Introduction to PyTorch

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Agenda

1. Introduction
2. Tensors
3. Autograd
4. Loss

Why use deep learning libraries?

- Quickly implement and test new ideas
- No need to implement your own neural networks, just use their (likely more efficient) implementation
- Automatically compute gradients (!!)
- Efficiently run on GPUs to speed up computations with few changes

Deep Learning Frameworks

Caffe
(UC Berkeley)

Torch
(NYU / Facebook)

Theano
(U Montreal)

2007-2015

Deep Learning Frameworks

Caffe (UC Berkeley)	→	Caffe2 (Facebook) ↓
Torch (NYU / Facebook)	→	PyTorch (Facebook)
Theano (U Montreal)	→	TensorFlow (Google)

2016-2020

Deep Learning Frameworks

Caffe (UC Berkeley) → Caffe2 (Facebook)

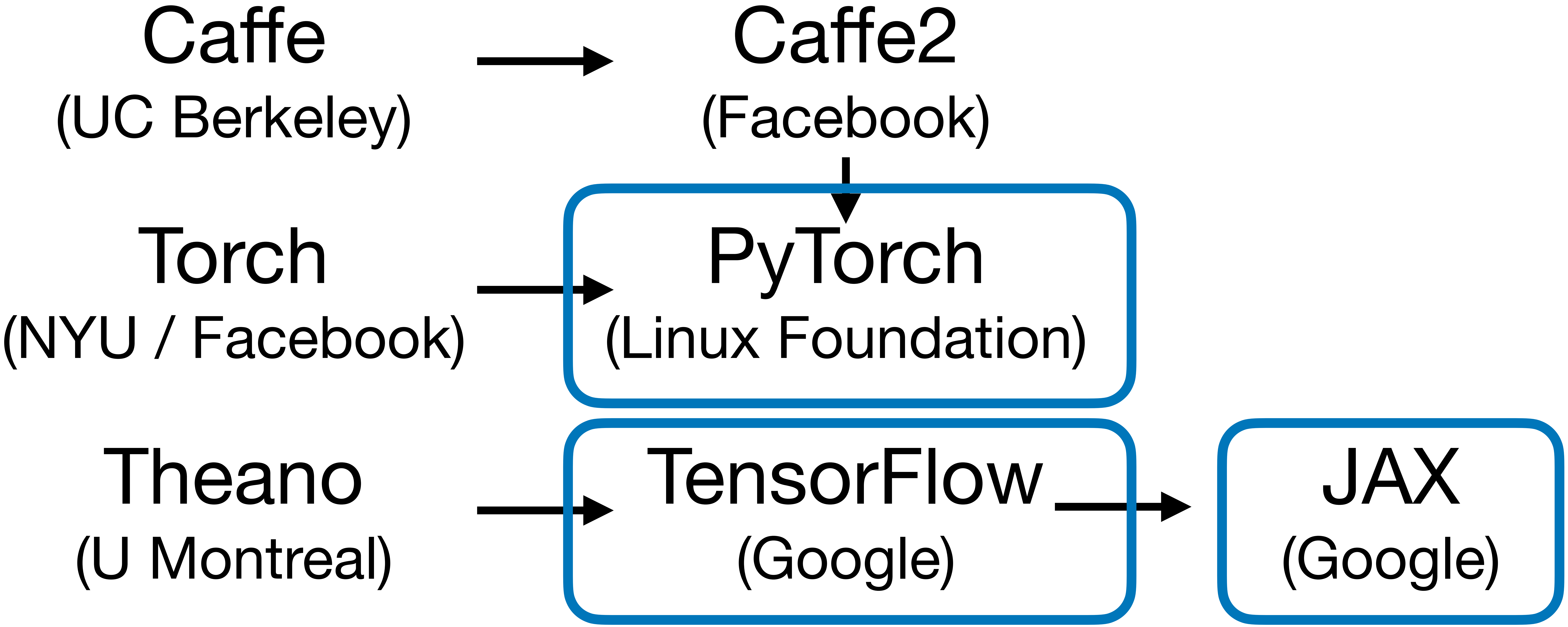
↓

Torch (NYU / Facebook) → PyTorch (Linux Foundation)

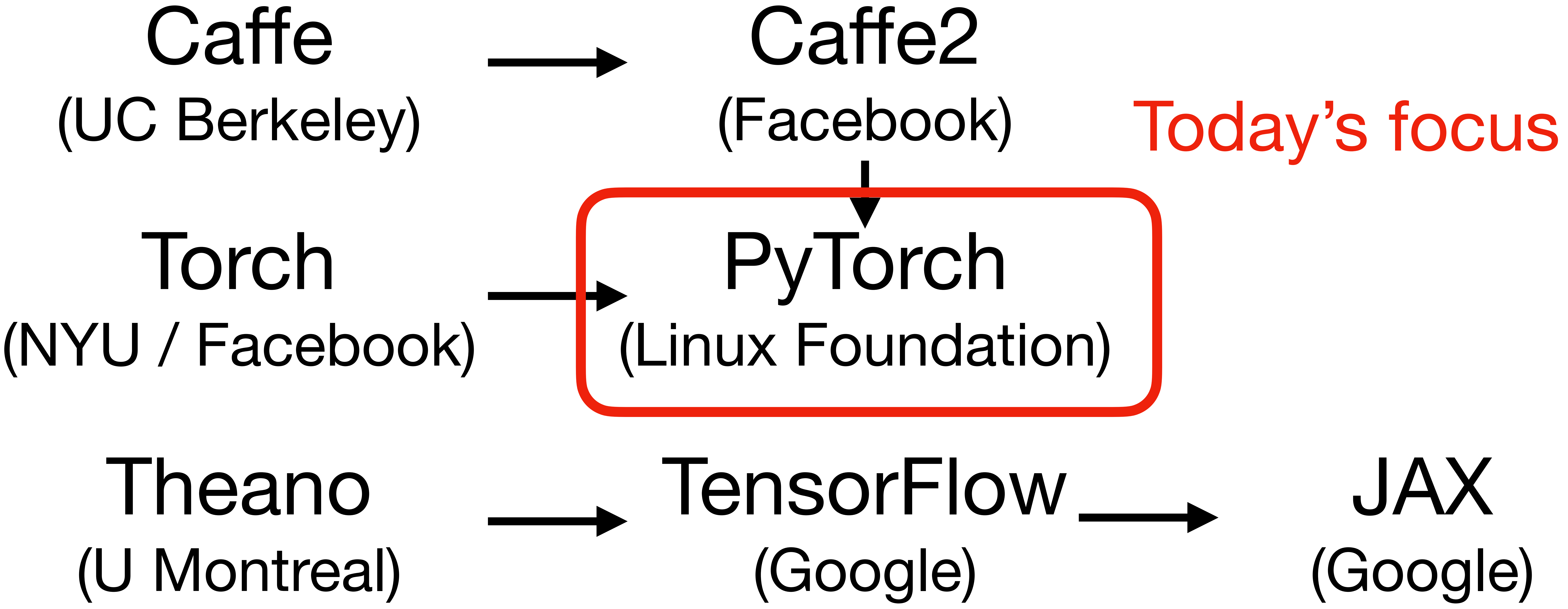
2020-present

Theano (U Montreal) → TensorFlow (Google) → JAX (Google)

Deep Learning Frameworks



Deep Learning Frameworks



Deep Learning Frameworks

DyNet
(CMU)

CNTK
(Microsoft)

Chainer
(Preferred Networks)

MXNet
(Amazon)

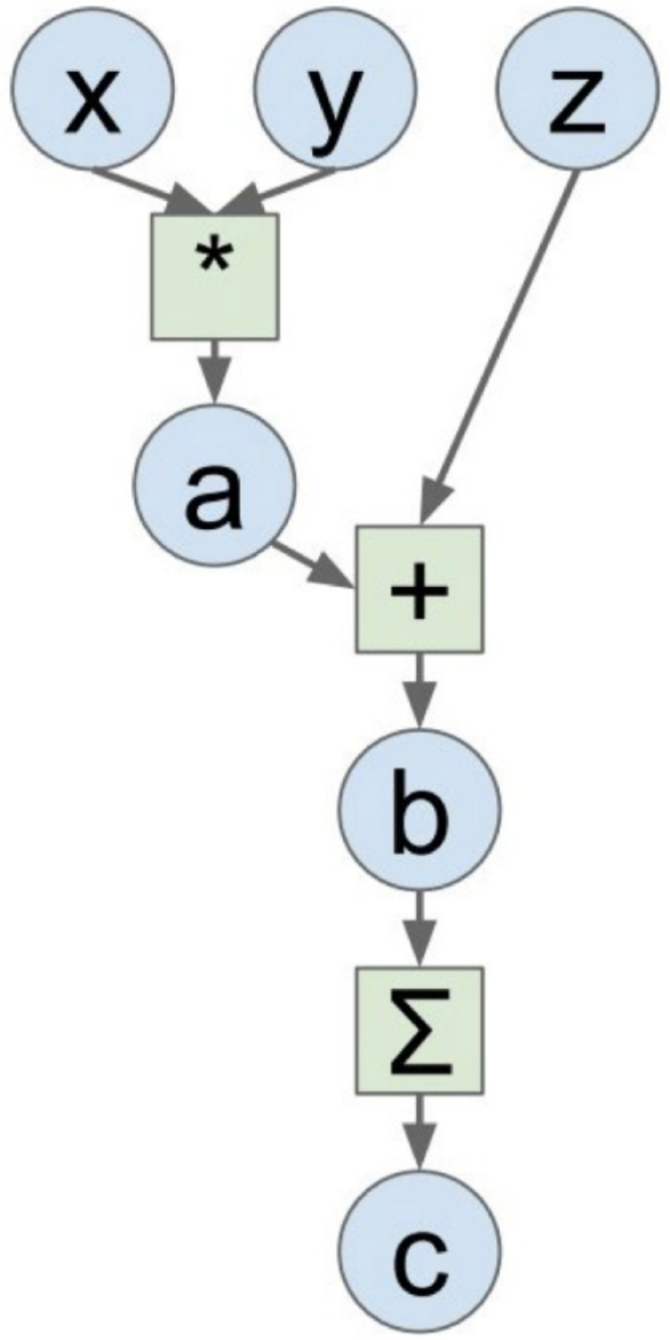
Other frameworks that tried to make a dent

Installing PyTorch: Google Colab

- We assume you'll be using Google Colab for your projects
- torch (PyTorch) should come pre-installed in the colab environment
    - *If* it isn't, you can always install outside packages using:
      `!pip install torch`

PyTorch Preview

- API is very clean and code is very readable
- No need to compute gradients, just use `.backward()` !



Computational Graph

```python
import numpy as np
np.random.seed(0)

N, D = 3, 4

x = np.random.randn(N, D)
y = np.random.randn(N, D)
z = np.random.randn(N, D)

a = x * y
b = a + z
c = np.sum(b)

grad_c = 1.0
grad_b = grad_c * np.ones((N, D))
grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
grad_y = grad_a * x
```

NumPy

```python
import torch
torch.manual_seed(0)

N, D = 3, 4

x = torch.rand((N, D), requires_grad=True)
y = torch.rand((N, D), requires_grad=True)
z = torch.rand((N, D), requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()
```

PyTorch

torch.Tensor: Introduction

- Exactly like NumPy arrays, but can be run efficiently on GPUs
- Supports the same operations like indexing, slicing, reshaping, transpose, cross product, matrix product, element-wise multiplication, …

```python
import numpy
# create a tensor
new_numpy = numpy.array([[1, 2], [3, 4]])
# create a 2 x 3 tensor with random values
empty_numpy = numpy.random.rand(2,3)
# create a 2 x 3 tensor with random values between -1 and 1
uniform_numpy = numpy.reshape(np.random.uniform(-1,1,6),[2,3])
# create a 2 x 3 tensor with random values from a uniform distribution on the interval [0, 1)
rand_numpy = numpy.random.rand(2, 3)
# create a 2 x 3 tensor of zeros
zero_numpy = numpy.zeros([2, 3])
```

NumPy

```python
import torch
# create a tensor
new_tensor = torch.Tensor([[1, 2], [3, 4]])
# create a 2 x 3 tensor with random values
empty_tensor = torch.Tensor(2, 3)
# create a 2 x 3 tensor with random values between -1and 1
uniform_tensor = torch.Tensor(2, 3).uniform_(-1, 1)
# create a 2 x 3 tensor with random values from a uniform distribution on the interval
rand_tensor = torch.rand(2, 3)
# create a 2 x 3 tensor of zeros
zero_tensor = torch.zeros(2, 3)
```

PyTorch

torch.Tensor: Gradients

`requires_grad` - Makes this a trainable parameter

- *False* by default
- Turn on:

  ```
  t.requires_grad_()
  t = torch.randn(1, requires_grad=True)
  ```
- Tensor value = `t.data`
- Gradient value = `t.grad`
- History of autograd operations = `t.grad_fn`

```python
import torch

N, D = 3, 4

x = torch.rand((N, D),requires_grad=True)
y = torch.rand((N, D),requires_grad=True)
z = torch.rand((N, D),requires_grad=True)

a = x * y
b = a + z
c=torch.sum(b)

c.backward()

print(c.grad_fn)
print(x.data)
print(x.grad)
```

```
<SumBackward0 object at 0x7fd0cb970cc0>
tensor([[0.4118, 0.2576, 0.3470, 0.0240],
        [0.7797, 0.1519, 0.7513, 0.7269],
        [0.8572, 0.1165, 0.8596, 0.2636]])
tensor([[0.6855, 0.9696, 0.4295, 0.4961],
        [0.3849, 0.0825, 0.7400, 0.0036],
        [0.8104, 0.8741, 0.9729, 0.3821]])
```

Note: Functions that end with an underscore _ modify the tensor in-place!

Tensors: Devices

Check if a GPU is available:

`torch.cuda.is_available()`

Convert a `numpy.array` to `torch.Tensor`:

`torch.from_numpy(x_train)`

this returns a cpu tensor

Convert back to `numpy`:

`t.numpy()`

Move tensor to a device:

`t.to('cuda')` or `t.to('cpu')`

Check tensor or array type:

`type(t)` or `t.type()`

```
import torch
import torch.optim as optim
import torch.nn as nn
from torchviz import make_dot

device = 'cuda' if torch.cuda.is_available() else 'cpu'

# Our data was in Numpy arrays, but we need to transform them into PyTorch's Tensors
# and then we send them to the chosen device
x_train_tensor = torch.from_numpy(x_train).float().to(device)
y_train_tensor = torch.from_numpy(y_train).float().to(device)

# Here we can see the difference - notice that .type() is more useful
# since it also tells us WHERE the tensor is (device)
print(type(x_train), type(x_train_tensor), x_train_tensor.type())
```

Autograd: Introduction

- Automatic differentiation package
- `t.backward()` calculates gradients along the computational graph
- Gradients are accumulated by default
    - Need to zero them out after each update
    - t.grad.zero_()
    - (Typically done with Optimizer!)

Autograd: Introduction

Automatic differentiation package

We can easily compute gradients with:

```
t.backward()  # computes along the computation graph
```

Gradients are accumulated by default

We can update the parameter weight using the gradient as:

```
w -= lr * w.grad
```

After updating, you need to reset the gradients by clearing their values:

```
w.grad_.zero()
```

Autograd: Manual Update Example

- Definition
- Forward pass
- Backward pass
- Weight update
- Reset grads

```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor
    error = y_train_tensor - yhat
    loss = (error ** 2).mean()

    loss.backward()

    with torch.no_grad():
        a -= lr * a.grad
        b -= lr * b.grad

    a.grad.zero_()
    b.grad.zero_()

print(a, b)
```

Optimizer

The `torch.optim` library makes updating the parameters easier:

We can use different optimization algorithms, like Adam, SGD, RMSprop.

We compute the gradients like before: `t.backward()`

But now we use the optimizer to apply param updates: `optimizer.step()`

Zero gradients with: `optimizer.zero_grad()`

```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)


# Defines a SGD optimizer to update the parameters
optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor
    error = y_train_tensor - yhat
    loss = (error ** 2).mean()

    loss.backward()

    optimizer.step()

    optimizer.zero_grad()
```

Loss Functions

- Use pre-implemented loss functions too!
- L1, MSE, Cross-Entropy, …

```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

# Defines a MSE loss function
loss_fn = nn.MSELoss(reduction='mean')

optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor

    loss = loss_fn(y_train_tensor, yhat)

    loss.backward()
    optimizer.step()
    optimizer.zero_grad()
```

Precept on Friday

- Model
- Dataset
- Evaluation