

Lec 22 - pytorch

Statistical Computing and Computation

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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_h h W_x 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

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

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

1	2
3	4

3d tensor

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

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

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

2	
1	4
3	

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

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()
```

