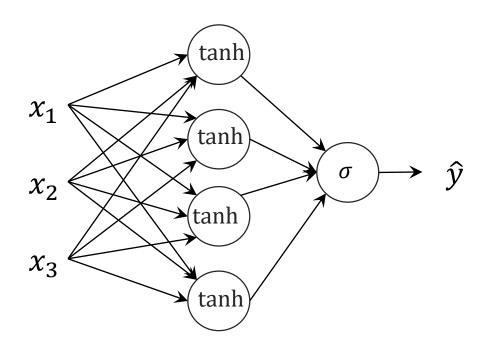
# Implementing Neural Networks in PyTorch



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#### Shallow Neural Network



$$\mathbf{z}^{[1]} = \mathbf{W}^{[1]} \mathbf{x} + \mathbf{b}^{[1]}$$
 $\mathbf{a}^{[1]} = \tanh \mathbf{z}^{[1]}$ 
 $\mathbf{z}^{[2]} = \mathbf{w}^{[2]} \mathbf{a}^{[1]} + \mathbf{b}^{[2]}$ 
 $\hat{y} = a^{[2]} = \sigma(\mathbf{z}^{[2]})$ 

Parameters:  $\boldsymbol{\theta} = \{ \boldsymbol{W}^{[1]}, \, \boldsymbol{b}^{[1]}, \boldsymbol{w}^{[2]}, \, b^{[2]} \}$ Loss  $L(\hat{y}, y)$ Cost  $J(\theta)$ 

Gradient descent

$$\boldsymbol{\theta} \coloneqq \boldsymbol{\theta} - \eta \nabla J = \boldsymbol{\theta} - \eta \frac{\nabla L}{m}$$

#### Basic operations in Neural Networks

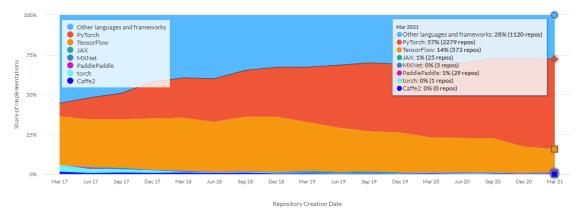
- Vector/Matrix multiplications
- Elementwise operations
  - Addition
  - Multiplication
  - Activation (Sigmoid, ReLU, Tanh, ...)
  - Loss computation (MSE, CrossEntropy,...)

# Building NNs using PyTorch

# PyTorch

- Open source DL framework
- Provides two high-level features
  - Tensor computing (like NumPy) with strong acceleration via GPU
  - Automatic differentiation system
- Easy to learn
- Growing ecosystem

#### https://paperswithcode.com/



T = 5 L Fi

Let's import torch

# Building NNs using PyTorch: Overview

- Tensor
- Tensor operations
- Autograd
- Module

# torch.Tensor

#### torch.Tensor

- Like tensors in linear algebra, PyTorch tensors are arrays which can be multi-dimensional
- PyTorch tensors are similar to NumPy ndarrays except for GPU acceleration
  - PyTorch provides most of tensor operations in NumPy

#### Initialize with Python lists

```
import torch
import numpy as np
arr = [[1,2],[2,3]]
                                             In [5]:
              In [4]:
             arr_n = np.array(arr)
                                             arr_t = torch.Tensor(arr)
             print(type(arr_n))
                                             print(type(arr_t))
             print(arr_n)
                                             print(arr_t)
             <class 'numpy.ndarray'>
                                             <class 'torch.Tensor'>
              [[1 2]
                                             tensor([[1., 2.],
               [2 3]]
                                                     [2., 3.]])
                                                     PyTorch
                      NumPy
```

#### Initialization: ones & zeros

PyTorch tensors are similar to NumPy ndarrays

NumPy

PyTorch

#### Initialization: ones\_like & zeros\_like

```
In [8]: print(np.ones_like(arr_n))
    print(np.zeros_like(arr_n))

[[1 1]
    [1 1]]
    [[0 0]
    [0 0]]
```

NumPy

PyTorch

### Two ways of specifying data type

1. Use keyword argument dtype

2. Use typed tensors

```
ft = torch.FloatTensor([1,2])
print(ft)
print(ft.dtype)

tensor([1., 2.])
torch.float32
```

Data type	dtype	CPU tensor	GPU tensor	_
32-bit floating point	torch.float32 OF torch.float	torch.FloatTensor	torch.cuda.FloatTensor	Default type
64-bit floating point	torch.float64 OF torch.double	torch.DoubleTensor	torch.cuda.DoubleTensor	
16-bit floating point 1	torch.float16 OF torch.half	torch.HalfTensor	torch.cuda.HalfTensor	
32-bit integer (signed)	torch.int32 OF torch.int	torch.IntTensor	torch.cuda.IntTensor	
64-bit integer (signed)	torch.int64 OF torch.long	torch.LongTensor	torch.cuda.LongTensor	
Boolean	torch.bool	torch.BoolTensor	torch.cuda.BoolTensor	

For more types, please refer to <a href="https://pytorch.org/docs/stable/tensors.html">https://pytorch.org/docs/stable/tensors.html</a>

# Tensor operations

#### Accessing elements

Access

```
In [42]: arr_t = torch.Tensor([[1,2],[2,3]])
In [43]: arr_t[0,1]
Out [43]: tensor(2.)
```

Similar to NumPy But, it always returns Tensor

- Get a Python number
  - torch.Tensor.item()
    - Get a Python number from a tensor containing a single value

In [44]: arr\_t[0,1].item()

Out [44]: 2.0

- Update
  - Same with NumPy

#### Slicing

- Taking elements from one given index to another index
  - Pass slice instead of index: [start: end]
    - Start (inclusive), end (exclusive)
    - Default values (start: 0, end: length)

### Negative slicing

Use minus operator to refer to an index from the end

Index	0	1	2	 N-2	N-1
Negative index	N-1	N-2	N-3	 -2	-1

# Shape & Transpose (matrix)

- Transpose of 2-D tensor (matrix)
  - Tensor.T

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

- Shape
  - A tuple of tensor dimensions

```
print(X.shape)
print(X.T.shape)

torch.Size([2, 3])
torch.Size([3, 2])
```

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

#### Sum

- torch.sum(*input*, \*, dtype=None) → Tensor
  - Parameters
    - **input** (Tensor): the input tensor
  - Keyword arguments
    - **dtype** (torch.dtype, *optional*): desired datatype (default: None)
      - If specified, the input tensor is casted to dtype before the operation is performed
- Equivalent representations: X.sum() and torch.sum(X)
- Example)

#### Sum

- torch.sum(input, dim, keepdim=False, \*, dtype=None) → Tensor
  - Parameters
    - input (Tensor): the input tensor
    - dim (int or tupke, optional): the dimensions to reduce
  - Keyword arguments
    - **dtype** (torch.dtype, *optional*): desired datatype (default: None)
    - keepdim (bool): whether the output tensor has dim retained or not

#### Example)

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

#### Mean

- torch.mean(input, dim, keepdim=False, \*) → Tensor
  - Parameters
    - **input** (Tensor): the input tensor
    - dim (int or tuple, optional): the dimensions to reduce
- Example)

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

```
print(X.mean())
print(X.mean(0))
print(X.mean(1))

tensor(3.5000)
tensor([2.5000, 3.5000, 4.5000])
tensor([2., 5.])
```

#### Max

- torch.max(input, dim, keepdim=False,
   \*) → Tensor
  - Parameters
    - input (Tensor): the input tensor
    - **dim** (int or tuple, *optional*): the dimensions to reduce
  - Output
    - out (Tensor, if dim is specified): the input tensor (max, max\_indices)
- You can use torch.argmax to get only max\_indices

```
X
tensor([[1., 7., 3.],
[4., 5., 6.]])
```

```
print(X.max())
print(X.max(0))
print(X.max(1))

tensor(7.)
torch.return_types.max(
values=tensor([4., 7., 6.]),
indices=tensor([1, 0, 1]))
torch.return_types.max(
values=tensor([7., 6.]),
indices=tensor([1, 2]))
```

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

#### 

#### Binary Operators

- Addition Z = X + Y
  - $z_{ij} = x_{ij} + y_{ij}$

$$\chi \textcolor{red}{+} \gamma$$

```
tensor([[2, 3, 4], [5, 6, 7]])
```

- Element-wise multiplication
  - $z_{ij} = x_{ij} * y_{ij}$

tensor([[1., 0., 6.], [4., 0., 6.]])

Matrix multiplication

torch.matmul(X,Y.T)

tensor([[ 7., 4.], [16., 10.]])

### Inner product

```
x = torch.FloatTensor([1,2])
y = torch.FloatTensor([1,1])
tensor(3.)
```

### Tensor manipulation

You will struggle with dimensions and shapes

```
RuntimeError Traceback (most recent call last)
<ipython-input-54-22cf2a5648e8> in <module>
----> 1 torch.matmul(X,Y)

RuntimeError: mat1 and mat2 shapes cannot be multiplied (2x3 and 2x3)
```

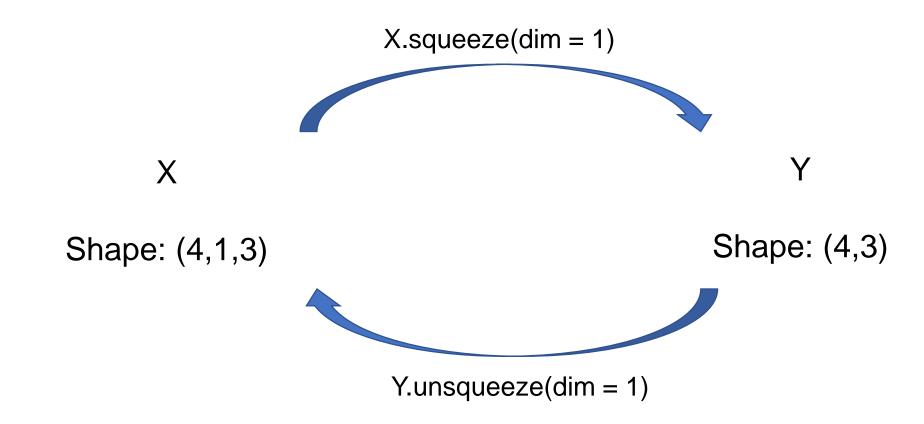
View, Squeeze, Unsqueeze, ...

#### View

- Returns a tensor with the same data and number of elements as self but with the specified shape
- X.view(\*shape)
  - shape (int or tuple): the desired shape

```
Y = X.view(6,3)
                               Y = X.view(3,2,3)
print(X.shape)
                                                               print(Y.shape)
                               print(Y.shape)
print(X)
                               print(Y)
                                                               print(Y)
                               torch.Size([3, 2, 3])
                                                               torch.Size([6, 3])
torch.Size([2, 3, 3])
                               tensor([[[1., 3., 1.],
tensor([[[1., 3., 1.],
                                                               tensor([[1., 3., 1.],
                                        [0., 2., 1.]]
          [0., 2., 1.],
                                                                        [0., 2., 1.],
                                                                        [1., 2., 5.],
          [1., 2., 5.]],
                                       [[1., 2., 5.],
                                                                        [0., 4., 2.],
                                        [0., 4., 2.]]
         [[0., 4., 2.],
                                                                        [1., 1., 2.],
                                                                        [3., 2., 1.]])
          [1., 1., 2.],
                                       [[1., 1., 2.],
         [3., 2., 1.]]])
                                        [3.. 2.. 1.]]])
```

### Squeeze/Unsqueeze

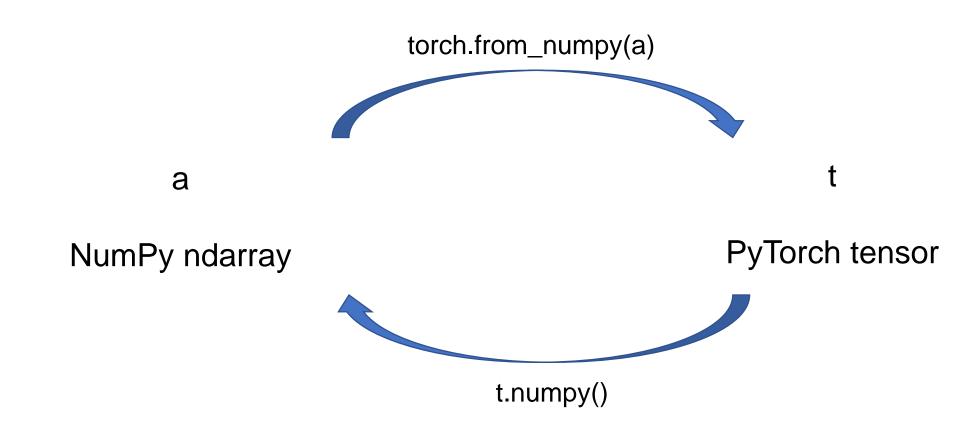


#### Broadcasting

- If a PyTorch operation supports broadcast, its Tensor arguments can be automatically expanded to be of equal sizes
- Two non-empty tensors are "broadcastable" if
  - When iterating over the dimension sizes, starting at the trailing dimension, the dimension sizes must either be
    - 1. one of them is 1
    - 2. one of them does not exist

```
print(X.shape)
                                                                                 Y+X
                                      Y = torch.ones((1,1,3))
print(X)
                                                                                 tensor([[[2., 4., 2.],
torch.Size([2, 3, 3])
                                                                                           [1., 3., 2.],
                                     Y = torch.ones((1.3))
tensor([[[1., 3., 1.],
                                                                                           [2., 3., 6.]],
        [0., 2., 1.],
        [1., 2., 5.]]
                                                                                          [[1., 5., 3.],
                                     Y = torch.ones(3)
       [[0...4...2.].
                                                                                           [2., 2., 3.],
        [1., 1., 2.],
                                                                                           [4.. 3.. 2.111)
        [3., 2., 1.]]])
```

### ndarray <->tensor



# Autograd

# Easy?

$$\begin{split} \frac{\partial L(a^{[2]},y)}{\partial b^{[2]}} &= \frac{\partial L(a^{[2]},y)}{\partial a^{[2]}} \frac{\partial a^{[2]}}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial b^{[2]}} \\ &= \left(\frac{-y}{a^{[2]}} + \frac{1-y}{1-a^{[2]}}\right) \sigma(z^{[2]}) \left(1-\sigma(z^{[2]})\right) \\ &= \left(\frac{-y}{a^{[2]}} + \frac{1-y}{1-a^{[2]}}\right) a^{[2]} \left(1-a^{[2]}\right) \\ &= -y \left(1-a^{[2]}\right) + a^{[2]} \left(1-y\right) = a^{[2]} - y \\ \\ \frac{\partial L(a^{[2]},y)}{\partial b^{[1]}_i} &= \frac{\partial L(a^{[2]},y)}{\partial a^{[2]}} \frac{\partial a^{[2]}}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial a^{[1]}_i} \frac{\partial a^{[1]}_i}{\partial z^{[1]}_i} \frac{\partial z^{[1]}_i}{\partial b^{[1]}_i} \\ &= \left(a^{[2]}-y\right) \frac{\partial z^{[2]}}{\partial a^{[1]}_i} \frac{\partial a^{[1]}_i}{\partial z^{[1]}_i} \frac{\partial z^{[1]}_i}{\partial b^{[1]}_i} \\ &= \left(a^{[2]}-y\right) w^{[2]}_i \left(1-\tanh^2 z^{[1]}_i\right) \cdot 1 \\ &= \left(a^{[2]}-y\right) w^{[2]}_i \left(1-a^{[1]}_i\right)^2 \end{split}$$

$$\frac{\partial L(a^{[2]},y)}{\partial w_i^{[2]}} = \frac{\partial L(a^{[2]},y)}{\partial a^{[2]}} \frac{\partial a^{[2]}}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial w_i^{[2]}}$$

$$= (a^{[2]} - y) \frac{\partial z^{[2]}}{\partial w_i^{[2]}}$$

$$= (a^{[2]} - y) a_i^{[1]}$$

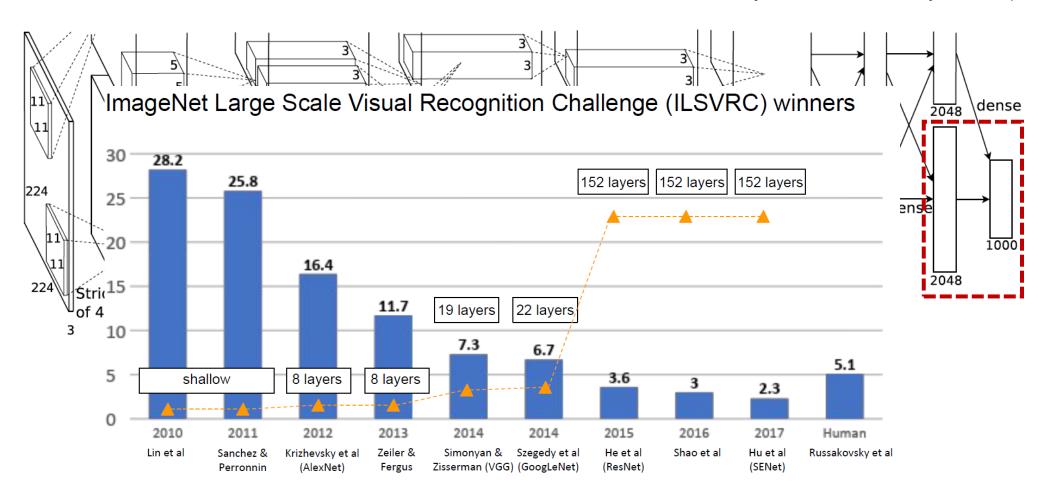
$$\frac{\partial L(a^{[2]},y)}{\partial w_{ij}^{[1]}} = \frac{\partial L(a^{[2]},y)}{\partial a^{[2]}} \frac{\partial a^{[2]}}{\partial z^{[2]}} \frac{\partial z^{[2]}}{\partial a_i^{[1]}} \frac{\partial a_i^{[1]}}{\partial z_i^{[1]}} \frac{\partial z_i^{[1]}}{\partial w_{ij}^{[1]}}$$

$$= (a^{[2]} - y) w_i^{[2]} \left(1 - a_i^{[1]^2}\right) \frac{\partial z_i^{[1]}}{\partial w_{ij}^{[1]}}$$

$$= (a^{[2]} - y) w_i^{[2]} \left(1 - a_i^{[1]^2}\right) x_j$$

#### How about this?

AlexNet, by Alex Krizhevsky et al. (2012)



#### Autograd

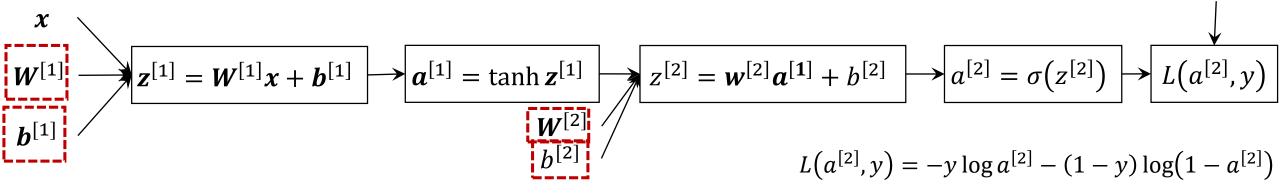
- torch.autograd is PyTorch's automatic differentiation engine that powers neural network training.
- Initialization
  - Set requires\_grad to True if you want to track the gradient

```
w = torch.randn(2, requires_grad = True)
x = torch.ones(2)

print("w", w.requires_grad)
print("x", x.requires_grad)
w True
x False
```

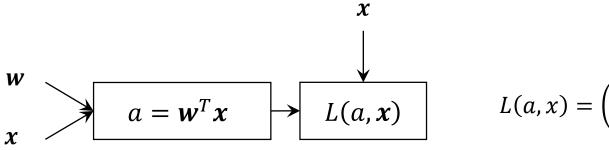
#### backward():

 Computes the sum of gradients of given tensors w.r.t. the leaves of computation graphs



- Accessing the gradient
  - w.grad
    - w is a tensor whose requires\_grad is True

# Example



# $L(a,x) = \left(a - \frac{x_1 + x_2}{2}\right)^2$

#### 1. Initialize

```
w = torch.randn(2, requires_grad = True)
x = torch.Tensor([1,2])
```

#### 2. Predict output

y\_hat = torch.inner(w,x)

#### 3. Compute loss

tensor(0.6281, grad\_fn=<PowBackward0>)

#### 4. Backpropagation

loss.backward()

#### 2-2. Intermediate results

```
print(x)
print(w)
print(y_hat)
```

tensor([1., 2.])
tensor([-0.0444, 0.3759], requires\_grad=True)
tensor(0.7075, grad\_fn=<ViewBackward>)

#### 4-2. Accessing the gradient

```
w.grad
tensor([-1.5851, -3.1701])
```

#### Update parameters

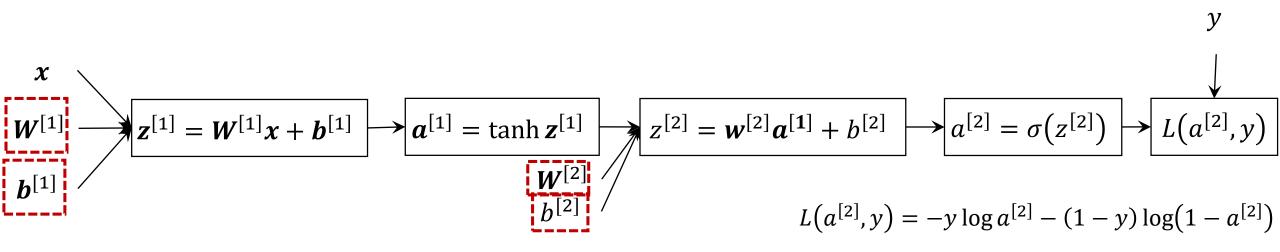
Torch.no\_grad disables gradient calculation

## In-place operations and Autograd

- An in-place operation is an operation that changes directly the content of a given Tensor without making a copy
  - EX) Y[1,2] = 3, A +=Y

Supporting in-place operations in autograd is a hard matter, and we discourage their use in most cases. - PyTorch -

# In-place operations and Autograd



Anyway, never use in-place operations to the tensors on the path from the parameters to the loss

# Avoiding in-place operations

In-place operations

1. 
$$A += X$$

1. 
$$a[i:] = 0$$

Without In-place operations

1. 
$$A = A + X$$

- mask = torch.ones\_like(a)
- 2. mask[i:] = 0
- 3. a = a\*mask

# Implement a Shallow NN with PyTorch autograd

## Data preparation & Import

```
In [1]: import numpy as np import torch
```

#### XOR data (numpy)

## Model

### Model (torch)

```
class shallow_neural_network():
   def __init__(self, num_input_features, num_hiddens):
        self.num_input_features = num_input_features
        self.num_hiddens = num_hiddens
       self.W1 = torch.randn((num_hiddens, num_input_features), requires_grad = True)
       self.b1 = torch.randn(num_hiddens, requires_grad = True)
       self.W2 = torch.randn(num_hiddens, requires_grad = True)
        self.b2 = torch.randn(1, requires_grad = True)
       self.tanh = torch.nn.Tanh()
       self.sigmoid = torch.nn.Sigmoid()
   def predict(self.x):
       z1 = torch.matmul(self.W1,x) + self.b1
       a1 = self.tanh(z1)
       z2 = torch.matmul(self.W2,a1)+ self.b2
       a2 = self.sigmoid(z2)
        return a2
```

## Training

```
def train(X, Y, model, Ir = 0.1):
    m = Ien(X)
   cost = 0.0
    for x,y in zip(X,Y):
       x_torch = torch.from_numpy(x)
        a2 = model.predict(x_torch)
        if v == 10
            loss = -torch.log(a2+0.0001)
        else:
            loss = -torch.log(1.0001-a2)
        loss.backward()
        cost += loss.item()
    with torch.no grad():
        model.W1 -= Ir * model.W1.grad/m
        model.b1 -= lr * model.b1.grad/m
        model.W2 -= Ir * model.W2.grad/m
        model.b2 -= lr * model.b2.grad/m
   model.W1.requires_grad = True
    model.b1.requires_grad = True
   model.W2.requires_grad = True
    model.b2.requires grad = True
    return cost/m
```

```
for epoch in range(100):
   cost = train(X,Y, model, 1.0)
   if epoch % 10 == 0:
      print(epoch, cost)
```

```
0 0.6836582199335098
10 0.3127332235444337
20 0.21746384638389588
30 0.23482400209485924
40 0.27920054577931797
50 0.29317299860637286
60 0.3011668978813414
70 0.28102042431628615
80 0.29269537733129686
90 0.2781521064764529
```

## **Testing**

```
print(model.predict(torch.Tensor((0,0))))
print(model.predict(torch.Tensor((0,1))))
print(model.predict(torch.Tensor((1,0))))
print(model.predict(torch.Tensor((1,1))))

tensor([1.8461e-35], grad_fn=<SigmoidBackward>)
tensor([1.], grad_fn=<SigmoidBackward>)
tensor([1.], grad_fn=<SigmoidBackward>)
tensor([0.1467], grad_fn=<SigmoidBackward>)
```

# nn.Module

## Modules

- PyTorch uses modules to represent neural networks
- Modules are:
  - Building blocks of computations
    - A module represents a node or a subgraph in a computation graph
  - Tightly integrated with autograd
    - Make it simple to specify learnable parameters
  - Easy to work with
    - Save, restore, transfer between CPU/GPU ...

## A simple custom module

```
import torch
from torch import nn

class MyLinear(nn.Module):
    def __init__(self, in_features, out_features):
        super().__init__()
        self.weight = nn.Parameter(torch.randn(in_features, out_features))
        self.bias = nn.Parameter(torch.randn(out_features))

def forward(self, input):
    return (input @ self.weight) + self.bias
```

Call forward

```
m = MyLinear(4, 3)
sample_input = torch.randn(4)
m(sample_input)
: tensor([-0.3037, -1.0413, -4.2057], grad_fn=<AddBackward0>)
```

## Modules as Building Blocks

```
import torch.nn.functional as F
class Net(nn.Module):
 def __init__(self):
    super().__init__()
    self.10 = nn.Linear(4,3)
    self.11 =
               nn.Linear(3,1)
 def forward(self, x):
   x = self.10(x)
   x = F.relu(x)
    x = self.11(x)
    return x
```

## Training with Modules

- Initialize
  - model = YourModel()
  - optimizer = torch.optim.SGD(model.parameters(), lr = <learning\_rate>
- Forward
  - y\_hat = model(input)
- Backward
  - loss = compute\_loss(y, y\_hat) //You need to implement compute\_loss
  - model.zero\_grad()
  - loss.backward()
  - optimizer.step()

# Implement a Shallow NN with autograd and nn.Module

## Model (torch.nn.Module)

```
class shallow_neural_network(nn.Module):
    def __init__(self, num_input_features, num_hiddens):
        super().__init__()
        self.num_input_features = num_input_features
        self.num_hiddens = num_hiddens
        self.linear1 = nn.Linear(num_input_features, num_hiddens)
        self.linear2 = nn.Linear(num_hiddens, 1)
        |self.tanh|=|torch.nn.Tanh()|
        self.sigmoid = torch.nn.Sigmoid()
    def forward(self,x):
        z1 = self.linear1(x)
       a1 = self.tanh(z1)
        z2 = self.linear2(a1)
        a2 = self.sigmoid(z2)
        return a2
```

## Training

```
num_epochs = 100
Ir = 1.0
num_hiddens = 3

model = shallow_neural_network(2,num_hiddens)
optimizer = optim.SGD(model.parameters(), Ir = Ir)
Ioss = nn.BCELoss()
```

```
for epoch in range(num_epochs):
   optimizer.zero_grad()
   cost = 0.0
    for x,y in zip(X,Y):
       x_torch = torch.from_numpy(x)
       v torch = torch.FloatTensor([v])
       y_hat = model(x_torch)
        loss_val = loss(y_hat, y_torch)
       cost += loss_val
   cost = cost / Ien(X)
   cost.backward()
   optimizer.step()
    if epoch %10==0:
       print(epoch, cost)
```

### Test

```
for x,y in zip(x_seeds,y_seeds):
    print(x)
    x_torch = torch.FloatTensor(x)
    y_hat = model(x_torch)
    print(y, y_hat.item())
[0, 0,]
0 0.19255302846431732
[1. 0.]
1 0.702729344367981
[0, 1,]
1 0.7534303665161133
0 0.1685885339975357
```

# PyTorch

Has much more powerful functions to build and train deep neural networks