Lecture

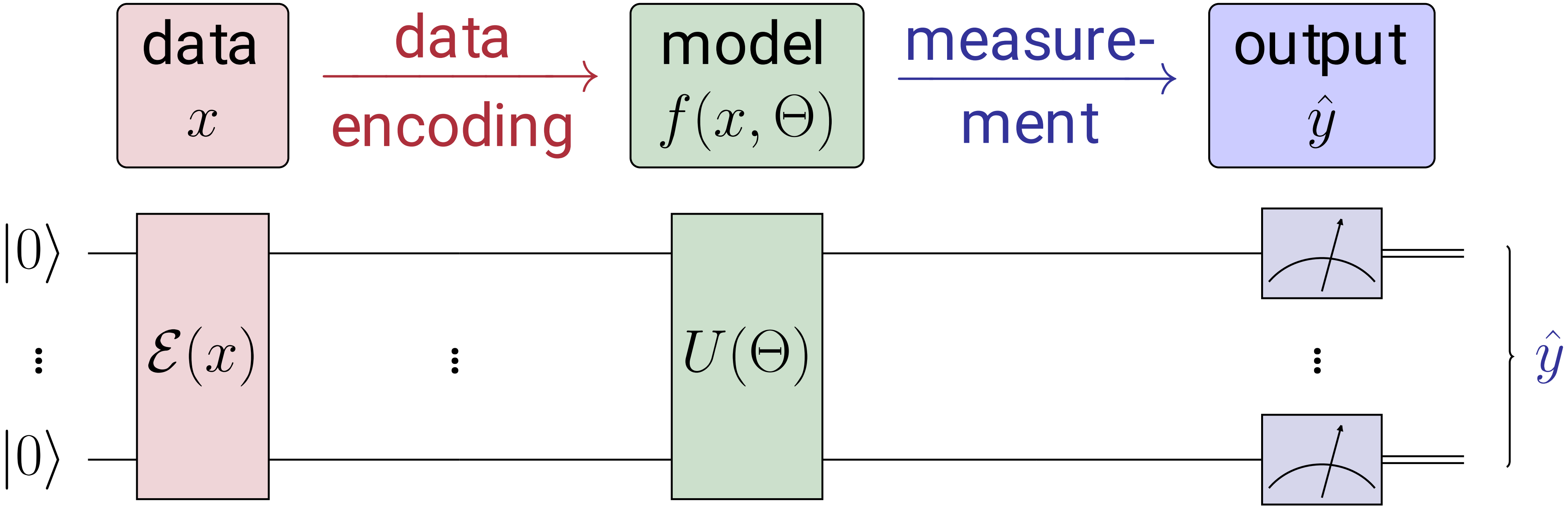
Quantum Computing

(CS5070)

Quantum Machine Learning: Optimization

Professor Dr. rer. nat. habil. Sven Groppe
https://www.ifis.uni-luebeck.de/index.php?id=groppe

Quantum Model



1. Encode classical data x into a quantum state $|\psi(x)\rangle = \mathcal{E}(x)|0\rangle$
2. Apply a parametrized unitary $|U_\psi(x, \Theta)\rangle = U(\Theta)|\psi(x)\rangle$
3. Measure classical data $z = (z_1, \dots, z_n)$
4. Do classical post-processing to get prediction $\hat{y} = g(z)$
5. Use **optimization techniques** (like gradient descent) to optimize Θ

Supervised Learning: Cost

- Classify whether the picture contains a cat or dog based on certain features of animals:
  3. For the t samples in the training dataset compute cost with
     a. Mean Squared Error (MSE): $C_{MSE} = \frac{1}{t} \cdot \sum_{i=1}^{t} (\hat{y}_1 - y_i)^2$
     b. Binary classification (e.g., "cat" or "dog") using cross-entropy loss:

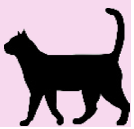
$y_i \in \{0, 1\}$, i.e., "true" label or two classes like **"cat"** and **"dog"**

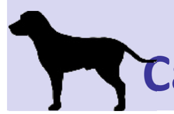
Probability for $y_i = 1$ (e.g., "cat")

$$C_{CE}(\Theta, (y_1, \ldots, y_t)) = -\frac{1}{t} \sum_{i=1}^{t} \left(y_i \cdot log(f(x_i, \Theta)) + (1 - y_i) \cdot log(1 - f(x_i, \Theta)) \right)$$

Probability for $y_i = 0$ (e.g., "dog")

Case $y_i = 1$, e.g. "cat"



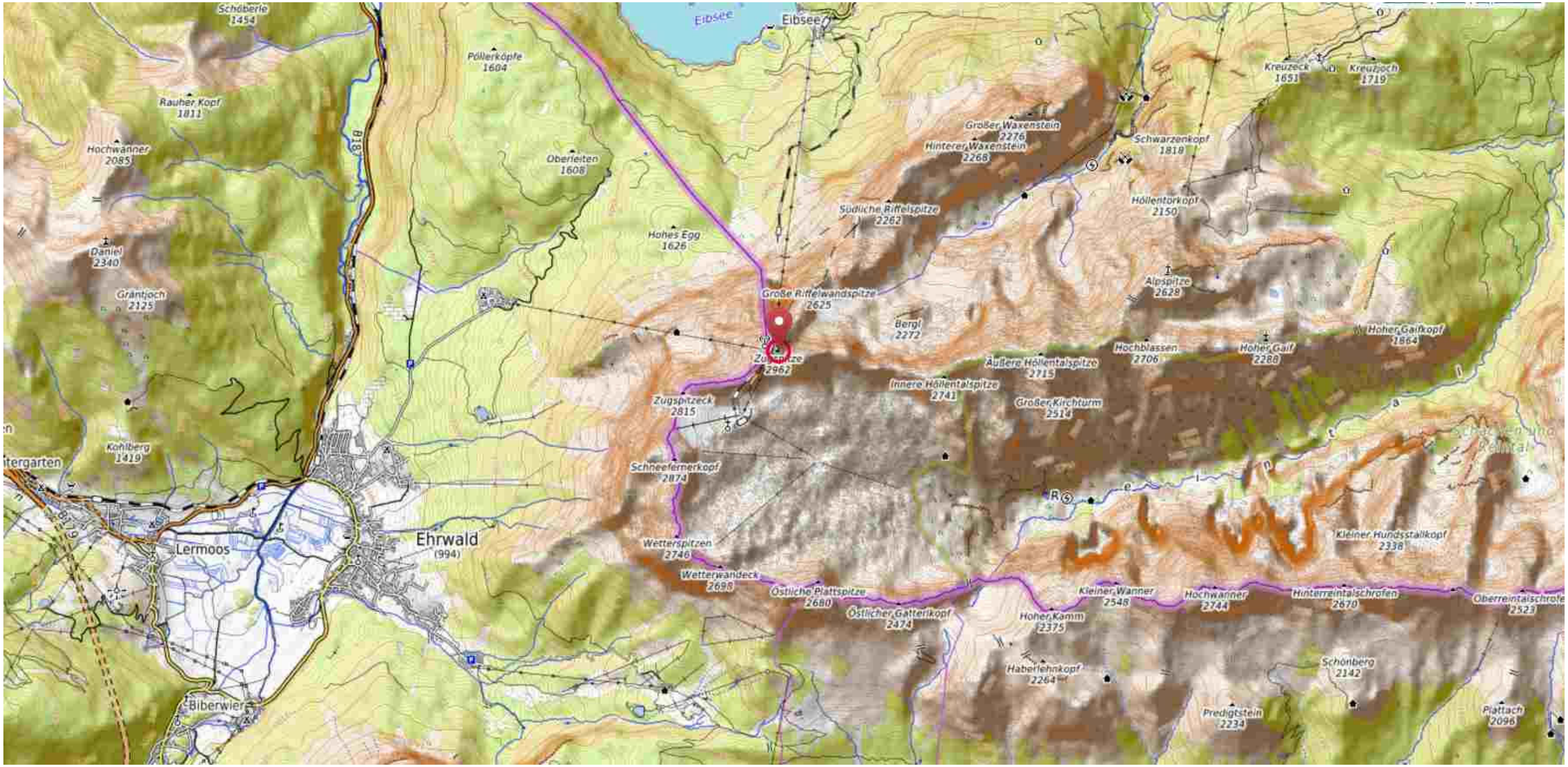


Case $y_i = 0$, e.g. "dog"

  4. ...

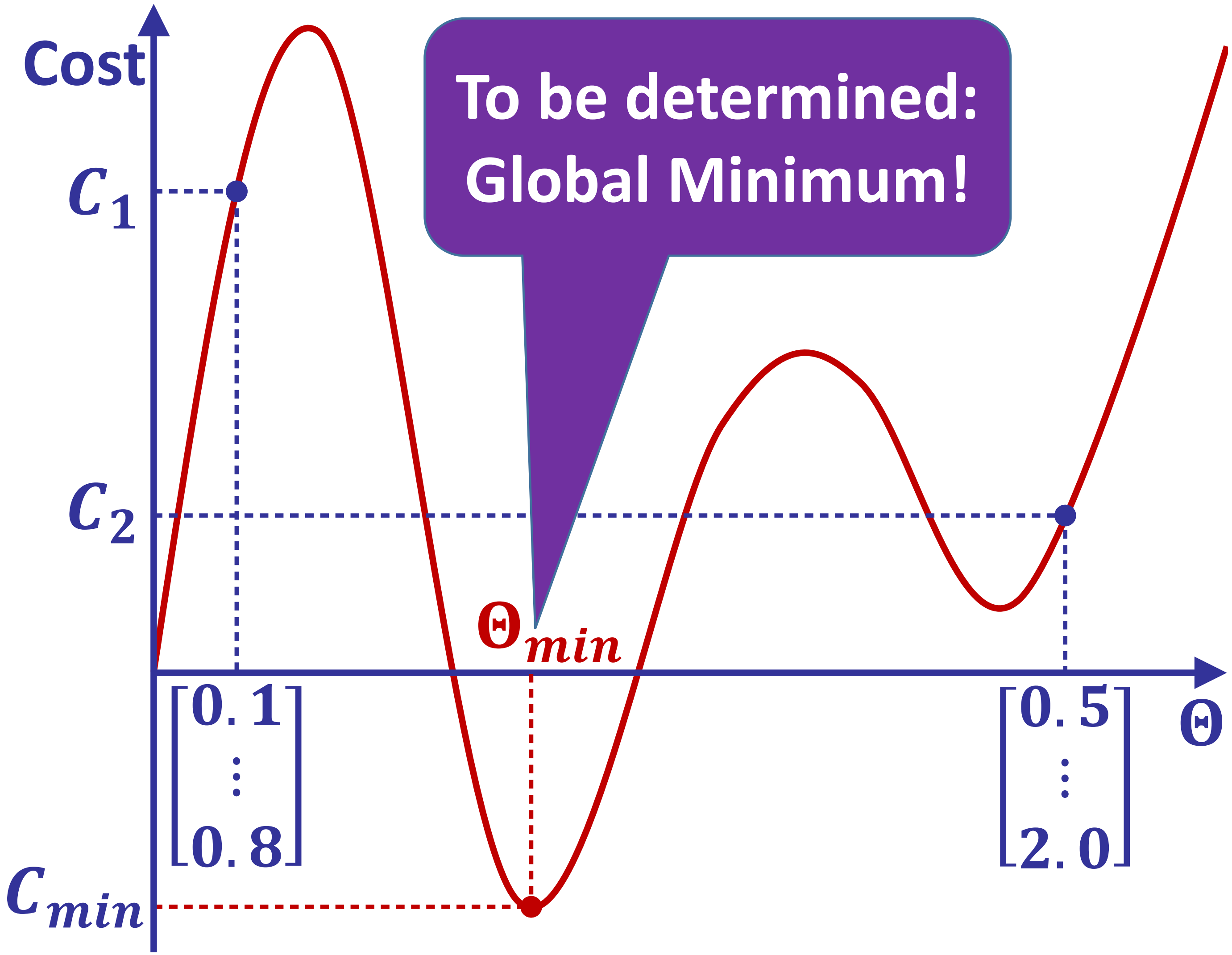
Minimize the chosen cost function to have a good model $f(x_i, \Theta)$

How to optimize the model?

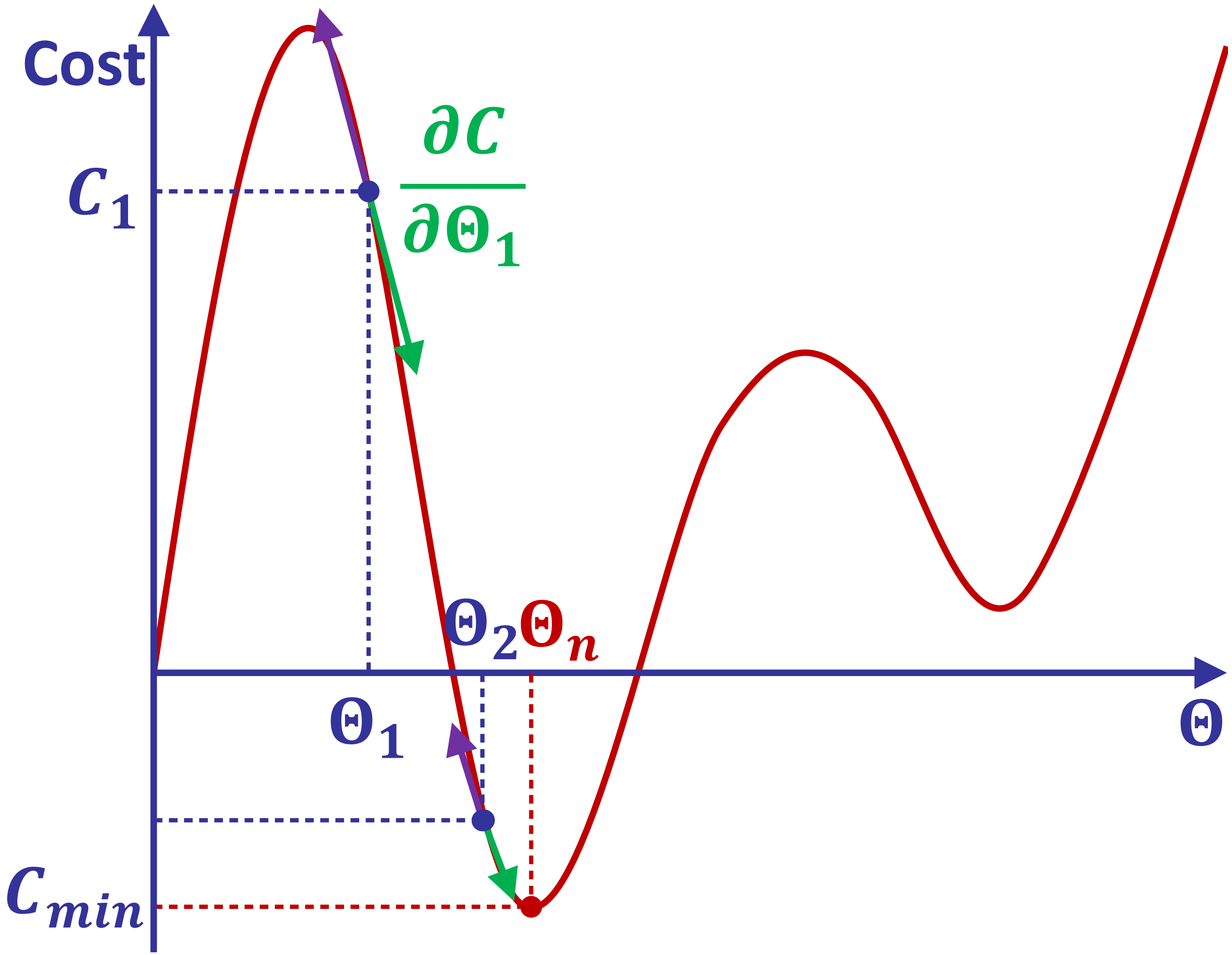


- Being on a mountain in fog (only seeing some few meters):
  Where to go to be on the fastest route to the valley?

How to optimize the model?

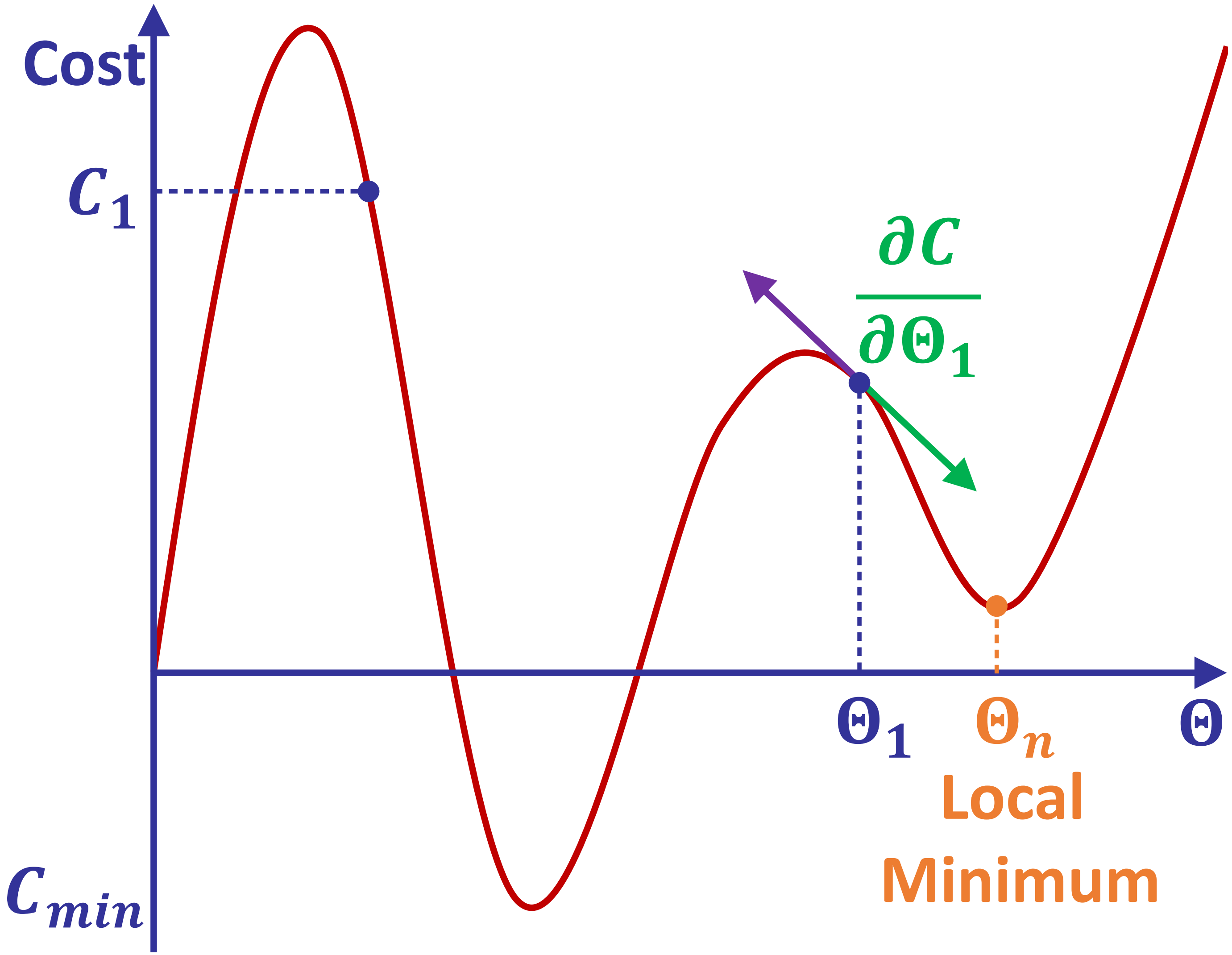


How to optimize the model?



Gradient descent algorithm:
$\Theta_{i+1} = \Theta_i - \eta \cdot \nabla C(\Theta_i)$
where η is the learning rate
(smaller for larger i)

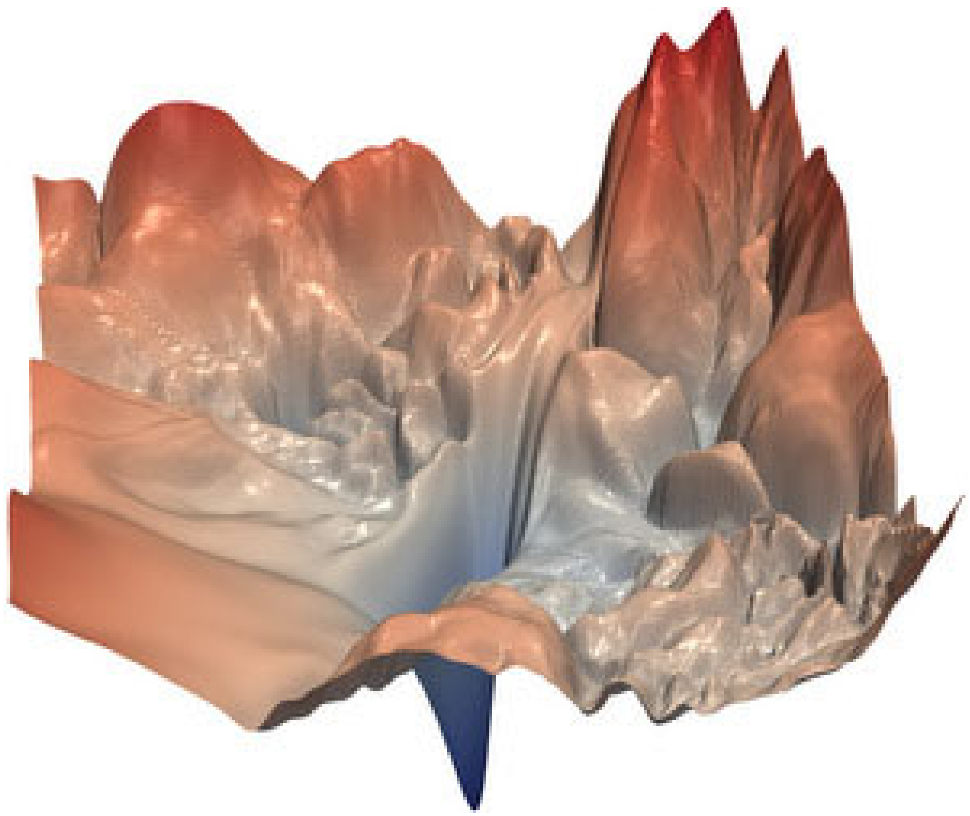
How to optimize the model?



Gradient descent algorithm:
$\Theta_{i+1} = \Theta_i - \eta \cdot \nabla C(\Theta_i)$
where η is the learning rate
(smaller for larger i)

How to optimize the model?

- Cost functions are often complicated in practice!



Loss surface of **ResNet-56** (residual network with 56 layers)

- In practice: Stochastic gradient-descent methods usually **avoid local minima**

How to optimize the model?

Training Data: X_{train}

Feed in the **samples** $(x_1, \ldots, x_n)$

How to optimize the model?

Training Data: X_{train} → Model: $f(X_{train}, \Theta) = \hat{y}$

Pick **random parameters Θ**

Compute **predicted labels** $(\hat{y}_1, \dots, \hat{y}_n)$

How to optimize the model?

Training Data: X_{train} → Model: $f(X_{train}, \Theta) = \hat{y}$ → Cost: $C(f(X_{train}, \Theta), y)$

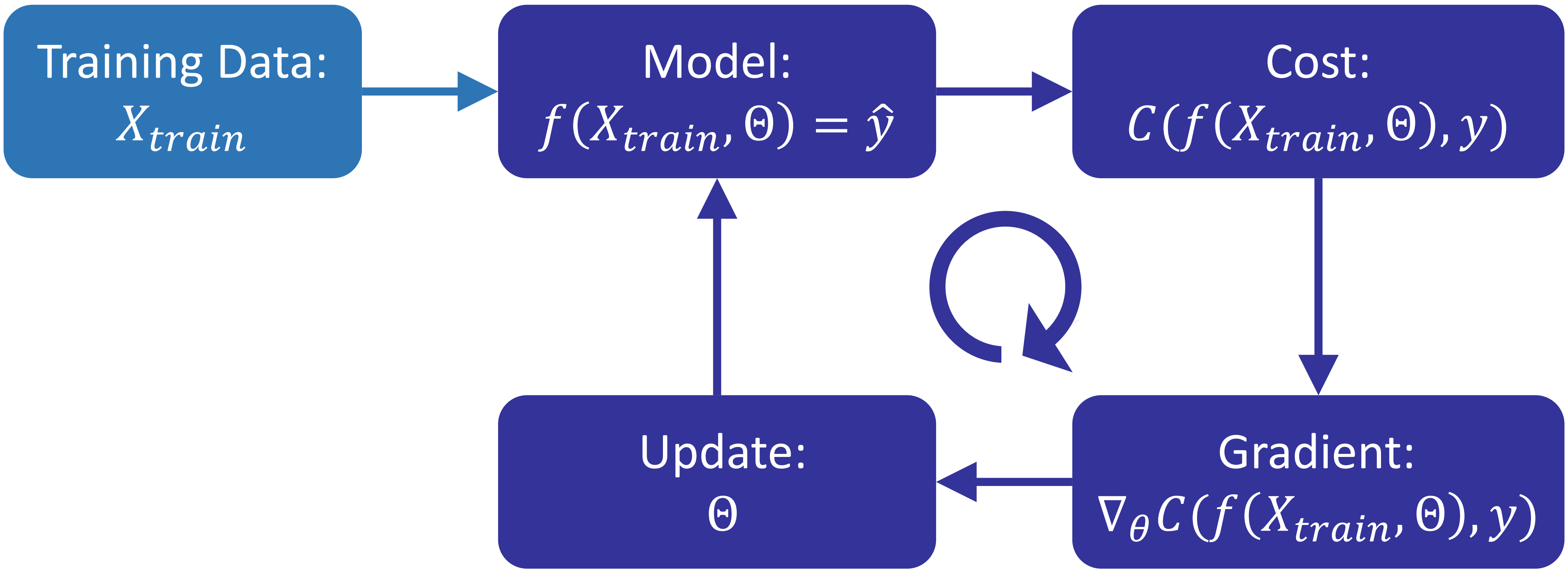
Compute **cost from predicted label $\hat{y}$ and ground truth y**

How to optimize the model?

Training Data: X_{train} → Model: $f(X_{train}, \Theta) = \hat{y}$ → Cost: $C(f(X_{train}, \Theta), y)$ → Gradient: $\nabla_\theta C(f(X_{train}, \Theta), y)$

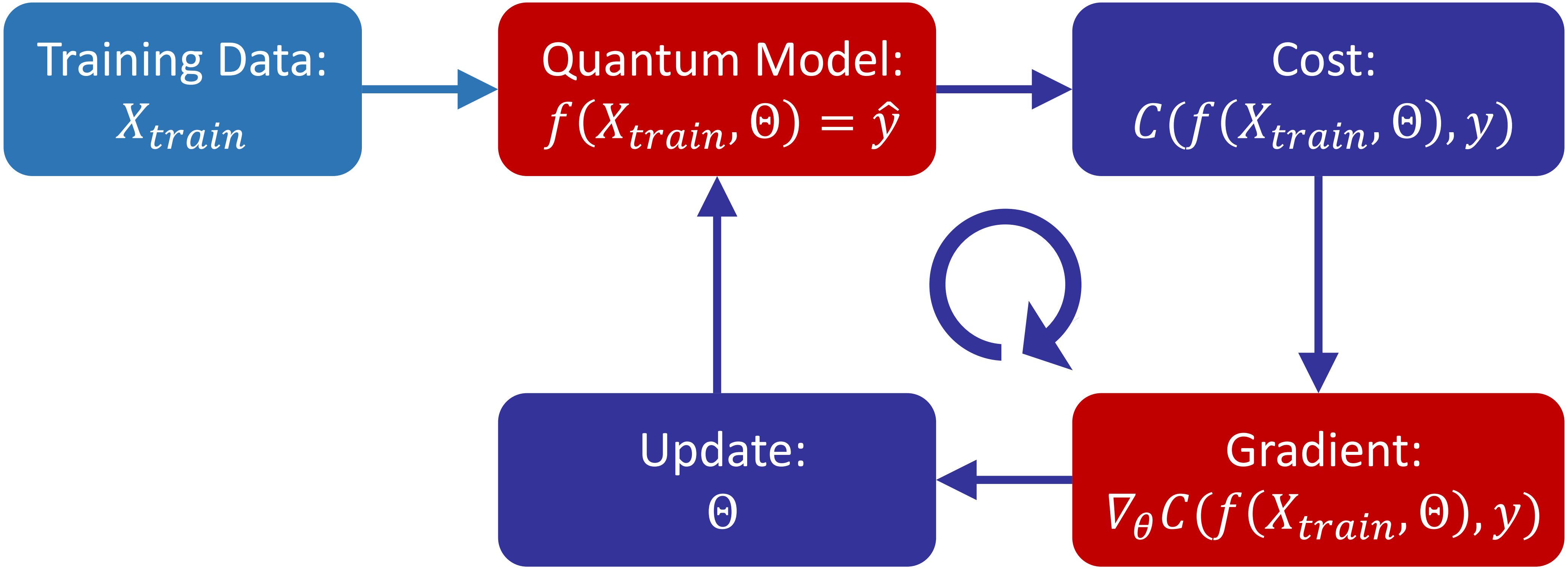
Compute **gradient** of the cost function for the samples of the dataset

How to optimize the model?



Update parameters Θ and start the **next iteration** of the optimization process

How to optimize the model?



How to compute gradients on quantum computer?

Optimization: **Gradient** Calculation

- **Example:** Binary classification using cross-entropy loss:

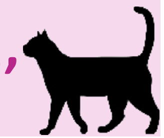
$y_i \in \{0, 1\}$, i.e., "true" label or two classes like **"cat"** and **"dog"**

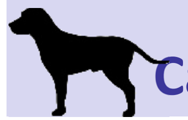
Probability for $y_i = 1$ (e.g., "cat")

$$C_{CE}(\Theta, (y_1, \dots, y_t)) = -\frac{1}{t}\sum_{i=1}^{t}\left(y_i \cdot log(f(x_i,\Theta)) + (1 - y_i) \cdot log(1 - f(x_i, \Theta))\right)$$

Probability for $y_i = 0$ (e.g., "dog")

Case $y_i = 1$, e.g. "cat"





Case $y_i = 0$, e.g. "dog"

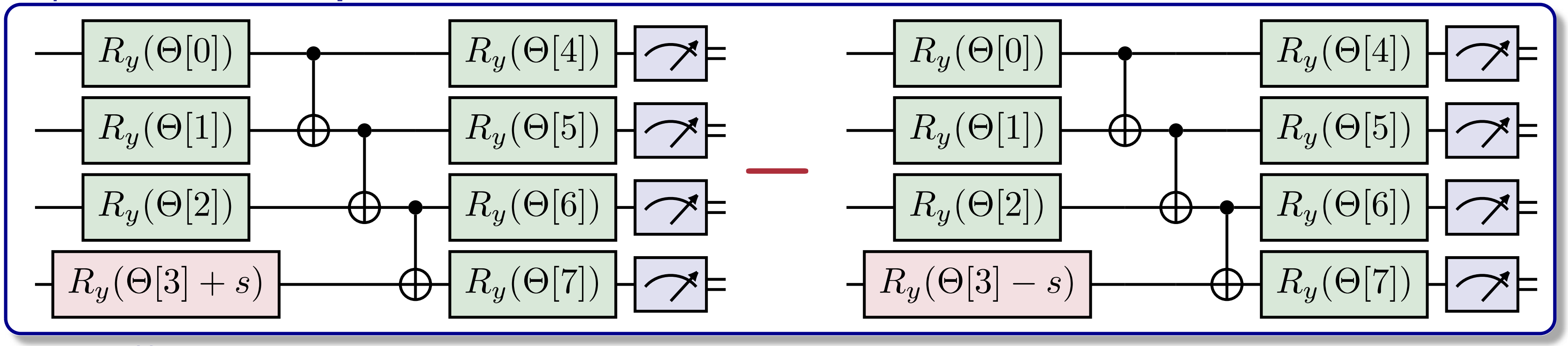
- **Gradient** Calculation:

Let $\Theta = \begin{bmatrix} \Theta[1] \\ \vdots \\ \Theta[r] \end{bmatrix}$, **then** $\frac{\partial C}{\partial \Theta} = \begin{bmatrix} \frac{\partial C}{\partial \Theta[1]} \\ \vdots \\ \frac{\partial C_{CE}}{\partial \Theta[r]} \end{bmatrix}$ **and** $\frac{\partial C}{\partial \Theta[k]} = -\sum_{i=1}^{t}\left(\frac{y_i}{f(x_i, \Theta)} - \frac{1 - y_i}{1 - f(x_i, \Theta)}\right) \cdot \boxed{\frac{\partial f(x_i, \Theta)}{\partial \Theta[k]}}$

to be evaluated on the quantum computer!

Quantum Gradient Calculation

- For expectation- & sample-based labels to be evaluated:
  a) $\frac{\partial}{\partial\Theta_k}\langle\psi(x_i,\Theta)|Z|\psi(x_i,\Theta)\rangle$ b) $|\psi(x_i,\Theta)\rangle = U(\Theta)\mathcal{E}(x_i)|0\rangle = U|\psi(x)\rangle$
- Options to determine gradient [S+'18]
  - Numerical differentiation
    - The gradient is approximated by black-box evaluations, i.e., in general $\nabla g(x) \approx \frac{g(x+s)-g(x-s)}{2\cdot s}$, where s is small shift
    - In quantum model via **parameter shift rule**:



  - Symbolic differentiation
    - ∇g via manual calculations or symbolic computer algebra package
  - Automatic differentiation of $g(x) := g_1(g_2(\cdots g_v(x)\cdots)))$
    - ∇g via accumulation of derivatives of $g_1 \cdots g_v$ following the chain rule [R'96]

Quantum Gradient Calculation

- Quantum computing frameworks often support many different approaches for gradient calculations
  - Qiskit Gradient Framework
  - PennyLane Optimizers
  - Cirq calculate gradients
  - ...

How do we assess our model? - Validation

Test Data:
X_{test}

Feed in the
test samples
$(x_1, \ldots, x_m)$

How do we assess our model? - Validation

Test Data: X_{test} → Quantum Model: $f(X_{test}, \Theta^*) = \hat{y}$

Use **parameter values Θ^* obtained in the optimization**

Compute **predicted labels** $(\hat{y}_1, \ldots, \hat{y}_n)$

How do we assess our model? - Validation

Test Data: X_{test} → **Quantum Model:** $f(X_{test}, \Theta^*) = \hat{y}$ → **Cost:** $C(f(X_{test}, \Theta^*), y)$

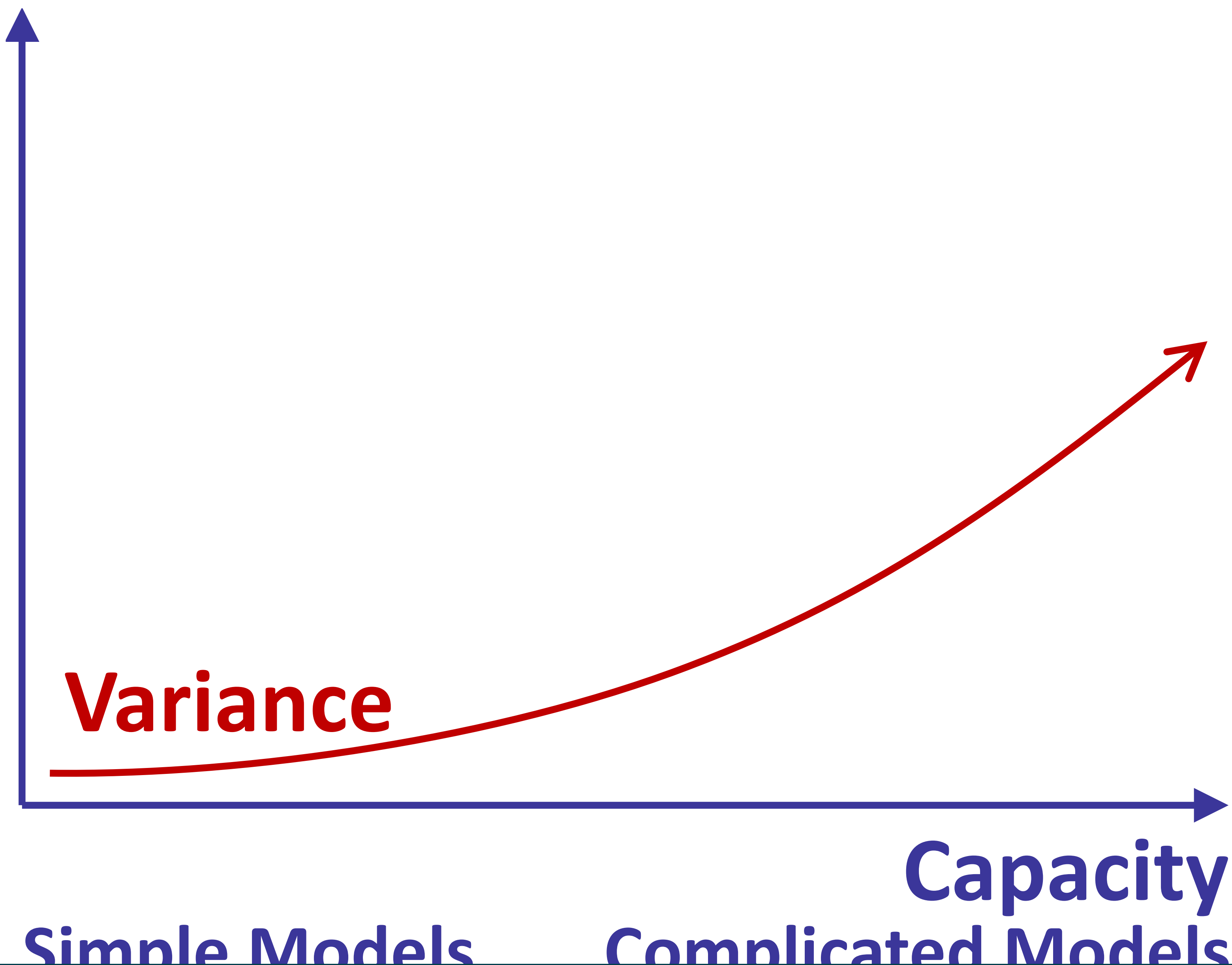
Compute **cost from predicted label $\hat{y}$ and ground truth y:**

How good is it?

What about unseen data?

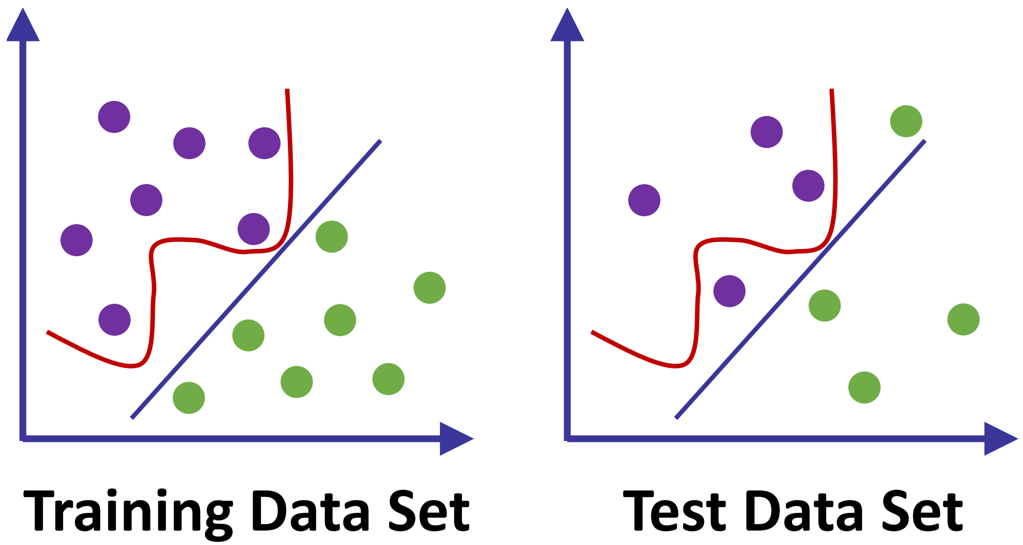
Image source: Lion

Generalization Error

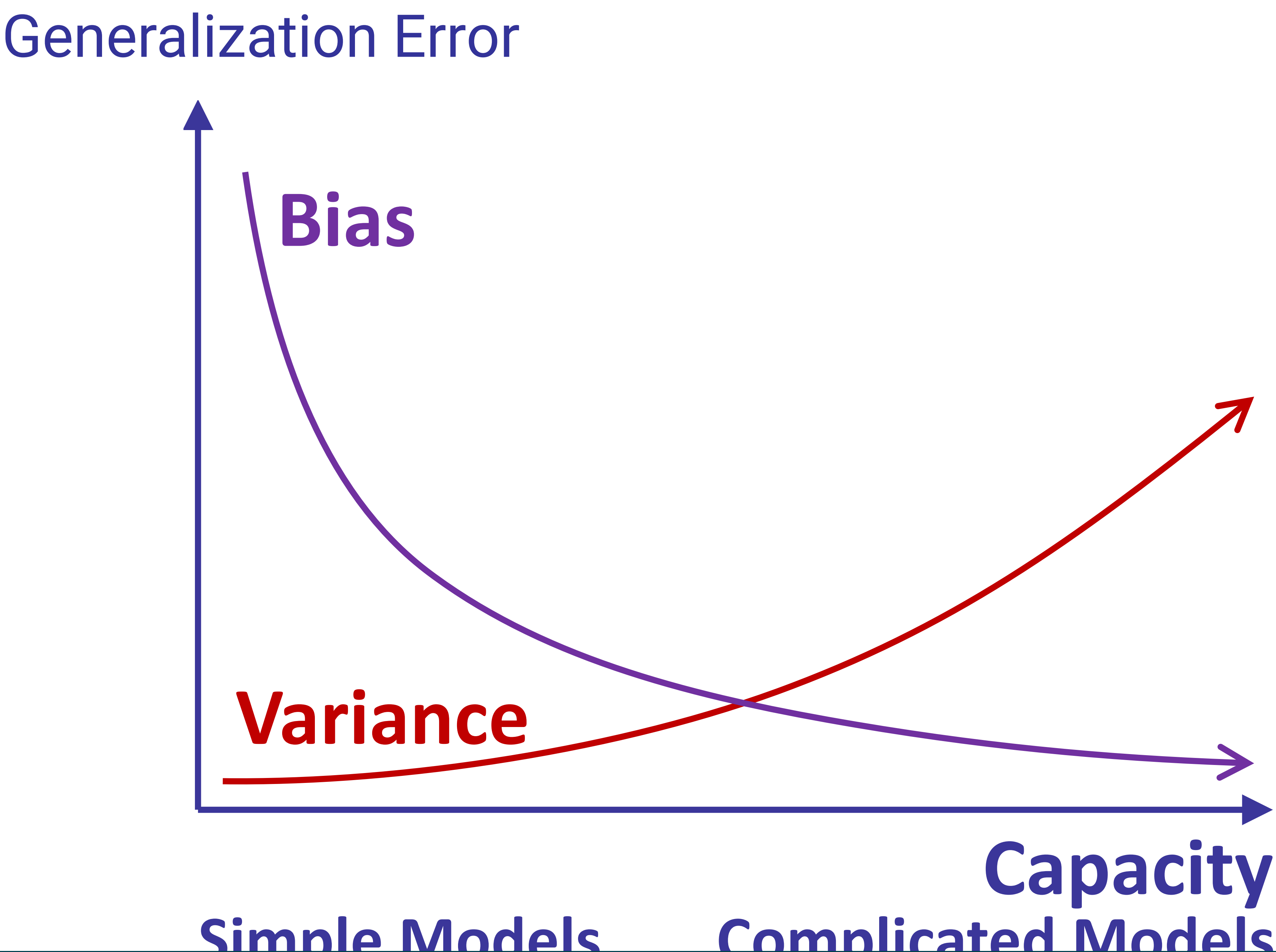


Variance

- refers to the changes in the model when using different portions of the training data set
- **Simply stated:** variability in the model prediction, i.e., how much the ML function can adjust depending on the given data set

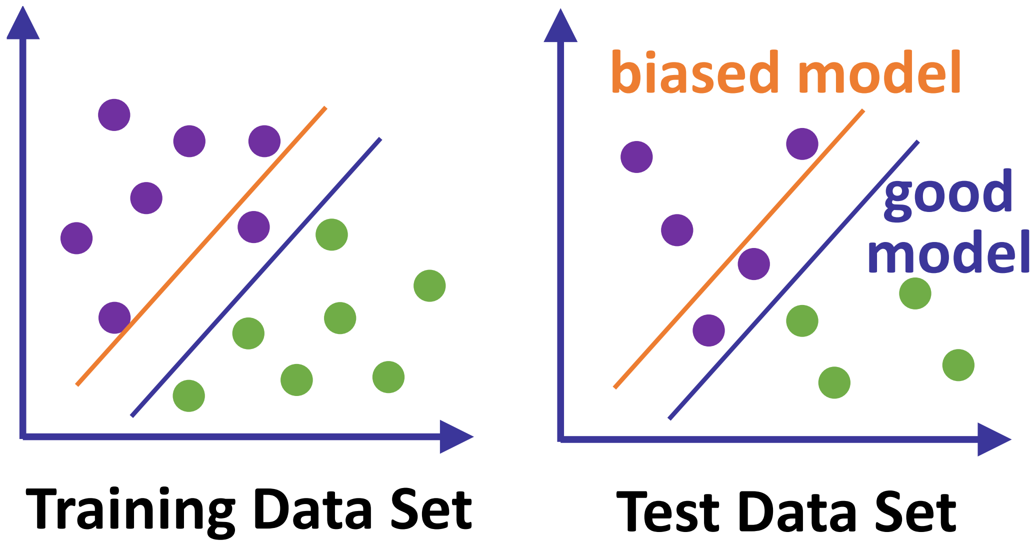


- Model captures a very specific pattern observed only in the training data and misclassifies the test data



Adapted from A. Dekusar, J. Gacon, Qiskit Machine Learning: Quantum algorithms for supervised learning, EQTC, 2022

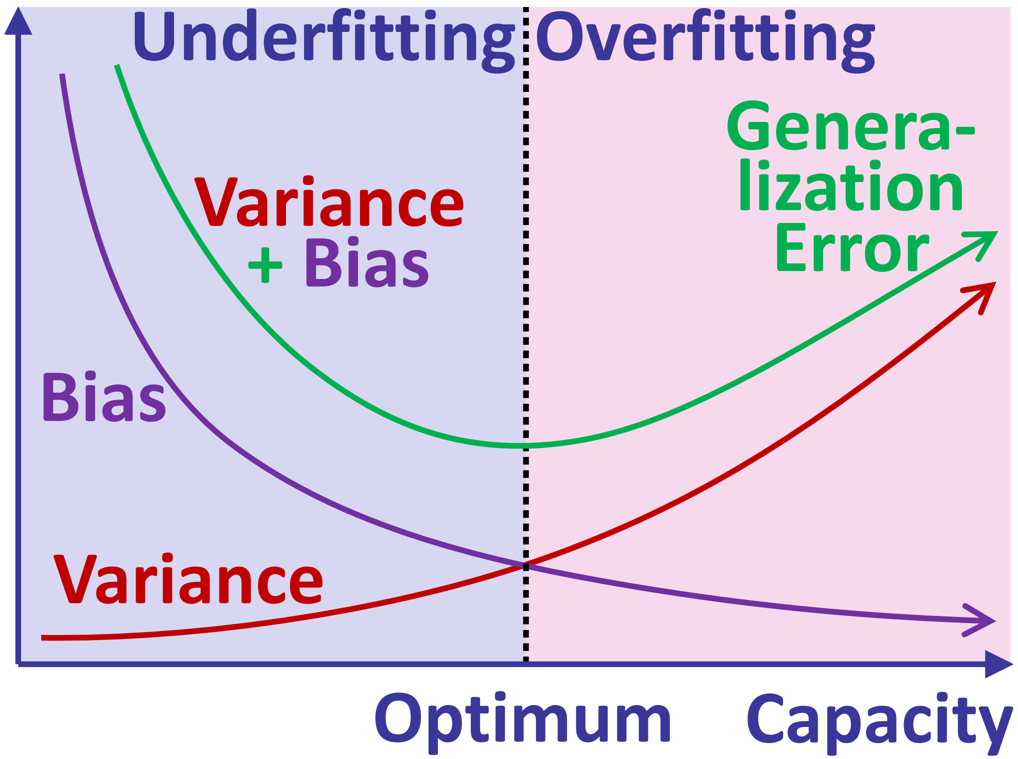
Bias



- Model does not capture enough patterns from data to produce correct results

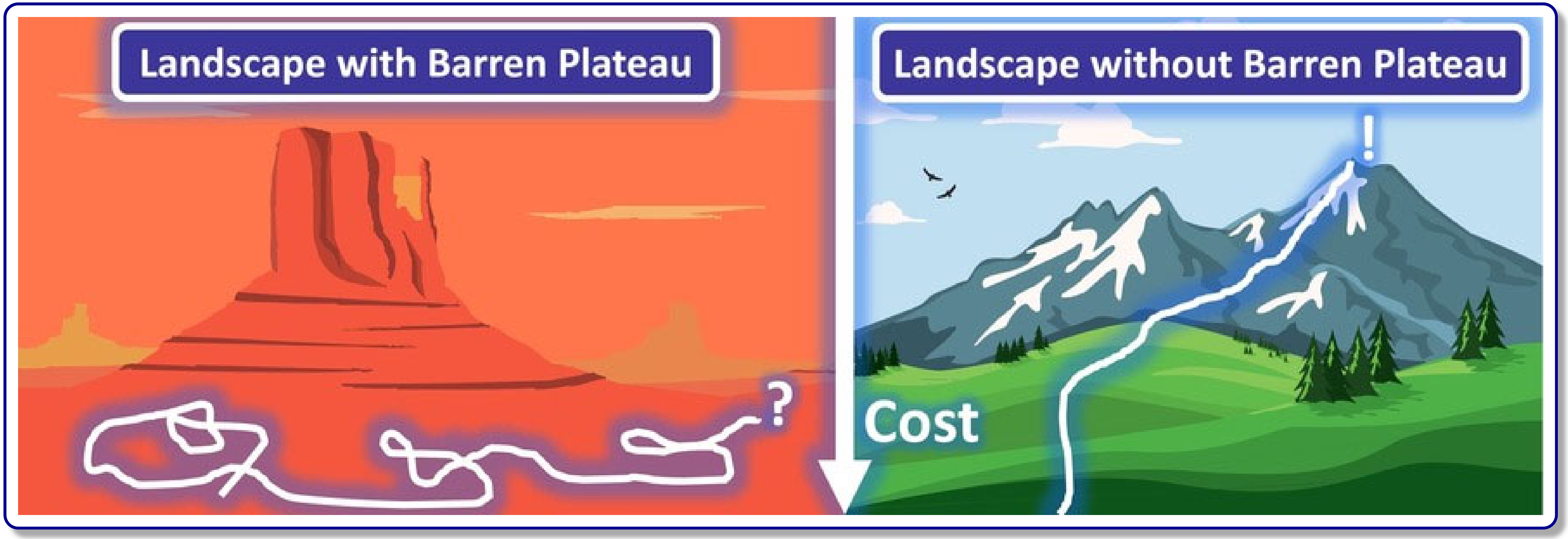
Generalization Error

Model is not complex enough to match all the available data and performs poorly with the training dataset ⇒ **Underfitting:** model is unable to match the input data to the target data



Highly complex models matching almost all the given data points and perform well in training datasets, **but**: model cannot generalize the data point in the test data set to predict the outcome accurately ⇒ **Overfitting:** model tries to match non-existent data

Barren Plateau hindering Optimization



- Many QML algorithms suffer from the dreaded "barren plateau" of unsolvability running into dead ends on optimization problems
- Trainability problem for flat problem-solving spaces
- Optimization algorithm can't find the downward slope in a "featureless" landscape with no clear path to the energy minimum

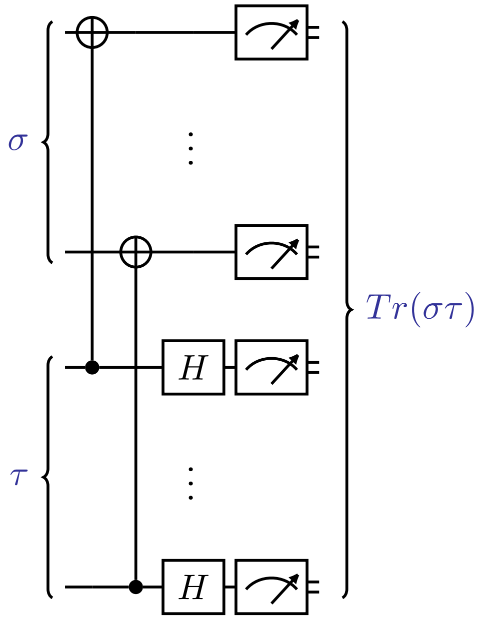
Barren Plateau hindering Optimization

- Barren plateau landscapes correspond to gradients that vanish exponentially in the number of qubits
  - An exponentially large precision is needed to navigate through the landscape
- A **cost function $C(\Theta)$ has a barren plateau iff the variance $Var \in O(\frac{1}{b^n})$ for some $b > 1$ with n number of qubits**
- In the absence of a barren plateau:
  - Determination of a minimizing direction in the cost function landscape does not require an exponentially large precision
    - One can always navigate through the landscape by measuring expectation values with a precision that grows at most polynomially with the system size
  - Speedup over classical algorithms often scaling exponentially for polynomial overhead of quantum algorithms
  - **Quantum speedup** often only in the absence of a barren plateau
- Although different approaches overcome the limitations arising from barren plateaus, there is not one simple way for it

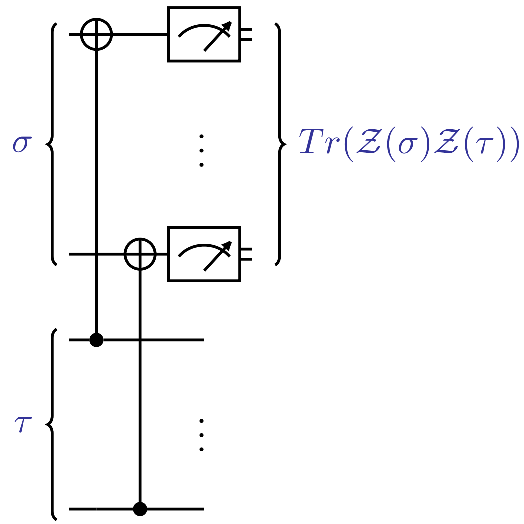
Local Cost Functions for Diagonalization

Goal is to find $\Theta_{\text{opt}} := argmin_\Theta(C(U_p(\Theta)))$, where $C(U_p(\Theta))$ quantifies how far the state $\rho_p(\Theta)$ is from being diagonal.
Cost functions: $C_1(U_p(\Theta)) = Tr(\rho^2) - Tr(\mathcal{Z}(\rho)^2)$ and $C_2(U_p(\Theta)) = Tr(\rho^2) - \frac{1}{n}\sum_{j=1}^{n} Tr(\mathcal{Z}_j(\rho)^2)$ using below given tests.
$\Rightarrow C_2$ **mitigates barren plateaus** for large n in comparison to C_1!
Correctness: Global minima of C_1 and C_2 coincide for $U_p(\Theta)$ diagonalizing ρ: $C_1(U_p(\Theta)) = 0 \Leftrightarrow C_2(U_p(\Theta)) = 0 \Leftrightarrow \rho = \mathcal{Z}(\rho)$

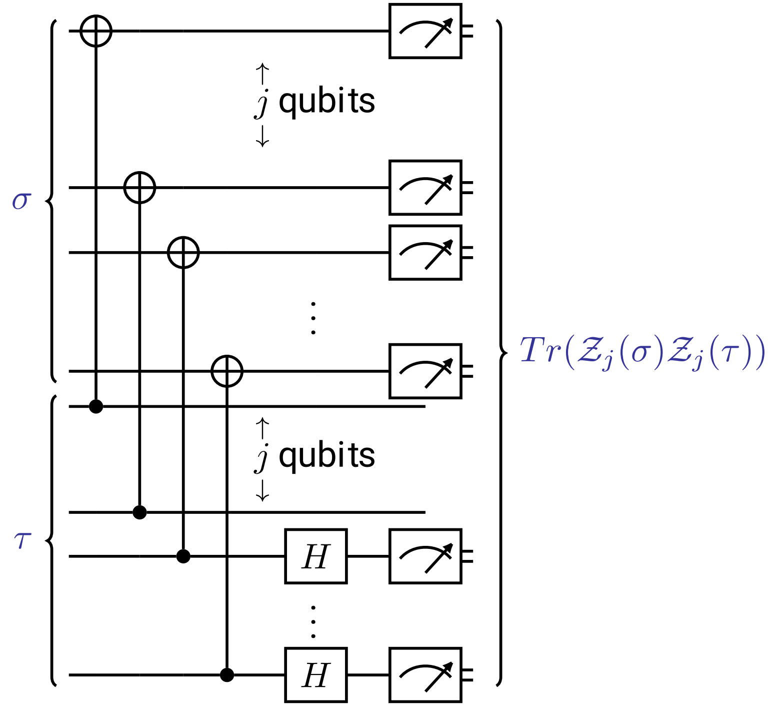
Tests: Destructive Swap



Diagonalized Inner Product (DIP)



Partially Diagonalized Inner Product (PDIP)



Postprocessing: scales $O(n)$ — no — scales $O(n)$

Notation:
$Tr(\rho^2)$: Purity of an n-qubit state ρ ranging from:
being completely mixed (i.e., the center of the Bloch sphere) $\frac{1}{2 \cdot n} \leq Tr(\rho^2) \leq 1$ pure state on the surface of the Bloch sphere
$\mathcal{Z}(\sigma)$ and $\mathcal{Z}_j(\sigma)$ are quantum channels that dephase (i.e., destroy the off-diagonal elements of σ) in the global standard basis
and in the local standard basis on a set j of qubits

Barren Plateau hindering Optimization

- "If you have a barren plateau, all hope of quantum speedup or quantum advantage is lost"
- "People have been proposing quantum neural networks and benchmarking them by doing small-scale simulations of 10s (or fewer) qubits. The trouble is, you won't see the barren plateau with a small number of qubits, but when you try to scale up to more qubits, it appears. Then the algorithm has to be reworked for a larger quantum computer."
- "We were able to prove that, if you choose a cost function that looks locally at each individual qubit, then we guarantee that the scaling won't result in an impossibly steep curve of time versus system size, and therefore can be trained"
- Most quantum variational algorithms initiate their search randomly and evaluate the cost function globally across every qubit, which often leads to a barren plateau.

Barren Plateau hindering Optimization

- Barren plateaus may occur for global cost functions and for circuits with large depth

Circuit Depth	$O(1)$	$O(log(n))$	$O(poly(log(n))$	$O(poly(n))$
Global Cost Function	maybe Barren Plateau	maybe Barren Plateau	maybe Barren Plateau	maybe Barren Plateau
Local Cost Function	Trainable	Trainable	Transition	maybe Barren Plateau

Quantum Neural Networks Variants

Classical Approach	Abbreviation	Quantum Counterpart
Boltzmann Machine	BM	QBM
Convolutional Neural Network	CVNN	QCVNN
Generative Adversarial Network	GAN	QGAN
		Quantum Space Graph Convolutional Neural Network (QSGCNN)
Random Walk Neural Networks	RWNN	Quantum Walking Neural Network (QWNN)
Recurrent Neural Network	RNN	QRNN
Tensor Neural Networks	TNN	QTNN
Perceptron	P	Quantum Perceptron (QP)
Competitive Neural Networks	CPNN	QCPNN
Self-Organizing Neural Network	SONN	QSONN
Cellular Neural Network	CELL	QCELL
Weightless Neural Network	WLNN	QWLNN
Graph Neural Network	GNN	QGNN

Summary & Conclusions

- Machine Learning
  - Basics: Optimization
- **Gradient** Descent Algorithm
  - Calculation
    - Numerical differentiation
      - In quantum model via parameter shift rule
    - Symbolic differentiation
    - Automatic differentiation
      - Chain rule
- Generalization Error
  - Variance, Bias
  - Underfitting, Overfitting
  - Barren Plateau
- Overview Quantum Neural Networks Variants