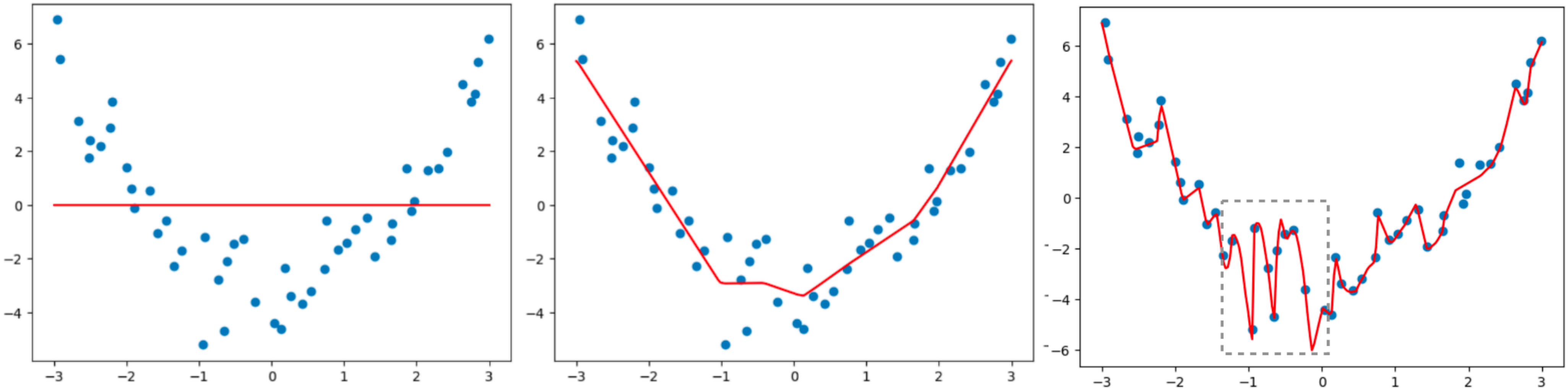


- Which function best fits this data? Why?

- What are some of the choices that we can make when designing a neural network?

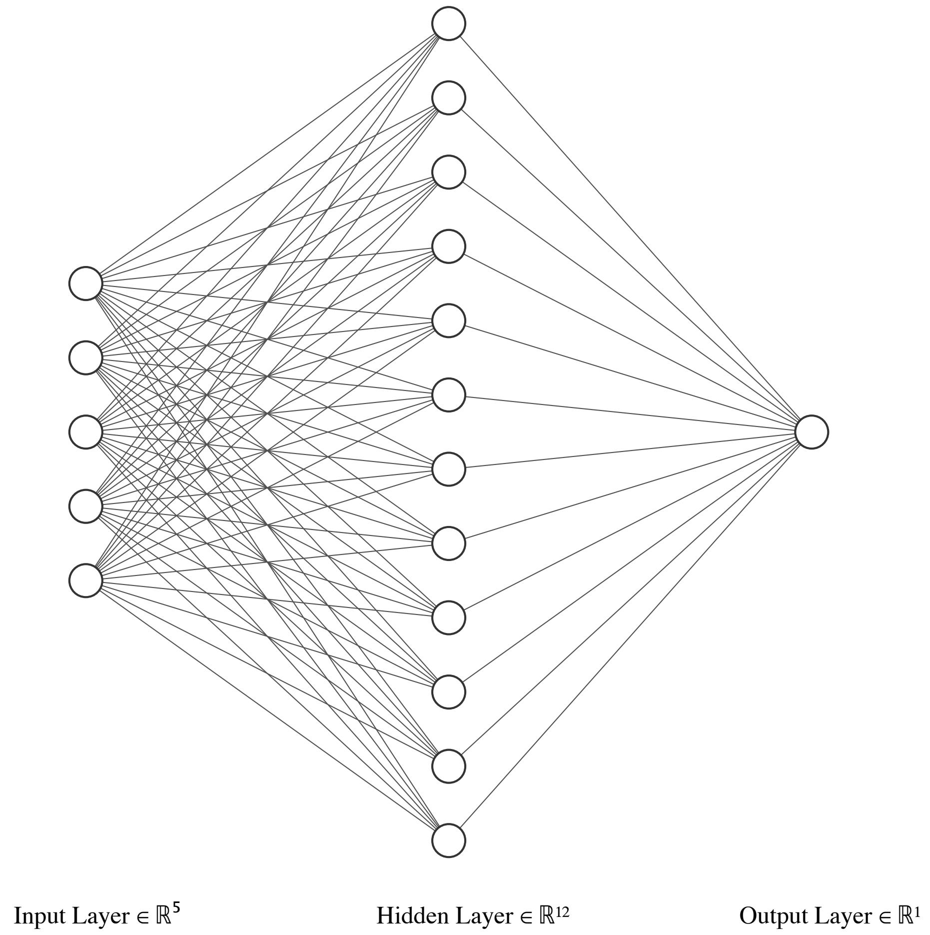
- What might we infer about the differences in the neural networks used for each function?

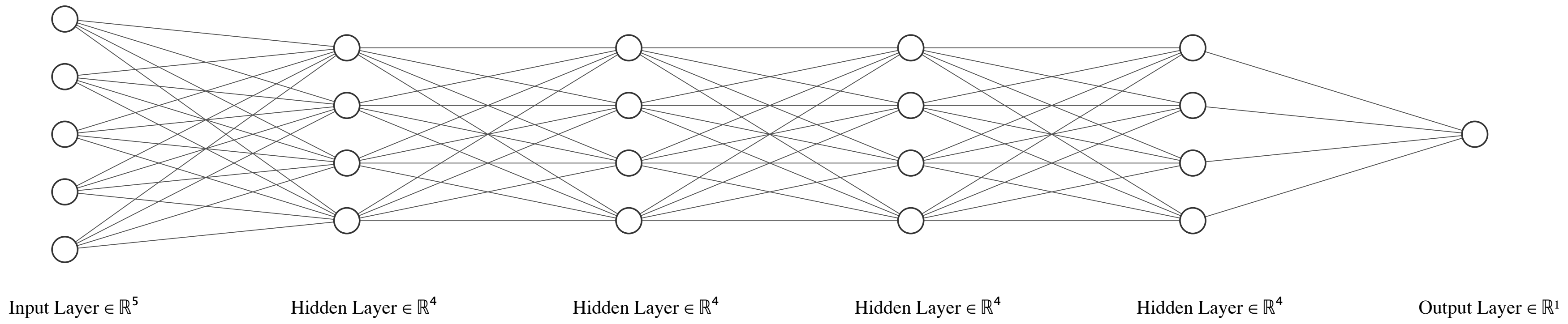
- What can we conclude about the neural network weights in the third figure from looking at the highlighted region?

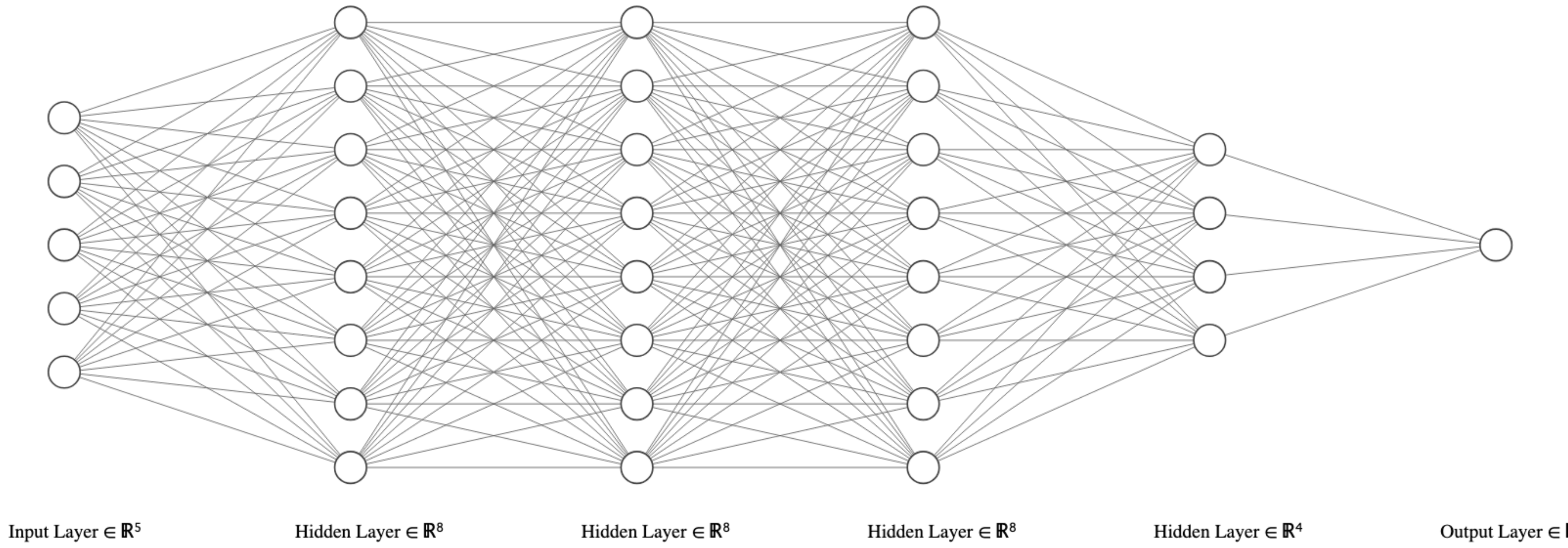
Evaluation

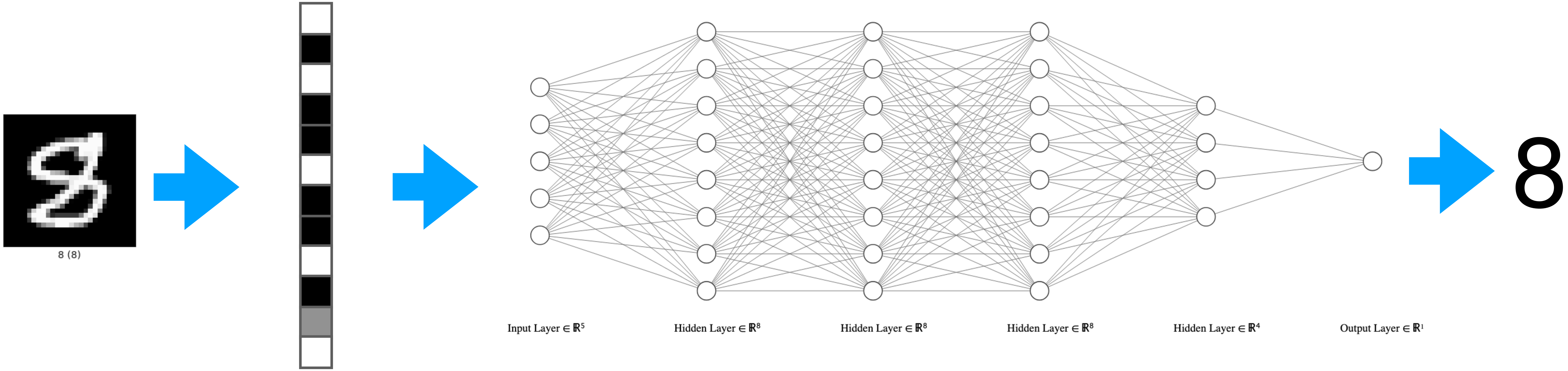
8 (8)

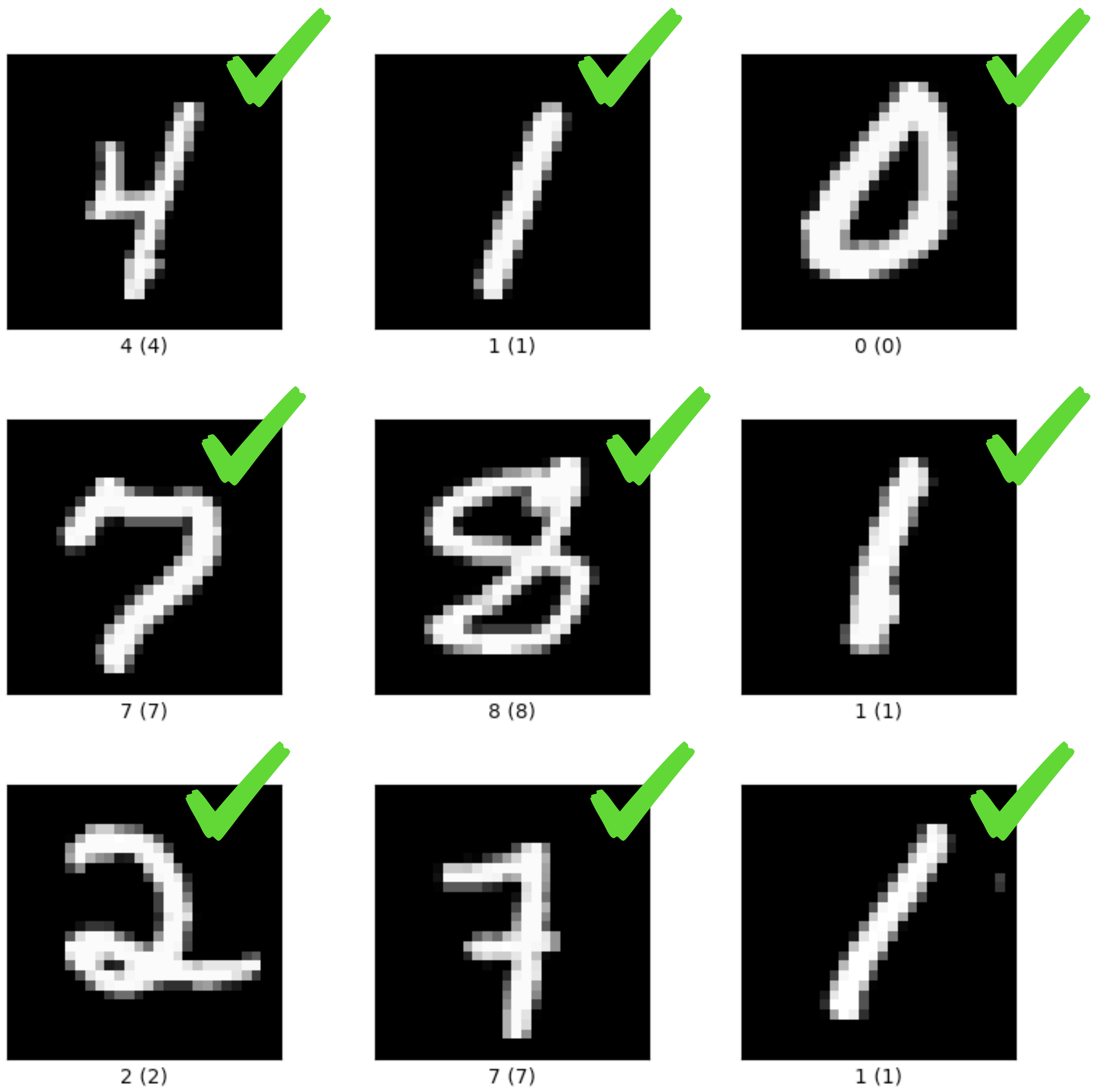
8

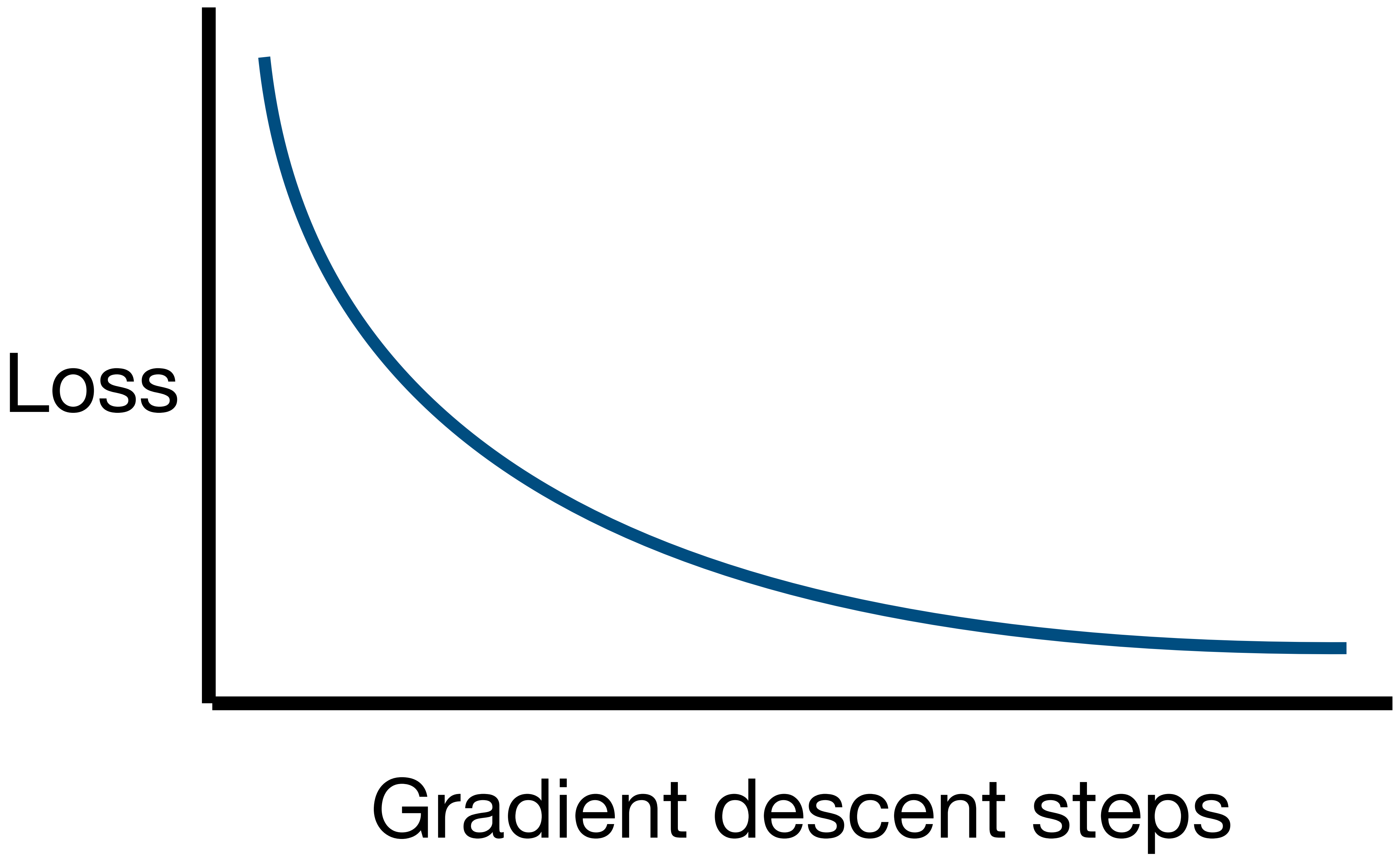

Input Layer ∈ $\mathbb{R}^5$
Hidden Layer ∈ $\mathbb{R}^{12}$
Output Layer ∈ $\mathbb{R}^1$


Input Layer ∈ $\mathbb{R}^5$
Hidden Layer ∈ $\mathbb{R}^4$
Hidden Layer ∈ $\mathbb{R}^4$
Hidden Layer ∈ $\mathbb{R}^4$
Hidden Layer ∈ $\mathbb{R}^4$
Output Layer ∈ $\mathbb{R}^1$

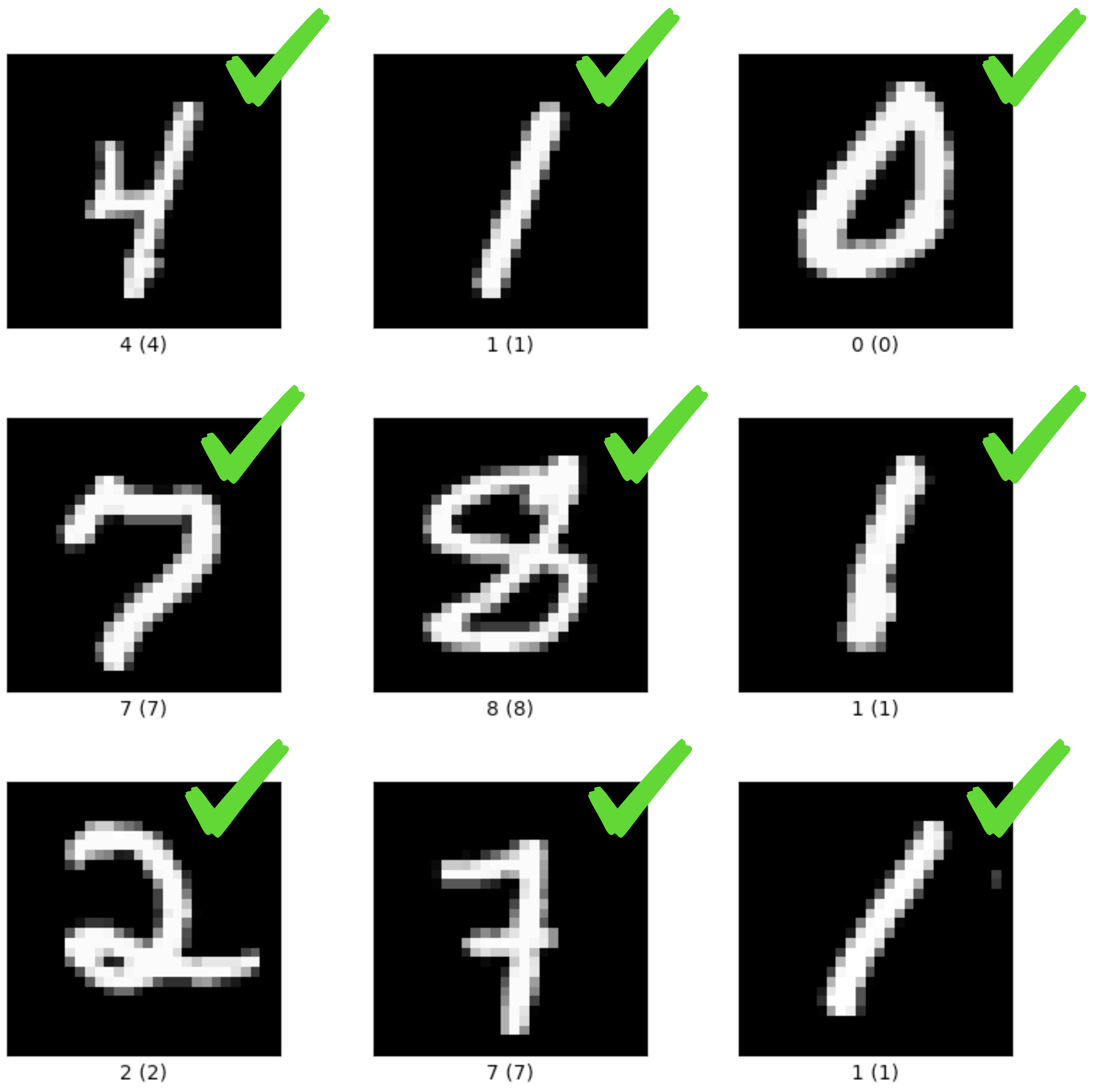

Input Layer ∈ $\mathbb{R}^5$
Hidden Layer ∈ $\mathbb{R}^8$
Hidden Layer ∈ $\mathbb{R}^8$
Hidden Layer ∈ $\mathbb{R}^8$
Hidden Layer ∈ $\mathbb{R}^4$

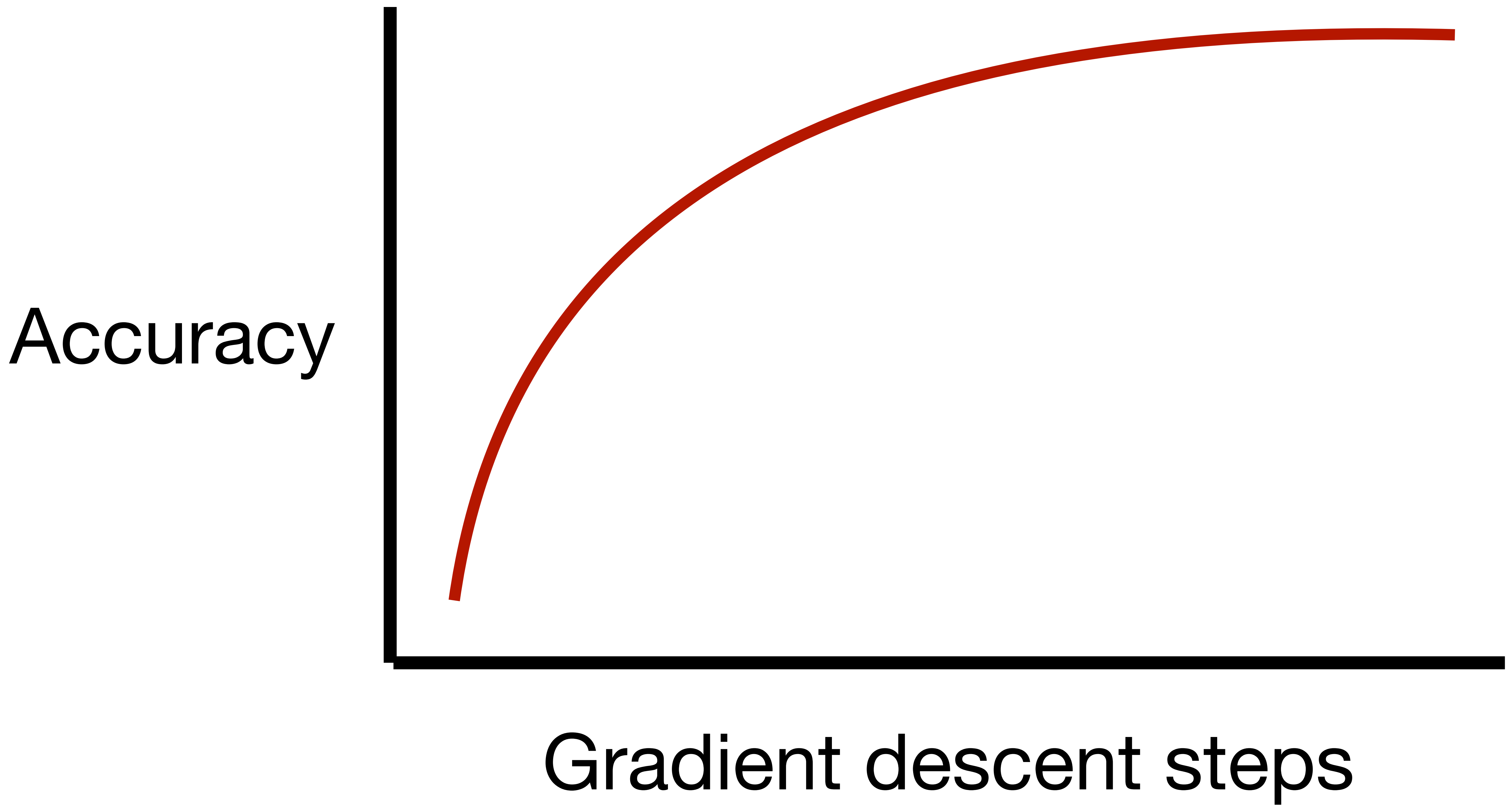

8 (8)
Input Layer ∈ $\mathbb{R}^5$
Hidden Layer ∈ $\mathbb{R}^8$
Hidden Layer ∈ $\mathbb{R}^8$
Hidden Layer ∈ $\mathbb{R}^8$
Hidden Layer ∈ $\mathbb{R}^4$
Output Layer ∈ $\mathbb{R}^1$
8





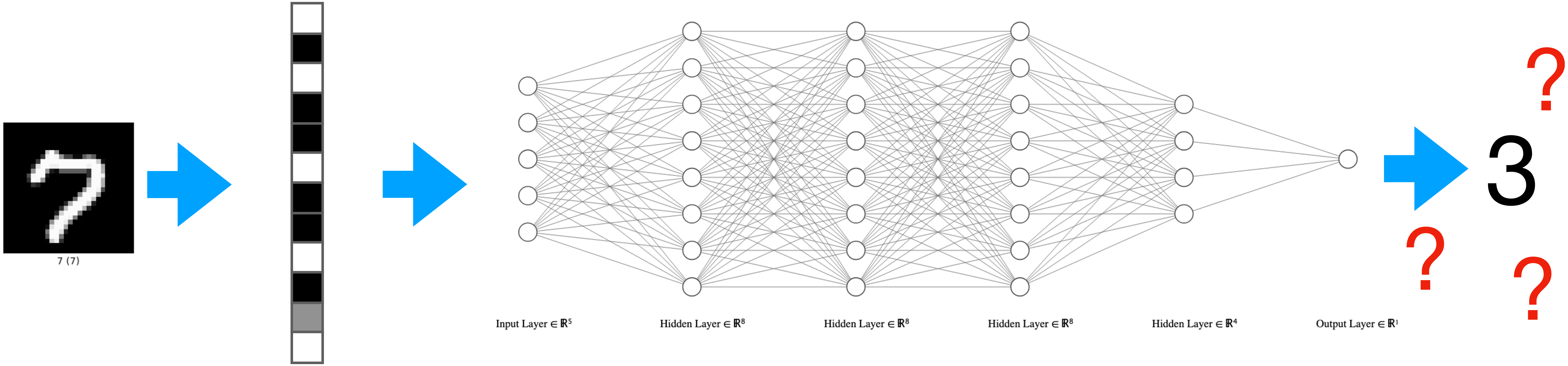
$$\mathbf{Loss}(\mathbf{w}) = \mathbf{NLL}(\mathbf{w}, \mathbf{X}, \mathbf{y}) = -\sum_{i=1}^{N} \log p(y_i \mid \mathbf{x}_i, \mathbf{w})$$



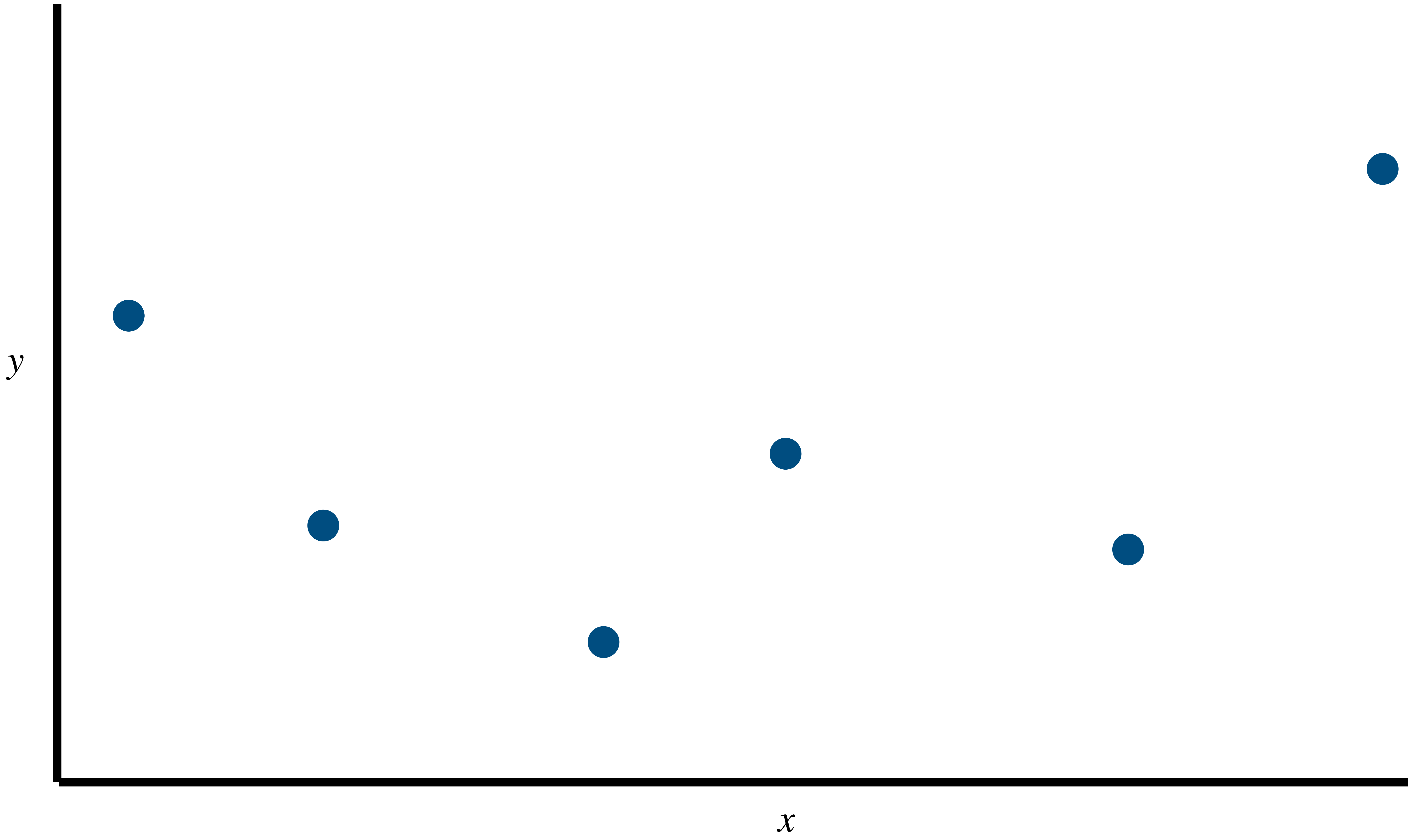


Accuracy: $\frac{\text{\# of correct predictions}}{\text{Total predictions}} = \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}\big(f(\mathbf{x}_i) = y_i\big)$

Are we done?

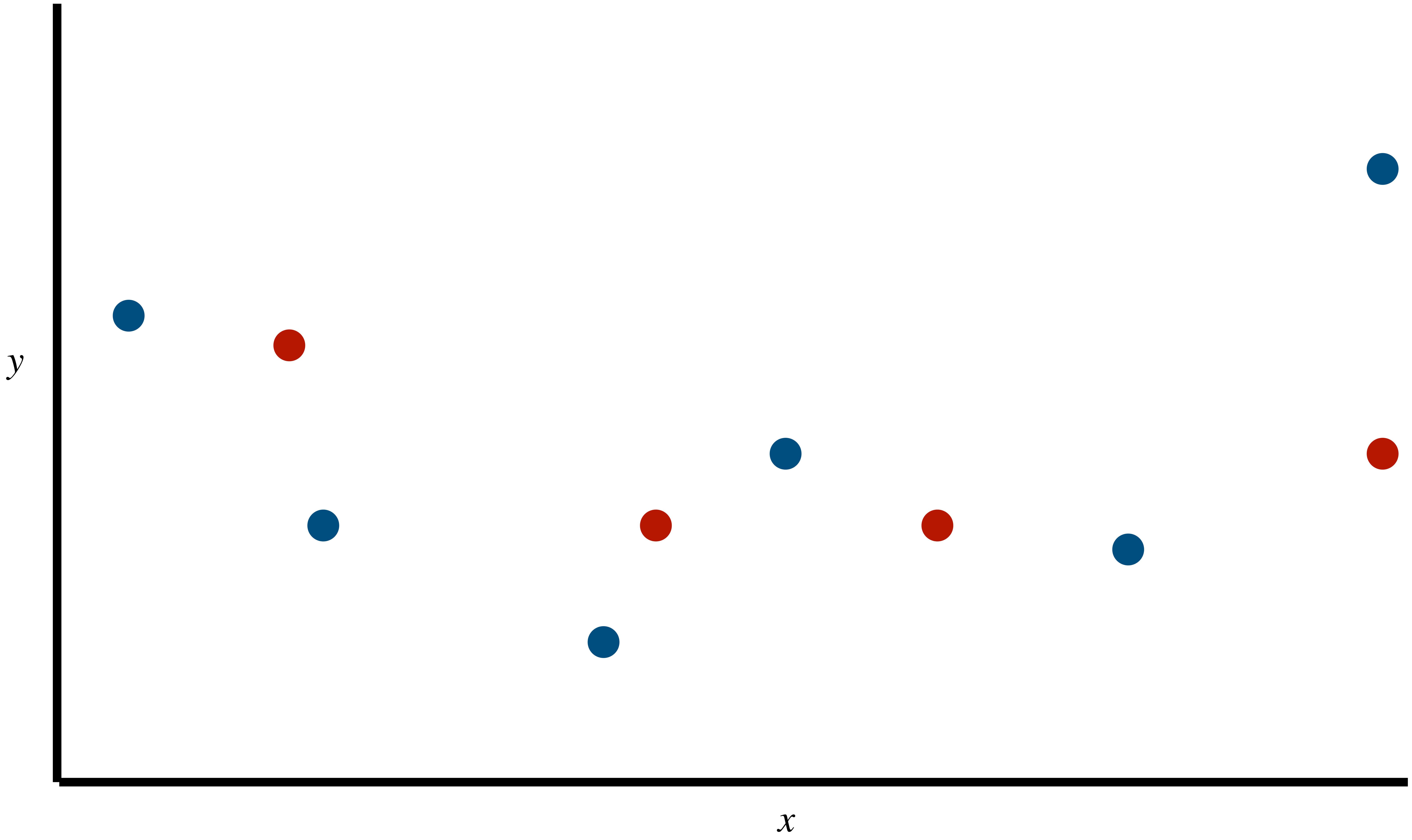

7 (7)
Input Layer ∈ ℝ⁵
Hidden Layer ∈ ℝ⁸
Hidden Layer ∈ ℝ⁸
Hidden Layer ∈ ℝ⁸
Hidden Layer ∈ ℝ⁴
Output Layer ∈ ℝ¹
3
?
?
?

How many functions have 0 loss?

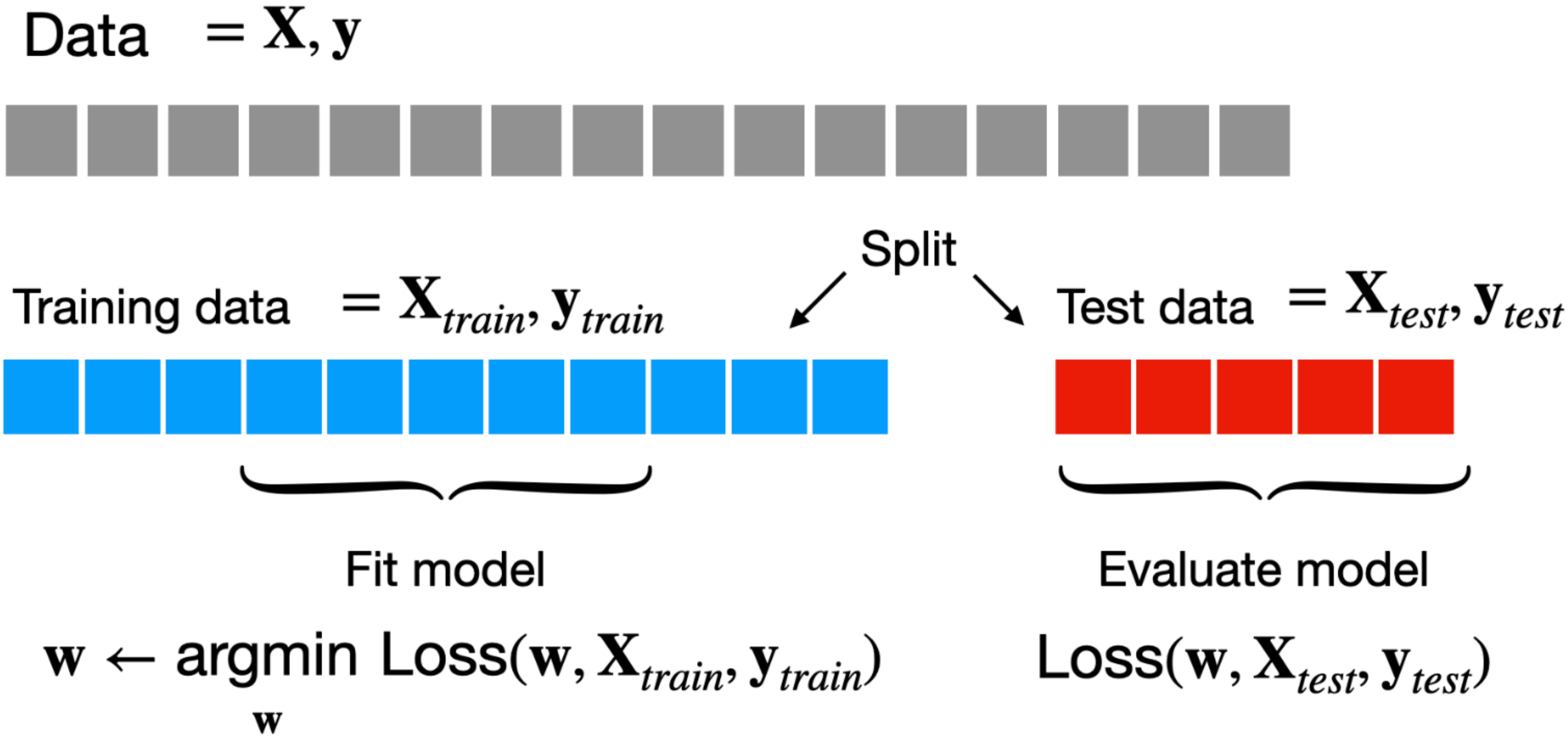


MSE Loss $= \frac{1}{N} \sum_{i=1}^{N} \left(f(x_i) - y_y\right)^2$

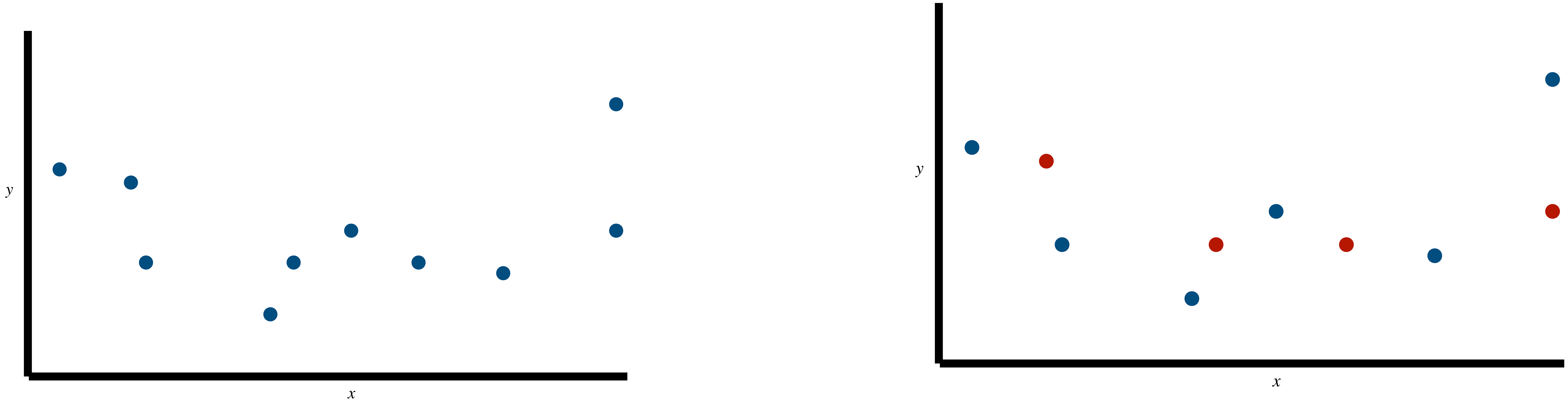
What if we then see new data?

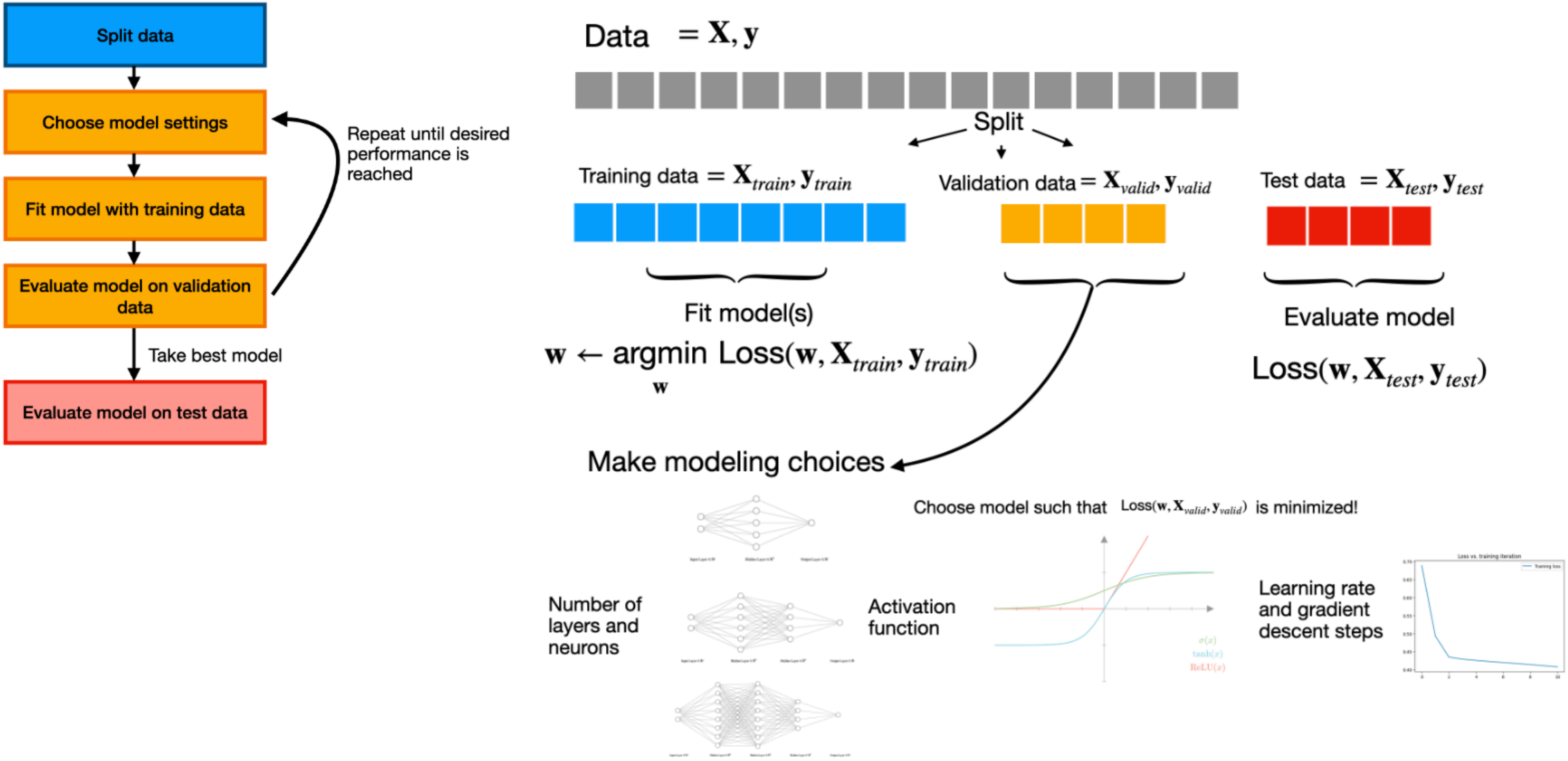


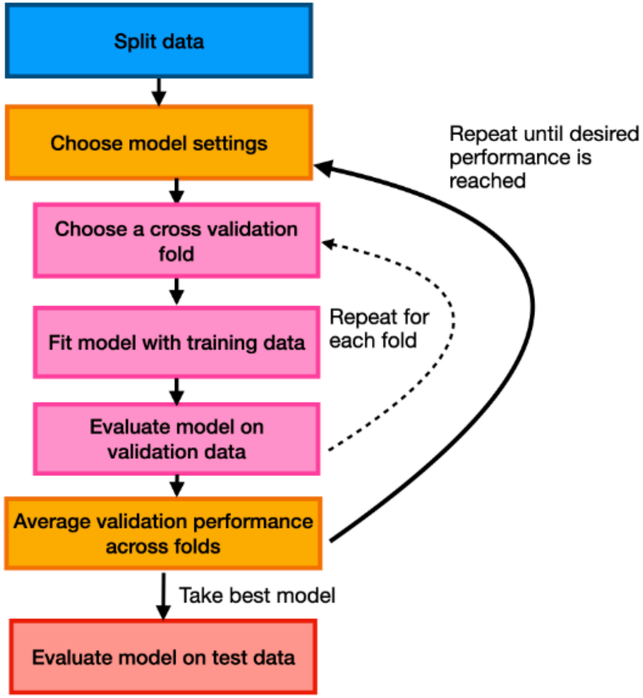
MSE Loss $= \frac{1}{N}\sum_{i=1}^{N}\left(f(x_i) - y_y\right)^2$

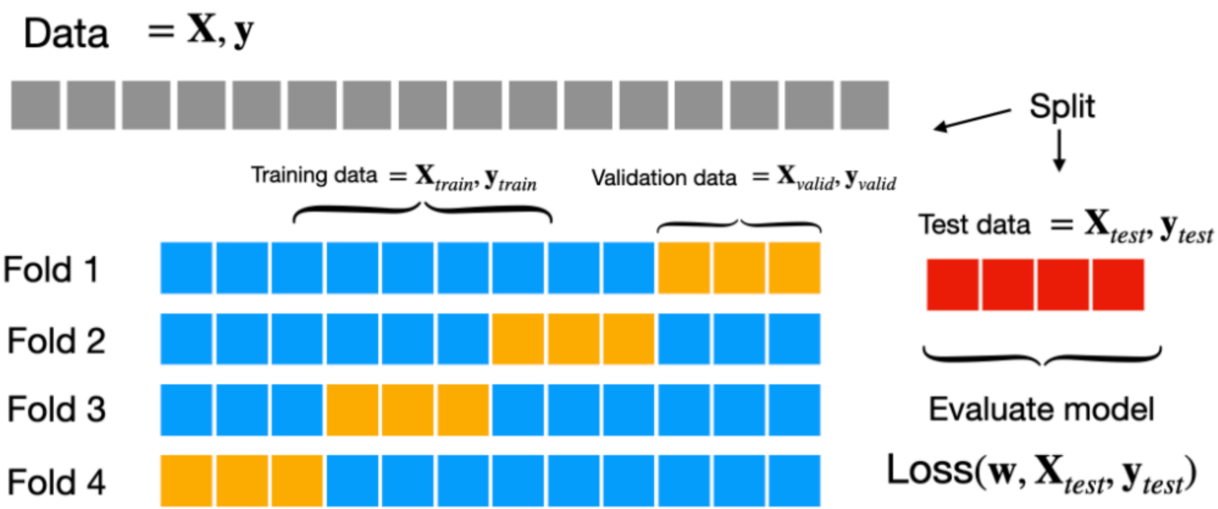

Data $= \mathbf{X}, \mathbf{y}$
Split
Training data $= \mathbf{X}_{train}, \mathbf{y}_{train}$
Test data $= \mathbf{X}_{test}, \mathbf{y}_{test}$
Fit model
Evaluate model
$\mathbf{w} \leftarrow \underset{\mathbf{w}}{\text{argmin}} \; \text{Loss}(\mathbf{w}, \mathbf{X}_{train}, \mathbf{y}_{train})$
$\text{Loss}(\mathbf{w}, \mathbf{X}_{test}, \mathbf{y}_{test})$

Train-test split




Split data
Choose model settings
Fit model with training data
Evaluate model on validation data
Take best model
Evaluate model on test data
Repeat until desired performance is reached
Data $= \mathbf{X}, \mathbf{y}$
Split
Training data $= \mathbf{X}_{train}, \mathbf{y}_{train}$
Validation data $= \mathbf{X}_{valid}, \mathbf{y}_{valid}$
Test data $= \mathbf{X}_{test}, \mathbf{y}_{test}$
Fit model(s)
$\mathbf{w} \leftarrow \operatorname{argmin}_{\mathbf{w}} \text{Loss}(\mathbf{w}, \mathbf{X}_{train}, \mathbf{y}_{train})$
Evaluate model
$\text{Loss}(\mathbf{w}, \mathbf{X}_{test}, \mathbf{y}_{test})$
Make modeling choices
Choose model such that $\text{Loss}(\mathbf{w}, \mathbf{X}_{valid}, \mathbf{y}_{valid})$ is minimized!
Number of layers and neurons
Activation function
$\sigma(x)$
$\tanh(x)$
$\text{ReLU}(x)$
Learning rate and gradient descent steps





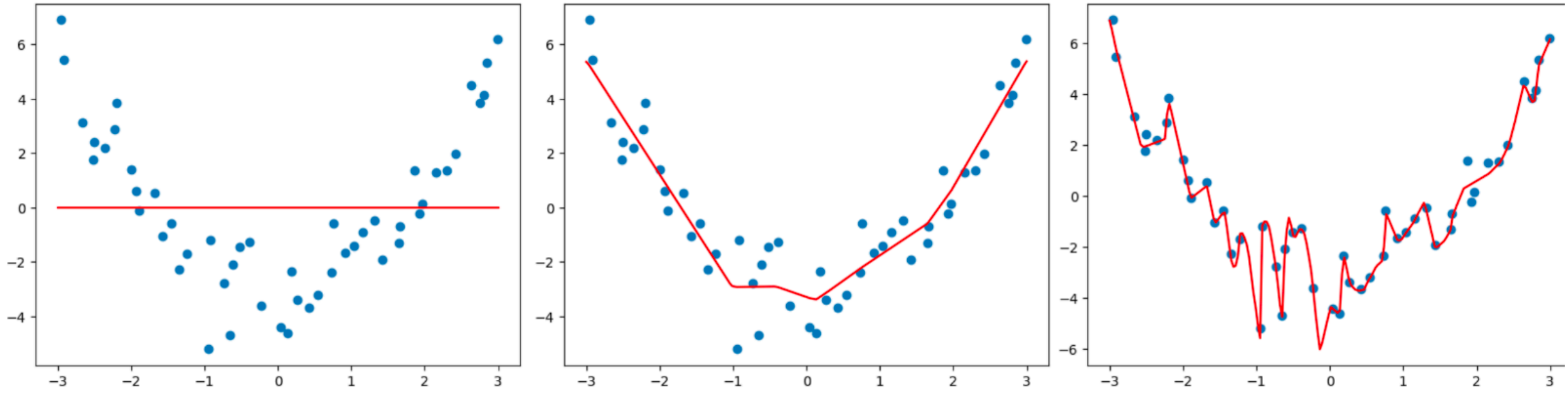
For *each* fold:

Fit model(s)

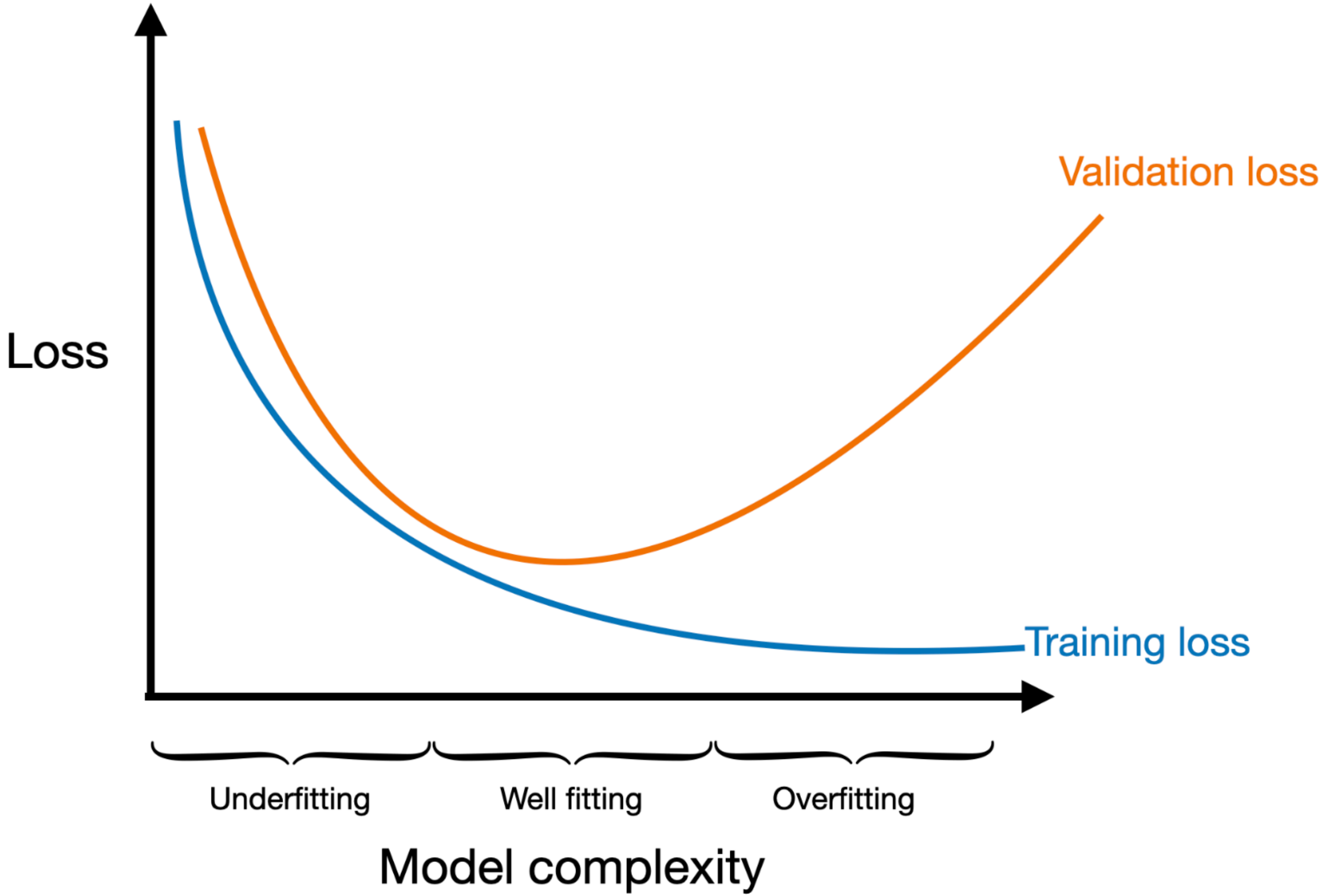
$$\mathbf{w} \leftarrow \underset{\mathbf{w}}{\text{argmin}}\ \text{Loss}(\mathbf{w}, \mathbf{X}_{train}, \mathbf{y}_{train})$$

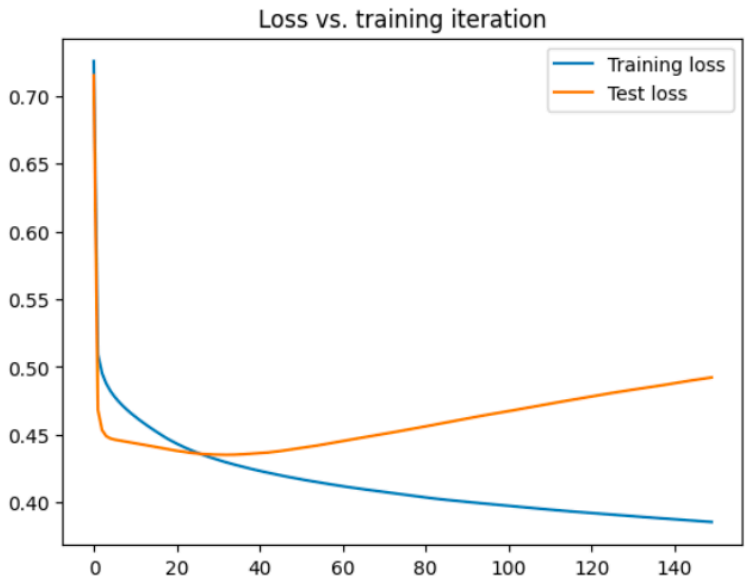
Evaluate model

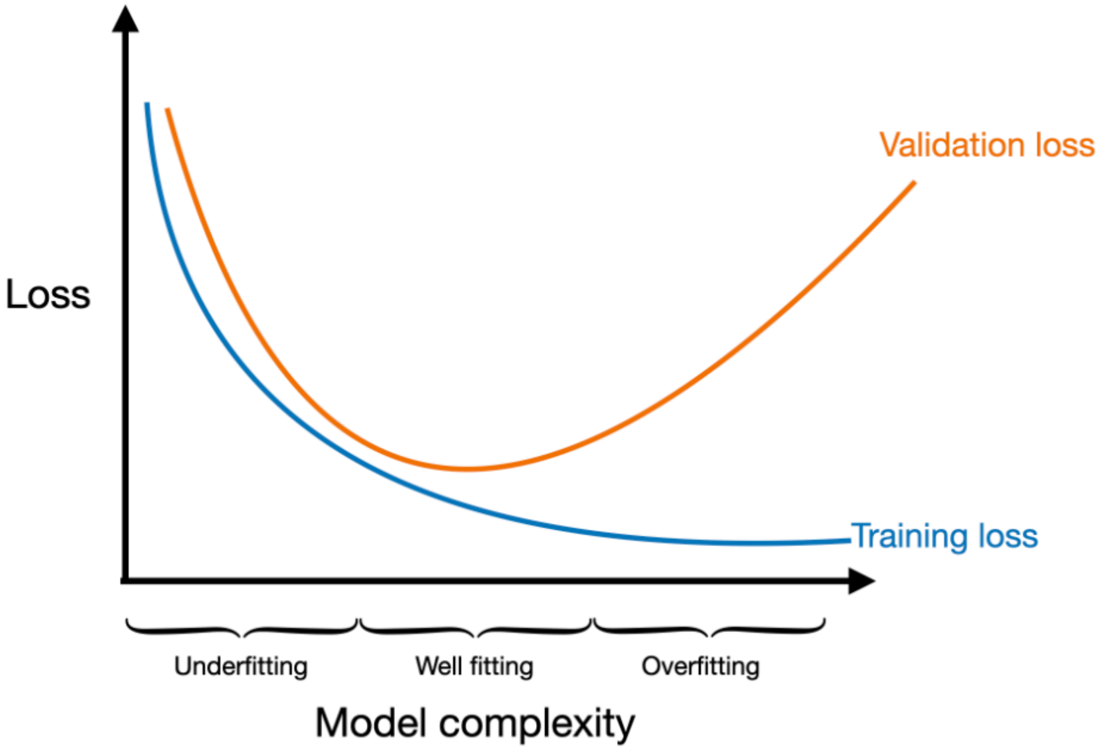
$$\text{Loss}(\mathbf{w}, \mathbf{X}_{valid}, \mathbf{y}_{valid})$$

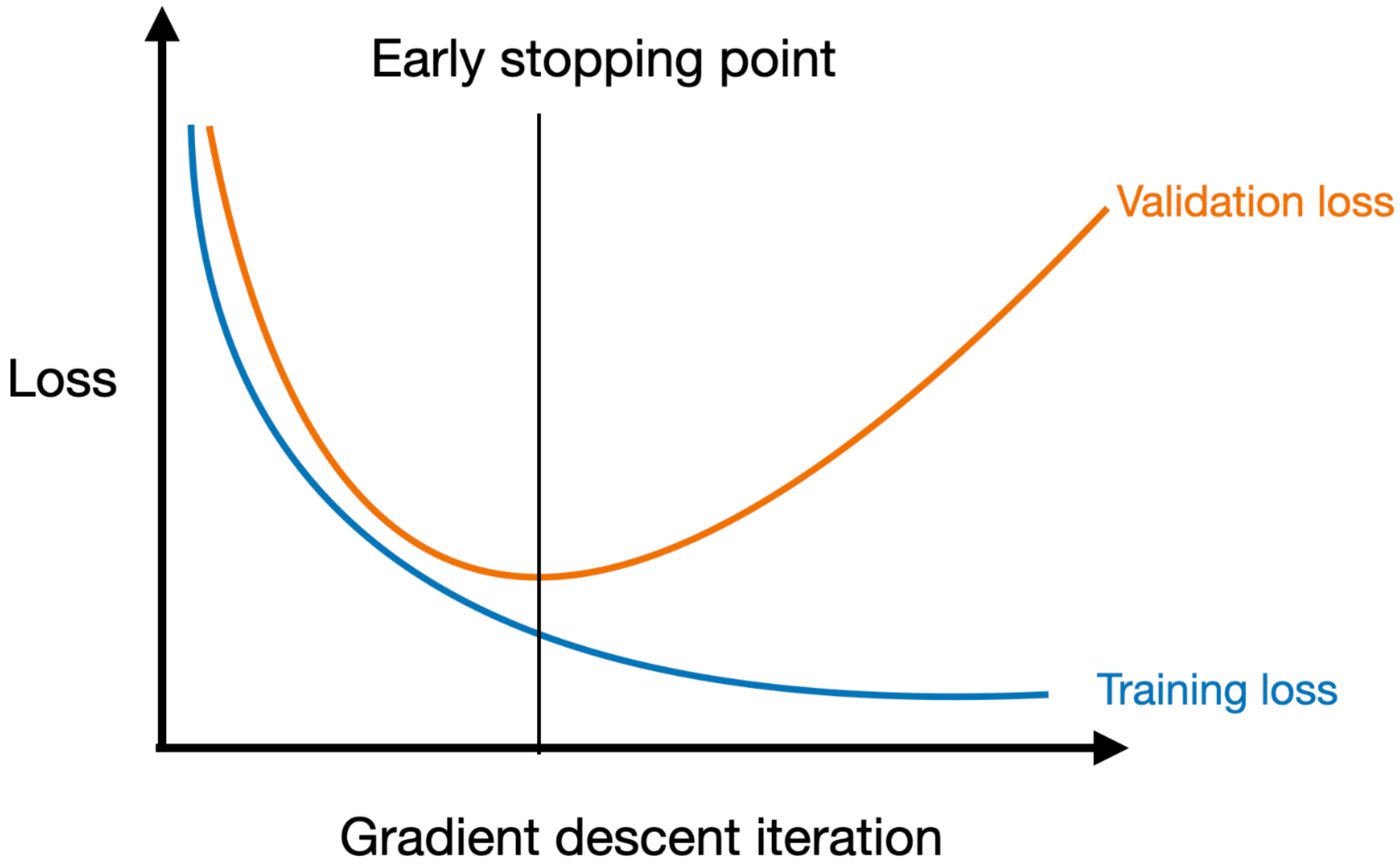


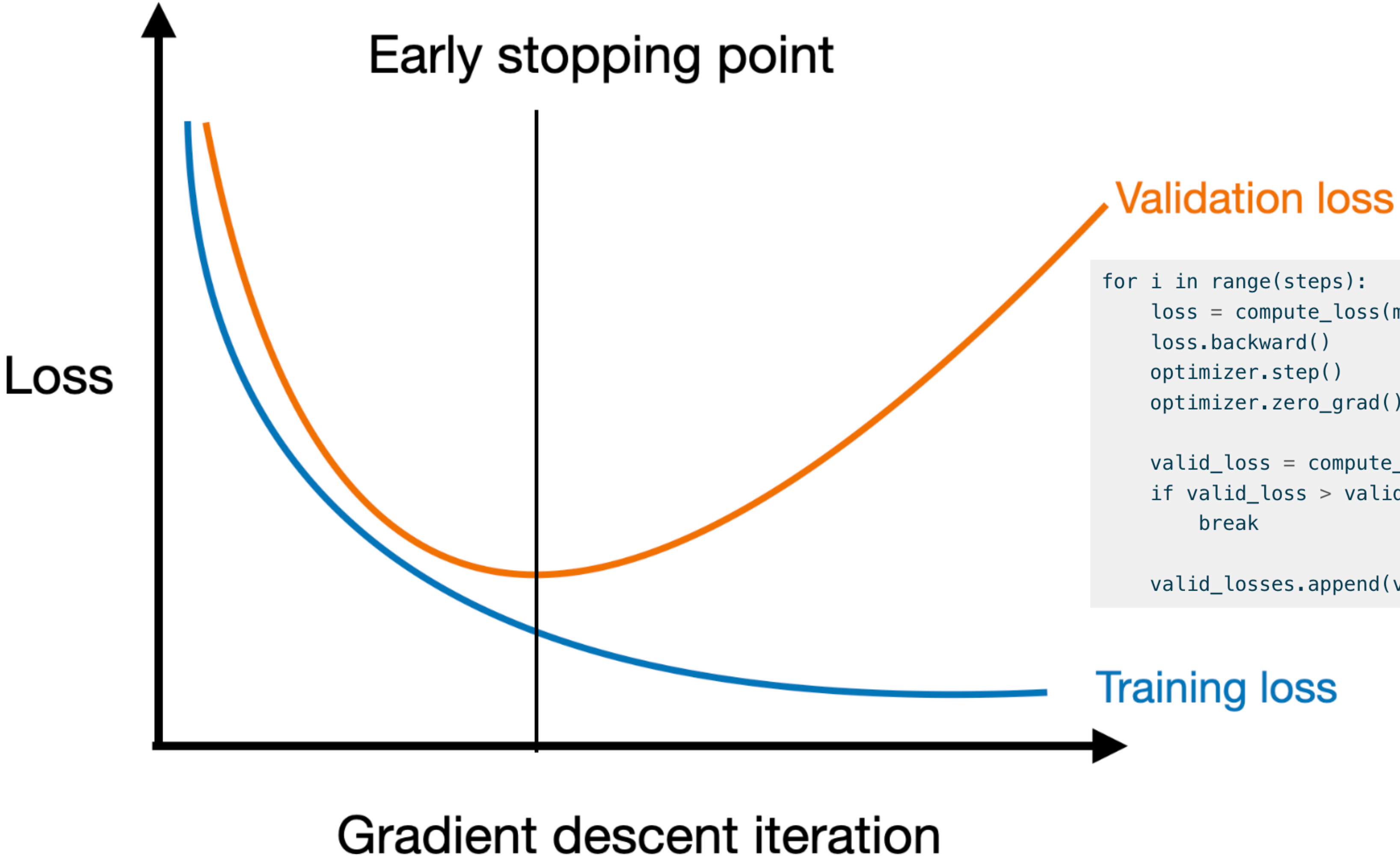
Underfitting Well-fit Overfit


Validation loss
Loss
Training loss
Underfitting
Well fitting
Overfitting
Model complexity

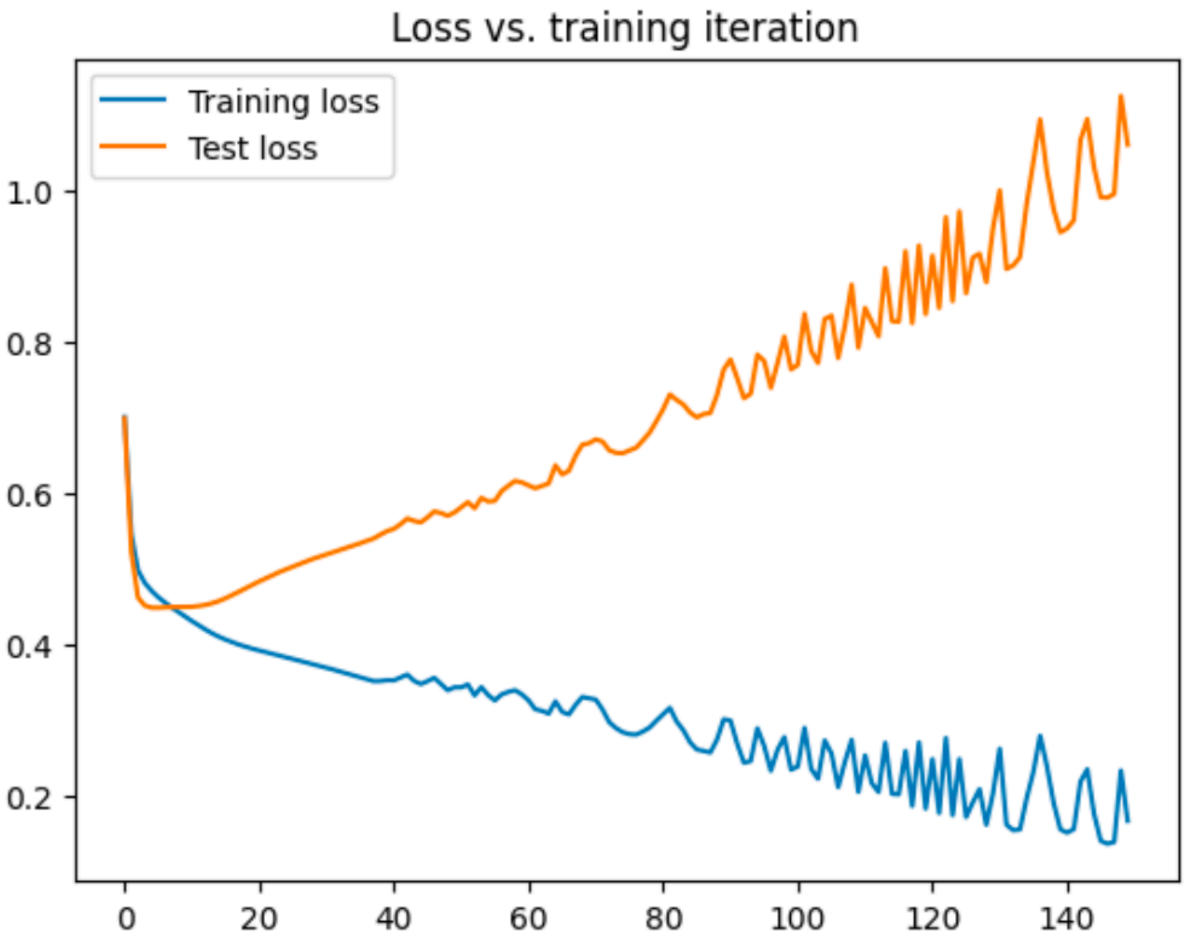

Loss vs. training iteration
Training loss
Test loss
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0
20
40
60
80
100
120
140


Loss
Validation loss
Training loss
Underfitting
Well fitting
Overfitting
Model complexity

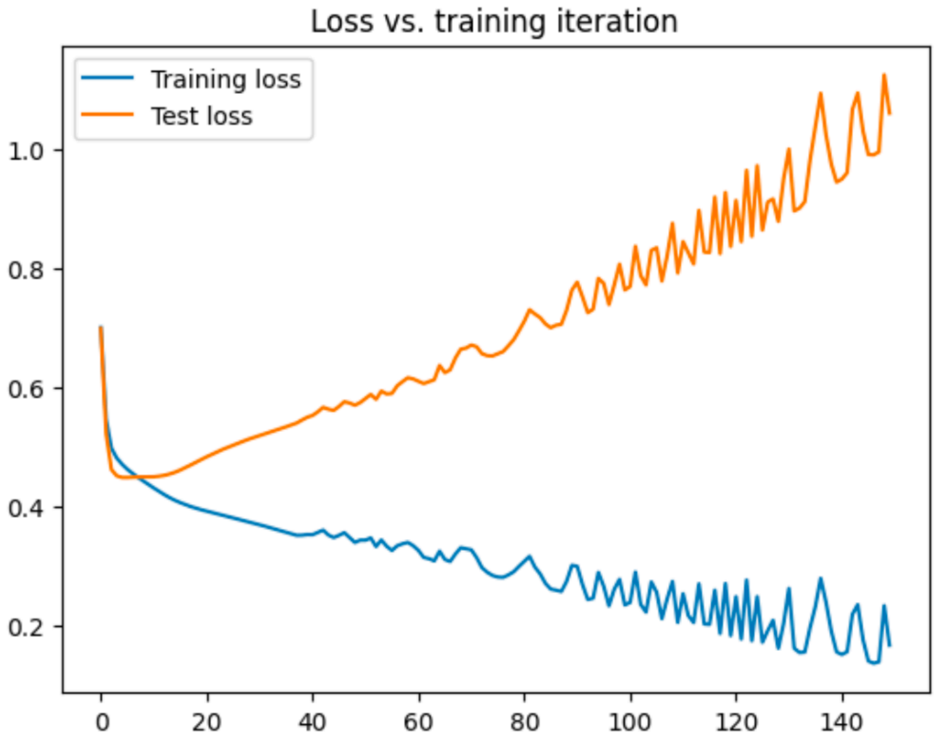

Early stopping point
Validation loss
Loss
Training loss
Gradient descent iteration



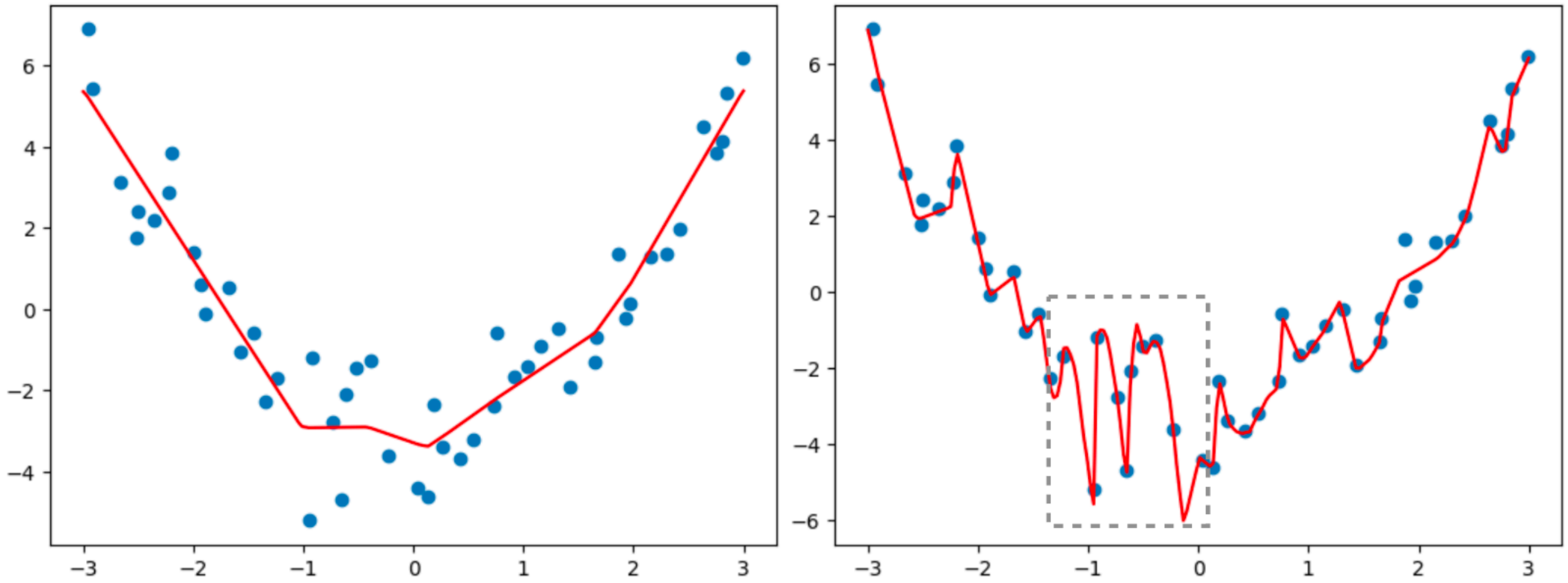

```python
for i in range(steps):
    loss = compute_loss(model, training_data)
    loss.backward()
    optimizer.step()
    optimizer.zero_grad()

    valid_loss = compute_loss(model, training_data)
    if valid_loss > valid_losses[-1]:
        break

    valid_losses.append(valid_loss)
```



Loss vs. training iteration
Training loss
Test loss
1.0
0.8
0.6
0.4
0.2
0
20
40
60
80
100
120
140

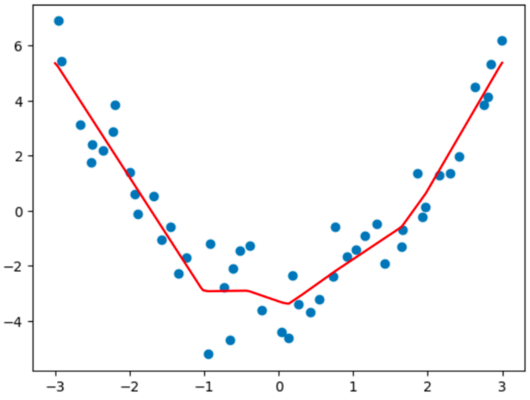



```
patience = 5                    # Number of steps to wait before stopping
steps_since_improvement = 0     # Steps since validation loss improved
min_loss = 1e8                  # Minimum loss seen so far (start large)

for i in range(steps):
    ...

    valid_loss = compute_loss(model, training_data)

    # If the validation loss improves reset the counter
    if valid_loss < min_loss:
        steps_since_improvement = 0
        min_loss = valid_loss

    # Otherwise increment the counter
    else:
        steps_since_improvement += 1

    # If its been patience steps since the last improvement, stop
    if steps_since_improvement == patience:
        break
```

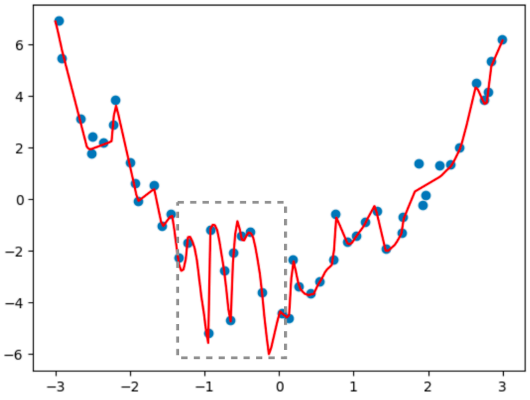


Well-fit Overfit

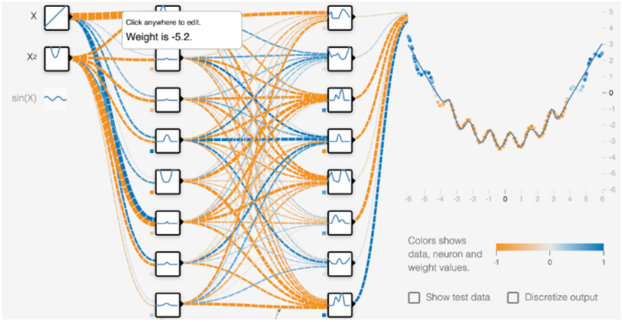
$$\mathbf{MSE}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} ((f(\mathbf{x}_i, \mathbf{w}) - y_i)^2)$$



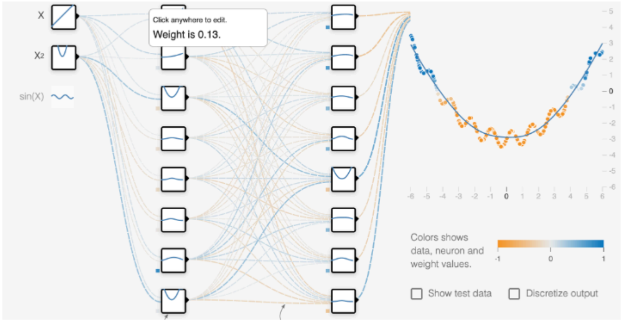
Well-fit



Overfit



An overfit network will have large weights to encode large slopes.



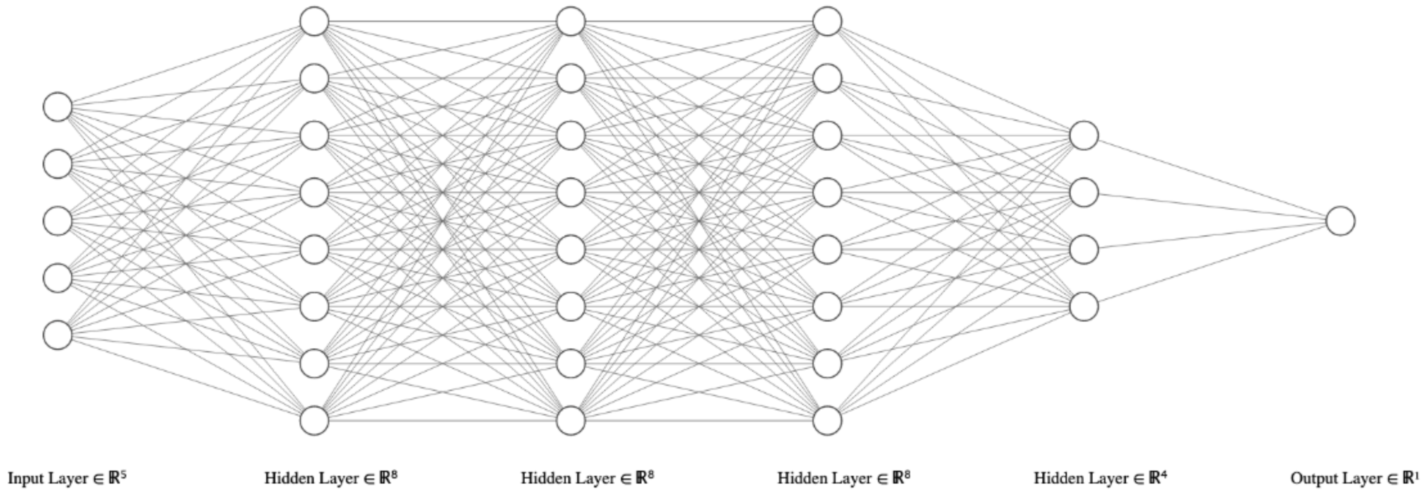
A regularized network will have smaller weights encoding a smooth function.

$$\mathbf{L}_2(\mathbf{w}) = \|\mathbf{w}\|_2^2 = \sum_{i=1}^{d} w_i^2$$

$$\mathbf{L}_2(\mathbf{W}) = \|\mathbf{W}\|_2^2 = \sum_{i=1}^{d} \sum_{j=1}^{e} w_{ij}^2$$

$$\mathbf{Loss}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \mathbf{MSE}(\mathbf{X}, \mathbf{y}, \mathbf{w}) + \lambda \mathbf{L}_2(\mathbf{w})$$

$$f(\mathbf{x}, \mathbf{w}_0, \dots) = \sigma(\sigma(\sigma(\sigma(\mathbf{x}^\mathbf{T}\mathbf{W}_4)^T\mathbf{W}_3)^T\mathbf{W}_2)^T\mathbf{W}_1)^T\mathbf{w}_0$$



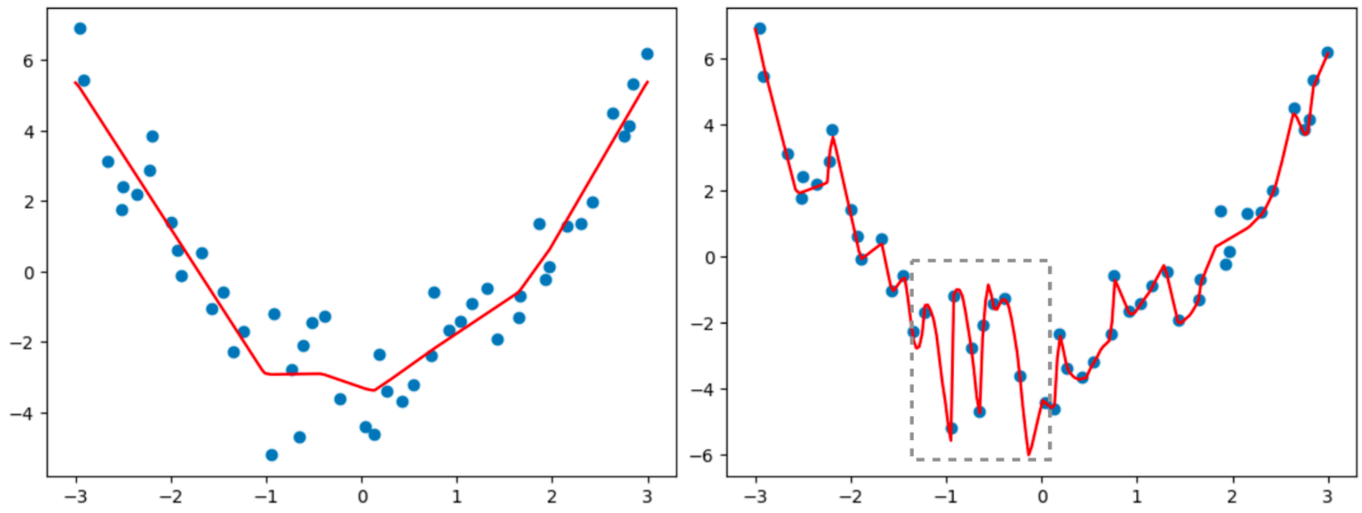
$$\mathbf{L}_2(\mathbf{w}_0, \mathbf{W}_1, \dots, \mathbf{W}_L) = \sum_{l=0}^{L} \|\mathbf{W}_l\|_2^2$$

In practice most networks also incorporate bias terms, so each linear function in our network can be written as:

$$\mathbf{x}^T\mathbf{W} + \mathbf{b}$$

And the full prediction function for a sigmoid-activation network might be:

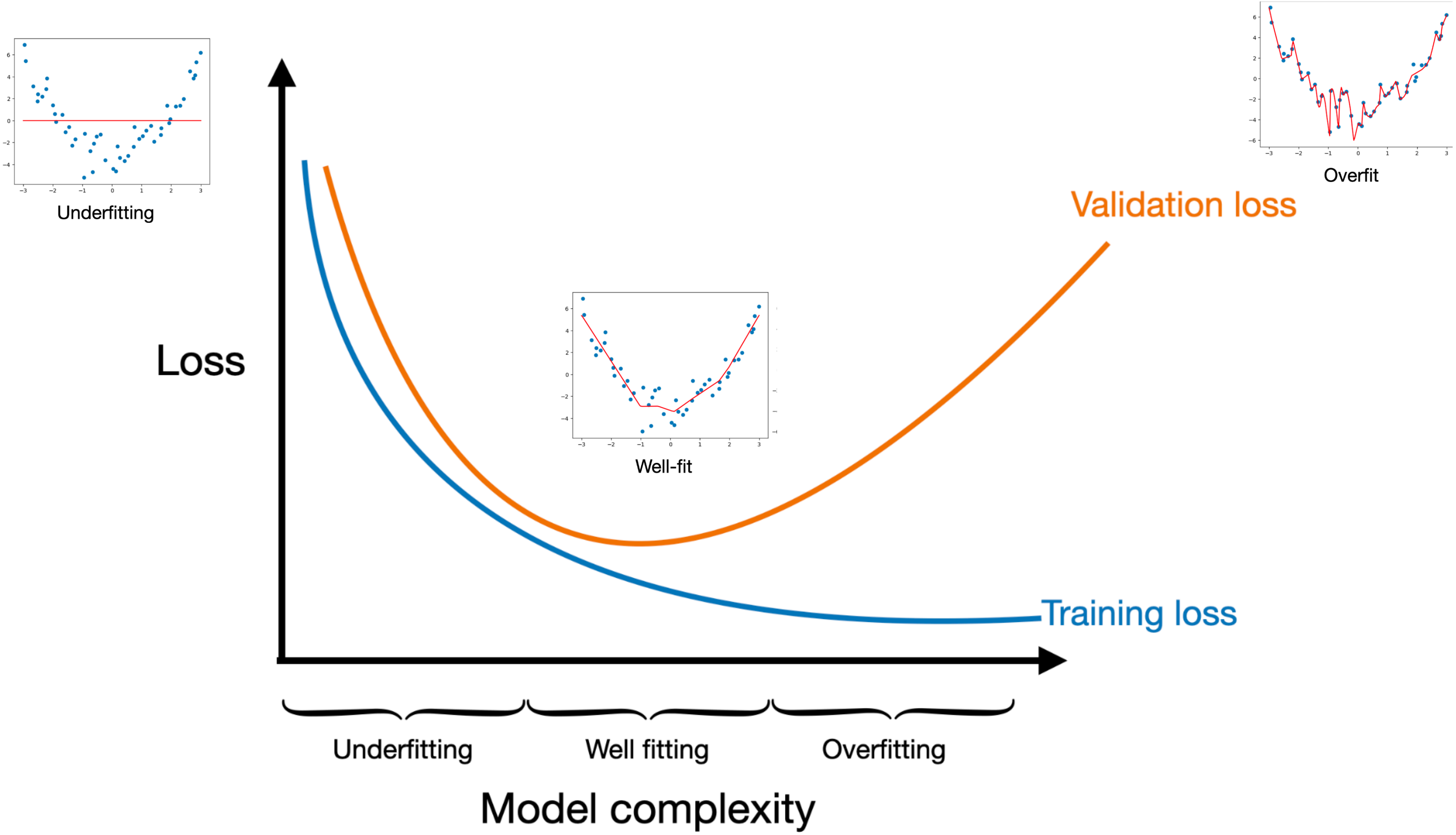
$$f(\mathbf{x}, \mathbf{w}_0, \ldots) = \sigma(\sigma(\sigma(\sigma(\mathbf{x}^{\mathbf{T}}\mathbf{W}_4 + \mathbf{b}_4)^T\mathbf{W}_3 + \mathbf{b}_3)^T\mathbf{W}_2 + \mathbf{b}_2)^T\mathbf{W}_1 + \mathbf{b}_1)^T\mathbf{w}_0 + \mathbf{b}_0$$



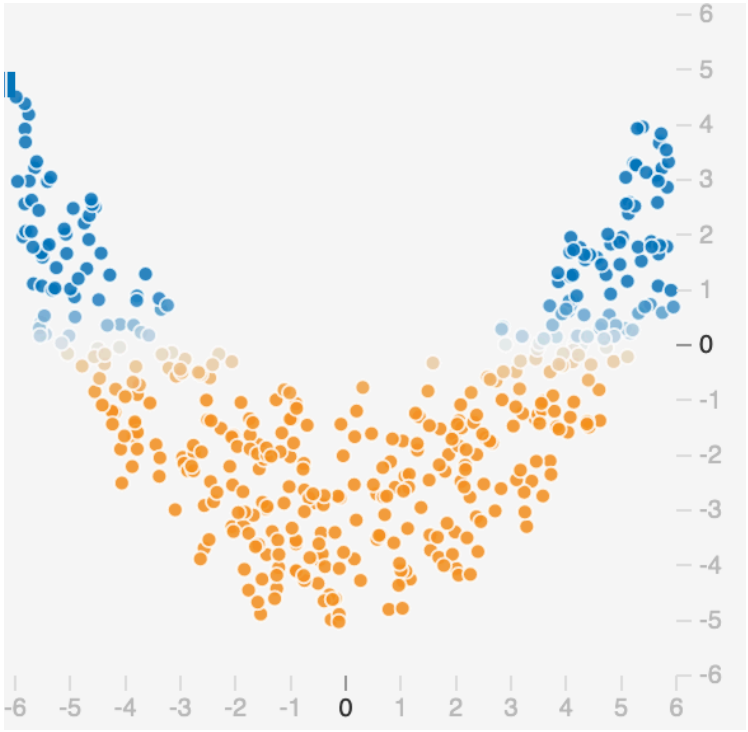
Well-fit

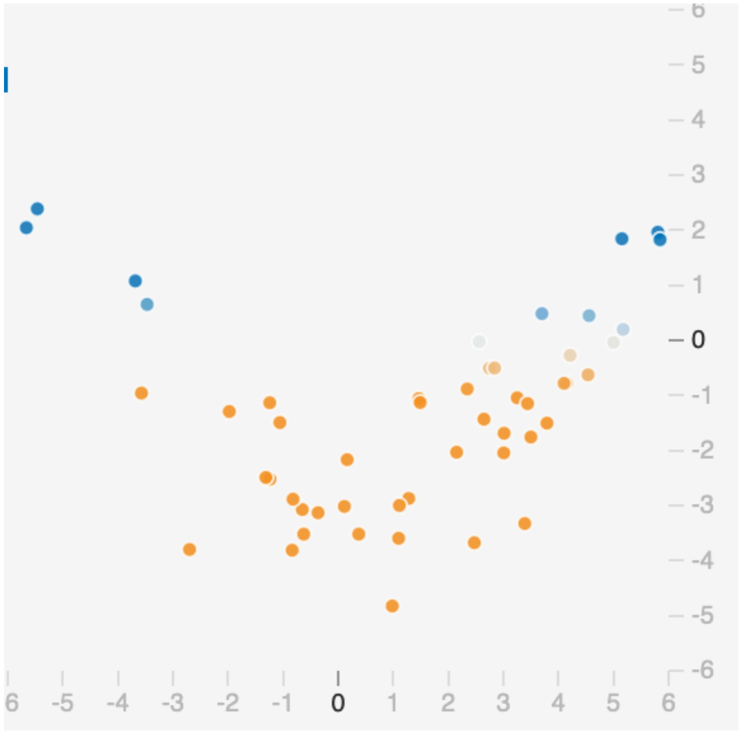
Overfit

Does the bias contribute to overfitting?

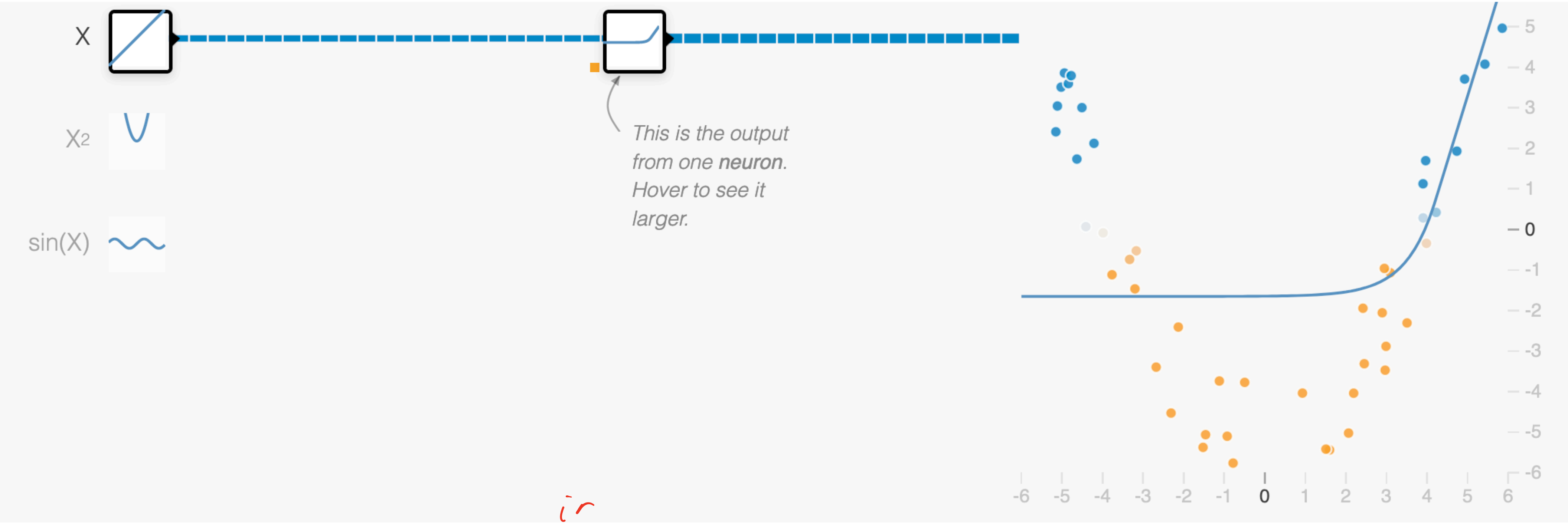

Underfitting
Overfit
Validation loss
Loss
Well-fit
Training loss
Underfitting
Well fitting
Overfitting
Model complexity

Sampling data

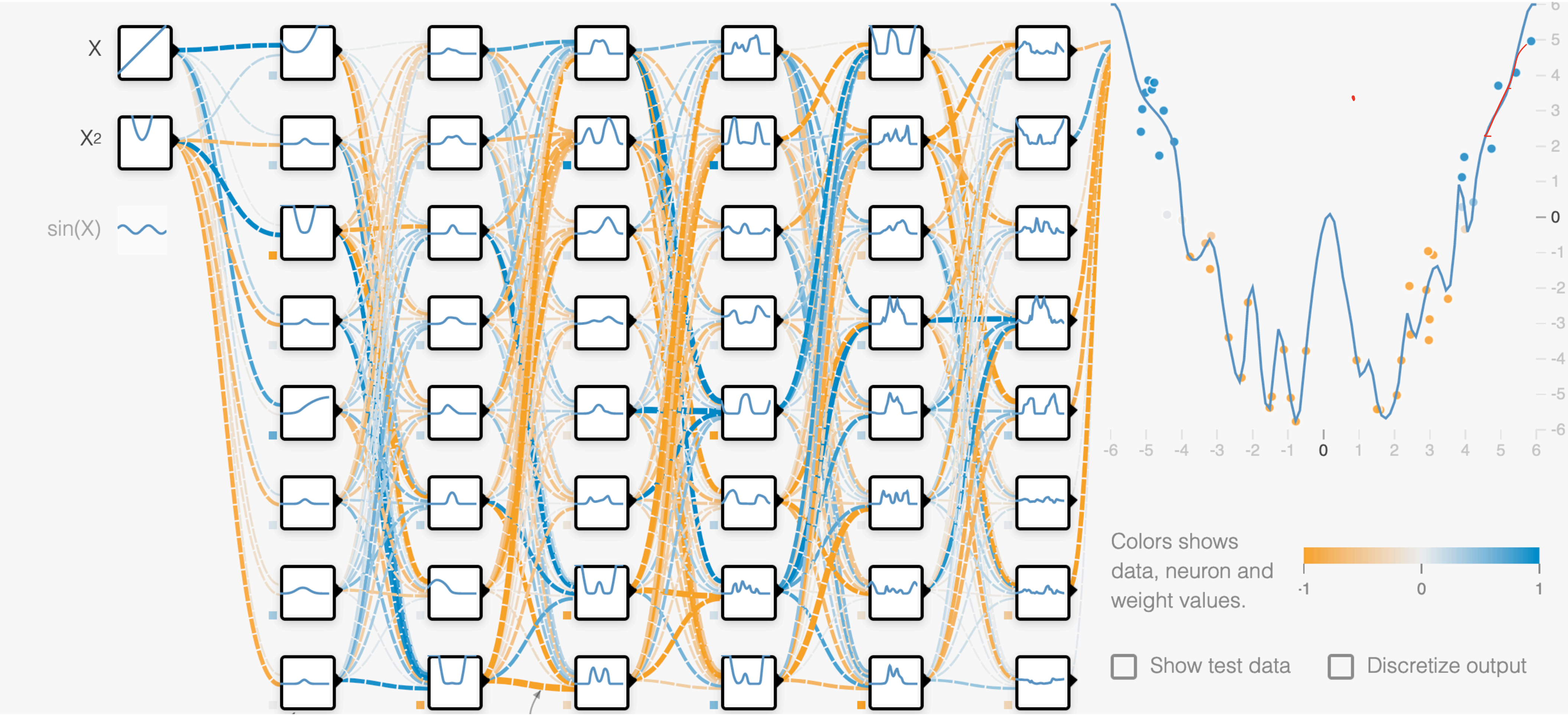




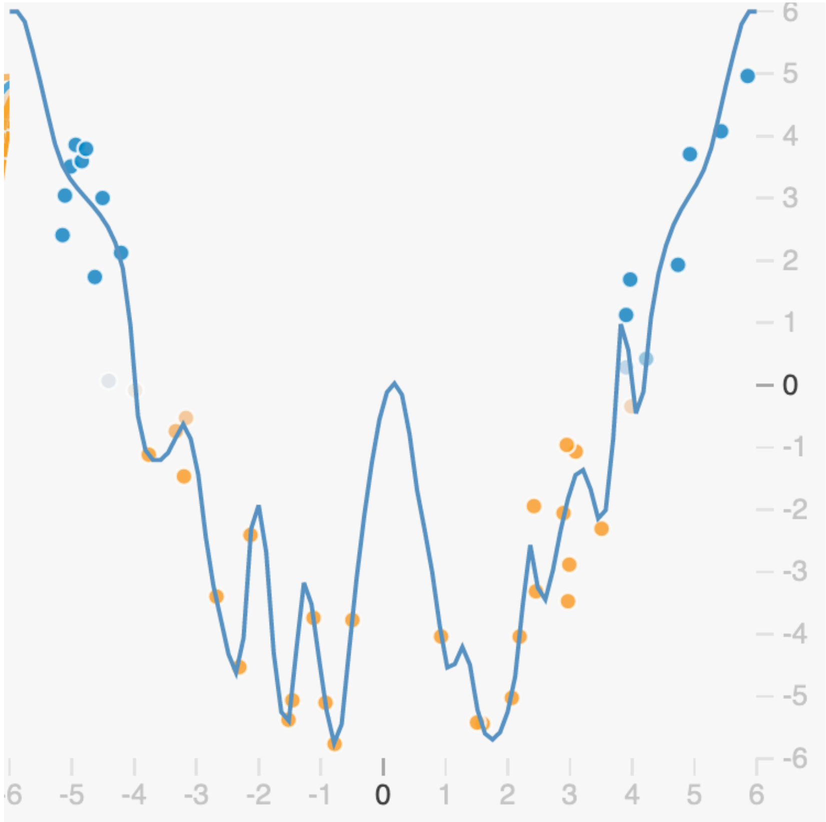
Underfitting

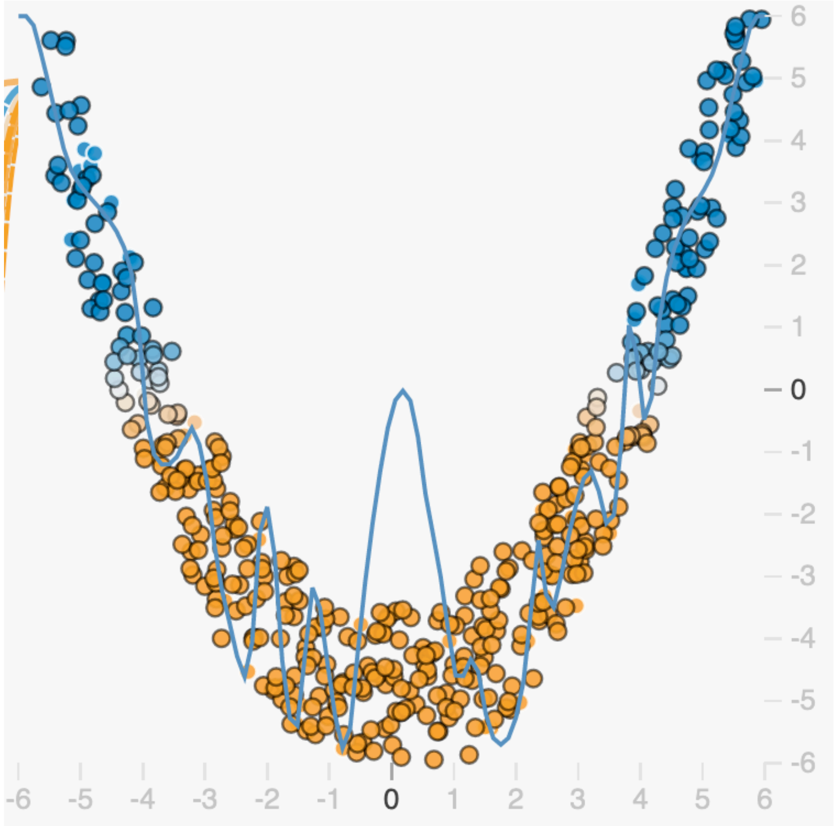


Overfitting

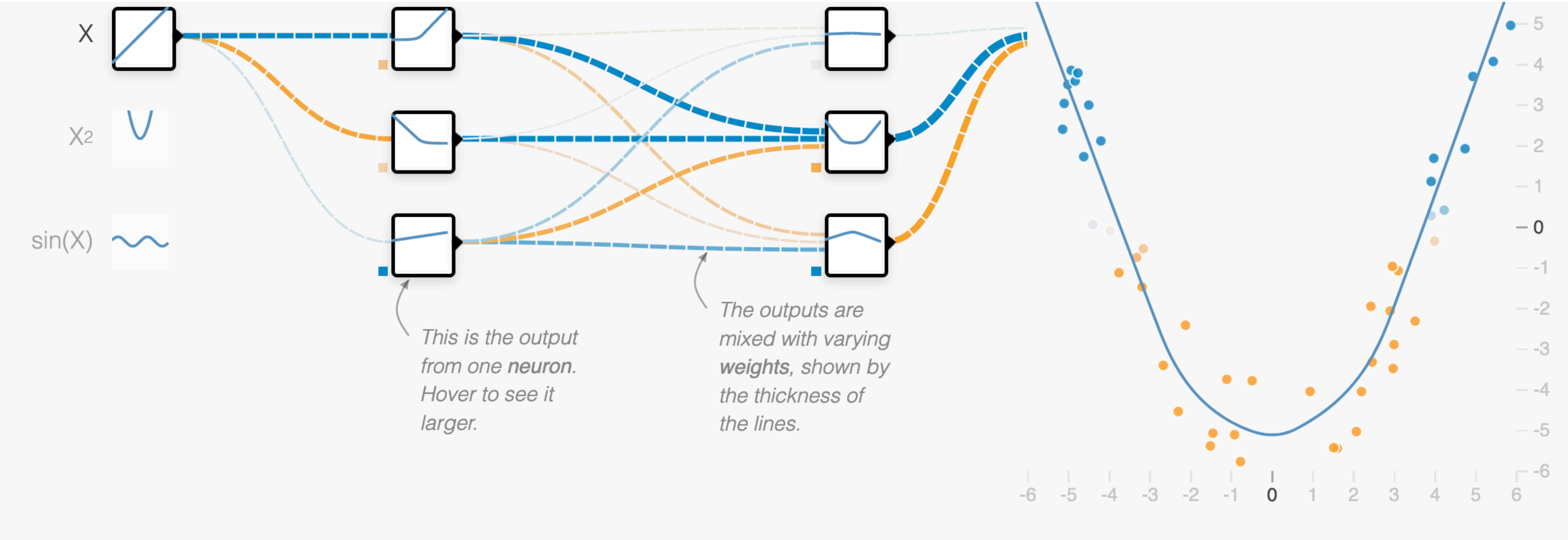


Overfitting

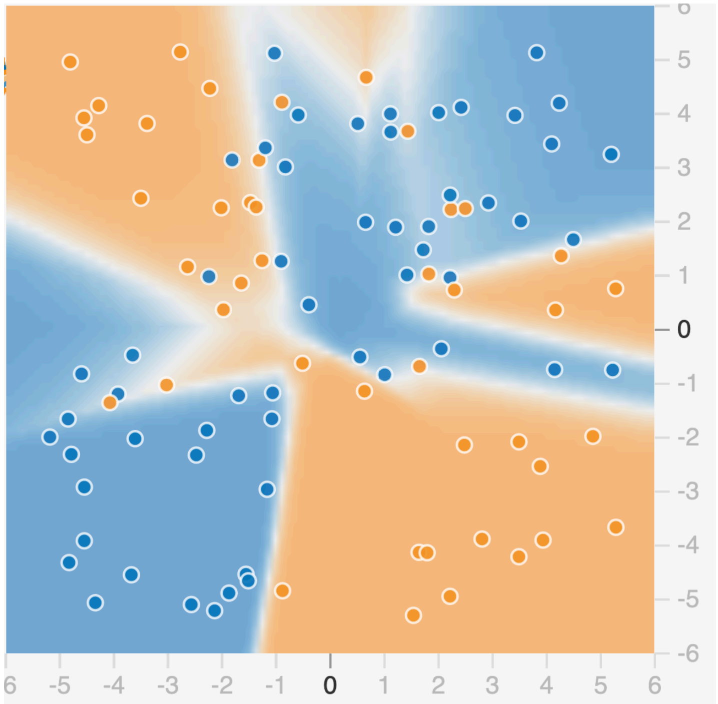


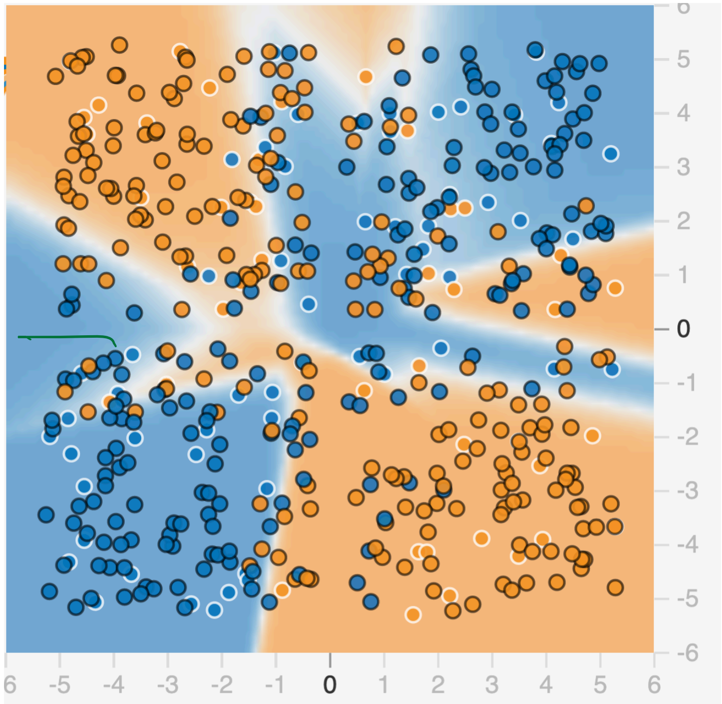


Good fit

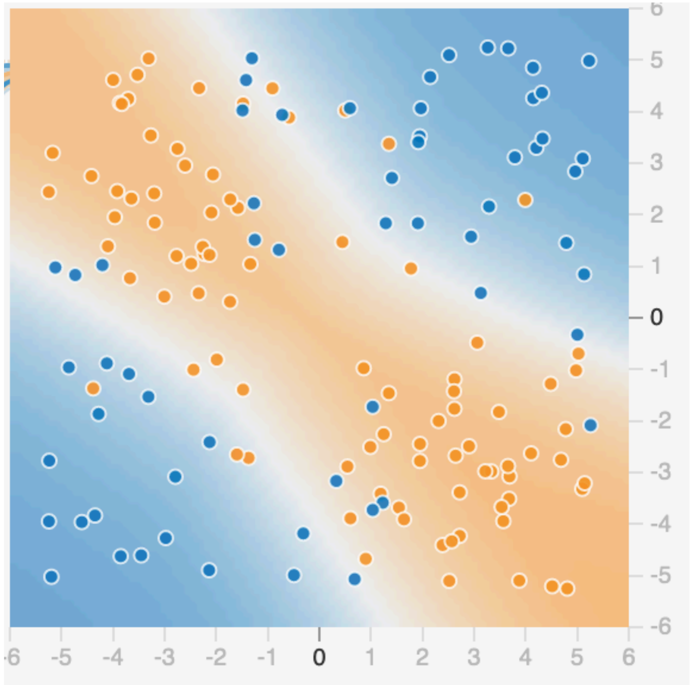

X
X2
sin(X)
This is the output from one **neuron**. Hover to see it larger.
The outputs are mixed with varying **weights**, shown by the thickness of the lines.
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6

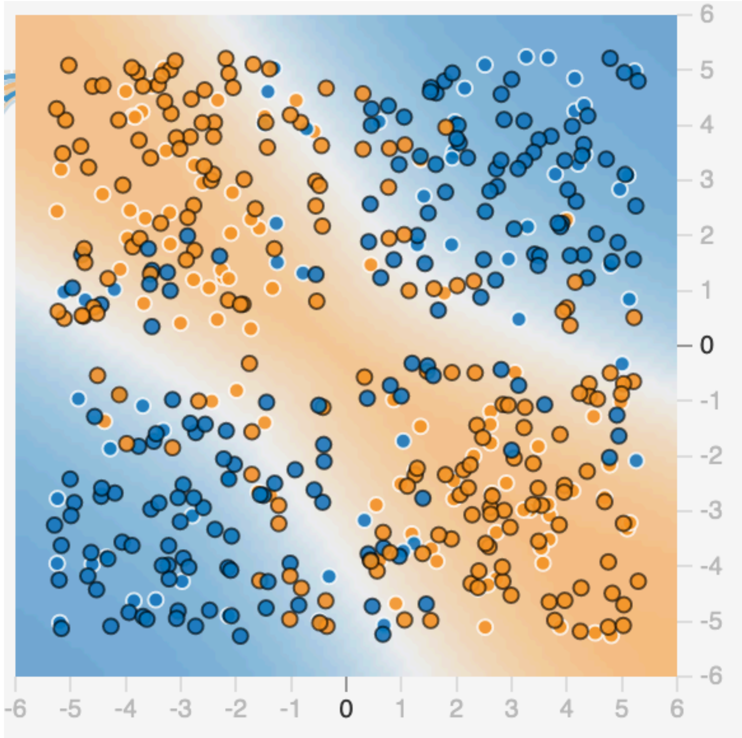
Overfitting

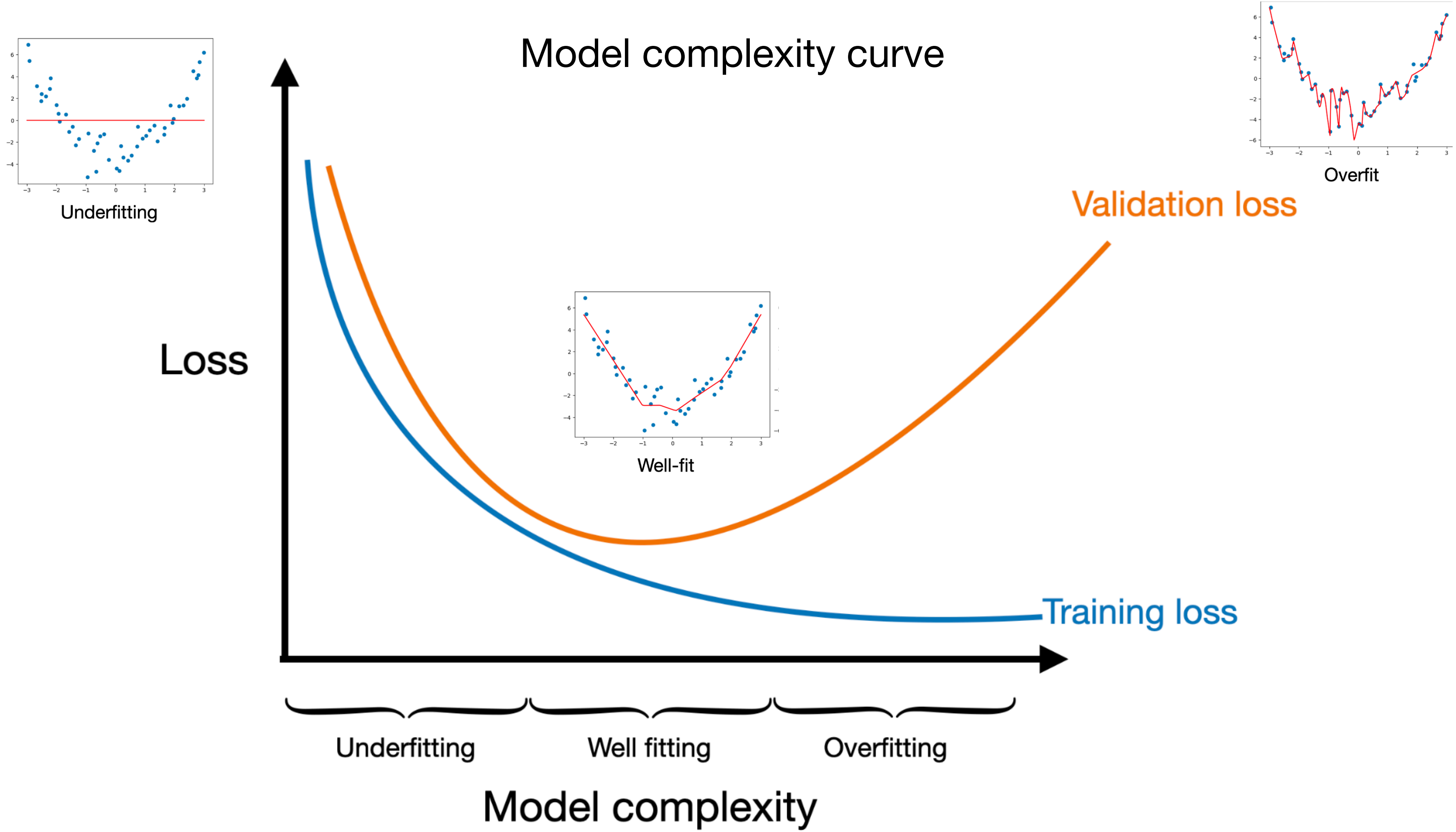




Better fit

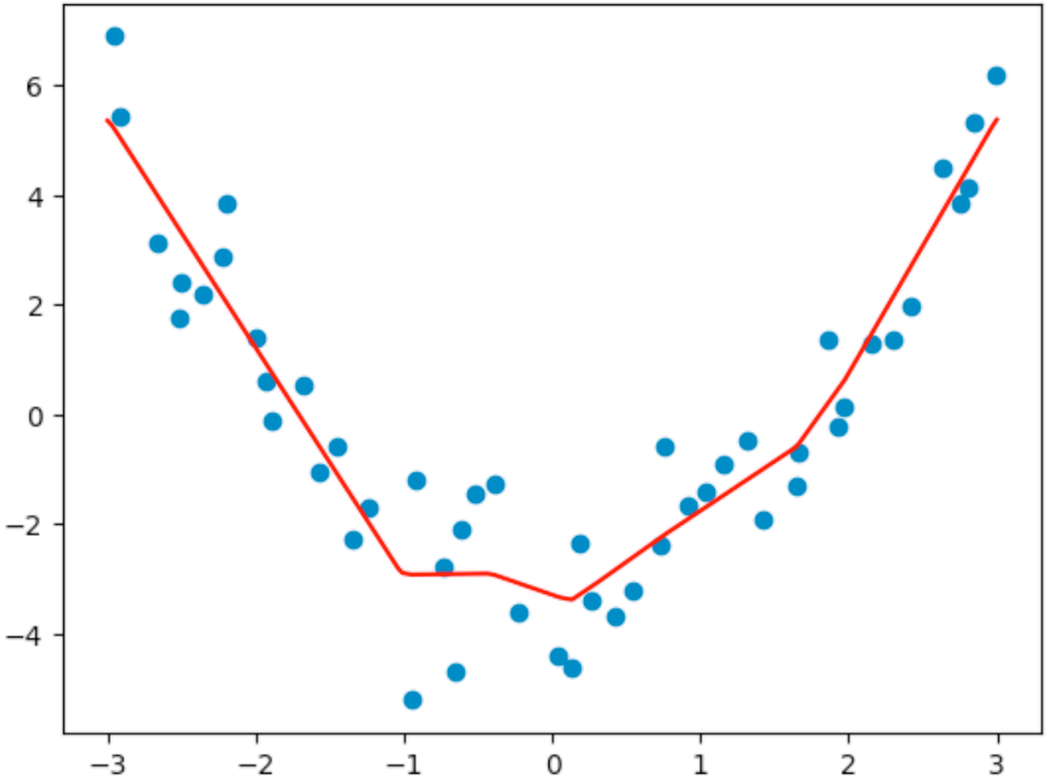

6
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6


6
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6

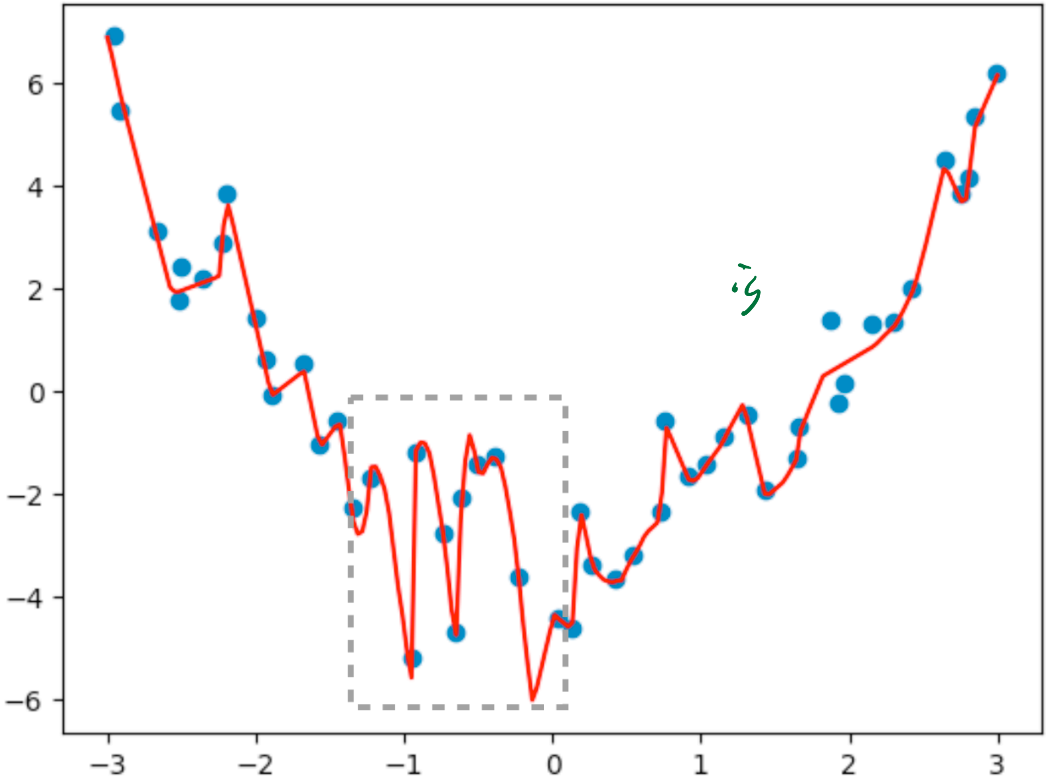

Model complexity curve
Underfitting
Overfit
Validation loss
Well-fit
Loss
Training loss
Underfitting
Well fitting
Overfitting
Model complexity

	Underfitting	Overfitting	Good fit
Training loss:			
Test loss:			

Overfitting with high weights

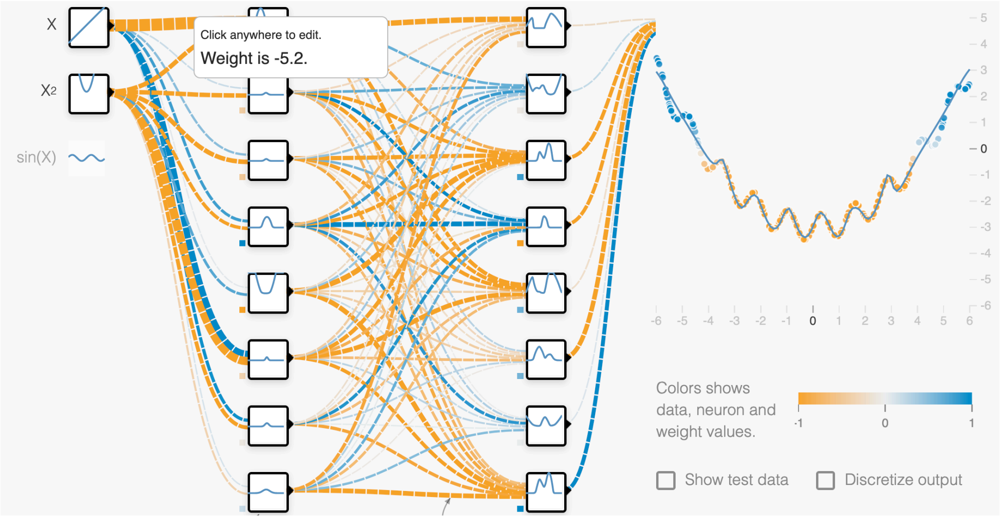


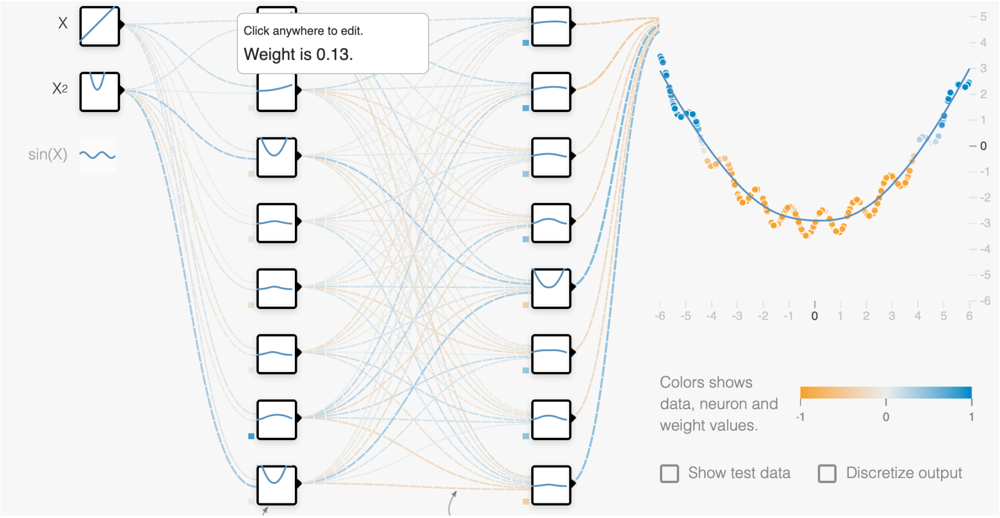
Well-fit



Overfit

Overfitting with high weights

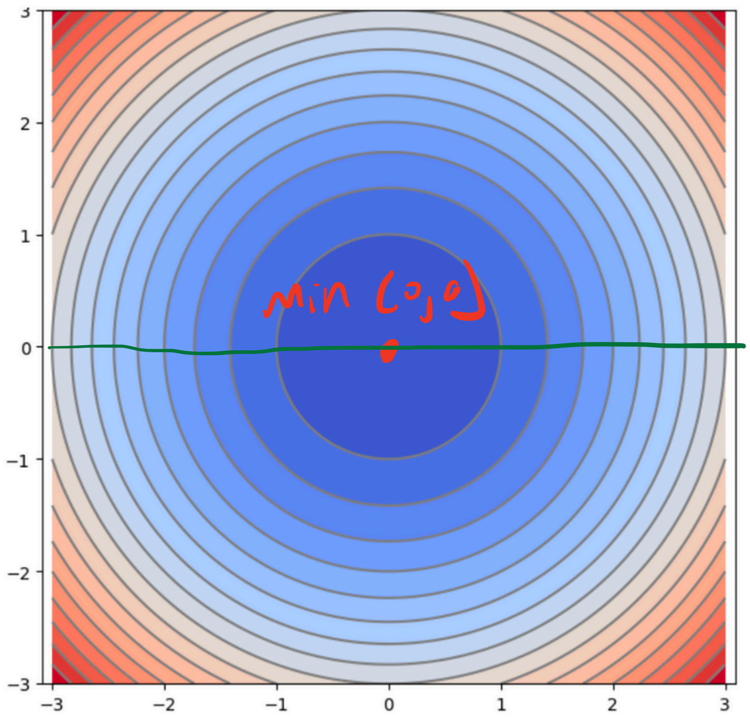




L2 Regularization

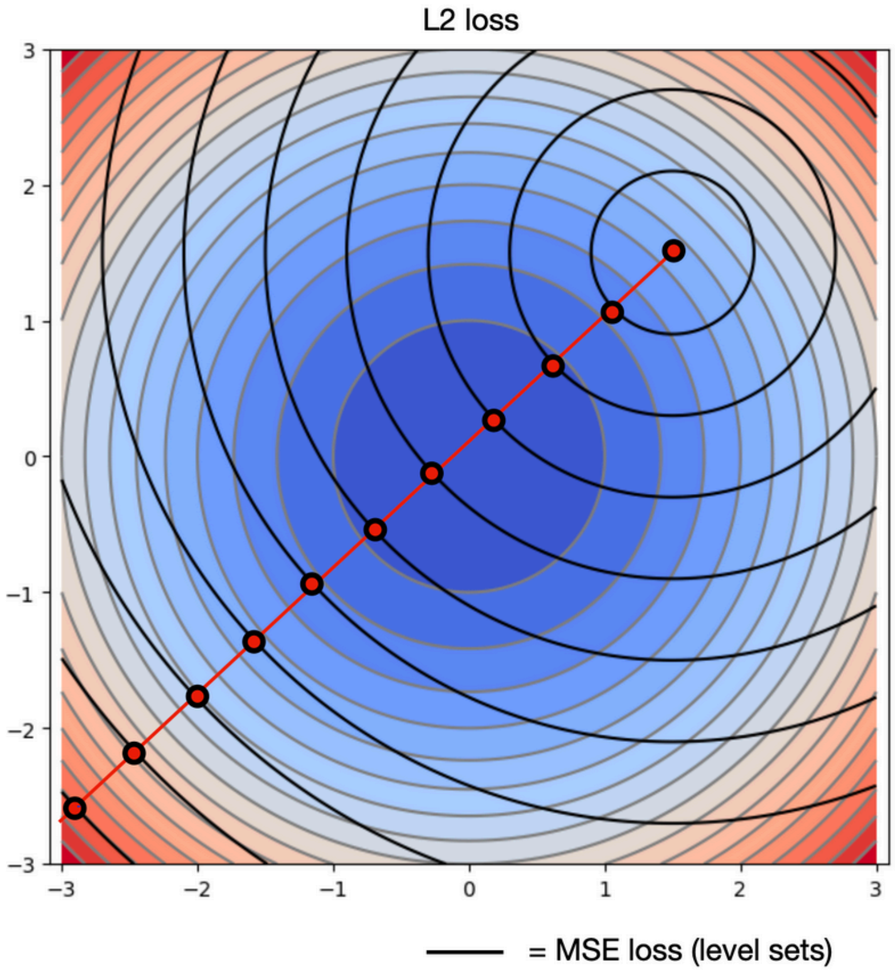
L2-Loss

$$\ell^2 = w_1^2 + w_2^2$$



$$\mathbf{L}_2(\mathbf{W}) = \|\mathbf{W}\|_2^2 = \sum_{i=1}^{d}\sum_{j=1}^{e} w_{ij}^2$$

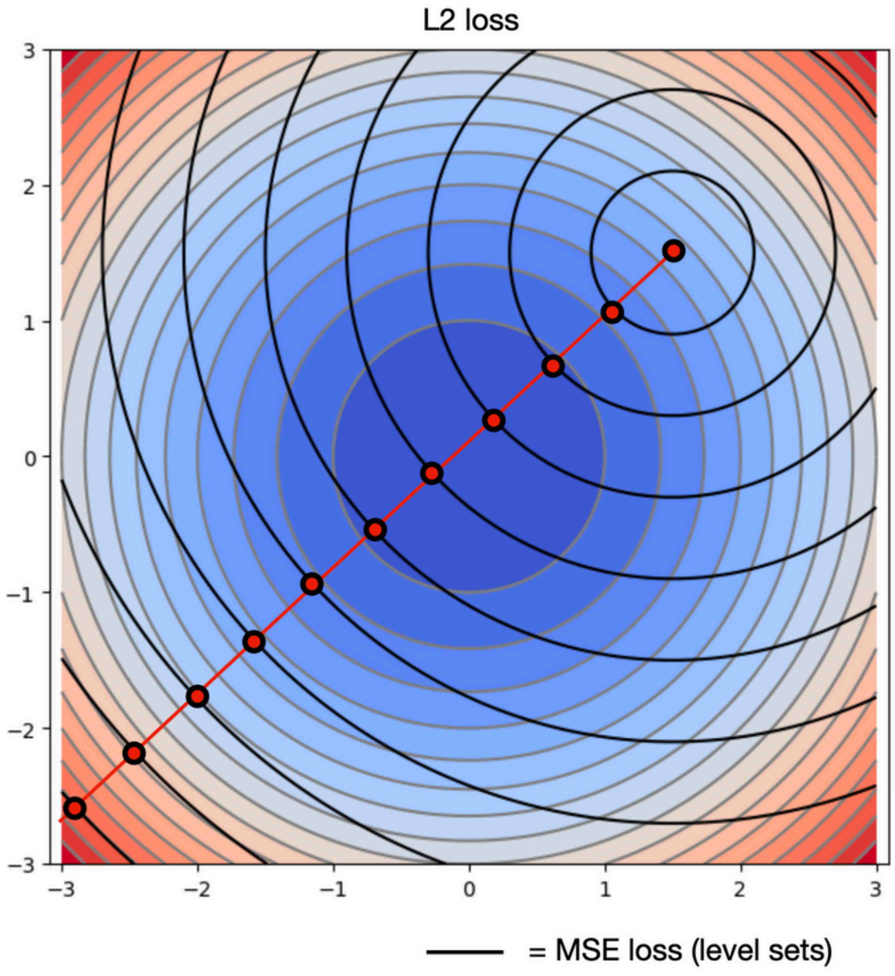
L2 Regularization



$$\mathbf{L}_2(\mathbf{W}) = \|\mathbf{W}\|_2^2 = \sum_{i=1}^{d}\sum_{j=1}^{e} w_{ij}^2$$

$$\mathbf{Loss}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \mathbf{MSE}(\mathbf{X}, \mathbf{y}, \mathbf{w}) + \lambda \mathbf{L}_2(\mathbf{w})$$

L2 Regularization



$$\mathbf{L}_2(\mathbf{W}) = \|\mathbf{W}\|_2^2 = \sum_{i=1}^{d}\sum_{j=1}^{e} w_{ij}^2$$

$$\mathbf{Loss}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \mathbf{MSE}(\mathbf{X}, \mathbf{y}, \mathbf{w}) + \lambda \mathbf{L}_2(\mathbf{w})$$

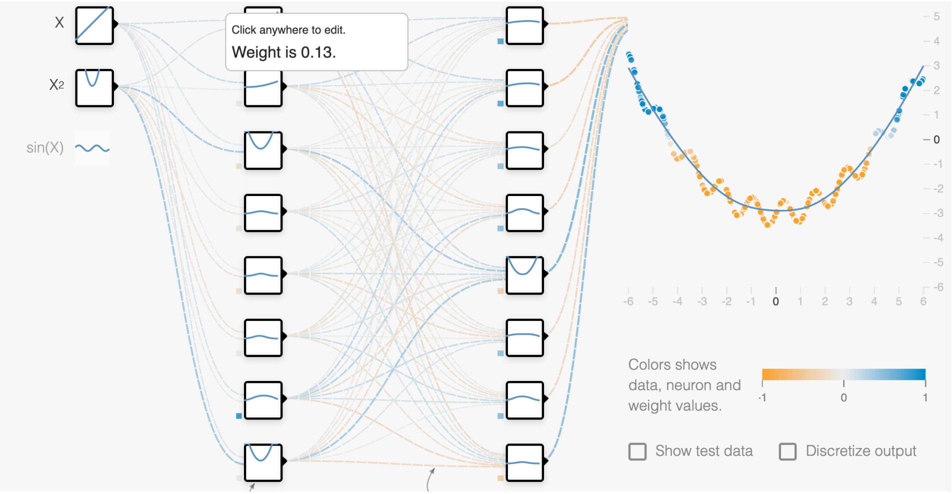
```
from torch import optim
optimizer = optim.SGD(model.parameters(), lr=0.1, weight_decay=0.01)
```

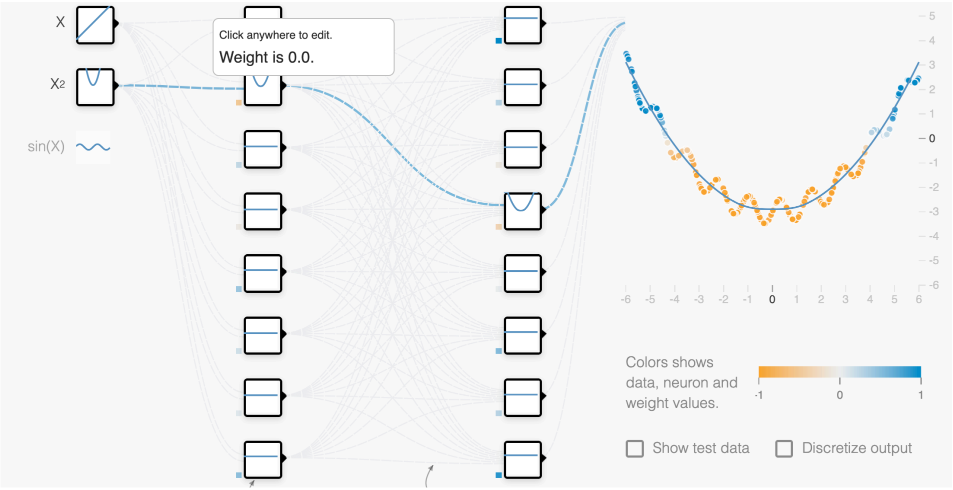
L1 Regularization

Vector: $\mathbf{L}_2(\mathbf{w}) = \|\mathbf{w}\|_2^2 = \sum_{i=1}^{d} w_i^2$ Matrix: $\mathbf{L}_2(\mathbf{W}) = \|\mathbf{W}\|_2^2 = \sum_{i=1}^{d} \sum_{j=1}^{e} w_{ij}^2$

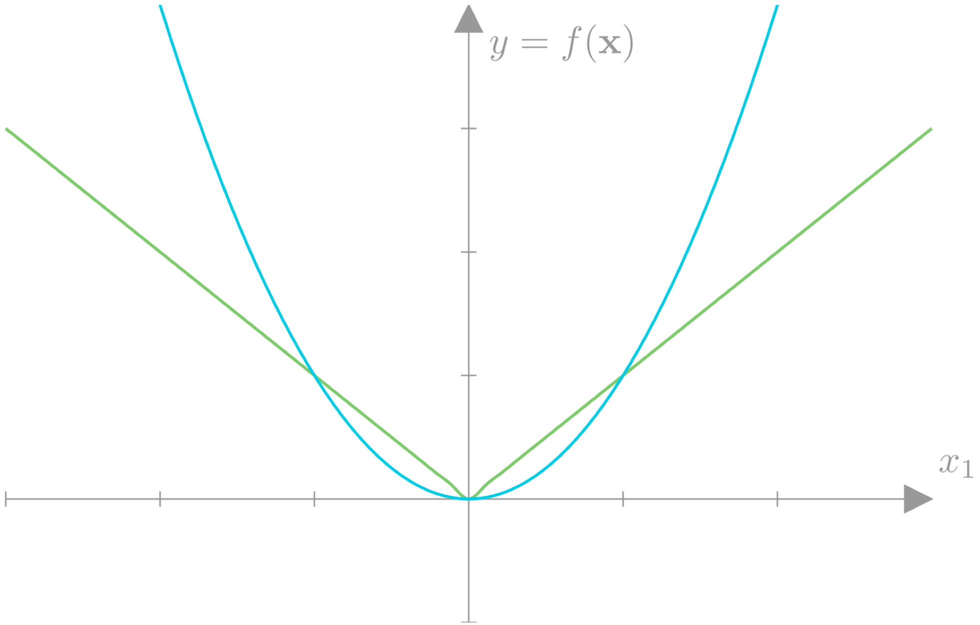
Vector: $\mathbf{L}_1(\mathbf{w}) = \|\mathbf{w}\|_1 = \sum_{i=1}^{d} |w_i|$, Matrix: $\mathbf{L}_1(\mathbf{W}) = \|\mathbf{W}\|_1 = \sum_{i=1}^{d} \sum_{j=1}^{e} |w_{ij}|$

L1 Regularization





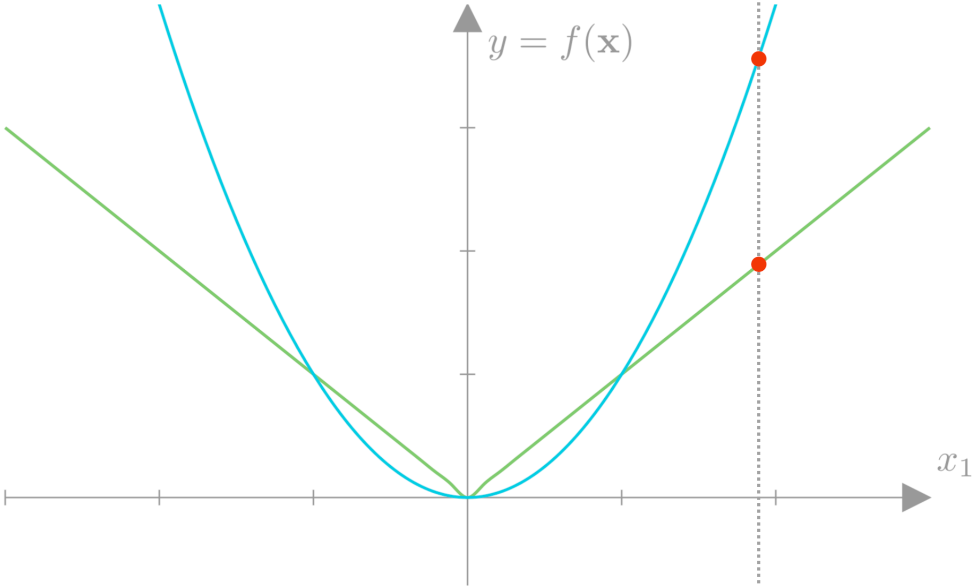
L1 Vs. L2 Regularization

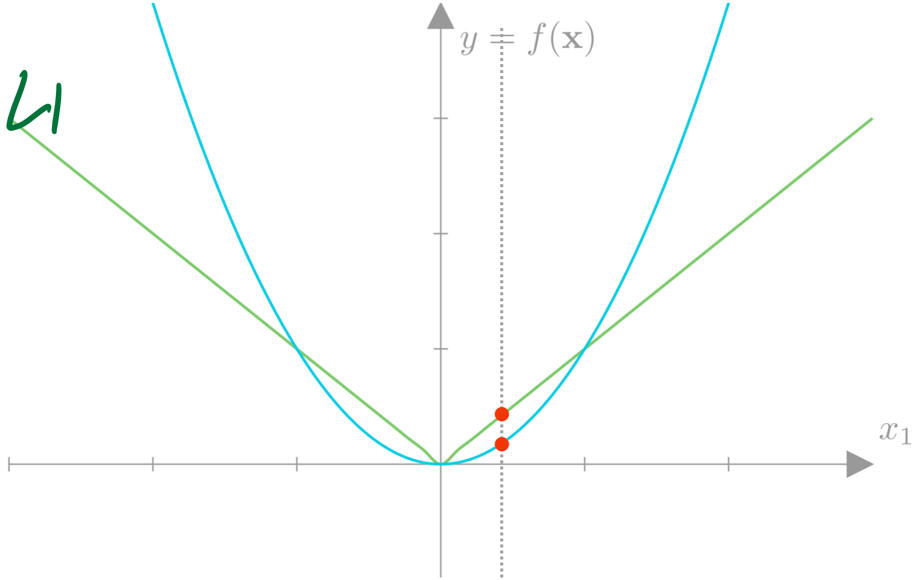


$$\text{Vector: } \mathbf{L}_2(\mathbf{w}) = \|\mathbf{w}\|_2^2 = \sum_{i=1}^{d} w_i^2$$

$$\text{Vector: } \mathbf{L}_1(\mathbf{w}) = \|\mathbf{w}\|_1 = \sum_{i=1}^{d} |w_i|,$$

L1 Vs. L2 Regularization

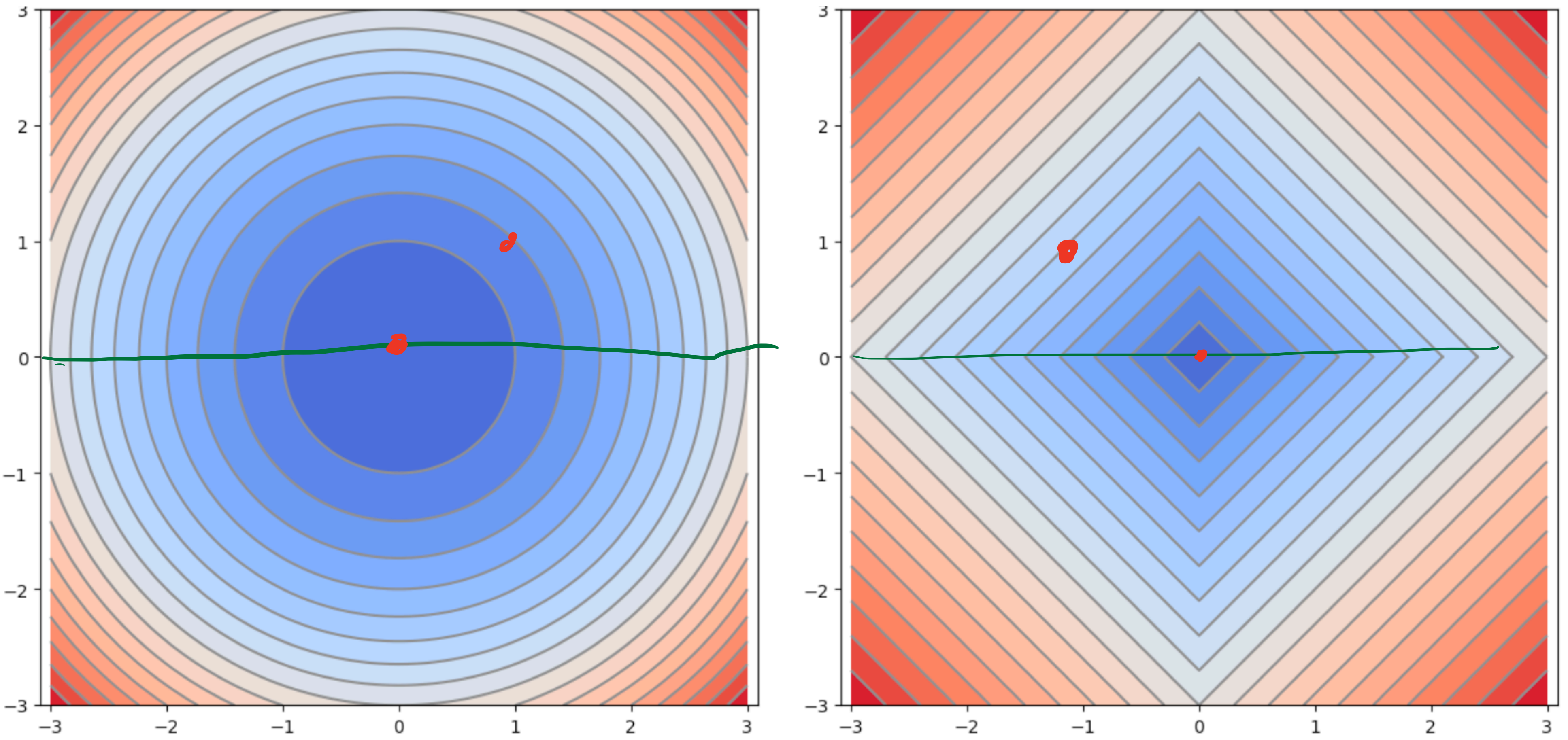




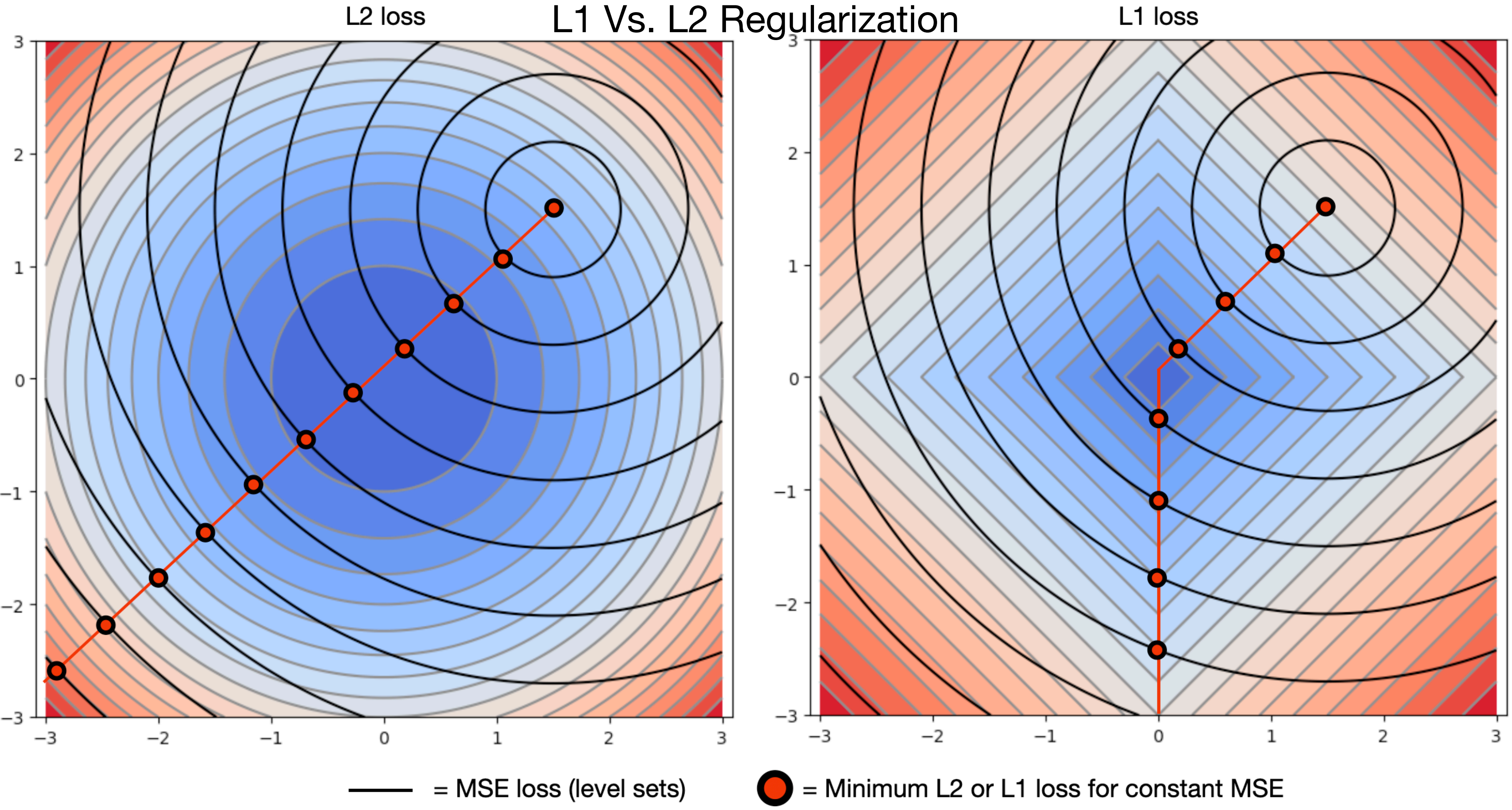
L2-Loss L1 Vs. L2 Regularization L1-Loss

$$\ell^2 = w_1^2 + w_2^2$$

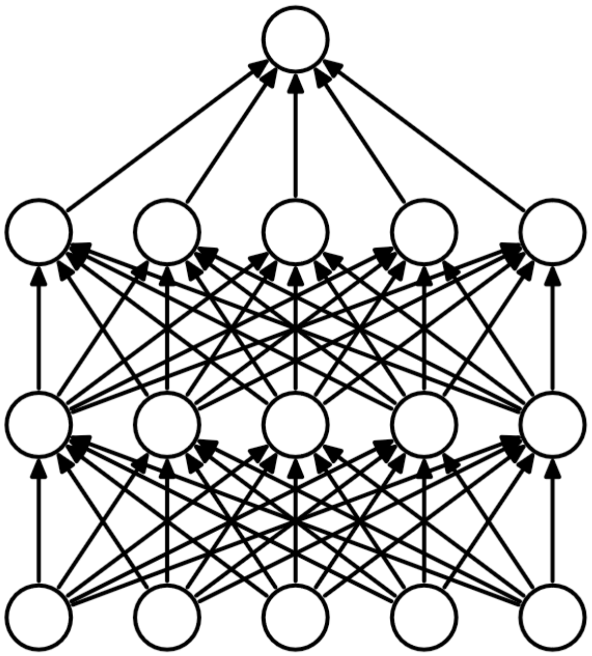
$$\ell^1 = |w_1| + |w_2|$$



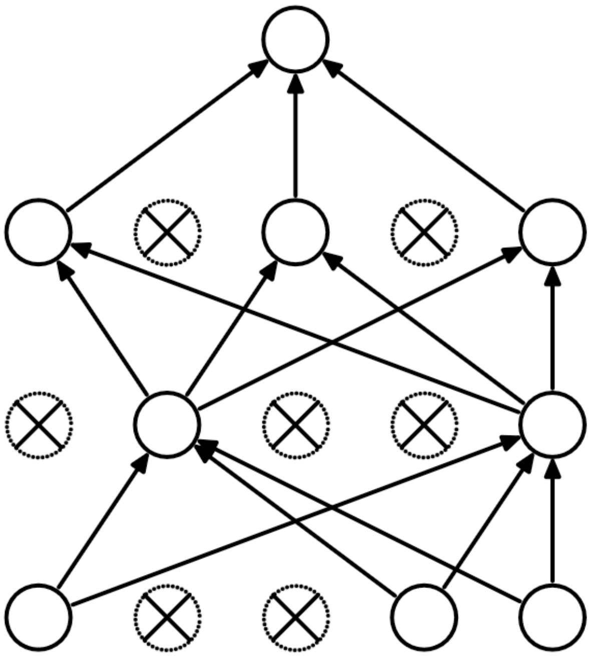
L1 Vs. L2 Regularization



Dropout



(a) Standard Neural Net



(b) After applying dropout.

Figure 1: Dropout Neural Net Model. **Left**: A standard neural net with 2 hidden layers. **Right**: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

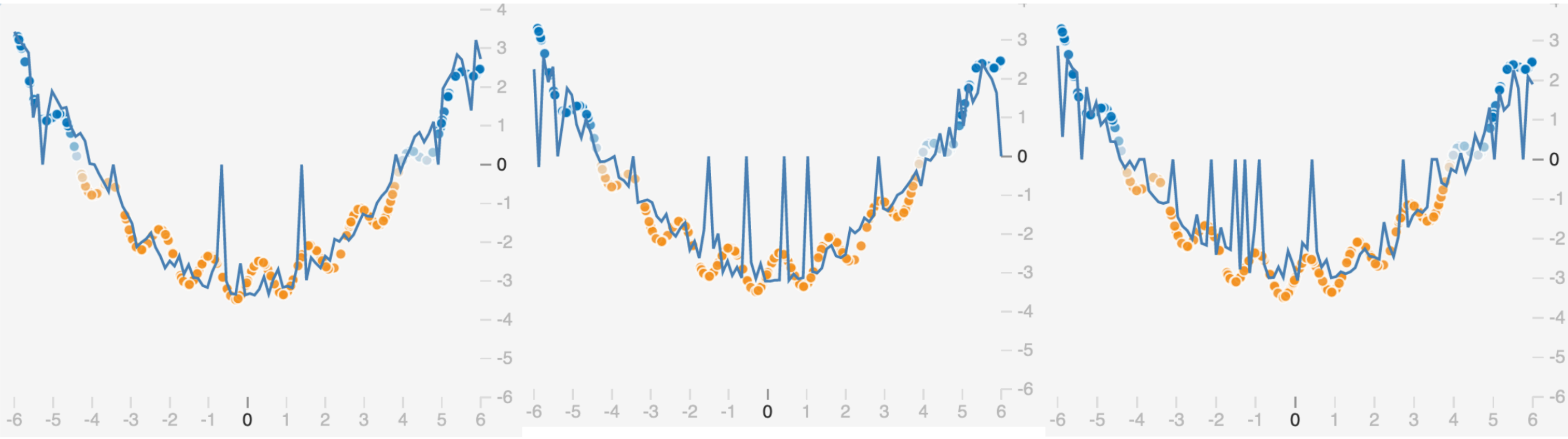
Dropout

$$\text{Dropout}(\mathbf{X}, r) = \mathbf{D} \odot \mathbf{X}, \quad \mathbf{D} = \begin{bmatrix} d_{11} & d_{12} & \dots & d_{1n} \\ d_{21} & d_{22} & \dots & d_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{m1} & d_{m2} & \dots & d_{mn} \end{bmatrix}, \; d_{ij} \sim \text{Bernoulli}(1 - r)$$

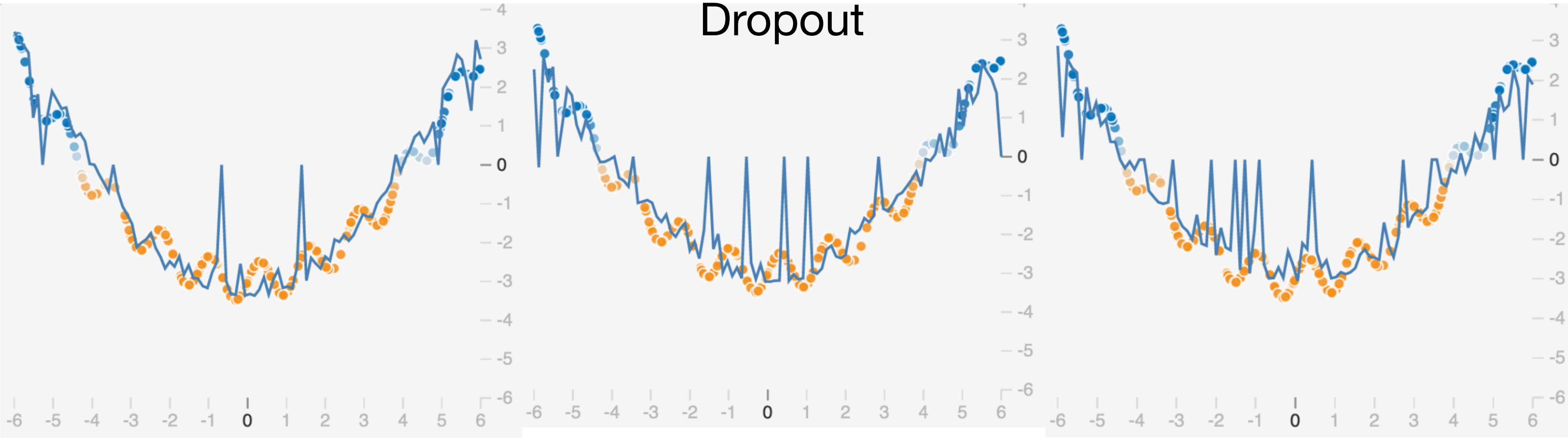
$$\phi(\mathbf{x}) = \sigma(\text{DO}_r(\mathbf{x})^T \mathbf{W} + \mathbf{b})$$

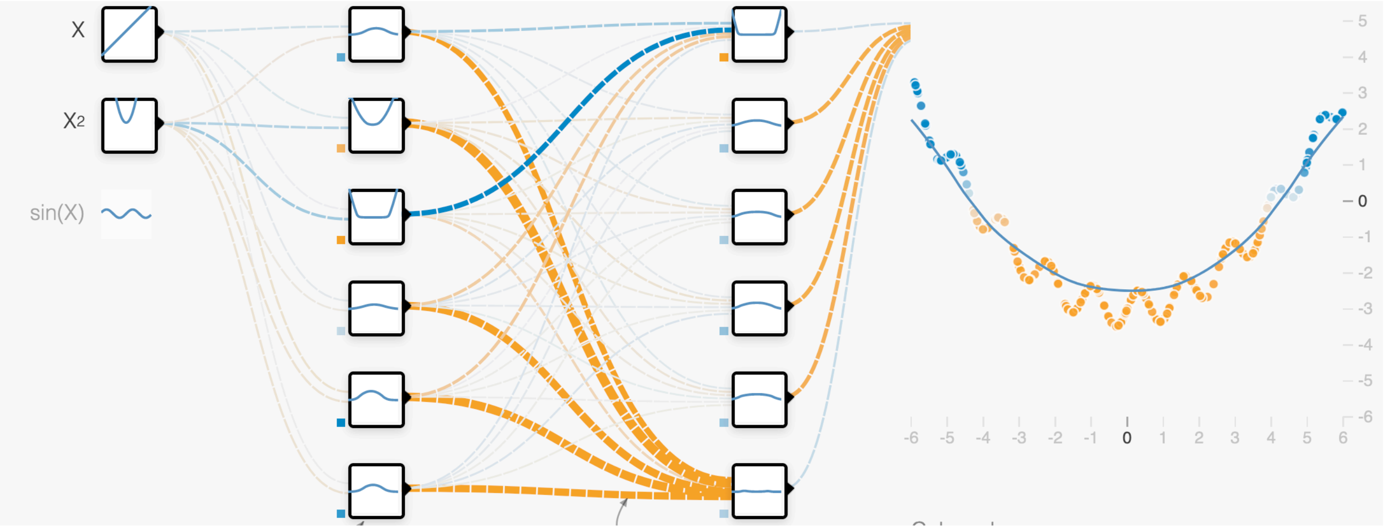
Dropout

$$\text{Dropout}(\mathbf{X}, r) = \mathbf{D} \odot \mathbf{X}, \quad \mathbf{D} = \begin{bmatrix} d_{11} & d_{12} & \dots & d_{1n} \\ d_{21} & d_{22} & \dots & d_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{m1} & d_{m2} & \dots & d_{mn} \end{bmatrix}, \; d_{ij} \sim \text{Bernoulli}(1 - r)$$



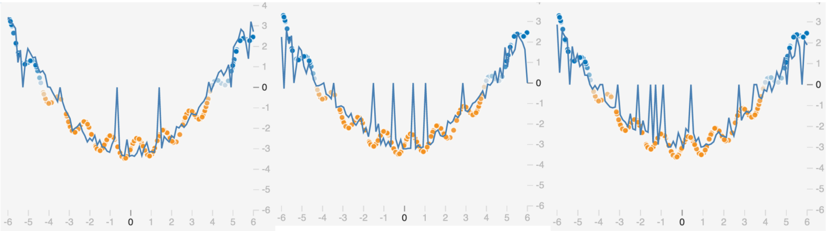
Dropout

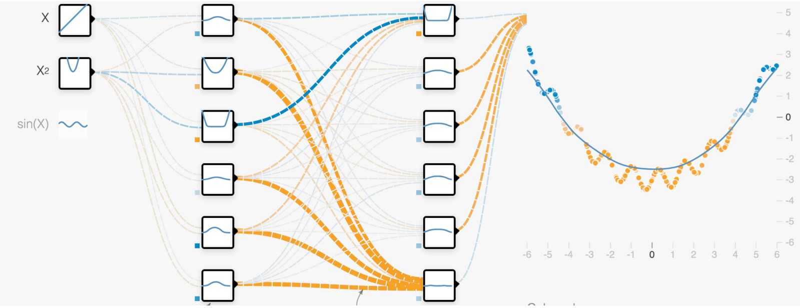




Dropout

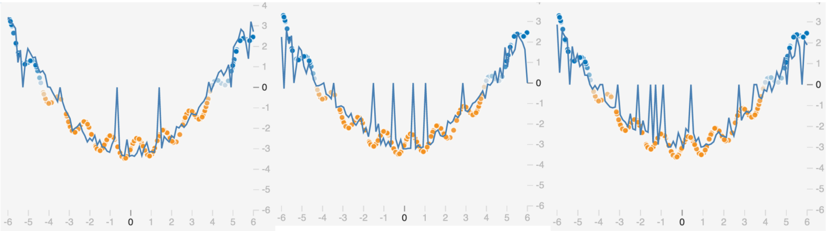
$$\phi(\mathbf{x})_{train} = \sigma(\mathrm{DO}_r(\mathbf{x})^T\mathbf{W} + \mathbf{b}) \quad \rightarrow \quad \phi(\mathbf{x})_{eval} = \sigma(\mathbf{x}^T\mathbf{W} + \mathbf{b})$$

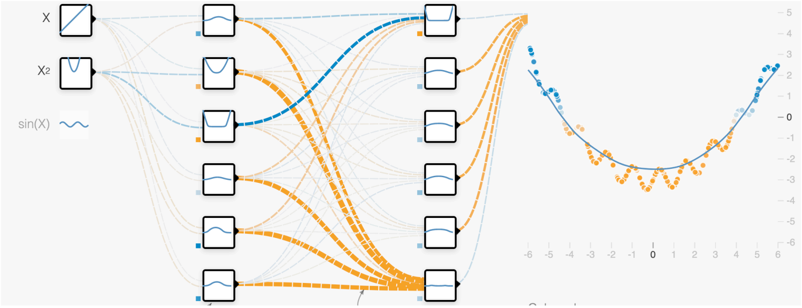




Dropout

$$\phi(\mathbf{x})_{train} = \sigma(\mathrm{DO}_r(\mathbf{x})^T\mathbf{W} + \mathbf{b}) \quad \rightarrow \quad \phi(\mathbf{x})_{eval} = \sigma(\mathbf{x}^T\mathbf{W} + \mathbf{b})$$





$$\mathbb{E}[\mathrm{DO}_r(\mathbf{x})^T\mathbf{w}] = \sum_i d_i x_i w_i, \quad d_i \sim \mathrm{Bernoulli}(1-r)$$

$$= \sum_i p(d_i = 1) x_i w_i = (1-r)\sum_i x_i w_i < \sum_i x_i w_i$$

Dropout

```
# 2 Hidden-layer network with dropout
model = nn.Sequential(nn.Dropout(0.5), nn.Linear(2, 10), nn.ReLU(),
                      nn.Dropout(0.5), nn.Linear(10, 10), nn.ReLU(),
                      nn.Dropout(0.5), nn.Linear(10, 1)
                     )
```