torch

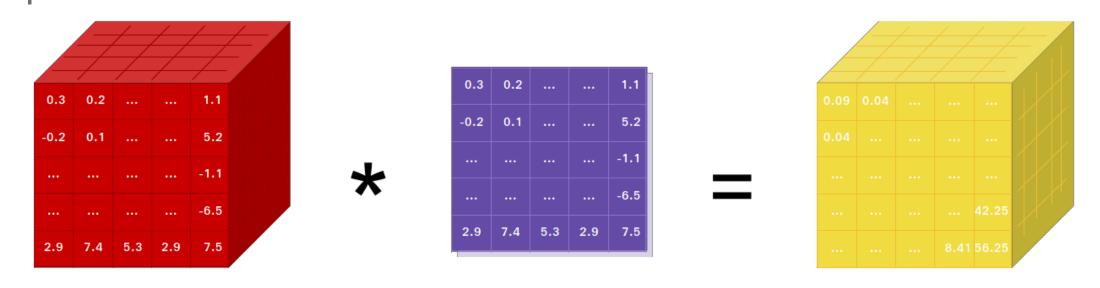
Lecture 17

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;2.6.0'

A graph is created on the fly

```
W_h h W_x x
```

```
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, jax, etc.)

```
1 torch.zeros(3)
                                                torch.manual_seed(1234)
tensor([0., 0., 0.])
                                            <torch. C.Generator object at
                                            0x30217f490>
 1 torch.ones(3,2)
                                              1 torch.rand(2,2,2,2)
tensor([[1., 1.],
        [1., 1.],
                                            tensor([[[[0.0290, 0.4019],
        [1., 1.]])
                                                       [0.2598, 0.3666]],
 1 torch.empty(2,2,2)
                                                      [[0.0583, 0.7006],
                                                       [0.0518, 0.4681]],
tensor([[[0., 0.],
         [0., 0.]],
                                                     [[0.6738, 0.3315],
                                                       [0.7837, 0.5631],
        [[0., 0.],
         [0., 0.]]
                                                      [[0.7749, 0.8208],
                                                       [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)
tensor(1)
                                            at dim 1 (got 2)
 1 torch.tensor((1,2))
tensor([1, 2])
 1 torch.tensor([[1,2,3], [4,5,6]])
tensor([[1, 2, 3],
        [4, 5, 6]])
                                             tensor([[True]])
 1 torch.tensor([(1,2,3), [4,5,6]])
tensor([[1, 2, 3],
        [4, 5, 6]])
```

```
ValueError: expected sequence of length 3
    torch.tensor([["A"]])
ValueError: too many dimensions 'str'
 1 torch.tensor([[True]])
```

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 a = torch.tensor([1,2,3]); a
                                                    1 c = torch.tensor([1.,2.,3.]); c
tensor([1, 2, 3])
                                                  tensor([1., 2., 3.])
 1 a.dtype
                                                    1 c.dtype
                                                  torch.float32
torch.int64
 1 b = torch.tensor([1,2,3], dtype=torch.float1
                                                    1 d = torch.tensor([1,2,3], dtype=torch.float(
tensor([1., 2., 3.], dtype=torch.float16)
                                                  tensor([1., 2., 3.], dtype=torch.float64)
                                                      d.dtype
    b.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)
RuntimeError: value cannot be converted to type
                                                  tensor(0.33325195, dtype=torch.float16)
int8 without overflow
                                                    1 torch.tensor(1/3, dtype=torch.float32)
  1 torch.tensor([128]).to(torch.int8)
                                                  tensor(0.33333334)
tensor([-128], dtype=torch.int8)
                                                    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(1/3, dtype=torch.bfloat16)
    torch.tensor([300]).to(torch.uint8)
                                                  tensor(0.33398438, dtype=torch.bfloat16)
tensor([44], dtype=torch.uint8)
  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)
                                               2 torch.ones(2,2) @ x
tensor([[6., 6.],
        [6., 6.]]
                                             tensor([[1.22126317, 1.36931109],
                                                     [1.22126317, 1.36931109]])
 1 torch.ones(2,2) + torch.tensor([[1,2],
                                               1 torch.clamp(x*2-1, -0.5, 0.5)
tensor([[2., 3.],
        [4., 5.]
                                             tensor([[-0.49049568, 0.25872374],
                                                     [ 0.50000000, 0.47989845]])
 1 2 ** torch.tensor([[1,2], [3,4]])
                                               1 torch.mean(x)
tensor([[ 2, 4],
        [ 8, 16]])
                                             tensor(0.64764357)
 1 2 ** torch.tensor([[1,2], [3,4]]) > 5
                                               1 torch.sum(x)
                                             tensor(2.59057426)
tensor([[False, False],
        [True, True]])
                                               1 torch.min(x)
                                             tensor(0.25475216)
                                     Sta 663 - Spring 2025
```

Broadcasting

Like NumPy, cases where tensor dimensions do not match use the broadcasting heuristic.

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 = torch.rand(2,2)
 2 print(a)
tensor([[0.31861043, 0.29080772],
        [0.41960979, 0.37281448]])
 1 print(torch.exp(a))
                                                print(torch.exp_(a))
tensor([[1.37521553, 1.33750737],
                                            tensor([[1.37521553, 1.33750737],
                                                     [1.52136779, 1.45181489]])
        [1.52136779, 1.45181489]])
 1 print(a)
                                              1 print(a)
tensor([[0.31861043, 0.29080772],
                                            tensor([[1.37521553, 1.33750737],
                                                     [1.52136779, 1.45181489]])
        [0.41960979, 0.37281448]])
```

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+b
                                              1 a.add_(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.

contiguous subspaces). Use

.reshape(...) instead.

```
1 \times = torch.zeros(3, 2)
 2 y = x.view(2, 3)
 1 y
tensor([[0., 0., 0.],
        [0., 0., 0.]
  1 x.fill_(1)
tensor([[1., 1.],
        [1., 1.],
        [1., 1.]])
 1 y
tensor([[1., 1., 1.],
        [1., 1., 1.]])
```

```
1 \times = torch.zeros(3, 2)
                                          z = y \cdot reshape(6)
  2 y = x_{\bullet}t()
                                       2 x.fill (1)
  3 \times \text{view}(6)
                                     tensor([[1., 1.],
tensor([0., 0., 0., 0., 0.,
                                              [1., 1.],
0.])
                                              [1., 1.]])
  1 y_* view(6)
                                       1 y
RuntimeError: view size is not
                                     tensor([[1., 1., 1.],
                                              [1., 1., 1.]])
compatible with input tensor's
size and stride (at least one
                                       1 z
dimension spans across two
```

0.])

tensor([0., 0., 0., 0., 0.,

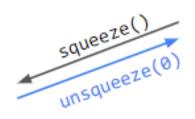
Adding or removing dimensions

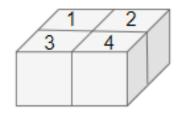
The squeeze() and unsqueeze() methods can be used to remove or add length 1 dimension(s) to a tensor.

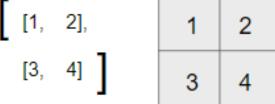
```
1 \times = torch.zeros(1,3,1)
                                               1 \times = torch.zeros(3,2)
 2 x.squeeze().shape
                                               2 x.unsqueeze(0).shape
                                             torch.Size([1, 3, 2])
torch.Size([3])
 1 x.squeeze(0).shape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

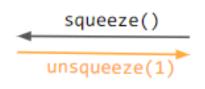
[[1, 2],

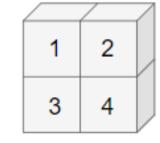


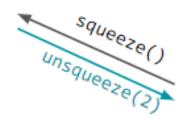


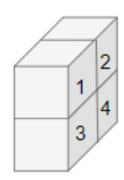


2d tensor









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).

```
1 x = torch.linspace(0, 2, steps=21, requires_grad=True)
 2 x
tensor([0.00000000, 0.10000000, 0.20000000, 0.30000001, 0.40000001, 0.50000000,
        0.60000002, 0.69999999, 0.80000001, 0.90000004, 1.00000000, 1.100000002,
        1.20000005, 1.29999995, 1.39999998, 1.50000000, 1.60000002, 1.70000005,
        1.79999995, 1.89999998, 2.00000000], requires grad=True)
 1 \quad v = 3*x + 2
tensor([2.00000000, 2.29999995, 2.59999990, 2.90000010, 3.20000005, 3.50000000,
        3.80000019, 4.09999990, 4.40000010, 4.69999981, 5.00000000, 5.30000019,
        5.60000038, 5.89999962, 6.19999981, 6.50000000, 6.80000019, 7.10000038,
        7.39999962, 7.69999981, 8.00000000], grad fn=<AddBackward0>)
```

Computational graph

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

```
1 y.grad_fn
<AddBackward0 object at 0x30981f730>
1 y.grad_fn.next_functions
((<MulBackward0 object at 0x11ff295a0>, 0), (None, 0))
1 y.grad_fn.next_functions[0][0].next_functions
((<AccumulateGrad object at 0x30981fa90>, 0), (None, 0))
1 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 *output* tensor (must be a scalar), this then makes the grad attribute available for the input (leaf) tensors.

A bit more complex

```
1 n = 21
 2 x = torch.linspace(0, 2, steps=n, requires_grad=True)
 3 m = torch.rand(n, requires_grad=True)
   v = m*x + 2
 7 y.backward(torch.ones(n))
 1 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])
 1 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, 1.29999995, 1.39999998, 1.50000000, 1.60000002, 1.70000005,
        1.79999995, 1.89999998, 2.00000000])
```

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

Sta 663 - Spring 2025

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):
 2 return 3*x + 1 + 2*y**2 + x*y
 1 for \times 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, inputs),"\n")
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.]]))
```

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

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

1 inputs = (torch.tensor([1.]), torch.tensor([1.]))

2 torch.autograd.functional.hessian(f, inputs)

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

Demo 1 - Linear Regression w/ PyTorch

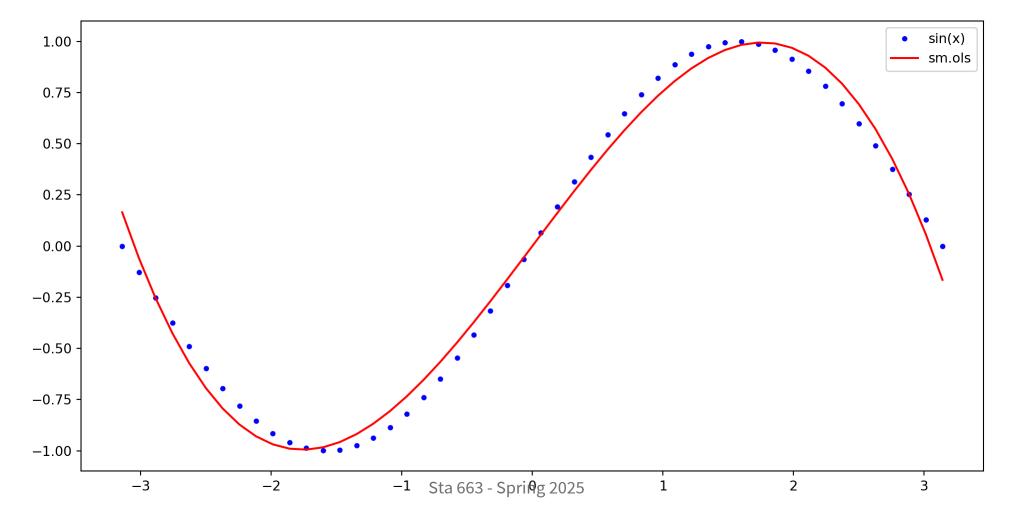
A basic model

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

OLS Regression Results Dep. Variable: Rsquared: 0.990 Model: 0LS Adj. Rsquared: 0.989 Method: Least Squares Fstatistic: 1455. Date: Tue, 18 Mar 2025 Prob (F-statistic): 1.44e-45 Time: 17:20:44 Log-Likelihood: 60.967 No. Observations: 50 AIC: -113.9Df Residuals: BIC: 46 -106.3Df Modol: 2

Predictions

```
1 plt.figure(figsize=(10,5), layout="constrained")
2 plt.plot(x, y, ".b", label="sin(x)")
3 plt.plot(x, lm.predict(), "-r", label="sm.ols")
4 plt.legend()
5 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,
                                            tensor([[ 1.00000000e+00,
-2.53654584e-01, -3.75267005e-01,
                                            -3.14159265e+00, 9.86960440e+00,
        -4.90717552e-01, -5.98110530e-01,
                                            -3.10062767e+01],
-6.95682551e-01, -7.81831482e-01,
                                                    [ 1.00000000e+00.
        -8.55142763e-01, -9.14412623e-01,
                                            -3.01336438e+00, 9.08036490e+00,
-9.58667853e-01, -9.87181783e-01,
                                            -2.73624482e+01],
        -9.99486216e-01, -9.95379113e-01,
                                                    [ 1.00000000e+00.
                                            -2.88513611e+00, 8.32401038e+00,
-9.74927912e-01, -9.38468422e-01,
        -8.86599306e-01, -8.20172255e-01,
                                            -2.40159029e+01].
-7.40277997e-01, -6.48228395e-01,
                                                    [ 1.00000000e+00,
        -5.45534901e-01, -4.33883739e-01,
                                            -2.75690784e+00, 7.60054083e+00,
-3.15108218e-01, -1.91158629e-01,
                                            -2.09539906e+01].
        -6.40702200e-02, 6.40702200e-02,
                                                    [ 1.00000000e+00,
1.91158629e-01, 3.15108218e-01,
                                            -2.62867957e+00, 6.90995627e+00,
         4.33883739e-01, 5.45534901e-01,
                                           -1.81640609e+01],
 40220205 - 01 7 40277007 - 01
                                                       \alpha
```

```
1 yt_pred = (Xt @ bt).squeeze()
```

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

2119.277704016523

Gradient descent

```
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
```

```
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)
   bt = torch.randn((Xt.shape[1], 1), dtype=torch.float64, requires_grad=True)
 4
   learning_rate = 1e-5
   for i in range(5000):
     yt_pred = Xt @ bt
 8
 9
     loss = (yt_pred - yt)_pow(2)_sum()
10
     if i % 500 == 0:
11
       print(f"Step: {i},\tloss: {loss.item()}")
12
13
     loss.backward()
14
15
16
     with torch.no grad():
17
       bt -= learning_rate * bt.grad
       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: 5.311942717260374
Step: 2000, loss: 3.2416251317783518
Step: 2500, loss: 2.020671792951764
Step: 3000, loss: 1.300022038356929
Step: 3500, loss: 0.8742816442183533
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

```
      1 lm.params
      1 bt

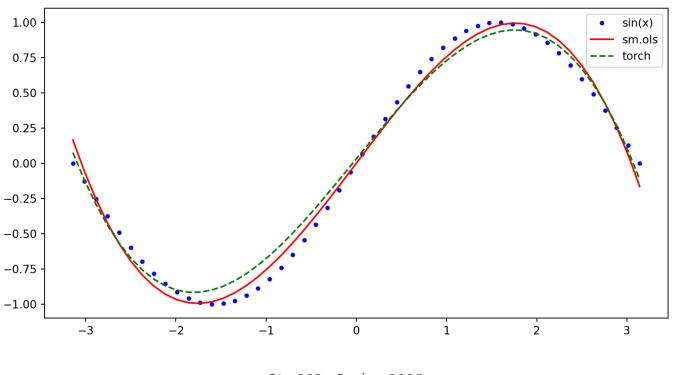
      Intercept -7.958044e-17
      tensor([[ 0.03143311],

      x
      8.476289e-01
      [ 0.78484316],

      I(x ** 2)
      3.691708e-17
      [-0.00520945],

      I(x ** 3)
      -9.120167e-02
      [-0.08260584]],

      dtype: float64
      dtype=torch.float64, requires_grad=True)
```



Demo 2 - Using a torch model

A sample model

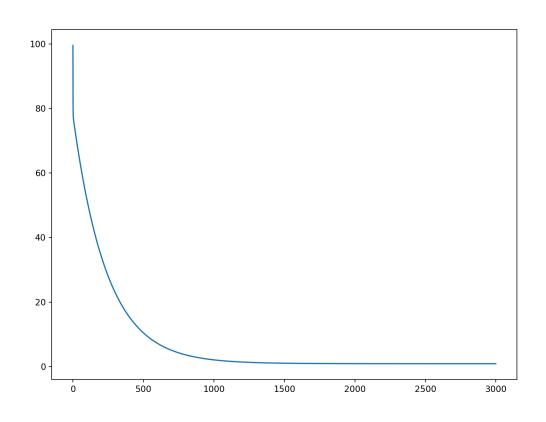
```
class Model(torch.nn.Module):
       def __init__(self, beta):
            super().__init__()
            beta.requires_grad = True
 4
            self.beta = torch.nn.Parameter(beta)
 6
       def forward(self, X):
            return X @ self.beta
 9
10
   def training_loop(model, X, y, optimizer,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

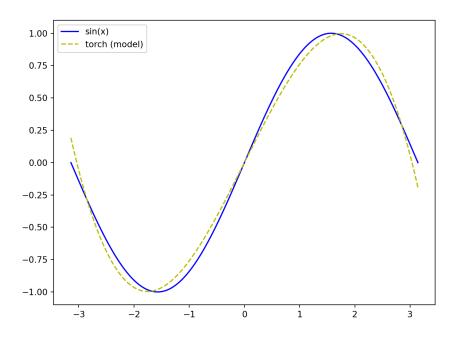
Fitting

Results

```
1 m.beta
```

Parameter containing: tensor([-4.07514189e-10, 8.52953434e-01, 1.22972355e-10, -9.25917700e-02], requires_grad=True)



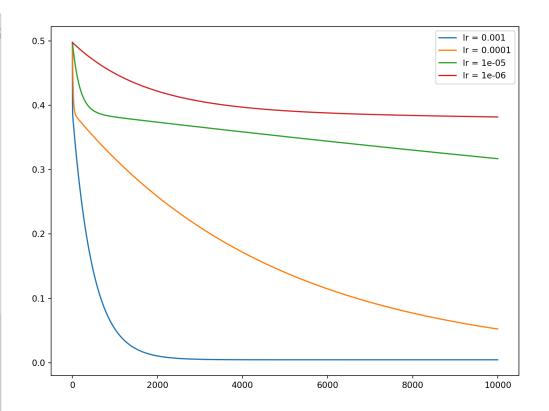


An all-in-one model

```
class Model(torch.nn.Module):
       def __init__(self, X, y, beta=None):
 2
            super().__init__()
 3
           self.X = X
 4
           self_y = y
           if beta is None:
 6
              beta = torch.zeros(X.shape[1])
           beta.requires_grad = True
            self.beta = torch.nn.Parameter(beta)
 9
10
11
       def forward(self, X):
12
            return X @ self.beta
13
14
       def fit(self, opt, n=1000, loss_fn = torch.nn.MSELoss()):
15
         losses = []
16
         for i in range(n):
17
              loss = loss_fn(self(self.X).squeeze(), self.y.squeeze())
              loss.backward()
18
19
              opt.step()
20
              opt.zero_grad()
              losses.append(loss.item())
21
```

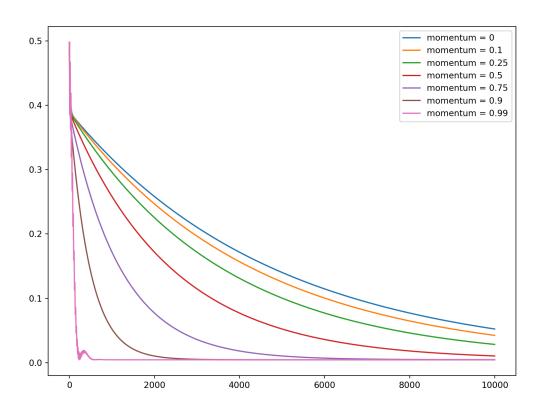
Learning rate and convergence

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



Momentum and convergence

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



Optimizers and convergence

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

