A shallow introduction to Deep Learning with

PYTORCH

DL4SCI 2020

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What to expect ?

Webinar format

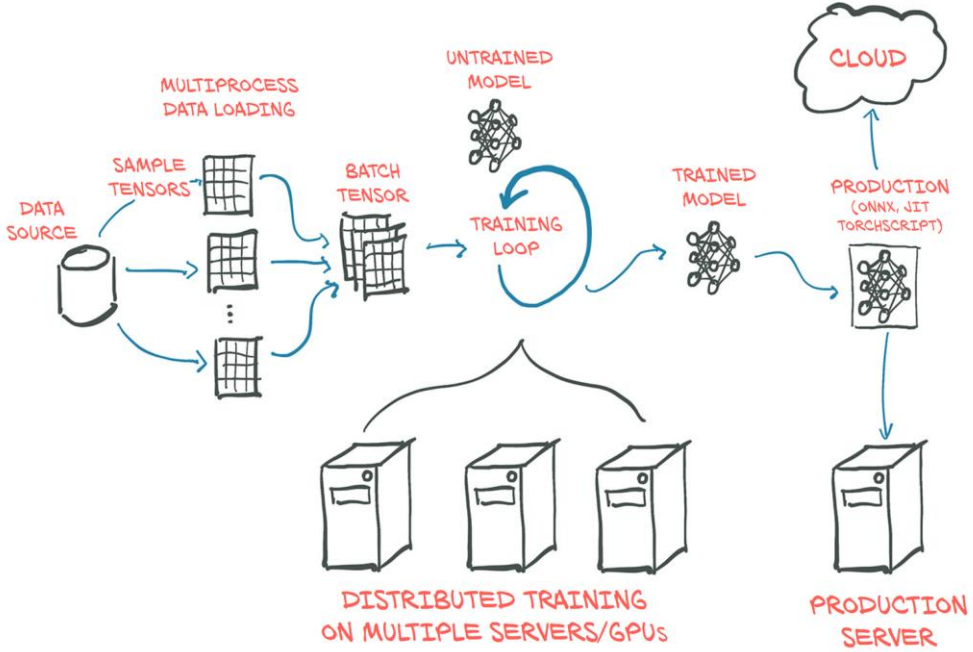
- 1 hour
- Prerequisites
  - Python
  - Gradient Based Machine Learning
  - A Numerical Computing Tool
- Slides & Notebooks

PyTorch

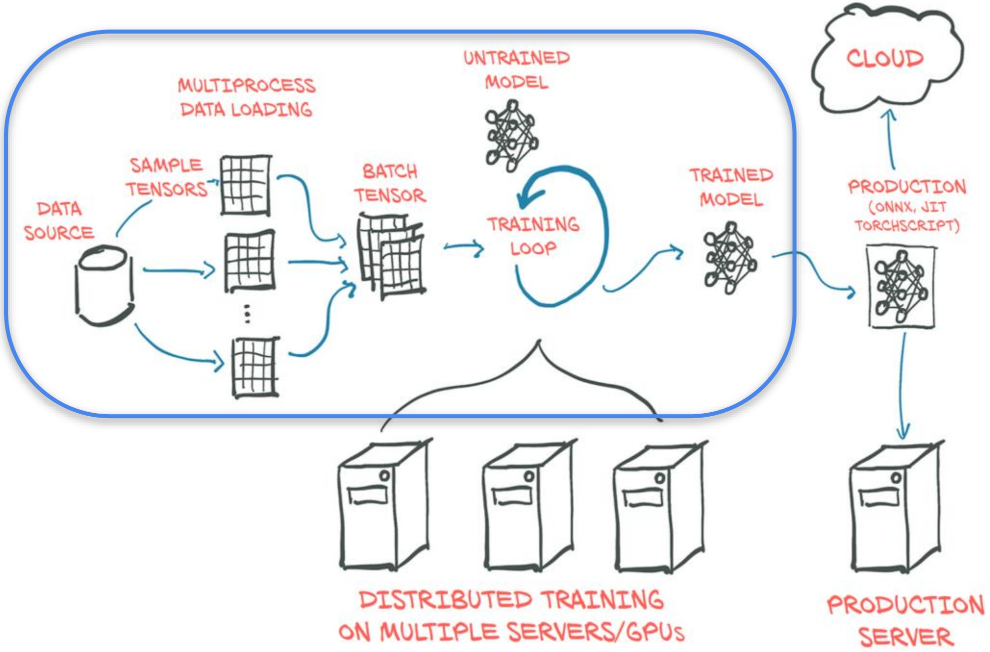
A library for scientific computing in Python, just like NumPy with:

- GPU support
- Automatic differentiation & Optimization algorithms
- All necessary tools for Deep Learning

Deep Learning pipeline with PyTorch



Deep Learning pipeline with PyTorch



Program Skeleton

INITIALISATION

- Create model
- Load data and prepare samples
- Initialise optimisation and training HP

TRAINING LOOP

- Get a batch of samples and labels from the dataset
- Move samples and labels to GPU
- Compute the model's predictions
- Compute the loss
- Compute the gradients with backpropagation
- Update the parameters

It’s all about Tensors

- Tensors are multi-dimensional arrays
- Very similar to NumPy for Tensor creation, indexing, masking

```
np.array([[1, 2, 3], [4, 5, 6]])

np.eye(2)

np.arange(1,5)

np.zeros(5)
```

```
torch.tensor([[1, 2, 3], [4, 5, 6]])

torch.eye(2)

torch.arange(1,5)

torch.zeros(5)
```

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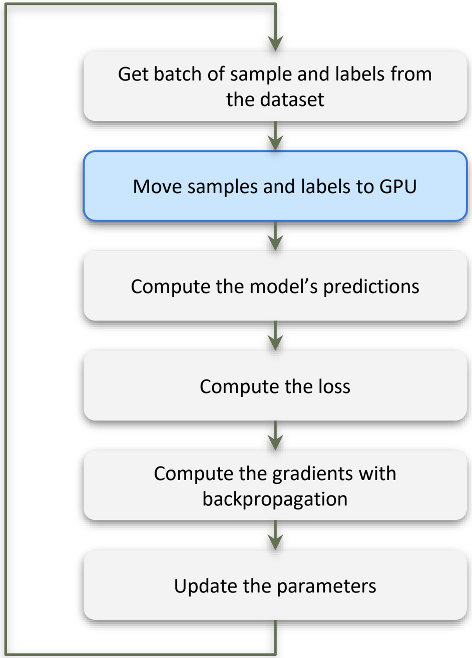
Tensors - Recap

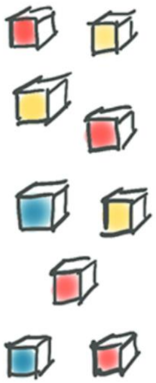
- Size and dimensions: `tensor.dim()` and `tensor.shape`
- Chain operations: `tensor.log().sum().exp()`
- In-place operations with underscore: `tensor.log_()`
- Reshape: `tensor.view(2,3)` and `tensor.view(-1, 3)`
- GPU ⇔ CPU: `torch.device` and `tensor.to(device)`

Building the Training Loop



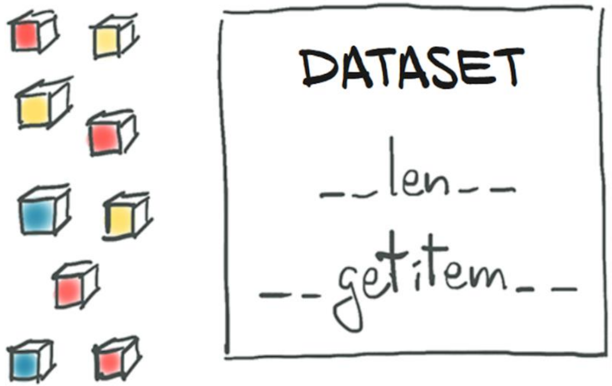

```
# TRAINING LOOP

# Loop through dataset to get batches of samples and labels
    samples = samples.to(device)
    labels = labels.to(device)
    # compute predictions with model
    # compute the loss
    # compute gradients
    # update model parameters
```

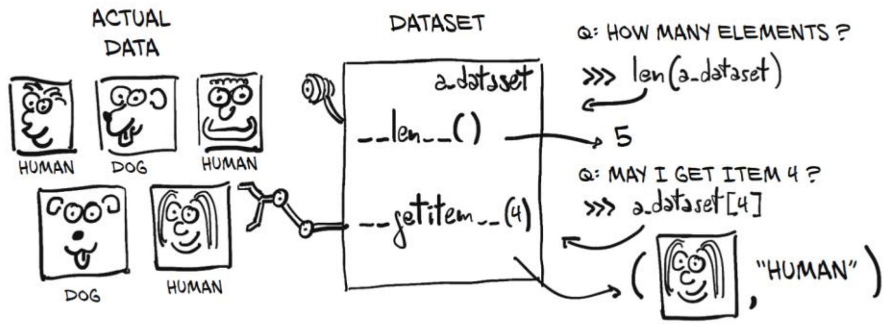
Working with data: Dataset & Dataloaders



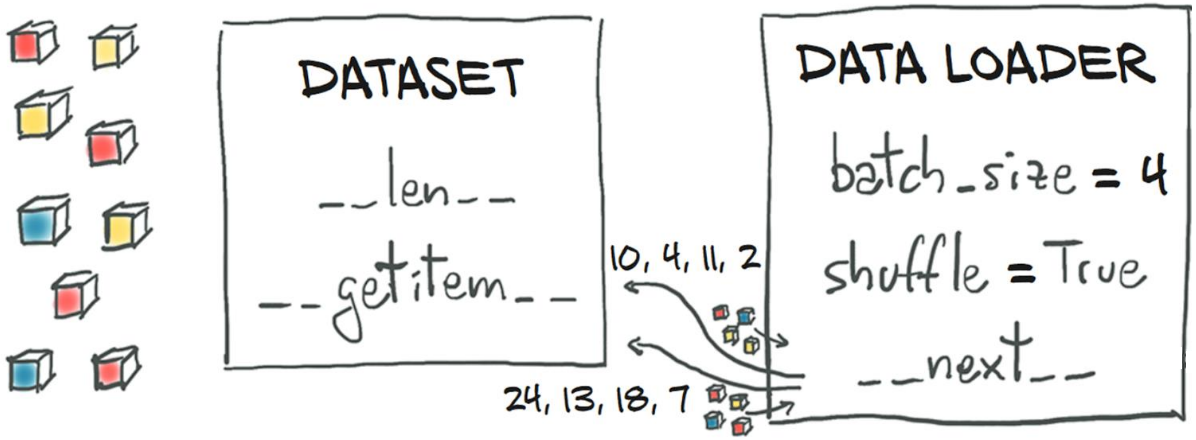
```
data/human-vs-dog
│
├──train
│     │
│     │──human
│     │       ├── 20.jpg
│     │       ├── 104.jpg
│     │       ├── ...
│     │
│     └──dog
│             │   1.jpg
│             │   78.jpg
│             ├── ...
│
└── validation
      ├── human
      │       │   233.jpg
      │       │   12.jpg
      │       ├── ...
      │
      └──dog
              │   22.jpg
              │   77.jpg
              ├── ...
```

Working with data: Dataset & Dataloaders

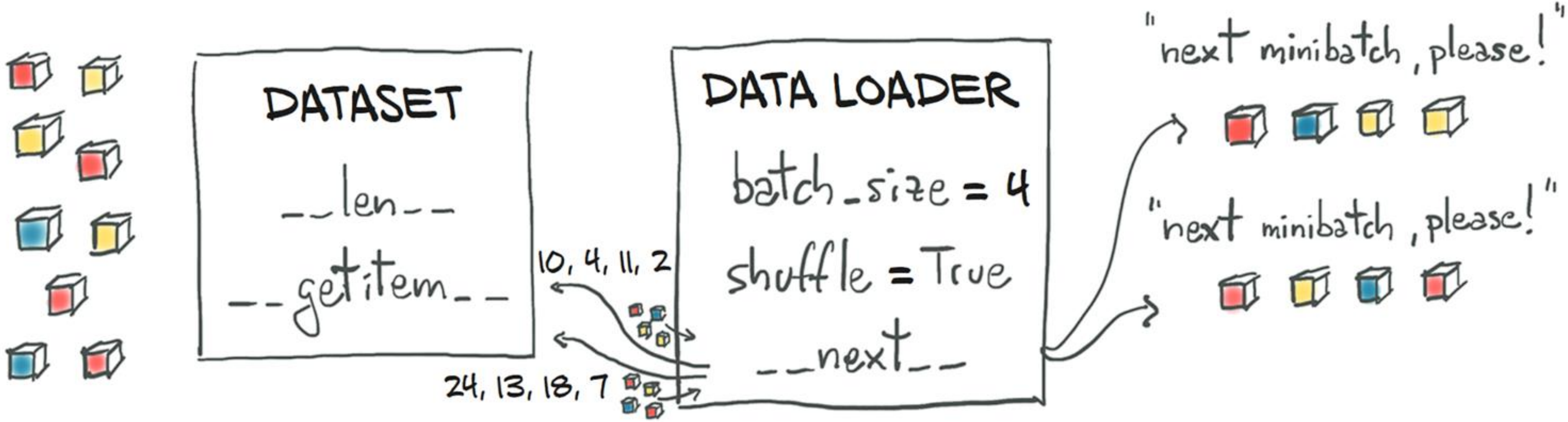




Working with data: Dataset & Dataloaders



Working with data: Dataset & Dataloaders



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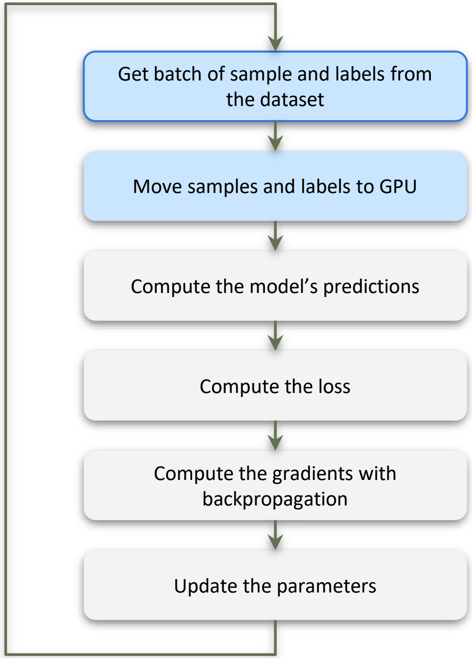
Building the Training Loop




```python
# TRAINING LOOP

for samples, labels in loader:
    samples = samples.to(device)
    labels = labels.to(device)
    # compute predictions with model
    # compute the loss
    # compute gradients
    # update model parameters
```

Modules - Overview

- Help building reusable model components
- Manage model parameters
- PyTorch provides lots of built-in modules

Modules - Managing Parameters

Modules help to:

- keep track of all parameters in your model.
- save/load your model
- reset all parameters gradients
- move all parameters to the gpu

Modules - torch.nn

Whole library dedicated to Neural Network, including:

- Linear / Convolution / Recurrent Layers
- Activation Functions (ReLU, Tanh, …)
- Loss Functions (MSE, CrossEntropy, ...)
- Pooling, Normalization, Dropout Layers

Modules - torch.nn.Module

- A class you inherit from to create a Module
- It needs to implement two methods:
  - The `__init__` function: What are the components of your model
  - The `forward` function: How these components are connected

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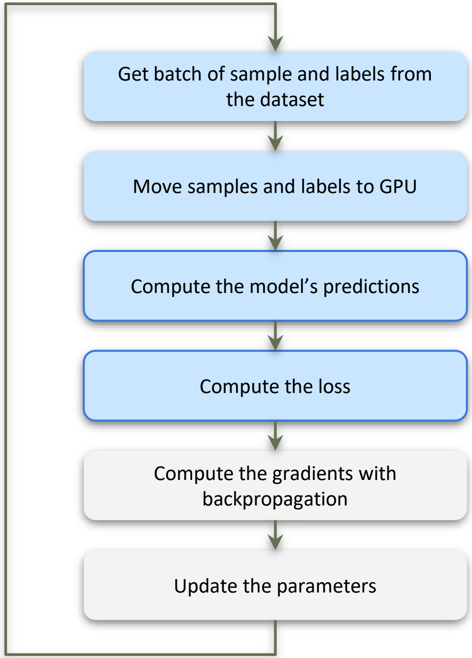
Building the Training Loop




```python
# TRAINING LOOP

for samples, labels in loader:
    samples = samples.to(device)
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    predictions = model(samples)
    loss = loss_fn(predictions, labels)
    # compute gradients
    # update model parameters
```

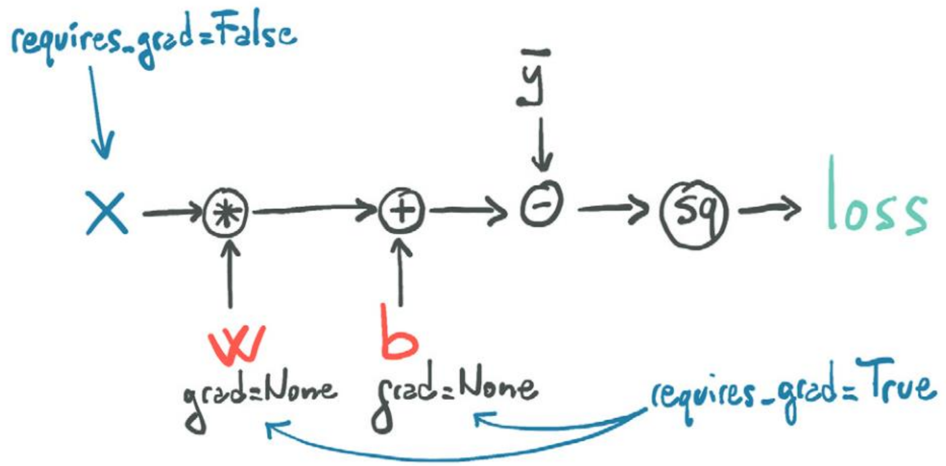
Computing gradients with Autograd

- Autograd: Automatic Differentiation package
- Each Tensor has a `requires_grad` boolean attribute
- Autograd creates a graph to record all operations during the computation
- Call `tensor.backward()` to compute all gradients automatically
- Gradients are accumulated into the `tensor.grad` attribute

Computing gradients with Autograd

```
loss = (x * W + b - y) ** 2
```

Computing gradients with Autograd



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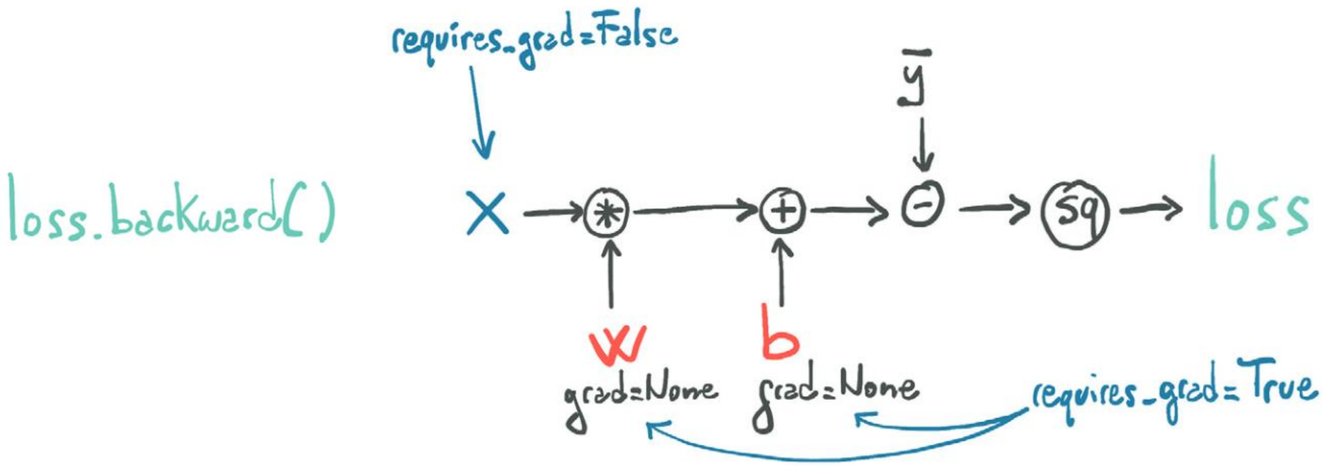
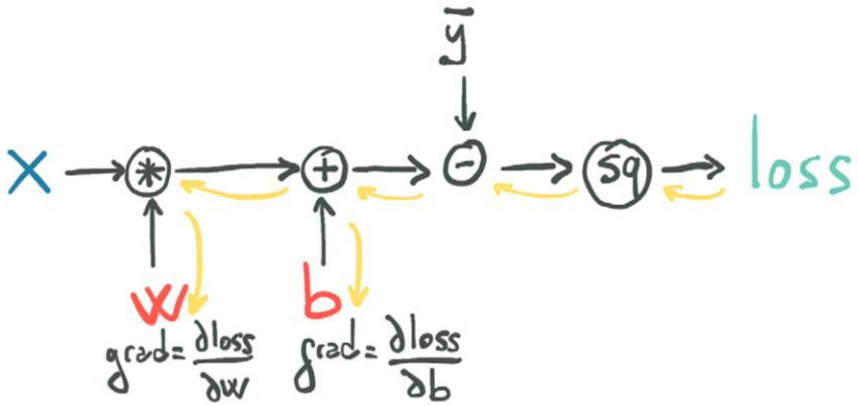


Computing gradients with Autograd

loss.backward()



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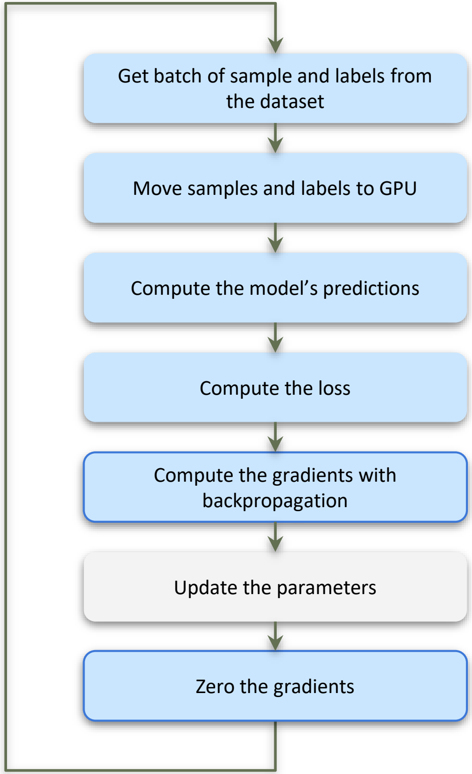
Building the Training Loop

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    predictions = model(samples)
    loss = loss_fn(predictions, labels)
    loss.backward()
    # update model parameters
    model.zero_grad()
```

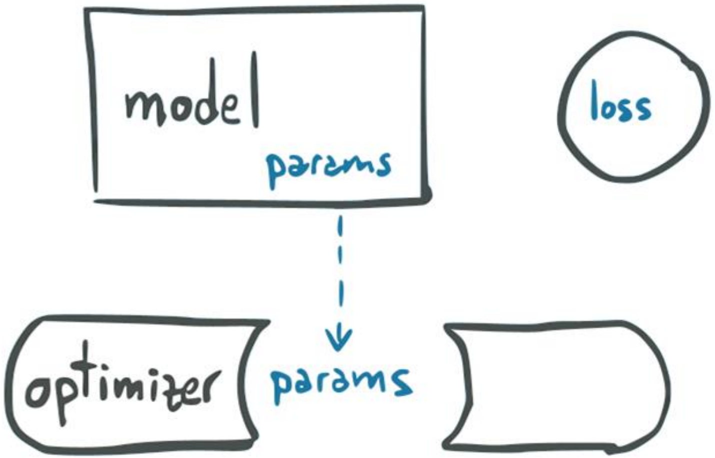
Optimizing parameters

- Use `torch.optim` submodule containing different optimizers
- The optimizer constructor takes a list of parameters
- A call to `optimizer.step()` updates the parameters

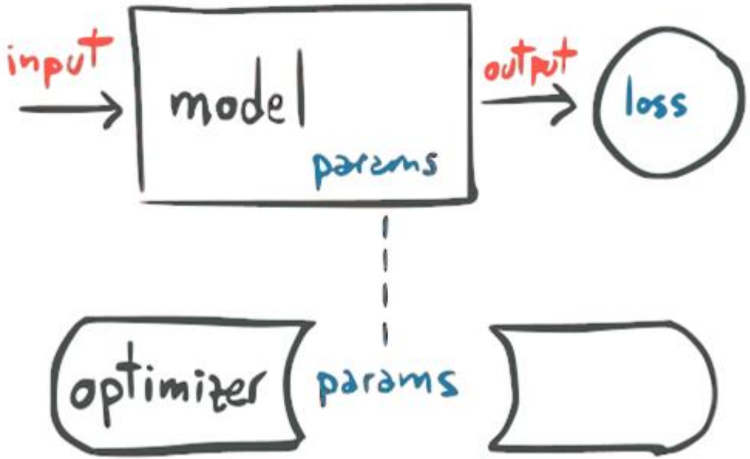
! Instead of `model.zero_grad()`,

you can use `optimizer.zero_grad()`

Optimizing parameters



Optimizing parameters



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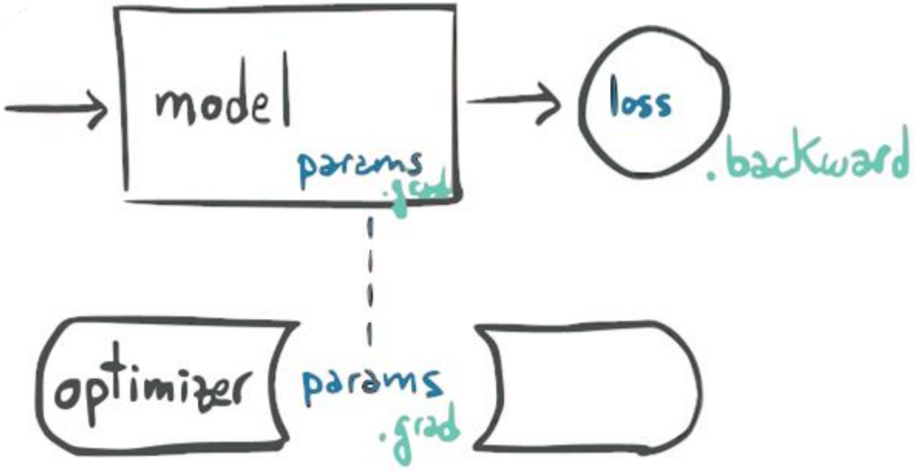

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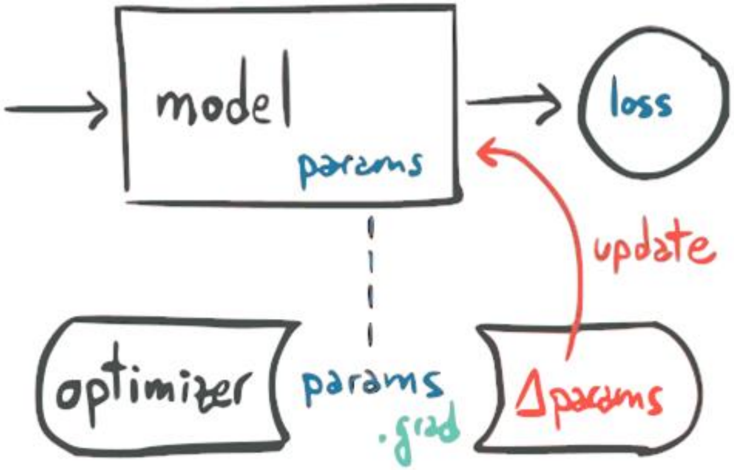

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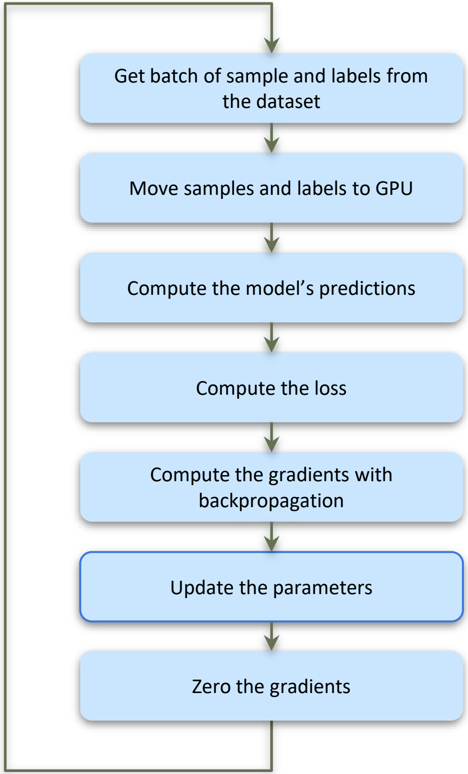
Building the Training Loop

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    optimizer.step()
    model.zero_grad()
```
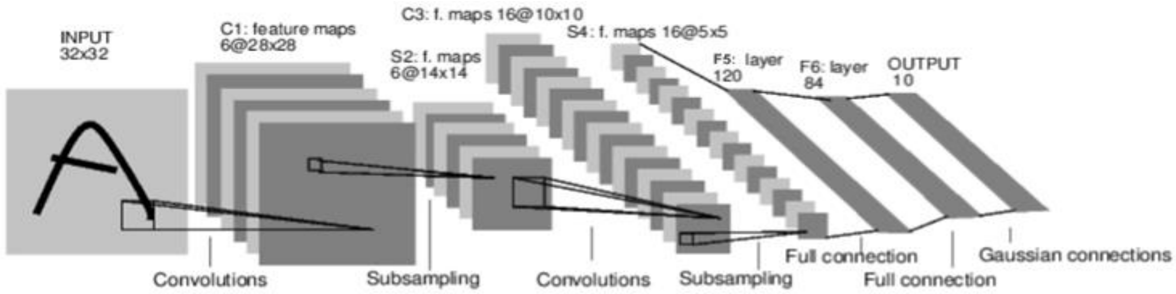

Walkthrough: Building and Training LeNet on MNIST

- Building LeNet5 with torch.nn.Module
- Loading MNIST dataset with TorchVision
- Training for multiple epochs with a custom train function



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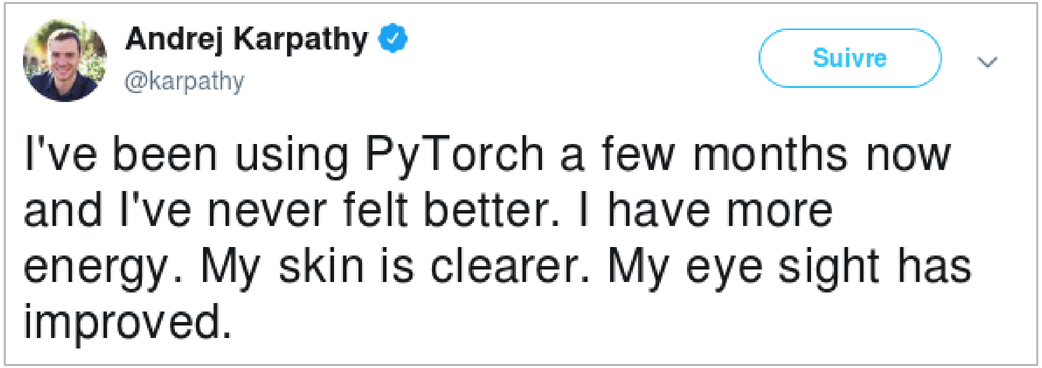
What you've still to discover

- Torchvision, Torchtext, Torchaudio
- Multi-GPU Distributed Training
- Quantisation & Pruning
- High-Performance with TorchScript + JIT
- Going to Production with ONNX, TorchElastic and TorchServe
- Organising your code with PyTorch Lightning

Still wondering why PyTorch?



Check our Material

Check github.com/theevann/dl4sci-pytorch-webinar for:

- Notebooks presented during this webinar (live-notebooks)
- Detailed notebooks for offline study (offline-notebooks)

Other References & Material

- Our notebooks at github.com/theevann/dl4sci-pytorch-webinar/
- Deep-Learning with PyTorch e-book
- Official tutorials at pytorch.org/tutorials/
- A good tutorial on towardsdatascience at bit.ly/38VgfaT/
- Advanced EPFL Deep Learning Course at fleuret.org/ee559/

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