

# Lec 22 - pytorch

**Statistical Computing and Computation**

**Sta 663 | Spring 2022**

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# PyTorch

PyTorch is a Python package that provides two high-level features:

- Tensor computation (like NumPy) with strong GPU acceleration
- Deep neural networks built on a tape-based autograd system

A graph is created on the fly

$W_h = \text{torch.randn}(20, 20, \text{requires_grad=True})$   
 $W_x = \text{torch.randn}(20, 10, \text{requires_grad=True})$   
 $x = \text{torch.randn}(1, 10)$   
 $\text{prev\_h} = \text{torch.randn}(1, 20)$

W<sub>h</sub>   h   W<sub>x</sub>   x

```
import torch  
torch.__version__
```

# Tensors

are the basic data abstraction in PyTorch and are implemented by the `torch.Tensor` class. They behave in much the same way as the other array libraries we've seen so far (`numpy`, `theano`, etc.)

```
torch.zeros(3)
```

```
## tensor([0., 0., 0.])
```

```
torch.ones(3,2)
```

```
## tensor([[1., 1.],  
##          [1., 1.],  
##          [1., 1.]])
```

```
torch.empty(2,2,2)
```

```
## tensor([[[ 0.0000e+00, -3.6893e+19],  
##          [ 4.2163e-29, -3.6893e+19]],  
##  
##          [[ 1.0000e+00,  1.0000e+00],  
##          [ 4.6725e+20,  1.4013e-45]]])
```

```
torch.manual_seed(1234)
```

```
## <torch._C.Generator object at 0x2aef26c50>
```

```
torch.rand(2,2,2,2)
```

```
## tensor([[[[0.0290,  0.4019],  
##           [0.2598,  0.3666]],  
##  
##           [[0.0583,  0.7006],  
##           [0.0518,  0.4681]]],  
##  
##           [[[0.6738,  0.3315],  
##             [0.7837,  0.5631]],  
##  
##             [[0.7749,  0.8208],  
##             [0.2793,  0.6817]]]])
```

# Constant values

As expected, tensors can be constructed from constant numeric values in lists or tuples.

```
torch.tensor(1)
```

```
## tensor(1)
```

```
torch.tensor((1,2))
```

```
## tensor([1, 2])
```

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

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

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

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

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

```
## ValueError: expected sequence of length 3 at dim 1 (
```

```
torch.tensor([["A"]])
```

```
## ValueError: too many dimensions 'str'
```

```
torch.tensor([[True]]).dtype
```

```
## torch.bool
```

Note using `tensor()` in this way results in a full copy of the data.

# Tensor Types

Data type	dtype	type()	Comment
32-bit float	float32 or float	FloatTensor	Default float type
64-bit float	float64 or double	DoubleTensor	
16-bit float	float16 or half	HalfTensor	
16-bit brain float	bfloat16	BFloat16Tensor	
64-bit complex float	complex64		
128-bit complex float	complex128 or cdouble		
8-bit integer (unsigned)	uint8	ByteTensor	
8-bit integer (signed)	int8	CharTensor	
16-bit integer (signed)	int16 or short	ShortTensor	
32-bit integer (signed) We've left off quantized integer types here	int32 or int	IntTensor	

# Specifying types

Just like NumPy and Pandas, types are specified via the `dtype` argument and can be inspected via the `dtype` attribute.

```
a = torch.tensor([1,2,3])  
a
```

```
## tensor([1, 2, 3])
```

```
a.dtype
```

```
## torch.int64
```

```
b = torch.tensor([1,2,3], dtype=torch.float16)  
b
```

```
## tensor([1., 2., 3.], dtype=torch.float16)
```

```
b.dtype
```

```
## torch.float16
```

```
c = torch.tensor([1.,2.,3.])  
c
```

```
## tensor([1., 2., 3.])
```

```
c.dtype
```

```
## torch.float32
```

```
d = torch.tensor([1,2,3], dtype=torch.float64)  
d
```

```
## tensor([1., 2., 3.], dtype=torch.float64)
```

```
d.dtype
```

```
## torch.float64
```

# Type precision

When using types with less precision it is important to be careful about underflow and overflow (ints) and rounding errors (floats).

```
torch.tensor([300], dtype=torch.int8)
```

```
## tensor([44], dtype=torch.int8)
```

```
torch.tensor([-300]).to(torch.int8)
```

```
## tensor([-44], dtype=torch.int8)
```

```
torch.tensor([-300]).to(torch.uint8)
```

```
## tensor([212], dtype=torch.uint8)
```

```
torch.tensor([300]).to(torch.int16)
```

```
## tensor([300], dtype=torch.int16)
```

```
torch.set_printoptions(precision=8)
```

```
torch.tensor(1/3, dtype=torch.float16)
```

```
## tensor(0.33325195, dtype=torch.float16)
```

```
torch.tensor(1/3, dtype=torch.float32)
```

```
## tensor(0.33333334)
```

```
torch.tensor(1/3, dtype=torch.float64)
```

```
## tensor(0.33333333, dtype=torch.float64)
```

# NumPy conversion

It is possible to easily move between NumPy arrays and Tensors via the `from_numpy()` function and `numpy()` method.

```
a = np.eye(3,3)
torch.from_numpy(a)

## tensor([[1., 0., 0.],
##         [0., 1., 0.],
##         [0., 0., 1.]], dtype=torch.float64)

b = np.array([1,2,3])
torch.from_numpy(b)

## tensor([1, 2, 3])

c = torch.rand(2,3)
c.numpy()

## array([[0.28367, 0.65673, 0.23876],
##        [0.73128, 0.60122, 0.30433]], dtype=float32)

d = torch.ones(2,2, dtype=torch.int64)
d.numpy()
```

# Math & Logic

Just like NumPy tensors support basic mathematical and logical operations with scalars and other tensors - the PyTorch library provides implementations of most commonly needed mathematical and related functions.

```
torch.ones(2,2) * 7 -1
```

```
## tensor([[6., 6.],  
##          [6., 6.]])
```

```
torch.ones(2,2) + torch.tensor([[1,2], [3,4]])
```

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

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

```
## tensor([[ 2,  4],  
##          [ 8, 16]])
```

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

```
## tensor([[False, False],
```

```
x = torch.rand(2,2)
```

```
torch.ones(2,2) @ x
```

```
## tensor([[1.22126317, 1.36931109],  
##          [1.22126317, 1.36931109]])
```

```
torch.clamp(x*2-1, -0.5, 0.5)
```

```
## tensor([[-0.49049568,  0.25872374],  
##          [ 0.50000000,  0.47989845]])
```

```
torch.mean(x)
```

```
## tensor(0.64764357)
```

```
torch.sum(x)
```

# Broadcasting

Like NumPy in cases where tensor dimensions do not match, the broadcasting algorithm is used. The rules for broadcasting are:

- Each tensor must have at least one dimension - no empty tensors.
- Comparing the dimension sizes of the two tensors, going from last to first:
  - Each dimension must be equal, or
  - One of the dimensions must be of size 1, or
  - The dimension does not exist in one of the tensors

# Exercise 1

Consider the following 6 tensors:

```
a = torch.rand(4, 3, 2)
b = torch.rand(3, 2)
c = torch.rand(2, 3)
d = torch.rand(0)
e = torch.rand(3, 1)
f = torch.rand(1, 2)
```

which of the above could be multiplied together and produce a valid result via broadcasting  
(e.g.  $a*b$ ,  $a*c$ ,  $a*d$ , etc.).

Explain why or why not broadcasting was able to be applied in each case.

# Inplace modification

In instances where we need to conserve memory it is possible to apply many functions in a way where a new tensor is not created but the original values are replaced. These functions share the same name with the original functions but have a \_ suffix.

```
a = torch.rand(2,2)
print(a)

## tensor([[0.31861043, 0.29080772],
##          [0.41960979, 0.37281448]])
```

```
print(torch.exp(a))

## tensor([[1.37521553, 1.33750737],
##          [1.52136779, 1.45181501]])
```

```
print(a)

## tensor([[0.31861043, 0.29080772],
##          [0.41960979, 0.37281448]])
```

For functions without a \_ variant, check if they have a to argument which can then be used instead - see `torch.matmul()`

```
print(torch.exp_(a))

## tensor([[1.37521553, 1.33750737],
##          [1.52136779, 1.45181501]])
```

```
print(a)

## tensor([[1.37521553, 1.33750737],
##          [1.52136779, 1.45181501]])
```

# Inplace arithmetic

All arithmetic functions are available as methods of the Tensor class,

```
a = torch.ones(2, 2)
b = torch.rand(2, 2)
```

a+b

```
## tensor([[1.37689185, 1.01077938],
##          [1.94549370, 1.76611161]])
```

print(a)

```
## tensor([[1., 1.],
##          [1., 1.]])
```

print(b)

```
## tensor([[0.37689191, 0.01077944],
##          [0.94549364, 0.76611167]])
```

a.add\_(b)

```
## tensor([[1.37689185, 1.01077938],
##          [1.94549370, 1.76611161]])
```

print(a)

```
## tensor([[1.37689185, 1.01077938],
##          [1.94549370, 1.76611161]])
```

print(b)

```
## tensor([[0.37689191, 0.01077944],
##          [0.94549364, 0.76611167]])
```

# Changing tensor shapes

The shape of a tensor can be changed using the `view()` or `reshape()` methods. The former guarantees that the result shares data with the original object (but requires contiguity), the latter may or may not copy the data.

```
x = torch.zeros(3, 2)
y = x.view(2, 3)
y
```

```
## tensor([[0., 0., 0.],
##          [0., 0., 0.]])
```

```
x.fill_(1)
```

```
## tensor([[1., 1.],
##          [1., 1.],
##          [1., 1.]])
```

```
y
```

```
## tensor([[1., 1., 1.],
##          [1., 1., 1.]])
```

```
x = torch.zeros(3, 2)
y = x.t()
z = y.view(6)
```

```
## RuntimeError: view size is not compatible with input
```

```
z = y.reshape(6)
x.fill_(1)
```

```
## tensor([[1., 1.],
##          [1., 1.],
##          [1., 1.]])
```

```
y
```

```
## tensor([[1., 1., 1.],
##          [1., 1., 1.]])
```

# Adding or removing dimensions

The `squeeze()` and `unsqueeze()` methods can be used to remove or add length 1 dimension(s) to a tensor.

```
x = torch.zeros(1,3,1)  
x.squeeze().shape
```

```
## torch.Size([3])
```

```
x.squeeze(0).shape
```

```
## torch.Size([3, 1])
```

```
x.squeeze(1).shape
```

```
## torch.Size([1, 3, 1])
```

```
x.squeeze(2).shape
```

```
## torch.Size([1, 3])
```

```
y = x.squeeze()  
x.fill_(1)
```

```
x = torch.zeros(3,2)  
x.unsqueeze(0).shape
```

```
## torch.Size([1, 3, 2])
```

```
x.unsqueeze(1).shape
```

```
## torch.Size([3, 1, 2])
```

```
x.unsqueeze(2).shape
```

```
## torch.Size([3, 2, 1])
```

```
y = x.unsqueeze(1)  
x.fill_(1)
```

```
## tensor([[1., 1.],  
##          [1., 1.],  
##          [1., 1.]])
```

$\begin{bmatrix} [1, 2], \\ [3, 4] \end{bmatrix}$

1	2
3	4

2d tensor

$\xleftarrow{\text{squeeze}()} \quad \xrightarrow{\text{unsqueeze}(0)}$

1	2
3	4

3d tensor

$\begin{bmatrix} [[1, 2], \\ [3, 4]] \end{bmatrix}$

$\xleftarrow{\text{squeeze}()} \quad \xrightarrow{\text{unsqueeze}(0)}$

1	2
3	4

$\begin{bmatrix} [[1, 2], \\ [3, 4]] \end{bmatrix}$

$\xleftarrow{\text{squeeze}()} \quad \xrightarrow{\text{unsqueeze}(2)}$

1	2
3	4
3	

$\begin{bmatrix} [[1, 2], \\ [3, 4]] \end{bmatrix}$

## Exercise 2

Given the following tensors,

```
a = torch.ones(4,3,2)  
b = torch.rand(3)  
c = torch.rand(5,3)
```

what reshaping is needed to make it possible so that  $a * b$  and  $a * c$  can be calculated via broadcasting?

# Autograd

# Tensor expressions

Gradient tracking can be enabled using the `requires_grad` argument at initialization, alternatively the `requires_grad` flag can be set on tensor or the `enable_grad()` context manager used.

```
x = torch.linspace(0, 2, steps=21, requires_grad=True)
x

## tensor([0.0000000, 0.1000000, 0.2000000, 0.3000001, 0.4000001, 0.5000000,
##         0.6000002, 0.6999999, 0.8000001, 0.9000004, 1.0000000, 1.1000002,
##         1.2000005, 1.3000007, 1.3999998, 1.5000000, 1.6000002, 1.7000005,
##         1.7999995, 1.8999998, 2.0000000], requires_grad=True)

y = 3*x + 2
y

## tensor([2.0000000, 2.2999995, 2.5999990, 2.90000010, 3.20000005, 3.5000000,
##         3.80000019, 4.09999990, 4.40000010, 4.69999981, 5.00000000, 5.30000019,
##         5.60000038, 5.90000010, 6.19999981, 6.50000000, 6.80000019, 7.10000038,
##         7.39999962, 7.69999981, 8.00000000], grad_fn=<AddBackward0>)
```

# Computational graph

```
y.grad_fn  
## <AddBackward0 object at 0x2b1c5d790>  
  
y.grad_fn.next_functions  
## ((<MulBackward0 object at 0x2b1c5d250>, 0), (None, 0))  
  
y.grad_fn.next_functions[0][0].next_functions  
## ((<AccumulateGrad object at 0x2b1c5d4f0>, 0), (None, 0))  
  
y.grad_fn.next_functions[0][0].next_functions[0][0].next_functions  
## ()
```

# Autogradient

In order to calculate the gradients we use the `backward()` method on the calculation output tensor (must be a scalar), this then makes the `grad` attribute available for the input (leaf) tensors.

```
out = y.sum()  
out.backward()  
out
```

```
## tensor(105., grad_fn=<SumBackward0>)
```

y.grad

```
## UserWarning: The .grad attribute of a Tensor that is not a leaf Tensor is being accessed. Its .grad attribute  
be populated during autograd.backward(). If you indeed want the .grad field to be populated for a non-leaf T  
use .retain_grad() on the non-leaf Tensor. If you access the non-leaf Tensor by mistake, make sure you acces  
leaf Tensor instead. See github.com/pytorch/pytorch/pull/30531 for more informations. (Triggered internally at  
Users/distiller/project/pytorch/build/aten/src/ATen/core/TensorBody.h:475.)  
##    return self._grad
```

```
##     return self._grad
```

x.grad

# A bit more complex

```
n = 21
x = torch.linspace(0, 2, steps=n, requires_grad=True)
m = torch.rand(n, requires_grad=True)

y = m*x + 2

y.backward(torch.ones(n))
```

```
x.grad
```

```
## tensor([0.23227984, 0.72686875, 0.11874896, 0.39512146, 0.71987736, 0.75950843,
##         0.53108865, 0.64494550, 0.72242016, 0.44158769, 0.36338443, 0.88182861,
##         0.98741043, 0.73160070, 0.28143251, 0.06507802, 0.00649202, 0.50345892,
##         0.30815977, 0.37417805, 0.42968810])
```

```
m.grad
```

```
## tensor([0.00000000, 0.10000000, 0.20000000, 0.30000001, 0.40000001, 0.50000000,
##         0.60000002, 0.69999999, 0.80000001, 0.90000004, 1.00000000, 1.10000002,
##         1.20000005, 1.30000007, 1.39999998, 1.50000000, 1.60000002, 1.70000005,
##         1.79999995, 1.89999998, 2.00000000])
```

# High-level autograd API

This allows for the automatic calculation and evaluation of the jacobian and hessian for a function defined used tensors.

```
def f(x, y):
    return 3*x + 1 + 2*y**2 + x*y
```

```
for x in [0.,1.]:
    for y in [0.,1.]:
        print("x =",x, "y = ",y)
inputs = (torch.tensor([x]), torch.tensor([y])
print(torch.autograd.functional.jacobian(f, i
```

```
## x = 0.0 y =  0.0
## ((tensor([[3.]]), tensor([[0.]]))
##
## x = 0.0 y =  1.0
## ((tensor([[4.]]), tensor([[4.]]))
##
## x = 1.0 y =  0.0
## ((tensor([[3.]]), tensor([[1.]]))
##
```

```
inputs = (torch.tensor([0.]), torch.tensor([0.]))
torch.autograd.functional.hessian(f, inputs)
## ((tensor([[0.]]), tensor([[1.]])), (tensor([[1.]]),
## inputs = (torch.tensor([1.]), torch.tensor([1.]))
torch.autograd.functional.hessian(f, inputs)
## ((tensor([[0.]]), tensor([[1.]])), (tensor([[1.]]),
```

# Demo 1 - Linear Regression w/ PyTorch

# A basic model

```
x = np.linspace(-math.pi, math.pi, 200)
y = np.sin(x)
```

```
lm = smf.ols("y~x+I(x**2)+I(x**3)", data=pd.DataFrame({"x": x, "y": y})).fit()
print(lm.summary())
```

```
##                                     OLS Regression Results
## =====
## Dep. Variable:                      y   R-squared:                 0.991
## Model:                            OLS   Adj. R-squared:             0.991
## Method:                          Least Squares   F-statistic:            7041.
## Date:                Tue, 29 Mar 2022   Prob (F-statistic):        2.96e-199
## Time:                    14:21:12   Log-Likelihood:            254.95
## No. Observations:                  200   AIC:                     -501.9
## Df Residuals:                      196   BIC:                     -488.7
## Df Model:                           3
## Covariance Type:            nonrobust
## =====
##              coef    std err          t      P>|t|      [0.025      0.975]
## -----
## Intercept  6.104e-17  0.007  8.42e-15  1.000    -0.014     0.014
## x           0.8546   0.007   128.977  0.000     0.842     0.868
## I(x ** 2)  4.93e-18  0.002  3.03e-15  1.000    -0.003     0.003
```



# Making tensors

```
yt = torch.tensor(y)
Xt = torch.tensor(lm.model.exog)
bt = torch.randn((Xt.shape[1], 1), dtype=torch.float64, requires_grad=True)

yt_pred = (Xt @ bt).squeeze()

loss = (yt_pred - yt).pow(2).sum()
loss.item()

## 8060.669052389756
```

# Gradient descent

Going back to our discussion of optimization and gradient descent awhile back - we can update our guess for  $b$  /  $bt$  by moving in the direction of the negative gradient. The step size is referred to as the learning rate which we will pick a relatively small value for.

```
learning_rate = 1e-6  
  
loss.backward() # Compute the backward pass  
  
with torch.no_grad():  
    bt -= learning_rate * bt.grad # Make the step
```

```
bt.grad = None # Reset the gradients
```

```
yt_pred = (Xt @ bt).squeeze()  
loss = (yt_pred - yt).pow(2).sum()  
loss.item()
```

```
## 7380.58278232608
```

# Putting it together

```
yt = torch.tensor(y).unsqueeze(1)
Xt = torch.tensor(lm.model.exog)
bt = torch.randn((Xt.shape[1], 1), dtype=torch.float64, requires_grad=True)

learning_rate = 1e-5
for i in range(5000):

    yt_pred = Xt @ bt

    loss = (yt_pred - yt).pow(2).sum()
    if i % 500 == 0:
        print(i, loss.item())

    loss.backward()

    with torch.no_grad():
        bt -= learning_rate * bt.grad
        bt.grad = None

## 0 257680.8304254537
## 500 13.07780707986047
## 1000 2.4863342128971935
## 1500 1.1208859061116399
## 2000 0.9423484068960166
```

# Comparing results

bt

```
## tensor([[ 4.79584652e-05,
##           [ 8.54550246e-01],
##           [-8.19655854e-06],
##           [-9.28168699e-02]], dtype=torch.float64, requires_grad=True)
```

lm.params

```
## Intercept    6.104058e-17
## x            8.545770e-01
## I(x ** 2)   4.929732e-18
## I(x ** 3)   -9.282065e-02
## dtype: float64
```



## **Demo 2 - Using a model**

# A sample model

```
class Model(torch.nn.Module):
    def __init__(self, beta):
        super().__init__()
        beta.requires_grad = True
        self.beta = torch.nn.Parameter(beta)

    def forward(self, X):
        return X @ self.beta

def training_loop(model, X, y, optimizer, n=1000):
    losses = []
    for i in range(n):
        y_pred = model(X)

        loss = (y_pred.squeeze() - y.squeeze()).pow(2).sum()
        loss.backward()

        optimizer.step()
        optimizer.zero_grad()

        losses.append(loss.item())

    return losses
```

# Fitting

```
x = torch.linspace(-math.pi, math.pi, 200)
y = torch.sin(x)

X = torch.vstack((
    torch.ones_like(x),
    x,
    x**2,
    x**3
)).T

m = Model(beta = torch.zeros(4))
opt = torch.optim.SGD(m.parameters(), lr=1e-5)

losses = training_loop(m, X, y, opt, n=3000)
```

# Results

```
m.beta
```

```
## Parameter containing:  
## tensor([-8.40055758e-09,  8.52953434e-01,  2.83126012e-09, -9.25917700e-02],  
##         requires_grad=True)
```

```
plt.figure(figsize=(8,6), layout="constrained")  
plt.plot(losses)  
plt.show()
```

