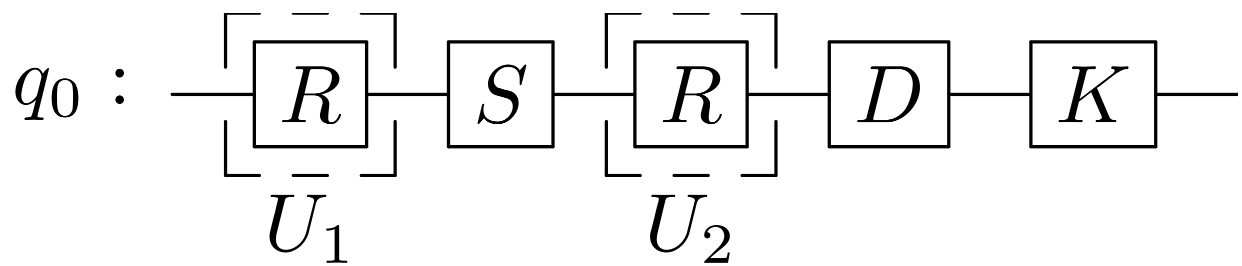
- Nonlinear transformation: use of a non-Gaussian transformation.
  - ✗ QO: the nonlinear Kerr effect. A Kerr medium has an index of refraction that is proportional to the total intensity of light going through.
  - ✗ QC: the nonlinear Kerr gate.

Continuous Variable q-NN

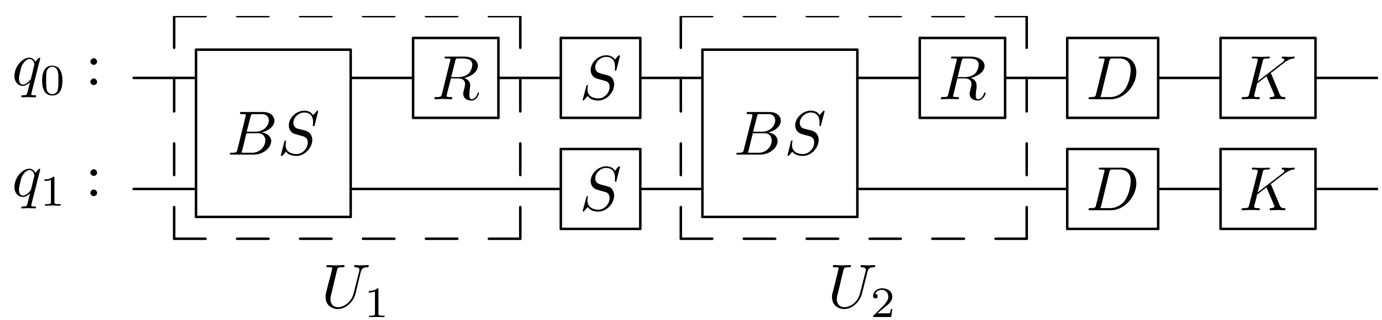
- Summary:



- Layer with 1 qumode :



- Layer with 2 qumodes:



Ending Thoughts

- Go through continuous variable measurements. Most common measurement is homodyne detection :
  - ✗ QO: beamsplitter + photodectectors.
  - ✗ QC: integrals.
- Implement the 1 layer circuit, that is:
  - ➢ Is PyQASM designed for continuous variables?
  - ➢ Implement custom gates: interferometers (beamsplitters and phase shifters), detection gate, squeezing gate, nonlinear Kerr gate.
  - ➢ Implement custom measurements: homodyne detection.
- Translate a simple classification task in the quantum equivalent.
- Run the circuit.
- Realization of a optical photon quantum computer? [1]
  - ➢ Single photons are easy to generate.
  - ➢ Single qumode operations are possible.
  - ➢ Main drawback: making photons interact (through the Kerr medium) is difficult

[1] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information