Deep Learning

Automatic Differentiation and Pytorch

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Recall: Optimizing ML Models

A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of these:
   - Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

   - Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:

(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Gradients

Backpropagation can compute this gradient!

And it's a **special case of a more general algorithm** called reverse-mode automatic differentiation that can compute the gradient of any differentiable function efficiently!

A Recipe for

Background

1. Given training dat

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of th

– Decision functio

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

opp site the gradient)

$$\boldsymbol{\theta}^{(t} \quad ^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

How to Compute Gradients

Motivations

- Backpropagation in NN models
  - Implementing Backprop by hand is like programming in Assembly. You can do it, but… why?
  - Still, if you know assembly you are better off!

Terminology

- Automatic differentiation (autodiff) refers to a general way of taking a program which computes a value, and automatically constructing a procedure for computing derivatives of that value.
    - In this lecture, we focus on reverse mode autodiff. There is also a forward mode, which is for computing directional derivatives.
- Backpropagation is the special case of autodiff applied to neural nets
    - But in machine learning, we often use backprop synonymously with autodiff
- Autograd is the name of a particular autodiff package.
    - But lots of people, including the PyTorch developers, got confused and started using “autograd” to mean “autodiff”

What Autodiff is not

- Autodiff is not finite differences.
  - Finite differences are expensive, since you need to do a forward pass for each derivative.
  - It also induces huge numerical error.
- Autodiff is both efficient (linear in the cost of computing the value) and numerically stable.

What Autodiff is not

- Autodiff is not symbolic differentiation (e.g. Mathematica).
    - Symbolic differentiation can result in complex and redundant expressions.
- The goal of autodiff is not a formula, but a procedure for computing derivatives.

What Autodiff is

- An autodiff system will convert the program into a sequence of primitive operations which have specified routines for computing derivatives.
    - In this representation, backprop can be done in a completely mechanical way.

Original program:

$$z = wx + b$$
$$y = \frac{1}{1 + \exp(-z)}$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

Sequence of primitive operations:

$$t_1 = wx$$
$$z = t_1 + b$$
$$t_3 = -z$$
$$t_4 = \exp(t_3)$$
$$t_5 = 1 + t_4$$
$$y = 1/t_5$$
$$t_6 = y - t$$
$$t_7 = t_6^2$$
$$\mathcal{L} = t_7/2$$

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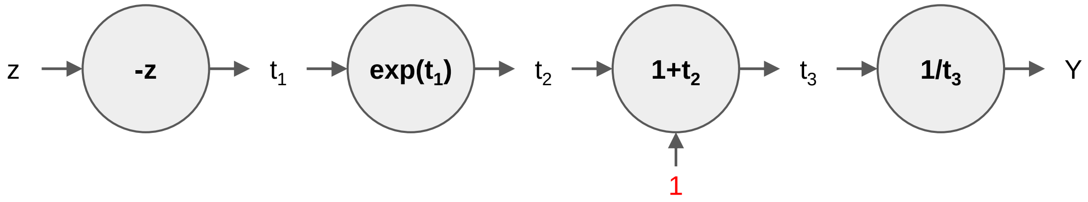
Computation Graph

Computation Graph: Logistic Regression

```
def logistic(z):
    return 1. / (1. + np.exp(z))
```

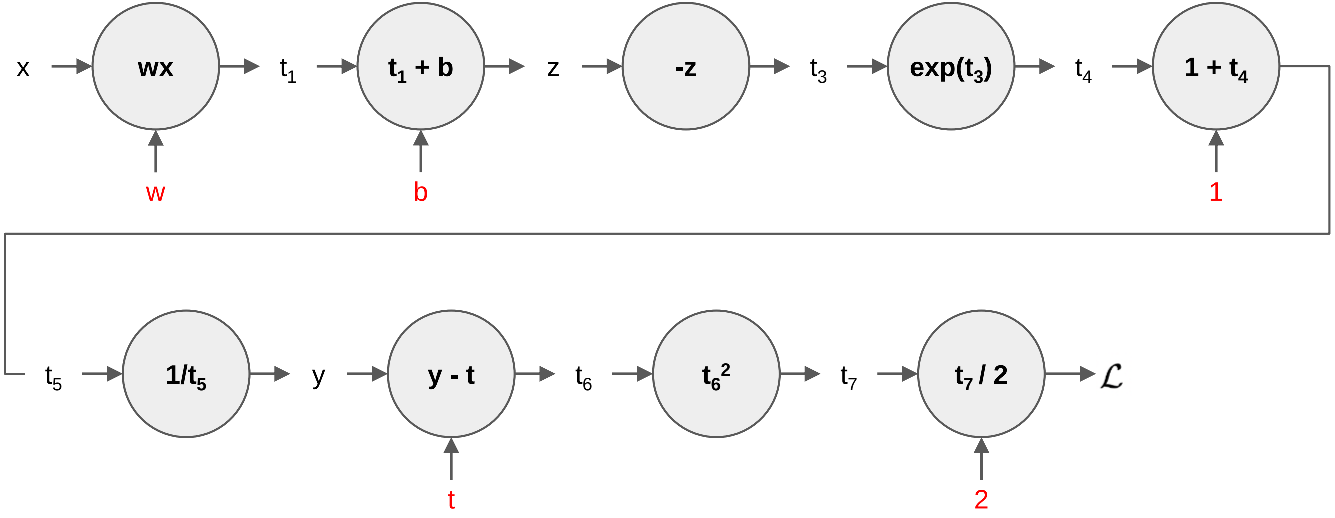
Z = 1.5
Y = logistic(1.5)



Computation Graph: Include the Loss

Original program:

$$z = wx + b$$
$$y = \frac{1}{1 + \exp(-z)}$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$



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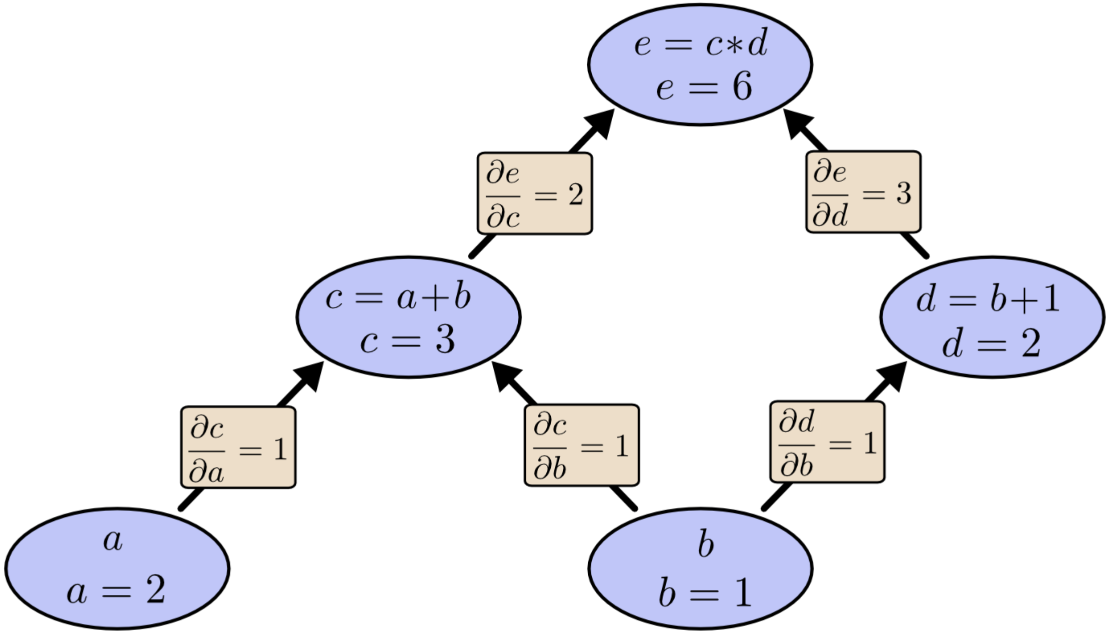
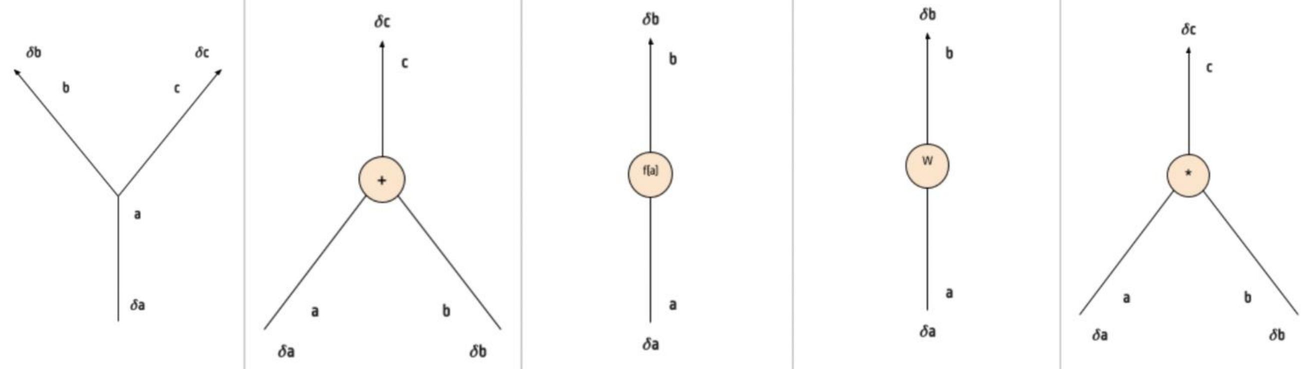
Backprop on the Computation Graph: Reverse Mode

- (Reverse Mode) Autodiff starts at an output of the graph and moves towards the beginning.
- At each node, it merges all paths which originated at that node.
- Example: (a+b)(b+1)

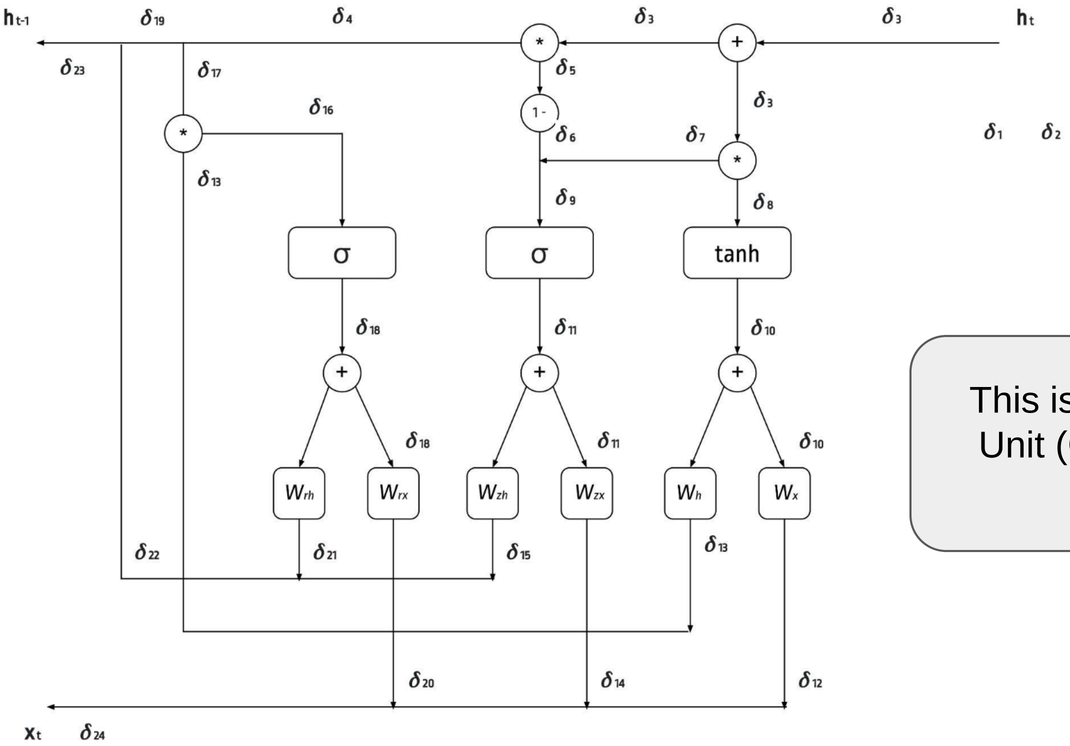


Backprop on the Computation Graph: Reverse Mode



SPLIT	ADDITION	FUNCTION	MATRIX MULTIPLY	HADAMARD PRODUCT
$c = a; b = a$	$c = a + b$	$b = f(a)$	$b = Wa$	$c = a * b$
$\delta_a = \delta_b + \delta_c$	$\delta_a = \delta_c; \delta_b = \delta_c$	$\delta_a = \delta_b * f'(a)$	$\delta_a = \delta_b * W^T$	$\delta_a = \delta_c * b$
				$\delta_b = \delta_c * a$

Things can get complicated :)



This is a Gated Recurrent Unit (GRU) Computation Graph

pyTorch

(slides inspired by this deck)

Do you have pyTorch installed?

```
>>> import numpy as np
>>> import torch
>>> import sys
>>> import matplotlib
>>> print(f'Python  version: {sys.version}')
Python  version: 3.8.1 | packaged by conda-forge | (default, Jan 29 2020, 14:55:04) [GCC 7.3.0]

>>> print(f'Numpy   version: {np.version.version}')
Numpy   version: 1.17.5

>>> print(f'PyTorch version: {torch.version.__version__}')
PyTorch version: 1.4.0

>>> print(f'Matplotlib version: {matplotlib.__version__}')
Matplotlib version: 3.1.2

>>> print(f'GPU present: {torch.cuda.is_available()}')
GPU present: False
```

pyTorch packages

Package	Description
torch	The top-level PyTorch package and tensor library.
torch.nn	A subpackage that contains modules and extensible classes for building neural networks.
torch.autograd	A subpackage that supports all the differentiable Tensor operations in PyTorch.
torch.nn.functional	A functional interface that contains typical operations used for building neural networks like loss functions, activation functions, and convolution operations.
torch.optim	A subpackage that contains standard optimization operations like SGD and Adam.
torch.utils	A subpackage that contains utility classes like data sets and data loaders that make data preprocessing easier.
torchvision	A package that provides access to popular datasets, model architectures, and image transformations for computer vision.

torch.tensor

- PyTorch ’s tensors are very similar to NumPy’s ndarrays
    - but they have a device attached, 'cpu', 'cuda', or 'cuda:X'
- They might require gradients

```
>>> t = torch.tensor([1,2,3], device='cpu',
...            requires_grad=False,dtype=torch.float32)
>>> print(t.dtype)
torch.float32
>>> print(t.device)
cpu
>>> print(t.requires_grad)
False
>>> t2 = t.to(torch.device('cuda'))
>>> t3 = t.cuda()  # or you can use shorthand
>>> t4 = t.cpu()
```

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pyTorch Data Types

Data type	dtype	CPU tensor	GPU tensor
32-bit floating point	torch.float32 or torch.float	torch.FloatTensor	torch.cuda.FloatTensor
64-bit floating point	torch.float64 or torch.double	torch.DoubleTensor	torch.cuda.DoubleTensor
16-bit floating point	torch.float16 or torch.half	torch.HalfTensor	torch.cuda.HalfTensor
8-bit integer (unsigned)	torch.uint8	torch.ByteTensor	torch.cuda.ByteTensor
8-bit integer (signed)	torch.int8	torch.CharTensor	torch.cuda.CharTensor
16-bit integer (signed)	torch.int16 or torch.short	torch.ShortTensor	torch.cuda.ShortTensor
32-bit integer (signed)	torch.int32 or torch.int	torch.IntTensor	torch.cuda.IntTensor
64-bit integer (signed)	torch.int64 or torch.long	torch.LongTensor	torch.cuda.LongTensor
Boolean	torch.bool	torch.BoolTensor	torch.cuda.BoolTensor

Conversion in numpy and in PyTorch:

```
new_array  = old_array.astype(np.int8)  # numpy array
new_tensor = old_tensor.to(torch.int8)  # torch tensor
```

Remarks: Almost always torch.float32 or torch.int64 are used.
Half does not work on CPUs and on many GPUs (hardware limitation).

Creating Tensors

- eye: creating diagonal matrix / tensor
- zeros: creating tensor filled with zeros
- ones: creating tensor filled with ones
- linspace: creating linearly increasing values
- arange: linearly increasing integers

```
>>> torch.eye(3, dtype=torch.double)
tensor([[1., 0., 0.],
        [0., 1., 0.],
        [0., 0., 1.]], dtype=torch.float64)
>>> torch.arange(6)
tensor([0, 1, 2, 3, 4, 5])
```

pyTorch functions, dimensionality

```
x.size()                      #* return tuple-like object of dimensions, old codes
x.shape                       #  return tuple-like object of dimensions, numpy style
x.ndim                        #  number of dimensions, also known as .dim()
x.view(a,b,...)               #* reshapes x into size (a,b,...)
x.view(-1,a)                  #* reshapes x into size (b,a) for some b
x.reshape(a,b,...)            # equivalent with .view()
x.transpose(a,b)              # swaps dimensions a and b
x.permute(*dims)              # permutes dimensions; missing in numpy
x.unsqueeze(dim)              # tensor with added axis; missing in numpy
x.unsqueeze(dim=2)            # (a,b,c) tensor -> (a,b,1,c) tensor; missing in numpy
torch.cat(tensor_seq, dim=0)  # concatenates tensors along dim
# For instance:
>>>t = torch.arange(6)
tensor([0, 1, 2, 3, 4, 5])
>>> t.reshape(2,3) # same as t.view(2,3 or t.view(2,-1)
tensor([[0, 1, 2],
        [3, 4, 5]])
>>> t.reshape(2,3).unsqueeze(1)
tensor([[[0, 1, 2]],
        [[3, 4, 5]]])
>>> t.reshape(2,3).unsqueeze(1).shape
torch.Size([2, 1, 3])
```

Indexing

- Standard numpy indexing works:

```
>>> t = torch.arange(12).reshape(3,4)
tensor([[ 0,  1,  2,  3],
[ 4,  5,  6,  7],
[ 8,  9, 10, 11]])
>>> t[1,1:3]
tensor([5, 6])
>>> t[:,:] = 0 # fill everything with 0, a.k.a. t.fill_(0)
tensor([[0, 0, 0, 0],
[0, 0, 0, 0],
[0, 0, 0, 0]])
```

Memory: Sharing vs. Copying

- Copy Data:
  - `torch.Tensor()`
  - `torch.tensor()`
  - `torch.clone()`
  - type casting
- Share Data
  - `torch.as_tensor()`
  - `torch.from_numpy()`
  - `torch.view()`
  - `torch.reshape()`

Most shape changing operators keep data.

Memory: Sharing vs. Copying

- How to test it?
  - create a tensor
  - copy/clone/view it
  - modify an element
  - compare the elements

```
>>> a = np.arange(6)                    #  [0,1,2,3,4,5]
>>> t = torch.from_numpy(a)
>>> t[2] = 11
>>> t
tensor([ 0,  1, 11,  3,  4,  5])
>>> a
array([ 0,  1, 11,  3,  4,  5])  # Changed the underlying numpy array too!
>>> b = a.copy()
>>> p = t.clone()
>>> t[0] = 7                            # a,t change, b, p remain intact.
```

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Creating Instances of `torch.Tensor` w/o Data

```
>>> torch.eye(2)
tensor([[1., 0.],
        [0., 1.]])
>>> torch.zeros(2,2)
tensor([[0., 0.],
        [0., 0.]])
>>> torch.ones(2,2)
tensor([[1., 1.],
        [1., 1.]])

>>> torch.rand(2,2)
tensor([[0.6849, 0.1091],
        [0.4953, 0.8975]])

>>> torch.empty(2,2) # NEVER USE IT! Creates uninitialized tensor.
tensor([[-2.2112e-16,  3.0693e-41],
        [-3.0981e-16,  3.0693e-41]])

>>> torch.arange(6)
tensor([0, 1, 2, 3, 4, 5])
```

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Interacting with numpy

```
>>> import imageio
>>> img = imageio.imread('example.png') #  reading data from disk
>>> t = torch.from_numpy(a)               #  input from numpy array
>>> out = model(t)                        #  processing
>>> result = out.numpy()                  #  converting back to numpy

# tuples, lists, arrays, etc. can be converted automatically:
>>> t2 = torch.tensor(...)
```

- Remarks:
  - arrays / tensors must be on the same device.
  - only detached arrays can be converted to numpy (see later)
  - if data types are not the same, casting might be needed (v1.1 or older)
    - E.g. adding an integer and a float tensor together.

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Autograd Example

```
>>> import torch
>>> from torch import autograd
>>> x1 = torch.tensor(2, requires_grad=True, dtype=torch.float32)
>>> x2 = torch.tensor(3, requires_grad=True, dtype=torch.float32)
>>> x3 = torch.tensor(1, requires_grad=True, dtype=torch.float32)
>>> x4 = torch.tensor(4, requires_grad=True, dtype=torch.float32)
>>> # Forward propagation
>>> z1 = x1 * x2
>>> z2 = x3 * x4
>>> f = z1 + z2
>>> df_dx = grad(outputs=f, inputs = [x1, x2, x3, x4])
>>> df_dx
(tensor(3.), tensor(2.), tensor(4.), tensor(1.))
```

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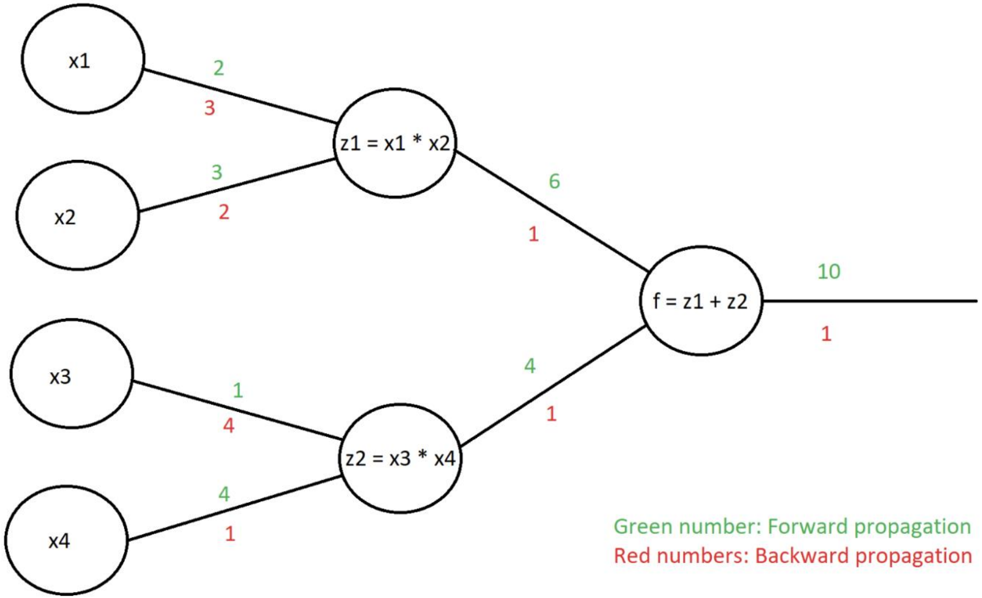
Under the Hood (a little bit)

```
>>> df_dx = grad(outputs=f, inputs = [x1, x2, x3, x4])
>>> df_dx
(tensor(3.), tensor(2.), tensor(4.), tensor(1.))
```



Autograd (a little bit better)

```
>>> import torch
>>> from torch import autograd
>>> x1 = torch.tensor(2, requires_grad=True, dtype=torch.float32)
>>> x2 = torch.tensor(3, requires_grad=True, dtype=torch.float32)
>>> x3 = torch.tensor(1, requires_grad=True, dtype=torch.float32)
>>> x4 = torch.tensor(4, requires_grad=True, dtype=torch.float32)
>>> # Forward propagation
>>> z1 = x1 * x2
>>> z2 = x3 * x4
>>> f = z1 + z2
>>> #  df_dx = grad(outputs=f, inputs = [x1, x2, x3, x4]) # inconvenient
>>> f.backward()                                              # that is better!
>>> print(f" f's derivative w.r.t. x1 is {x.grad}")
tensor(3.)
```

Autograd (a little bit better)

```
>>> import torch
>>> from torch import autograd
>>> x1 = torch.tensor(2, requires_grad=True, dtype=torch.float32)
>>> x2 = torch.tensor(3, requires_grad=True, dtype=torch.float32)
>>> x3 = torch.tensor(1, requires_grad=True, dtype=torch.float32)
>>> x4 = torch.tensor(4, requires_grad=True, dtype=torch.float32)
>>> # Forward propagation
>>> z1 = x1 * x2
>>> z2 = x3 * x4
>>> f = z1 + z2
>>> #  df_dx = grad(outputs=f, inputs = [x1, x2, x3, x4]) # inconvenient
>>> f.backward()                                            # that is better!
>>> print(f" f's derivative w.r.t. x1 is {x.grad}")
tensor(3.)
```

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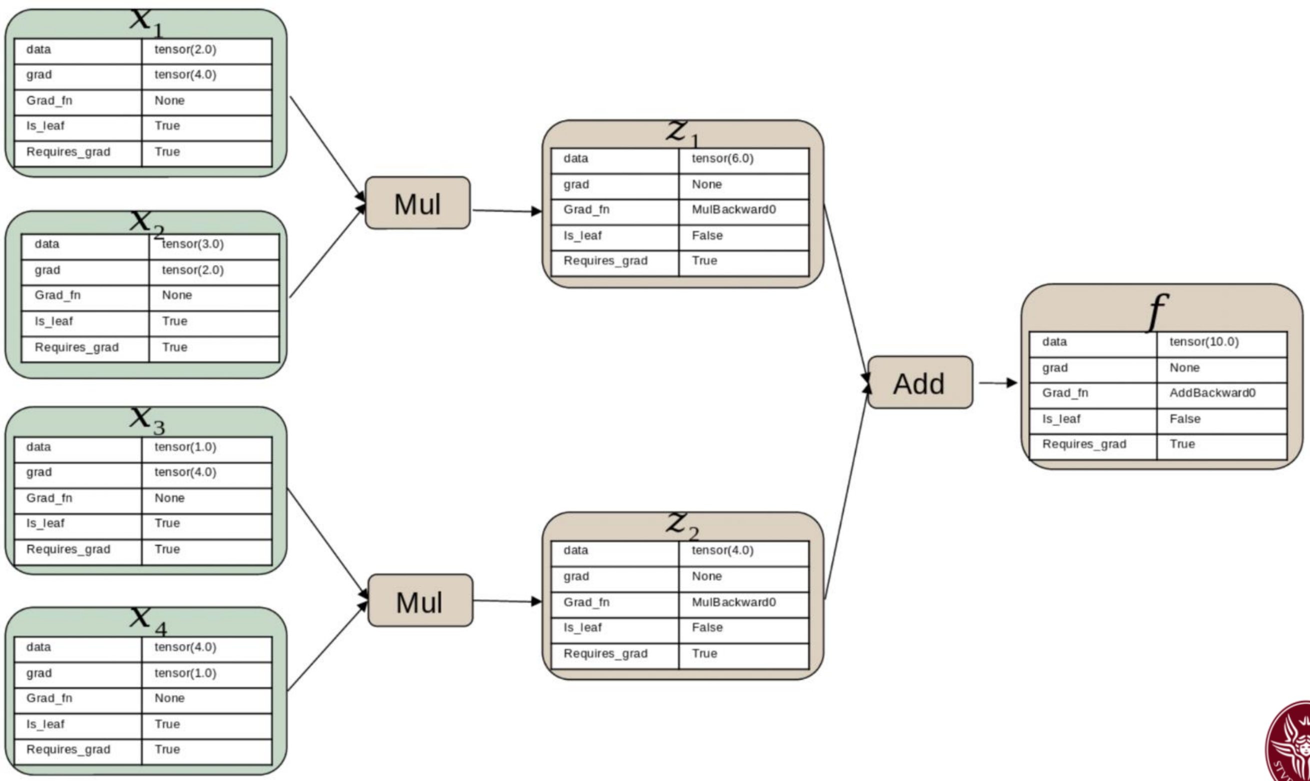
Under the Hood (a little bit)



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Context managers, decorators

- We can locally disable/enable gradient calculation with
  - `torch.no_grad()`
  - `torch.enable_grad()`
- or using the `@torch.no_grad` `@torch.enable_grad` decorators

```
>>> x = torch.tensor([1], requires_grad=True)
>>> with torch.no_grad():
...     y = x * 2
>>> y.requires_grad
False

>>> with torch.no_grad():
...     with torch.enable_grad():
...         y = x * 2
>>> y.requires_grad
True
```

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Example: Linear Regression

- Generating data:

```
>>> a_ref = -1.5
>>> b_ref = 8
>>> noise = 0.2 * np.random.randn(50)
>>> x = np.linspace(1, 4, 50)
>>> y = a_ref * x + b_ref + noise
```

- Defining loss function:

```
>>> def MSE_loss(prediction, target):
...     return (prediction-target).pow(2).mean()
```

Example: Linear Regression

- Data as torch tensors and the unknown variables:

```
xx = torch.tensor(x, dtype = torch.float32)
yy = torch.tensor(y, dtype = torch.float32)

a = torch.tensors(0, requires_grad = True, dtype=torch.float32)
b = torch.tensors(5, requires_grad = True, dtype=torch.float32)
```

Example: Linear Regression

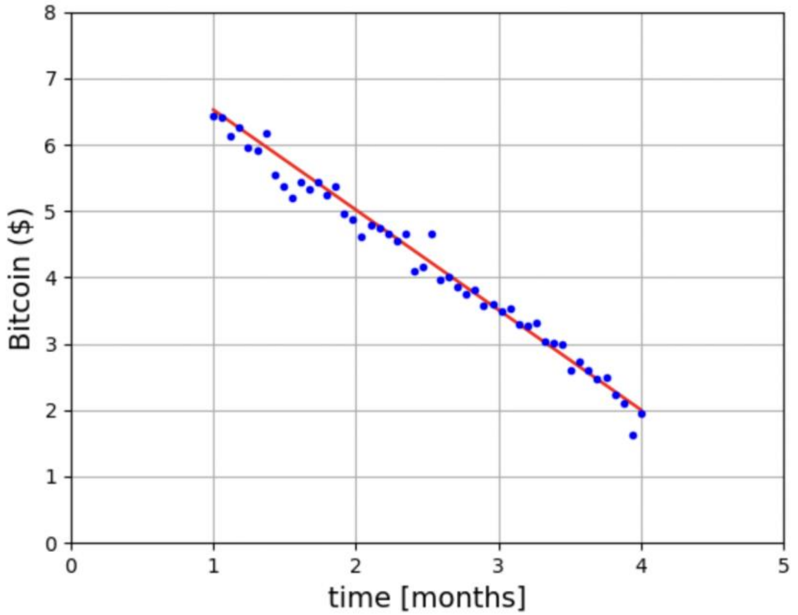
- Training Loop:

```
number_of_epochs = 1000
learning_rate = 0.01
for iteration in range(number_of_epochs):
    y_pred = a * xx + b
    loss = MSE_loss(y_pred, yy)
    loss.backward()
    with torch.no_grad():
        a = a - learning_rate * a.grad
        b = b - learning_rate * b.grad
    a.requires_grad = True
    b.requires_grad = True
print(a)
print(b)
```

Example: Linear Regression

- Result:

```
tensor(-1.5061, requires_grad=True)
tensor(8.0354, requires_grad=True)
```



Other useful pyTorch’s tensor functions

- If you want to detach a tensor from the graph, you can use « `detach()` »
- If you want to get a python number from a tensor, you can use « `item()` »
- But if you just take an element, it still will be part of the computational graph!

```
>>> x=torch.tensor([2.5,3.5], requires_grad=True)
tensor([2.5000, 3.5000], requires_grad=True)
>>> x.detach()
tensor([2.5000, 3.5000])
>>> x[0]     # still part of the graph!
tensor(2.5000, grad_fn=<SelectBackward>)
>>> x[0].item()
2.5

>>> #  a frequent line when you go back to numpy:
>>> x.detach().cpu().numpy()
array([2.5, 3.5], dtype=float32)
```

Functional

- The «torch.nn.functional» package is the functional interface for Pytorch features.
- Most feature exist both as a function and as a class.
- Structural parts, or objects with internal state usually used as objects
- Stateless or simple expressions are usually used in functional form.
- Activation functions, losses, convolutions, etc. It is a huge module.

```python
import torch
import torch.nn as nn
import torch.nn.functional as F
x = torch.rand(2,2)
y = F.relu(x)
relu = nn.ReLU()  # creating the object first
z = relu(x)       # then using it
y == z            # they should be the same

# Similarly:
mseloss = nn.MSELoss()

F.mseloss(...) == mseloss(...)
```

A typical (pyTorch) ML Workflow

1. creating dataset
2. creating a neural network (model)
3. defining a loss function
4. loading samples (data loader)
5. predicting with the model
6. comparison of the prediction and the target (loss)
7. backpropagation: calculating gradients from the error
8. updating the model (optimizer)
9. checking the loss: if low enough, stop training

Data Loading

Data loading and preprocessing

- The «`torch.utils.data`» package have two useful classes for loading and preprocessing data:
  - `torch.utils.data.Dataset`
  - `torch.utils.data.DataLoader`
- For more information visit:
  - https://pytorch.org/tutorials/beginner/data_loading_tutorial.html

torch.utils.data.Dataset: Regression Ex. revisited

```python
import torch
class LinearRegressionDataset(torch.utils.data.Dataset):

    def __init__(self,N = 50, m = -3, b = 2, *args,**kwargs):
        # N: number of samples, e.g. 50
        # m: slope
        # b: offset
        super().__init__(*args,**kwargs)

        self.x = torch.rand(N)
        self.noise = torch.rand(N)*0.2
        self.m = m
        self.b = b

    def __getitem__(self, idx):
        y = self.x[idx] * self.m + self.b + self.noise[idx]
        return {'input': self.x[idx], 'target': y}

    def __len__(self):
        return len(self.x)
```

torch.utils.data.Dataset: Image Datasets

```python
import torch
import imageio
class ImageDataset(torch.utils.data.Dataset):
    def __init__(self, root, N, *args,**kwargs):
        super().__init__(*args,**kwargs)

        self.input, self.target = [], []
        for i in range(N):
            t = imageio.imread(f'{root}/train_{i}.png')
            t = torch.from_numpy(t).permute(2,0,1)
            l = imageio.imread(f'target_{i}.png')
            l = torch.from_numpy(l).permute(2,0,1)
            self.input.append(t)
            self.target.append(l)

    def __getitem__(self, idx):
        return {'input': self.input[idx], 'target': self.target[idx]}

    def __len__(self):
        return len(self.input)
```

torch.utils.data.Dataset: Image Datasets

```
import torch
import ImageDataset

datapath = 'data_directory'
myImageDataset = ImageDataset(dataPath, 50)
# iterating through the samples
for sample in myImageDataset:
    input = sample['input'].cpu()  # or .cuda()
    target = sample['target'].cpu()  # or .to(device)
    ....
```

Never ever use .cuda() in the dataset or data loaders!

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torch.utils.data.Dataloader

```
import torch
import ImageDataset
datapath = 'data_directory'
myImageDataset = ImageDataset(dataPath, 50)
# iterating through the samples
train_loader = DataLoader(dataset=myImageDataset, batch_size=32,
                          shuffle=False, num_workers=2)
for sample in train_loader:
    ...
```

- «DataLoader» is used to:
  - Batching the dataset
  - Shuffling the dataset
  - Utilizing multiple CPU cores/ threads

Data augmentation

- modifying the dataset for better training (more robust, etc.)
- data set can have a a transform parameter

More details can be found here:
https://pytorch.org/tutorials/beginner/data_loading_tutorial.html

Data augmentation

```
import torch
import imageio
class ImageDataset(torch.utils.data.Dataset):
    def __init__(self, root, N, transform = None, *args,**kwargs):
        super().__init__(*args,**kwargs)
        self.transform = transform
        ...
    def __getitem__(self, idx):
        sample = {'input': self.input[idx], 'target': self.target[idx]}
        if self.transform:
            sample = self.transform(sample)
        return sample

    def __len__(self):
        return len(self.input)
```

Data transformation

```
import torchvision.transforms as T
composed = transforms.Compose([T.Rescale(256),
                               T.RandomCrop(224),
                               T.ToTensor()]
                               )
...
dataset = Mydataset(..., transform = composed)

# another version, needs different dataset
dataset = Mydataset(..., transform = {'input'  : composed,
                                       'target' : None} )
```

Creating the Model

nn.Module

- A model is of a `nn.Module` class type. A model can contain other models. E.g. we can create the class "Model" based on the stacking `nn.Modules` of type `nn.Linear()`
- The `nn.Module`'s weights as called "Parameters", and are similar to tensors with "`requires_grad=True`".
- A `nn.Module` consists of an initialization of the Parameters and a `forward` function.

```python
class Model(nn.Module):
    def __init__(self):
        super().__init__()
        # structure definition and initialization

    def forward(self, x):
        # actual forward propagation
        result = processing(x)
        return result
```

Model

```python
class Model(nn.Module):
    def __init__(self):
        super().__init__()
        # let's assume 28x28 input images, e.g. MNIST characters
        self.fc1 = nn.Linear(in_features = 28 * 28, out_features = 128, bias=True)
        self.fc2 = nn.Linear(in_features = 128, out_features = 64, bias=True)
        self.fc3 = nn.Linear(in_features = 64, out_features = 10, bias=True)

    def forward(self, x):
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

Model: Alternative Declaration

```python
class Model2(nn.Module):
    def __init__(self):
        super().__init__()
        # let's assume 28x28 input images, e.g. MNIST characters
        self.fc1 = nn.Linear(in_features = 28 * 28, out_features = 128, bias=True)
        self.activation1 = nn.ReLU()
        self.fc2 = nn.Linear(in_features = 128, out_features = 64, bias=True)
        self.activation2 = nn.ReLU()
        self.fc3 = nn.Linear(in_features = 64, out_features = 10, bias=True)
        self.activation3 = nn.ReLU()

    def forward(self, x):
        x = self.activation1(self.fc1(x))
        x = self.activation2(self.fc2(x))
        x = self.activation3(self.fc3(x))
        return x
```

What is the difference?

`nn.Module`’s member functions

- Access model information

```
>>> model = Model()
>>> model.eval() # see below
>>> list(model.children())
[Linear(in_features=784, out_features=128, bias=True),
Linear(in_features=128, out_features=64, bias=True),
Linear(in_features=64, out_features=10, bias=True)]
```

- Children: the parameters and modules / layers defined in the constructor.
- Parts defined in the forward method will not be listed.
- Forward is called many times, expensive objects should not be recreated.

Some layers as e.g. "dropout" and "batch_norm" should operate differently during training and evaluation of the model. We can set the model in different state by the `.train()` and `.eval()` functions.

Model’s Parameters

```
>>> for key, value in model.state_dict().items():
...     print(f'layer = {key:10s} | feature shape = {value.shape}')

layer = fc1.weight | feature shape = torch.Size([128, 784])
layer = fc1.bias   | feature shape = torch.Size([128])
layer = fc2.weight | feature shape = torch.Size([64, 128])
layer = fc2.bias   | feature shape = torch.Size([64])
layer = fc3.weight | feature shape = torch.Size([10, 64])
layer = fc3.bias   | feature shape = torch.Size([10])
```

- The .state_dict() contains all the trainable parameters of the model, this is used for optimization and saving/restoring the model.

So far…

```
device = torch.device('cpu')
dataset = CustomDataset()
dataloader = DataLoader(dataset, ...)
model = MyModel()
model.to(device)
for i in range(epochs):
    training_loss = 0
    for sample in dataloader:
        input = sample['input'].to(device)
        target = sample['target'].to(device)
        prediction = model(input)
        loss = loss_function(prediction, target)
        training_loss += loss.item()
        loss.backward()
        # updating the model
    print(f'Current training loss: {training_loss}')
    # validation loop
    ...
# saving the model
```

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Optimizers

Choosing an Optimizer

Using PyTorch's optimizers is easy!

```
import torch
optimizer = torch.optim.SGD(model.parameters(), lr = 0.01)
...
for sample in dataloader:
    input = sample['input'].to(device)
    target = sample['target'].to(device)
    prediction = model(input)
    loss = loss_fn(prediction, target)

    optimizer.zero_grad() # clears the gradients
    loss.backward()
    optimizer.step()      # performs the optimization
```

Accumulating Gradients (a Trick)

- If we don't clear the gradients, they sum up.
- This is often source of bugs, but it can be exploited for larger effective batch sizes:

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

optimizer.zero_grad()
for idx, sample in enumerate(dataloader):
    input = sample['input'].to(device)
    target = sample['target'].to(device)

    prediction = model(input)
    loss = loss_fn(prediction, target)

    loss.backward()
    if idx % 10 = 9:
        optimizer.step()
        optimizer.zero_grad()
```

Save/Load Models

Saving the internal state of a pyTorch model

- Saving and loading can easily be done using “`torch.save`” and “`torch.load`”
- pyTorch uses “pickling” to serialize the data.

```
>>> state = {'model_state' : model.state_dict(),
             'optimizer': optimizer.state_dict()}
>>> torch.save(state, 'state.pt')
```

Restoring state:

```
>>> model = Model()
>>> optimizer = optim.SGD(model_parameters(), lr=0.01)
>>> checkpoint = torch.load('state.pt')
>>> model.load_state_dict(checkpoint['model_state'])
>>> optimizer.load_state_dict(checkpoint['optimizer_state'])
```

A Typical ML Pipeline

All the pieces together, part 1

```
import json
config = json.load(open('config.cfg'))
device = torch.device(config['device'])
training_data = CustomDataset(..., **config['train'])
validation_data = CustomDataset(..., **config['valid'])
train_loader = DataLoader(training_data, **config['loader'])
validation_loader = DataLoader(validation_data, **config['loader'])
model = MyModel(**config['model'])
model.to(device)
optimizer = Optimizer(model.parameters(), **config['optimizer'])
for i in range(config['epochs']):
    model.train()
    for sample in train_loader:
        optimizer.zero_grad()
        input, target = sample['input'].to(device), sample['target'].to(device)
        prediction = model(input)
        loss = loss_function(prediction, target)
        print(f'Current training loss: {loss.item()}')
        loss.backward()
        optimizer.step()
```

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All the pieces together, part 2

```
    # validation loop
    model.eval()
    validation_loss = 0
    for sample in validation_loader:
        input, target = sample['input'].to(device), sample['target'].to(device)
        prediction = model(input)
        loss = loss_function(prediction, target)
        validation_loss += loss.item()
    print(f'Current validation loss: {validation_loss}')
    if validation_loss < config['loss_threshold']: # or other condition
        break
full_state = {'model_state' : model.state_dict(), 'optimizer': optimizer.state_dict()}
torch.save(full_state, 'parameters.pt')
```

Reproducibility

- Sometimes it is hard to reproduce bugs because of the randomness in the training. The solution is using fixed random seeds.
- For debugging purposes, you should start your codes with these lines:

```
import numpy as np
np.random.seed(42)                                    # your favourite integer

import torch
torch.manual_seed(42)                                # your favourite integer
torch.backends.cudnn.deterministic = True            # disable optimizations
torch.backends.cudnn.benchmark = False
```

But remove them when you are done with debugging,
otherwise all the models will be the same!
See: https://pytorch.org/docs/stable/notes/randomness.html

Colab Example

https://colab.research.google.com/drive/1HUWge-hdUQZMdIQX0fys77c9pUycxSPj#scrollTo=Y9gcgKUmyBXD

Deep Learning

Automatic Differentiation and Pytorch

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