

Computing quantum systems

Pre-colloquium

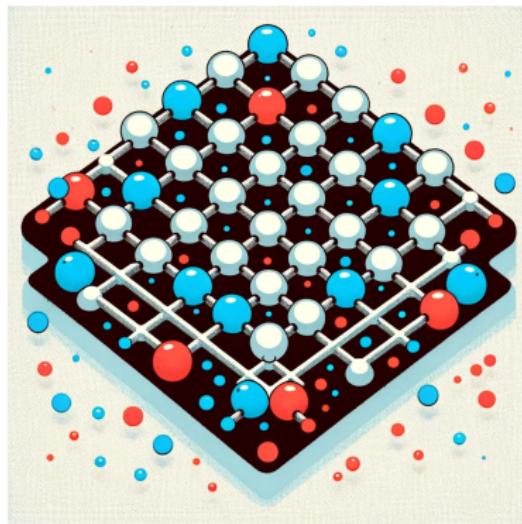
Matteo Robbiati
February 2024



Compute quantum mechanics

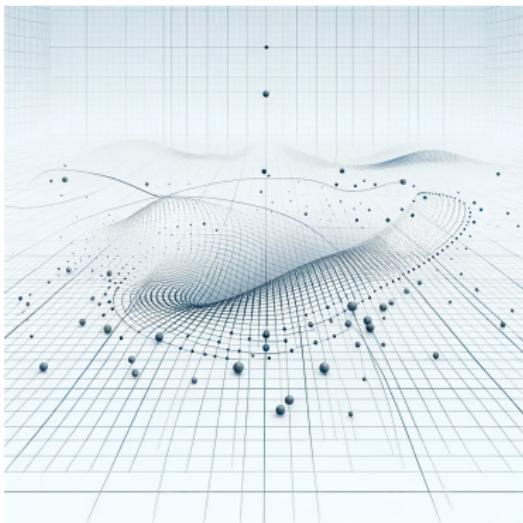
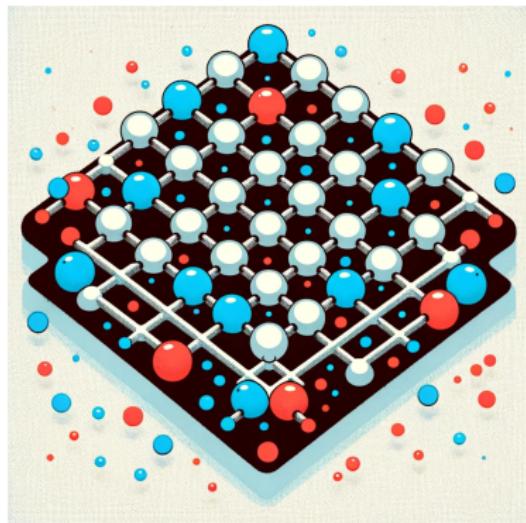
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- ✿ Representing N particles is difficult;
- ✿ considering N spins (\uparrow, \downarrow), we deal with a 2^N dimensional Hilbert space!



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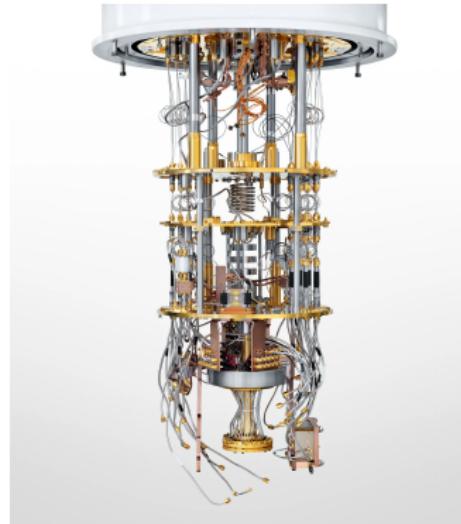
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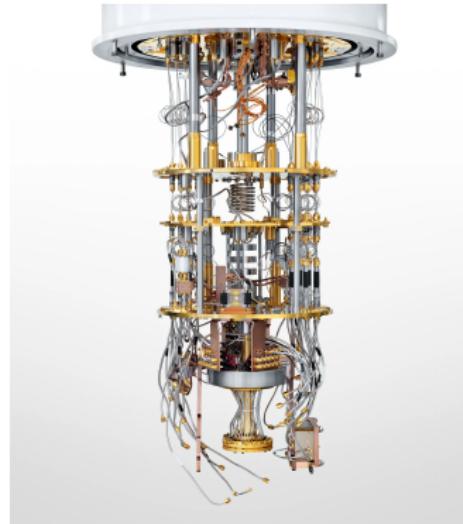


Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

— Richard Feynman, 1982, Simulating Physics with Computers

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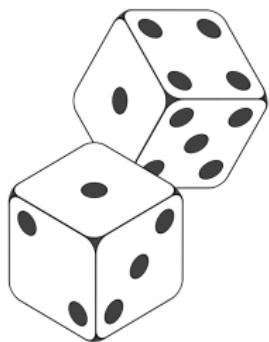


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1. Variational Monte Carlo (VMC): given a wave function $\Psi(x|\theta)$ and a target H , MC methods are used to minimize:

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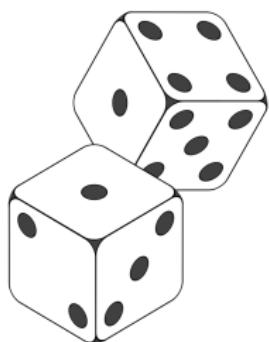
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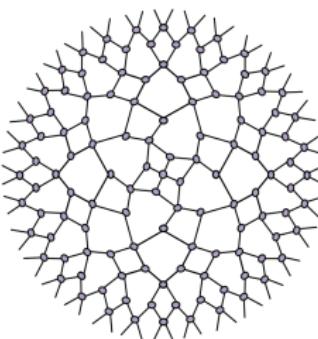
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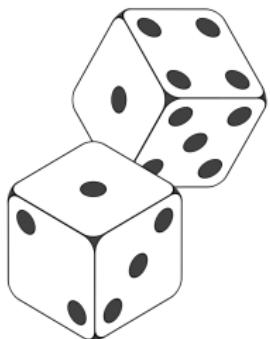
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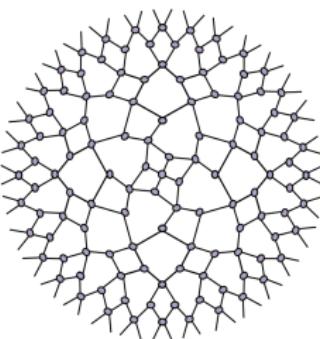
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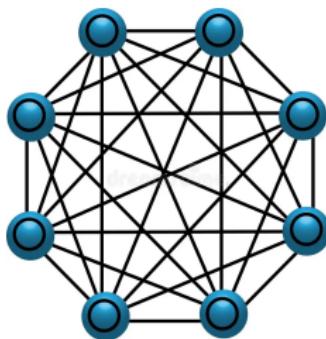
2. Tensor Networks (TNs): contraction of complex systems into simpler structures;
3. Neural Network Quantum States: use complex ANNs to represent the state.



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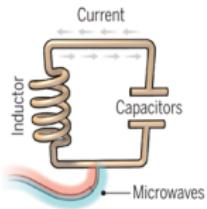
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A snapshot of quantum computing

Qubits

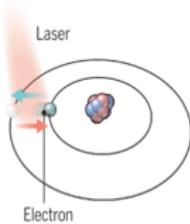
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Superconducting loops

A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into superposition states.



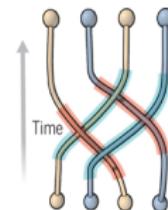
Trapped ions

Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.



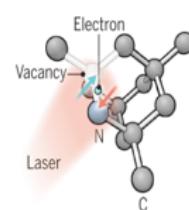
Silicon quantum dots

These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.



Topological qubits

Quasiparticles can be seen in the behavior of electrons channeled through semiconductor structures. Their braided paths can encode quantum information.

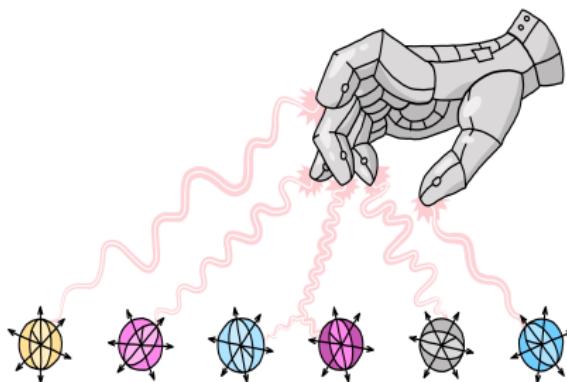


Diamond vacancies

A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.

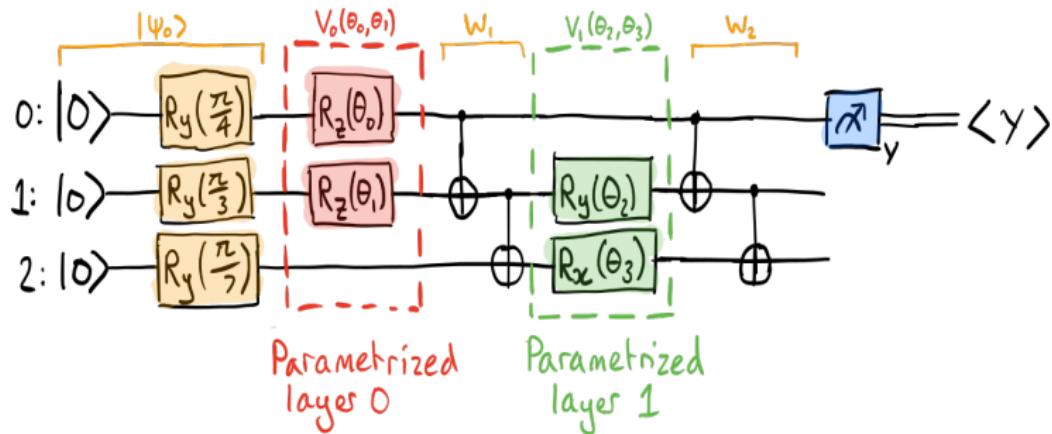
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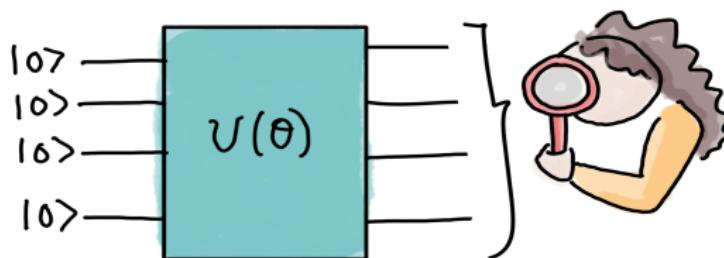
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4. to access the information we need to measure the system.



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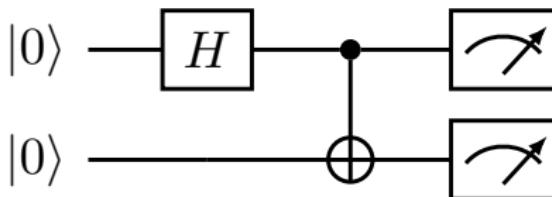
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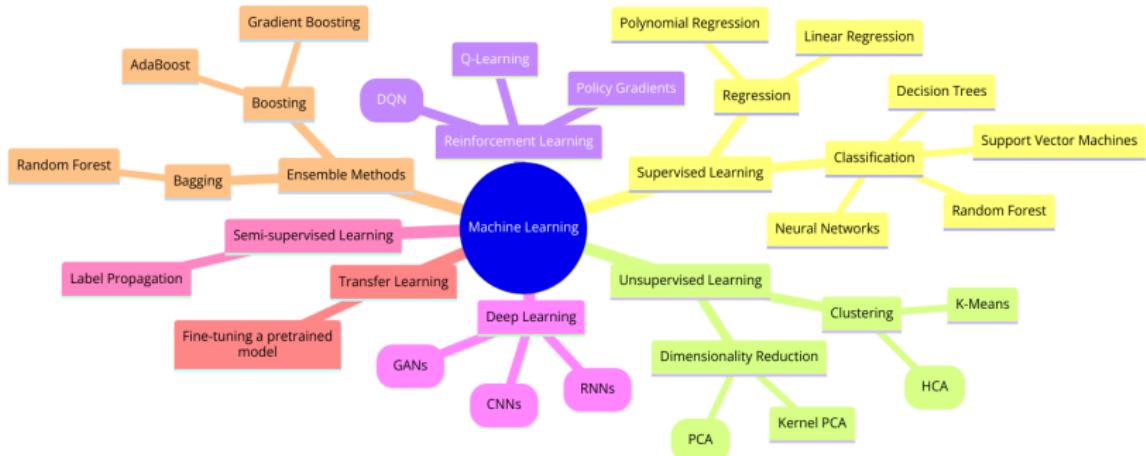
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Quantum Machine Learning

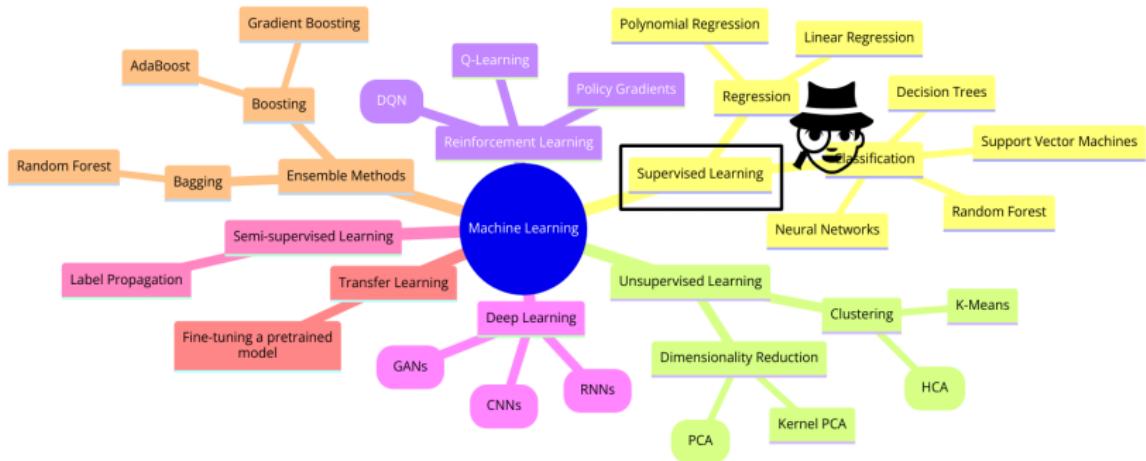
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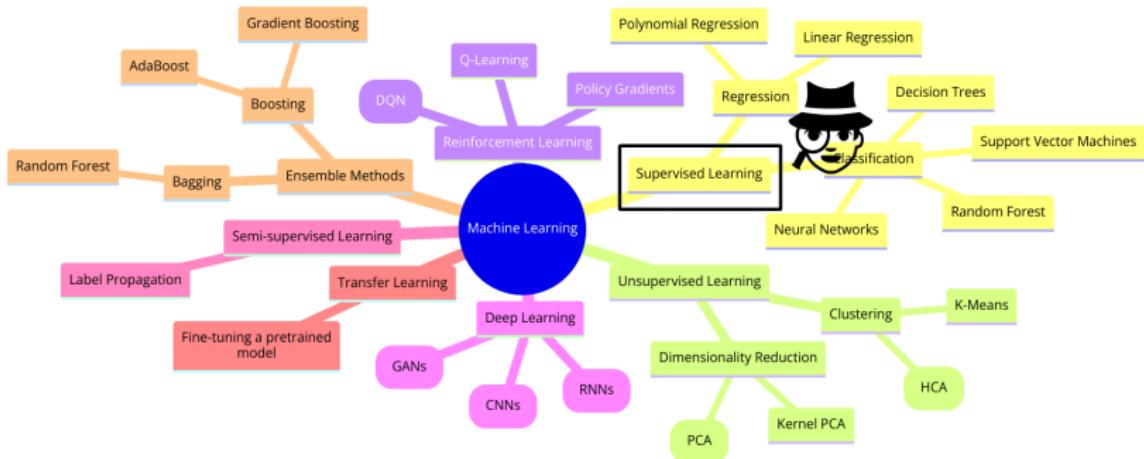
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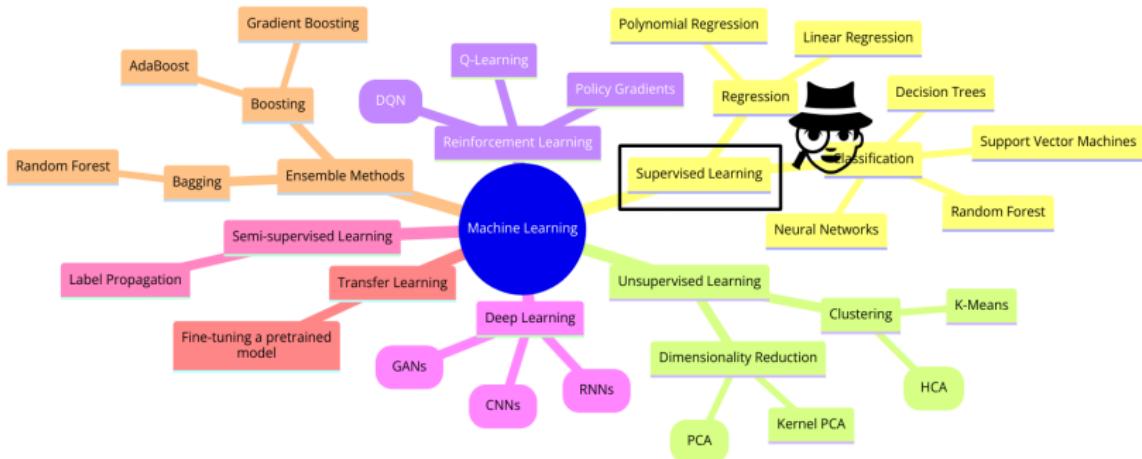


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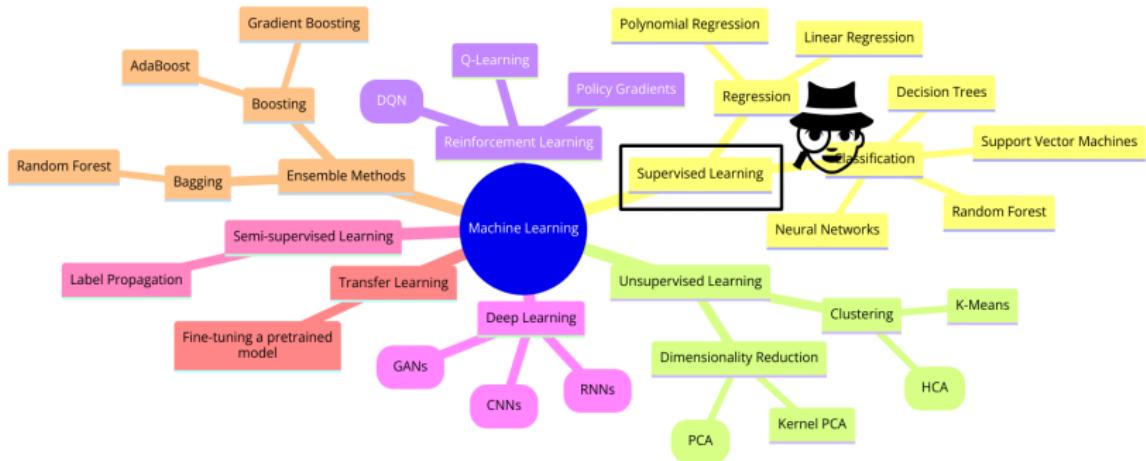


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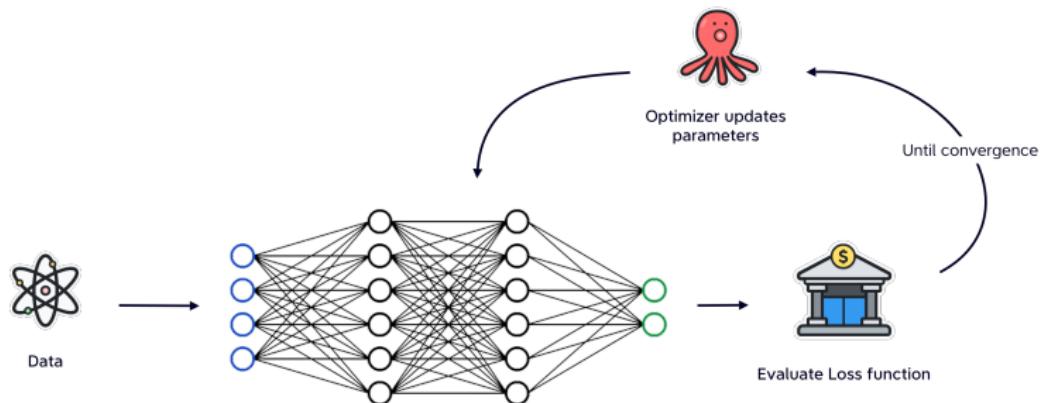
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- 📊 we define a parameteric model which returns $\hat{y}_{\text{est}} = f_{\text{est}}(x; \theta)$;
- 🔭 we define an optimizer, which task is to compute $\operatorname{argmin}_{\theta} [J(y_{\text{meas}}, \hat{y}_{\text{est}})]$.

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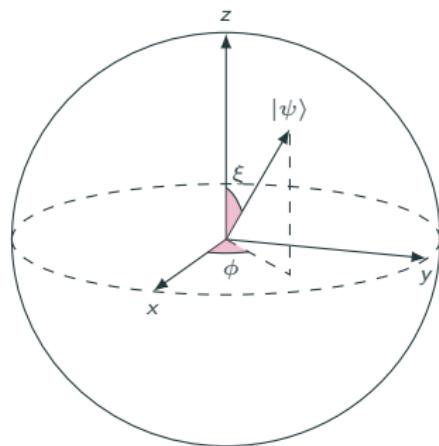
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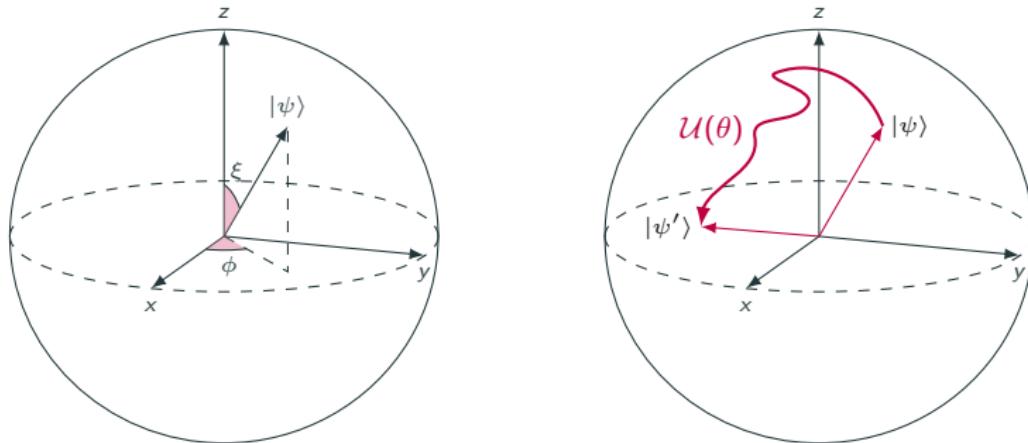


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We can use as parametric gates the rotation around the axis of the block sphere:

$$R_k(\theta) = \exp[-i\theta\sigma_k], \quad \text{with} \quad \sigma_k \in \{I, \sigma_x, \sigma_y, \sigma_z\}.$$

Machine Learning

\mathcal{M} : model;

\mathcal{O} : optimizer;

\mathcal{J} : loss function.

(x, y) : data

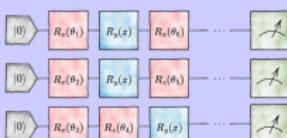
Quantum Computation

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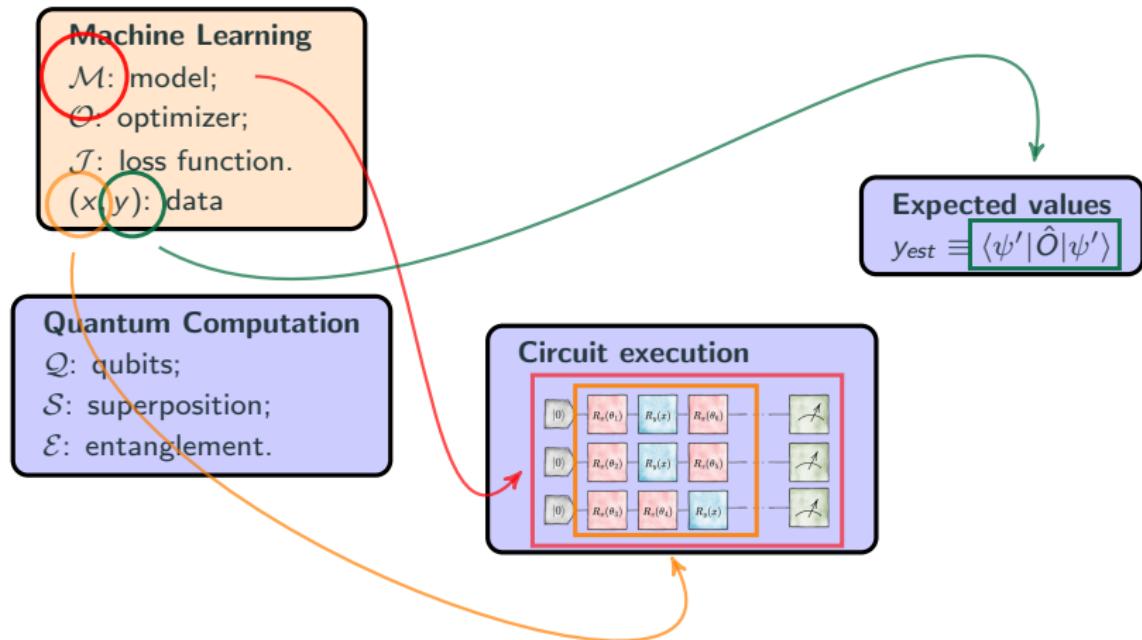
\mathcal{S} : superposition;

\mathcal{E} : entanglement.

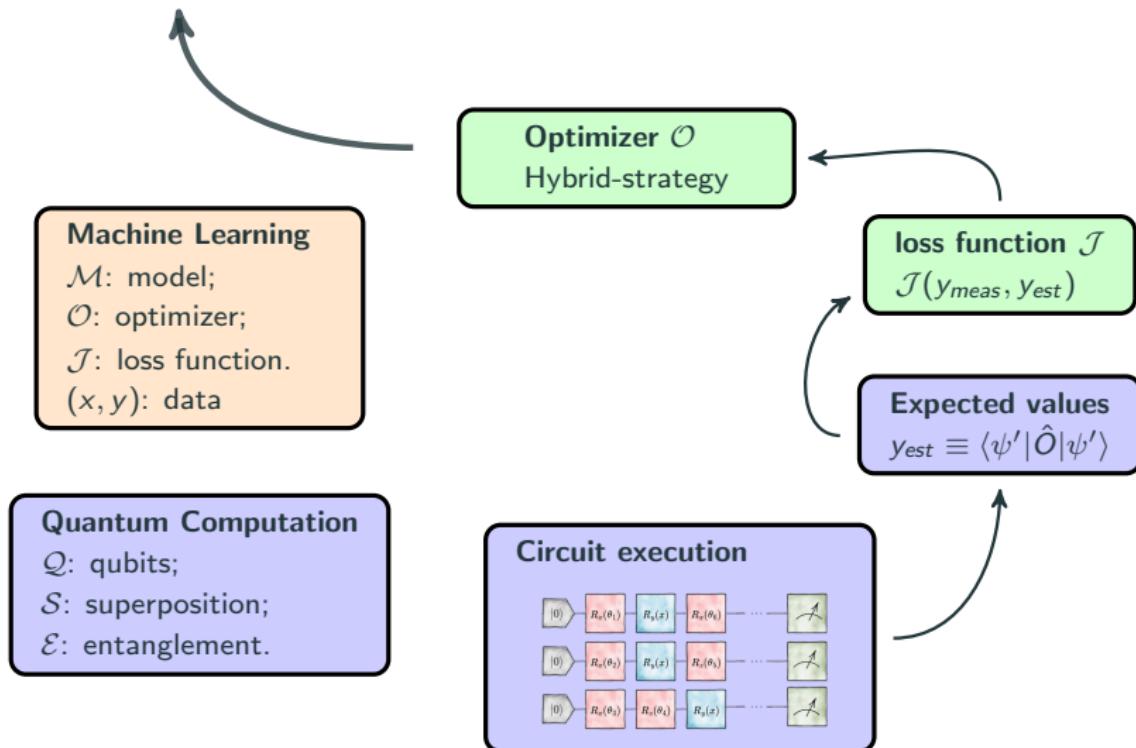
Circuit execution

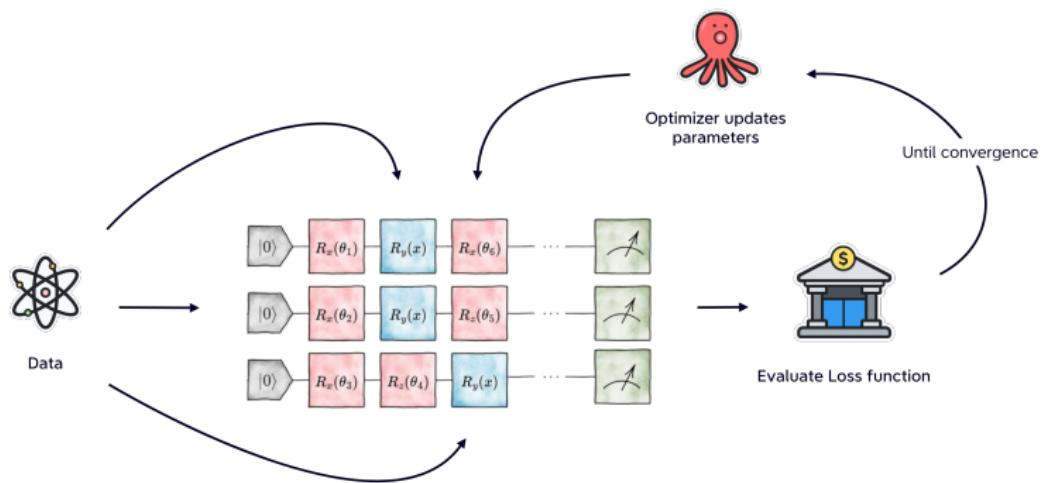


Expected values
 $y_{est} \equiv \langle \psi' | \hat{O} | \psi' \rangle$



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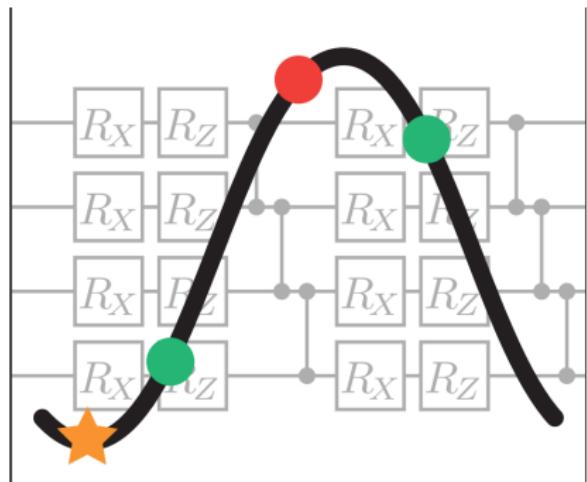
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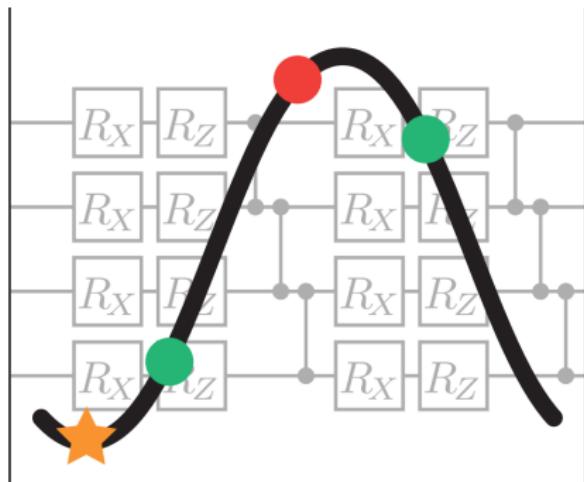


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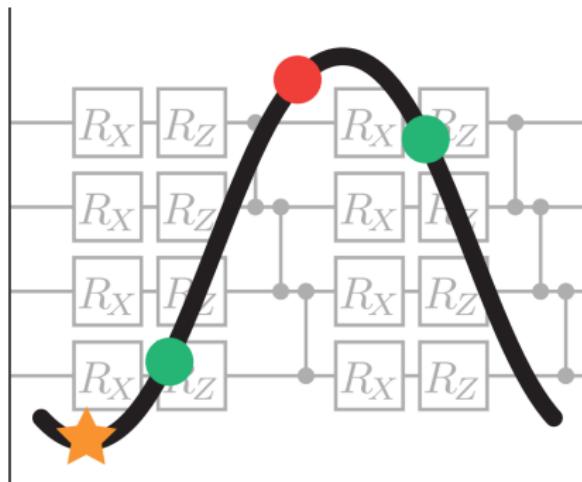


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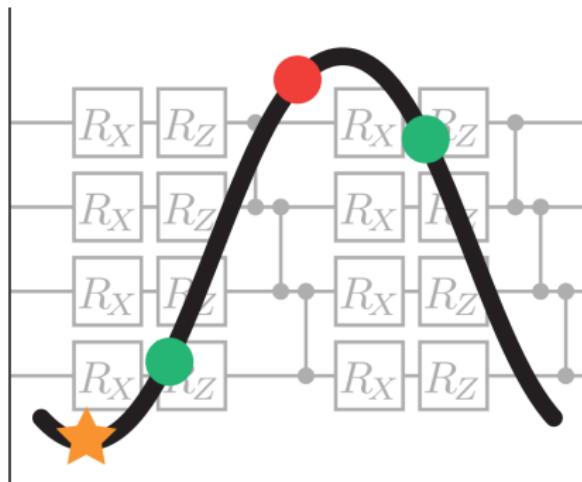


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3. **Solovay-Kitaev theorem:** the number of gates needed by \mathcal{U} to represent V with precision δ is $\mathcal{O}(\log^c \delta^{-1})$, where $c < 4$.



A practical example

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If adiabatic enough, you'll remain in the ground state.

Approximating ground states - Adiabatic Computing

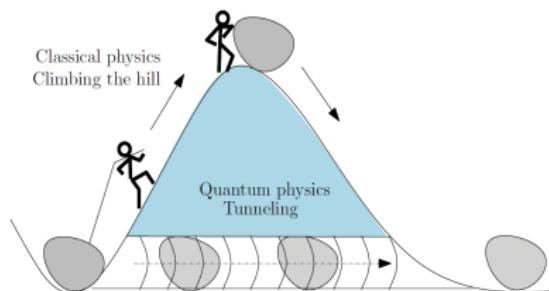
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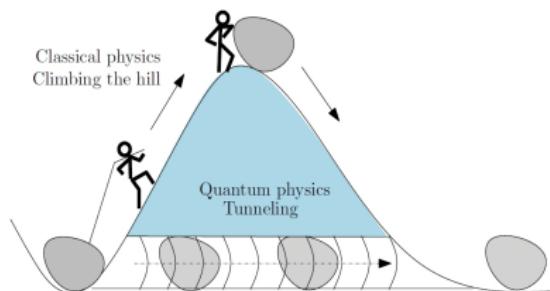
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<https://www.dwavesys.com/>

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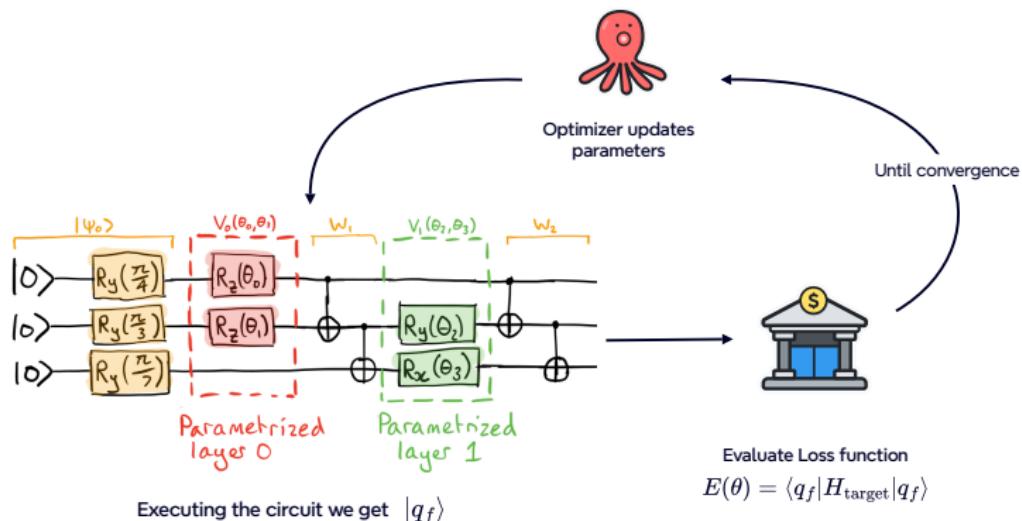
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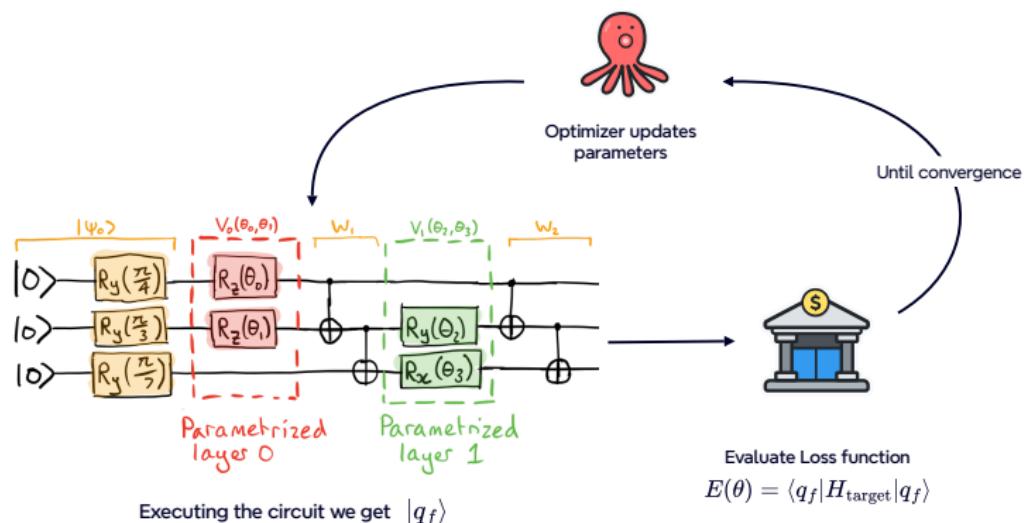
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> Let's code it!

