KMI School 2024

Quantum Computing for Particle Physics and Astrophysics
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Variational Quantum Algorithm and Quantum Machine Learning

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Ground State of Physical System

Charactering fundamental properties of a physical system often requires to know the ground state and its energy eigenvalue of the system

For an arbitrary state $|\psi\rangle$, the expectation value of a given Hamiltonian H is bounded by the ground state energy $\lambda_{\min}$:

$$\langle\psi|H|\psi\rangle \geq \lambda_{\min}$$

➡ Variational Method in Quantum Mechanics

Capability of quantum computer for calculating the expectation value of a Hamiltonian enables us to use the variational method to find the ground state

Variational Method

Let us consider a problem of approximating the energy eigenvalue for a certain system expressed by a matrix

For an eigenstate $|\psi_i\rangle$ and the eigenvalue λ_i of a given operator A:

$$A|\psi_i\rangle = \lambda_i|\psi_i\rangle$$

$\lambda_i = \lambda_i^*$ is real if A is a Hermitian observable ($A = A^\dagger$)

Considering the Hamiltonian H of a given physical system, the Hamiltonian can be expressed with eigenvalues λ_i and eigenvectors $|\psi_i\rangle$ in a diagonal form:

$$\Rightarrow H = \sum_{i=1}^{N} \lambda_i|\psi_i\rangle\langle\psi_i| \qquad \langle\psi_i|\psi_j\rangle = 0 \quad \forall i \neq j$$

Variational Method

For Hamiltonian $H = \sum_{i=1}^{N} \lambda_i |\psi_i\rangle\langle\psi_i|$, the expectation value of the Hamiltonian for an arbitrary state $|\psi\rangle$ is $\langle\psi|H|\psi\rangle =: \langle H\rangle_\psi$

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$$\langle H\rangle_\psi = \langle\psi| \left(\sum_{i=1}^{N} \lambda_i |\psi_i\rangle\langle\psi_i| \right) |\psi\rangle$$

$$= \sum_{i=1}^{N} \lambda_i \langle\psi|\psi_i\rangle\langle\psi_i|\psi\rangle$$

$$= \sum_{i=1}^{N} \lambda_i |\langle\psi_i|\psi\rangle|^2$$

Variational Method

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$$= \sum_{i=1}^{N} \lambda_i |\langle\psi_i|\psi\rangle|^2$$

Since $|\langle\psi_i|\psi\rangle|^2 \geq 0$

$$\langle H\rangle_\psi = \sum_{i=1}^{N} \lambda_i |\langle\psi_i|\psi\rangle|^2 \geq \lambda_{min}$$

Equality holds if $|\psi\rangle = |\psi_{\min}\rangle$

Variational Method

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If one can take $|\psi\rangle$ to be as close as possible to $|\psi_{\min}\rangle$,
$\lambda_{\min}$ can be well approximated by $\langle H \rangle_\psi$

Variational Method

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λ_{min} can be well approximated by $\langle H \rangle_\psi$

But how can we do that?

We cannot take $|\psi\rangle$ in an arbitrary manner because the overlap with $|\psi_{\mathrm{min}}\rangle$ is exponentially small with increasing system size

State Preparation in Variational Method

How can we take $|\psi\rangle$ to be close to $|\psi_{\min}\rangle$?

<u>Strategy:</u>

- Consider a certain initial state $|\psi_0\rangle$
- Generate a trial state $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|\psi_0\rangle$ by applying a unitary $U(\boldsymbol{\theta})$ (called **Ansatz**) to $|\psi_0\rangle$
- Calculate $\lambda(\boldsymbol{\theta}) := \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle$
- Find the smallest value of $\lambda(\boldsymbol{\theta})$ by varying the parameter $\boldsymbol{\theta}$

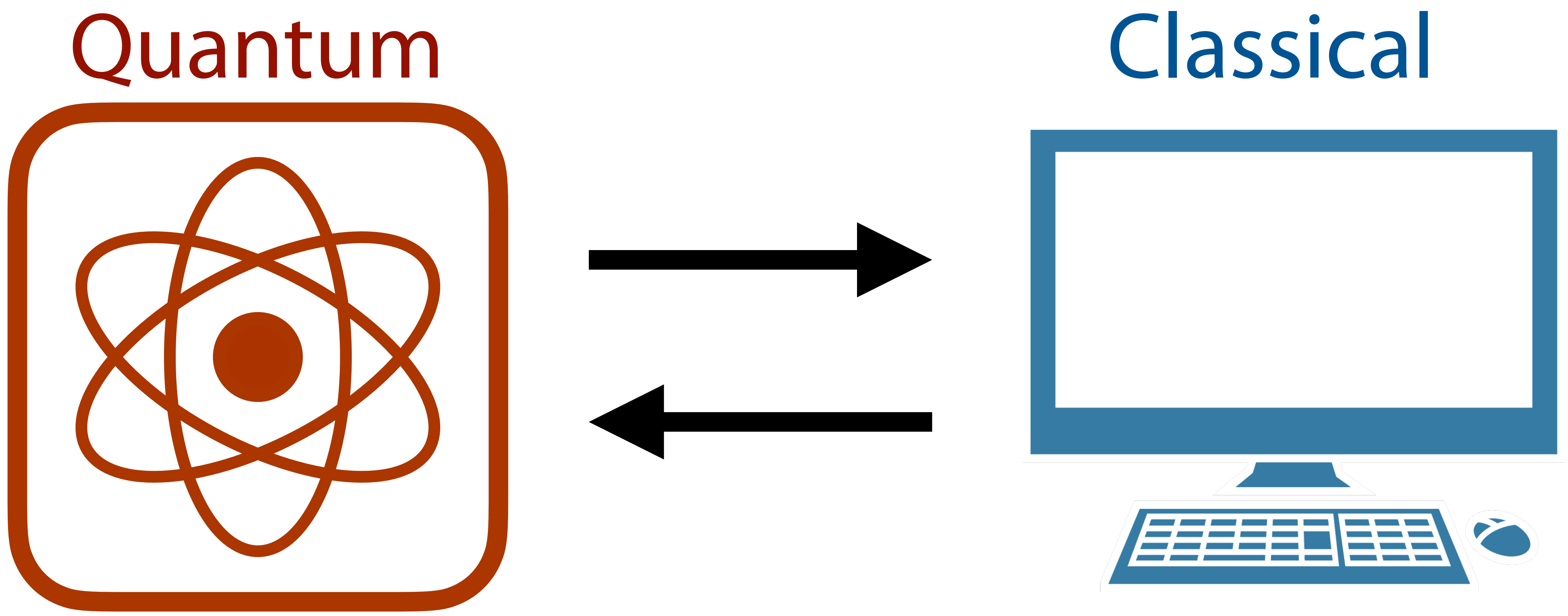
$$\boldsymbol{\theta} \to \boldsymbol{\theta}^* \Longrightarrow \lambda(\boldsymbol{\theta}^*) = \langle\psi(\boldsymbol{\theta}^*)|H|\psi(\boldsymbol{\theta}^*)\rangle \sim \langle\psi_{\min}|H|\psi_{\min}\rangle = \lambda_{\min}$$

State Preparation in Variational Method

$$\boldsymbol{\theta} \to \boldsymbol{\theta}^* \;\Rightarrow\; \lambda(\boldsymbol{\theta}^*) = \langle \psi(\boldsymbol{\theta}^*) \,|\, H \,|\, \psi(\boldsymbol{\theta}^*) \rangle \sim \langle \psi_{\mathrm{min}} \,|\, H \,|\, \psi_{\mathrm{min}} \rangle = \lambda_{\mathrm{min}}$$

⇒ Variational Quantum Eigensolver (VQE)

Find optimized parameter $\boldsymbol{\theta}^*$ by repeating the calculation of $\lambda(\boldsymbol{\theta})$ using quantum computer and parameter update using classical computer



Quantum-Classical hybrid algorithm

Relatively robust against hardware noise in the present quantum computer

Variational Quantum Eigensover

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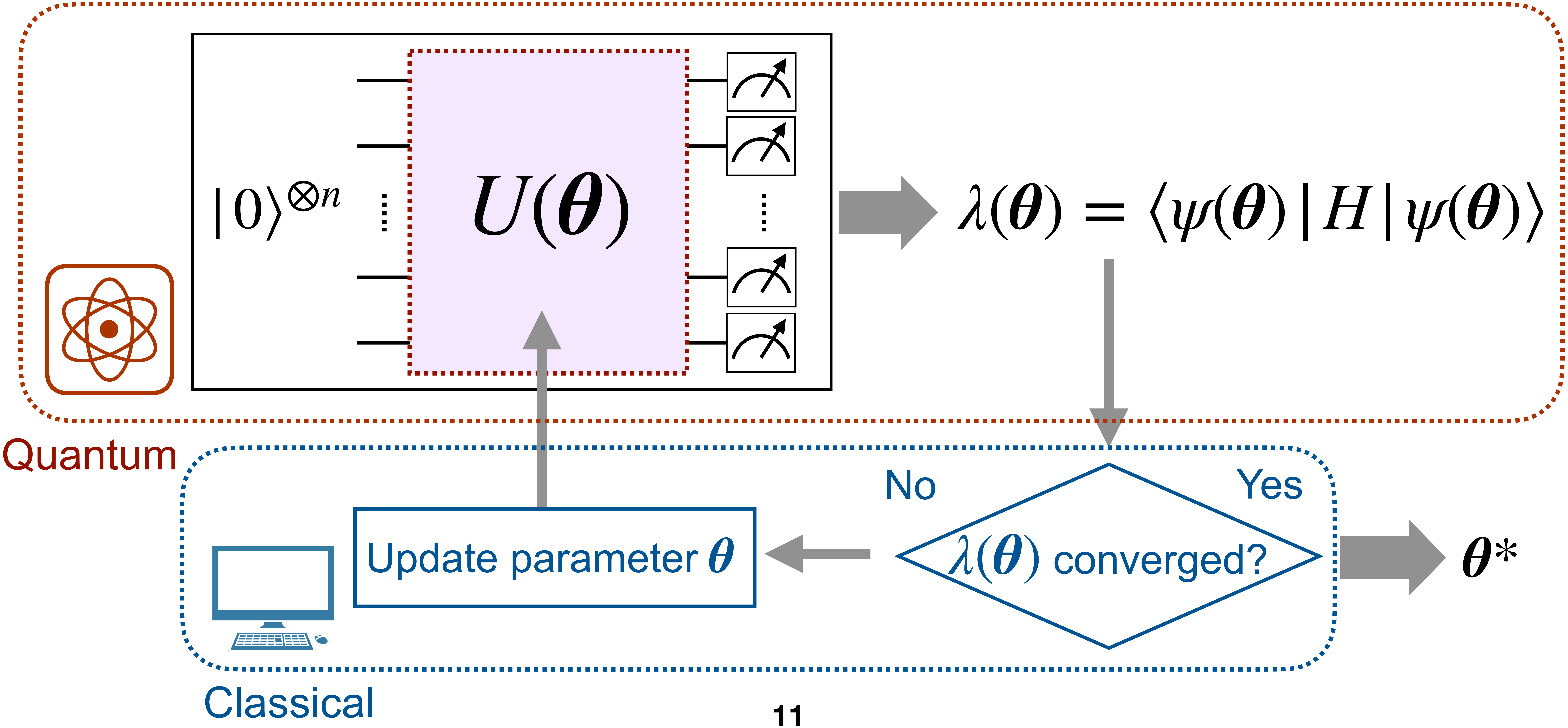

Parameter Optimization

Optimize parameter $\boldsymbol{\theta}$ so that $\lambda(\boldsymbol{\theta}) := \langle \psi(\boldsymbol{\theta}) \,|\, H \,|\, \psi(\boldsymbol{\theta}) \rangle$ becomes the smallest

$$\boldsymbol{\theta} \rightarrow \boldsymbol{\theta}^* \quad \Rightarrow \quad \lambda(\boldsymbol{\theta}^*) = \langle \psi(\boldsymbol{\theta}^*) \,|\, H \,|\, \psi(\boldsymbol{\theta}^*) \rangle \sim \langle \psi_{\mathrm{min}} \,|\, H \,|\, \psi_{\mathrm{min}} \rangle = \lambda_{\mathrm{min}}$$

➡ **Gradient descent** to find parameter $\boldsymbol{\theta}^*$ that minimizes $\lambda(\boldsymbol{\theta})$

Calculate the gradient $\partial \lambda(\boldsymbol{\theta}) / \partial \theta_j$ with respect to each θ_j and update the parameter θ_j so that $\lambda(\boldsymbol{\theta})$ decreases

$$\theta_j \; \rightarrow \; \theta_j' = \theta_j - \epsilon \frac{\partial \lambda(\boldsymbol{\theta})}{\partial \theta_j}$$

$\epsilon(>0)$ = Learning rate

Parameter Optimization

So-called "**Parameter Shift Rule**" used to obtain the gradient for certain type of unitaries

Consider a unitary $U(\boldsymbol{\theta}) = \prod_{j=1}^{L} U_j(\theta_j)$ with $U_j(\theta_j) = e^{-i\theta_j P_j/2}$ $\quad P_j \in \{X, Y, Z\}$

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Expectation value of observable M

$$\langle M(\boldsymbol{\theta})\rangle = \mathrm{Tr}\left[MU(\boldsymbol{\theta})\rho U(\boldsymbol{\theta})^\dagger\right]$$

$$\Rightarrow \frac{\partial}{\partial\theta_j}\langle M(\boldsymbol{\theta})\rangle = \frac{1}{2}\left[\left\langle M\left(\boldsymbol{\theta} + \frac{\pi}{2}\boldsymbol{e}_j\right)\right\rangle - M\left\langle\left(\boldsymbol{\theta} - \frac{\pi}{2}\boldsymbol{e}_j\right)\right\rangle\right]$$

$\boldsymbol{e}_j$ = unit vector with 1 in j-th element, 0 otherwise

Gradient of the expectation value can be obtained as a difference between two expectation values with $\theta_j \pm \pi/2$

Caveat:

Need to calculate expectation values twice per parameter

Variational Quantum Algorithm

VQE is a typical example of Variational Quantum Algorithm (VQA)

Variational Quantum Algorithm

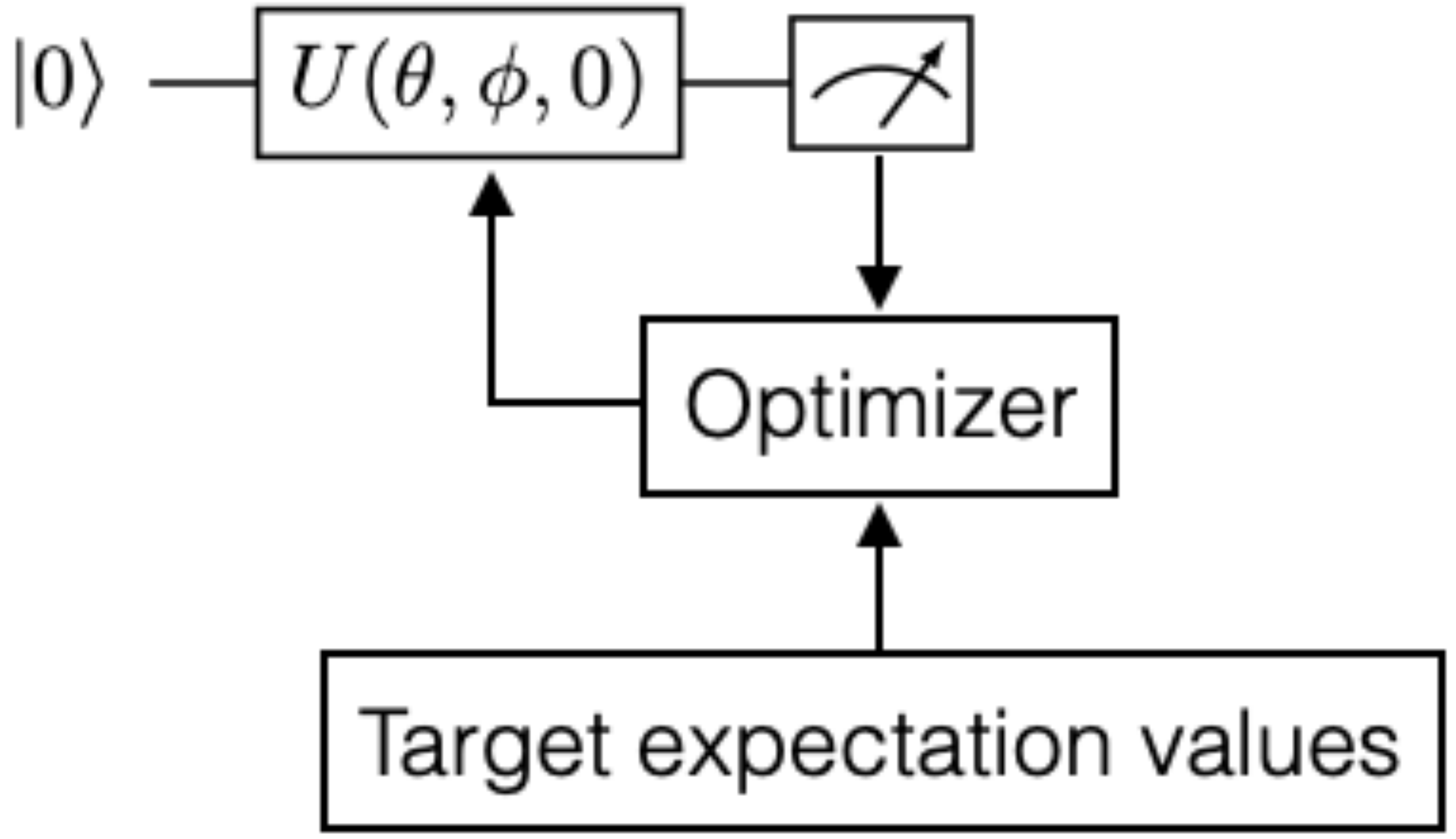
- Implement unitary operator $U(\boldsymbol{\theta})$ with parameterized quantum circuit (called *variational quantum circuit* or *variational form*)
- Generate output state $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|\psi_0\rangle$ by applying $U(\boldsymbol{\theta})$ to an initial state $|\psi_0\rangle$
- Optimize parameter $\boldsymbol{\theta}$ so that the output state approximates the desired state

Exercise of VQA

Let us try to approximate randomly chosen quantum state using VQA

- Generate a random single-qubit state $|\psi_0\rangle$
- Approximate $|\psi_0\rangle$ with a trial state $|\psi(\theta,\phi)\rangle = U(\theta,\phi,0)|0\rangle$
- Use $U(\theta,\phi,\lambda=0)$ gate as a single-qubit variational form:

$$U(\theta,\phi,\lambda) = \begin{pmatrix} \cos\frac{\theta}{2} & -e^{i\lambda}\sin\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} & e^{i\lambda+i\phi}\cos\frac{\theta}{2} \end{pmatrix}$$



Single-qubit state fully determined by the expectation values of Pauli X, Y and Z operators

➡ Optimize (θ,ϕ) so that

$$\langle P\rangle_{|\psi_0\rangle} \approx \langle P\rangle_{|\psi(\theta,\phi)\rangle}\ {}^\forall P \in \{X,Y,Z\}$$

Exercise of VQE

Consider a problem of minimizing the expectation value of an observable using parameter shift rule

- Generate a trial state $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|0\rangle$ with

$$U(\boldsymbol{\theta}) = \prod_l \left(\prod_j R_j^Z(\theta_{j2}^l) R_j^Y(\theta_{j1}^l) \right)$$

- Calculate the expectation value $\langle\psi(\boldsymbol{\theta})|O|\psi(\boldsymbol{\theta})\rangle$ with $O = ZXY$
- Minimize it in a quantum-classical optimization loop

We will try another VQE exercise in a later session

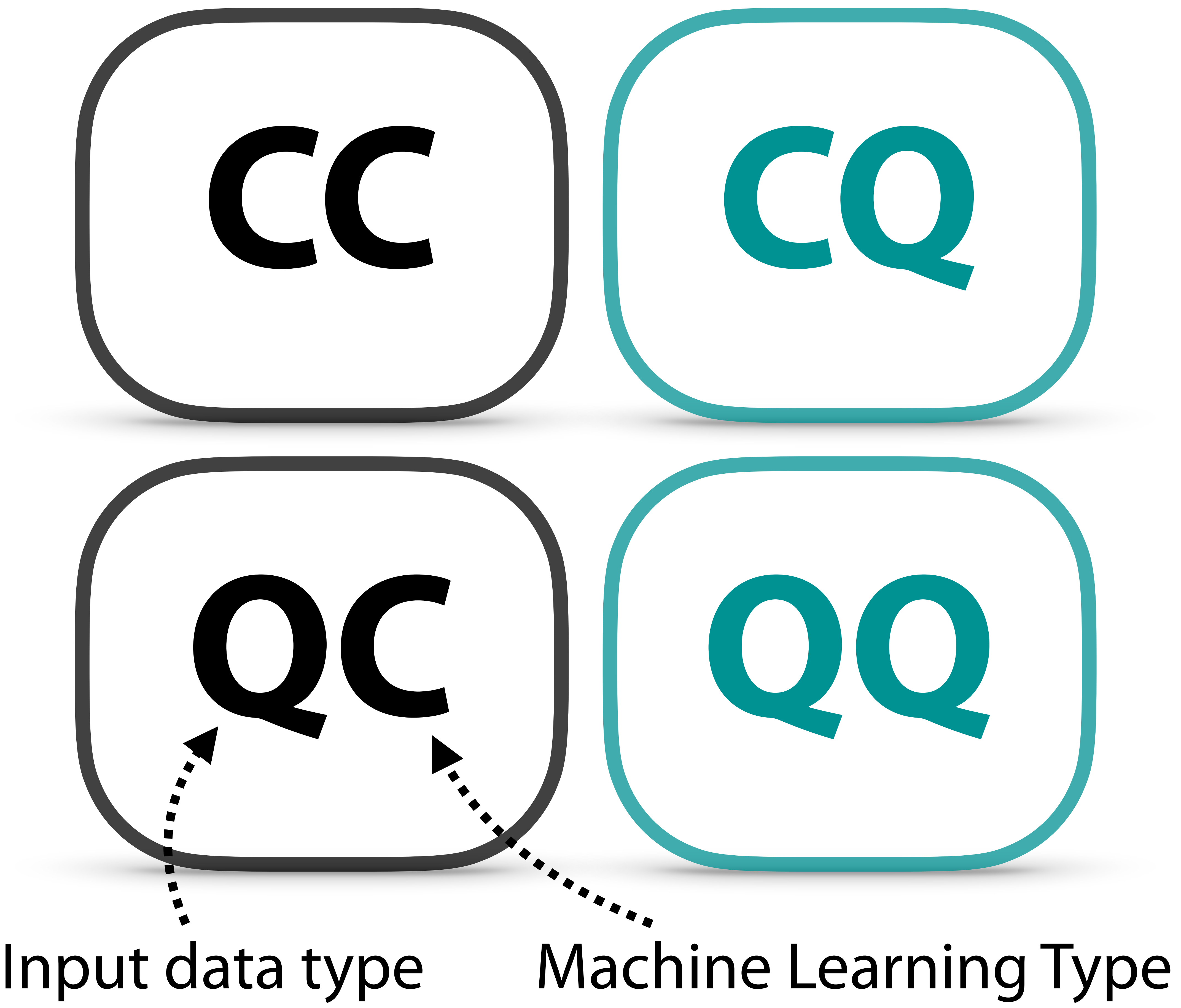
Hands-on Exercise (I)

- Variations Quantum Algorithm :
  - Approximate randomly chosen quantum state
- Variational Quantum Eigensolver :
  - Minimize expectation value of an observable

Quantum Machine Learning

Performing machine learning task by including quantum computing technology in the training and/or inference processes

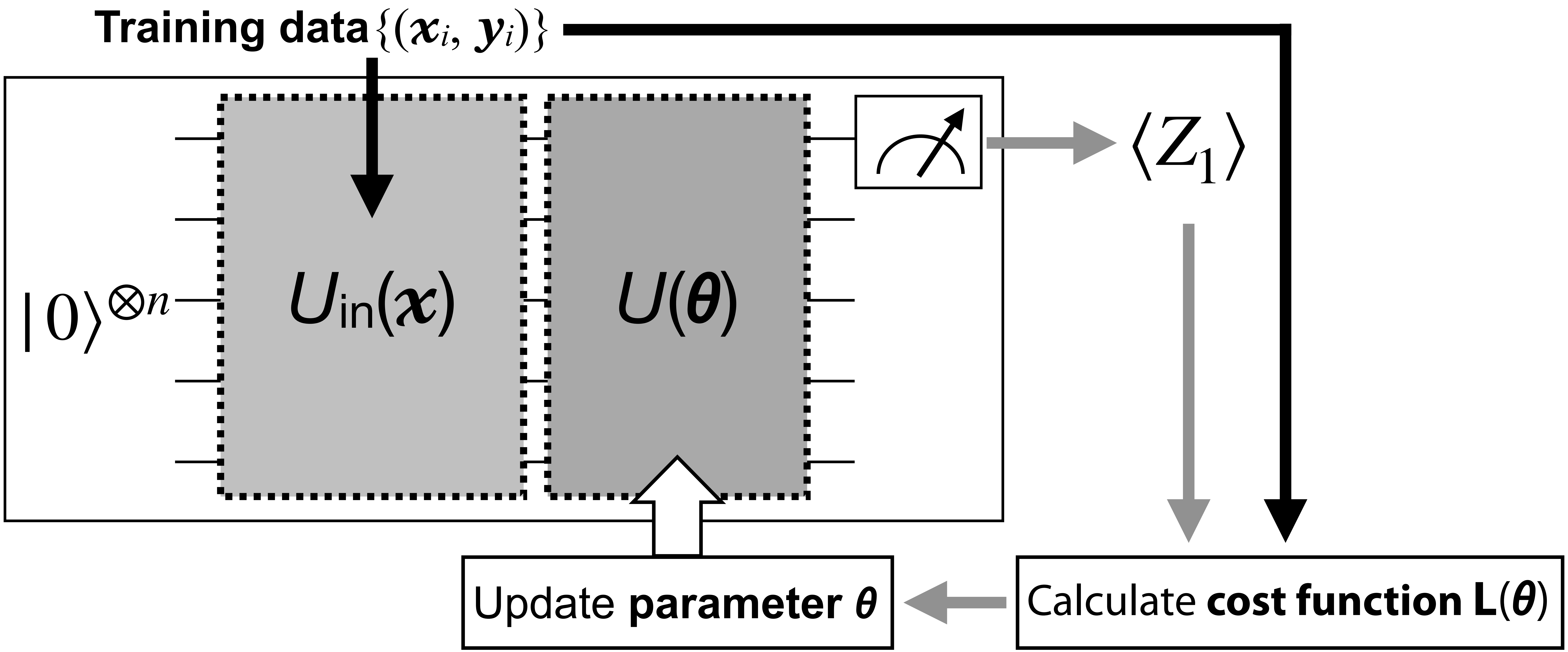
➡ **Quantum Machine Learning**



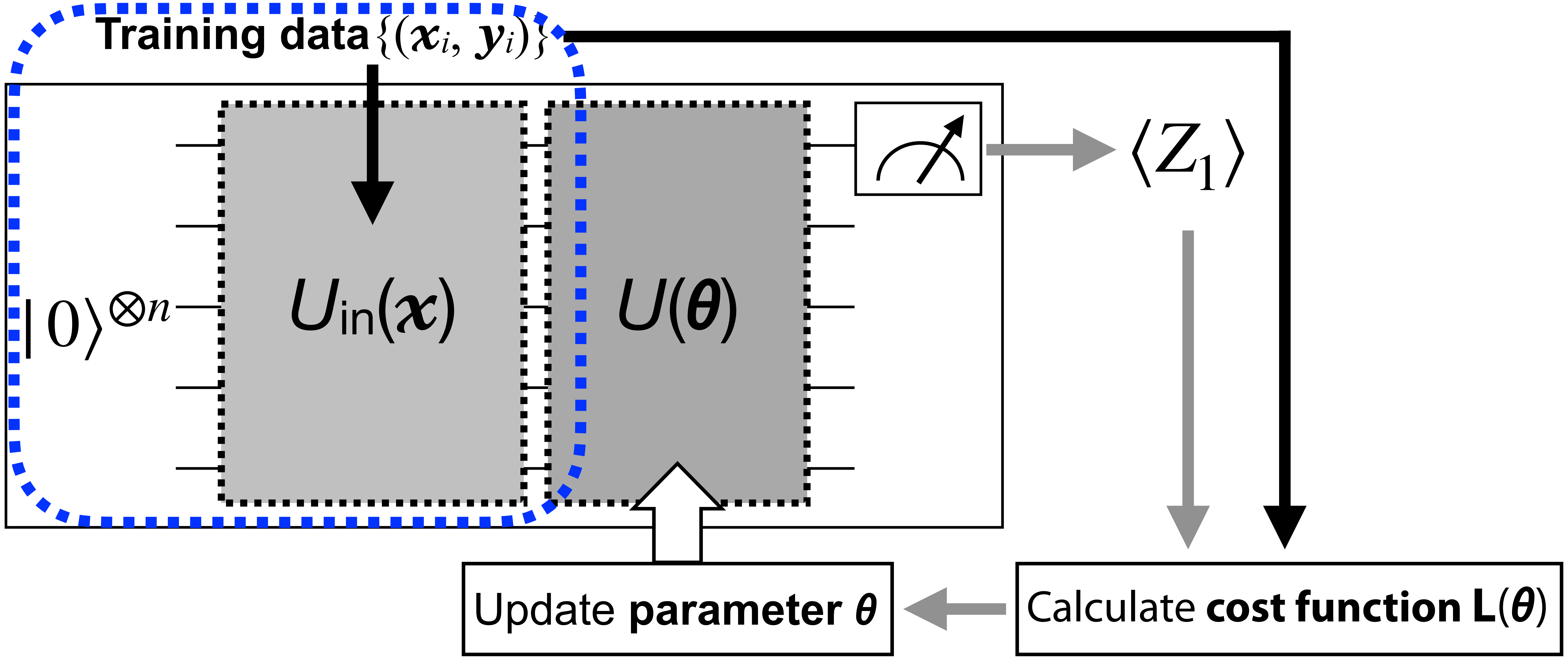
Classical = **C**
Quantum = **Q**

In the hands-on exercise, we will try QML in both CQ and QQ settings

Conventional **Quantum Neural Network (QNN)** model for supervised machine learning task



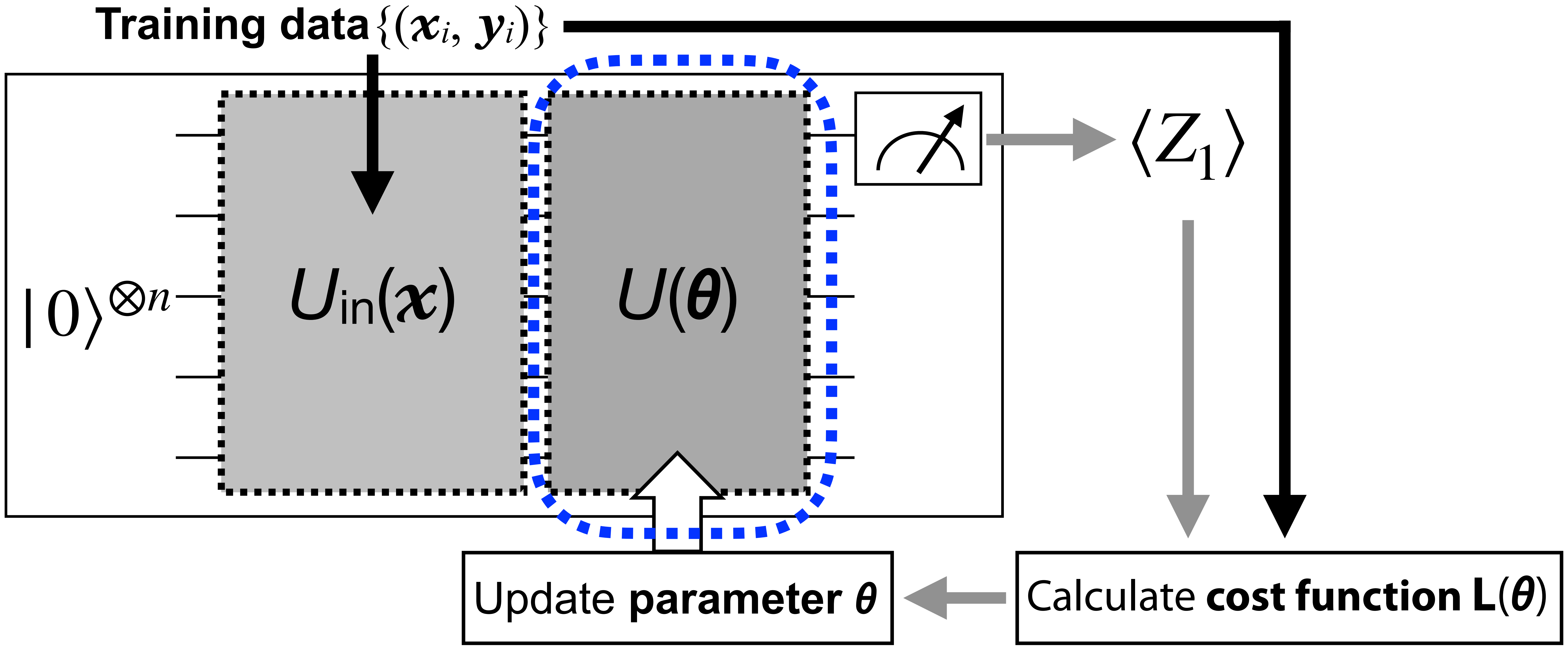
QML with Quantum Neural Networks



1. Prepare $|\psi_{\text{in}}(\boldsymbol{x}_i)\rangle = U_{\text{in}}(\boldsymbol{x}_i)|0\rangle^{\otimes n}$ using unitary $U_{\text{in}}(\boldsymbol{x})$ with input data $\boldsymbol{x}_i$ as parameter

$U_{\text{in}}(\boldsymbol{x})$ called feature map

QML with Quantum Neural Networks



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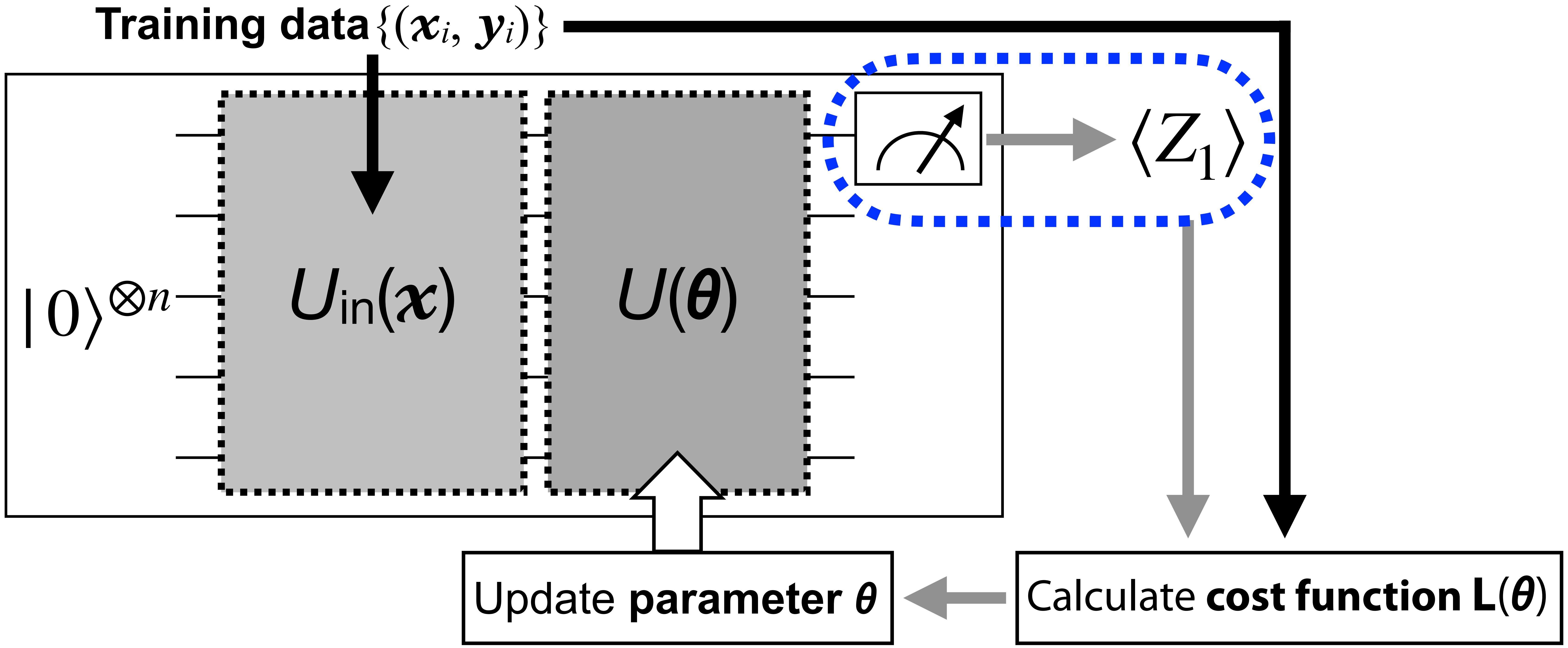
2. Generate output state $|\psi_{\rm out}(\boldsymbol{x}_i, \boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|\psi_{\rm in}(\boldsymbol{x}_i)\rangle$ by processing $|\psi_{\rm in}(\boldsymbol{x}_i)\rangle$ with $U(\boldsymbol{\theta})$

QML with Quantum Neural Networks



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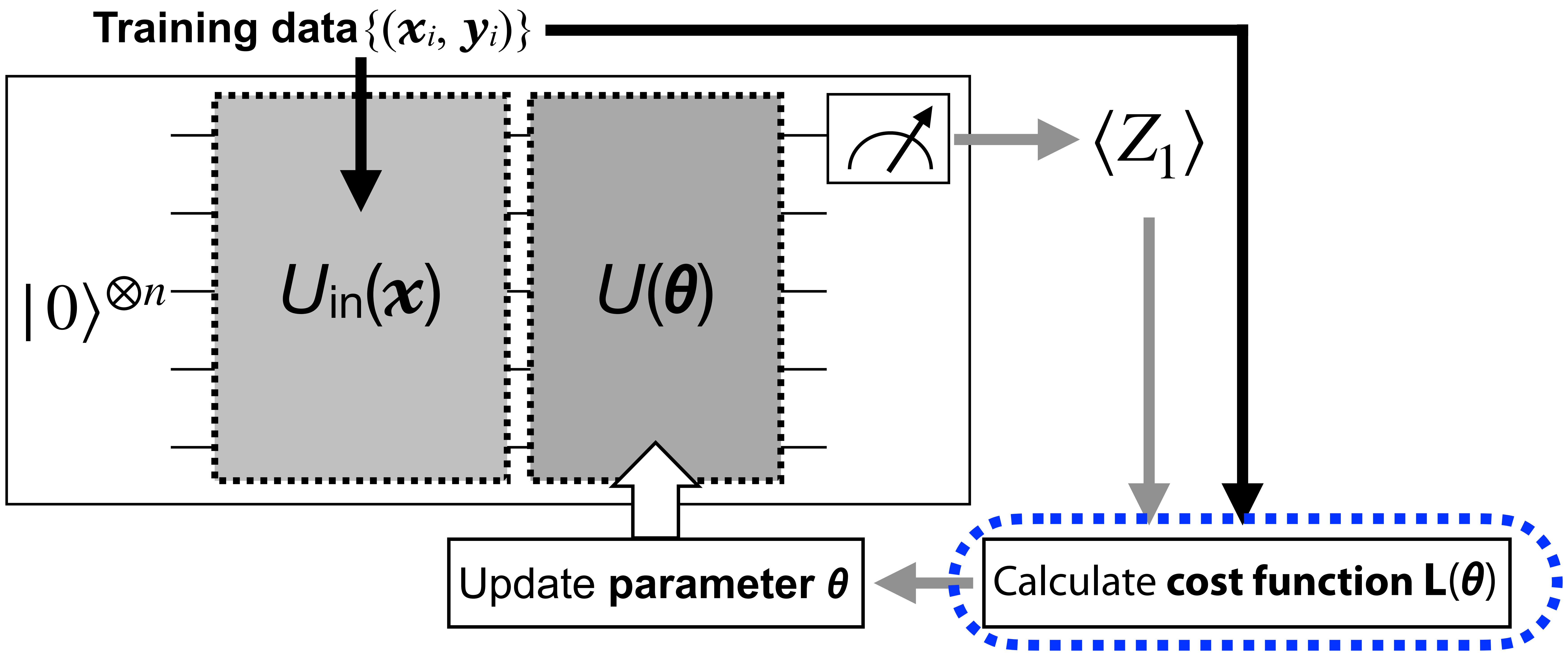

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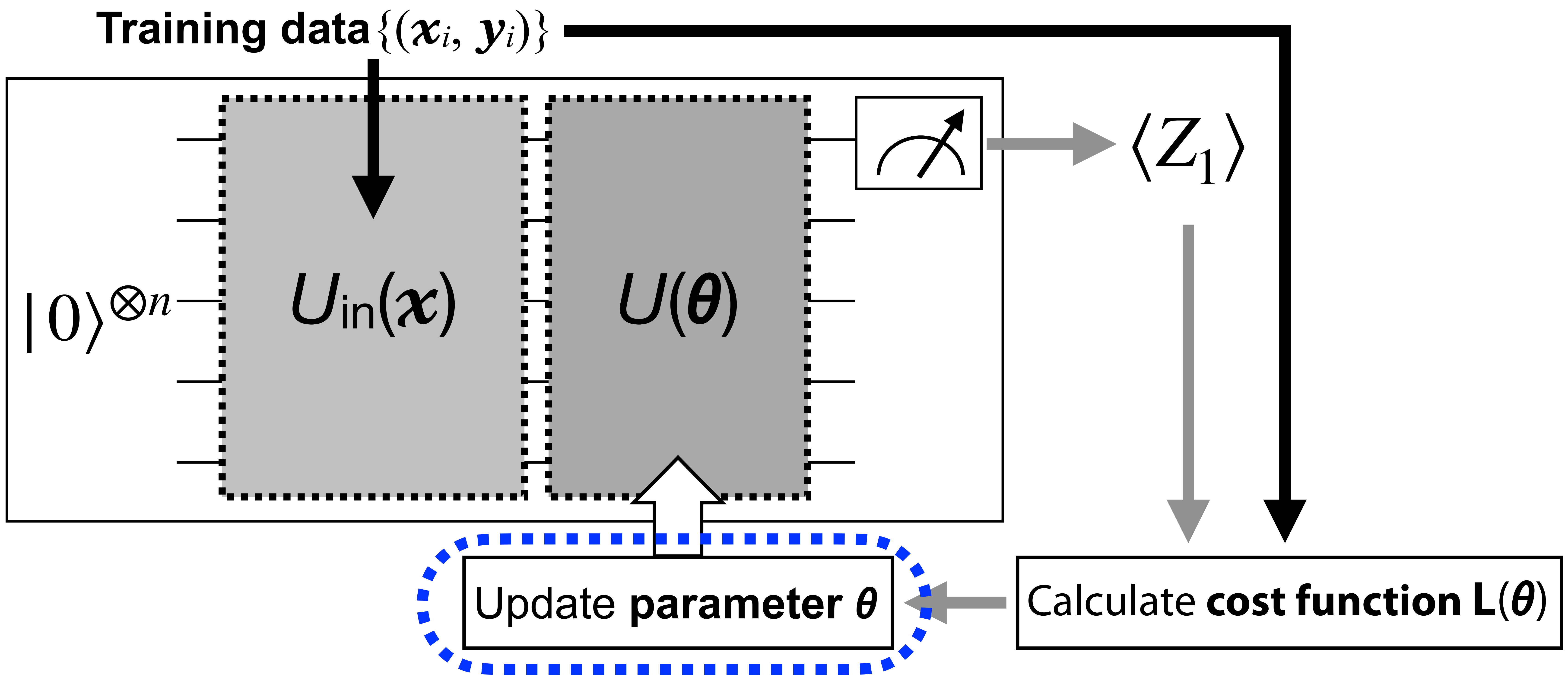
QML with Quantum Neural Networks



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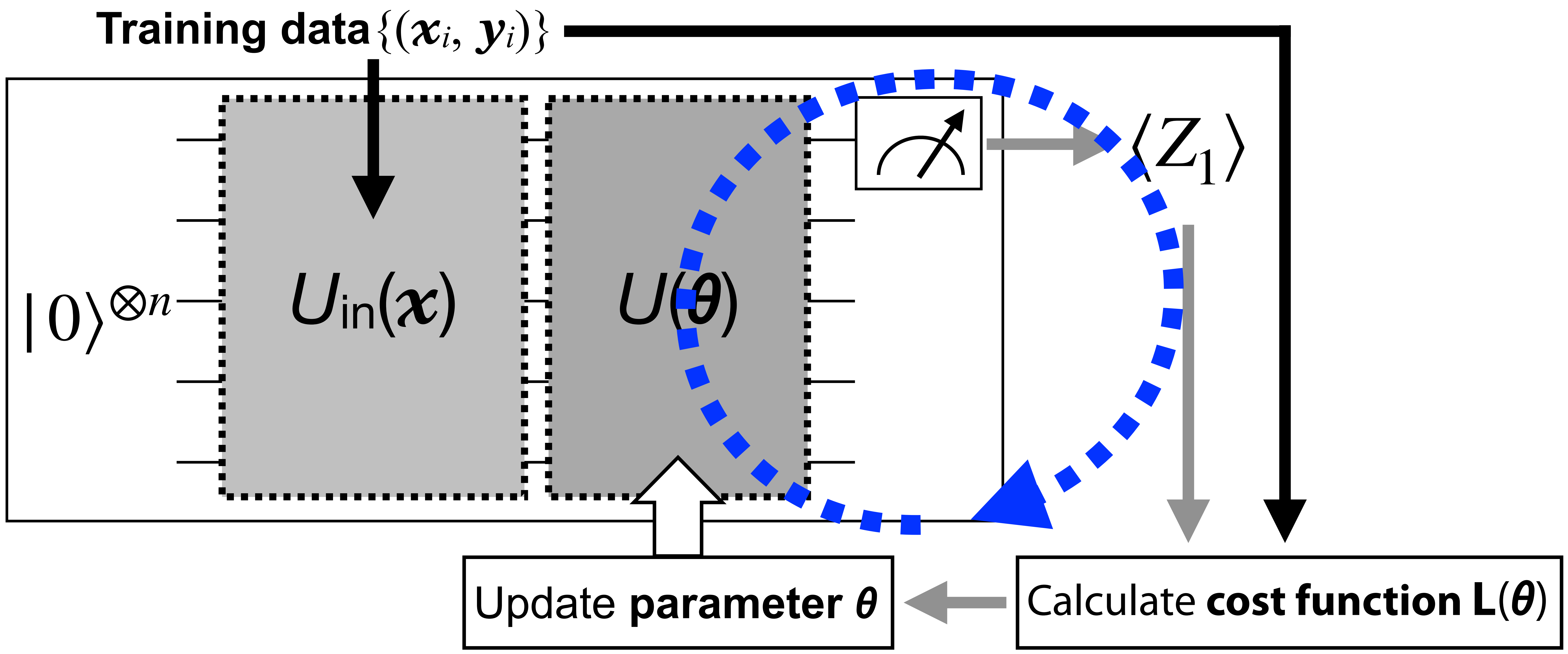
QML with Quantum Neural Networks



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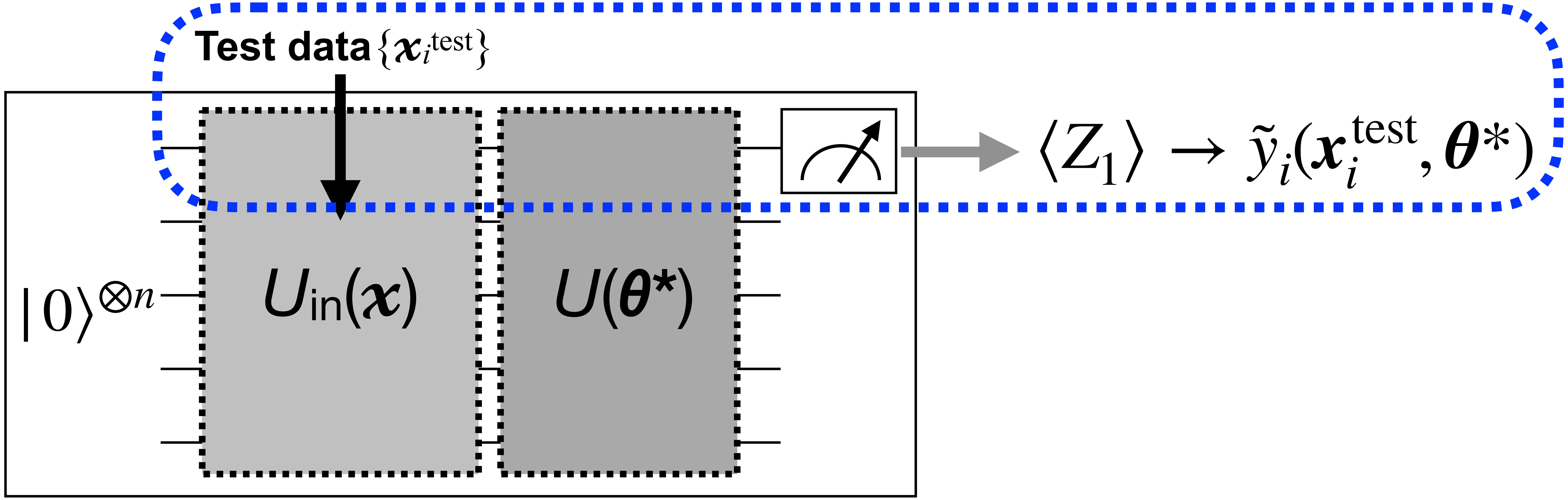
QML with Quantum Neural Networks



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5. Update parameter $\boldsymbol{\theta}$ so that $L(\boldsymbol{\theta})$ becomes smaller
6. Determine optimized parameter $\boldsymbol{\theta}^*$ that minimizes $L(\boldsymbol{\theta})$ by iterating the 2-5 steps
7. Predict the label $\tilde{y}_i(\boldsymbol{x}_i^{\text{test}}, \boldsymbol{\theta}^*)$ for unseen test data $\boldsymbol{x}_i^{\text{test}}$ using the trained model

Simple Example of QML

Let us consider an *inverse problem* to find a function f when only input data x_i and the output $y_i = f(x_i)$ are given

- Feature map: $U_{\text{in}}(x_i) = \prod_j R_j^Z(\cos^{-1}(x^2))R_j^Y(\sin^{-1}(x))$
- Variational form: $U(\boldsymbol{\theta}) : U(\{\theta_j^l\}) = \prod_{l=1}^{d}\left(\left(\prod_{j=1}^{n} U_{\text{rot}}(\theta_j^l)\right)\cdot U_{\text{ent}}\right)\cdot \prod_{j=1}^{n} U_{\text{rot}}(\theta_j^0)$

  Apply U_{rot} first, then use d times a pair of U_{ent} and U_{rot}

  $U_{\text{rot}}(\theta_j^l) = R_j^Y(\theta_{j3}^l)R_j^Z(\theta_{j2}^l)R_j^Y(\theta_{j1}^l)$: Single-qubit rotation gates with $\theta's$ as parameters

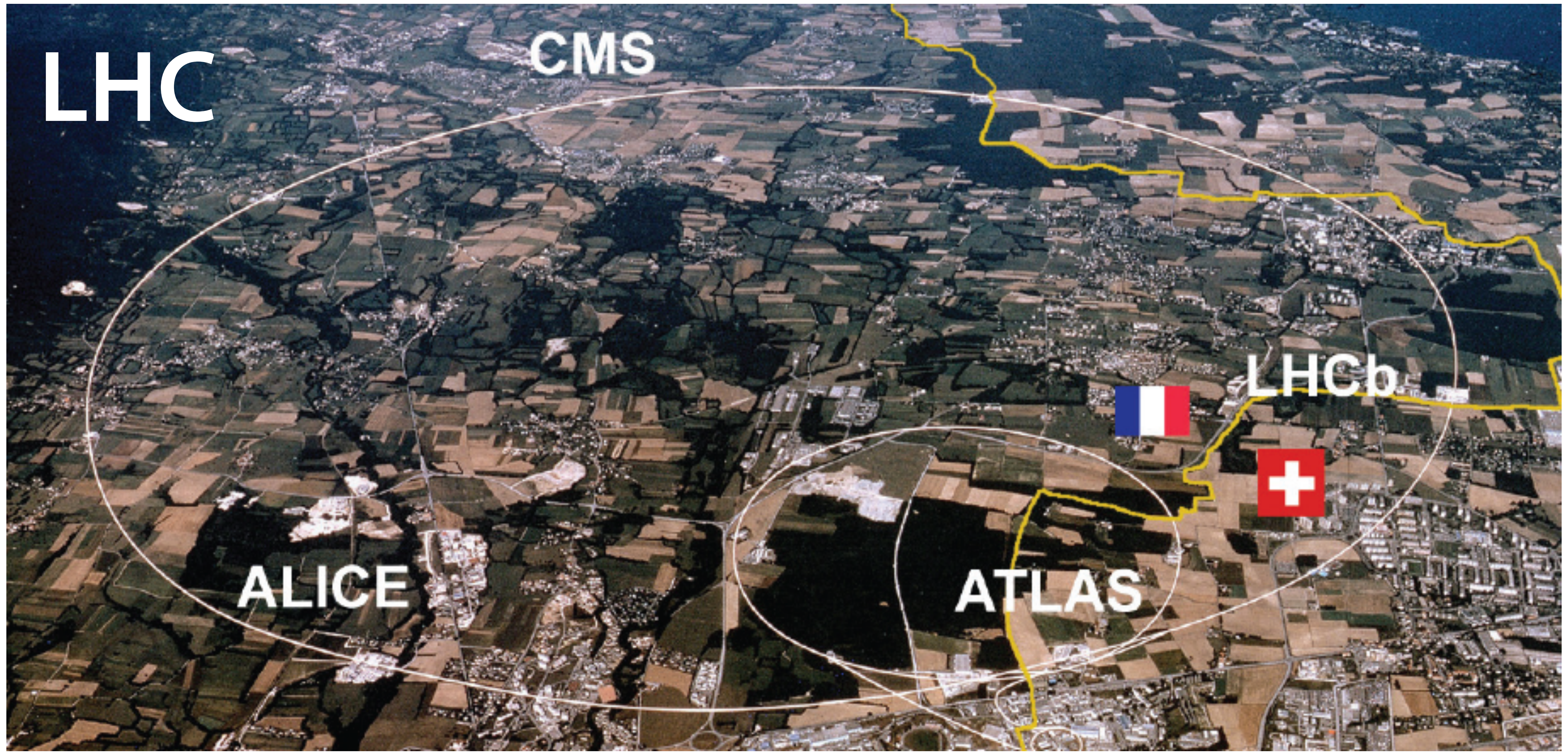
  $U_{\text{ent}} = \prod_{j=1}^{n} C_{j\%n+1}^{j}[Z]$: Controlled-Z gate as an entangling gate

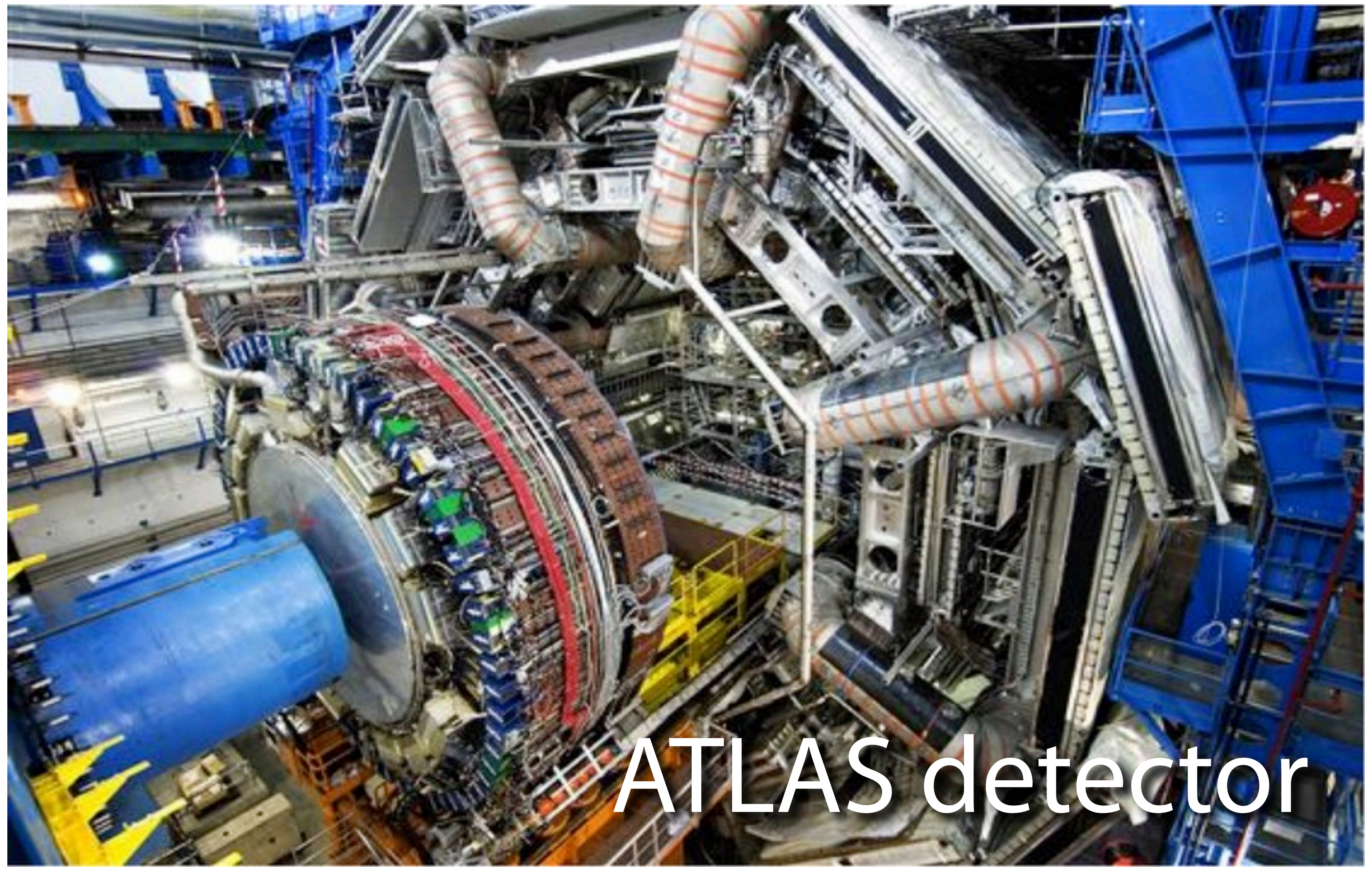
Hands-on Exercise (II)

- Quantum Machine Learning :
  - Learn a function from input and output data from the function

Application to High-Energy Physics

Learn more complex data from high-energy physics (HEP) experiment
(though actually "truth-level" simulation data)





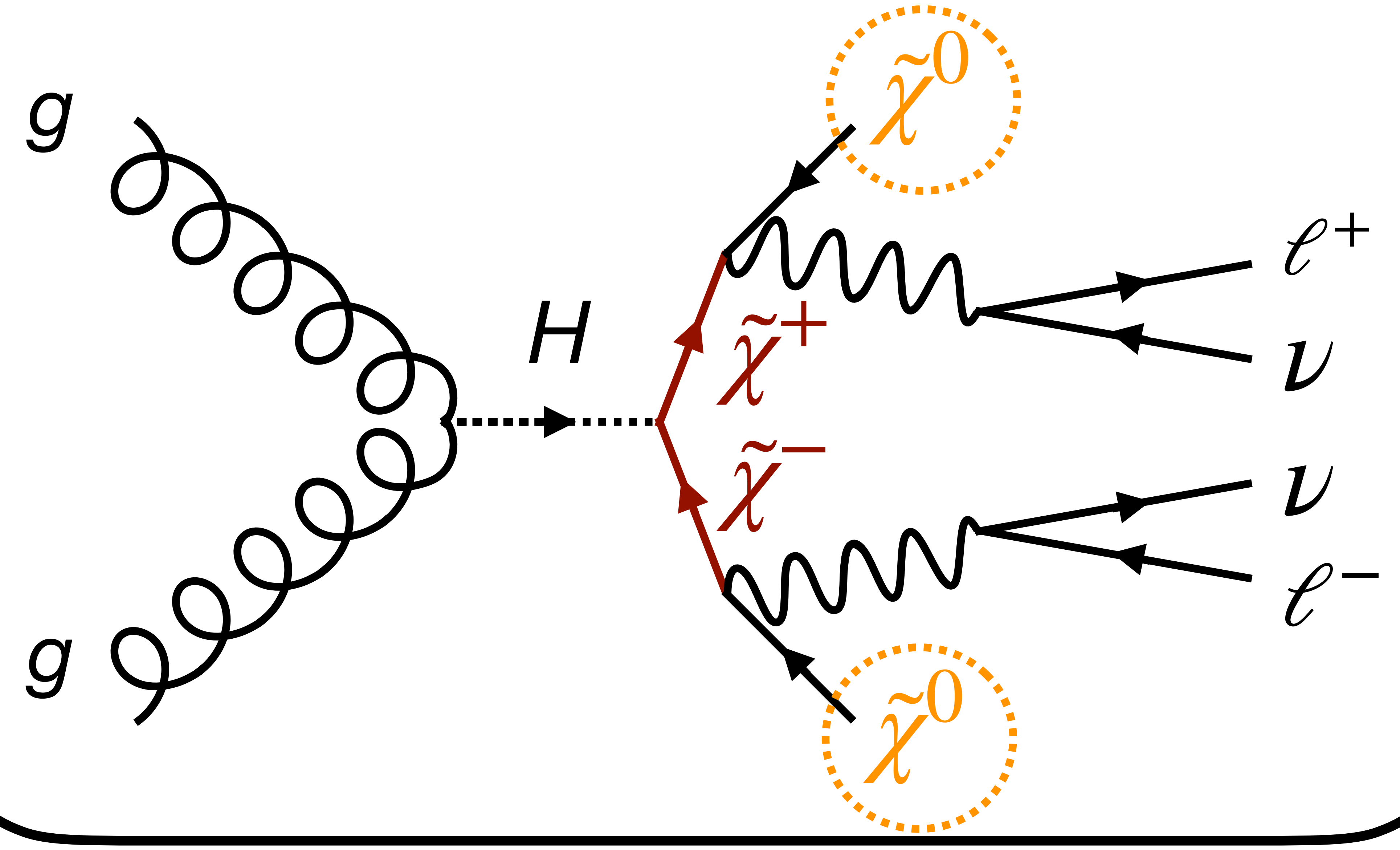
Machine learning technique is ubiquitous in HEP experiment

Detector reconstruction, simulation, data analysis, trigger, …

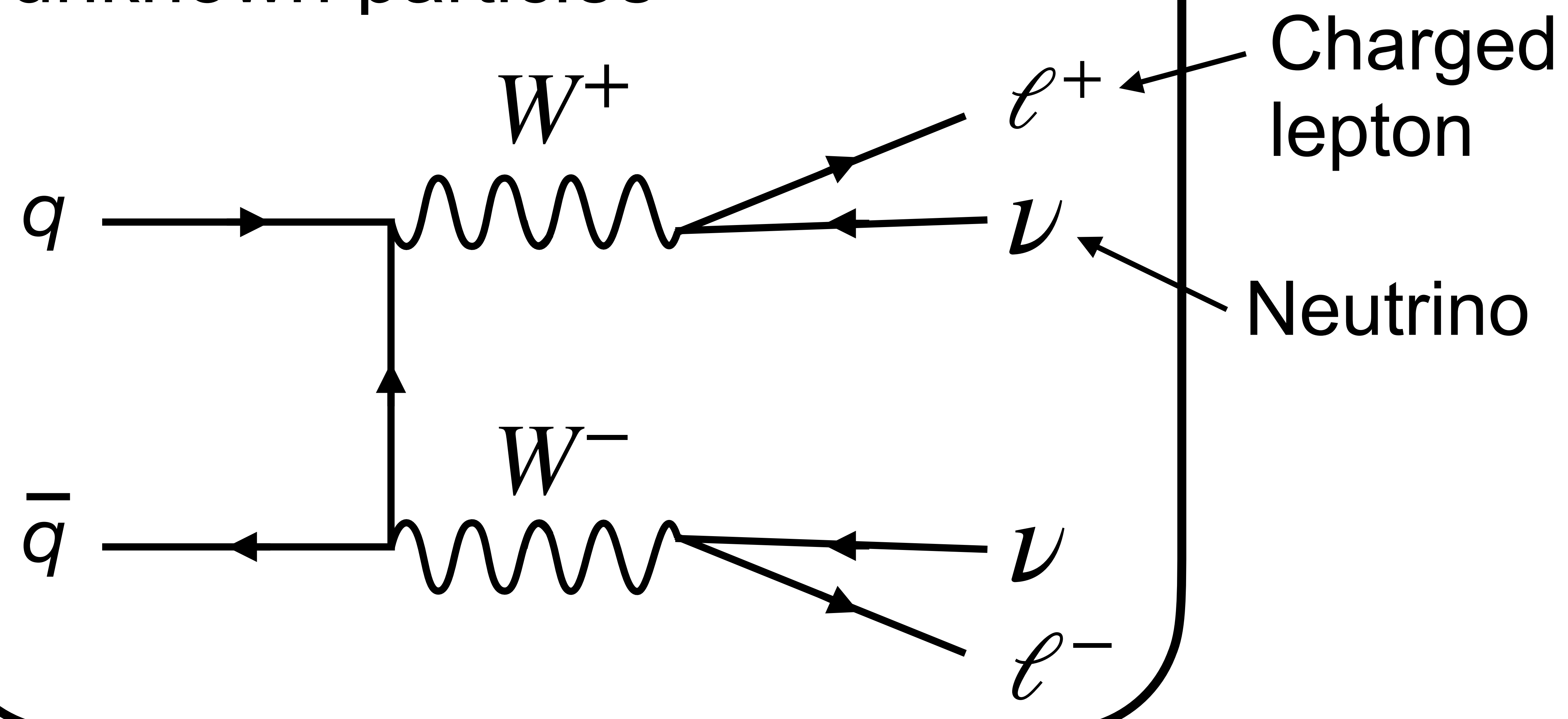
QML Application to Event Classification

Classify events that contain new physics signal from background events

Signal event with unknown particles



Background event without unknown particles



Neutralino ➡ Not observed by the detector, like SM neutrino

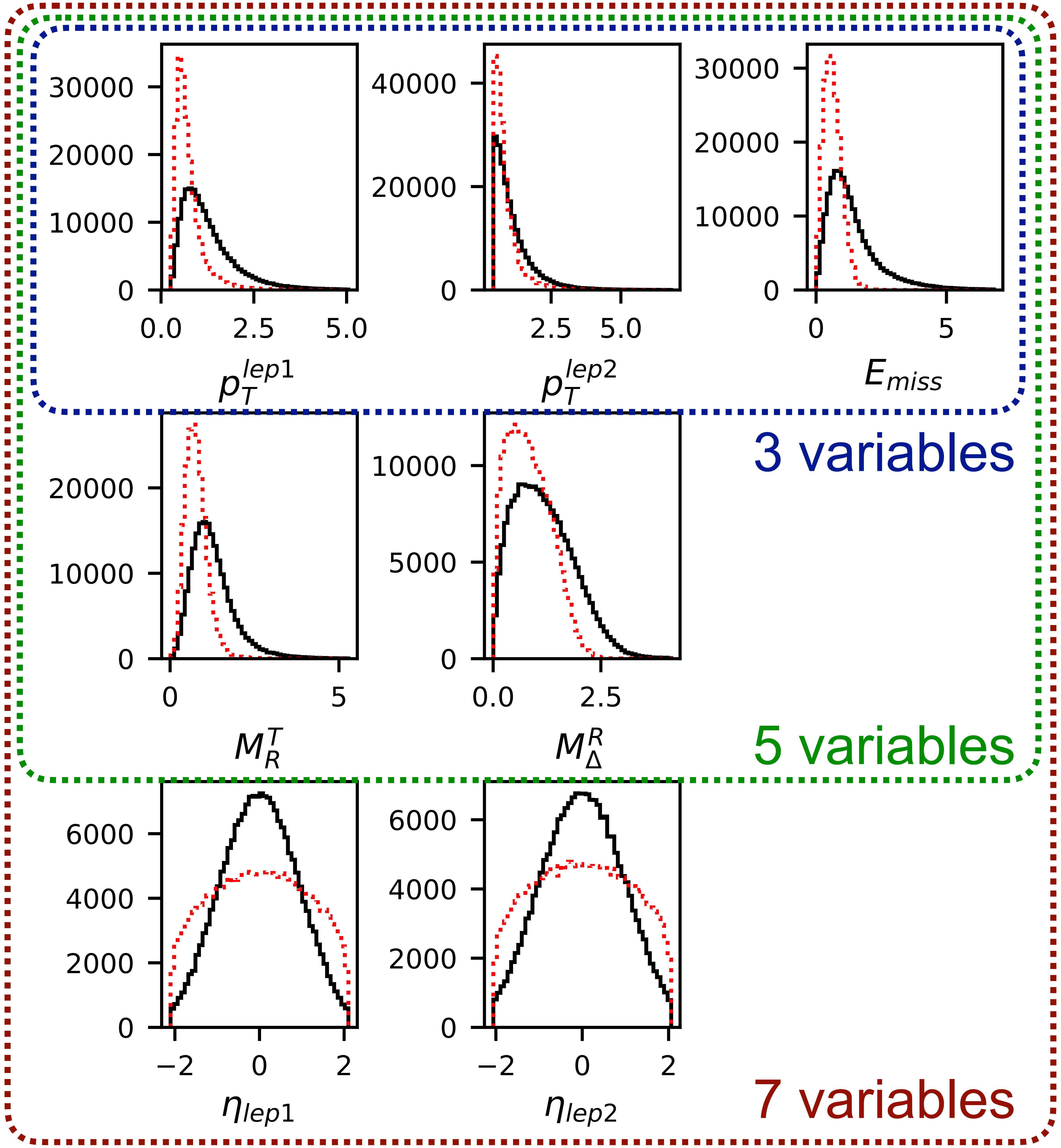
Use differences in kinematical properties due to the presence of *H* and $\tilde{\chi}^{\pm}/\tilde{\chi}^0$ to classify signal from background

Training Data

Use SUSY dataset in machine learning repository by University of California, Irvine

Signal (red histogram) and **background** (black histogram) differ in kinematical features of final state particles

Use these features as input data and classify signal and background events



Quantum Neural Network Model

- Feature map: $U_{\text{in}}(\boldsymbol{x}_i) = U_\phi(\boldsymbol{x}_i)H^{\otimes n}$

$$U_\phi(\boldsymbol{x}_i) = \exp\left(i \sum_{k=1}^{n} \phi_{\{k,k+1\}}(\boldsymbol{x}_i) Z_k Z_{k\%n+1} + i \sum_{k=1}^{n} \phi_{\{k\}}(\boldsymbol{x}_i) Z_k \right)$$

$$\phi_{\{k\}}(\boldsymbol{x}_i) = x_i^{\{k\}},\ \phi_{\{k,k+1\}}(\boldsymbol{x}_i) = (\pi - x_i^{\{k\}})(\pi - x_i^{\{k\%n+1\}})$$

➡ called ZZ feature map

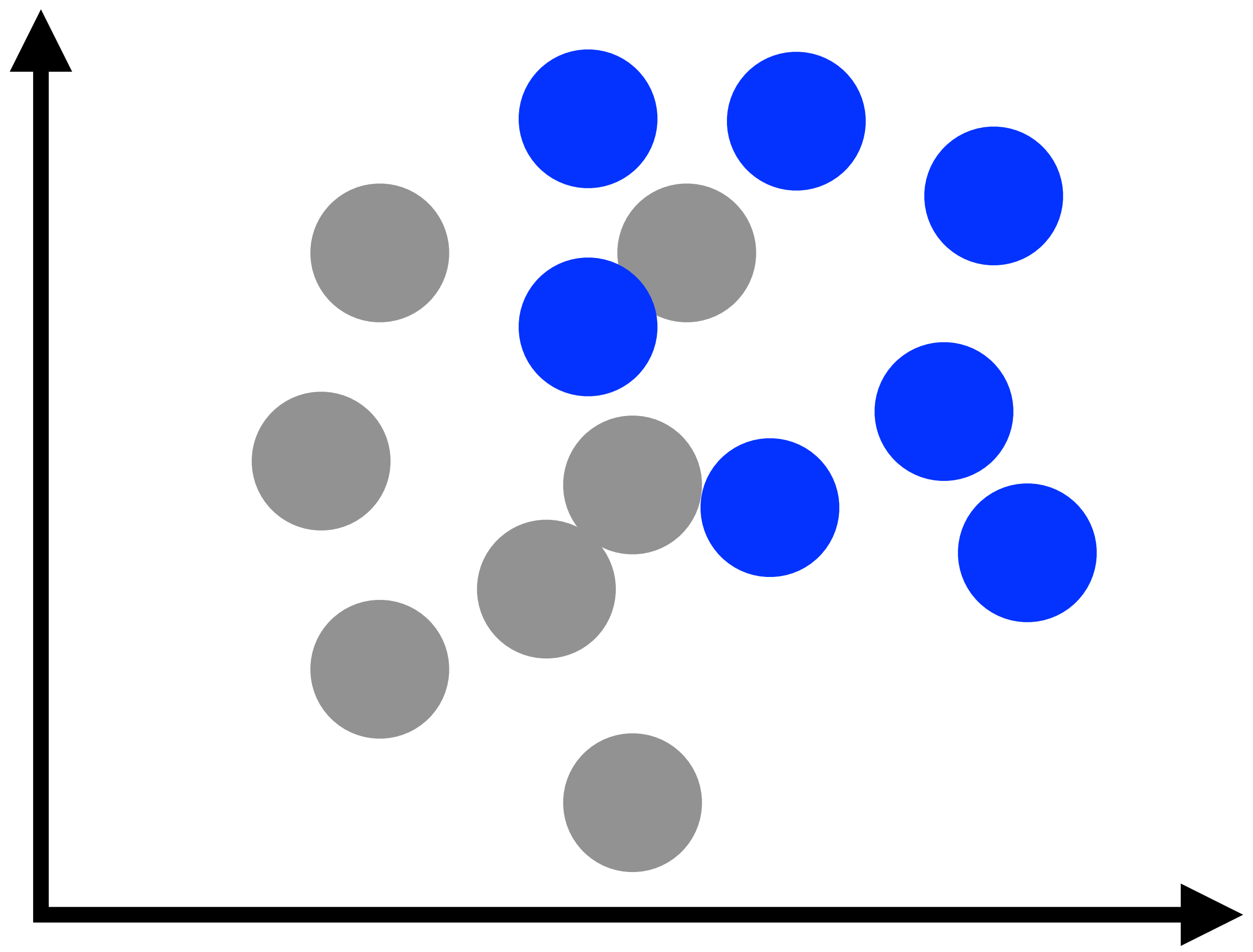
- Variational form:

$$U(\{\theta_j^l\}) = \prod_{l=1}^{d} \left(\left(\prod_{j=1}^{n} U_{\text{rot}}(\theta_j^l) \right) \cdot U_{\text{ent}} \right) \cdot \prod_{j=1}^{n} U_{\text{rot}}(\theta_j^0)$$

$$U_{\text{rot}}(\theta_j^l) = R_j^Z(\theta_{j2}^l) R_j^Y(\theta_{j1}^l) \qquad U_{\text{ent}} = \prod_{j=1}^{n} C_{j\%n+1}^{j}[Z]$$

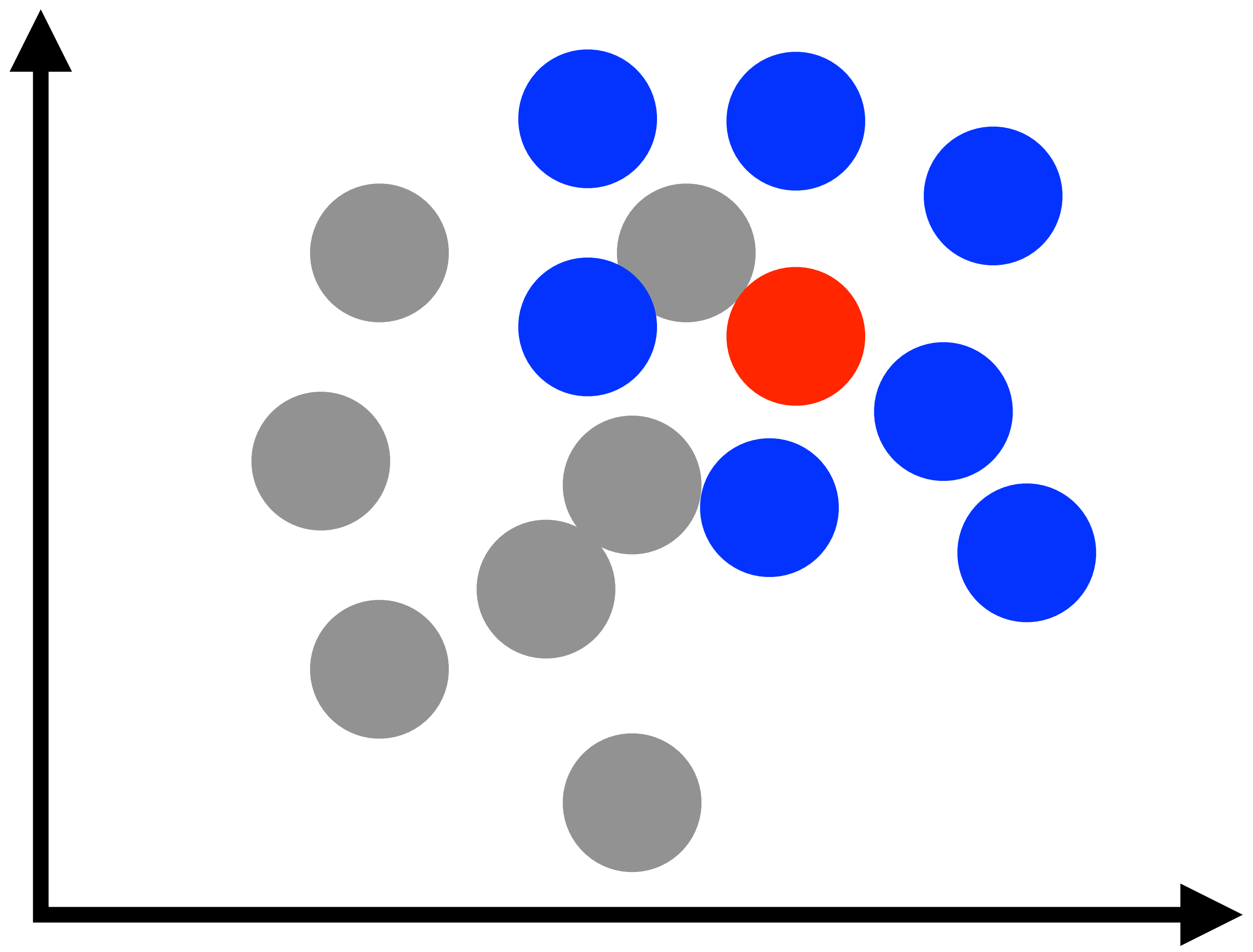
Kernel Method for Machine Learning

Assuming there are two classes of data: and



There is a new data

➡ Which class of or does the new data belong to?



Likely

➡ *Distance* or *Similarity* between data can be used to judge

Kernel Method for Machine Learning

Function to quantify the distance measure $\kappa : D \times D \to \mathbb{R}$

Consider a matrix with elements $K_{m,m'} = \kappa(\boldsymbol{x}^m, \boldsymbol{x}^{m'})$ constructed from two different training points $\boldsymbol{x}^m, \boldsymbol{x}^{m'}$ in the training sample D

Kernel Matrix

The closer the data points are, the larger the matrix elements

Representative kernel function is

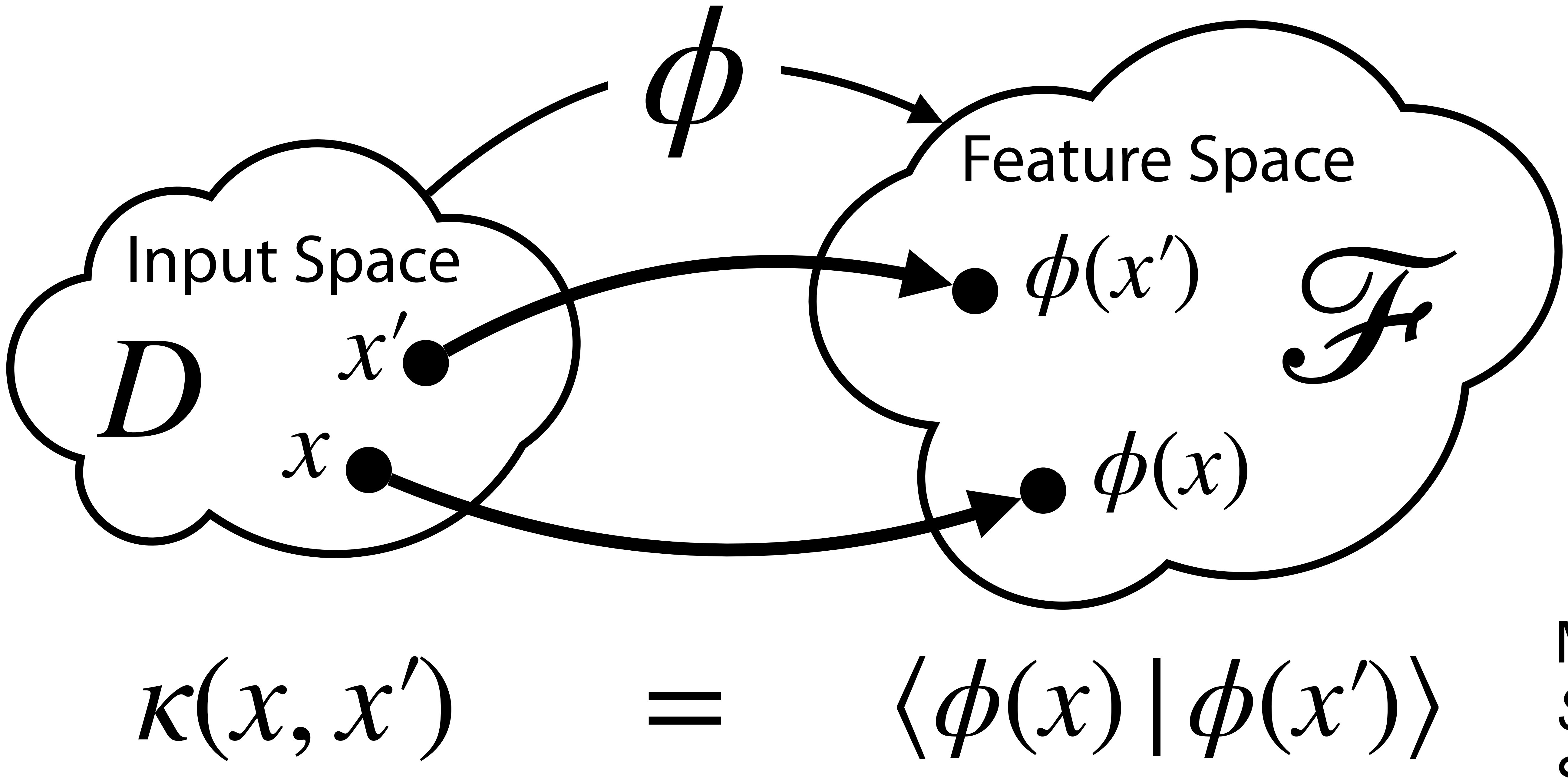
- Linear kernel : $\boldsymbol{x}^T \boldsymbol{x}'$
- Gaussian kernel : $e^{-\gamma \|\boldsymbol{x} - \boldsymbol{x}'\|^2}$

Kernel Method for Machine Learning

Input data encoded in high-dimensional Hilbert space using feature map in QML

➡ Inner products of encoded states can be used as a kernel function

$\kappa(\boldsymbol{x}^m, \boldsymbol{x}^{m'}) = \langle \phi(\boldsymbol{x}) \,|\, \phi(\boldsymbol{x}') \rangle$ for a feature map $\phi : D \to \mathscr{F}$



For positive definite kernel, there is a feature space $\mathscr{F}$ created by ϕ such that the kernel κ in D is equal to inner product in $\mathscr{F}$

M. Schuld, F. Petruccione, *Supervised Learning with Quantum Computers*, Springer Nature

Kernel Method for Machine Learning

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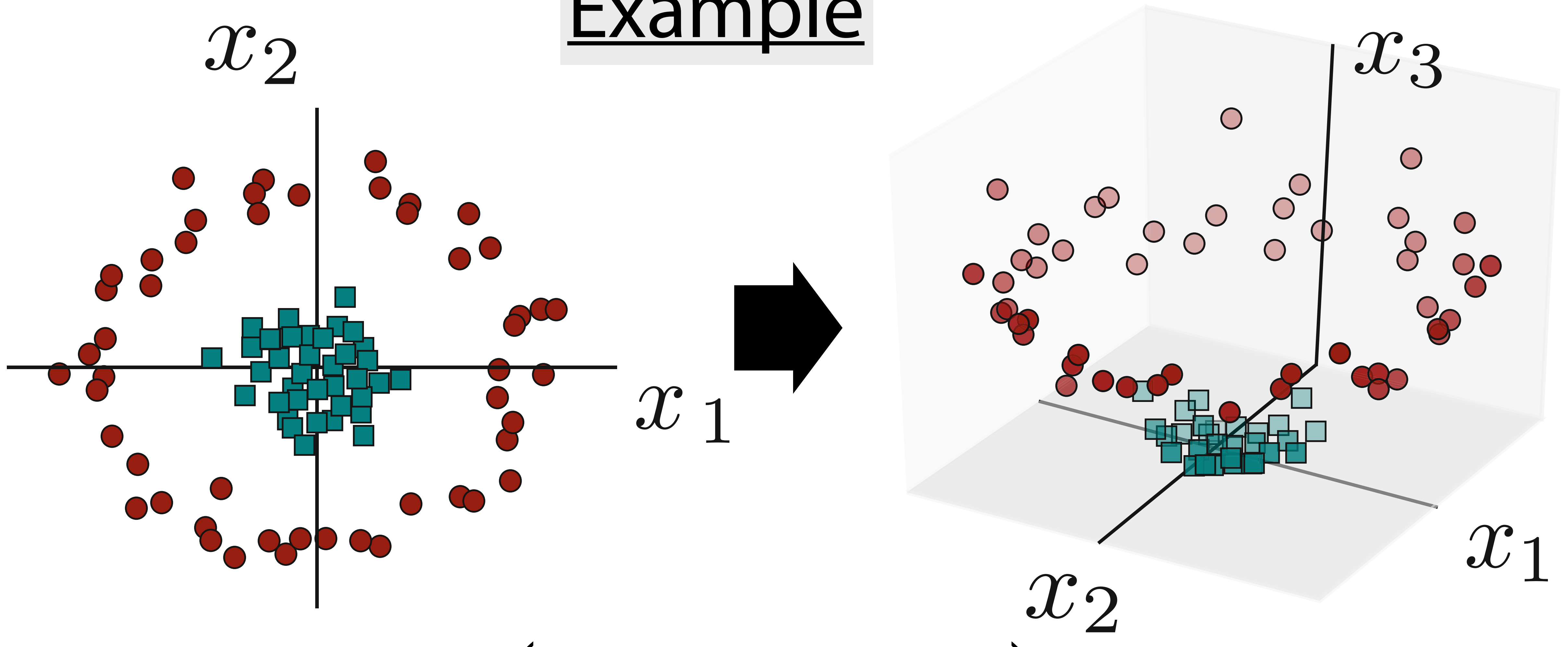
$$\kappa(\boldsymbol{x}^m, \boldsymbol{x}^{m'}) = \langle \phi(\boldsymbol{x}) \,|\, \phi(\boldsymbol{x}') \rangle \text{ for a feature map } \phi : D \to \mathscr{F}$$

Example



$$\phi(x_1, x_2) = \left(x_1, x_2, \frac{(x_1^2 + x_2^2)}{2} \right)$$

Data classification can often improve when the input data are encoded into higher-dimensional feature space

M. Schuld, F. Petruccione, *Supervised Learning with Quantum Computers*, Springer Nature

How can we find a good feature map?

Kernel Method for Machine Learning

Input data encoded in high-dimensional Hilbert space using feature map in QML

➡ Inner products of encoded states can be used as a kernel function

$\kappa(\boldsymbol{x}^m, \boldsymbol{x}^{m'}) = \langle \phi(\boldsymbol{x}) \,|\, \phi(\boldsymbol{x}') \rangle$ for a feature map $\phi : D \rightarrow \mathscr{F}$

Quantum Kernel

How can we find a good feature map?

This is of course a problem and data dependent

Modifying kernel function would result in *non-trivial* changes in feature space

➡ called **Kernel Trick**

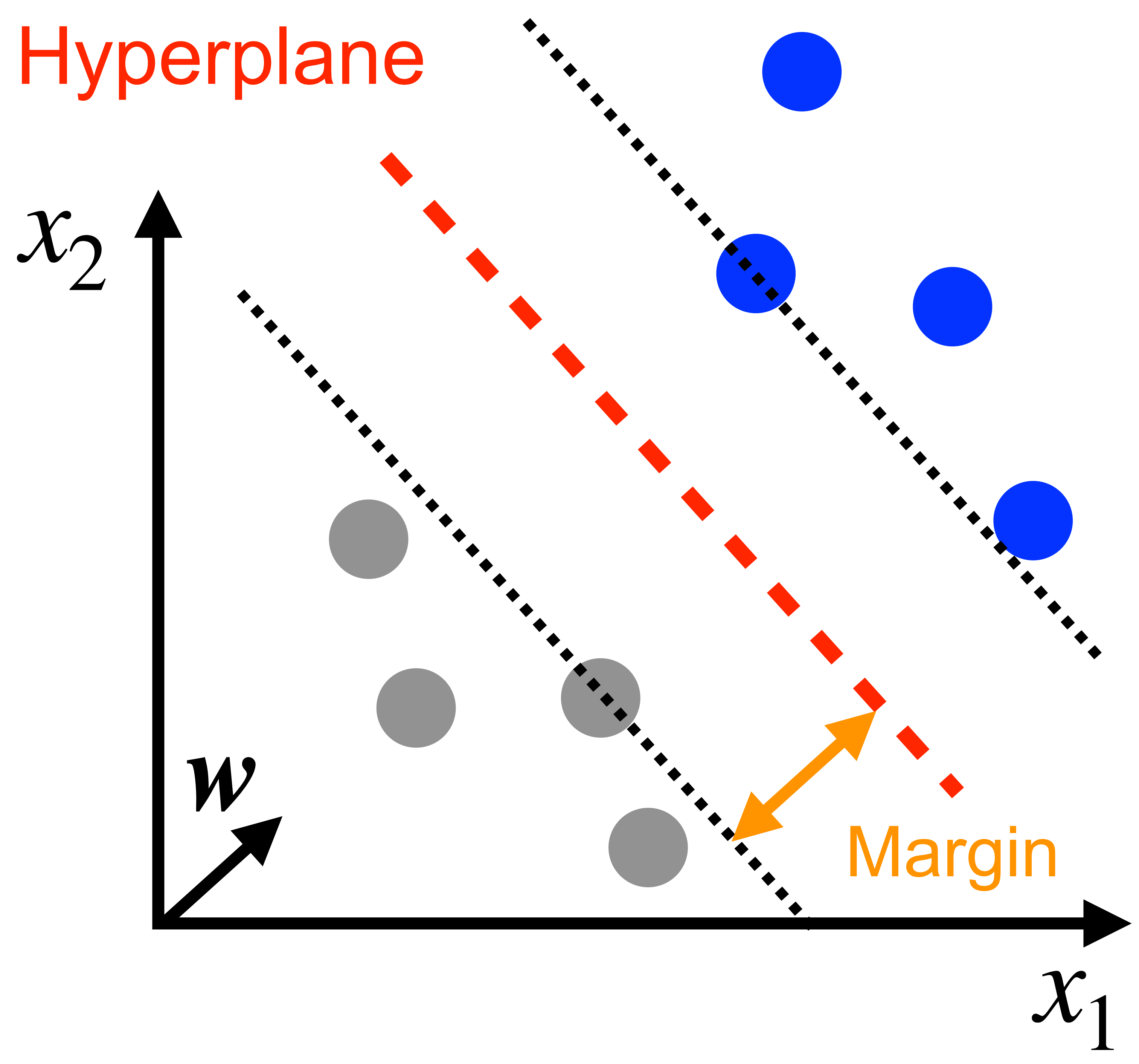
ML Classification in Feature Space

Consider a 2-class classification problem:

$$\{(\boldsymbol{x}_i, y_i)\}(i = 1, \cdots, N)\ \ \boldsymbol{x}_i \in \mathbb{R}^d, y_i \in \{+1, -1\}$$

Define ***hyperplane*** as the points $\{\boldsymbol{x} \,|\, \boldsymbol{x} \in \mathbb{R}^d, \boldsymbol{w} \cdot \boldsymbol{x} + b = 0\}$

➡ Separate the feature space linearly into two data regions with different labels by a hyperplane



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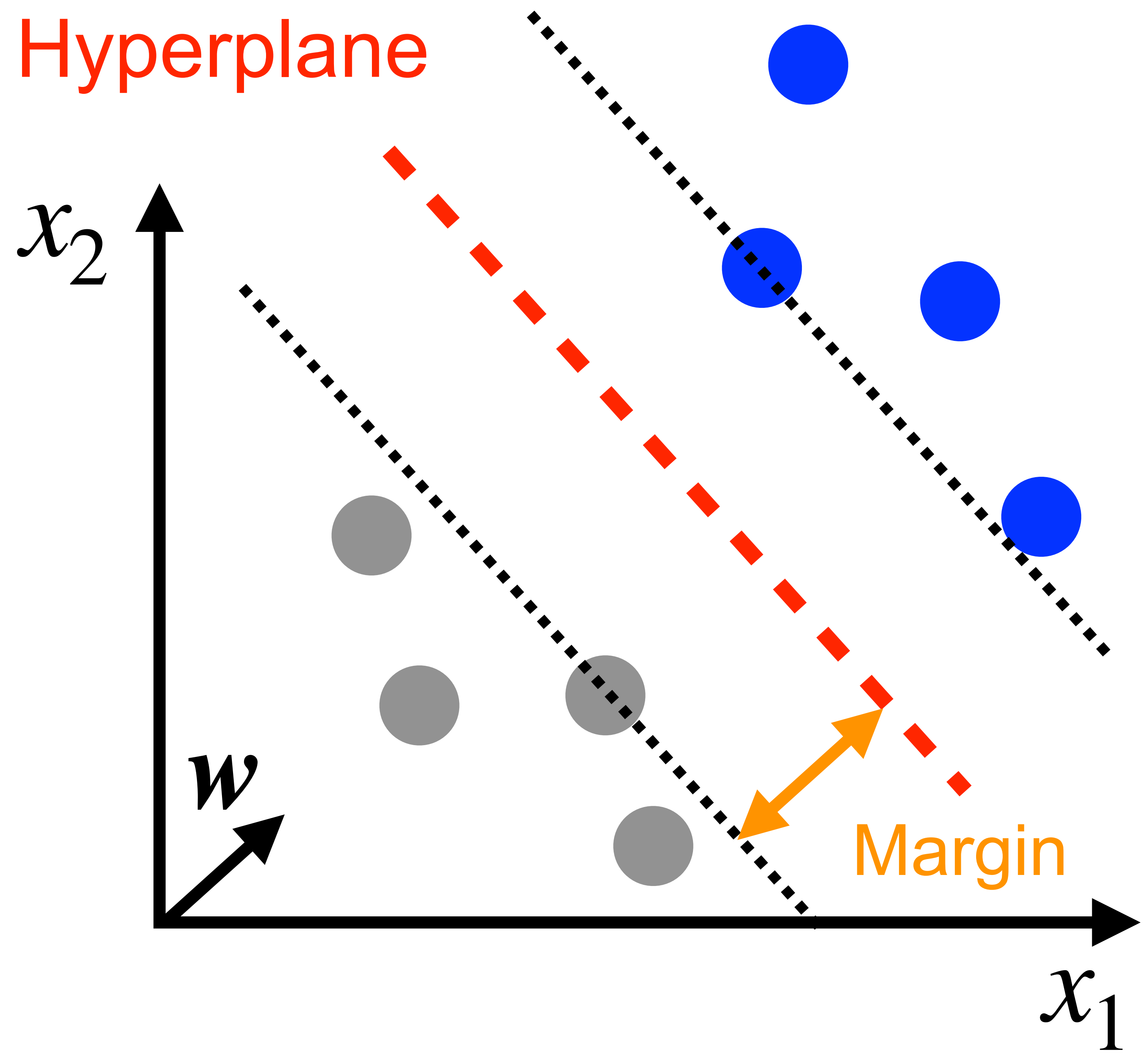


<u>Machine Learning task:</u>

- Training : Find a hyperplane $(\boldsymbol{w}, b)$ that satisfies $y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) \geq 1 \;\; \forall i$
- Inference : Sign of $\boldsymbol{w} \cdot \boldsymbol{x}_i' + b$ gives a label prediction for unseen new data $\boldsymbol{x}_i'$

Support Vector Machine

Find a hyperplane that maximizes the margin ($\propto 1/ \|\boldsymbol{w}\|$) between hyperplane and the nearest data point

Quantum SVM

Linear separation of data points in Hilbert space ➡ **Finding the minimum of** $\| \boldsymbol{w} \|^2$

➡ Further translated to a problem of finding parameters $\{\alpha_i\}$ that minimize

$$L(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

under the conditions $\sum_{i=1}^{N} \alpha_i y_i = 0, \alpha_i \geq 0$ for parameters $\{\alpha_i\}(i = 1, \cdots, N)$

More details in [QML workbook]

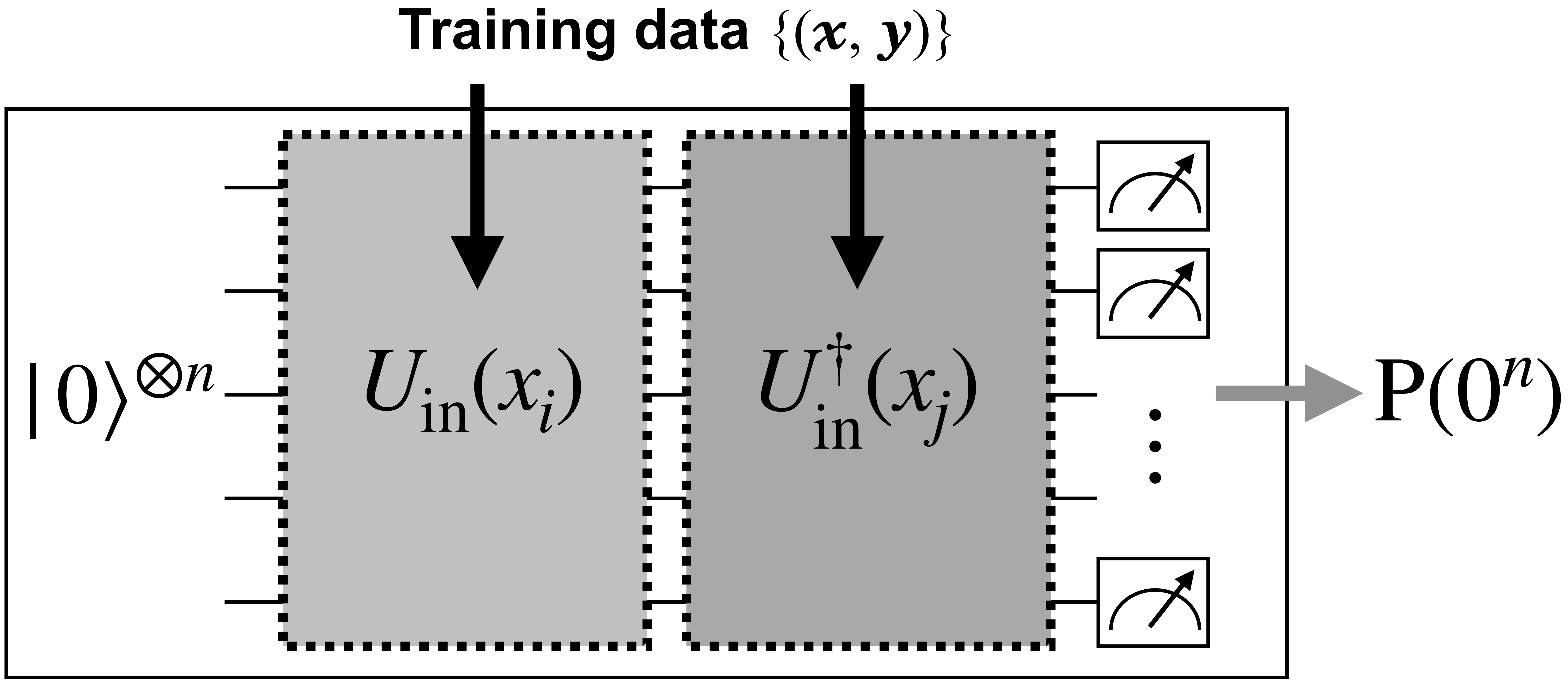
Calculate ***Quantum Kernel*** $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ using quantum computer

Sign of $\sum_{i=1}^{N} y_i \alpha_i^* K(\boldsymbol{x}_i, \boldsymbol{x}') + b^*$ with optimized parameters $\{\alpha_i^*, b^*\}$

➡ Label prediction for test data $\boldsymbol{x}'$

Quantum Circuit for QSVM

Quantum kernel can be obtained as inner product for a given feature map $U_{\text{in}}(x)$



Quantum Kernel $K(x_i, x_j) := |\langle\phi(x_j)|\phi(x_i)\rangle|^2 = |\langle 0^{\otimes n}|U^{\dagger}_{\text{in}}(x_j)|U_{\text{in}}(x_i)|0^{\otimes n}\rangle|^2$

➡ Probability of measuring 0 in all n-qubits with the initial state $|0\rangle^{\otimes n}$

Hands-on Exercise (III)

- Quantum Machine Learning :
  - Event classification using quantum neural network model
  - Event classification using quantum kernel method