Title: Quantum Machine Learning

Speakers: Alvaro Ballon Bordo

Collection: Navigating Quantum and AI Career Trajectories: A Beginnerâ€™s Mini-Course on Computational Methods and their Applications

Date: May 23, 2024 - 9:30 AM

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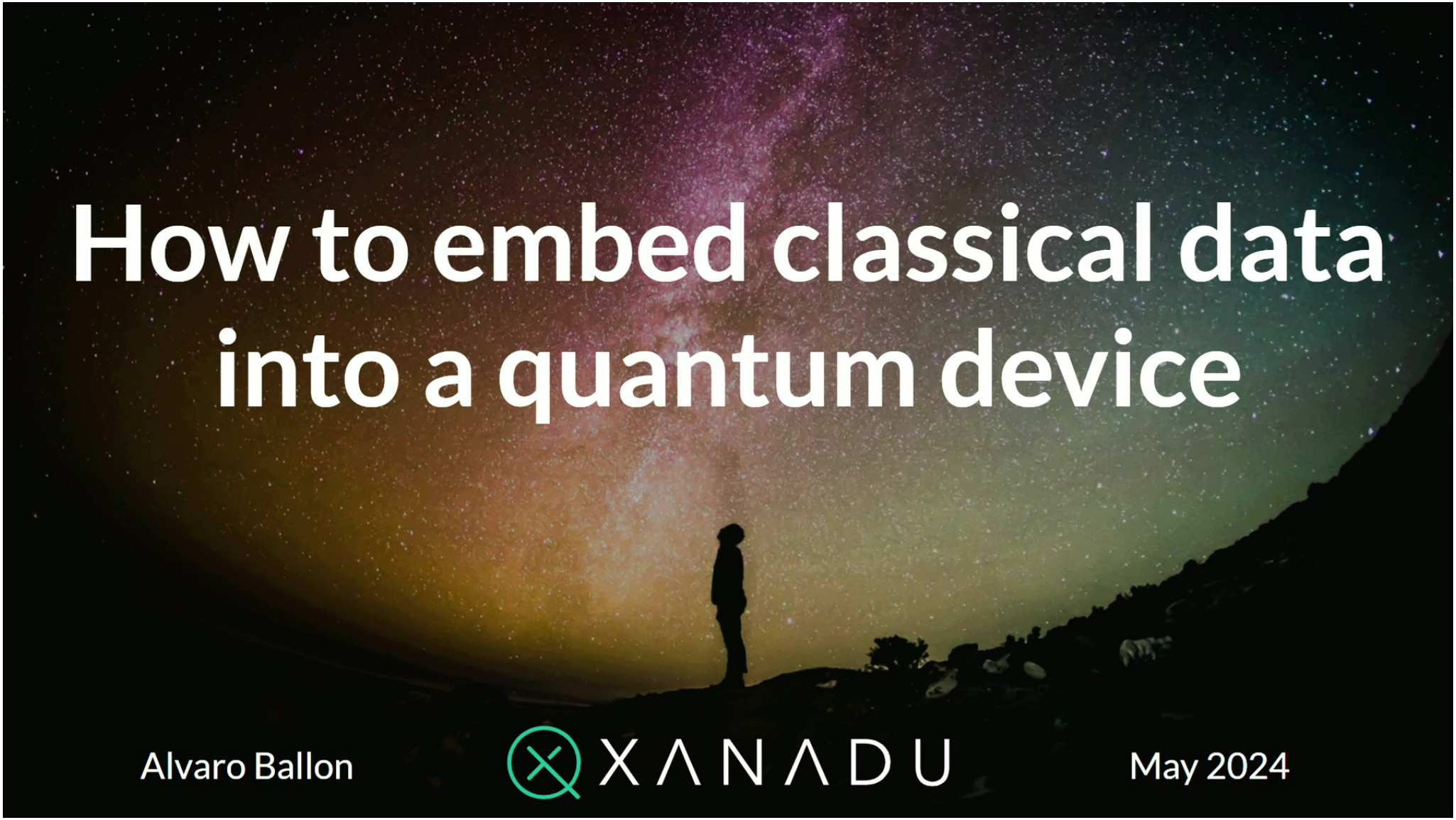
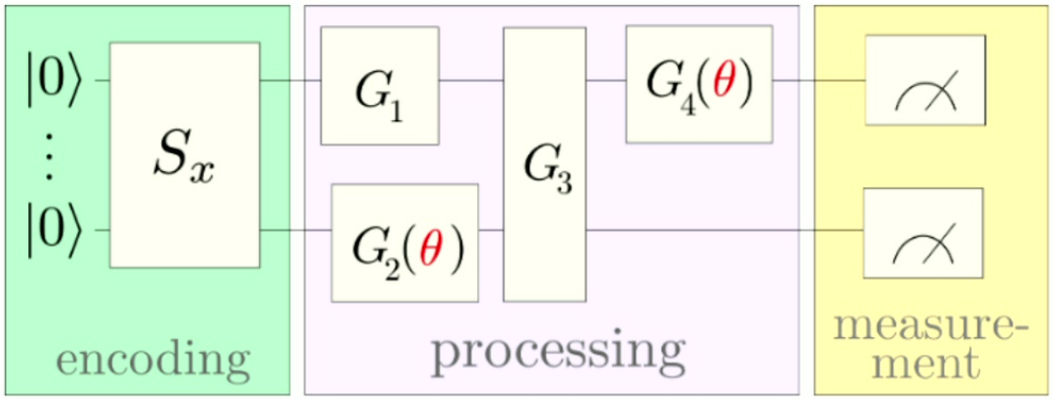

How to embed classical data into a quantum device
Alvaro Ballon
XANADU
May 2024

Data embedding



Basis Embedding

Used for discrete data, encoded as binary strings

```
N = 3
wires = range(N)
dev = qml.device("default.qubit", wires)

@qml.qnode(dev)
def circuit(b):
    qml.BasisEmbedding(b, wires)
    return qml.state()
>>> circuit([1, 1, 1])
[0.+0.j 0.+0.j 0.+0.j 0.+0.j 0.+0.j 0.+0.j 0.+0.j 1.+0.j]
```

Angle Embedding

Used for real-valued data. Normalize, then embed as rotation angles.

$$x \mapsto R_k(x)|0\rangle = e^{-ix\sigma_k/2}|0\rangle,$$

```
@qml.qnode(dev)
def circuit(val_list):
    qml.AngleEmbedding(val_list, wires)
    return [qml.expval(qml.PauliZ(w)) for w in wires]
>>> circuit([0.0, np.pi / 2, np.pi])
tensor([ 1.0,  0.0, -1.0], requires_grad=True)
```

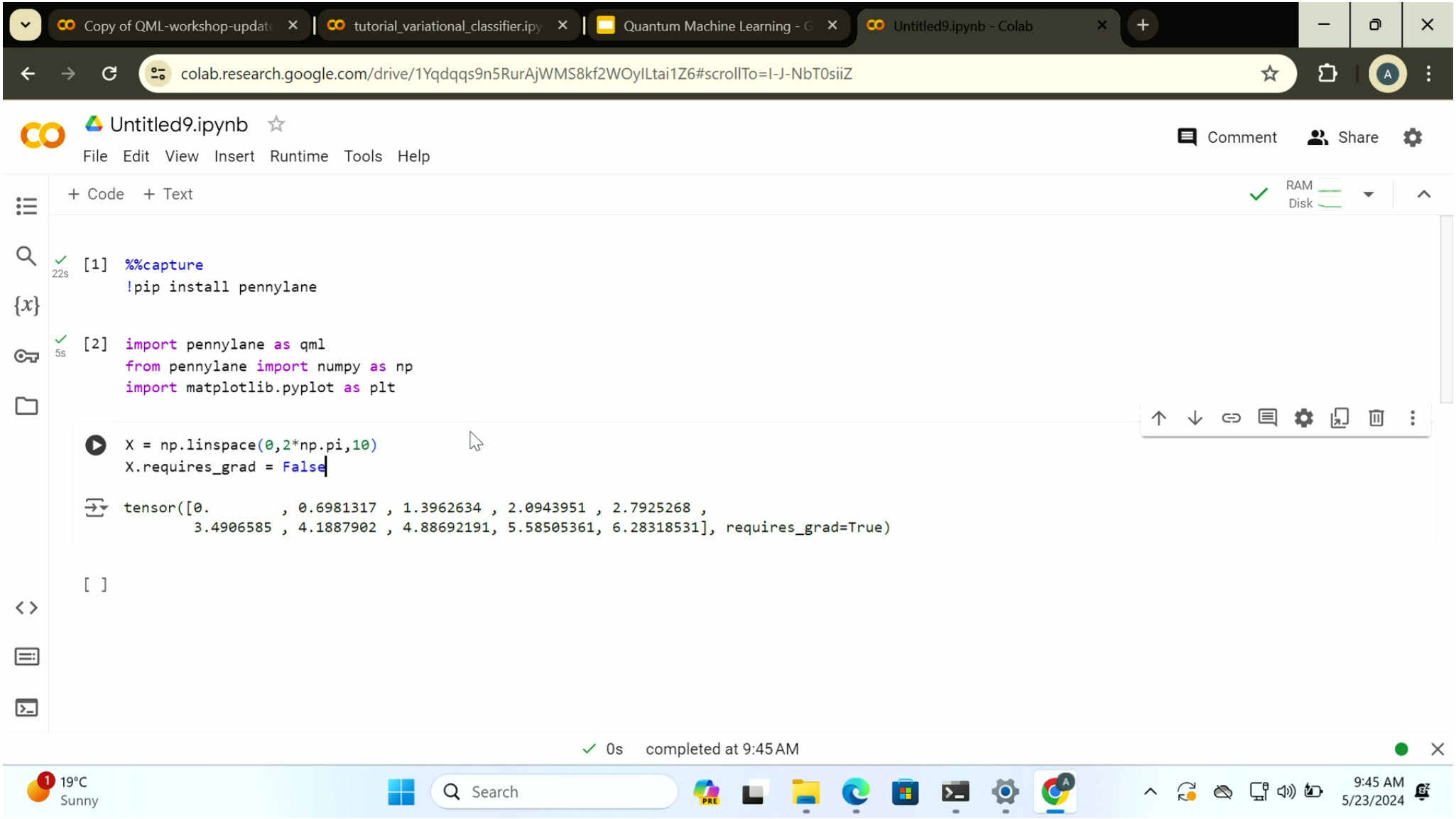
Amplitude Embedding

Used for complex- valued data.

$$\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_{2^N-1}) \mapsto \sum_{k=0}^{2^N-1} \alpha_k |k\rangle$$

```
N = 3
wires = range(N)
dev = qml.device("default.qubit", wires)

@qml.qnode(dev)
def circuit(features):
    qml.AmplitudeEmbedding(features, wires)
    return qml.state()
>>> circuit([0.625, 0.0, 0.0, 0.0, 0.625j, 0.375, 0.25, 0.125])
tensor([0.625+0.j   , 0.   +0.j   , 0.   +0.j   , 0.   +0.j   ,
        0.   +0.625j, 0.375+0.j   , 0.25 +0.j   , 0.125+0.j   ], requires_grad=True)
```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22s
[1] %%capture
!pip install pennylane
5s
[2] import pennylane as qml
from pennylane import numpy as np
import matplotlib.pyplot as plt
X = np.linspace(0,2*np.pi,10)
X.requires_grad = False
tensor([0. , 0.6981317 , 1.3962634 , 2.0943951 , 2.7925268 ,
3.4906585 , 4.1887902 , 4.88692191, 5.58505361, 6.28318531], requires_grad=True)
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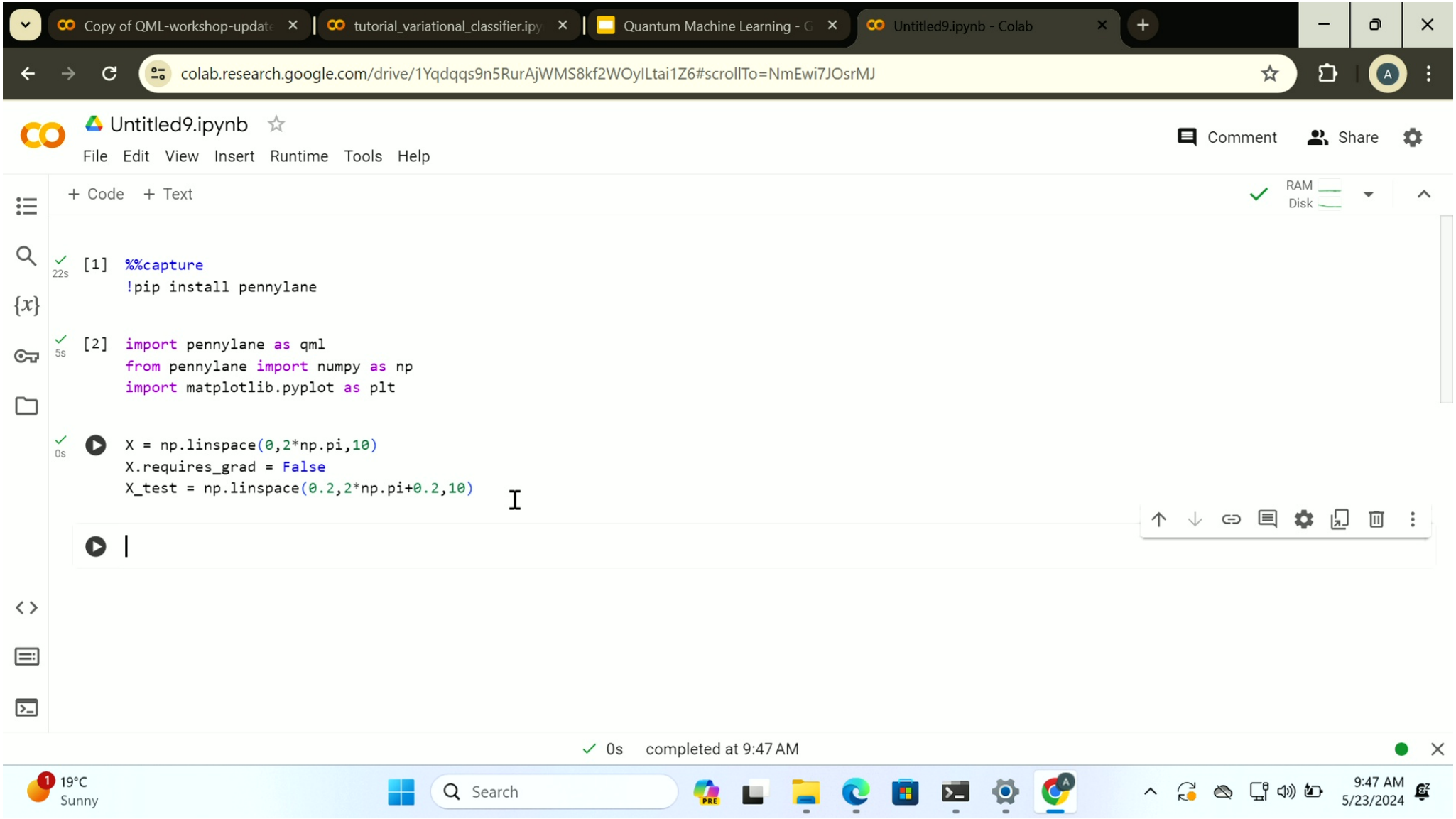
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22s [1] %%capture
!pip install pennylane
5s [2] import pennylane as qml
from pennylane import numpy as np
import matplotlib.pyplot as plt
0s X = np.linspace(0,2*np.pi,10)
X.requires_grad = False
X_test = np.linspace(0.2,2*np.pi+0.2,10)
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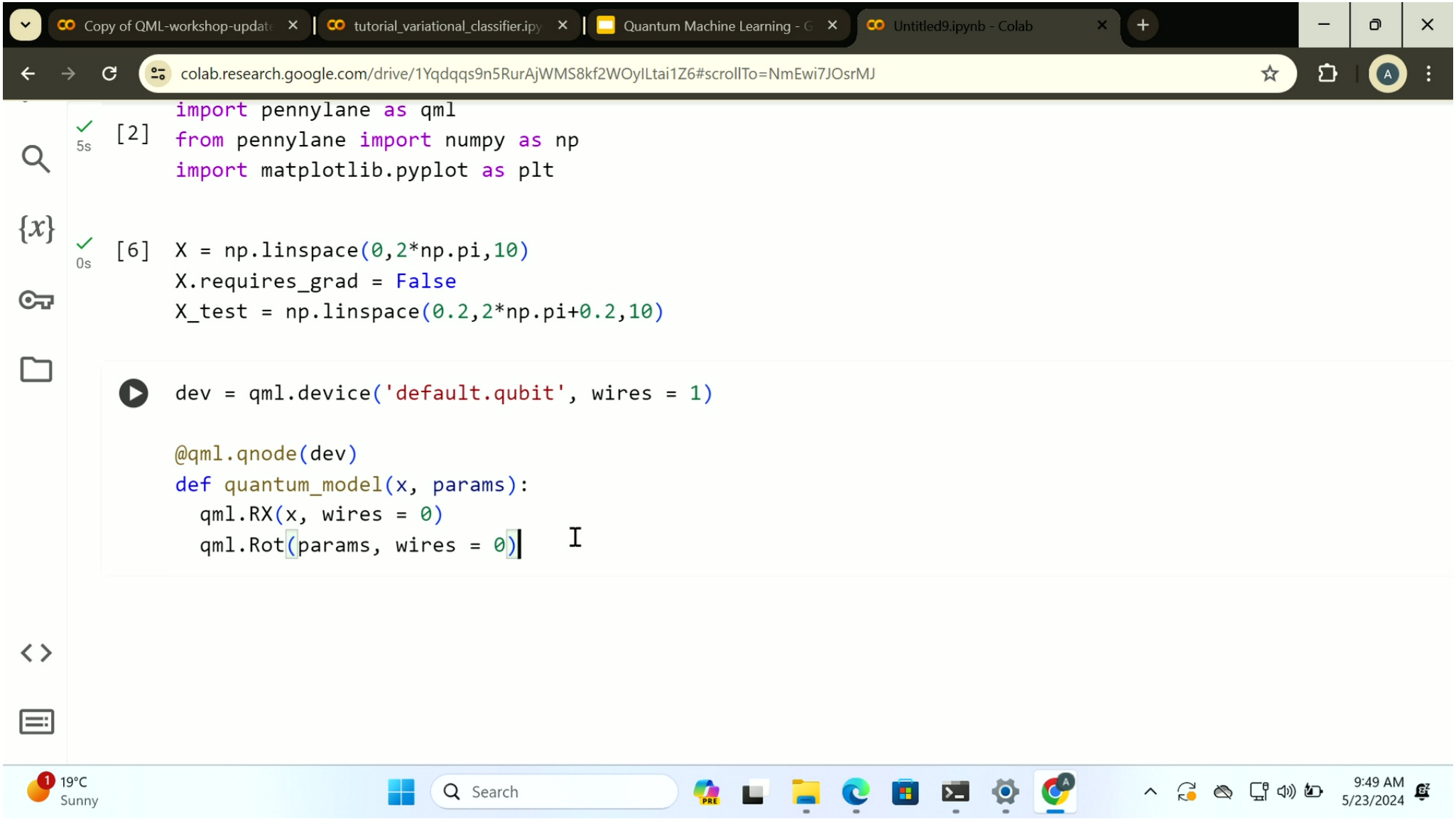
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import pennylane as qml
[2]
5s
from pennylane import numpy as np
import matplotlib.pyplot as plt
[6]
0s
X = np.linspace(0,2*np.pi,10)
X.requires_grad = False
X_test = np.linspace(0.2,2*np.pi+0.2,10)
dev = qml.device('default.qubit', wires = 1)
@qml.qnode(dev)
def quantum_model(x, params):
qml.RX(x, wires = 0)
qml.Rot(params, wires = 0)
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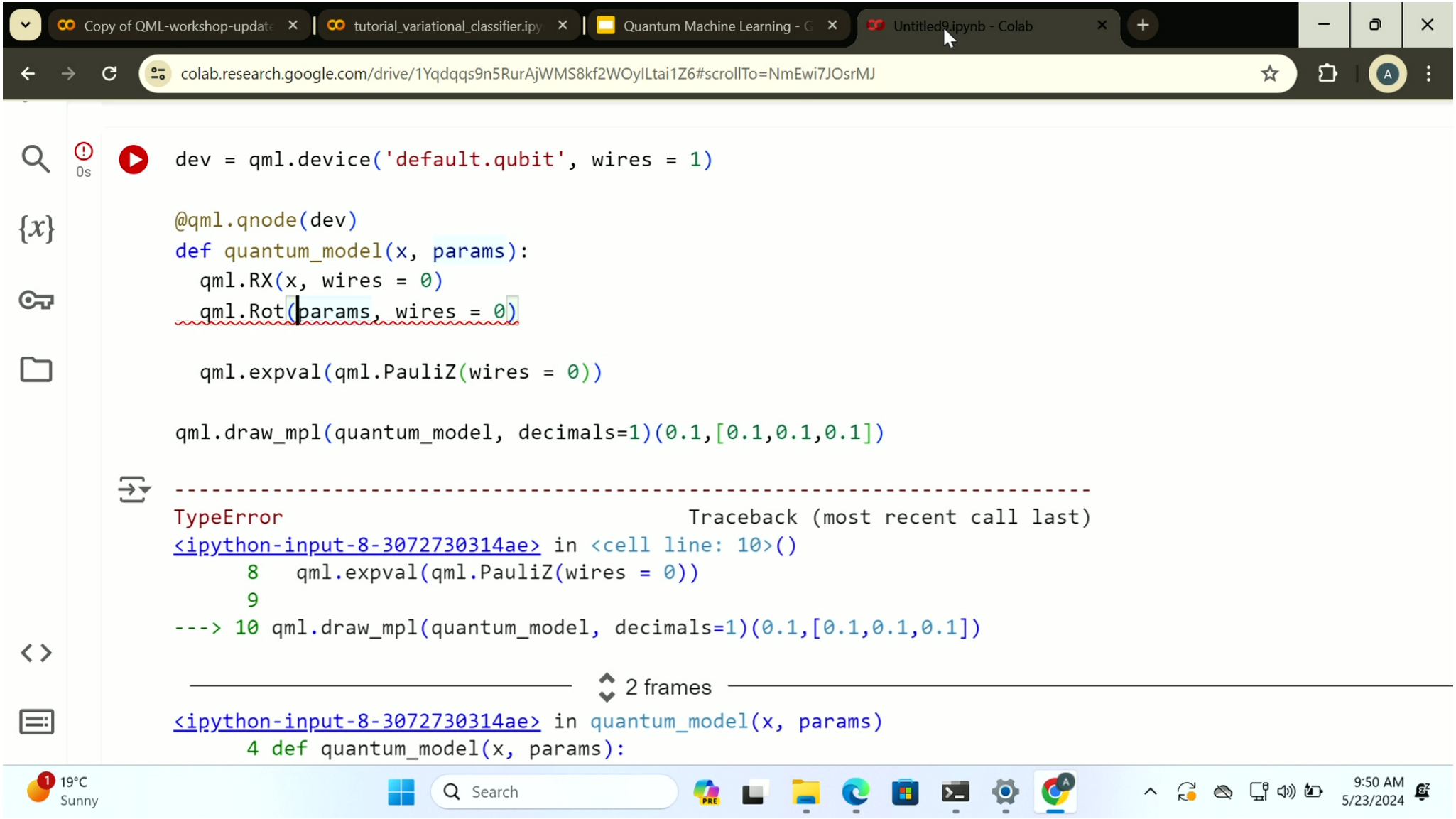
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dev = qml.device('default.qubit', wires = 1)
@qml.qnode(dev)
def quantum_model(x, params):
qml.RX(x, wires = 0)
qml.Rot(params, wires = 0)
qml.expval(qml.PauliZ(wires = 0))
qml.draw_mpl(quantum_model, decimals=1)(0.1,[0.1,0.1,0.1])
TypeError Traceback (most recent call last)
<ipython-input-8-3072730314ae> in <cell line: 10>()
8 qml.expval(qml.PauliZ(wires = 0))
9
---> 10 qml.draw_mpl(quantum_model, decimals=1)(0.1,[0.1,0.1,0.1])
2 frames
<ipython-input-8-3072730314ae> in quantum_model(x, params)
4 def quantum_model(x, params):
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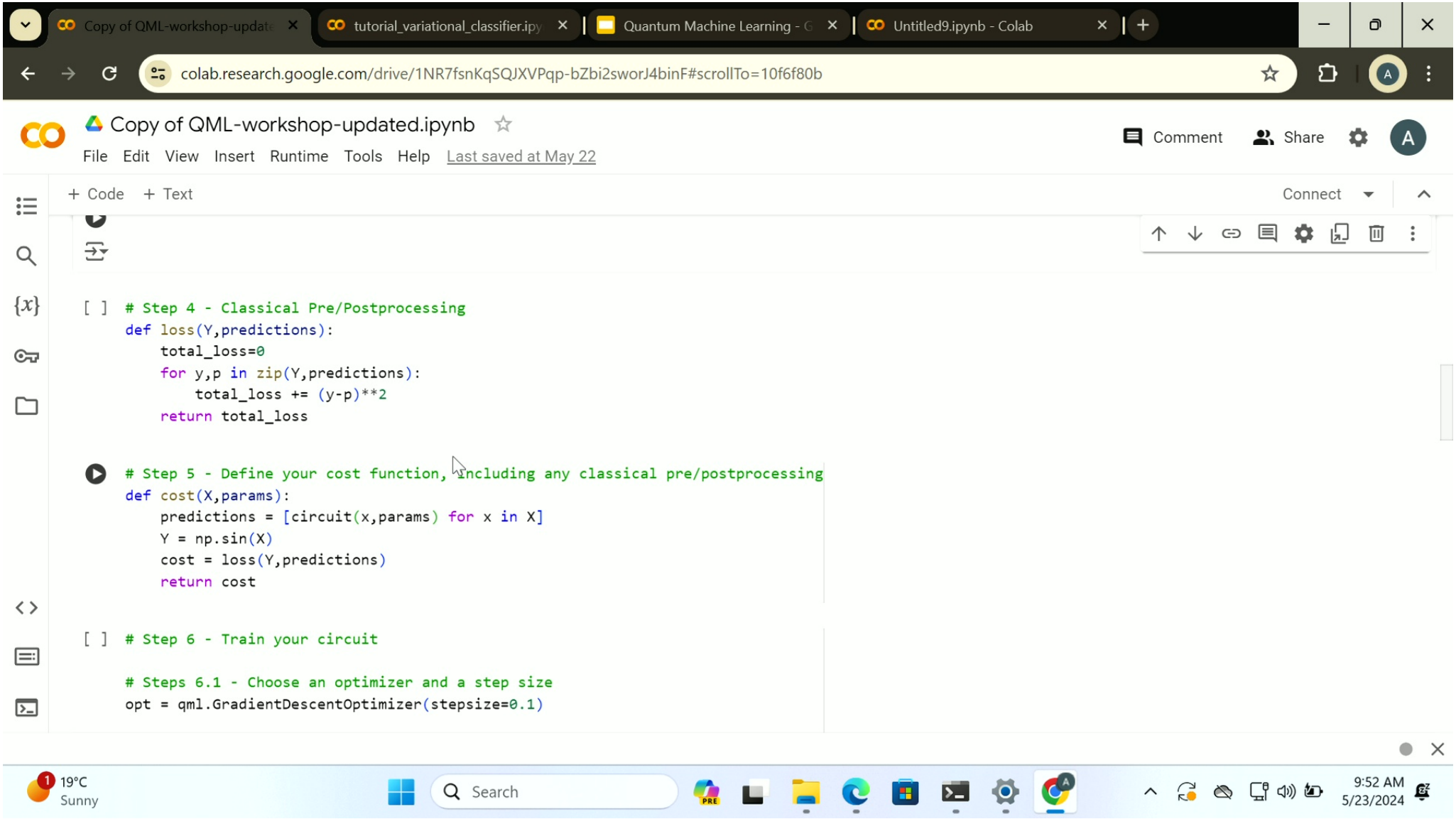
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[ ] # Step 4 - Classical Pre/Postprocessing
def loss(Y,predictions):
total_loss=0
for y,p in zip(Y,predictions):
total_loss += (y-p)**2
return total_loss
# Step 5 - Define your cost function, including any classical pre/postprocessing
def cost(X,params):
predictions = [circuit(x,params) for x in X]
Y = np.sin(X)
cost = loss(Y,predictions)
return cost
[ ] # Step 6 - Train your circuit
# Steps 6.1 - Choose an optimizer and a step size
opt = qml.GradientDescentOptimizer(stepsize=0.1)
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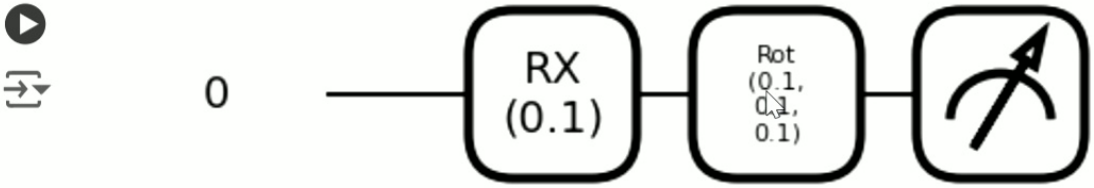


```
def loss(Y,predictions):
    total_loss=0
    for y,p in zip(Y,predictions):
        total_loss += (y-p)**2
    return total_loss
```

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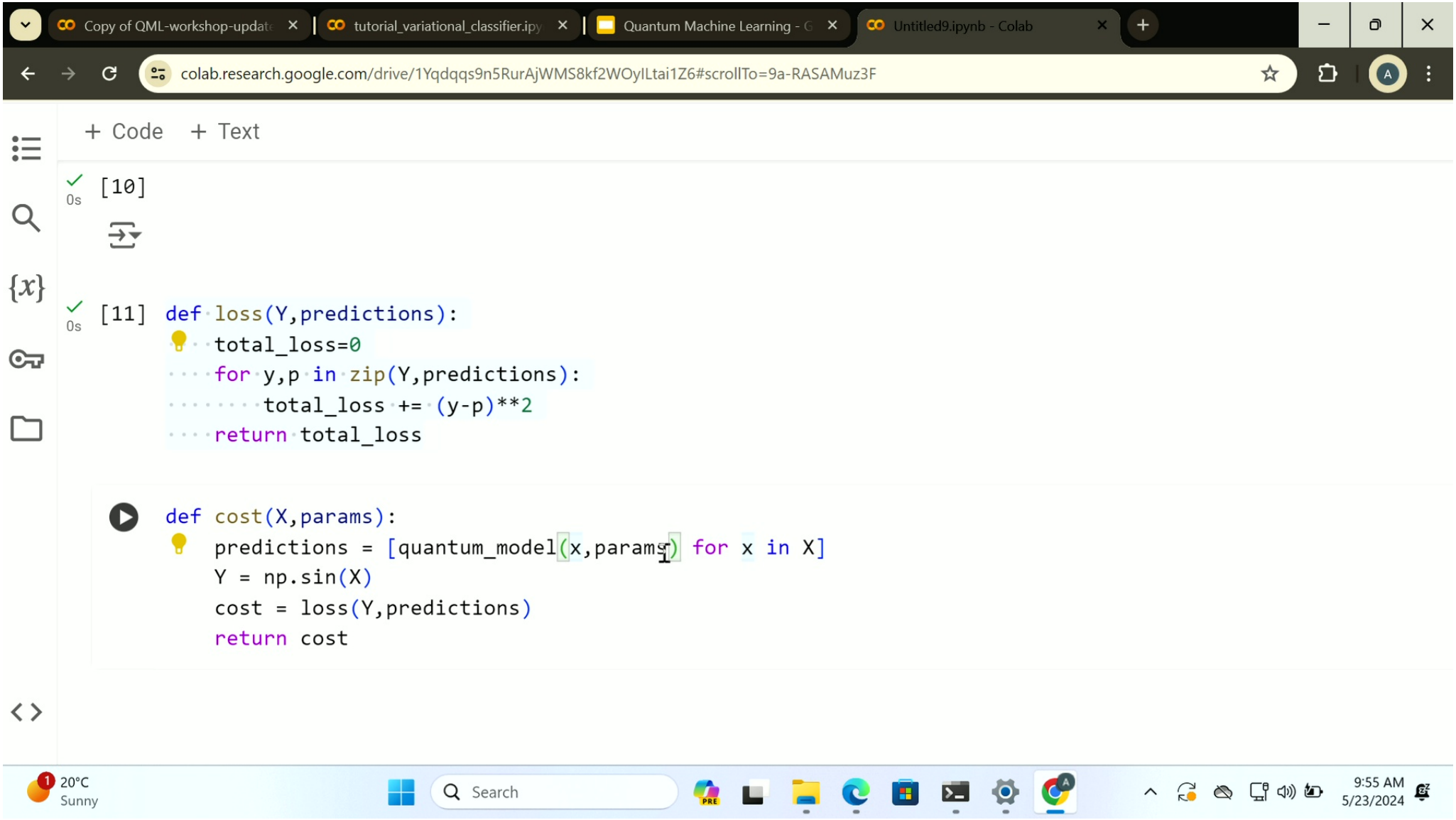
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def loss(Y,predictions):
total_loss=0
for y,p in zip(Y,predictions):
total_loss += (y-p)**2
return total_loss
def cost(X,params):
predictions = [quantum_model(x,params) for x in X]
Y = np.sin(X)
cost = loss(Y,predictions)
return cost
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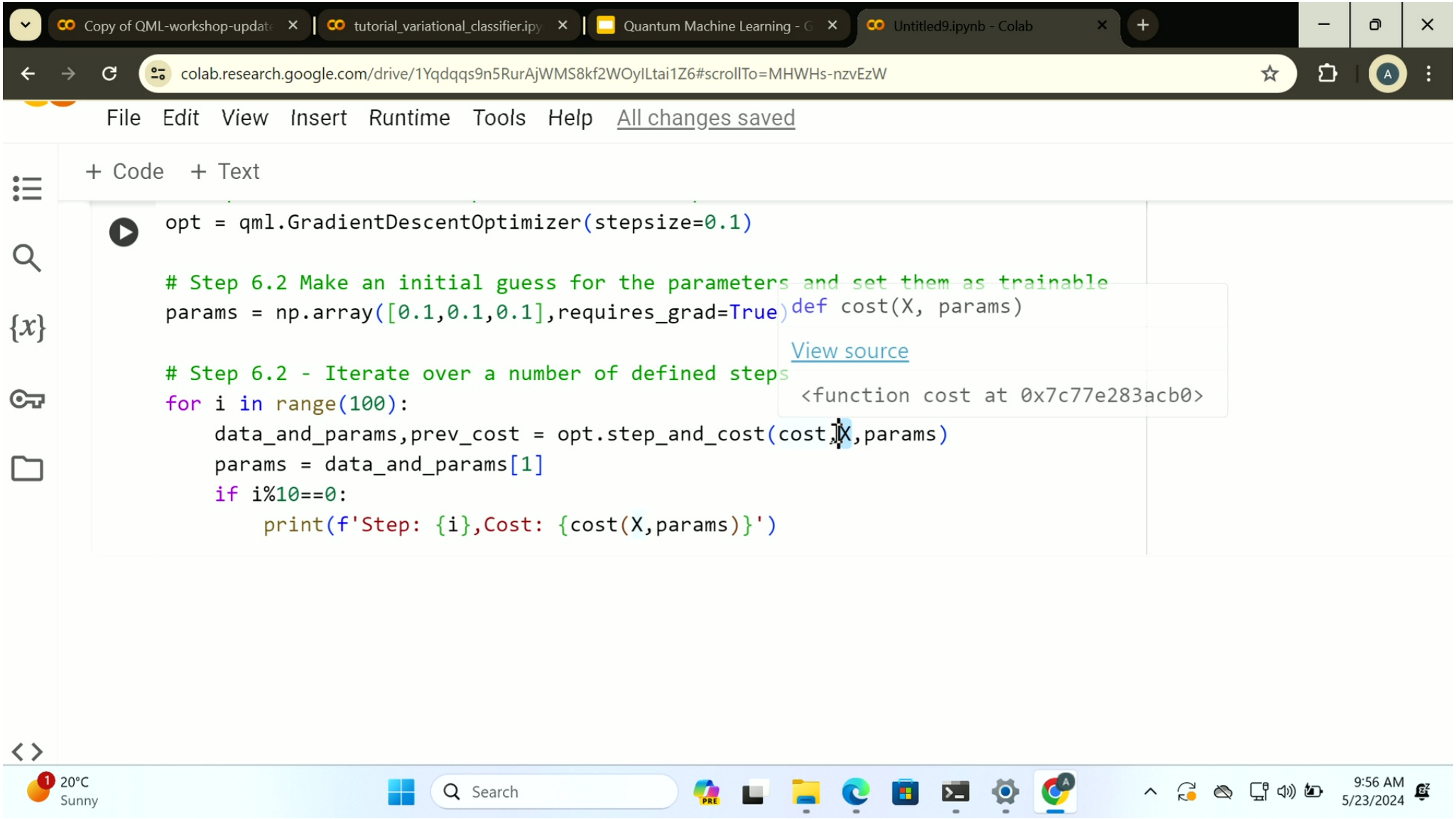
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opt = qml.GradientDescentOptimizer(stepsize=0.1)
# Step 6.2 Make an initial guess for the parameters and set them as trainable
params = np.array([0.1,0.1,0.1],requires_grad=True)
# Step 6.2 - Iterate over a number of defined steps
for i in range(100):
data_and_params,prev_cost = opt.step_and_cost(cost,X,params)
params = data_and_params[1]
if i%10==0:
print(f'Step: {i},Cost: {cost(X,params)}')
def cost(X, params)
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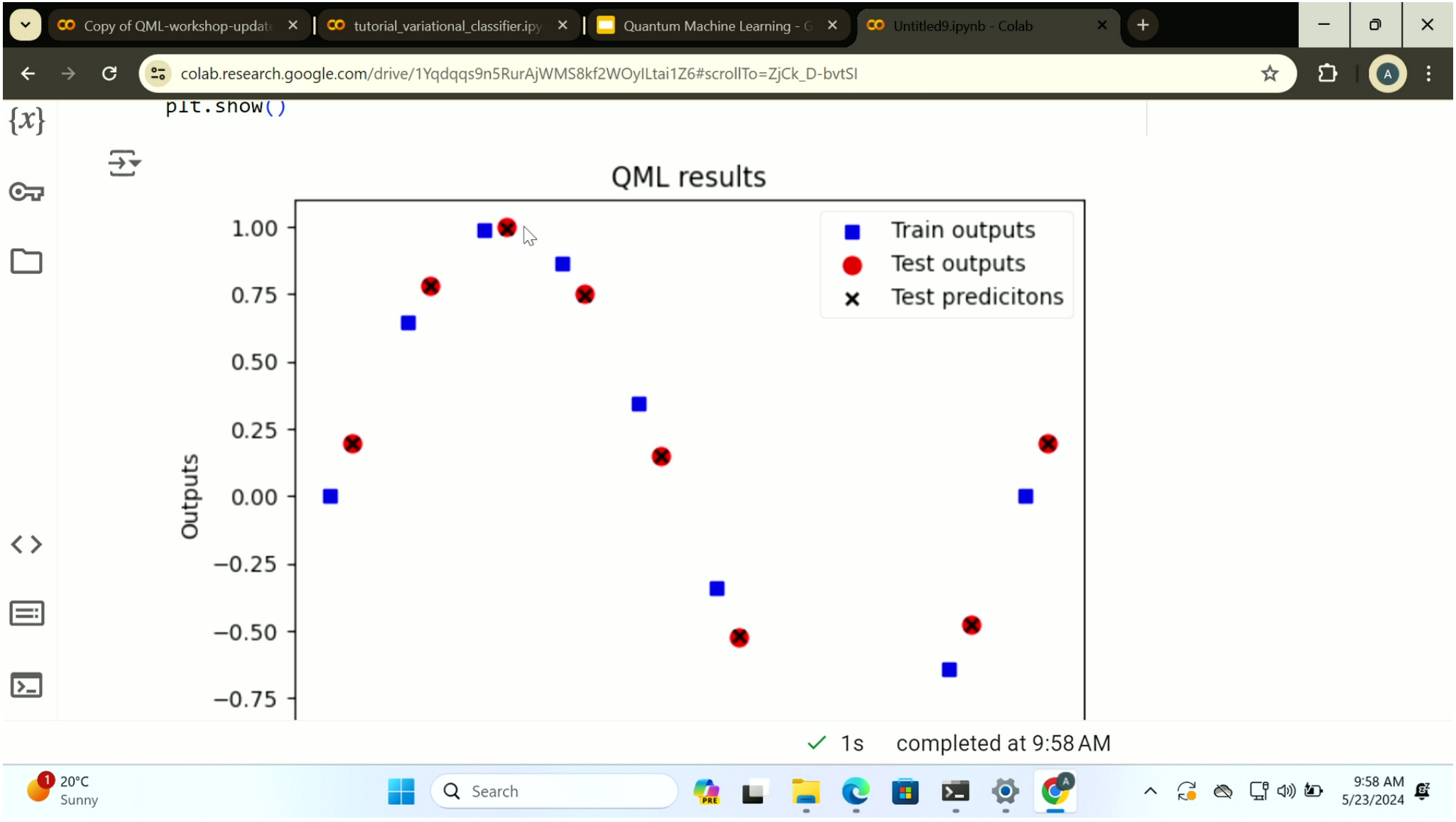
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plt.show()
QML results
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Test outputs
Test predicitons
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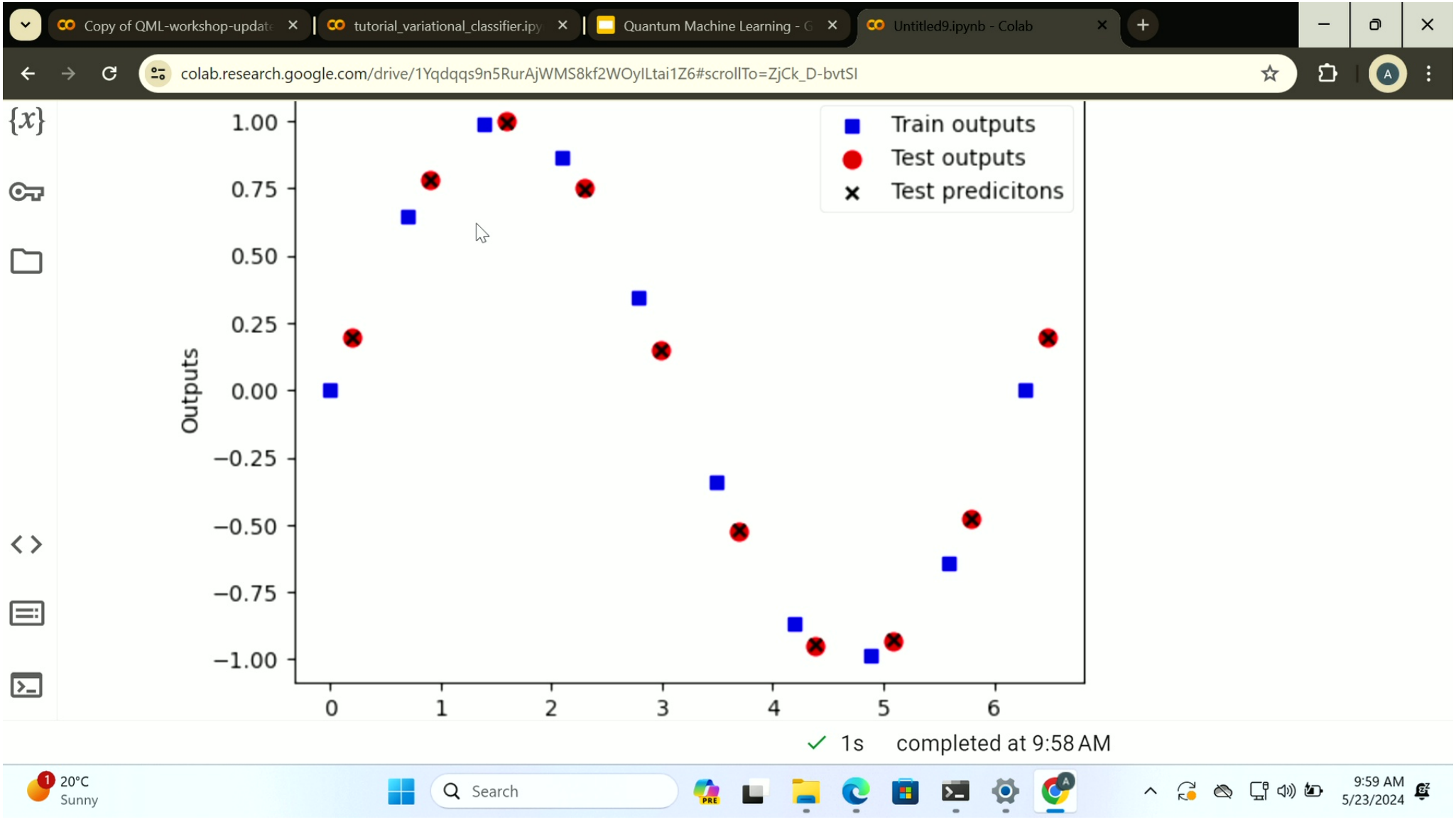
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Train outputs
Test outputs
Test predicitons
Outputs
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4 Angle embedding

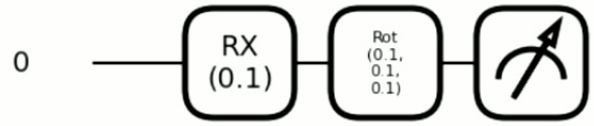
5 Amplitude Embedding

6 A simple QML model

7 Variational Quantum Classifier

A simple QML model

Let's do something super simple to warm up



RX here is the angle embedding. Rot is the model

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Variational Quantum Classifier (VQC)

Aim: Classify **discrete** data.

As per the Machine Learning supervised learning paradigm, we train with labelled data, and then extend to unknown data

In this example, we classify bit strings according to their parity.

$$f : x \in \{0,1\}^{\otimes n} \rightarrow y = \begin{cases} 1 \text{ if uneven number of 1's in } x \\ 0 \text{ else.} \end{cases}$$

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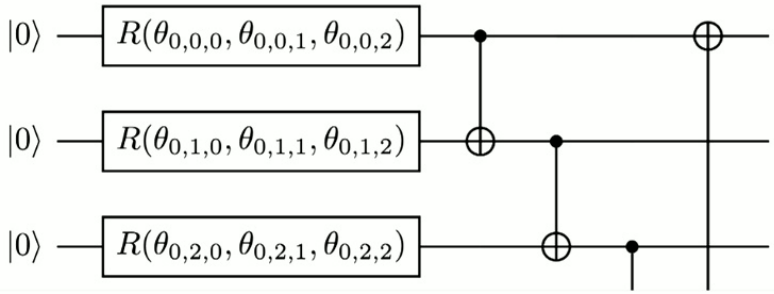
We then create a quantum device that will run our circuits.

```
[ ]  dev = qml.device("default.qubit")
```

Variational classifiers usually define a "layer" or "block", which is an elementary circuit architecture that gets repeated to build the full variational circuit.

Our circuit layer will use four qubits, or wires, and consists of an arbitrary rotation on every qubit, as well as a ring of CNOTs that entangles each qubit with its neighbour. Borrowing from machine learning, we call the parameters of the layer `weights`. Let's take a look on how this quantum circuit looks like:



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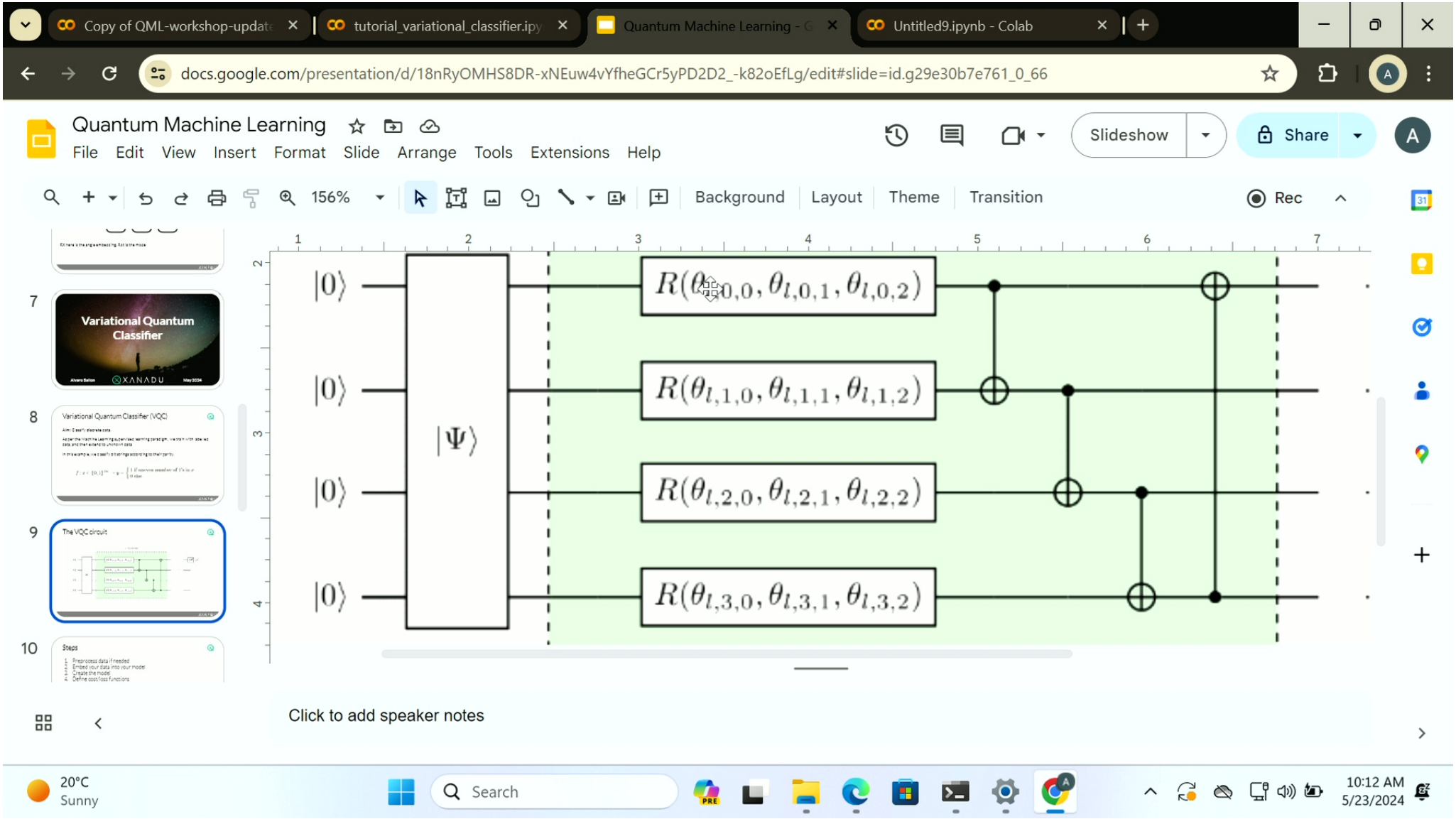
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Variational Quantum Classifier
8
Variational Quantum Classifier (VQC)
9
The VQC circuit
10
Steps
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$|0\rangle$
$|0\rangle$
$|0\rangle$
$|\Psi\rangle$
$R(\theta_{l,0,0}, \theta_{l,0,1}, \theta_{l,0,2})$
$R(\theta_{l,1,0}, \theta_{l,1,1}, \theta_{l,1,2})$
$R(\theta_{l,2,0}, \theta_{l,2,1}, \theta_{l,2,2})$
$R(\theta_{l,3,0}, \theta_{l,3,1}, \theta_{l,3,2})$
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```
[ ]
```

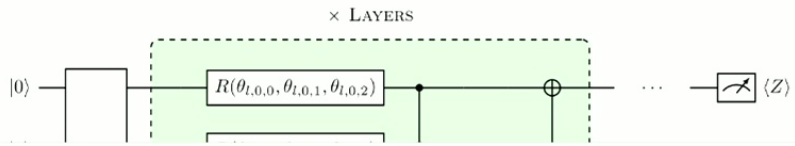
We also need a way to encode data inputs x into the circuit, so that the measured output depends on the inputs. In this first example, the inputs are bitstrings, which we encode into the state of the qubits. The quantum state ψ after state preparation is a computational basis state that has 1s where x has 1s, for example

$$x = 0101 \rightarrow |\psi\rangle = |0101\rangle.$$

The `pennylane.BasisState` function provided by PennyLane is made to do just this. It expects `x` to be a list of zeros and ones, i.e. `[0,1,0,1]`.

```
def state_preparation(x):
    qml.BasisState(x, wires=[0, 1, 2, 3])
```

Now we define the variational quantum circuit as this state preparation routine, followed by a repetition of the layer structure. This circuit should look like this:



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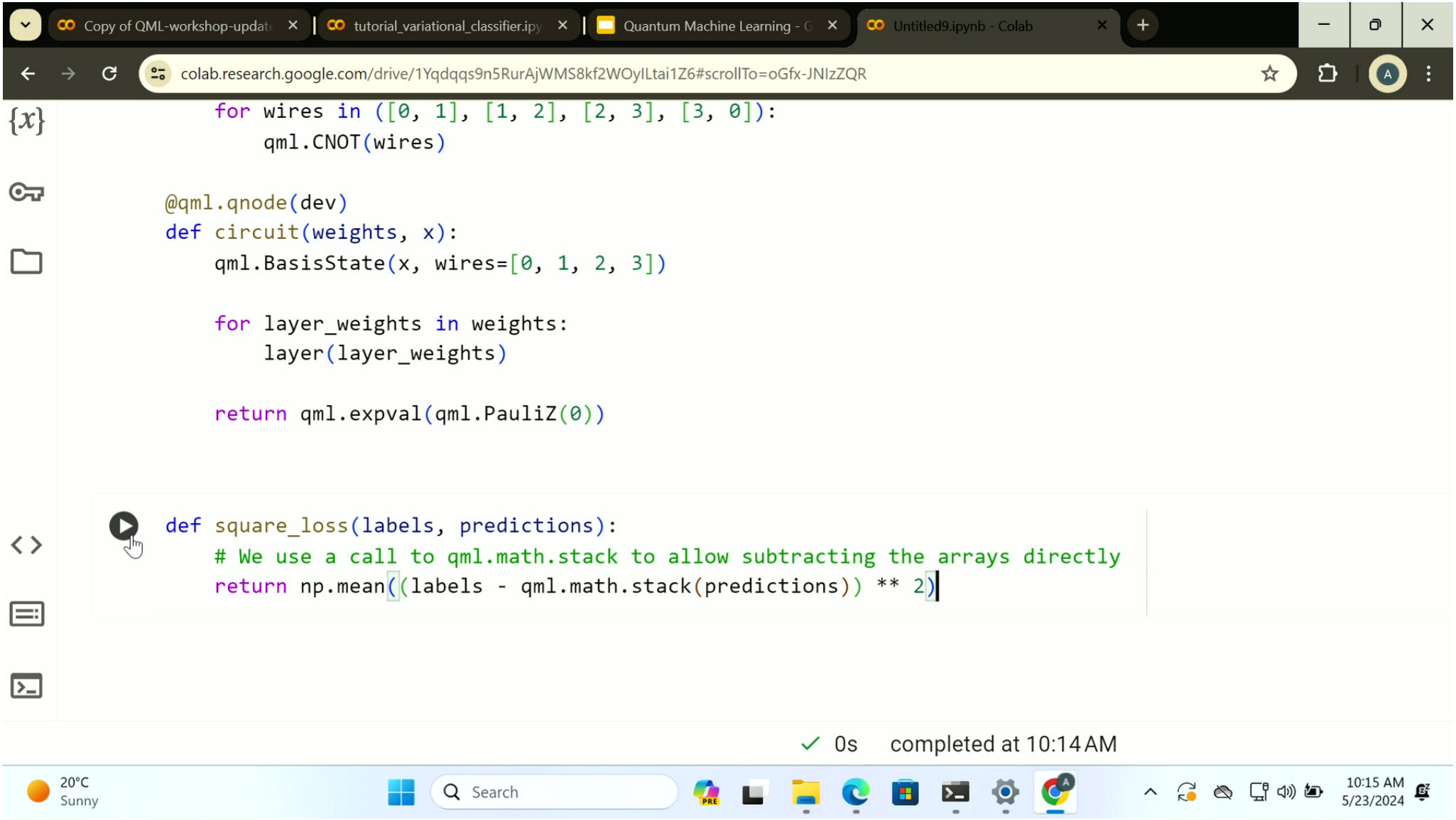
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for wires in ([0, 1], [1, 2], [2, 3], [3, 0]):
qml.CNOT(wires)
@qml.qnode(dev)
def circuit(weights, x):
qml.BasisState(x, wires=[0, 1, 2, 3])
for layer_weights in weights:
layer(layer_weights)
return qml.expval(qml.PauliZ(0))
def square_loss(labels, predictions):
# We use a call to qml.math.stack to allow subtracting the arrays directly
return np.mean((labels - qml.math.stack(predictions)) ** 2)
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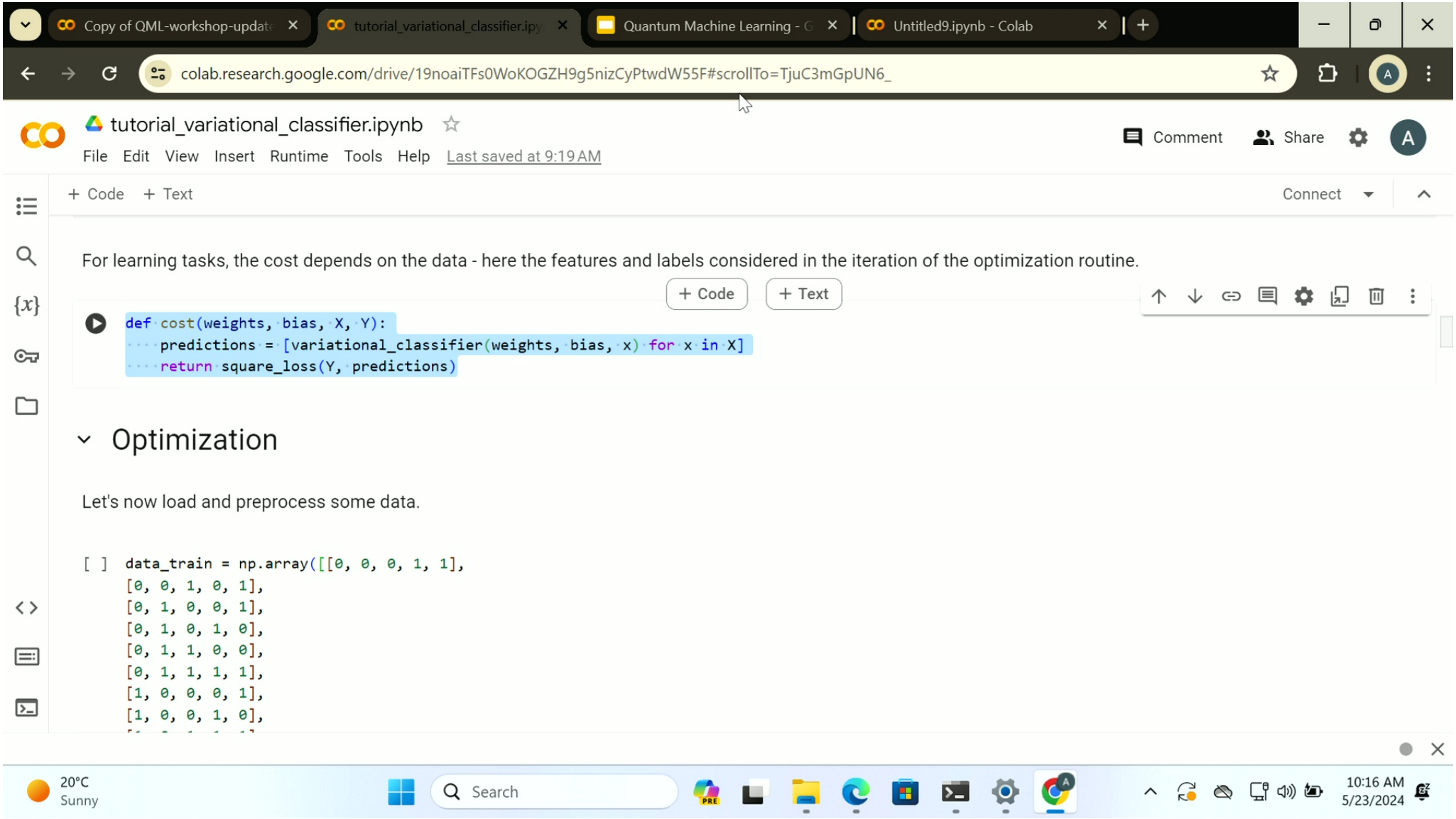
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For learning tasks, the cost depends on the data - here the features and labels considered in the iteration of the optimization routine.
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def cost(weights, bias, X, Y):
predictions = [variational_classifier(weights, bias, x) for x in X]
return square_loss(Y, predictions)
Optimization
Let's now load and preprocess some data.
[ ] data_train = np.array([[0, 0, 0, 1, 1],
[0, 0, 1, 0, 1],
[0, 1, 0, 0, 1],
[0, 1, 0, 1, 0],
[0, 1, 1, 0, 0],
[0, 1, 1, 1, 1],
[1, 0, 0, 0, 1],
[1, 0, 0, 1, 0],
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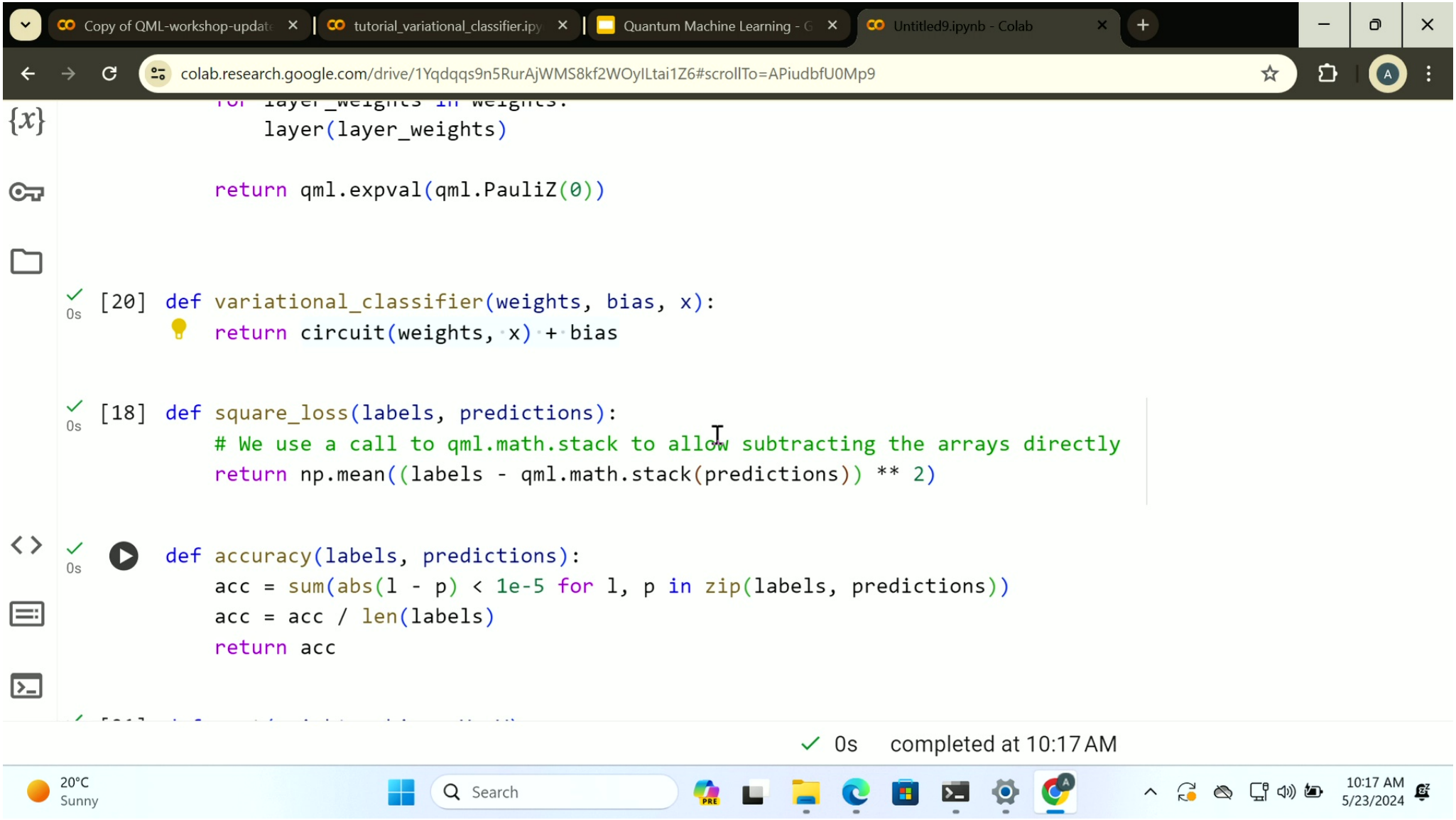
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layer(layer_weights)
return qml.expval(qml.PauliZ(0))
[20] def variational_classifier(weights, bias, x):
return circuit(weights, x) + bias
[18] def square_loss(labels, predictions):
We use a call to qml.math.stack to allow subtracting the arrays directly
return np.mean((labels - qml.math.stack(predictions)) ** 2)
def accuracy(labels, predictions):
acc = sum(abs(l - p) < 1e-5 for l, p in zip(labels, predictions))
acc = acc / len(labels)
return acc
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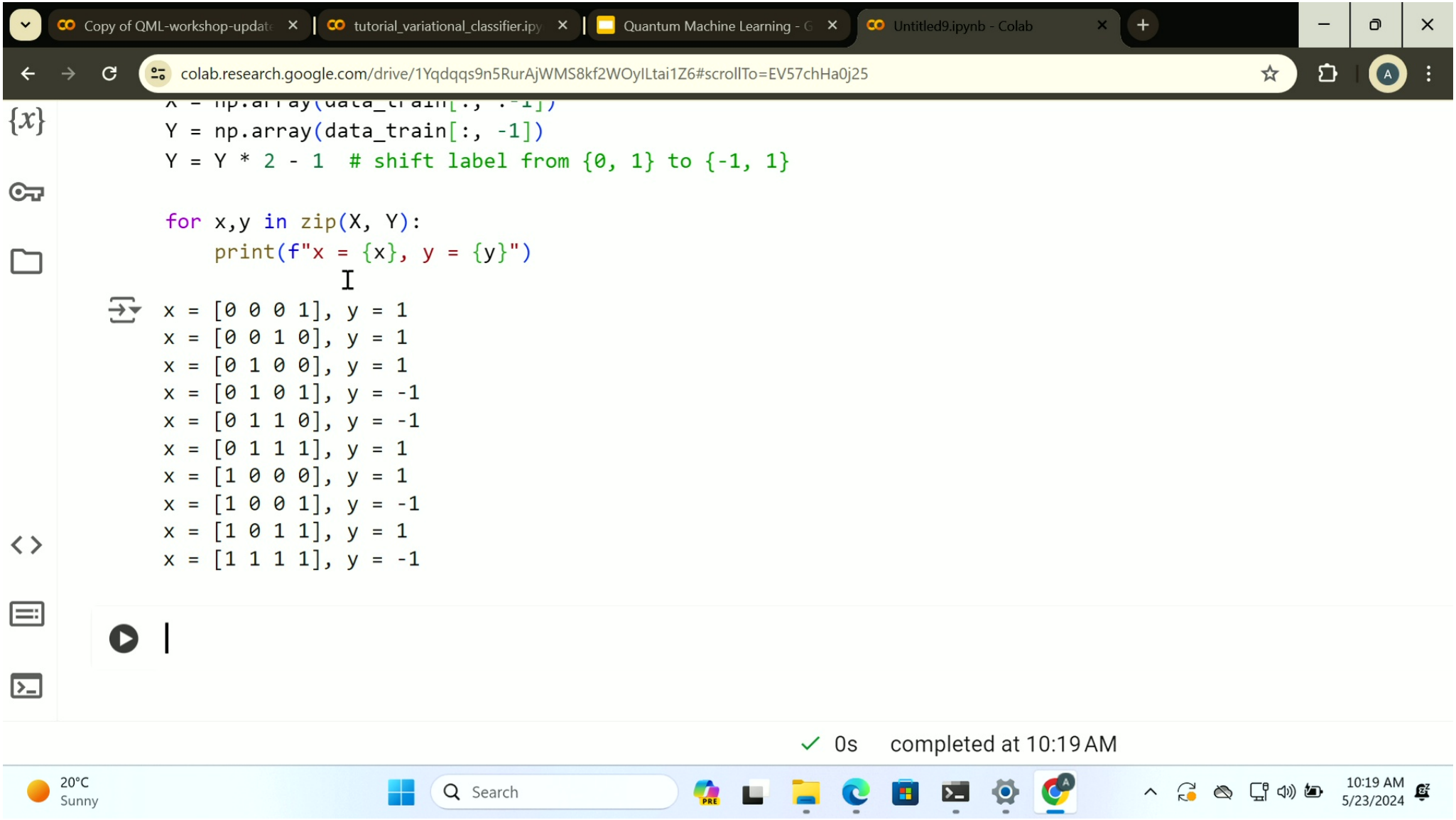
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Y = np.array(data_train[:, -1])
Y = Y * 2 - 1 # shift label from {0, 1} to {-1, 1}
for x,y in zip(X, Y):
print(f"x = {x}, y = {y}")
x = [0 0 0 1], y = 1
x = [0 0 1 0], y = 1
x = [0 1 0 0], y = 1
x = [0 1 0 1], y = -1
x = [0 1 1 0], y = -1
x = [0 1 1 1], y = 1
x = [1 0 0 0], y = 1
x = [1 0 0 1], y = -1
x = [1 0 1 1], y = 1
x = [1 1 1 1], y = -1
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tutorial_variational_classifier.ipynb

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```
import pennylane as qml
from pennylane import numpy as np
from pennylane.optimize import NesterovMomentumOptimizer
```

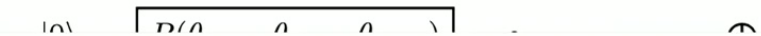
Quantum and classical nodes

We then create a quantum device that will run our circuits.

```
[ ]  dev = qml.device("default.qubit")
```

Variational classifiers usually define a "layer" or "block", which is an elementary circuit architecture that gets repeated to build the full variational circuit.

Our circuit layer will use four qubits, or wires, and consists of an arbitrary rotation on every qubit, as well as a ring of CNOTs that entangles each qubit with its neighbour. Borrowing from machine learning, we call the parameters of the layer `weights`. Let's take a look on how this quantum circuit looks like:



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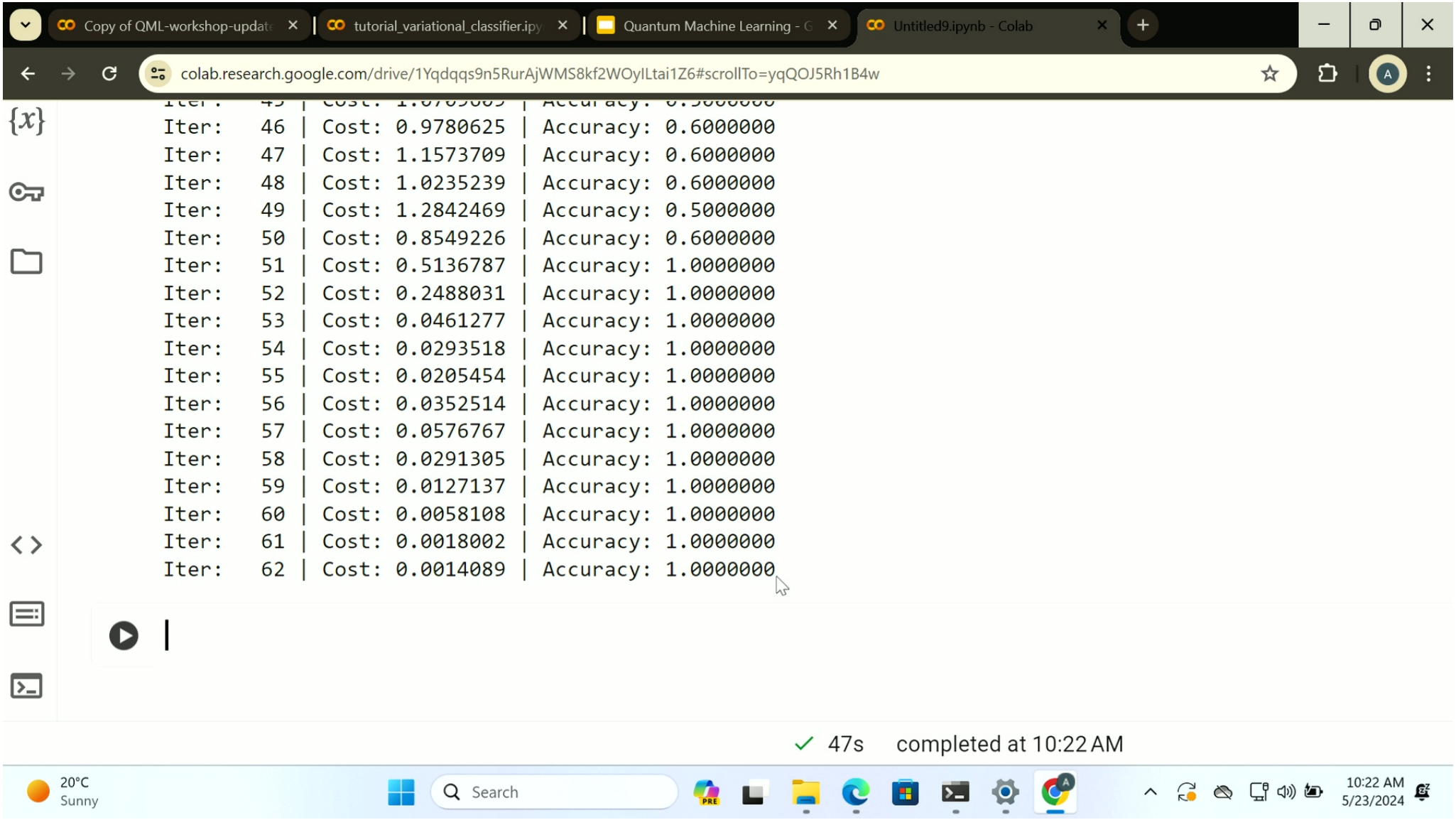
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colab.research.google.com/drive/1Yqdqqs9n5RurAjWMS8kf2WOyILtai1Z6#scrollTo=yqQOJ5Rh1B4w
Iter: 46 | Cost: 0.9780625 | Accuracy: 0.6000000
Iter: 47 | Cost: 1.1573709 | Accuracy: 0.6000000
Iter: 48 | Cost: 1.0235239 | Accuracy: 0.6000000
Iter: 49 | Cost: 1.2842469 | Accuracy: 0.5000000
Iter: 50 | Cost: 0.8549226 | Accuracy: 0.6000000
Iter: 51 | Cost: 0.5136787 | Accuracy: 1.0000000
Iter: 52 | Cost: 0.2488031 | Accuracy: 1.0000000
Iter: 53 | Cost: 0.0461277 | Accuracy: 1.0000000
Iter: 54 | Cost: 0.0293518 | Accuracy: 1.0000000
Iter: 55 | Cost: 0.0205454 | Accuracy: 1.0000000
Iter: 56 | Cost: 0.0352514 | Accuracy: 1.0000000
Iter: 57 | Cost: 0.0576767 | Accuracy: 1.0000000
Iter: 58 | Cost: 0.0291305 | Accuracy: 1.0000000
Iter: 59 | Cost: 0.0127137 | Accuracy: 1.0000000
Iter: 60 | Cost: 0.0058108 | Accuracy: 1.0000000
Iter: 61 | Cost: 0.0018002 | Accuracy: 1.0000000
Iter: 62 | Cost: 0.0014089 | Accuracy: 1.0000000
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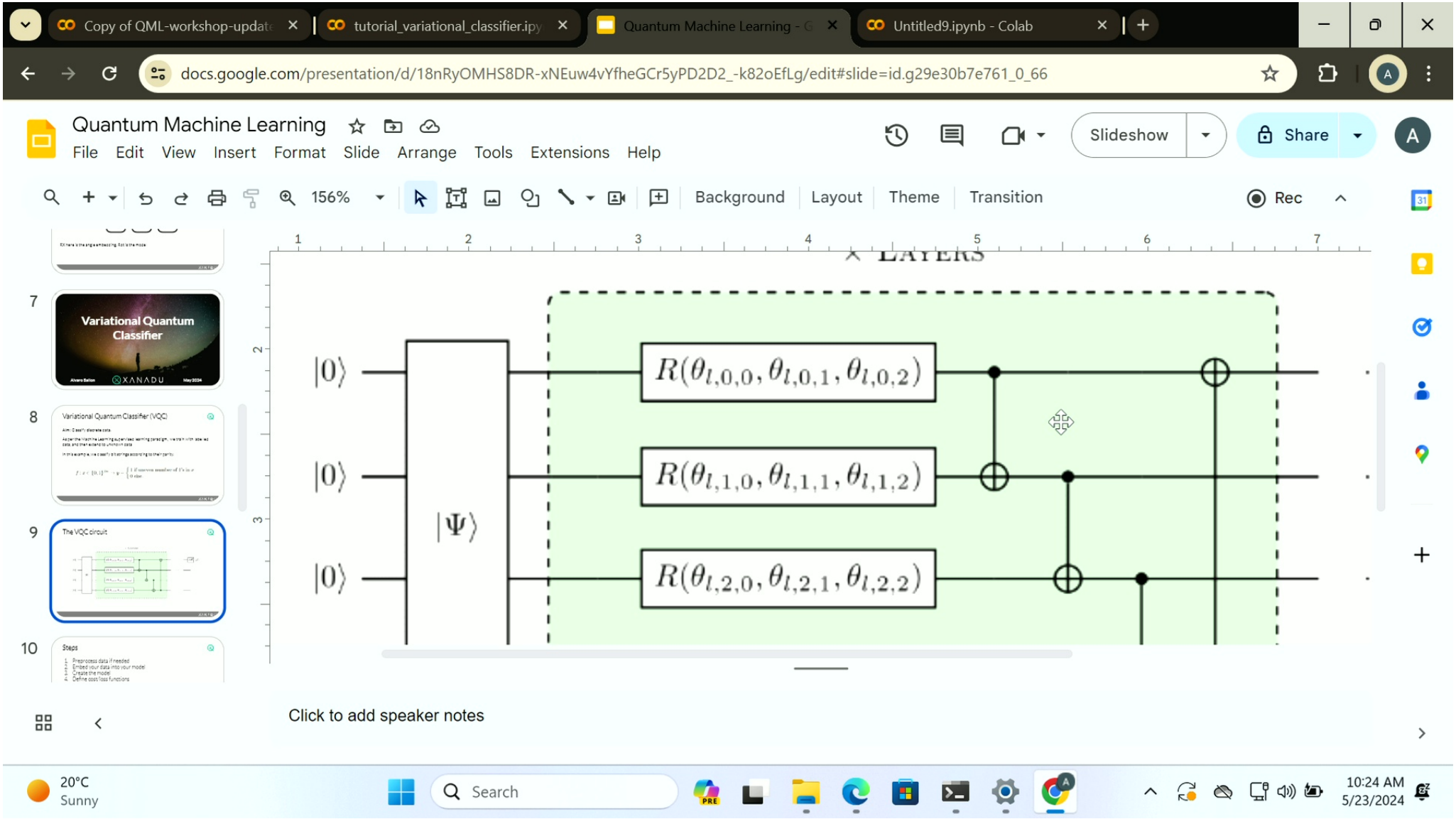
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Rec
7
Variational Quantum Classifier
8
Variational Quantum Classifier (VQC)
9
The VQC circuit
10
Steps
$|0\rangle$
$|0\rangle$
$|0\rangle$
$|\Psi\rangle$
$R(\theta_{l,0,0}, \theta_{l,0,1}, \theta_{l,0,2})$
$R(\theta_{l,1,0}, \theta_{l,1,1}, \theta_{l,1,2})$
$R(\theta_{l,2,0}, \theta_{l,2,1}, \theta_{l,2,2})$
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```
for x,y,p in zip(X_test, Y_test, predictions_test):
    print(f"x = {x}, y = {y}, pred={p}")

acc_test = accuracy(Y_test, predictions_test)
print("Accuracy on unseen data:", acc_test)
```

```
x = [0 0 0 0], y = -1, pred=-1.0
x = [0 0 1 1], y = -1, pred=-1.0
x = [1 0 1 0], y = -1, pred=-1.0
x = [1 1 1 0], y = 1, pred=1.0
x = [1 1 0 0], y = -1, pred=-1.0
x = [1 1 0 1], y = 1, pred=1.0
Accuracy on unseen data: 1.0
```

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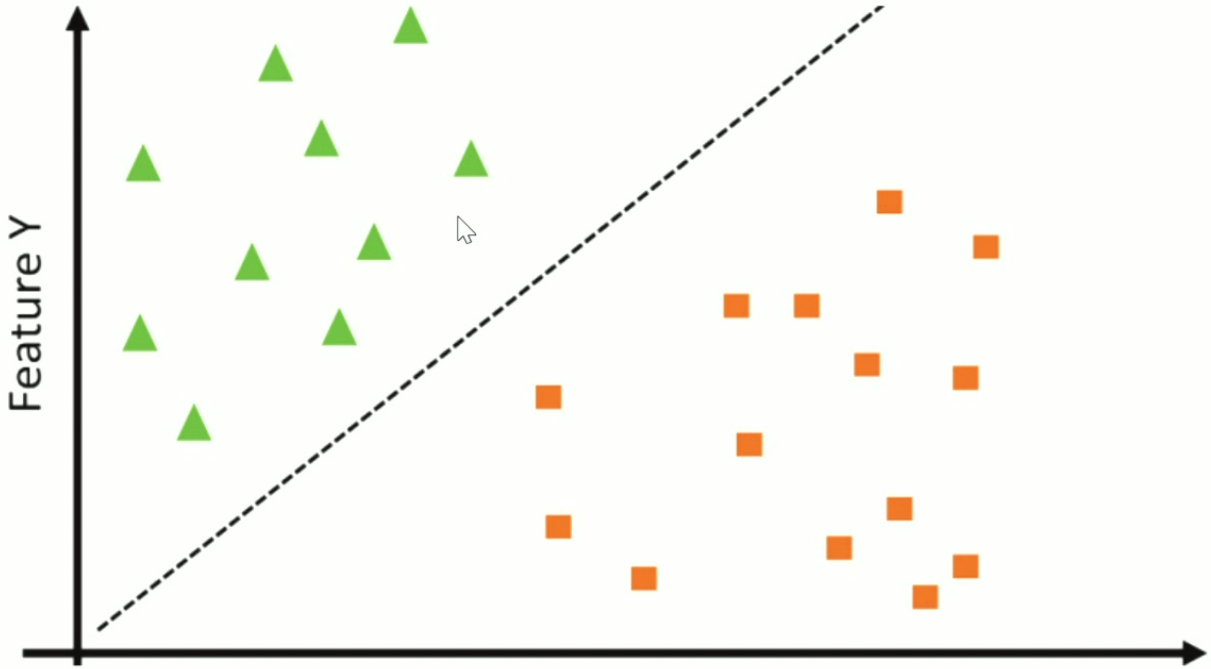
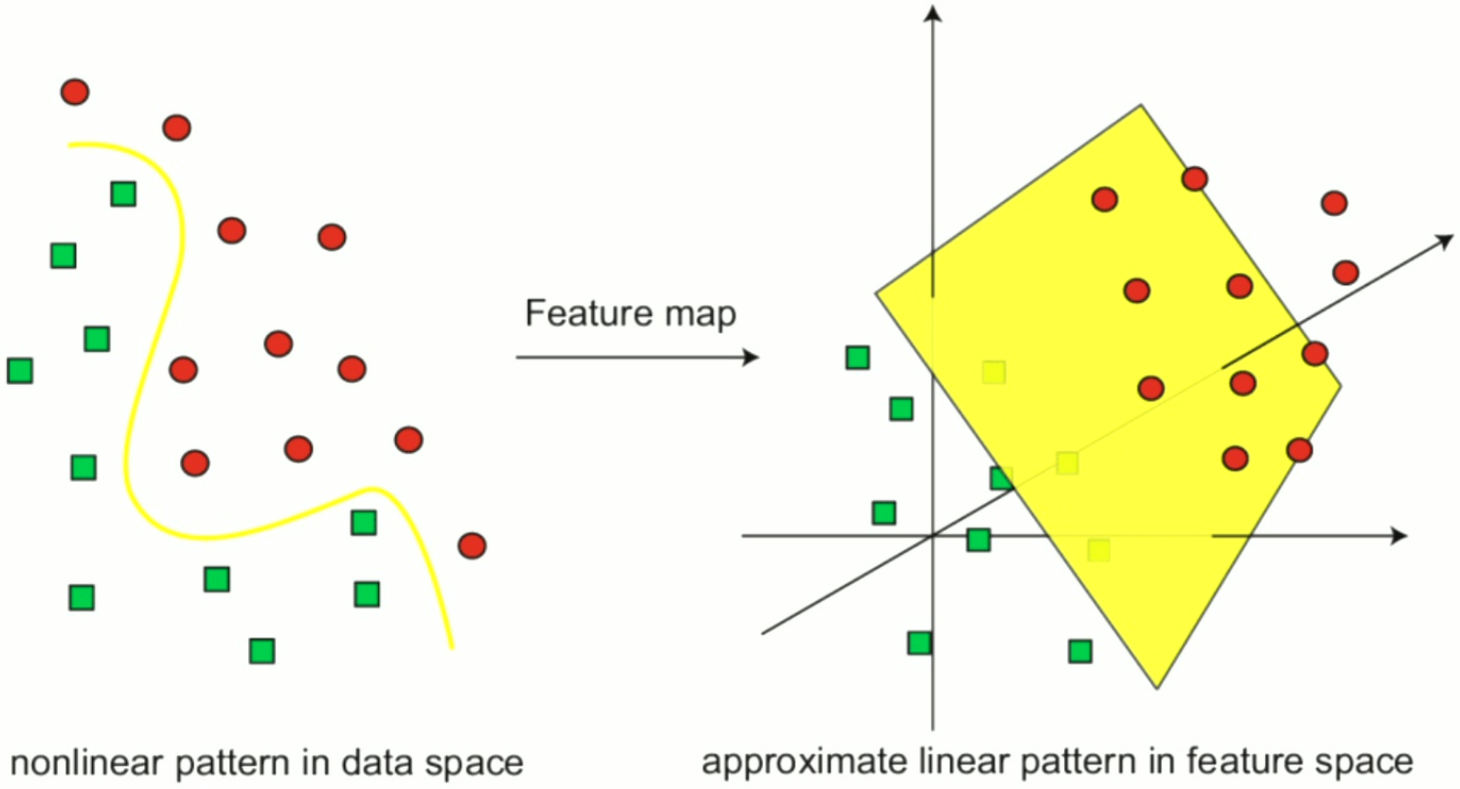
Support vector machine



Feature map


Feature map
nonlinear pattern in data space
approximate linear pattern in feature space

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PI_QML_Tutorial_2.ipynb

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(iv) The way an SVM with a custom kernel is implemented in scikit-learn requires us to pass a function that computes a matrix of kernel evaluations for samples in two different datasets A, B. If A=B, this is the Gram matrix. **Complete the `kernel_matrix` function below to build this matrix of kernel evaluations.**

```
def kernel_matrix(A, B):
    """Compute the matrix whose entries are the kernel
       evaluated on pairwise data from sets A and B."""
    return # Return the kernel matrix
```

(v) Training the SVM optimizes internal parameters that basically weigh kernel functions. It is a breeze in scikit-learn, which is designed as a high-level machine learning library. **Run the cell below to fit the Support Vector Machine**. (I'm aware this is kind of black-boxy, but if you're interested in how this work, do read up on *normal* Machine Learning. You will find that one is very black-boxy too though).

```
[ ]  svm = SVC(kernel=kernel_matrix).fit(X_train, y_train)
```

Now run the cell below to compute the accuracy on the test set

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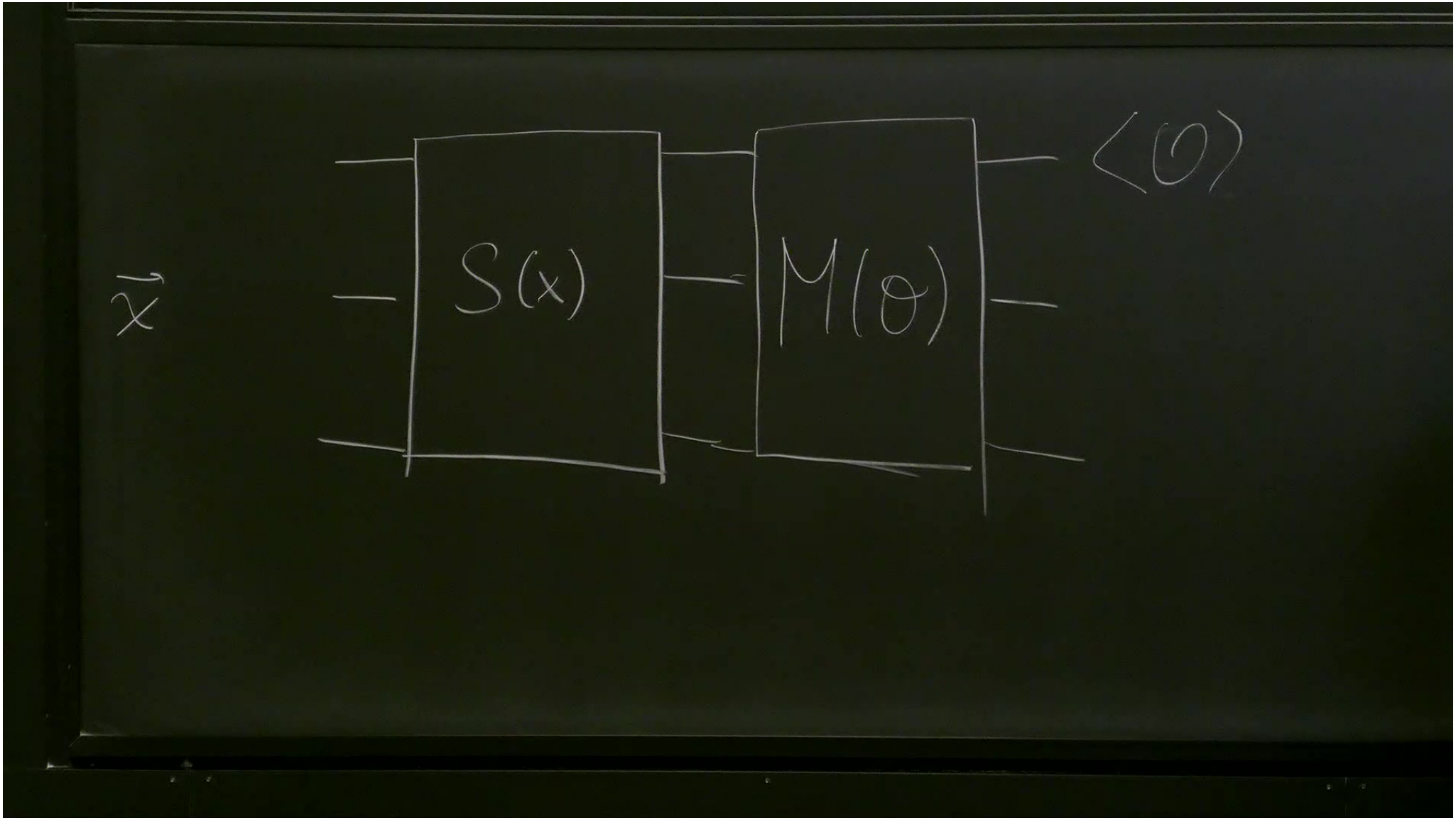
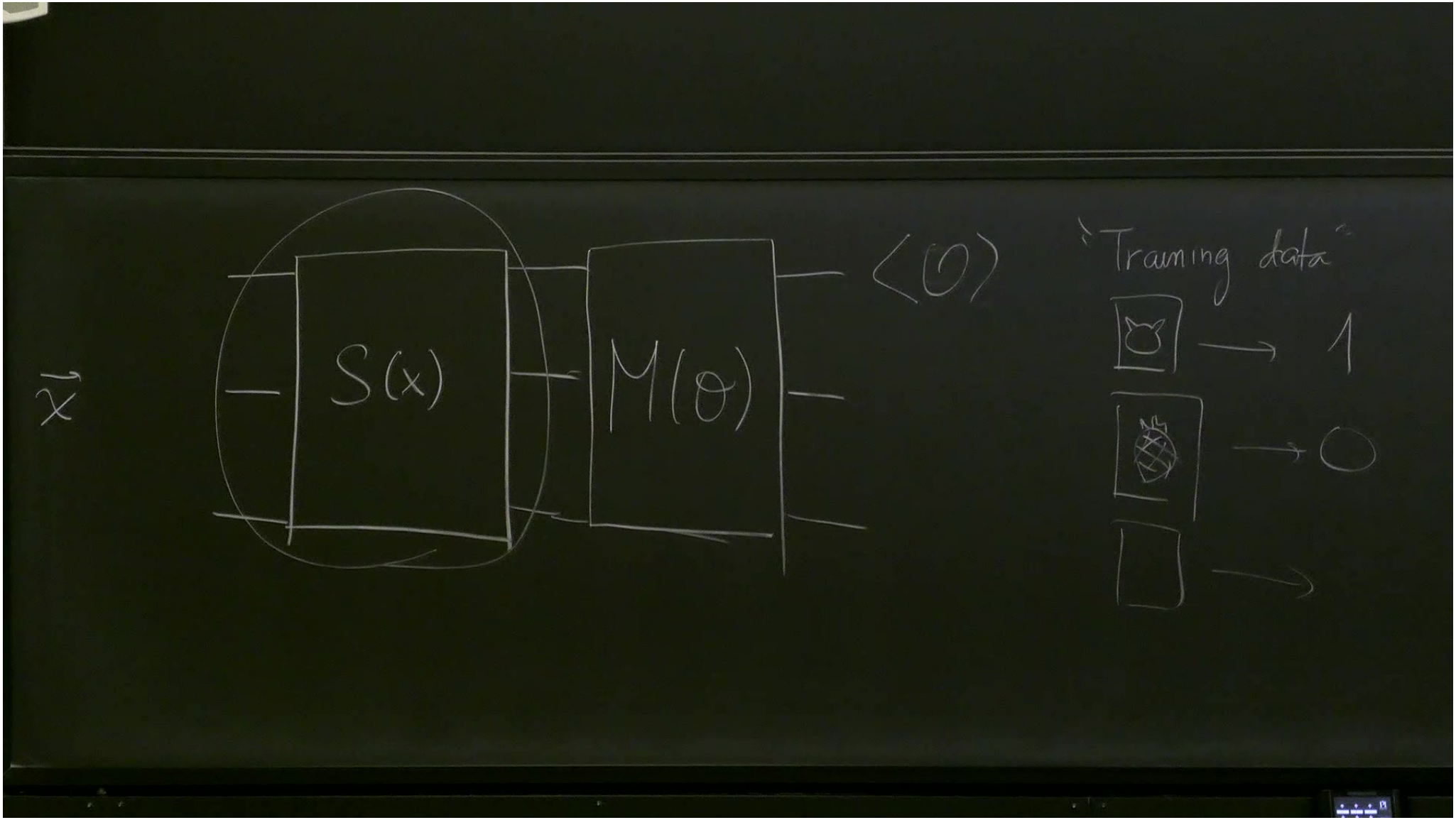
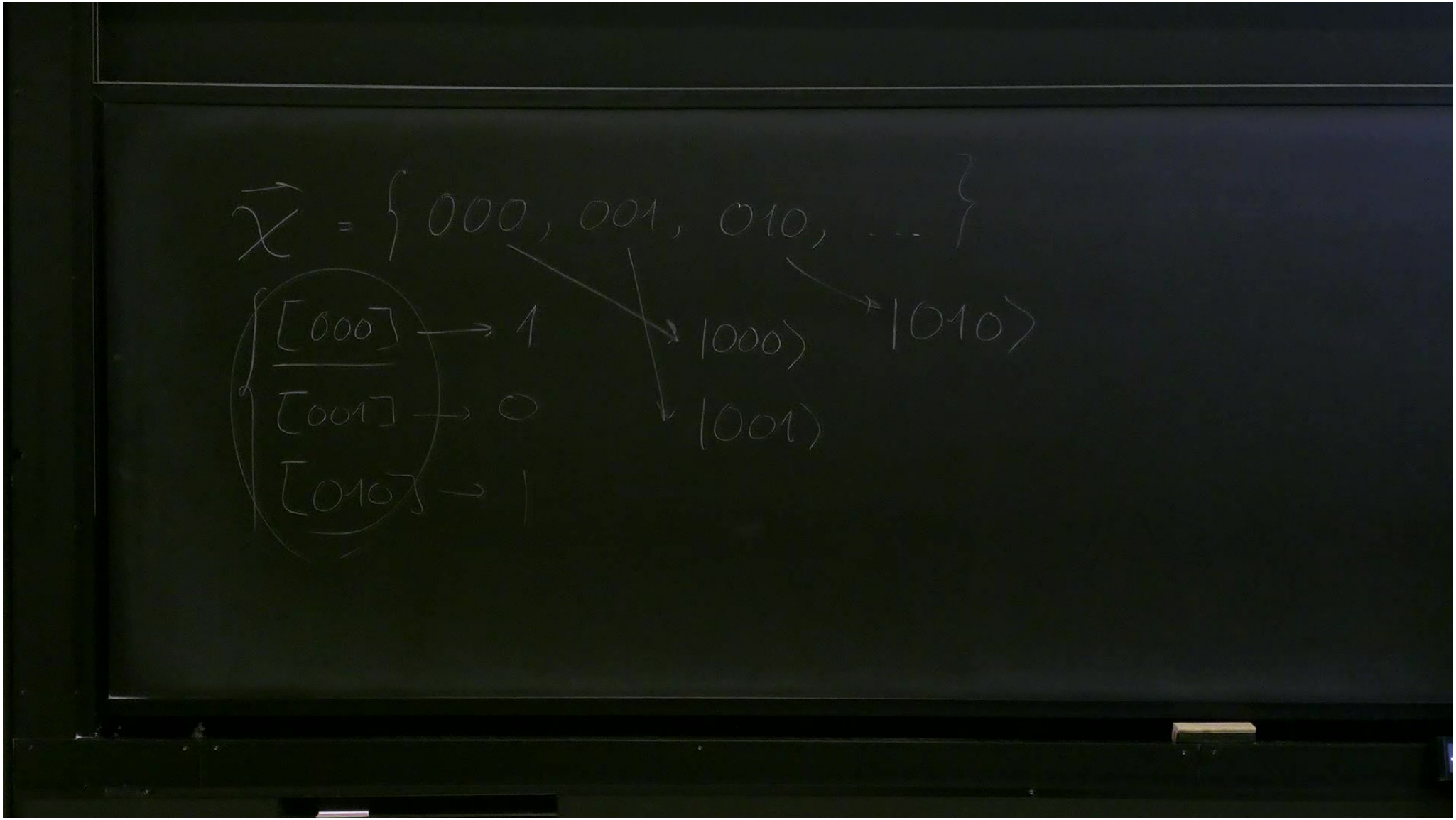
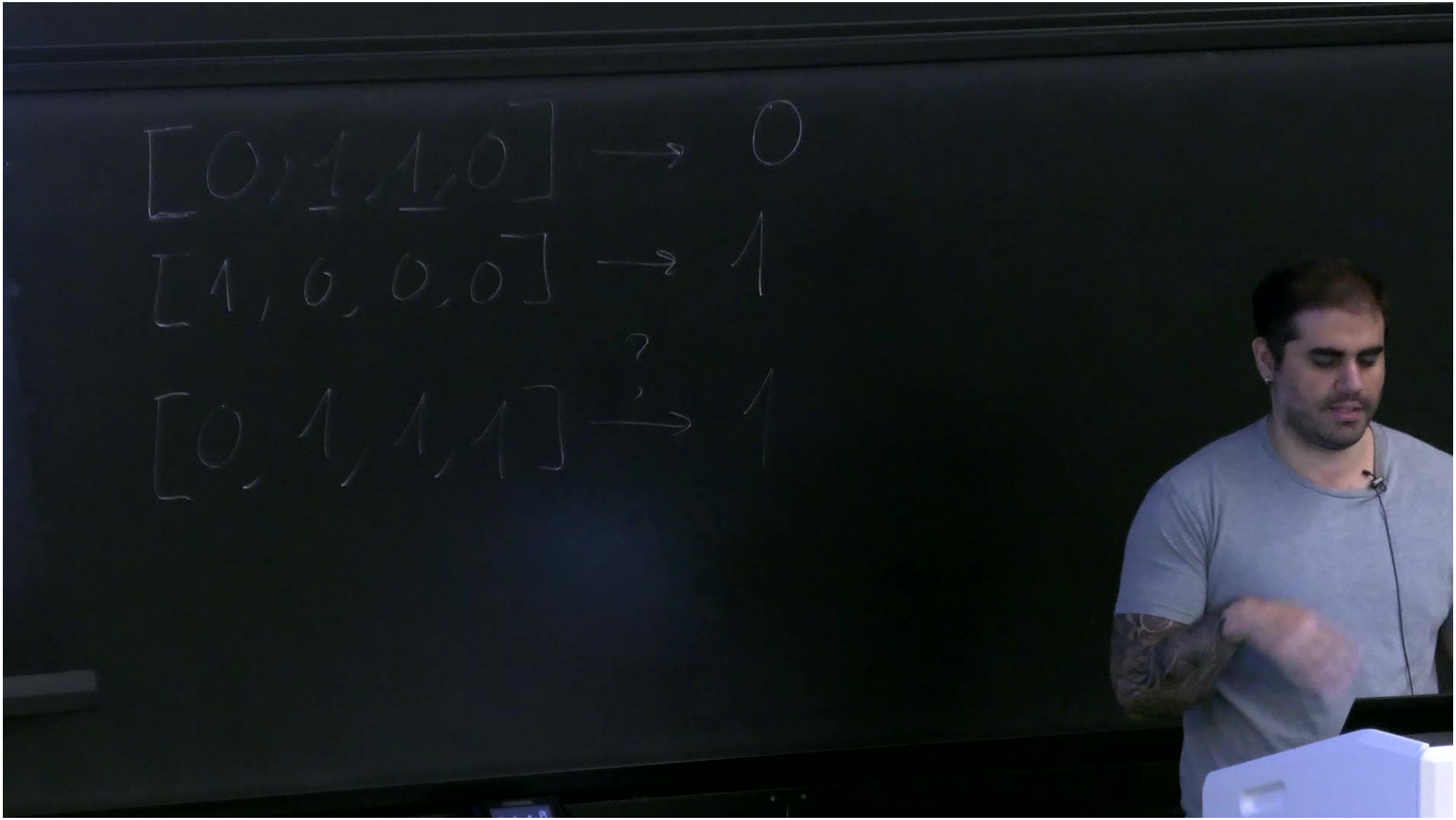
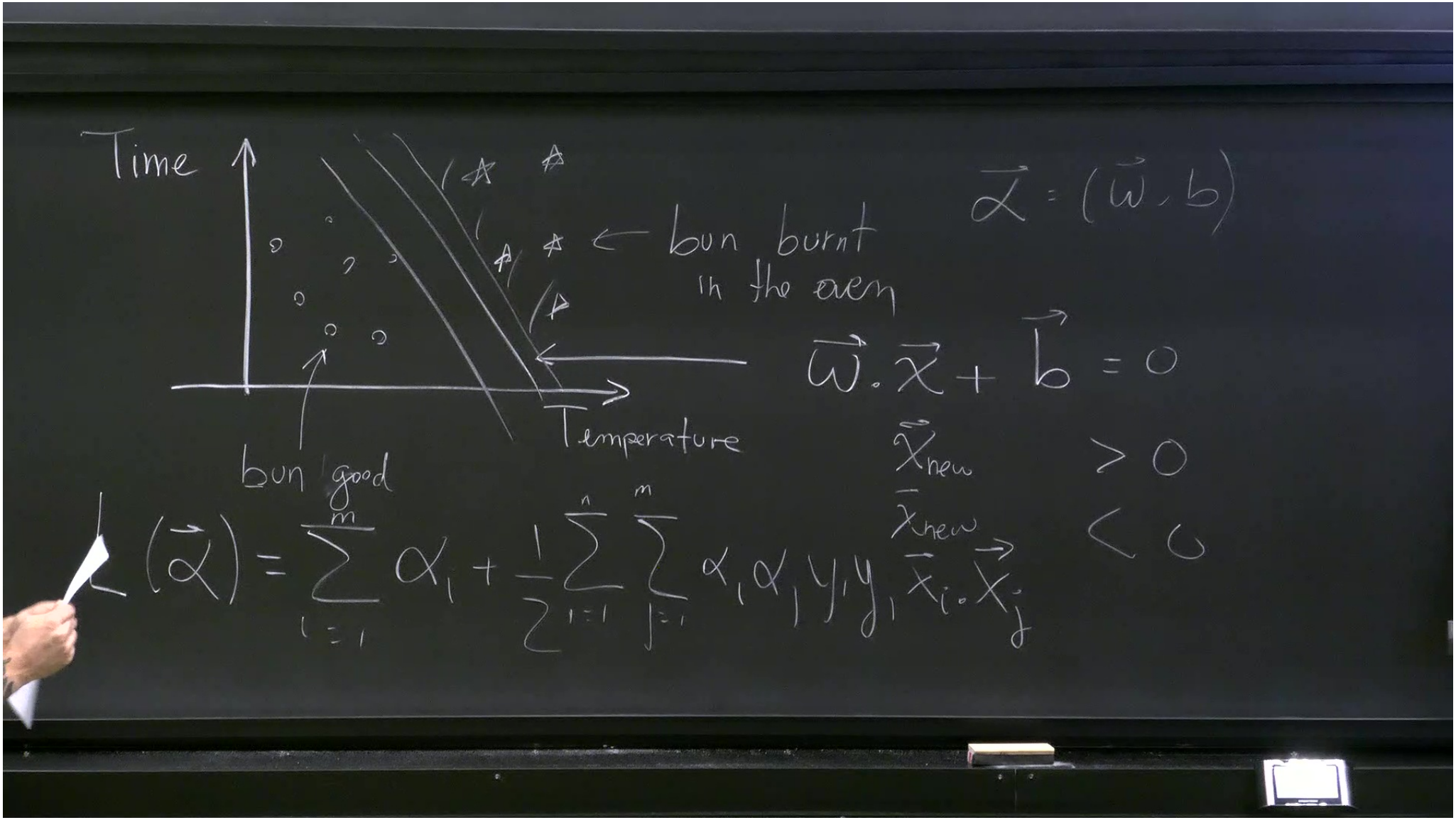
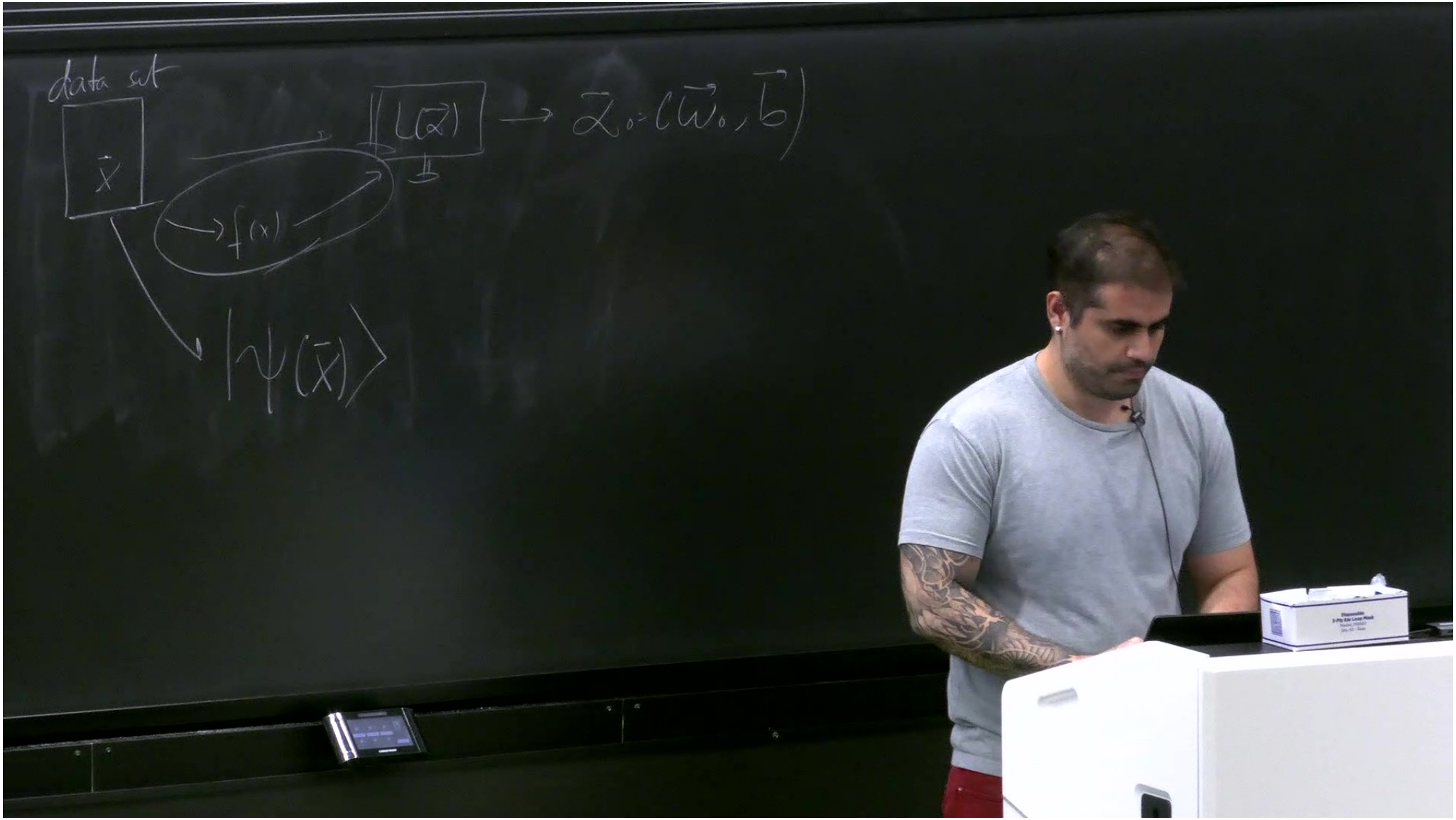

$\vec{x}$
S(x)
M(θ)
⟨O⟩


$\vec{x}$
S(x)
M(θ)
<O>
"Traning data"
1
0


$\vec{x} = \{000, 001, 010, \ldots\}$
[000] → 1
[001] → 0
[010] → 1
|000⟩
|001⟩
|010⟩


[0,1,1,0] → 0
[1,0,0,0] → 1
[0,1,1,1] → ? 1


Time
bun burnt in the oven
Temperature
bun good
$\vec{\alpha} = (\vec{w}, b)$
$\vec{w} \cdot \vec{x} + b = 0$
$\vec{x}_{new} > 0$
$\vec{x}_{new} < 0$
$L(\vec{\alpha}) = \sum_{i=1}^{m} \alpha_i + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \vec{x}_i \cdot \vec{x}_j$


data set
$\vec{x}$
$L(\vec{x})$
$\vec{z}_0 = (\vec{w}_0, \vec{b})$
$f(x)$
$|\psi(\vec{x})\rangle$