torch

Lecture 17

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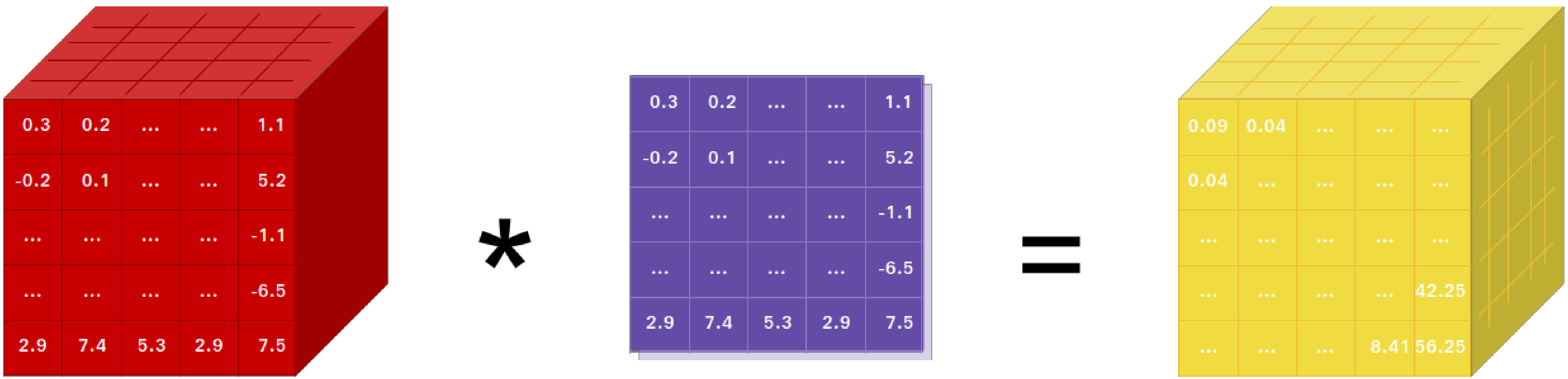
PyTorch

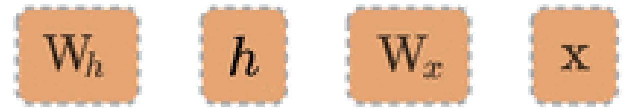
> PyTorch is a Python package that provides two high-level features:
>
> - Tensor computation (like NumPy) with strong GPU acceleration
> - Deep neural networks built on a tape-based autograd system




```python
import torch
torch.__version__
```

```
'2.6.0'
```

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`, `jax`, 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., 0.],
         [0., 0.]],

        [[0., 0.],
         [0., 0.]]])
```

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

```
<torch._C.Generator object at
0x3015a3410>
```

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

```
tensor([[[[0.02898, 0.40190],
          [0.25984, 0.36664]],

         [[0.05830, 0.70064],
          [0.05180, 0.46814]]],


        [[[0.67381, 0.33146],
          [0.78371, 0.56306]],

         [[0.77485, 0.82080],
          [0.27928, 0.68171]]]])
```

Constants

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

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

```
tensor(1)
```

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

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

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

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

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

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

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

```
ValueError: expected sequence of length 3 at dim 1 (got 2)
```

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

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

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

```
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.

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

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

```
a.dtype
```

```
torch.int64
```

```
b = torch.tensor([1,2,3], dtype=torch.float1
```

```
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.float6
```

```
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([128], dtype=torch.int8)
```

```
RuntimeError: value cannot be converted to type
int8 without overflow
```

```
torch.tensor([128]).to(torch.int8)
```

```
tensor([-128], dtype=torch.int8)
```

```
torch.tensor([255]).to(torch.uint8)
```

```
tensor([255], dtype=torch.uint8)
```

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

```
tensor([44], dtype=torch.uint8)
```

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

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

```
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)
```

```
torch.tensor(1/3, dtype=torch.bfloat16)
```

```
tensor(0.33398438, dtype=torch.bfloat16)
```

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()
```

```
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.

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

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

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

```
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],
        [ True,  True]])
```

```
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)
```

```
tensor(2.59057426)
```

```
torch.min(x)
```

```
tensor(0.25475216)
```

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:

```
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.

```
countdown::countdown(5)
```

05:00

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.

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

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

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

```
tensor([[1.37521553, 1.33750737],
        [1.52136779, 1.45181489]])
```

```python
print(a)
```

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

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

```
tensor([[1.37521553, 1.33750737],
        [1.52136779, 1.45181489]])
```

```python
print(a)
```

```
tensor([[1.37521553, 1.33750737],
        [1.52136779, 1.45181489]])
```

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()
```

```
x.view(6)
```

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

```
y.view(6)
```

```
RuntimeError: view size is not
compatible with input tensor's
size and stride (at least one
dimension spans across two
   contiguous subspaces). Use
.reshape(...) instead.
```

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

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

```
y
```

```
tensor([[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.

```python
x = torch.zeros(1,3,1)
```

```python
x.squeeze().shape
```

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

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

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

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

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

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

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

```python
x = torch.zeros(3,2)
```

```python
x.unsqueeze(0).shape
```

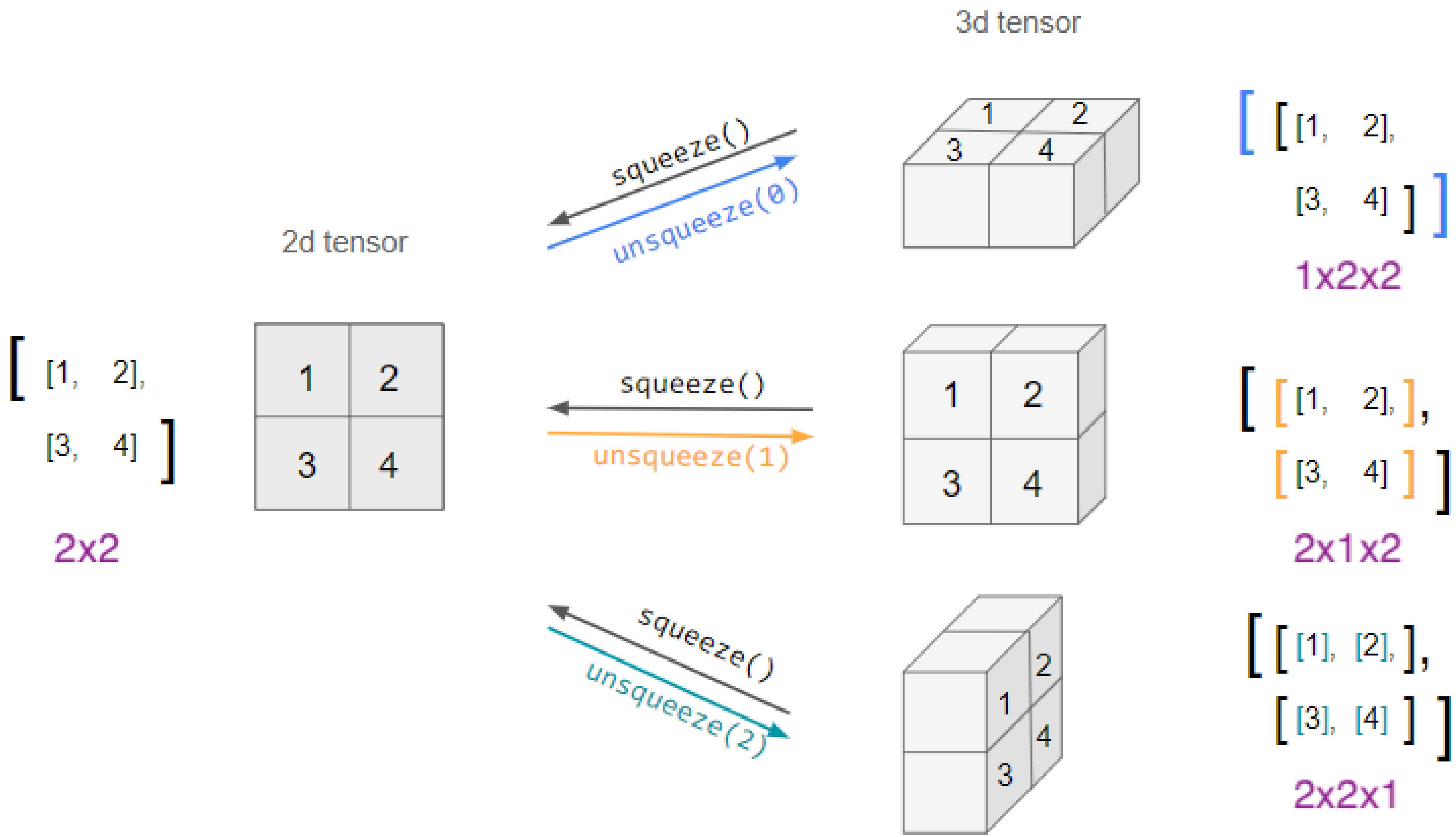
```
torch.Size([1, 3, 2])
```

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

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

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

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


3d tensor
2d tensor
squeeze()
unsqueeze(0)
squeeze()
unsqueeze(1)
squeeze()
unsqueeze(2)
[[1, 2],
[3, 4]]
2x2
1x2x2
2x1x2
2x2x1
[[[1, 2],
[3, 4]]]
[[[1, 2]],
[[3, 4]]]
[[[1], [2]],
[[3], [4]]]

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?

```
countdown::countdown(3)
```

03:00

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`).

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

```
tensor([0.00000000, 0.10000000, 0.20000000, 0.30000001, 0.40000001, 0.50000000,
0.60000002, 0.69999999, 0.80000001,
   0.90000004, 1.00000000, 1.10000002, 1.20000005, 1.29999995, 1.39999998,
1.50000000,
        1.60000002, 1.70000005, 1.79999995, 1.89999998, 2.00000000],
requires_grad=True)
```

```
y = 3*x + 2
y
```

```
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

```
y.grad_fn
```

```
<AddBackward0 object at 0x30c815390>
```

```
y.grad_fn.next_functions
```

```
((<MulBackward0 object at 0x30bb8e740>, 0), (None, 0))
```

```
y.grad_fn.next_functions[0][0].next_functions
```

```
((<AccumulateGrad object at 0x30c817f10>, 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 *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
```

```
x.grad
```

```
tensor([3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3., 3.,
3., 3.])
```

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, 1.29999995, 1.39999998,
1.50000000,
        1.60000002, 1.70000005, 1.79999995, 1.89999998, 2.00000000])
```

High-level autograd API

allows for the automatic calculation and evaluation of the jacobian and hessian for a function defined using 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, 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.]]))
```

```
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

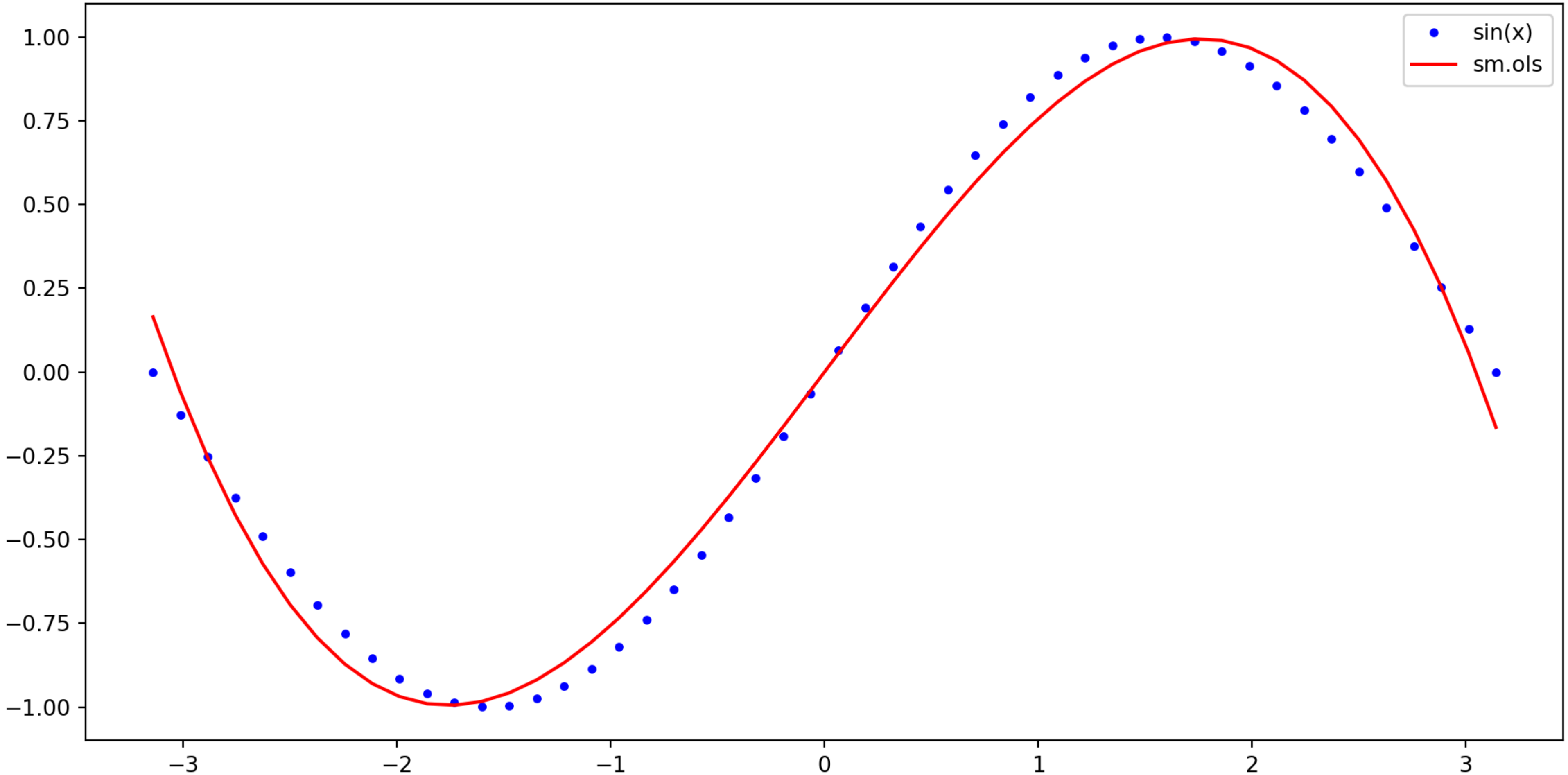
A basic model

```python
x = np.linspace(-math.pi, math.pi, 50)
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:                       0.990
Model:                            OLS   Adj. R-squared:                  0.989
Method:                 Least Squares   F-statistic:                     1455.
Date:                Wed, 19 Mar 2025   Prob (F-statistic):           1.44e-45
Time:                        09:33:38   Log-Likelihood:                 60.967
No. Observations:                  50   AIC:                            -113.9
Df Residuals:                      46   BIC:                            -106.3
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept  -7.958e-17      0.016  -5.03e-15      1.000      -0.032       0.032
x              0.8476      0.014     59.444      0.000       0.819       0.876
I(x ** 2)   3.692e-17      0.003   1.07e-14      1.000      -0.007       0.007
I(x ** 3)     -0.0912      0.002    -42.977      0.000      -0.095      -0.087
==============================================================================
```

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

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

```
yt.shape
```

```
torch.Size([50])
```

```
Xt.shape
```

```
torch.Size([50, 4])
```

```
bt.shape
```

```
torch.Size([4, 1])
```

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

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

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

```
2069.4881821807053
```

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(5001):

  yt_pred = Xt @ bt

  loss = (yt_pred - yt).pow(2).sum()
  if i % 500 == 0:
    print(f"Step: {i},\tloss: {loss.item()}")

  loss.backward()

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

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
Step: 5000, loss: 0.38513809895450724
```

```
print(bt)
```

```
tensor([[ 0.03141952],
        [ 0.78487683],
        [-0.00520719],
        [-0.08261045]], dtype=torch.float64,
requires_grad=True)
```

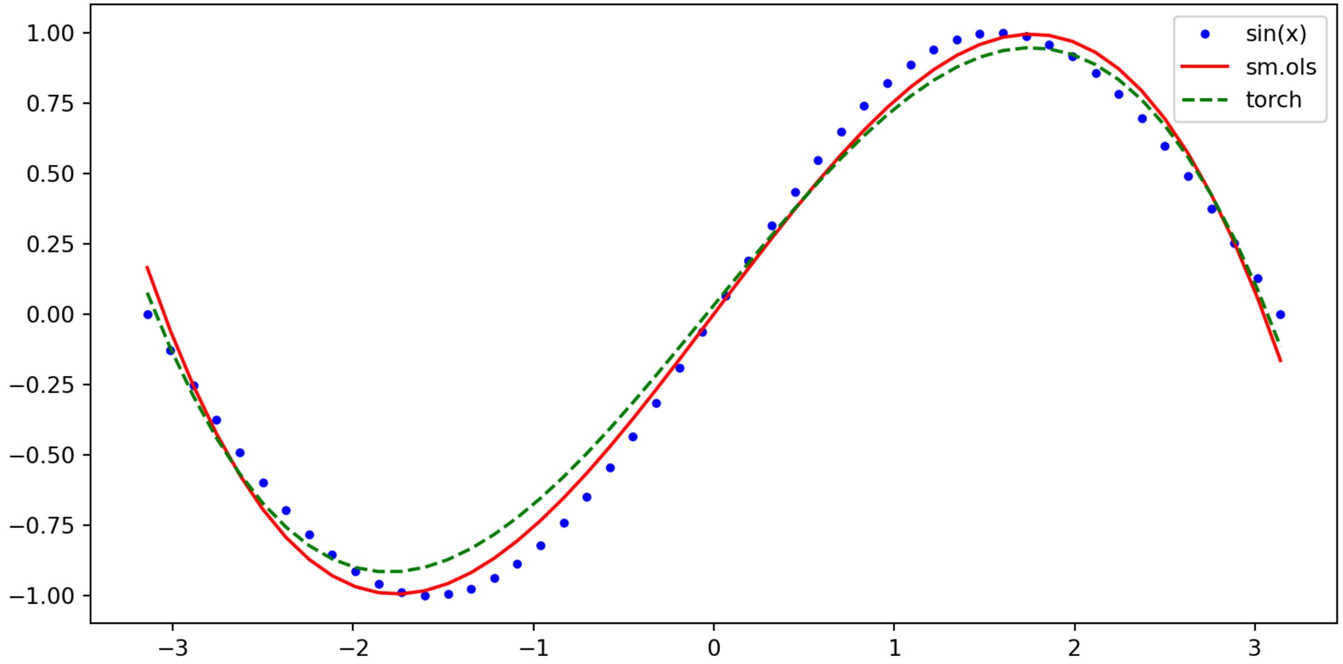
Comparing results

```
lm.params
```

```
Intercept   -7.958044e-17
x            8.476289e-01
I(x ** 2)    3.691708e-17
I(x ** 3)   -9.120167e-02
dtype: float64
```

```
bt
```

```
tensor([[ 0.03141952],
        [ 0.78487683],
        [-0.00520719],
        [-0.08261045]],
dtype=torch.float64, requires_grad=True)
```



Demo 2 - Using a torch model

A simple 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
```

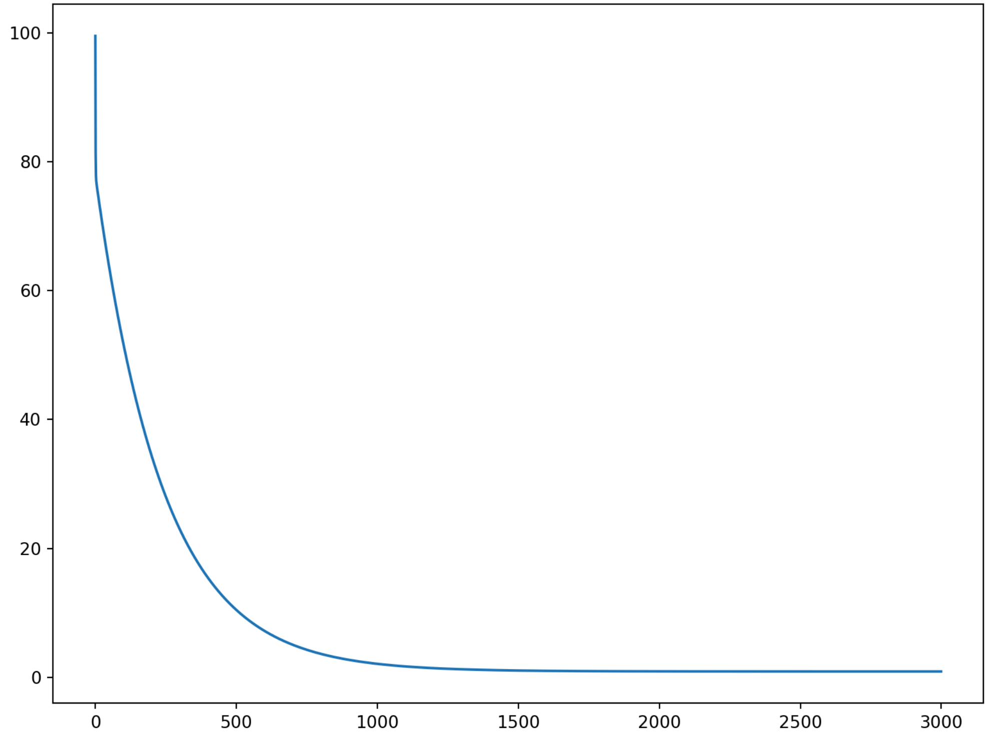
Fitting

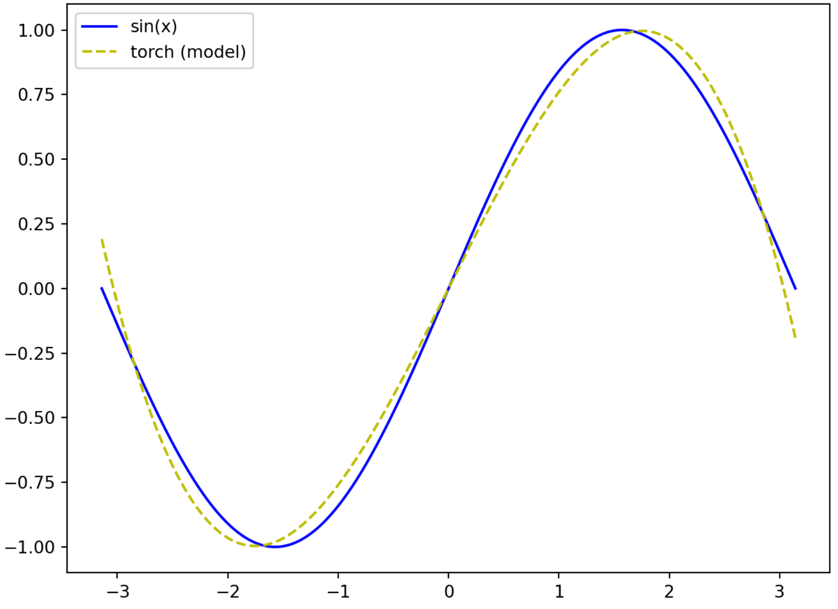
```python
x = torch.linspace(-math.pi, math.pi, 200)
y = torch.sin(x)

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

```
1  m.beta
```

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



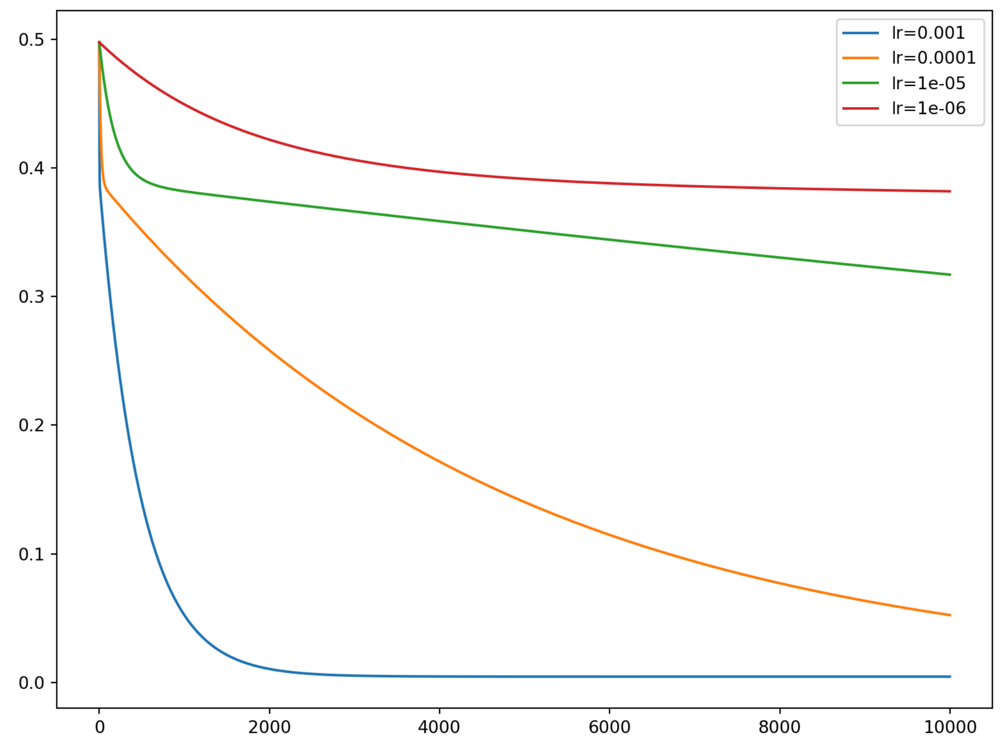


An all-in-one model

```python
class Model(torch.nn.Module):
    def __init__(self, X, y, beta=None):
        super().__init__()
        self.X = X
        self.y = y
        if beta is None:
          beta = torch.zeros(X.shape[1])
        beta.requires_grad = True
        self.beta = torch.nn.Parameter(beta)

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

    def fit(self, opt, n=1000, loss_fn = torch.nn.MSELoss()):
      losses = []
      for i in range(n):
          loss = loss_fn(self.forward(self.X).squeeze(), self.y.squeeze())
          loss.backward()
          opt.step()
          opt.zero_grad()
          losses.append(loss.item())
```

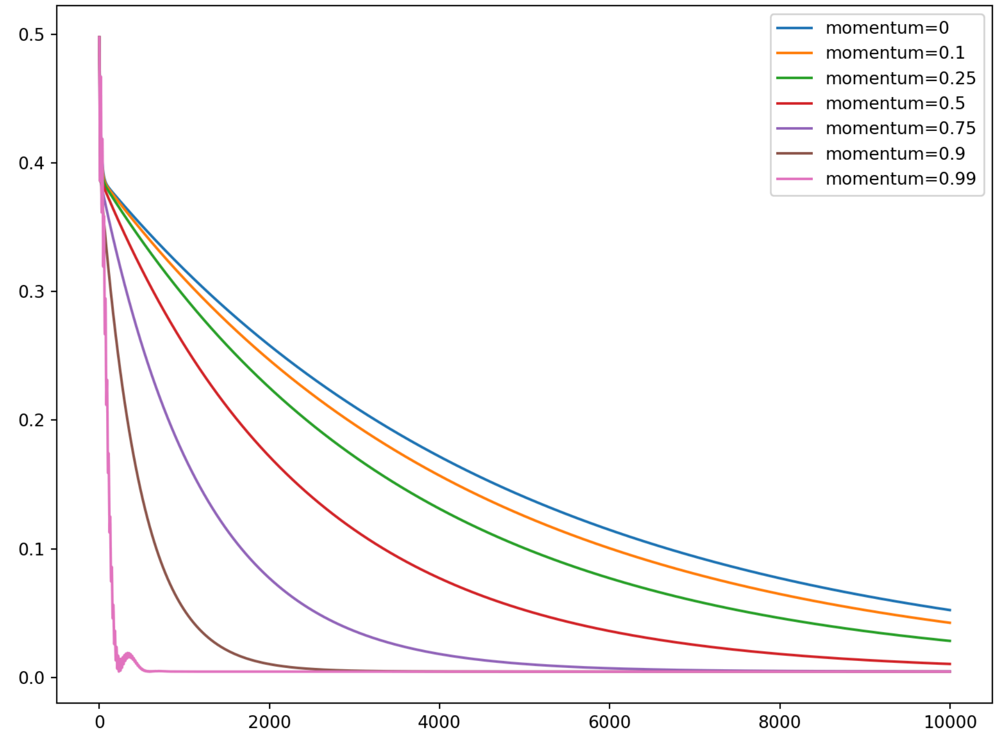
Learning rate and convergence

```
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=}")
  
plt.legend()
plt.show()
```



Momentum and convergence

```python
plt.figure(figsize=(8,6), layout="constraine

for momentum 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 = momentum
  )
  losses = m.fit(opt, n=10000)

  plt.plot(losses, label=f"{momentum=}")

plt.legend()
plt.show()
```



Optimizers and convergence

```python
plt.figure(figsize=(8,6), layout="constraine

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)

  plt.plot(losses, label=f"{opt_fn=}")

plt.legend()
plt.show()
```