Training Neural Networks in PyTorch

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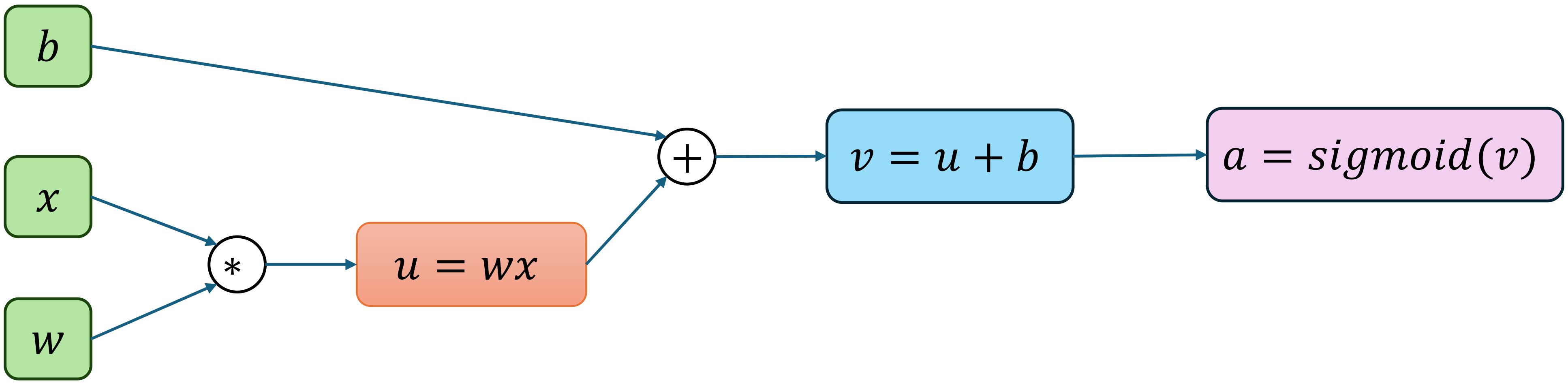
Section-1: Autograd in Pytorch

Autograd in PyTorch

Let's consider the computation graph of following:

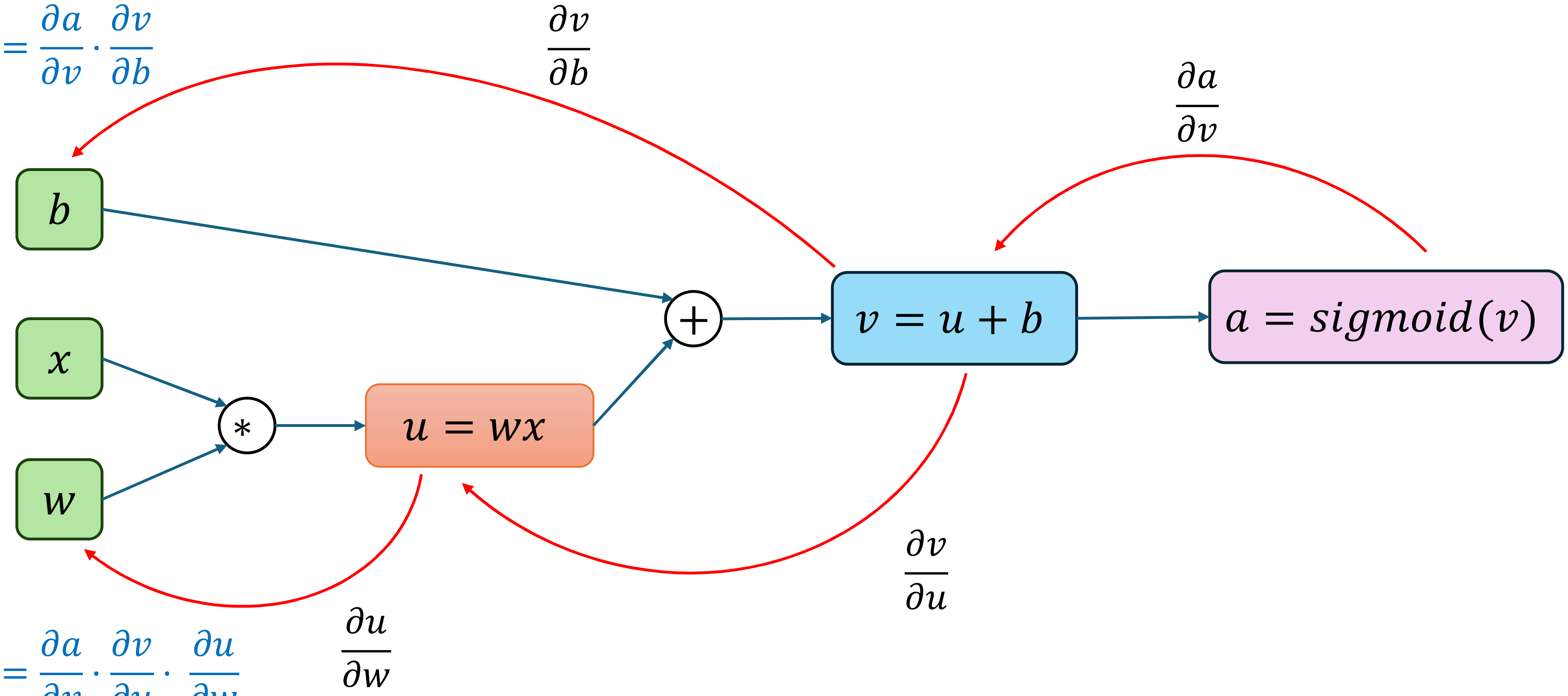
$$a(x, w, b) = sigmoid(\underbrace{\underbrace{w.x}_{u} + b}_{v})$$

Where, $sigmoid(z) = \frac{1}{1+e^{-z}}$



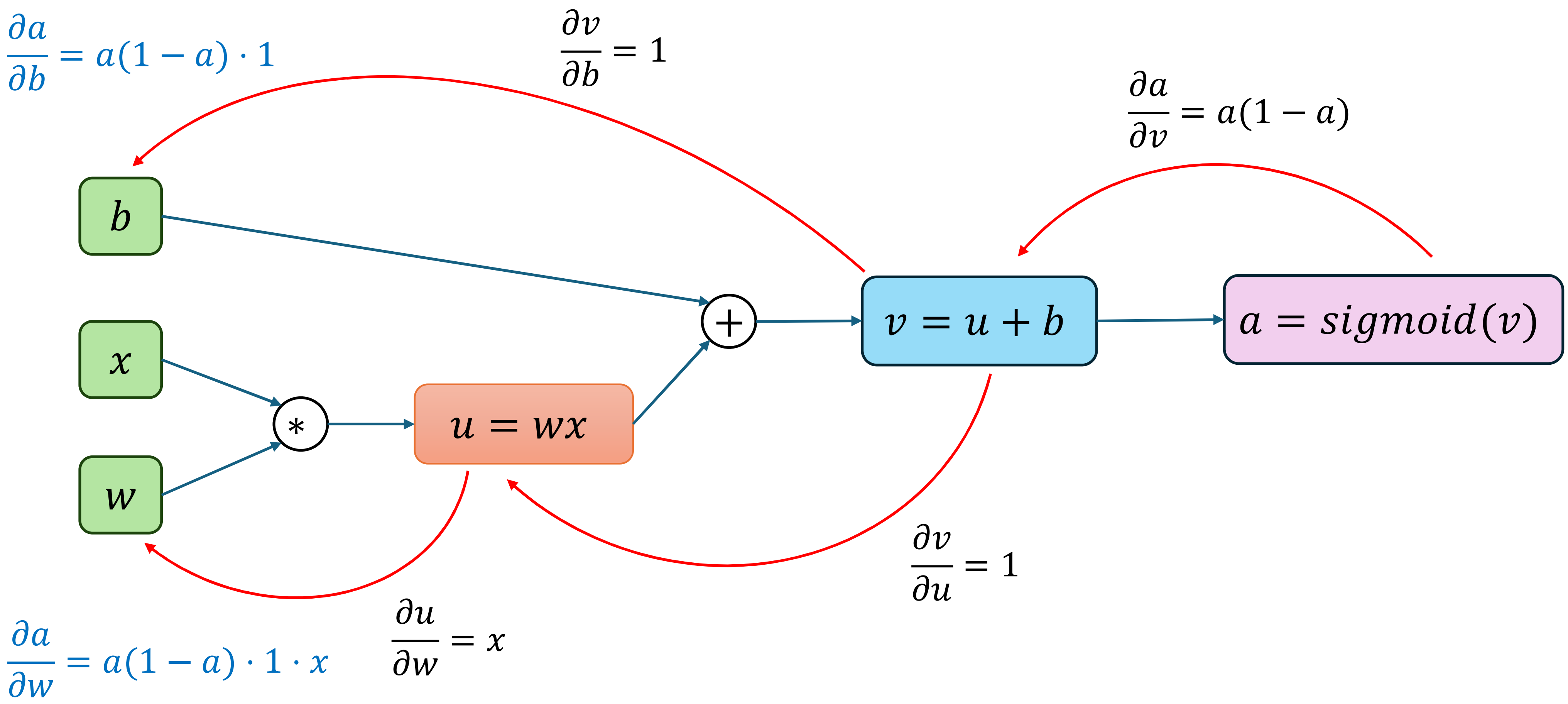
Autograd in PyTorch

$$\frac{\partial a}{\partial b} = \frac{\partial a}{\partial v} \cdot \frac{\partial v}{\partial b}$$

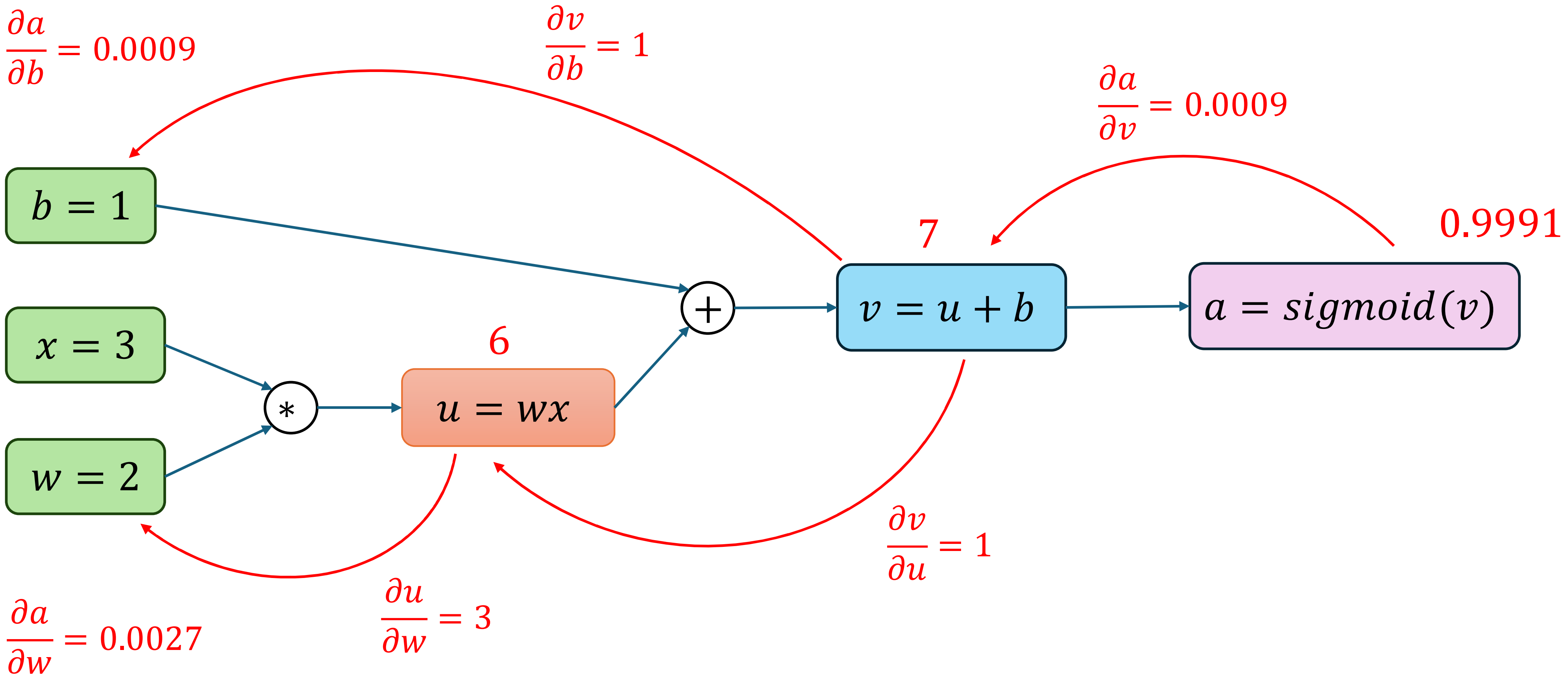


$$\frac{\partial a}{\partial w} = \frac{\partial a}{\partial v} \cdot \frac{\partial v}{\partial u} \cdot \frac{\partial u}{\partial w}$$

Autograd in PyTorch



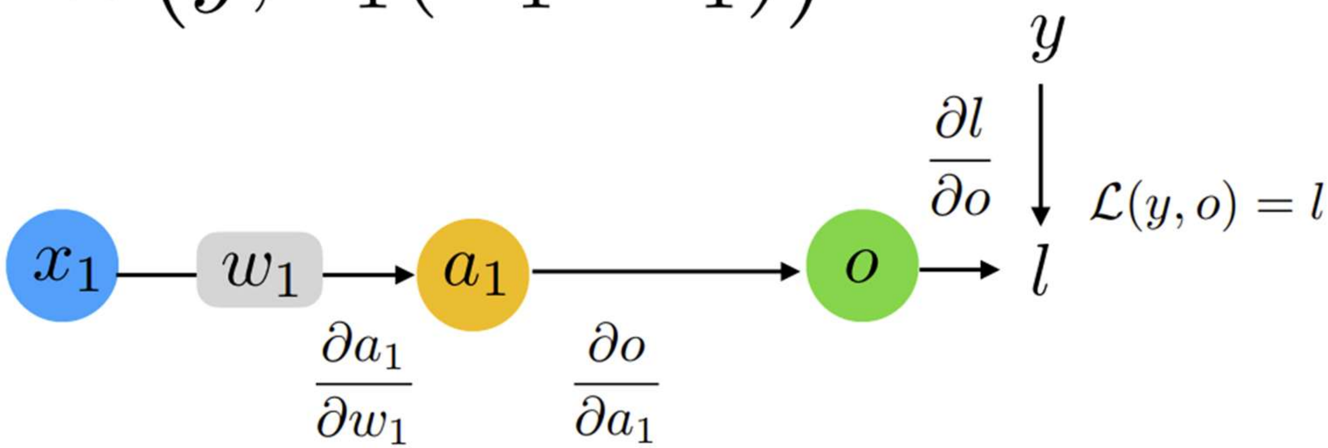
Autograd in PyTorch



Some More Computation Graphs

Graphs with Single Path

$$\mathcal{L}\big(y, \sigma_1(w_1 \cdot x_1)\big)$$

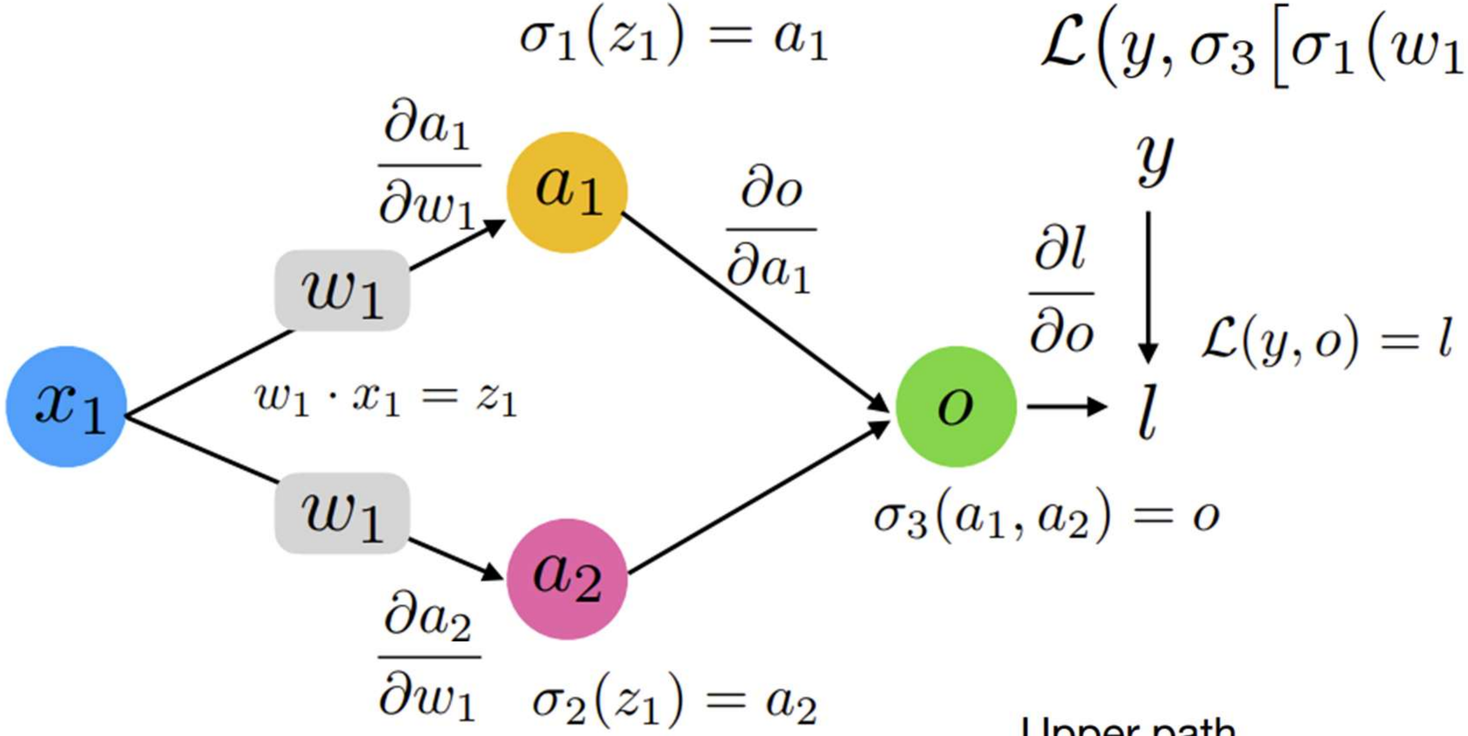


$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1} \cdot \frac{\partial a_1}{\partial w_1} \quad \text{(univariate chain rule)}$$

Some More Computation Graphs

Graphs with Weight Sharing

$$\mathcal{L}\Big(y, \sigma_3\big[\sigma_1(w_1 \cdot x_1), \sigma_2(w_1 \cdot x_1)\big]\Big)$$



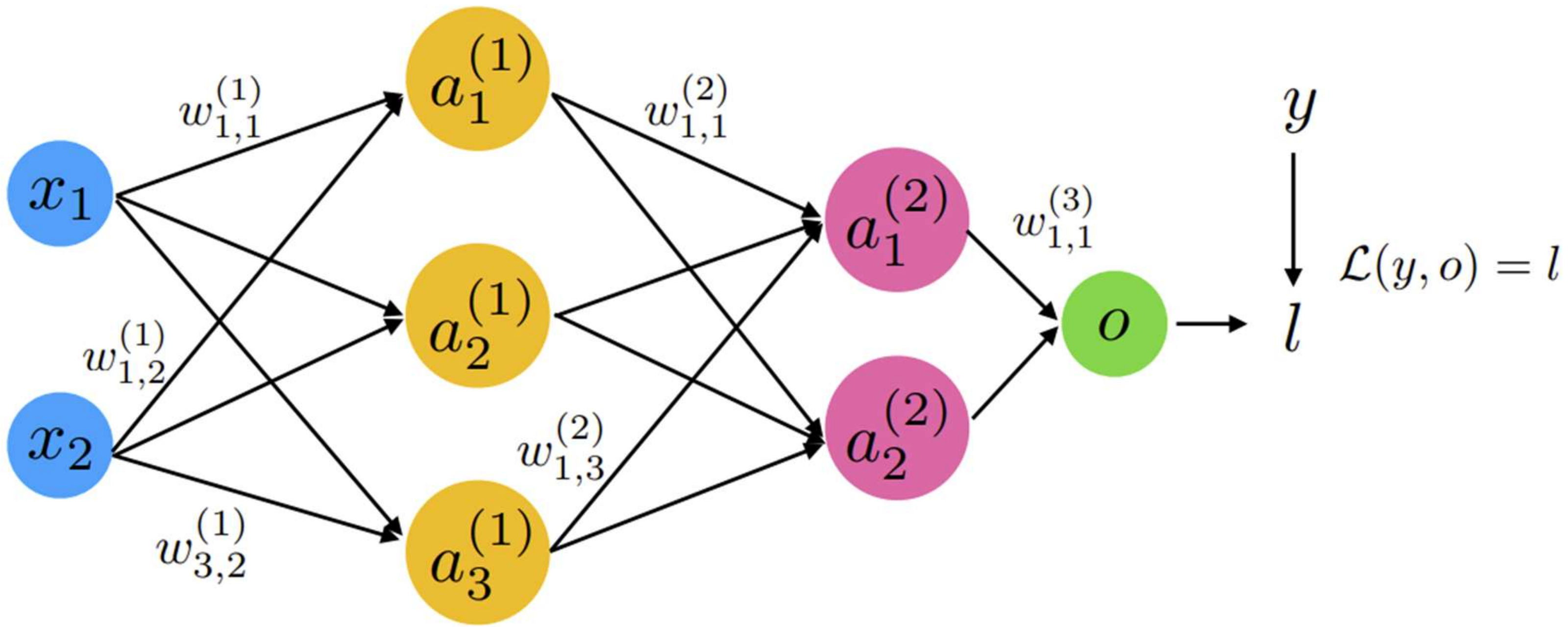
Upper path

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1} \cdot \frac{\partial a_1}{\partial w_1} + \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_2} \cdot \frac{\partial a_2}{\partial w_1}$$ (multivariable chain rule)

Lower path

Some More Computation Graphs

Graphs with Fully Connected Layers (MLP)



$$\frac{\partial l}{\partial w_{1,1}^{(1)}} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1^{(2)}} \cdot \frac{\partial a_1^{(2)}}{\partial a_1^{(1)}} \cdot \frac{\partial a_1^{(1)}}{\partial w_{1,1}^{(1)}}$$
$$+ \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_2^{(2)}} \cdot \frac{\partial a_2^{(2)}}{\partial a_1^{(1)}} \cdot \frac{\partial a_1^{(1)}}{\partial w_{1,1}^{(1)}}$$

Section-2: Important Modules in PyTorch

`torch.nn` module in PyTorch

What is `torch.nn`?

- `torch.nn` = **Neural Network** building blocks in PyTorch.
- Provides layers, activations, loss functions, and utilities for deep learning.
- Designed to work seamlessly with **autograd** for gradient computation.
- Helps organize models into **modular**, reusable components.
- Central abstraction: `nn.Module` – base class for all neural network layers/ models.

Key features of `torch.nn`

- **Predefined Layers:** `nn.Linear`, `nn.Conv2d`, `nn.LSTM`, etc.
- **Activation Functions:** `nn.ReLU`, `nn.Sigmoid`, `nn.Tanh`, etc.
- **Loss Functions:** `nn.CrossEntropyLoss`, `nn.BCELoss`, `nn.MSELoss`, etc.
- **Container Modules:** `nn.Sequential`, `nn.ModuleList`, `nn.ModuleDict`, etc. for structuring models.
- **Parameter Management:** automatically tracks model parameters (weights, biases) for optimization.
- **Integration with Optimizers:** works smoothly with `torch.optim` for training.

`torch.optim` module in PyTorch

What is `torch.optim`?

- `torch.optim` = **Optimization Algorithms** for training neural networks in PyTorch.
- Works with parameters tracked by `nn.Module`.
- Updates model weights based on computed gradients from **autograd**.
- Separates **model definition** (`torch.nn`) from **training logic** (`torch.optim`) maintaining **modular** components.
- Central abstraction: `torch.optim.Optimizer` class. All optimizers inherit from this base class.

Key features of `torch.optim`

- **Popular Optimizers Available:**
  - Gradient descent (SGD).
  - Adaptive methods: Adam, RMSprop, Adagrad etc. (we will learn more about these adaptive methods)
- **Parameter Management:** Takes model parameters (`model.parameters()`) as input.
- **Hyper parameters:** learning rate, momentum, weight decay, etc.
- **Zeroing Gradients:** `optimizer.zero_grad()` prevents accumulation.
- **Updating model parameters:** `optimizer.step()` automatically updates model parameters.
- **Scheduler Support:** `torch.optim.lr_scheduler` for learning rate adjustment during training.

torch.utils.data.Dataset and DataLoader

What are `torch.utils.data.Dataset` and `DataLoader`?

- **Dataset**
  - Represents your data (images, text, tabular, etc.)
  - Defines how to access a single sample and its label.
  - Custom datasets are created by subclassing `torch.utils.data.Dataset`

- **DataLoader**
  - Wraps a Dataset and provides batching, shuffling, and parallel loading.
  - Iterates over data efficiently during training.

Together: Provide an easy and scalable way to feed data into neural networks.

Key features

- **Dataset**
  - `__len__` : returns dataset size
  - `__getitem__` : fetches one data sample.
  - **Flexible**: can load from csv, images, databases etc.

- **Dataloader**
  - Batches data automatically by given `batch_size`.
  - Shuffles data each epoch (`shuffle = True`)
  - Supports parallelism (`num_workers`) for speed.
  - Returns data as an iterator for training loops.

Loading a csv dataset in PyTorch

```python
import torch
from torch.utils.data import Dataset, DataLoader
import pandas as pd

# Custom Dataset for CSV
class CSVDataset(Dataset):
    def __init__(self, csv_file):
        # Load CSV into a Pandas DataFrame
        self.data = pd.read_csv(csv_file)

        # Separate features (X) and labels (y)
        self.X = self.data.iloc[:, :-1].values   # all columns except last
        self.y = self.data.iloc[:, -1].values    # last column as label

    def __len__(self):
        return len(self.data)   # number of rows

    def __getitem__(self, idx):
        # Convert to tensors
        features = torch.tensor(self.X[idx], dtype=torch.float32)
        label = torch.tensor(self.y[idx], dtype=torch.long)
        return features, label


# Usage
dataset = CSVDataset("my_data.csv")
loader = DataLoader(dataset, batch_size=32, shuffle=True)

# Iterate through batches
for batch_X, batch_y in loader:
    print(batch_X.shape, batch_y.shape)
```

Creating a custom dataset (`CSVDataset`) by inheriting from `torch.utils.data.Dataset`

Separate features (X) with labels (y). This can be done in different ways for different datasets.

Using the class to load the data. Then using DataLoader on top of it to provide batching , shuffling

Functional vs Object Oriented APIs

Object Oriented API (`nn.Module` based)

- Layers are defined as **objects** (e.g. `nn.Linear`, `nn.Conv2d` etc.)
- Object oriented representations are state-full. Parameters (weights and biased) are stored internally as `torch.nn.Parameter`.
- Automatically integrated with the model's parameter management (`model.parameters()`).
- Typically used when building standard models (MLPs, CNNs, RNNs etc.)
- Useful for automatic parameter registration, saving / loading the models.

Functional API (torch.nn.`functional` based)

- Layers are defined as **functions.** (e.g. `F.linear`, `F.relu` etc.)
- Functional representations are state-less. Requires to explicitly pass weights and biases.
- Doesn't create persistent parameters – it just performs computation.
- Useful for building custom layers, experimenting.
- Functional APIs give low level controls, enabling the manipulation of the weights dynamically (e.g. weight sharing, custom initialization).

Functional vs Object Oriented APIs

Example of Object-Oriented API

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

# Define an input tensor (batch_size=2, input_dim=3)
x = torch.tensor([[1.0, 2.0, 3.0],
                  [4.0, 5.0, 6.0]])

# Define a linear layer: input features=3, output features=2
linear_layer = nn.Linear(in_features=3, out_features=2)

# Forward pass (automatically uses internal weights & bias)
output = linear_layer(x)
```

- `nn.Linear` stores weights and bias as Parameters.
- You can get them by `linear_layer.weight` and `linear_layer.bias`
- When you call `linear_layer(x)`, it applies:

$$y = xW^T + b$$

Example of Functional API

```python
import torch
import torch.nn as nn
import torch.nn.functional as F

# Define an input tensor (batch_size=2, input_dim=3)
x = torch.tensor([[1.0, 2.0, 3.0],
                  [4.0, 5.0, 6.0]])

# Explicitly register parameters
weights = nn.Parameter(torch.randn(out_features, in_features, dtype=torch.float),
                       requires_grad=True)

bias = nn.Parameter(torch.randn(out_features, dtype=torch.float),
                    requires_grad=True)

# Functional call: explicitly provide weight and bias
output_func = F.linear(x, weights, bias)
```

- `F.linear(x, weights, bias)` is just a function.
- Doesn’t track parameter by itself.
- Good for custom forward definitions in `nn.Module`.

Section-3: Different Loss Functions in PyTorch

Different Loss Functions in PyTorch

Loss function usually takes two sets of inputs: predicted values (inputs) and target values.
Here, we will talk about few widely used loss functions defined in PyTorch.
We will see both functional and object-oriented forms of loss functions.

Mean Square Error loss function:

- Object oriented form: **`nn.MSELoss()`**
- Functional form: **`nn.functional.mse_loss(inputs, targets)`**
- Used for regression (like: linear regression) or reconstruction (like: Auto-Encoders) type problems.
- The input and target needs to be torch tensors of same size.

```
import torch.nn as nn
import torch.nn.functional as F

# object oriented representation
loss_func = nn.MSELoss()

loss = loss_func(inputs, targets)

# functional representation

loss = F.mse_loss(inputs, targets)
```

`loss_func` defined as object of the class

Different Loss Functions in PyTorch

Binary Cross Entropy Loss:

- Object oriented form: **`nn.BCELoss()`**
- Functional form: **`nn.functional.binary_cross_entropy(inputs, targets)`**
- Used for binary classification problems.
- This takes logistic sigmoid values (i.e. probabilities) as inputs.
- The target needs to be encoded in 0 and 1.

```python
import torch.nn as nn
import torch.nn.functional as F

# object oriented representation
loss_func = nn.BCELoss()

loss = loss_func(inputs, targets)

# functional representation

loss = F.binary_cross_entropy(inputs, targets)
```

`loss_func` defined as object of the class

Different Loss Functions in PyTorch

Binary Cross Entropy With Logits Loss:

- Object oriented form: **`nn.BCEWithLogitsLoss()`**
- Functional form: **`nn.functional.binary_cross_entropy_with_logits(inputs, targets)`**
- Used for binary classification problems.
- This takes logits (before applying sigmoid) as inputs. It has built-in sigmoid layer that applies sigmoid internally.
- The target needs to be encoded in 0 and 1.

```python
import torch.nn as nn
import torch.nn.functional as F

# object oriented representation
loss_func = nn.BCEWithLogitsLoss()

loss = loss_func(logits, targets)

# functional representation

loss = F.binary_cross_entropy_with_logits(logits, targets)
```

`loss_func` defined as object of the class

Different Loss Functions in PyTorch

Cross Entropy Loss:

- Object oriented form: **`nn.CrossEntropyLoss()`**
- Functional form: **`nn.functional.cross_entropy (inputs, targets)`**
- Used for multi-class classification problems.
- This takes logits (before applying softmax) as inputs. It has built-in softmax layer that applies softmax internally.
- The target needs to be label-encoded i.e. in 0,1,2,….,C-1. [where C is the number of class]

```python
import torch.nn as nn
import torch.nn.functional as F

# object oriented representation
loss_func = nn.CrossEntropyLoss()

loss = loss_func(logits, targets)

# functional representation

loss = F.cross_entropy(logits, targets)
```

`loss_func` defined as object of the class

Different Loss Functions in PyTorch

Negative Log Likelihood Loss:

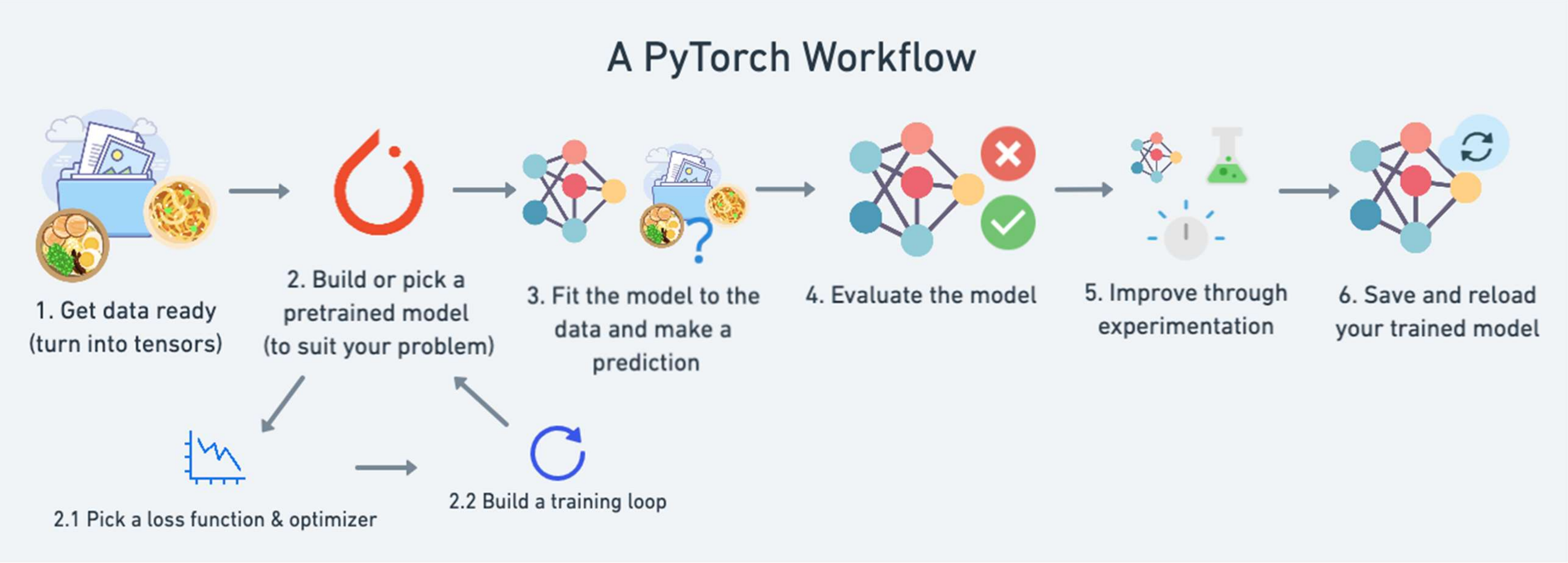
- Object oriented form: **`nn.NLLLoss()`**
- Functional form: **`nn.functional.nll_loss (inputs, targets)`**
- Used for multi-class classification problems.
- This takes log-softmax (logarithm of softmax) as inputs.
- The target needs to be label-encoded i.e. in 0,1,2,….,C-1. [where C is the number of class]

```
import torch.nn as nn
import torch.nn.functional as F

inputs = torch.log_softmax(logits, dim=1)

# object oriented representation
loss_func = nn.NLLLoss()

loss = loss_func(inputs, targets)

# functional representation

loss = F.nll_loss(inputs, targets)
```

`loss_func` defined as object of the class

Section-4: Defining, Creating, Training, and Evaluating Neural Networks in PyTorch

A PyTorch Workflow



MLP in PyTorch: Step-1 (Definition)

```python
import torch
import torch.nn as nn
import torch.nn.functional as F

class MultiLayerPerceptron(nn.module):

    def __init__(self, input_size, hidden_size_1, hidden_size_2, num_classes):

        super(MultiLayerPerceptron, self).__init__()

        # 1st hidden layer
        self.fc1 = nn.Linear(input_size, hidden_size_1)

        # 2nd hidden layer
        self.fc2 = nn.Linear(hidden_size_1, hidden_size_2)

        # Output layer
        self.linear_out = nn.Linear(hidden_size_2, num_classes)

    def forward(self, x):

        # passing through 1st hidden layer
        out = self.fc1(x)

        # activation function of 1st hidden layer
        out = F.relu(out)

        # passing through 2nd hidden layer
        out = self.fc2(out)

        # activation function of 2nd hidden layer
        out = F.relu(out)

        logits = self.linear_out(out)

        # Softmax to get probabilities
        probas = F.softmax(logits, dim=1)

        return logits, probas
```

Functional API to call the activation functions.

`MultilayerPerceptron` class which inherits **`torch.nn.Module.`**

Initializing the super (parent) class. `super().__init__()` will also do.

Defining the architecture of the feedforward neural network (MLP). The layers are defined by **`torch.nn.Linear`**, which are also called fully connected layers or dense layers.

The **`forward`** method defines the forward pass of the neural network. When inheriting from **`torch.nn.Module`** we need to explicitly create the **`forward`** method. This is a fundamental requirement in pytorch's architecture.

Pre and post activation of first hidden layer.

Pre and post activation of second hidden layer.

Logits / pre-activation of final classification layer.

Converting final classification layer's output to probability using `softmax`. This is optional.

MLP in PyTorch: Step-1 (Definition)

There is another neat way of creating the neural network using **`torch.nn.Sequential`** container module.

```python
import torch
import torch.nn as nn
import torch.nn.functional as F

class MultiLayerPerceptron(nn.module):

    def __init__(self, input_size, hidden_size_1, hidden_size_2, num_classes):

        super(MultiLayerPerceptron, self).__init__()

        # All layers within Sequential container step by step
        self.my_network = nn.Sequential(
            nn.Linear(input_size, hidden_size_1),
            nn.ReLU(),
            nn.Linear(hidden_size_1, hidden_size_2),
            nn.ReLU(),
            nn.Linear(hidden_size_2, num_classes)
        )

    def forward(self, x):

        # Forward pass through the network
        logits = self.my_network(x)

        # Softmax to get probabilities
        probas = F.softmax(logits, dim=1)

        return logits, probas
```

This code is more clear and more compact.

Note that how the activation functions are called as layers (object-oriented representation) in contrast to functional representation earlier.

But there are few caveats:

1. We can't use this, if you want to define your neural network with custom activation function and layers.
2. `forward` may be harder to debug if there are errors, as we can't simply add breakpoints or insert print statements within the `Sequential` block.

MLP in PyTorch: Step-2 (Creation)

```
torch.manual_seed(random_seed) # for reproducability

if torch.cuda.is_available():
    device = "cuda" # Use NVIDIA GPU (if available)
elif torch.backends.mps.is_available():
    device = "mps" # Use Apple Silicon GPU (if available)
else:
    device = "cpu" # Default to CPU if no GPU is available

# Defining model
model = MultilayerPerceptron(input_size, hidden_size_1, hidden_size_2, num_classes)

# move the model parameters to CPU/GPU/Apple Silicon GPU
model = model.to(device)

# Stochastic Gradient Descent (SGD) optimizer
learning_rate = 0.01
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate)
```

Instantiate model (creates the model parameters)

Moving the model to the available device (GPU / CPU)

Defining an optimization method

MLP in PyTorch: Step-3 (Training)

```python
train_data_loader = DataLoader(dataset=train_dataset, batch_size=32, shuffle=True)

num_epochs = 100

for epoch in range(num_epochs):

    model.train()  # set the model to training mode

    for batch_idx, (features, labels) in enumerate(train_data_loader):
        # move the features and labels to CPU/GPU/Apple Silicon GPU
        features = features.to(device)
        labels = labels.to(device)

        # Forward pass: compute predicted outputs by passing inputs to the model
        logits, probas = model(features)

        # Calculate the loss
        loss = F.cross_entropy(logits, labels)

        # Zero the gradients before running the backward pass.
        optimizer.zero_grad()

        # Backward pass: compute gradient of the loss with respect to model parameters
        loss.backward()

        # Perform a single optimization step (parameter update)
        optimizer.step()

```

Specifying a `DataLoader` for training dataset

Run for a specified number of epochs

Iterate over mini-batches in each epoch

Make sure your data is in the same hardware (device) as model.

`y = model(x)` calls `__call__` and then `.forward()`. Don't run `y = model.forward(x)` directly.

Specify loss function based on the problem. Notice, how the `cross_entropy` loss is applied to `logits` and not on `probas`.

To prevent gradient accumulation, we need to zero them before each backward pass

These two steps calculates the loss gradients w.r.t. model parameters and then updates the parameter. i.e. these two steps together perform gradient descent operation.

MLP in PyTorch: Step-4 (Evaluation)

Training / Validation / Test Split

- Training data set is used for training the neural networks. It's not necessary to plot the training loss / accuracy during training but it can be useful.
- Validation set accuracy provides a rough estimate of the generalization performance and then can be used to tune the hyper-parameters of the model.
- Test set should only be used once to get an unbiased estimate of the generalization performance.
- The **train : validation : test** ratio depends on dataset size, but usually for the large dataset the 80:5:15 split is a good idea.
- Sometimes validation data is not present, only train and test datasets are available. Then usually it is a good idea to split the train dataset further (like 90:10 split), where the larger part will be used for training and smaller part for validation.
- In many cases, with the absence of validation dataset, people often skip the validation part entirely and evaluate the generalization performance of the model on the test dataset.

MLP in PyTorch: Step-4 (Evaluation)

```
def compute_loss(net, data_loader):
    net.eval() # evaluation mode
    total_loss, total_samples = 0.0, 0
    with torch.no_grad(): # no gradient tracking
        for features, targets in data_loader:
            features = features.to(device),
            targets = targets.to(device)
            logits = net(features)
            loss = F.cross_entropy(logits, targets, reduction="sum")  # sum, not mean
            total_loss += loss.item()
            total_samples += targets.size(0)
    return total_loss / total_samples

def compute_accuracy(net, data_loader):
    net.eval()  # evaluation mode
    correct_pred, num_examples = 0, 0
    with torch.no_grad():  # no gradient tracking
        for features, targets in data_loader:
            features = features.to(device)
            targets = targets.to(device)

            logits = net(features)
            predicted_labels = torch.argmax(logits, dim=1)

            num_examples += targets.size(0)
            correct_pred += (predicted_labels == targets).sum().item()

    return correct_pred / num_examples * 100
```

By default, the cross-entropy loss computes the mean or average loss over entire mini-batch.

However, here we are trying to compute the sum of the loss for entire dataset and then compute average.

Hence, `cross_entropy` loss is used with reduction “`sum`”.

MLP in PyTorch: Step-4 (Evaluation)

```python
training_loss = []
validation_loss = []

for epoch in range(num_epochs):
    model.train()
    ### training codes ###

    # training loss
    loss_train = compute_loss(model, train_data_loader)
    training_loss.append(loss_train)

    # validation loss
    loss_val = compute_loss(model, validation_data_loader)
    validation_loss.append(loss_val)

    # training accuracy for each epoch
    training_accuracy = compute_accuracy(model, train_data_loader)

    # validation accuracy for each epoch
    validation_accuracy = compute_accuracy(model, validation_data_loader)

# compute test accuracy after completeing the training
test_accuracy = compute_accuracy(model, test_data_loader)
```

Keep track of training and validation loss and accuracy in each epoch / training loop

Test accuracy is computed only when training is complete

Few Important Notes

`model.train()` vs `model.eval()`

In PyTorch, **`model.train()`** and **`model.eval()`** are essential for managing the behavior of specific layers during the training and inference phases, primarily affecting layers like **Dropout** and **Batch Normalization**.

The **`model.train()`** method sets the model to training mode, but it doesn't perform the training. The **`model.eval()`** method switches the model to evaluation mode. In this mode, the behavior of the Dropout and Batch Normalization layer changes.

We will learn about dropout and batch normalization in details later.

`torch.no_grad()` vs `torch.inference_mode()`

Similarities:

- Both disables gradient tracking.
- Reduce memory usage and improve inference speed.
- Used during evaluation / inference, not training.

Differences:

- **`torch.no_grad()`** temporarily disables autograd but still maintains some autograd metadata internally. However, **`torch.inference_mode()`** is the stronger version which completely disables autograd and related metadata.
- While **`torch.no_grad()`** is good for "one-off" inference or validation step, **`torch.inference_mode()`** is more optimized and faster, especially on large models.
- **`torch.inference_mode()`** was introduced in PyTorch 1.9 for production grade inferences.

Section-5: Saving and Loading Neural Networks in PyTorch

Saving and Loading `state_dict`

- In PyTorch, saving and loading models is very flexible. You can save either the **entire model** or just its **learned parameters (`state_dict`)**.
- `state_dict` is usually smaller in size.
- It avoids issues with pickling (i.e. serializing the data).

```python
import torch

### Saving the model's state_dict ###

# Assume 'model' is an instance of nn.Module
torch.save(model.state_dict(), "model_weights.pth")

### Loading the model's state_dict ###

# Initialize the model class first which should be similar to the saved model
model = MyModel()
model.load_state_dict(torch.load("model_weights.pth"))
model.eval()
```

Saving and Loading Entire Model

- We can also save the entire model (model architecture + learned parameters)
- Tightly coupled with code structure. (can break if the class definition changes)
- It usually takes larger memory to store.

```python
import torch

### Saving theentire model ###

torch.save(model, "entire_model.pth")

### Loading the entire model ###

model = torch.load("entire_model.pth")
model.eval()
```

Saving and Loading With Checkpoint

- Checkpoint saves learned parameters + optimizer + epoch.
- Sometimes model trains for hours (or even days or weeks). For any hardware / software failure the model might stop training. In that case it is a good idea to periodically save the checkpoints and resume the training from the last saved checkpoint. It is like keeping a bookmark while reading.

```python
import torch

### Saving Checkpoints ###

torch.save({
    "epoch": epoch,
    "model_state_dict": model.state_dict(),
    "optimizer_state_dict": optimizer.state_dict(),
    "loss": loss,
}, "checkpoint.pth")

### Loading checkpoints ##

checkpoint = torch.load("checkpoint.pth")
model.load_state_dict(checkpoint["model_state_dict"])
optimizer.load_state_dict(checkpoint["optimizer_state_dict"])
epoch = checkpoint["epoch"]
loss = checkpoint["loss"]

model.train()  # or .eval(), depending on usage
```

Saving and Loading With TorchScript

- **TorchScript** converts PyTorch models into a form independent of python code (useful for C++ deployment or model serving in some servers / mobile devices / edge devices)
- It uses Just-In-Time (JIT) compiler which exports models for deployment in C++ or other runtimes.

```python
import torch

### Saving the script ###

scripted = torch.jit.script(model)
scripted.save("scripted_model.pt")

### Loading the script ###

loaded_model = torch.jit.load("scripted_model.pt")

# Set to evaluation mode if needed
loaded_model.eval()
```

Thank You