pytorch

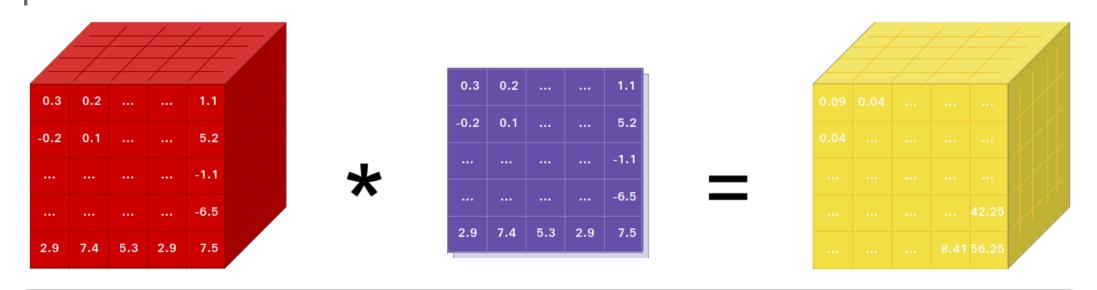
Lecture 22

Dr. Colin Rundel

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



- 1 import torch
- 2 torch.__version__

^{&#}x27;2.0.0'

A graph is created on the fly

```
W_h = torch.randn(20, 20, requires_grad=True)
W_x = torch.randn(20, 10, requires_grad=True)
x = torch.randn(1, 10)
prev_h = torch.randn(1, 20)
```



Tensors

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

```
1 torch.zeros(3)
                                                          1 torch.manual seed(1234)
tensor([0., 0., 0.])
                                                        <torch. C.Generator object at 0x29951c510>
                                                          1 torch.rand(2,2,2,2)
  1 torch.ones(3,2)
tensor([[1., 1.],
                                                        tensor([[[[0.0290, 0.4019],
                                                                   [0.2598, 0.3666]],
        [1., 1.],
        [1., 1.]])
                                                                 [[0.0583, 0.7006],
  1 torch.empty(2,2,2)
                                                                   [0.0518, 0.4681]]],
tensor([[[0., 0.],
                                                                [[[0.6738, 0.3315],
         [0., 0.]],
                                                                   [0.7837, 0.5631]],
        [[0., 0.],
                                                                 [[0.7749, 0.8208],
         [0., 0.]])
                                                                   [0.2793, 0.6817]]])
```

Constants

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

```
1 torch.tensor([(1,1,1), [4,5]])
  1 torch.tensor(1)
                                                        Error: ValueError: expected sequence of length 3 at (
tensor(1)
                                                          1 torch.tensor([["A"]])
  1 torch.tensor((1,2))
                                                        Error: ValueError: too many dimensions 'str'
tensor([1, 2])
  1 torch.tensor([[1,2,3], [4,5,6]])
                                                          1 torch.tensor([[True]]).dtype
                                                        torch.bool
tensor([[1, 2, 3],
       [4, 5, 6]])
  1 torch.tensor([(1,2,3), [4,5,6]])
tensor([[1, 2, 3],
        [4, 5, 6]])
```

Tensor Types

Data type	dtype	type()	Comment			
32-bit float	float32 or float	FloatTensor	Default float			
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)	int32 or int	IntTensor				
64-bit integer (signed)	int64 or long	LongTensor	Default integer			
Boolean	bool	BoolTensor				

Specifying types

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

```
1 c = torch.tensor([1.,2.,3.]); c
  1 a = torch.tensor([1,2,3]); a
tensor([1, 2, 3])
                                                       tensor([1., 2., 3.])
                                                         1 c.dtype
  1 a.dtype
                                                       torch.float32
torch.int64
 1 b = torch.tensor([1,2,3], dtype=torch.float16);
                                                            d = torch.tensor([1,2,3], dtype=torch.float64);
tensor([1., 2., 3.], dtype=torch.float16)
                                                       tensor([1., 2., 3.], dtype=torch.float64)
  1 b.dtype
                                                         1 d.dtype
torch.float16
                                                       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).

```
1 torch.tensor([128], dtype=torch.int8)
                                                         1 torch.tensor(1/3, dtype=torch.float16)
Error: RuntimeError: value cannot be converted to type
                                                       tensor(0.33325195, dtype=torch.float16)
  1 torch.tensor([128]).to(torch.int8)
                                                         1 torch.tensor(1/3, dtype=torch.float32)
tensor([-128], dtype=torch.int8)
                                                       tensor(0.33333334)
                                                         1 torch.tensor(1/3, dtype=torch.float64)
  1 torch.tensor([255]).to(torch.uint8)
                                                       tensor(0.33333333, dtype=torch.float64)
tensor([255], dtype=torch.uint8)
  1 torch.tensor([300]).to(torch.uint8)
                                                         1 torch.tensor(1/3, dtype=torch.bfloat16)
tensor([44], dtype=torch.uint8)
                                                       tensor(0.33398438, dtype=torch.bfloat16)
  1 torch.tensor([300]).to(torch.int16)
tensor([300], dtype=torch.int16)
```

NumPy conversion

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

```
1 \quad a = np.eye(3,3)
  2 torch.from numpy(a)
tensor([[1., 0., 0.],
        [0., 1., 0.],
        [0., 0., 1.]], dtype=torch.float64)
  1 b = np.array([1,2,3])
  2 torch.from numpy(b)
tensor([1, 2, 3])
 1 c = torch.rand(2,3)
  2 c.numpy()
array([[0.28367, 0.65673, 0.23876],
       [0.73128, 0.60122, 0.30433]], dtype=float32)
  1 d = torch.ones(2,2, dtype=torch.int64)
  2 d.numpy()
array([[1, 1],
       [1, 1]]
```

Math & Logic

Just like NumPy torch tensor objects support basic mathematical and logical operations with scalars and other tensors - torch provides implementations of most commonly needed mathematical functions.

```
1 torch.ones((2,2) * 7-1
                                                           1 \times = torch.rand(2,2)
tensor([[6., 6.],
                                                           3 \text{ torch.ones}(2,2) @ x
        [6., 6.11)
                                                         tensor([[1.22126317, 1.36931109],
  1 torch.ones(2,2) + torch.tensor([[1,2], [3,4]])
                                                                 [1.22126317, 1.36931109]])
tensor([[2., 3.],
                                                           1 torch.clamp(x*2-1, -0.5, 0.5)
        [4., 5.11)
                                                         tensor([[-0.49049568, 0.25872374],
  1 2 ** torch.tensor([[1,2], [3,4]])
                                                                 [0.50000000, 0.47989845]])
tensor([[ 2, 4],
                                                           1 torch.mean(x)
        [ 8, 16]])
                                                         tensor(0.64764357)
  1 2 ** torch.tensor([[1,2], [3,4]]) > 5
                                                           1 torch.sum(x)
tensor([[False, False],
                                                         tensor(2.59057426)
        [ True, True]])
                                                           1 torch.min(x)
                                                         tensor(0.25475216)
```

Sta 663 - Spring 2023

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:

```
1  a = torch.rand(4, 3, 2)
2  b = torch.rand(3, 2)
3  c = torch.rand(2, 3)
4  d = torch.rand(0)
5  e = torch.rand(3, 1)
6  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 such that a new tensor is not created but the original value(s) are replaced. These functions share the same name with the original functions but have a _ suffix.

```
1 a = torch.rand(2,2)
  2 print(a)
tensor([[0.31861043, 0.29080772],
        [0.41960979, 0.37281448]])
  1 print(torch.exp(a))
                                                          1 print(torch.exp (a))
tensor([[1.37521553, 1.33750737],
                                                        tensor([[1.37521553, 1.33750737],
                                                                [1.52136779, 1.45181501]])
        [1.52136779, 1.45181501]])
  1 print(a)
                                                          1 print(a)
tensor([[0.31861043, 0.29080772],
                                                        tensor([[1.37521553, 1.33750737],
        [0.41960979, 0.37281448]])
                                                                [1.52136779, 1.45181501]])
```

Inplace arithmetic

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

```
1 a = torch.ones(2, 2)
  2 b = torch.rand(2, 2)
                                                          1 a.add (b)
  1 a+b
tensor([[1.37689185, 1.01077938],
                                                        tensor([[1.37689185, 1.01077938],
        [1.94549370, 1.76611161]])
                                                                [1.94549370, 1.76611161]])
  1 print(a)
                                                          1 print(a)
tensor([[1., 1.],
                                                        tensor([[1.37689185, 1.01077938],
        [1., 1.]]
                                                                [1.94549370, 1.76611161]])
  1 print(b)
                                                          1 print(b)
tensor([[0.37689191, 0.01077944],
                                                        tensor([[0.37689191, 0.01077944],
        [0.94549364, 0.76611167]])
                                                                [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.

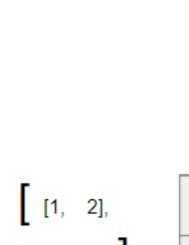
```
1 \times = torch.zeros(3, 2)
                                                          1 x = torch.zeros(3, 2)
 2 y = x.view(2, 3)
                                                          2 y = x.t()
                                                          3 z = y.view(6)
  3 y
tensor([[0., 0., 0.],
                                                        Error: RuntimeError: view size is not compatible with
        [0., 0., 0.11)
                                                          1 z = y.reshape(6)
  1 x.fill (1)
                                                          2 x.fill (1)
tensor([[1., 1.],
                                                        tensor([[1., 1.],
        [1., 1.],
                                                                [1., 1.],
        [1., 1.]]
                                                                [1., 1.]])
                                                          1 y
 1 y
tensor([[1., 1., 1.],
                                                        tensor([[1., 1., 1.],
        [1., 1., 1.]]
                                                                [1., 1., 1.]]
                                                          1 z
                                                        tensor([0., 0., 0., 0., 0., 0.])
```

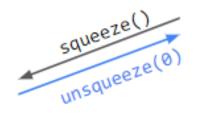
Adding or removing dimensions

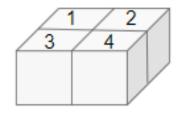
The squeeze() and unsqueeze() methods can be used to remove or add length 1 dimension(s) to a tensor.

```
1 \times = torch.zeros(1,3,1)
                                                          1 x = torch.zeros(3,2)
  2 x.squeeze().shape
                                                          2 x.unsqueeze(0).shape
torch.Size([3])
                                                        torch.Size([1, 3, 2])
  1 x.squeeze(0).shape
                                                          1 x.unsqueeze(1).shape
torch.Size([3, 1])
                                                        torch.Size([3, 1, 2])
  1 x.squeeze(1).shape
                                                          1 x.unsqueeze(2).shape
torch.Size([1, 3, 1])
                                                        torch.Size([3, 2, 1])
  1 x.squeeze(2).shape
torch.Size([1, 3])
```

3d tensor

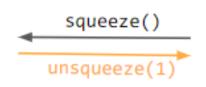


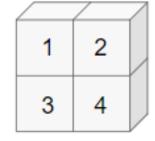


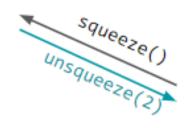


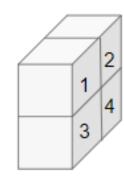


2d tensor









Exercise 2

Given the following tensors,

```
1  a = torch.ones(4,3,2)
2  b = torch.rand(3)
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 the tensor or the enable_grad() context manager used (via with).

Computational graph

Basics of the computation graph can be explored via the next_functions attribute

```
1 y.grad_fn
<AddBackward0 object at 0x29cee8520>
1 y.grad_fn.next_functions
((<MulBackward0 object at 0x29cee8640>, 0), (None, 0))
1 y.grad_fn.next_functions[0][0].next_functions
((<AccumulateGrad object at 0x29cee8490>, 0), (None, 0))
1 y.grad_fn.next_functions[0][0].next_functions
()
```

Autogradient

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

```
1 out = y.sum()
2 out.backward()
3 out
```

tensor(105., grad_fn=<SumBackward0>)

```
1 y.grad
```

<string>:1: UserWarning: The .grad attribute of a Tensor that is not a leaf Tensor is being accessed. Its .c
 attribute won't be populated during autograd.backward(). If you indeed want the .grad field to be populat
 non-leaf Tensor, use .retain_grad() on the non-leaf Tensor. If you access the non-leaf Tensor by mistake,
 you access the leaf Tensor instead. See github.com/pytorch/pytorch/pytorch/pull/30531 for more informations. (Tri
 internally at /Users/runner/work/pytorch/pytorch/pytorch/build/aten/src/ATen/core/TensorBody.h:491.)

A bit more complex

In context you can interpret x.grad and m.grad as the gradient of y with respect to x or m respectively.

High-level autograd API

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

```
1 def f(x, y):
      return 3*x + 1 + 2*y**2 + x*y
  1 for x in [0.,1.]:
      for y in [0.,1.]:
     print("x = ", x, "y = ", y)
  3
     inputs = (torch.tensor([x]), torch.tensor([y]))
        print(torch.autograd.functional.jacobian(f, inputs),"\n")
  5
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.]]))
x = 1.0 y = 1.0
(tensor([[4.]]), tensor([[5.]]))
```

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

((tensor([[0.]]), tensor([[1.]])), (tensor([[1.]]), tensor([[4.]])))
inputs = (torch.tensor([1.]), torch.tensor([1.]))
torch.autograd.functional.hessian(f, inputs)

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

Demo 1 - Linear Regression w/ PyTorch

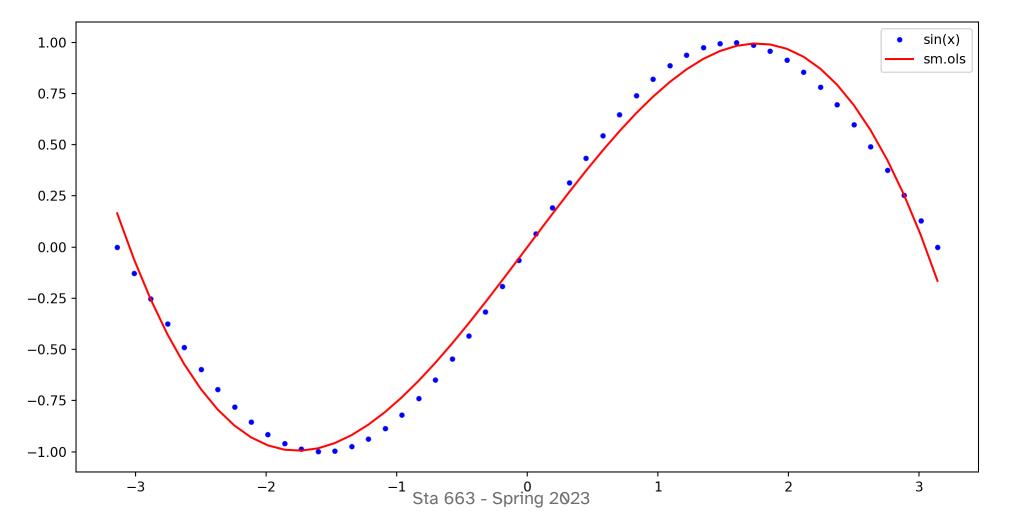
A basic model

```
1 x = np.linspace(-math.pi, math.pi, 50)
2 y = np.sin(x)
  lm = smf.ols(
   "y\sim x+I(x**2)+I(x**3)",
    data=pd.DataFrame({"x": x, "y": y})
  ).fit()
8
9 print(lm.summary())
```

========		(egress		
Dep. Varia	ble:			У	R-squ	ared:
Model:				OLS	Adj.	R-square
Method:		Leas.	t Squ	ares	F-sta	tistic:
Date:		Fri, 07	Apr	2023	Prob	(F-stati
Time:			12:4	3:41	Log-L	ikelihoo
No. Observ	ations:			50	AIC:	
Df Residua	ls:			46	BIC:	
Df Model:				3		
Covariance	Type:	1	nonro	bust		
========	=======	-=====		=====	=====	======
	coef	std	err		t	P> 1
Intercept	3.161e-16	5 0	.016	2	e-14	1.00
х	0.8476	5 0	.014	59	. 444	0.00
I(x ** 2)	-4.949e-17	0	.003	-1.44	e-14	1.00
I(x ** 3)	-0.0912	2 0	.002	-42	.977	0.00
========	=======	======	====	=====	=====	======
Omnibus:			3	.322	Durbi	n-Watsor
Prob(Omnibus):			0.190		Jarque-Bera	
Skew:			0	.000	Prob(JB):
Kurtosis:			2	.111	Cond.	No.

Predictions

```
plt.figure(figsize=(10,5), layout="constrained")
plt.plot(x, y, ".b", label="sin(x)")
plt.plot(x, lm.predict(), "-r", label="sm.ols")
plt.legend()
plt.show()
```



Making tensors

```
1 yt = torch.tensor(y)
 2 Xt = torch.tensor(lm.model.exog)
  3 bt = torch.randn((Xt.shape[1], 1), dtype=torch.float64, requires grad=True)
  1 yt
                                                         1 Xt
tensor([-1.22464680e-16, -1.27877162e-01, -2.53654584
                                                       tensor([[ 1.00000000e+00, -3.14159265e+00,
                                                                                                   9.8696044
        -4.90717552e-01, -5.98110530e-01, -6.9568255
                                                               [ 1.00000000e+00, -3.01336438e+00,
                                                                                                   9.0803649
        -8.55142763e-01, -9.14412623e-01, -9.5866785
                                                               [ 1.00000000e+00, -2.88513611e+00, 8.3240103
        -9.99486216e-01, -9.95379113e-01, -9.74927912
                                                               [ 1.00000000e+00, -2.75690784e+00,
                                                                                                  7.6005408
        -8.86599306e-01, -8.20172255e-01, -7.4027799
                                                               [ 1.00000000e+00, -2.62867957e+00,
                                                                                                   6.9099562
        -5.45534901e-01, -4.33883739e-01, -3.1510821
                                                               [ 1.00000000e+00, -2.50045130e+00, 6.2522566
        -6.40702200e-02, 6.40702200e-02, 1.91158629
                                                               [ 1.00000000e+00, -2.37222302e+00, 5.6274420
         4.33883739e-01, 5.45534901e-01, 6.4822839!
                                                               [ 1.00000000e+00, -2.24399475e+00,
                                                                                                  5.0355124
         0 00170000 01
                          0 00000000 01
                                         0 20460421
                                                                1 000000000000
  1 yt pred = (Xt @ bt).squeeze()
  1 loss = (yt pred - yt).pow(2).sum()
    loss.item()
```

2119.2777040165224

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 refered to as the *learning rate* which we will pick a relatively small value for.

```
learning_rate = le-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
```

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

2069.4881821807053

Putting it together

```
1 yt = torch.tensor(y).unsqueeze(1)
 2 Xt = torch.tensor(lm.model.exog)
 3 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
 8
 9
10
     loss = (yt_pred - yt).pow(2).sum()
     if i % 500 == 0:
11
12
       print(f"Step: {i},\tloss: {loss.item()}")
13
     loss.backward()
14
15
     with torch.no grad():
16
       bt -= learning rate * bt.grad
17
       bt.grad = None
18
```

Putting it together

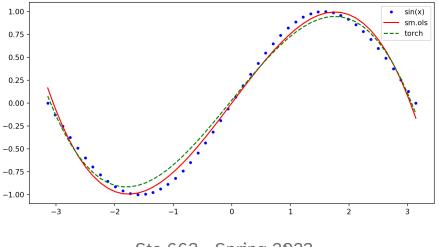
```
Step: 0, loss: 70161.1580804254
Step: 500, loss: 14.791178300540242
Step: 1000, loss: 8.825181658035252
Step: 1500, loss: 5.311942717260375
Step: 2000, loss: 3.2416251317783518
Step: 2500, loss: 2.020671792951764
Step: 3000, loss: 1.3000220383569292
Step: 3500, loss: 0.8742816442183534
Step: 4000, loss: 0.6225166364100523
Step: 4500, loss: 0.473473387453477
 1 print(bt)
tensor([[ 0.03143311],
```

```
[ 0.78484316],

[-0.00520945],

[-0.08260584]], dtype=torch.float64, requires grad=True)
```

Comparing results



Demo 2 - Using a torch model

A sample model

```
class Model(torch.nn.Module):
       def init (self, beta):
           super(). init ()
 3
           beta.requires grad = True
 4
            self.beta = torch.nn.Parameter(beta)
 6
       def forward(self, X):
 7
           return X @ self.beta
 8
 9
   def training_loop(model, X, y, optimizer, n=1000):
10
       losses = []
11
12
       for i in range(n):
           y pred = model(X)
13
14
15
           loss = (y pred.squeeze() - y.squeeze()).pow(2).sum()
           loss.backward()
16
17
           optimizer.step()
18
19
           optimizer.zero_grad()
20
21
           losses.append(loss.item())
22
23
       return losses
```

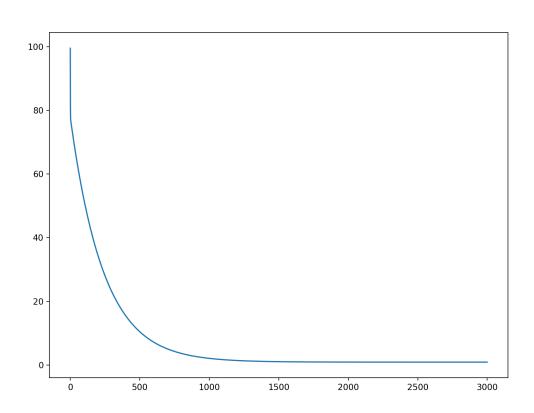
Fitting

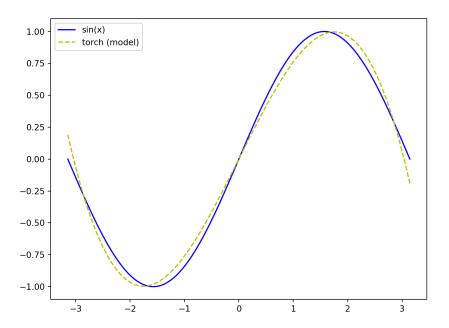
```
1  x = torch.linspace(-math.pi, math.pi, 200)
2  y = torch.sin(x)
3
4  X = torch.vstack((
5    torch.ones_like(x),
6    x,
7    x**2,
8    x**3
9  )).T
10
11  m = Model(beta = torch.zeros(4))
12  opt = torch.optim.SGD(m.parameters(), lr=le-5)
13
14  losses = training_loop(m, X, y, opt, n=3000)
```

Results

```
1 m.beta
```

```
Parameter containing:
tensor([ 2.66870664e-10, 8.52953434e-01, 6.79866718e-11, -9.25917700e-02],
requires_grad=True)
```



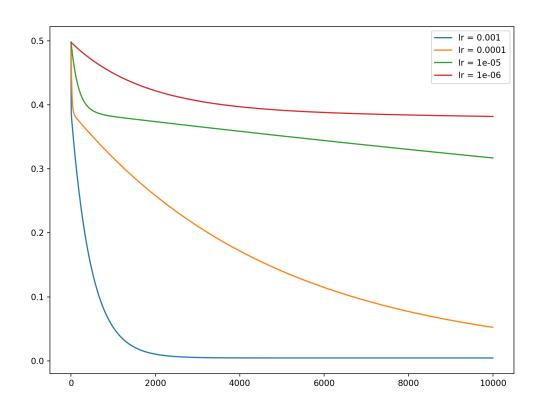


An all-in-one model

```
1 class Model(torch.nn.Module):
       def init (self, X, y, beta=None):
           super(). init ()
 3
           self.x = x
 4
           self.y = y
          if beta is None:
 6
 7
            beta = torch.zeros(X.shape[1])
           beta.requires grad = True
 8
           self.beta = torch.nn.Parameter(beta)
9
10
       def forward(self, X):
11
12
           return X @ self.beta
13
       def fit(self, opt, n=1000, loss_fn = torch.nn.MSELoss()):
14
         losses = []
15
16
         for i in range(n):
             loss = loss fn(self(self.X).squeeze(), self.y.squeeze())
17
             loss.backward()
18
19
             opt.step()
20
             opt.zero_grad()
             losses.append(loss.item())
21
22
23
         return losses
```

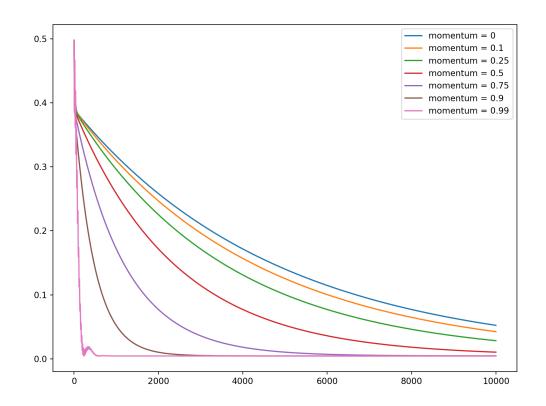
Learning rate and convergence

```
1 plt.figure(figsize=(8,6), layout="constrained")
   for lr in [1e-3, 1e-4, 1e-5, 1e-6]:
     m = Model(X, y)
     opt = torch.optim.SGD(m.parameters(), lr=lr)
     losses = m.fit(opt, n=10000)
 6
     plt.plot(losses, label=f"lr = {lr}")
 8
 9
   plt.legend()
11 plt.show()
```



Momentum and convergence

```
1 plt.figure(figsize=(8,6), layout="constrained")
   for mt in [0, 0.1, 0.25, 0.5, 0.75, 0.9, 0.99]:
     m = Model(X, y)
 4
     opt = torch.optim.SGD(
 6
       m.parameters(),
       lr = 1e-4
 8
       momentum = mt
 9
     losses = m.fit(opt, n=10000)
10
11
12
     plt.plot(losses, label=f"momentum = {mt}")
13
   plt.legend()
15 plt.show()
```



Optimizers and convergence

```
plt.figure(figsize=(8,6), layout="constrained")
 2
   opts = (torch.optim.SGD,
           torch.optim.Adam,
           torch.optim.Adagrad)
   for opt fn in opts:
     m = Model(X, y)
 8
     opt = opt fn(m.parameters(), lr=1e-4)
     losses = m.fit(opt, n=10000)
10
11
12
     plt.plot(losses, label=f"opt = {opt fn}")
13
   plt.legend()
15 plt.show()
```

