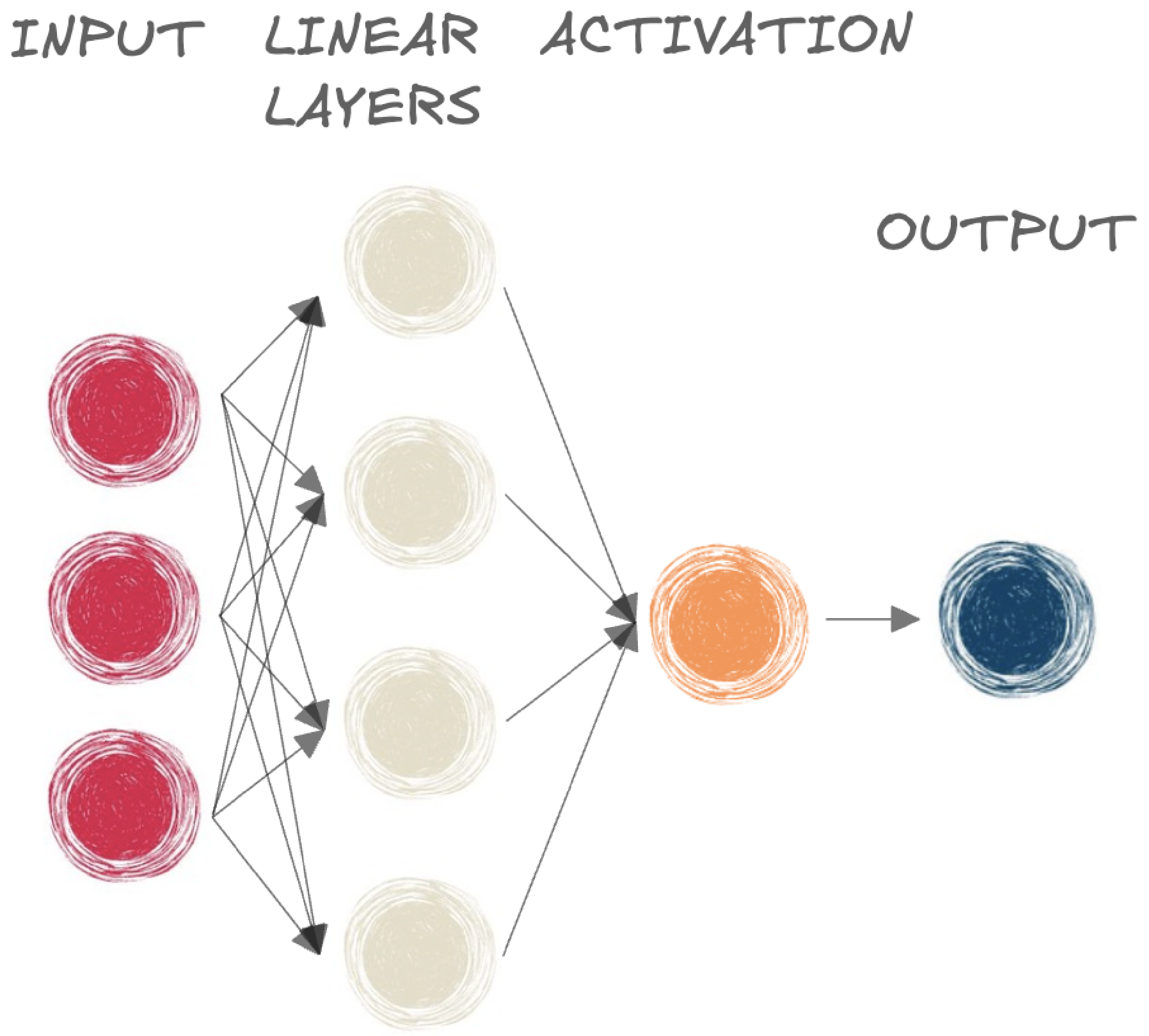
Discovering activation functions

INTRODUCTION TO DEEP LEARNING WITH PYTORCH

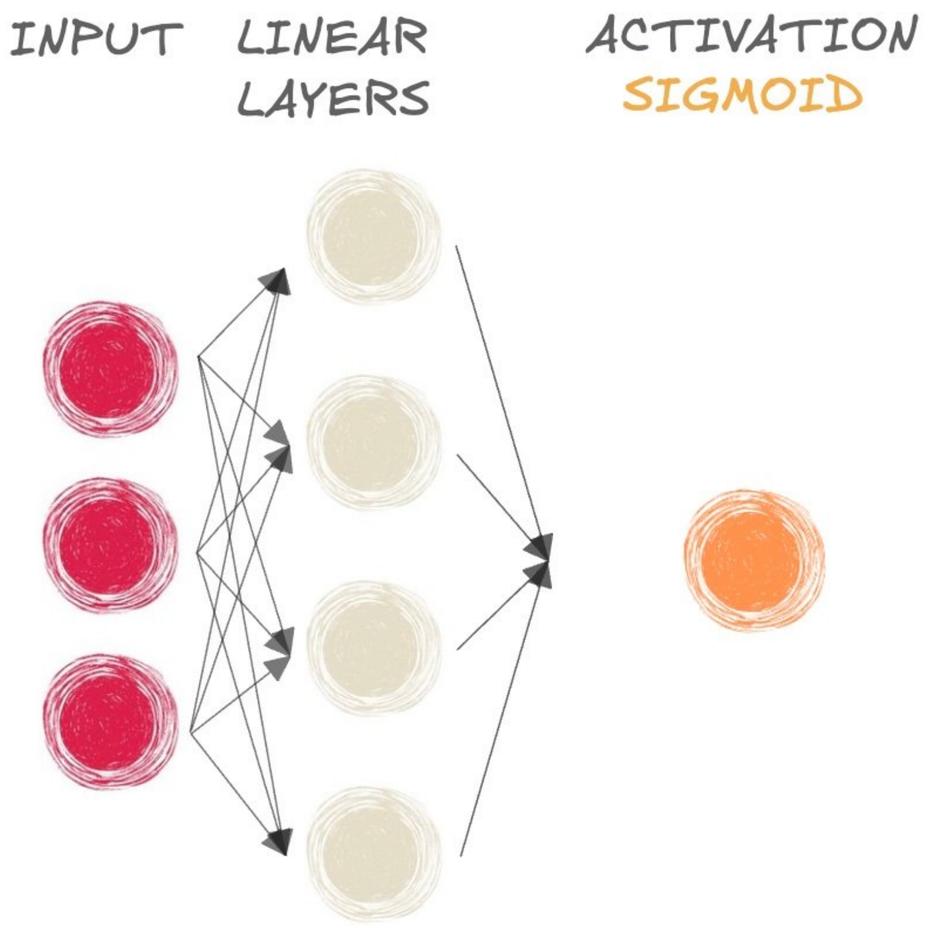
Jasmin Ludolf
Senior Data Science Content Developer, DataCamp

Activation functions

- **Activation functions** add **non-linearity** to the network
  - **Sigmoid** for binary classification
  - **Softmax** for multi-class classification
- A network can learn more **complex** relationships with non-linearity
- "Pre-activation" output passed to the activation function

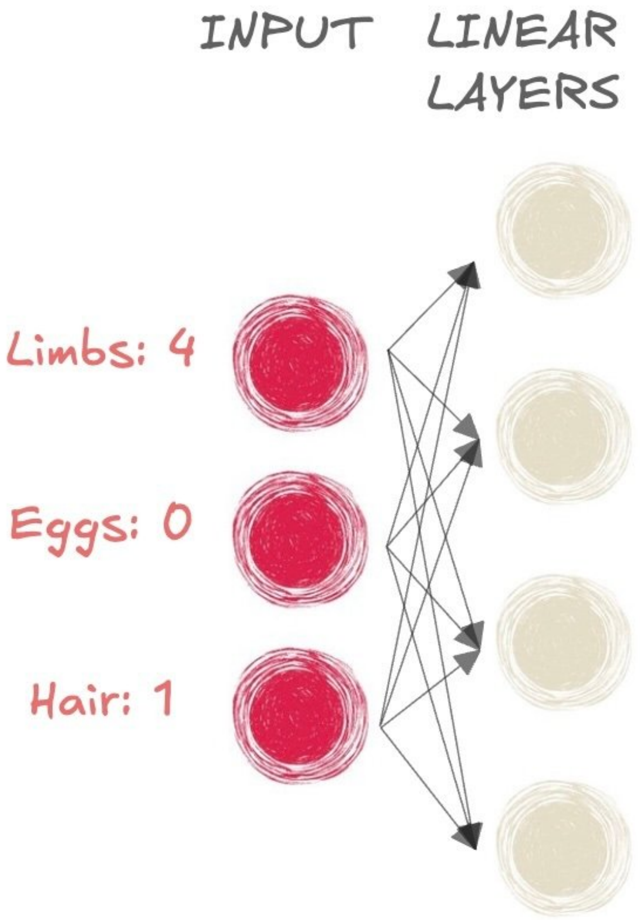


Meet the sigmoid function



- Mammal or not?

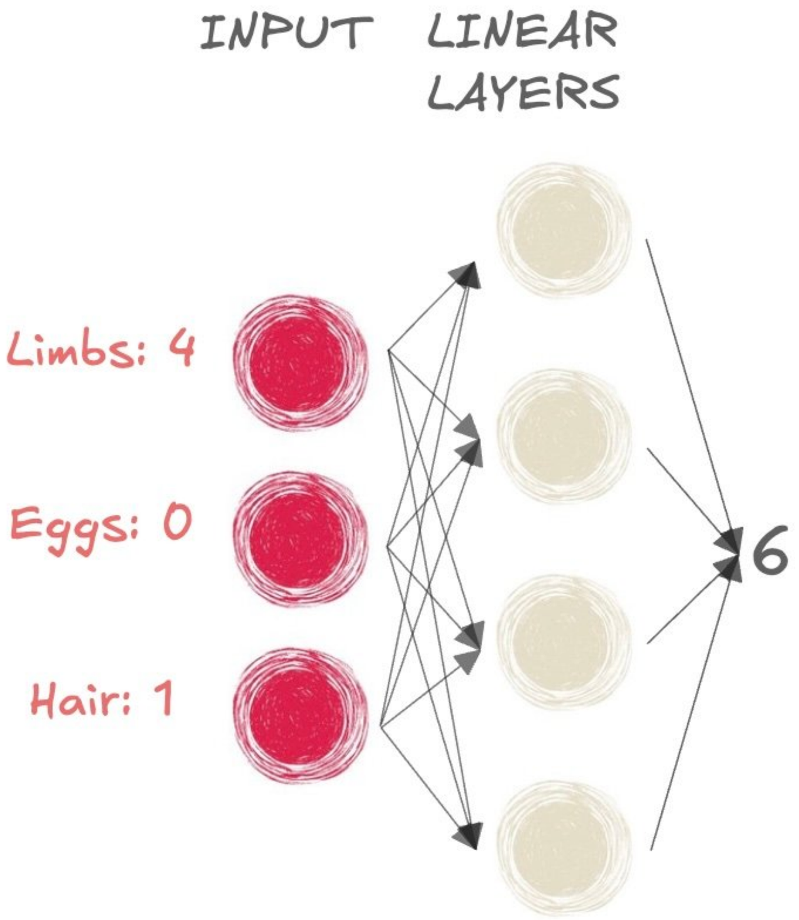
Meet the sigmoid function



- Mammal or not?

- Input:
  - Limbs: 4
  - Eggs: 0
  - Hair: 1

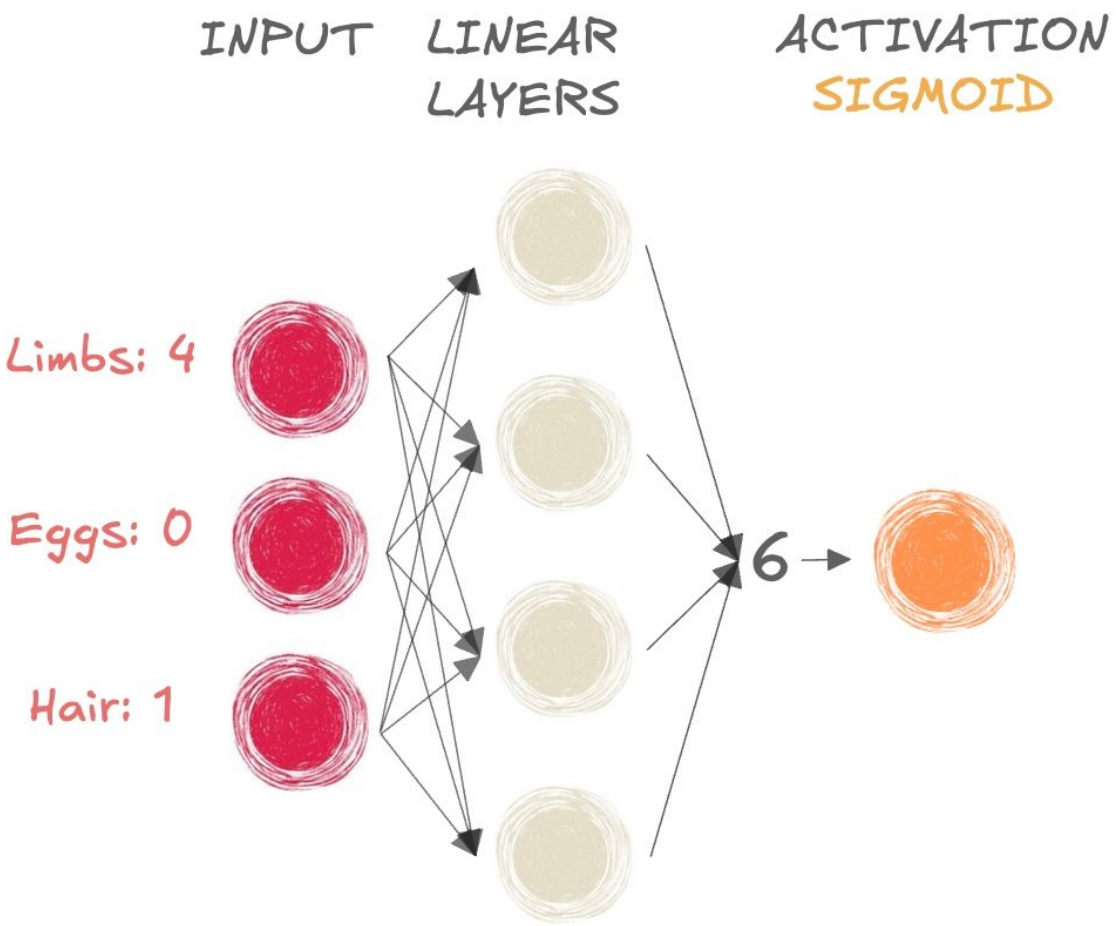
Meet the sigmoid function



- Mammal or not?

- Output to the linear layers is 6

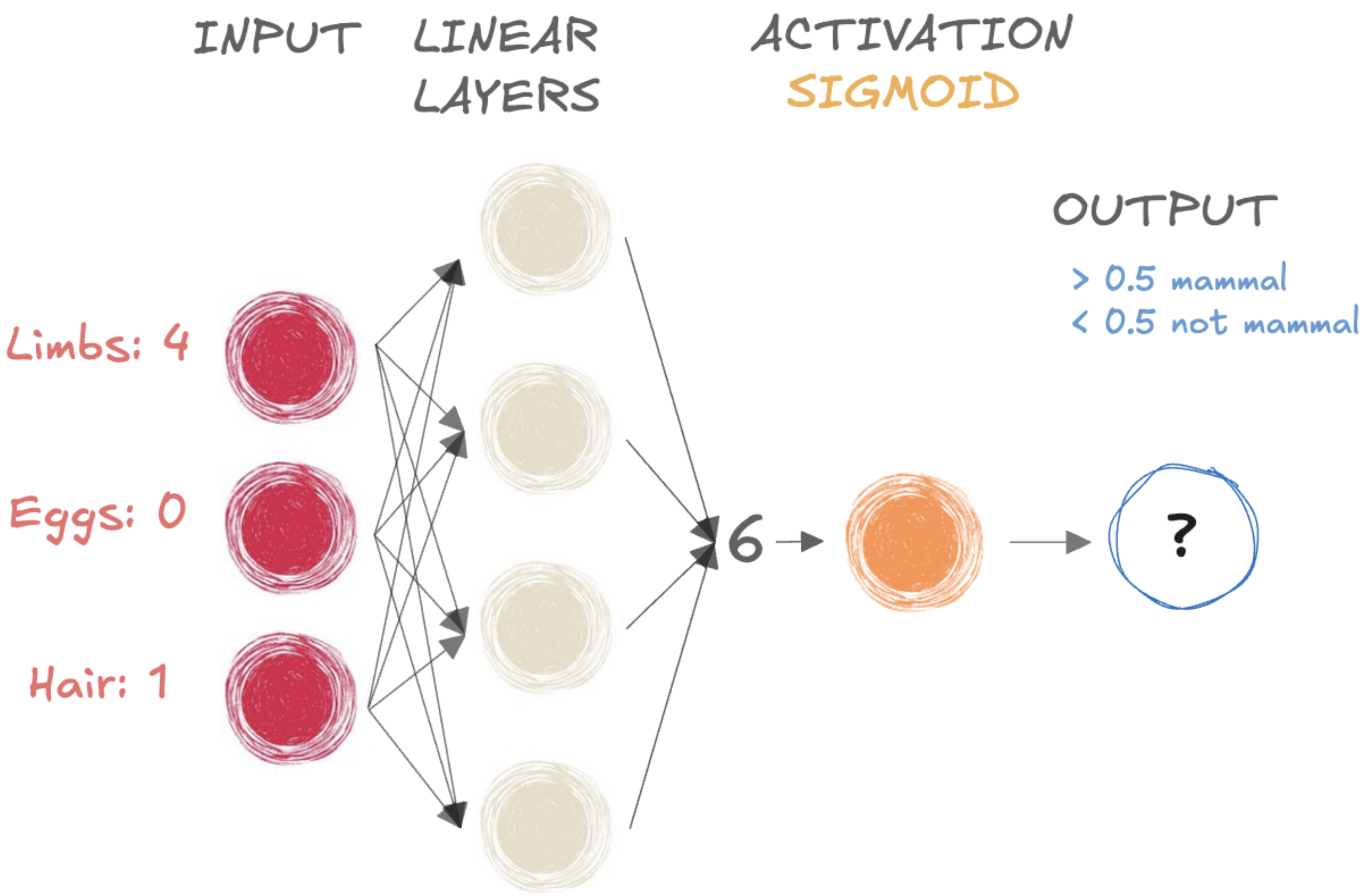
Meet the sigmoid function



- Mammal or not?

- We take the pre-activation output (6) and pass it to the sigmoid function

Meet the sigmoid function



- Mammal or not?

- We take the pre-activation output (6) and pass it to the sigmoid function
- Obtain a value between 0 and 1
- If output is > 0.5, class label = **1 (mammal)**
- If output is <= 0.5, class label = **0 (not mammal)**

Meet the sigmoid function

```python
import torch
import torch.nn as nn

input_tensor = torch.tensor([[6]])
sigmoid = nn.Sigmoid()
output = sigmoid(input_tensor)
print(output)
```

```
tensor([[0.9975]])
```

Activation as the last layer

```
model = nn.Sequential(
  nn.Linear(6, 4), # First linear layer
  nn.Linear(4, 1), # Second linear layer
  nn.Sigmoid() # Sigmoid activation function
)
```

Sigmoid as last step in network of linear layers is **equivalent** to traditional logistic regression

Getting acquainted with softmax

- Three classes:

Getting acquainted with softmax

- Three classes:

BIRD (0)

Getting acquainted with softmax

- Three classes:

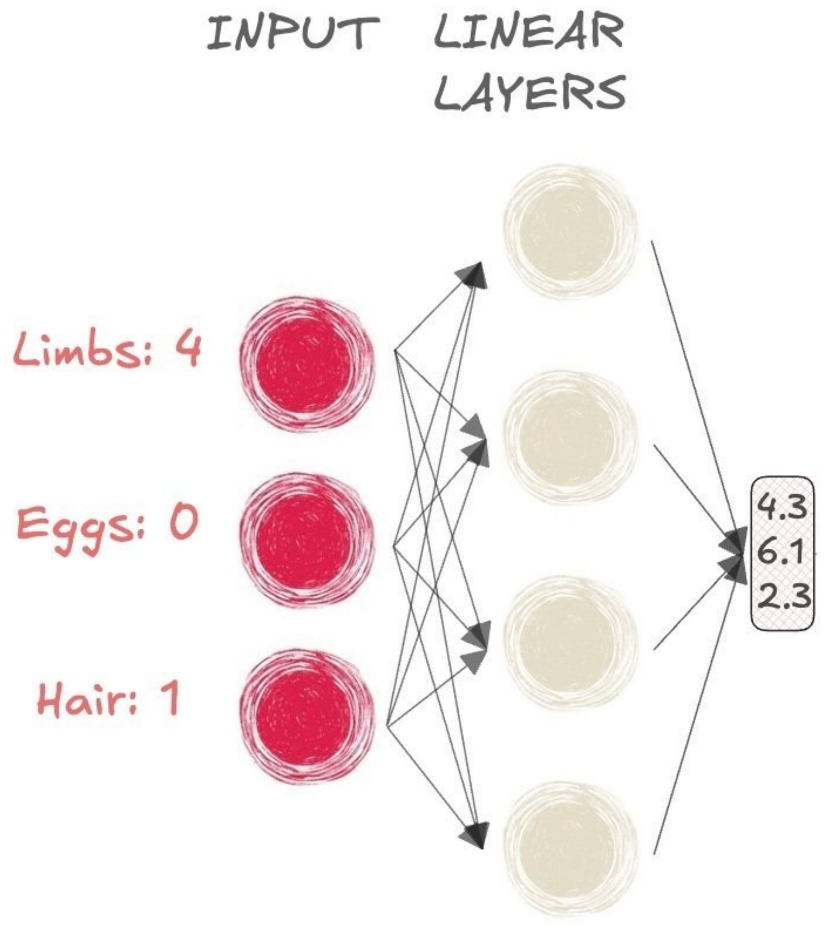
BIRD (0)

? MAMMAL (1)

Getting acquainted with softmax

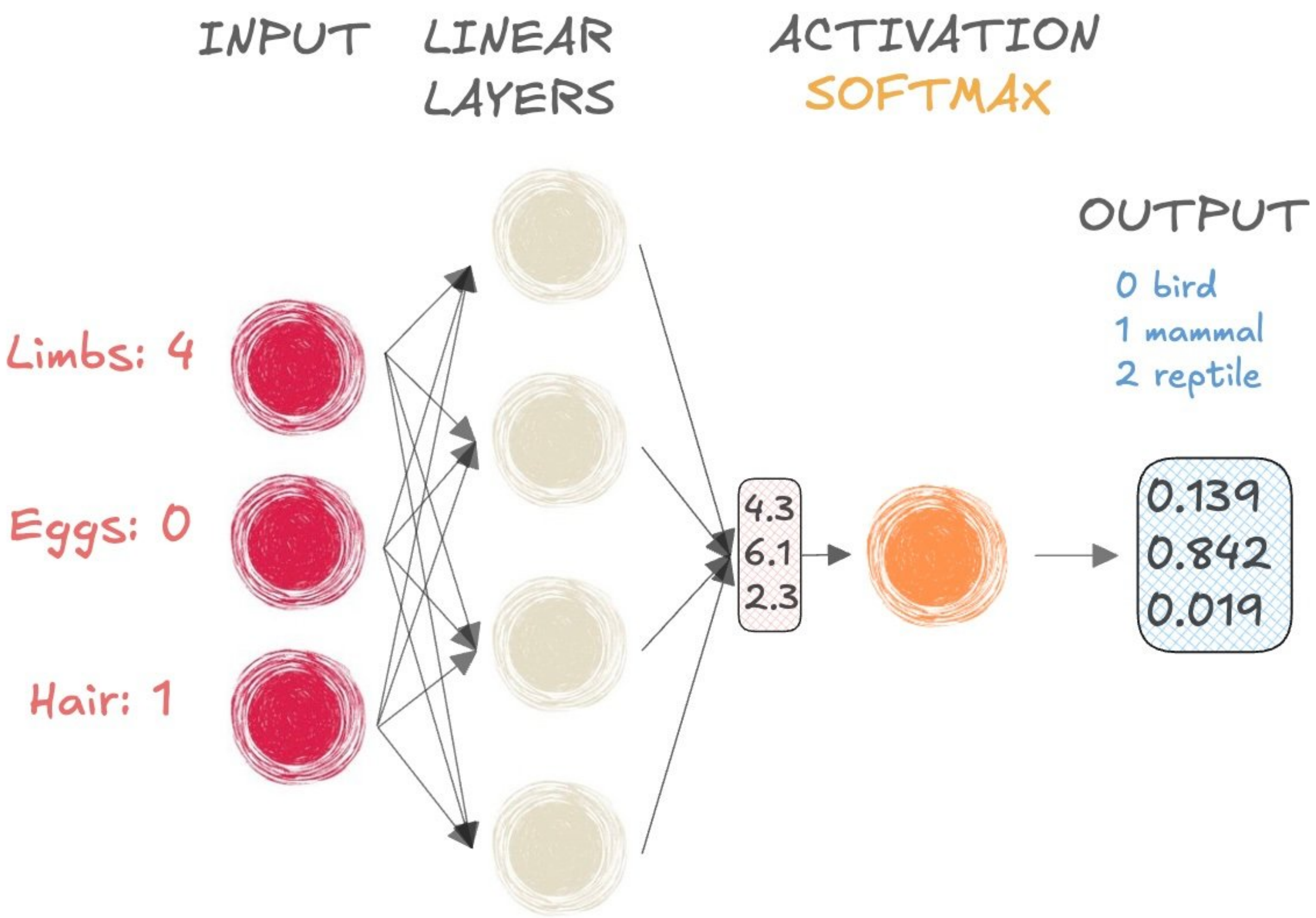
- Three classes:

Getting acquainted with softmax



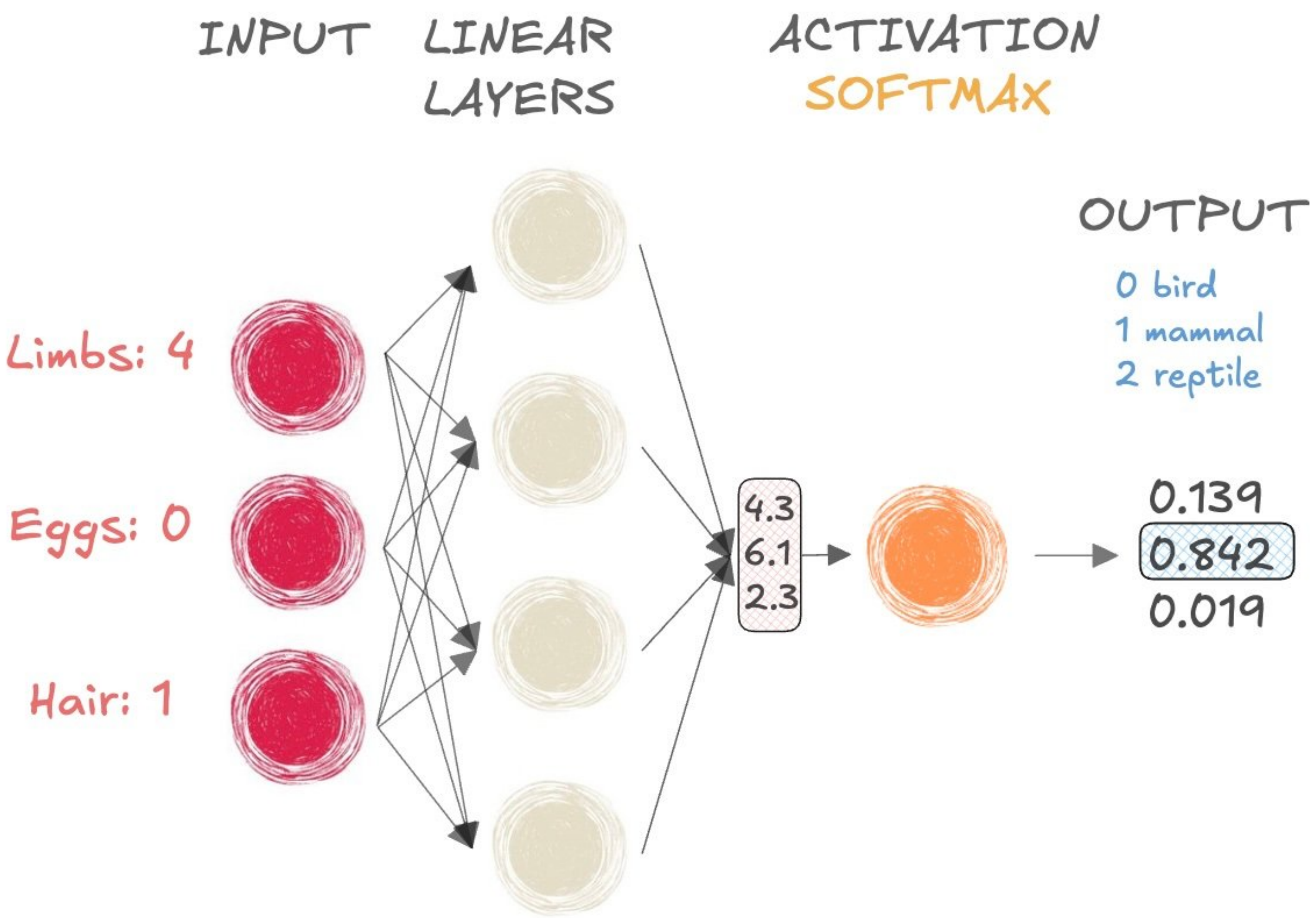
- Takes three-dimensional as input and outputs the same shape

Getting acquainted with softmax



- Takes three-dimensional as input and outputs the same shape
- Outputs a probability distribution:
  - Each element is a probability (it's bounded between 0 and 1)
  - The sum of the output vector is equal to 1

Getting acquainted with softmax



- Takes N-element vector as input and outputs vector of same size
- Outputs a probability distribution:
  - Each element is a probability (it's bounded between 0 and 1)
  - The sum of the output vector is equal to 1

Getting acquainted with softmax

```python
import torch
import torch.nn as nn

# Create an input tensor
input_tensor = torch.tensor(
    [[4.3, 6.1, 2.3]])

# Apply softmax along the last dimension
probabilities = nn.Softmax(dim=-1)
output_tensor = probabilities(input_tensor)
print(output_tensor)
```

```
tensor([[0.1392, 0.8420, 0.0188]])
```

- `dim = -1` indicates softmax is applied to the input tensor's last dimension
- `nn.Softmax()` can be used as last step in `nn.Sequential()`

Let's practice!

INTRODUCTION TO DEEP LEARNING WITH PYTORCH

Running a forward pass

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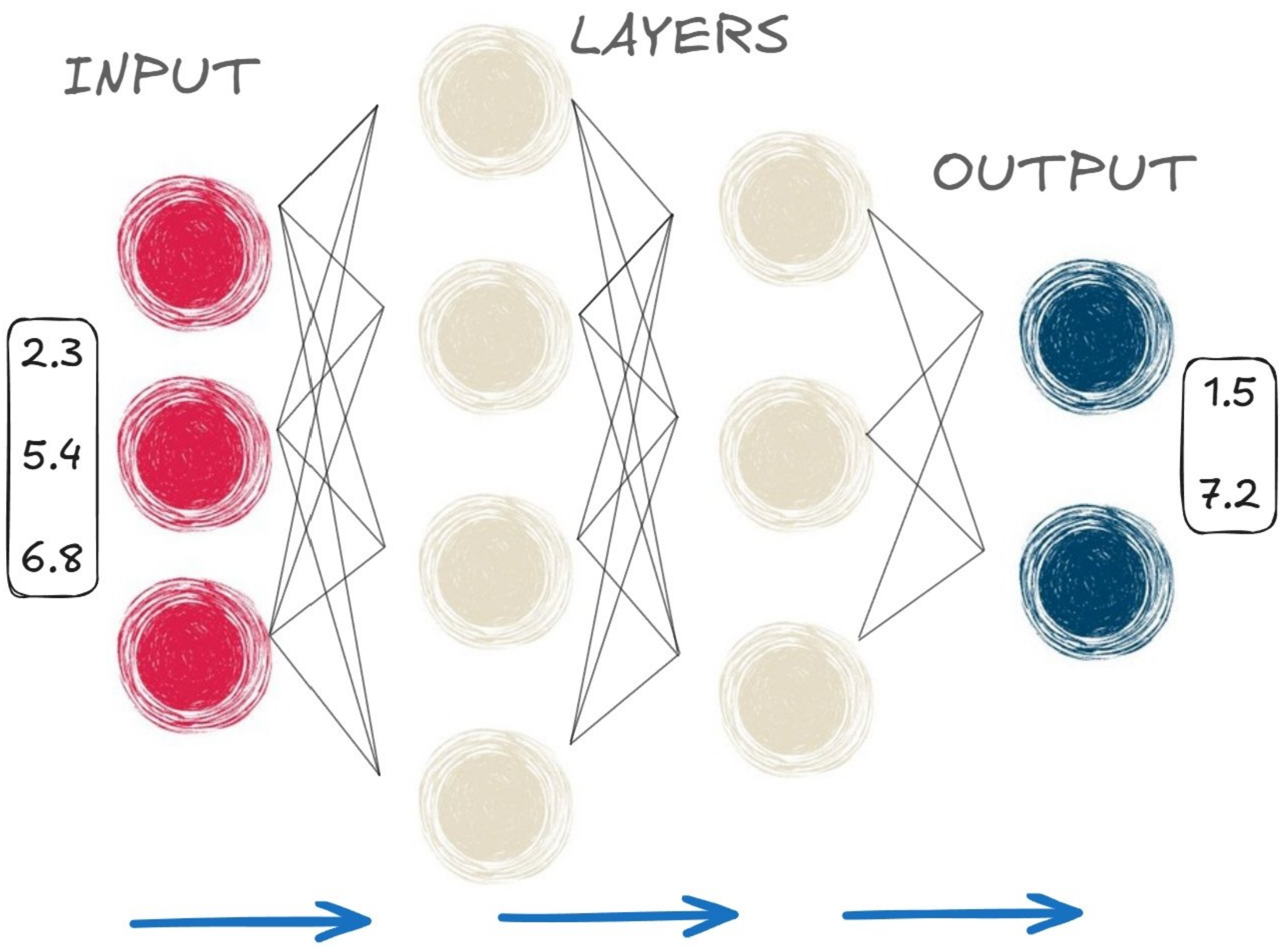
Jasmin Ludolf
Senior Data Science Content Developer, DataCamp

What is a forward pass?

- Input data **flows** through layers
- **Calculations** performed at each layer
- Final layer generates **outputs**

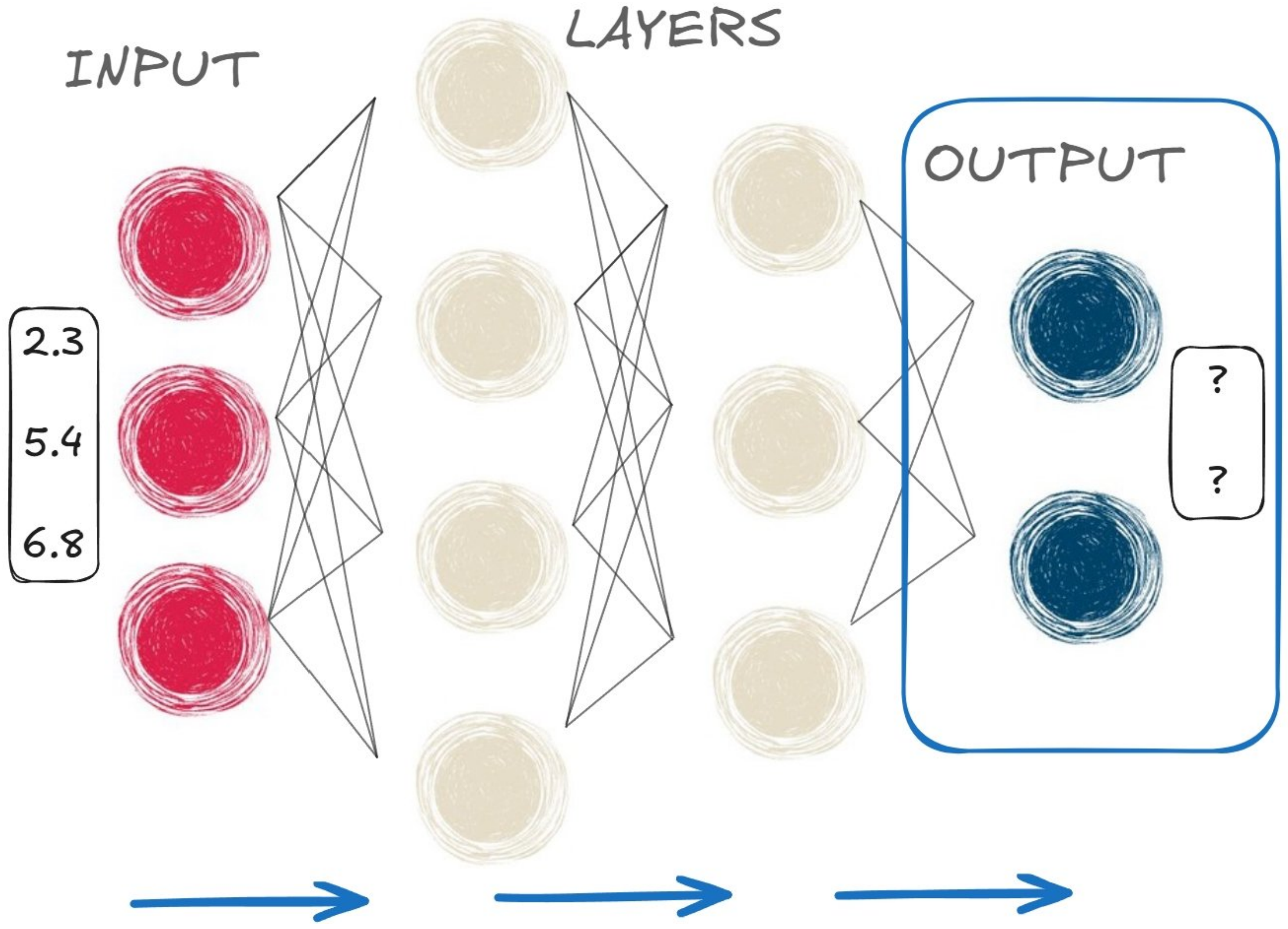
- Outputs produced based on **weights** and **biases**
- Used for **training** and making **predictions**



What is a forward pass?

Possible outputs:

- Binary classification
- Multi-class classification
- Regressions



Binary classification: forward pass

```
# Create input data of shape 5x6
input_data = torch.tensor(
        [[-0.4421,  1.5207,  2.0607, -0.3647,  0.4691,  0.0946],
        [-0.9155, -0.0475, -1.3645,  0.6336, -1.9520, -0.3398],
        [ 0.7406,  1.6763, -0.8511,  0.2432,  0.1123, -0.0633],
        [-1.6630, -0.0718, -0.1285,  0.5396, -0.0288, -0.8622],
        [-0.7413,  1.7920, -0.0883, -0.6685,  0.4745, -0.4245]])
```

5 animals

6 features

```
# Create binary classification model
model = nn.Sequential(
  nn.Linear(6, 4), # First linear layer
  nn.Linear(4, 1), # Second linear layer
  nn.Sigmoid() # Sigmoid activation function
)
```

Binary classification: forward pass

```
# Pass input data through model
output = model(input_data)
print(output)
```

```
tensor([[0.5188], [0.3761], [0.5015], [0.3718], [0.4663]],
    grad_fn=<SigmoidBackward0>)
```

- Output: five probabilities between 0 and 1, one for each animal
- Classification (0.5 threshold):
  - Class = 1 (mammal) for values ≥ 0.5 (`0.5188`, `0.5015`)
  - Class = 0 (not mammal) for values < 0.5 (`0.3761`, `0.3718`, `0.4633`)

Multi-class classification: forward pass

- Class 1 - **mammal**, class 2 - **bird**, class 3 - **reptile**

```
n_classes = 3

# Create multi-class classification model
model = nn.Sequential(
  nn.Linear(6, 4), # First linear layer
  nn.Linear(4, n_classes), # Second linear layer
  nn.Softmax(dim=-1) # Softmax activation
)

# Pass input data through model
output = model(input_data)
print(output.shape)
```

```
torch.Size([5, 3])
```

Multi-class classification: forward pass

```
print(output)
```

```
tensor([[0.4969, 0.3606, 0.1425],
        [0.5105, 0.3262, 0.1633],
        [0.3253, 0.3174, 0.3572],
        [0.5499, 0.3361, 0.1141],
        [0.4117, 0.3366, 0.2517]], grad_fn=<SoftmaxBackward0>)
```

5 animals

probabilities for each class

- Each row sums to one
- Predicted label = class with the highest probability
- Row 1 = class 1 (mammal), row 2 = class 1 (mammal), row 3 = class 3 (reptile)

Regression: forward pass

```
# Create regression model
model = nn.Sequential(
  nn.Linear(6, 4), # First linear layer
  nn.Linear(4, 1) # Second linear layer
)

# Pass input data through model
output = model(input_data)

# Return output
print(output)
```

```
tensor([[0.3818],
        [0.0712],
        [0.3376],
        [0.0231],
        [0.0757]],
        grad_fn=<AddmmBackward0>)
```

Let's practice!

INTRODUCTION TO DEEP LEARNING WITH PYTORCH

Using loss functions to assess model predictions

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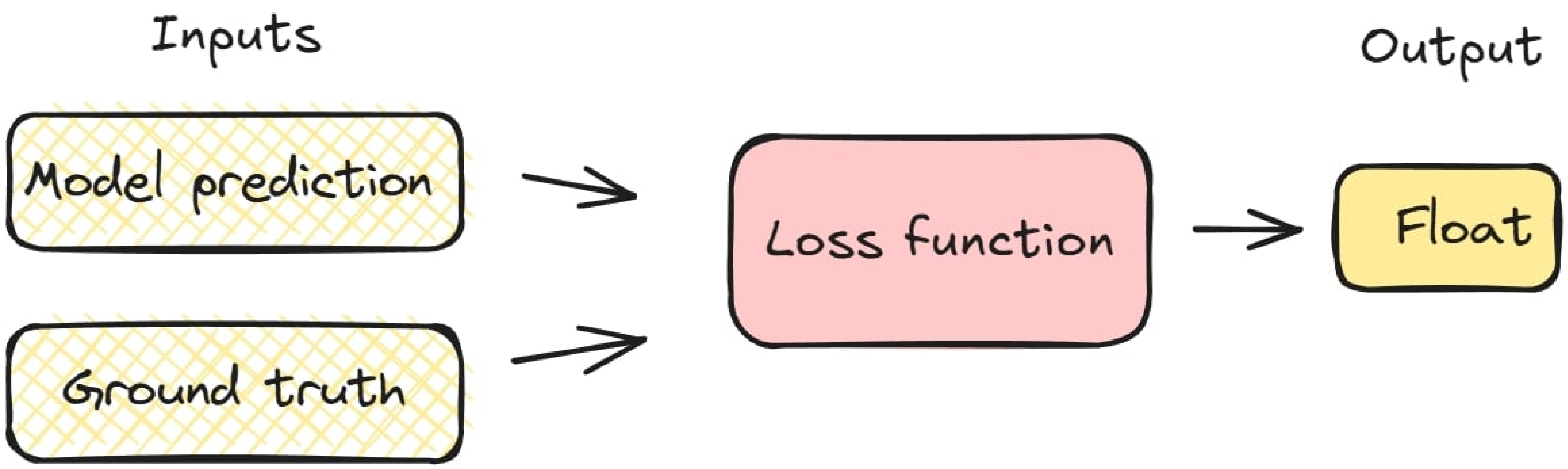
Why do we need a loss function?

- Tells us how good our model is during training
- Takes a model **prediction** $\hat{y}$ and **ground truth** y
- Outputs a float



Why do we need a loss function?

- Class 0 - **mammal**, class 1 - **bird**, class 2 - **reptile**

Hair	Feathers	Eggs	Milk	Fins	Legs	Tail	Domestic	Catsize	Class
1	0	0	1	0	4	0	0	1	0

- Predicted class = 0 -> **correct** = low loss
- Predicted class = 1 -> **wrong** = high loss
- Predicted class = 2 -> **wrong** = high loss

- Our goal is to **minimize loss**

One-hot encoding concepts

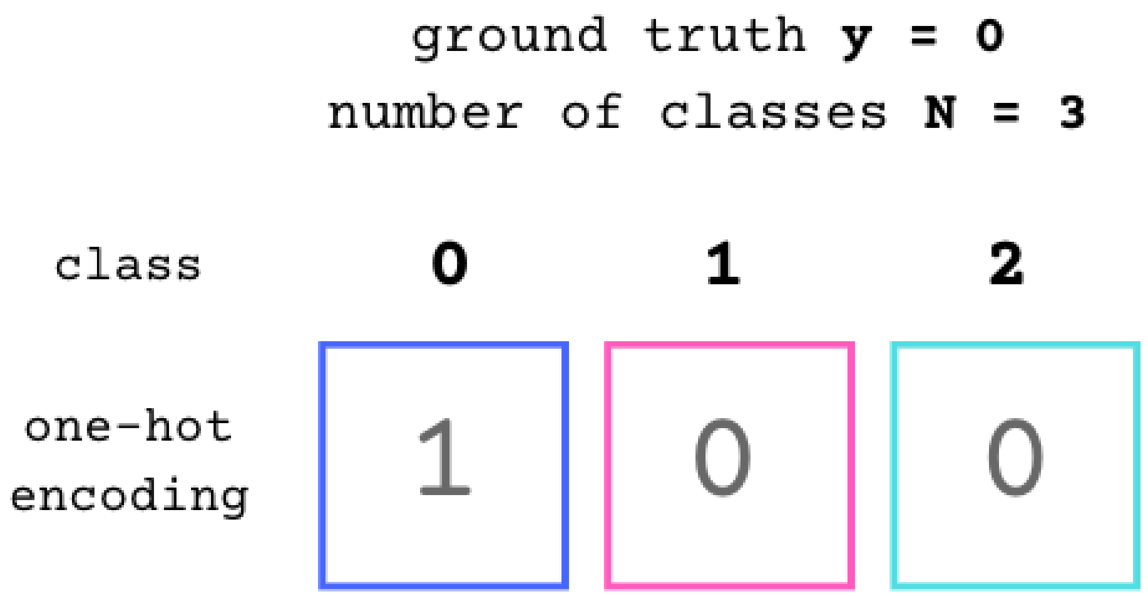
- $loss = F(y, \hat{y})$

- y is a single **integer** (class label)
  - e.g. $y = 0$ when y is a mammal

- $\hat{y}$ is a **tensor** (prediction before softmax)
  - If N is the number of classes, e.g. N = 3
  - $\hat{y}$ is a tensor with N dimensions,
    - e.g. $\hat{y}$ = `[-5.2, 4.6, 0.8]`

One-hot encoding concepts

- Convert an **integer** y to a **tensor** of zeros and ones



Transforming labels with one-hot encoding

```
import torch.nn.functional as F

print(F.one_hot(torch.tensor(0), num_classes = 3))
```

```
tensor([1, 0, 0])
```

```
print(F.one_hot(torch.tensor(1), num_classes = 3))
```

```
tensor([0, 1, 0])
```

```
print(F.one_hot(torch.tensor(2), num_classes = 3))
```

```
tensor([0, 0, 1])
```

Cross entropy loss in PyTorch

```python
from torch.nn import CrossEntropyLoss

scores = torch.tensor([-5.2, 4.6, 0.8])
one_hot_target = torch.tensor([1, 0, 0])

criterion = CrossEntropyLoss()
print(criterion(scores.double(), one_hot_target.double()))
```

```
tensor(9.8222, dtype=torch.float64)
```

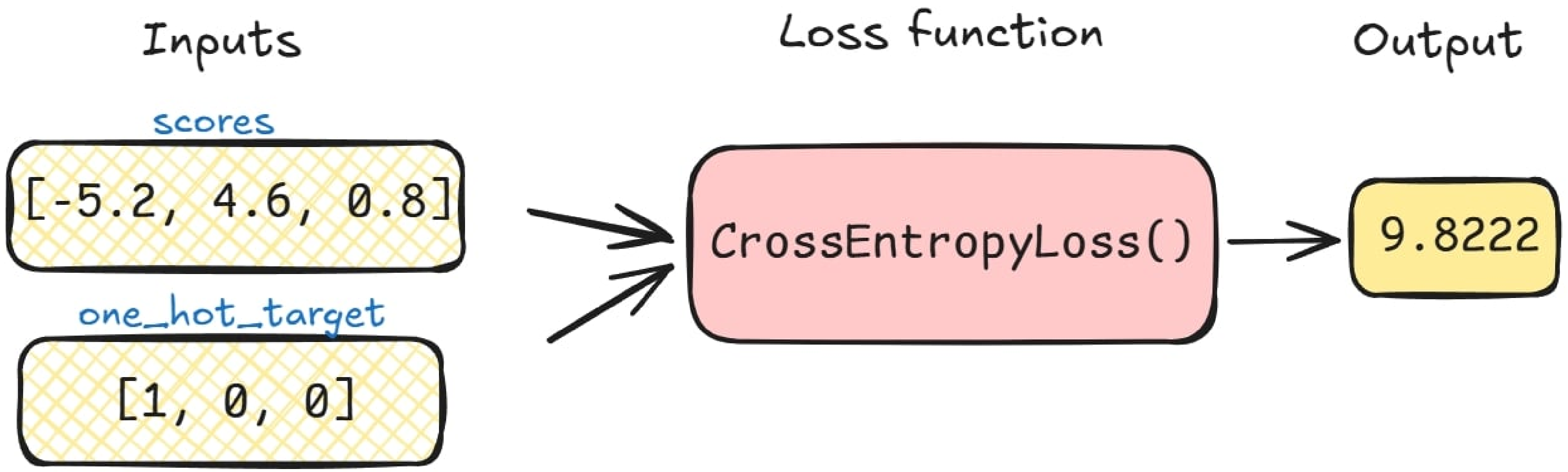
Bringing it all together

Loss function takes:

- **scores** - model predictions **before** the final softmax function
- **one_hot_target** - one hot encoded ground truth label

Loss function outputs:

- **loss** - a single **float**



Let's practice!

INTRODUCTION TO DEEP LEARNING WITH PYTORCH

Using derivatives to update model parameters

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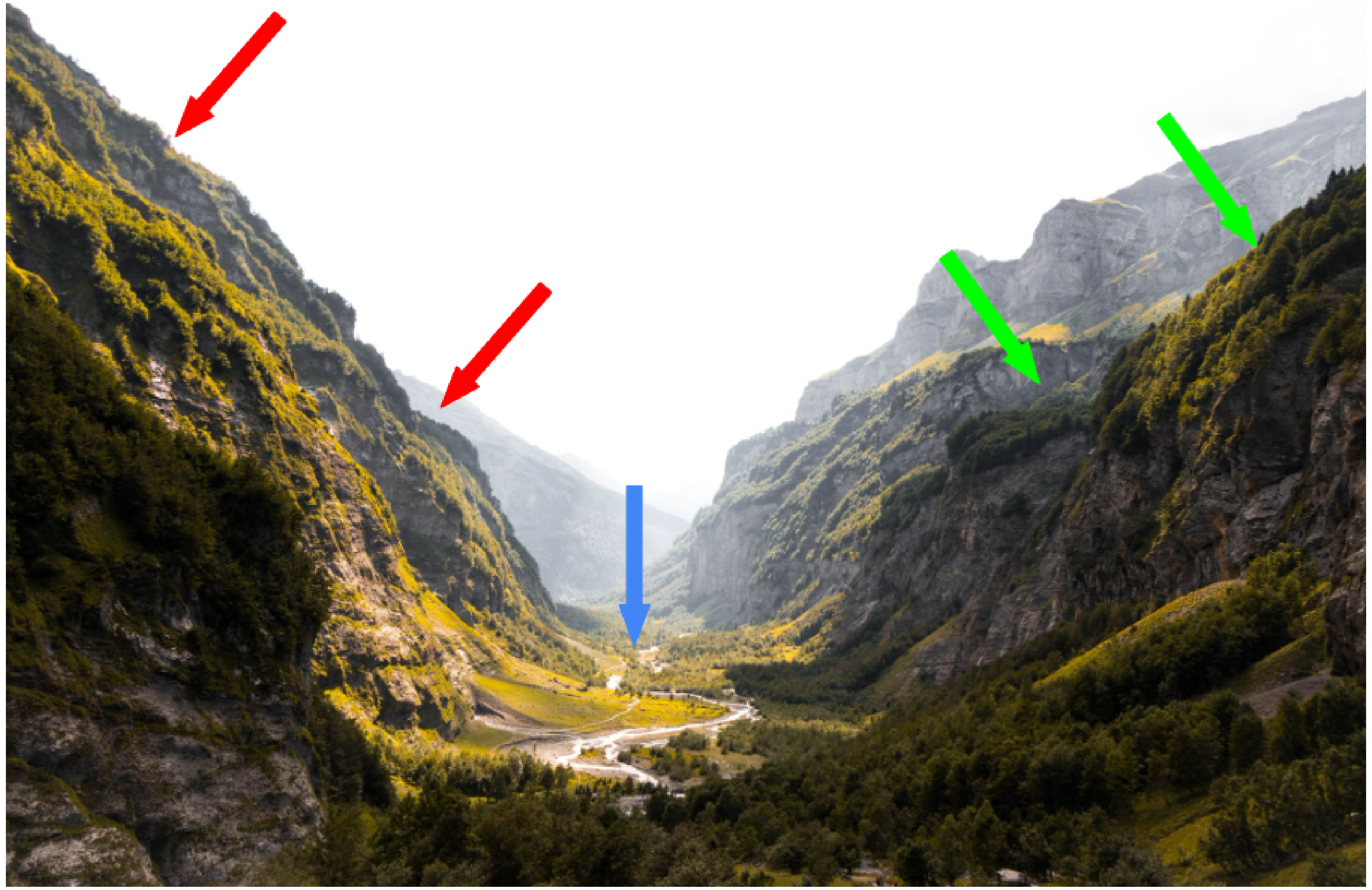
An analogy for derivatives

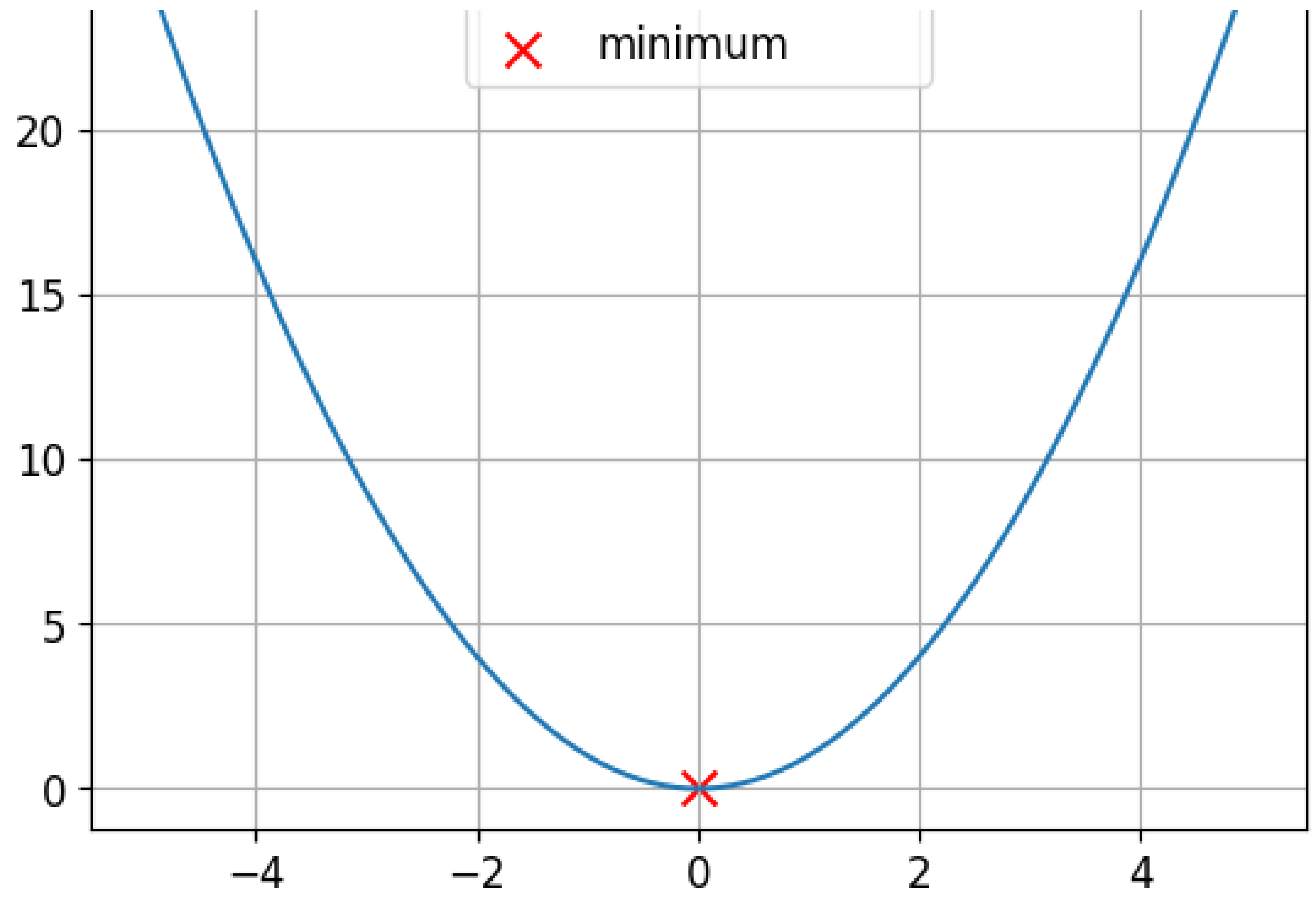
Derivative represents the **slope of the curve**

- **Steep slopes** (red arrows):
  - Large steps, **derivative is high**
- **Gentler slopes** (green arrows):
  - Small steps, **derivative is low**
- **Valley floor** (blue arrow):
  - Flat, **derivative is zero**

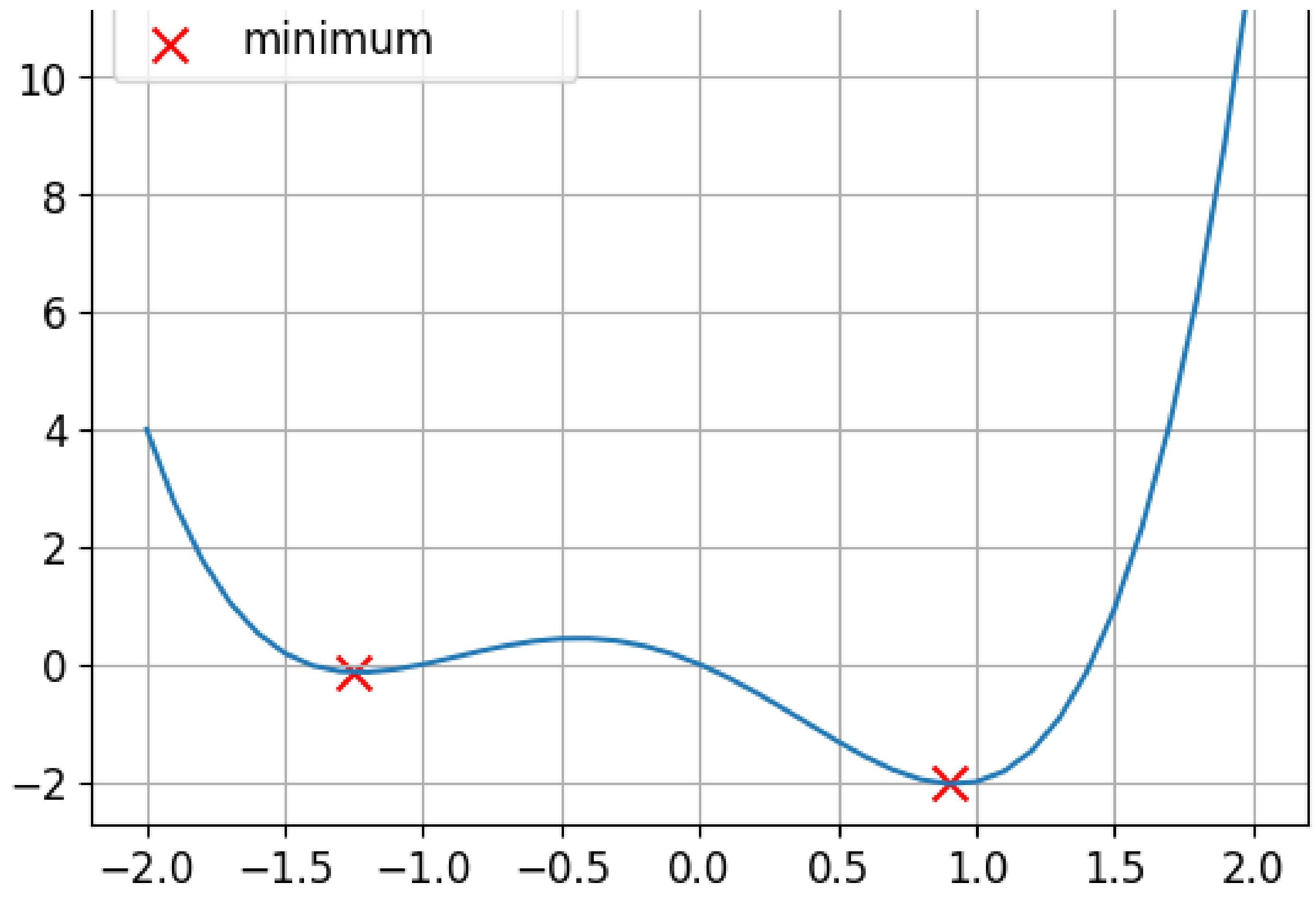


Convex and non-convex functions

This is a **convex function**

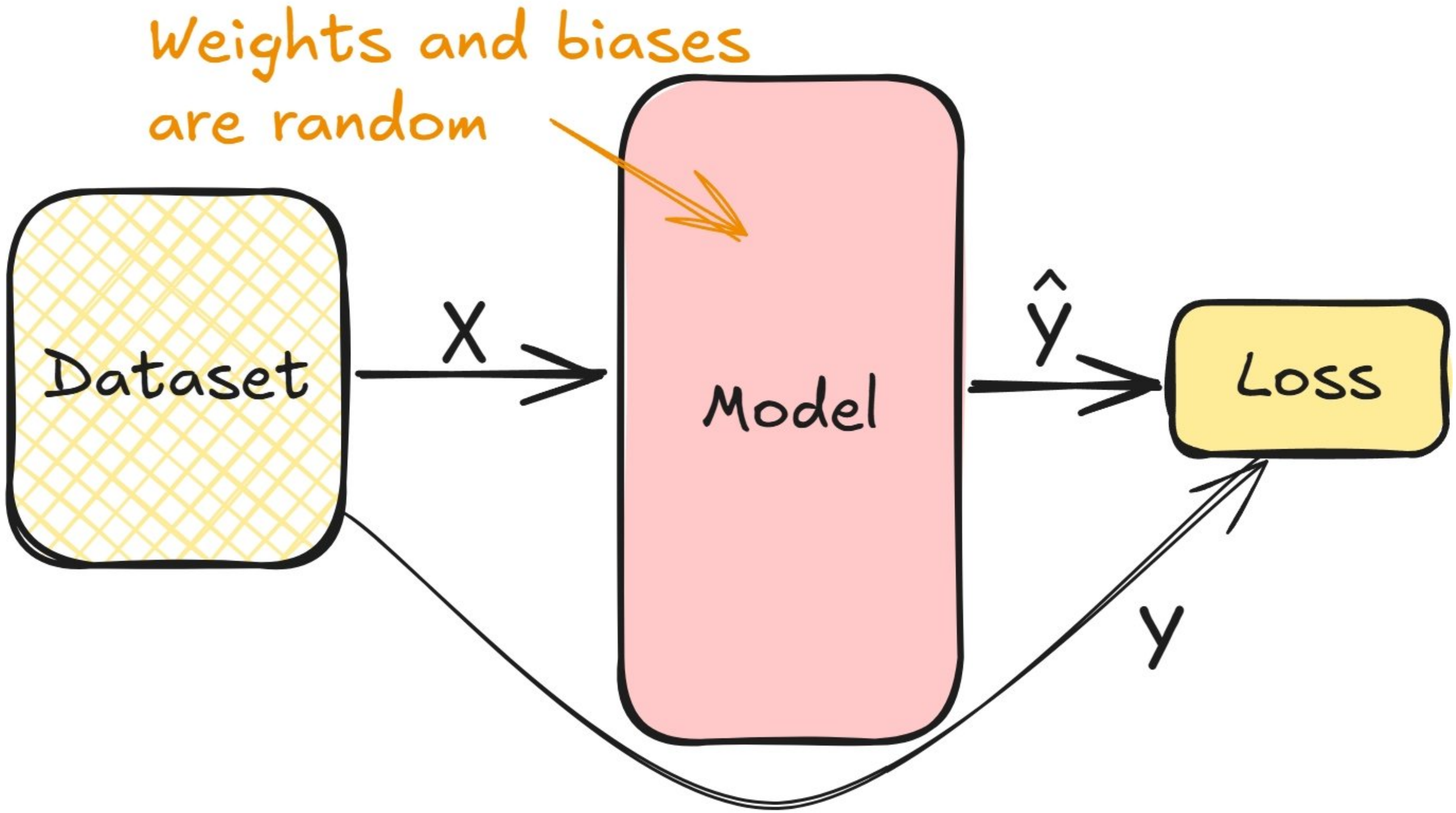


This is a **non-convex function**



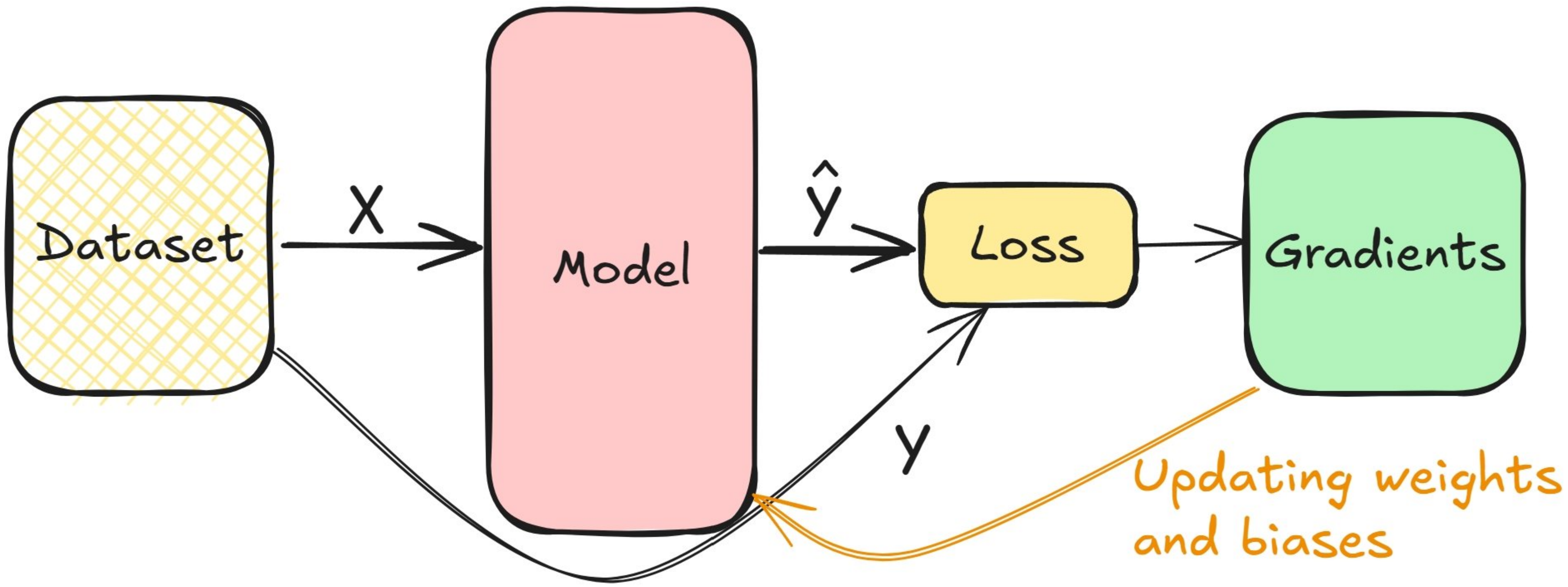
Connecting derivatives and model training

- Compute the loss in the forward pass during training



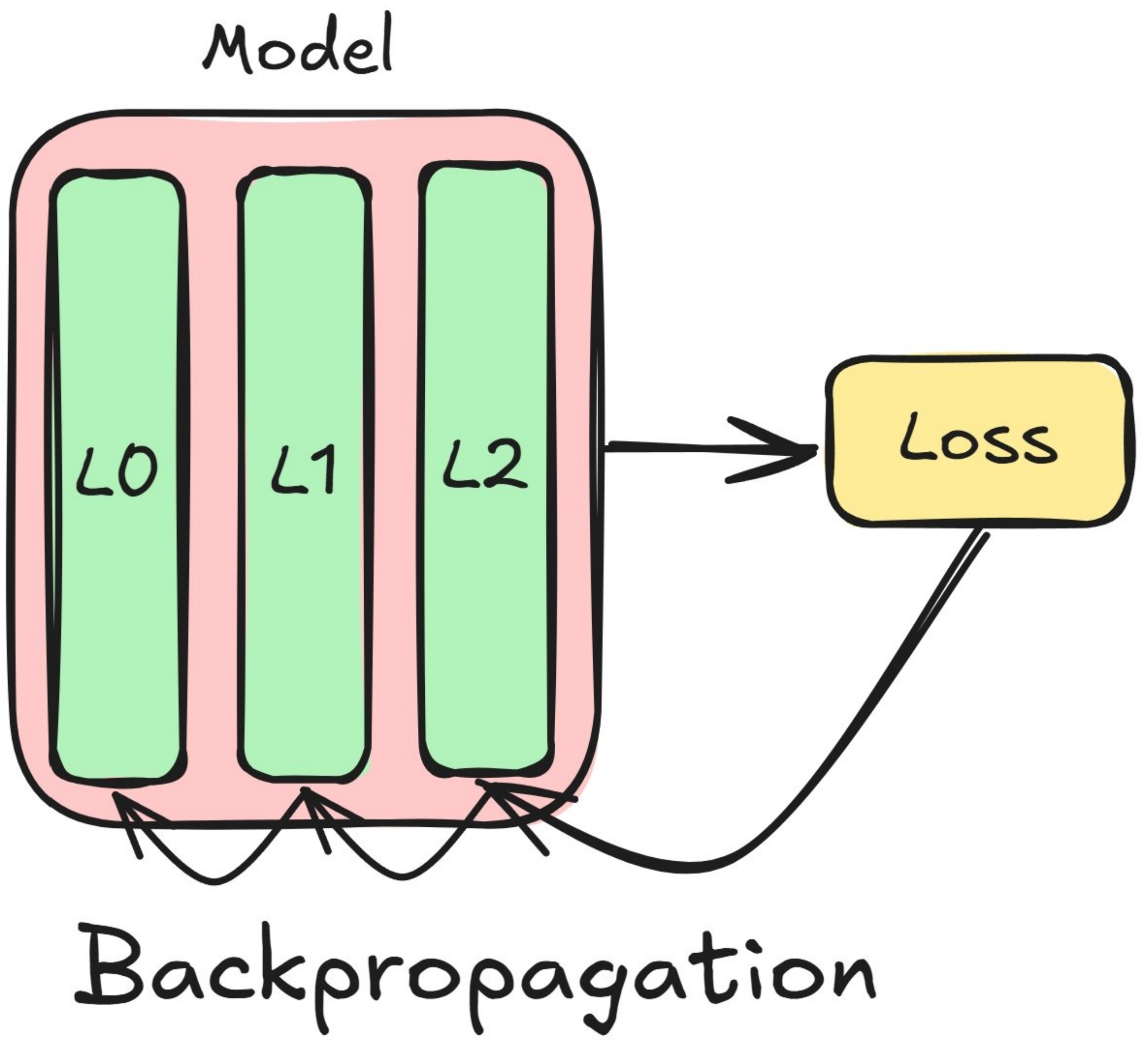
Connecting derivatives and model training

- Gradients help minimize **loss**, tune layer **weights** and **biases**
- Repeat until the layers are **tuned**



Backpropagation concepts

- Consider a network made of three layers:
  - Begin with loss gradients for $L2$
  - Use $L2$ to compute $L1$ gradients
  - Repeat for all layers ($L1$, $L0$)



Backpropagation in PyTorch

```
# Run a forward pass
model = nn.Sequential(nn.Linear(16, 8),
                      nn.Linear(8, 4),
                      nn.Linear(4, 2))
prediction = model(sample)

# Calculate the loss and gradients
criterion = CrossEntropyLoss()
loss = criterion(prediction, target)
loss.backward()
```

```
# Access each layer's gradients
model[0].weight.grad
model[0].bias.grad
model[1].weight.grad
model[1].bias.grad
model[2].weight.grad
model[2].bias.grad
```

Updating model parameters manually

```
# Learning rate is typically small
lr = 0.001

# Update the weights
weight = model[0].weight
weight_grad = model[0].weight.grad

weight = weight - lr * weight_grad

# Update the biases
bias = model[0].bias
bias_grad = model[0].bias.grad
bias = bias - lr * bias_grad
```

- Access each layer gradient
- Multiply by the learning rate
- Subtract this product from the weight

Gradient descent

- For non-convex functions, we will use **gradient descent**
- PyTorch simplifies this with **optimizers**
  - Stochastic gradient descent (SGD)

```
import torch.optim as optim

# Create the optimizer
optimizer = optim.SGD(model.parameters(), lr=0.001)

# Perform parameter updates
optimizer.step()
```

Let's practice!

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