Understanding PyTorch with an example: a step-by-step tutorial

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Introduction

PyTorch is the **fastest growing** Deep Learning framework and it is also used by **Fast.ai** in its MOOC, Deep Learning for Coders and its library.

PyTorch is also very *pythonic*, meaning, it feels more natural to use it if you already are a Python developer.

Besides, using PyTorch may even *improve your health*, according to Andrej Karpathy :-)

Motivation

There are *many many* PyTorch tutorials around and its documentation is quite complete and extensive. So, **why** should you keep reading this step-by-step tutorial?

Well, even though one can find information on pretty much *anything* PyTorch can do, I missed having a **structured**, **incremental** and **from first principles** approach to it.

In this post, I will guide you through the *main reasons* why PyTorch makes it much **easier** and more **intuitive** to build a Deep Learning model in Python—**autograd**, **dynamic computation graph**, **model classes** and more—and I will also show you **how to avoid** some **common pitfalls** and **errors** along the way.

Moreover, since this is quite a **long** post, I built a *Table of Contents* to make navigation easier, should you use it as a **mini-course** and work your way through the content one topic at a time.

Table of Contents

A Simple Regression Problem

Most tutorials start with some nice and pretty *image classification problem* to illustrate how to use PyTorch. It may seem cool, but I believe it **distracts** you from the **main goal**: **how PyTorch works**?

For this reason, in this tutorial, I will stick with a **simple** and **familiar** problem: a **linear regression with a single feature *x***! It doesn't get much simpler than that...

$$y = a + bx + \epsilon$$

Simple Linear Regression model

Data Generation

Let's start **generating** some synthetic data: we start with a vector of 100 points for our **feature *x*** and create our **labels** using ***a* = *1***, ***b* = *2*** and some Gaussian noise.

Next, let's **split** our synthetic data into **train** and **validation** sets, shuffling the array of indices and using the first 80 shuffled points for training.

```python
# Data Generation
np.random.seed(42)
x = np.random.rand(100, 1)
y = 1 + 2 * x + .1 * np.random.randn(100, 1)

# Shuffles the indices
idx = np.arange(100)
np.random.shuffle(idx)

# Uses first 80 random indices for train
train_idx = idx[:80]
# Uses the remaining indices for validation
```

Generating synthetic train and validation sets for a linear regression

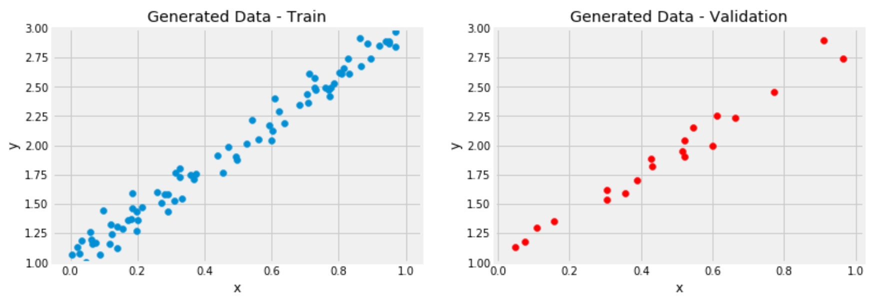


Figure 1: Synthetic data — Train and Validation sets

We **know** that a = 1 and b = 2, but now let's see how close we can get to the true values by using **gradient descent** and the 80 points in the **training set**…

Gradient Descent

If you are comfortable with the inner workings of gradient descent, *feel free to skip* this section. It goes beyond the scope of this post to fully explain how gradient descent works, but I'll cover the **four basic steps** you'd need to go through to compute it.

Step 1: Compute the Loss

For a regression problem, the **loss** is given by the **Mean Square Error (MSE)**, that is, the average of all squared differences between **labels** (y) and **predictions** (a + bx).

> *It is worth mentioning that, if we use **all points** in the training set (N) to compute the loss, we are performing a **batch** gradient descent. If we were to use a **single point** at each time, it would be a **stochastic** gradient descent. Anything else (n) **in-between 1 and N** characterizes a **mini-batch** gradient descent.*

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - a - bx_i)^2$$

Loss: Mean Squared Error (MSE)

Step 2: Compute the Gradients

A **gradient** is a **partial derivative**—*why partial*? Because one computes it with respect to (w.r.t.) a **single parameter**. We have two parameters, ***a*** and ***b***, so we must compute two partial derivatives.

A **derivative** tells you *how much* **a given quantity changes** when you *slightly vary* some **other quantity**. In our case, how much does our ***MSE*** **loss** change when we vary **each one of our two parameters**?

The *right-most* part of the equations below is what you usually see in implementations of gradient descent for a simple linear regression. In the **intermediate step**, I show you **all elements** that pop-up from the application of the chain rule, so you know how the final expression came to be.

$$\frac{\partial MSE}{\partial a} = \frac{\partial MSE}{\partial \hat{y}_i}\cdot\frac{\partial \hat{y}_i}{\partial a} = \frac{1}{N}\sum_{i=1}^{N}2(y_i - a - bx_i)\cdot(-1) = -2\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)$$

$$\frac{\partial MSE}{\partial b} = \frac{\partial MSE}{\partial \hat{y}_i}\cdot\frac{\partial \hat{y}_i}{\partial b} = \frac{1}{N}\sum_{i=1}^{N}2(y_i - a - bx_i)\cdot(-x_i) = -2\frac{1}{N}\sum_{i=1}^{N}x_i(y_i - \hat{y}_i)$$

Computing gradients w.r.t coefficients a and b

Step 3: Update the Parameters

In the final step, we **use the gradients to update** the parameters. Since we are trying to **minimize** our **losses**, we **reverse the sign** of the gradient for the update.

There is still another parameter to consider: the **learning rate**, denoted by the *Greek letter* ***eta*** (that looks like the letter ***n***), which is the **multiplicative factor** that we need to apply to the gradient for the parameter update.

$$a = a - \eta \frac{\partial MSE}{\partial a}$$
$$b = b - \eta \frac{\partial MSE}{\partial b}$$

Updating coefficients a and b using computed gradients and a learning rate

How to **choose** a learning rate? That is a topic on its own and beyond the scope of this post as well.

Step 4: Rinse and Repeat!

Now we use the **updated parameters** to go back to **Step 1** and restart the process.

> ***An epoch is complete whenever every point has been already used for computing the loss***. *For* ***batch*** *gradient descent, this is trivial, as it uses all points for computing the loss—* ***one epoch*** *is the same as* ***one update***. *For* ***stochastic*** *gradient descent,* ***one epoch*** *means* ***N updates***, *while for* ***mini-batch*** *(of size n),* ***one epoch*** *has* ***N/n updates***.

Repeating this process over and over, for **many epochs**, is, in a nutshell, **training** a model.

Linear Regression in Numpy

It's time to implement our linear regression model using gradient descent using **Numpy only**.

> *Wait a minute… I thought this tutorial was about PyTorch!*

Yes, it is, but this serves **two purposes**: *first*, to introduce the **structure** of our task, which will remain largely the same and, *second*, to show you the main **pain points** so you can fully appreciate how much PyTorch makes your life easier :-)

For training a model, there are **two initialization steps**:

- Random initialization of parameters/weights (we have only two, *a* and *b*)—lines 3 and 4;
- Initialization of hyper-parameters (in our case, only *learning rate* and *number of epochs*)—lines 9 and 11;

Make sure to *always initialize your random seed* to ensure **reproducibility** of your results. As usual, the random seed is 42, the *least random* of all random seeds one could possibly choose :-)

For each epoch, there are **four training steps**:

- Compute model's predictions—this is the **forward pass**—line 15;
- Compute the loss, using *predictions* and and *labels* and the appropriate **loss function** for the task at hand—lines 18 and 20;
- Compute the **gradients** for every parameter—lines 23 and 24;
- **Update** the parameters—lines 27 and 28;

Just keep in mind that, if you *don't* use batch gradient descent (our example does),you'll have to write an **inner loop** to perform the **four training steps** for either each **individual point** (**stochastic**) or ***n* points** (**mini-batch**). We'll see a mini-batch example later down the line.

```python
# Initializes parameters "a" and "b" randomly
np.random.seed(42)
a = np.random.randn(1)
b = np.random.randn(1)

print(a, b)

# Sets learning rate
lr = 1e-1
# Defines number of epochs
n_epochs = 1000

for epoch in range(n_epochs):
    # Computes our model's predicted output
    yhat = a + b * x_train

    # How wrong is our model? That's the error!
    error = (y_train - yhat)
    # It is a regression, so it computes mean squared
    loss = (error ** 2).mean()

    # Computes gradients for both "a" and "b" paramete
    a_grad = -2 * error.mean()
    b_grad = -2 * (x_train * error).mean()
```

Implementing gradient descent for linear regression using Numpy

Just to make sure we haven't done any mistakes in our code, we can use *Scikit-Learn's Linear Regression* to fit the model and compare the coefficients.

```
# a and b after initialization
[0.49671415] [-0.1382643]
# a and b after our gradient descent
[1.02354094] [1.96896411]
# intercept and coef from Scikit-Learn
[1.02354075] [1.96896447]
```

They **match** up to 6 decimal places—we have a *fully working implementation of linear regression* using Numpy.

Time to **TORCH** it :-)

PyTorch

First, we need to cover a **few basic concepts** that may throw you off-balance if you don't grasp them well enough before going full-force on modeling.

In Deep Learning, we see **tensors** everywhere. Well, Google's framework is called *TensorFlow* for a reason! *What is a tensor, anyway?*

Tensor

In *Numpy*, you may have an **array** that has **three dimensions**, right? That is, technically speaking, a **tensor**.

A **scalar** (a single number) has **zero** dimensions, a **vector has one** dimension, a **matrix has two** dimensions and a **tensor has three or more** dimensions. That's it!

But, to keep things simple, it is commonplace to call vectors and matrices tensors as well—so, from now on, **everything is either a scalar or a tensor**.

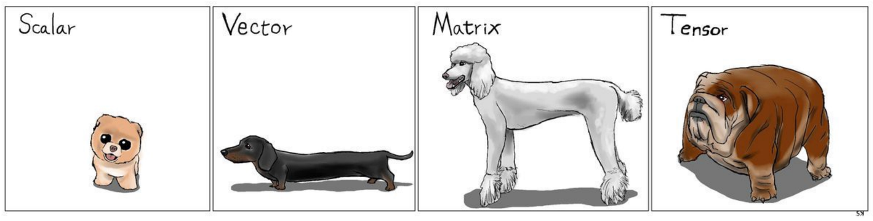


Figure 2: Tensors are just higher-dimensional matrices :-) Source

Loading Data, Devices and CUDA

"*How do we go from Numpy's arrays to PyTorch's tensors*", you ask? That's what `from_numpy` is good for. It returns a **CPU tensor**, though.

"*But I want to use my fancy GPU...*", you say. No worries, that's what `to()` is good for. It sends your tensor to whatever **device** you specify, including your **GPU** (referred to as `cuda` or `cuda:0`).

"*What if I want my code to fallback to CPU if no GPU is available?*", you may be wondering... PyTorch got your back once more—you can use `cuda.is_available()` to find out if you have a GPU at your disposal and set your device accordingly.

You can also easily **cast** it to a lower precision (32-bit float) using `float()`.

```
import torch
import torch.optim as optim
import torch.nn as nn
from torchviz import make_dot

device = 'cuda' if torch.cuda.is_available() else 'cpu

# Our data was in Numpy arrays, but we need to transfo
# and then we send them to the chosen device
x_train_tensor = torch.from_numpy(x_train).float().to(
y_train_tensor = torch.from_numpy(y_train).float().to(
```

Loading data: turning Numpy arrays into PyTorch tensors

If you compare the **types** of both variables, you'll get what you'd expect: `numpy.ndarray` for the first one and `torch.Tensor` for the second one.

But where does your nice tensor "live"? In your CPU or your GPU? You can't say... but if you use PyTorch's `type()`, it will reveal its **location**— `torch.cuda.FloatTensor` —a GPU tensor in this case.

We can also go the other way around, turning tensors back into Numpy arrays, using `numpy()`. It should be easy as `x_train_tensor.numpy()` **but**...

```
TypeError: can't convert CUDA tensor to numpy. Use
Tensor.cpu() to copy the tensor to host memory first.
```

Unfortunately, Numpy **cannot** handle GPU tensors... you need to make them CPU tensors first using `cpu()`.

Creating Parameters

What distinguishes a *tensor* used for *data*—like the ones we've just created—from a **tensor** used as a (*trainable*) **parameter/weight**?

The latter tensors require the **computation of its gradients**, so we can **update** their values (the parameters' values, that is). That's what the `requires_grad=True` argument is good for. It tells PyTorch we want it to compute gradients for us.

You may be tempted to create a simple tensor for a parameter and, later on, send it to your chosen device, as we did with our data, right? Not so fast...

```
# FIRST
# Initializes parameters "a" and "b" randomly, ALMOST
# since we want to apply gradient descent on these par
# to set REQUIRES_GRAD = TRUE
a = torch.randn(1, requires_grad=True, dtype=torch.flo
b = torch.randn(1, requires_grad=True, dtype=torch.flo
print(a, b)

# SECOND
# But what if we want to run it on a GPU? We could jus
a = torch.randn(1, requires_grad=True, dtype=torch.flo
b = torch.randn(1, requires_grad=True, dtype=torch.flo
print(a, b)
# Sorry, but NO! The to(device) "shadows" the gradient

# THIRD
```

Trying to create variables for the coefficients...

The first chunk of code creates two nice tensors for our parameters, gradients and all. But they are **CPU** tensors.

```
# FIRST
tensor([-0.5531], requires_grad=True)
tensor([-0.7314], requires_grad=True)
```

In the second chunk of code, we tried the **naive** approach of sending them to our GPU. We succeeded in sending them to another device, but we ”**lost**” the **gradients** somehow…

```
# SECOND
tensor([0.5158], device='cuda:0', grad_fn=
<CopyBackwards>) tensor([0.0246], device='cuda:0',
grad_fn=<CopyBackwards>)
```

In the third chunk, we **first** send our tensors to the **device** and **then** use **`requires_grad_()`** method to set its `requires_grad` to `True` in place.

```
# THIRD
tensor([-0.8915], device='cuda:0', requires_grad=True)
tensor([0.3616], device='cuda:0', requires_grad=True)
```

> *In PyTorch, every method that **ends** with an **underscore** (_) makes changes **in-place**, meaning, they will **modify** the underlying variable.*

Although the last approach worked fine, it is much better to **assign** tensors to a **device** at the moment of their **creation**.

```
# We can specify the device at the moment of creation -
torch.manual_seed(42)
a = torch.randn(1, requires_grad=True, dtype=torch.floa
b = torch.randn(1, requires_grad=True, dtype=torch.floa
```

Actually creating variables for the coefficients :-)

```
tensor([0.6226], device='cuda:0', requires_grad=True)
tensor([1.4505], device='cuda:0', requires_grad=True)
```

Much easier, right?

Now that we know how to create tensors that require gradients, let's see how PyTorch handles them—that's the role of the…

Autograd

Autograd is PyTorch's *automatic differentiation package*. Thanks to it, we **don't need to worry** about *partial derivatives, chain rule* or anything like it.

So, how do we tell PyTorch to do its thing and **compute all gradients**? That's what **`backward()`** is good for.

Do you remember the **starting point** for **computing the gradients**? It was the **loss**, as we computed its partial derivatives w.r.t. our parameters. Hence, we need to invoke the `backward()` method from the corresponding Python variable, like, `loss.backward().`

What about the **actual values** of the **gradients**? We can inspect them by looking at the **`grad`** **attribute** of a tensor.

If you check the method's documentation, it clearly states that **gradients are accumulated**. So, every time we use the **gradients** to **update** the parameters, we need to **zero the gradients afterwards**. And that's what **`zero_()`** is good for.

What does the **underscore** (_) at the **end of the method name** mean? Do you remember? If not, scroll back to the previous section and find out.

So, let's **ditch** the **manual computation of gradients** and use both `backward()` and `zero_()` methods instead.

That's it? Well, pretty much… but, there is always a **catch**, and this time it has to do with the **update** of the **parameters**…

```
lr = 1e-1
n_epochs = 1000

torch.manual_seed(42)
a = torch.randn(1, requires_grad=True, dtype=torch.flo
b = torch.randn(1, requires_grad=True, dtype=torch.flo

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor
    error = y_train_tensor - yhat
    loss = (error ** 2).mean()

    # No more manual computation of gradients!
    # a_grad = -2 * error.mean()
    # b_grad = -2 * (x_tensor * error).mean()

    # We just tell PyTorch to work its way BACKWARDS f
    loss.backward()
    # Let's check the computed gradients...
    print(a.grad)
    print(b.grad)

    # What about UPDATING the parameters? Not so fast.

    # FIRST ATTEMPT
    # AttributeError: 'NoneType' object has no attribu
    # a = a - lr * a.grad
    # b = b - lr * b.grad
    # print(a)

    # SECOND ATTEMPT
```

In the first attempt, if we use the same update structure as in our *Numpy* code, we'll get the weird **error** below... but we can get a *hint* of what's going on by looking at the tensor itself—once again we **"lost"** the **gradient** while reassigning the update results to our parameters. Thus, the `grad` attribute turns out to be `None` and it raises the error...

```
# FIRST ATTEMPT
tensor([0.7518], device='cuda:0', grad_fn=
<SubBackward0>)
AttributeError: 'NoneType' object has no attribute
'zero_'
```

We then change it slightly, using a familiar **in-place Python assignment** in our second attempt. And, once again, PyTorch complains about it and raises an **error**.

```
# SECOND ATTEMPT
RuntimeError: a leaf Variable that requires grad has
been used in an in-place operation.
```

> *Why?! It turns out to be a case of **"too much of a good thing"**. The culprit is PyTorch's ability to build a **dynamic computation graph** from every **Python operation** that involves any **gradient-computing tensor** or **its dependencies**.*

> *We'll go deeper into the inner workings of the dynamic computation graph in the next section.*

So, how do we tell PyTorch to **"back off"** and let us **update our parameters** without messing up with its *fancy dynamic computation graph*? That's what `torch.no_grad()` is good for. It allows us to **perform regular Python operations on tensors**, **independent of PyTorch's computation graph**.

Finally, we managed to successfully run our model and get the **resulting parameters**. Surely enough, they **match** the ones we got in our *Numpy*-only implementation.

```
# THIRD ATTEMPT
tensor([1.0235], device='cuda:0', requires_grad=True)
tensor([1.9690], device='cuda:0', requires_grad=True)
```

Dynamic Computation Graph

> *"Unfortunately, no one can be told what the dynamic computation graph is. You have to see it for yourself." Morpheus*

How great was "*The Matrix*"? Right, right? But, jokes aside, I want **you** to **see the graph for yourself** too!

> *The PyTorchViz package and its* `make_dot(variable)` *method allows us to easily visualize a graph associated with a given Python variable.*

So, let's stick with the **bare minimum**: two (*gradient computing*) **tensors** for our parameters, predictions, errors and loss.

```
torch.manual_seed(42)
a = torch.randn(1, requires_grad=True, dtype=torch.floa
b = torch.randn(1, requires_grad=True, dtype=torch.floa

yhat = a + b * x_train_tensor
error = y_train_tensor - yhat
```

Computing MSE in three steps

If we call `make_dot(yhat)` we'll get the **left-most graph** on Figure 3 below:

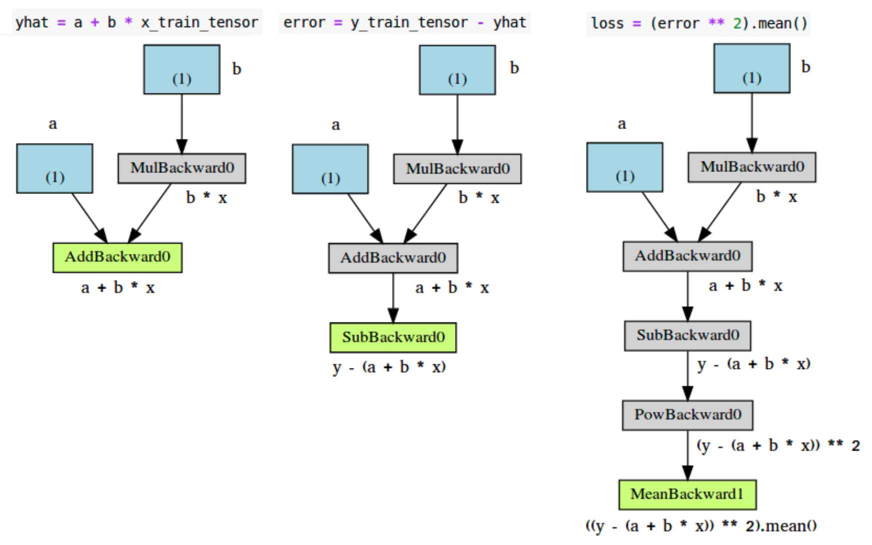


Figure 3: Computation graph for every step in computing MSE

Let’s take a closer look at its components:

- **blue boxes**: these correspond to the **tensors** we use as **parameters**, the ones we’re asking PyTorch to **compute gradients** for;
- **gray box**: a **Python operation** that involves a **gradient-computing tensor** or **its dependencies**;
- **green box**: the same as the gray box, except it is the **starting point for the computation** of gradients (assuming the `backward()` method is called from the **variable used to visualize** the graph)— they are computed from the **bottom-up** in a graph.

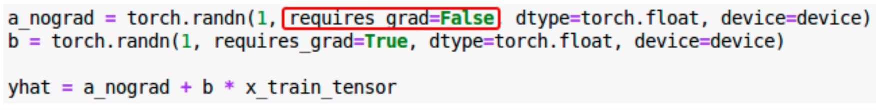
If we plot graphs for the `error` (center) and `loss` (right) **variables**, the **only difference** between them and the first one is the number of **intermediate steps** (**gray boxes**).

Now, take a closer look at the **green box** of the **left-most** graph: there are **two arrows** pointing to it, since it is **adding** up **two variables**, `a` and `b*x` . Seems obvious, right?

Then, look at the **gray box** of the same graph: it is performing a **multiplication**, namely, `b*x` . But there is only one arrow pointing to it! The arrow comes from the **blue box** that corresponds to our **parameter b**.

Why don't we have a box for our **data x**? The answer is: we **do not compute gradients** for it! So, even though there are *more* tensors involved in the operations performed by the computation graph, it **only** shows **gradient-computing tensors** and **its dependencies**.

What would happen to the computation graph if we set `requires_grad` to `False` for our **parameter a**?



```
a_nograd = torch.randn(1, requires_grad=False, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

yhat = a_nograd + b * x_train_tensor
```

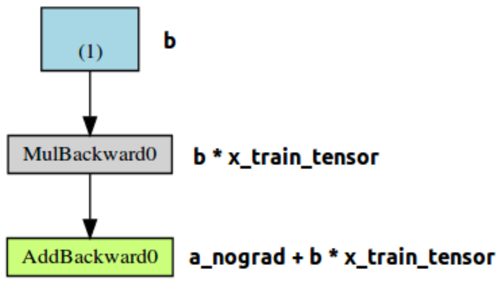


Figure 4: now variable a does NOT have its gradient computed anymore. But it is STILL used in computation

Unsurprisingly, the **blue box** corresponding to the **parameter a** is no more! Simple enough: **no gradients, no graph**.

The **best** thing about the *dynamic computing graph* is the fact that you can make it **as complex as you want** it. You can even use *control flow statements* (e.g., if statements) to **control the flow of the gradients** (obviously!) :-)

Figure 5 below shows an example of this. And yes, I do know that the computation itself is *completely nonsense*…

```
yhat = a + b * x_train_tensor
error = y_train_tensor - yhat

loss = (error ** 2).mean()

if loss > 0:
    yhat2 = b * x_train_tensor
    error2 = y_train_tensor - yhat2

loss += error2.mean()
```

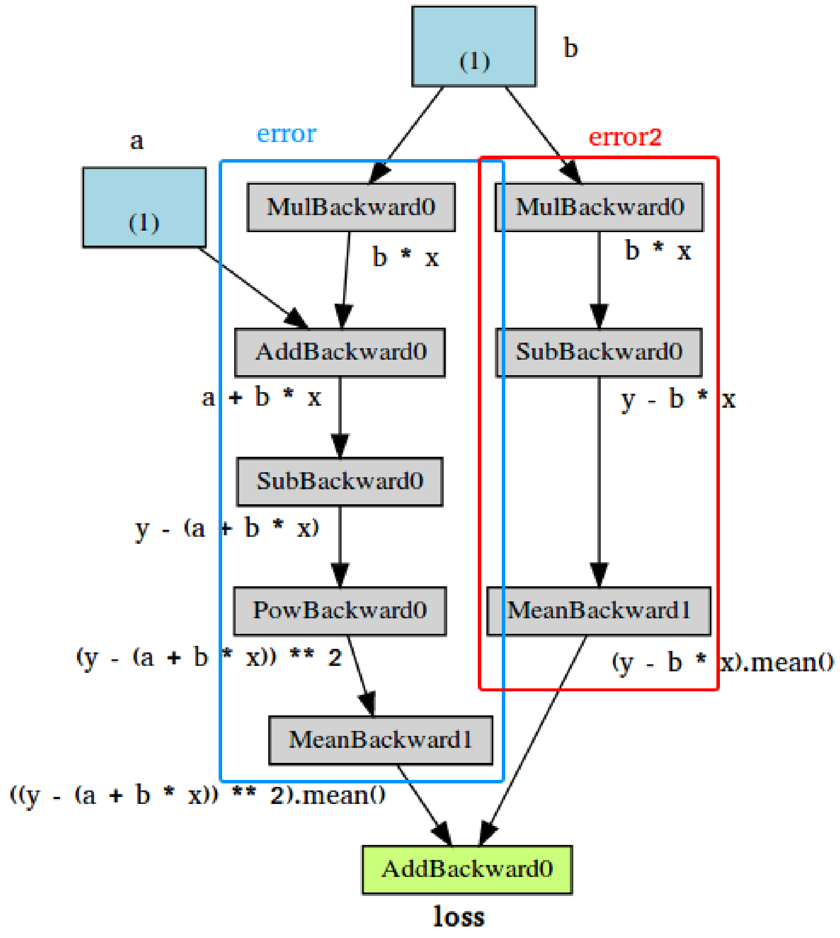


Figure 5: Complex computation graph just to make a point :-)

Optimizer

So far, we've been **manually** updating the parameters using the computed gradients. That's probably fine for *two parameters*... but what if we had a **whole lot of them**?! We use one of PyTorch's **optimizers**, like **SGD** or **Adam**.

An optimizer takes the **parameters** we want to update, the **learning rate** we want to use (and possibly many other hyper-parameters as well!) and **performs the updates** through its `step()` method.

Besides, we also don't need to zero the gradients one by one anymore. We just invoke the optimizer's `zero_grad()` method and that's it!

In the code below, we create a *Stochastic Gradient Descent* (SGD) optimizer to update our parameters **a** and **b**.

> *Don't be fooled by the **optimizer**'s name: if we use **all training data** at once for the update—as we are actually doing in the code—the optimizer is performing a **batch** gradient descent, despite of its name.*

```
torch.manual_seed(42)
a = torch.randn(1, requires_grad=True, dtype=torch.flo
b = torch.randn(1, requires_grad=True, dtype=torch.flo
print(a, b)

lr = 1e-1
n_epochs = 1000

# Defines a SGD optimizer to update the parameters
optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor
    error = y_train_tensor - yhat
    loss = (error ** 2).mean()

    loss.backward()

    # No more manual update!
    # with torch.no_grad():
```

PyTorch's optimizer in action—no more manual update of parameters!

Let's check our two parameters, before and after, just to make sure everything is still working fine:

```
# BEFORE: a, b
tensor([0.6226], device='cuda:0', requires_grad=True)
tensor([1.4505], device='cuda:0', requires_grad=True)
# AFTER: a, b
tensor([1.0235], device='cuda:0', requires_grad=True)
tensor([1.9690], device='cuda:0', requires_grad=True)
```

Cool! We've *optimized* the **optimization** process :-) What's left?

Loss

We now tackle the **loss computation**. As expected, PyTorch got us covered once again. There are many loss functions to choose from, depending on the task at hand. Since ours is a regression, we are using the Mean Square Error (MSE) loss.

> *Notice that* `nn.MSELoss` *actually* ***creates a loss function*** *for us—* ***it is NOT the loss function itself****. Moreover, you can specify a* ***reduction method*** *to be applied, that is,* ***how do you want to aggregate the results for individual points****—you can average them (reduction='mean') or simply sum them up (reduction='sum').*

We then **use** the created loss function later, at line 20, to compute the loss given our **predictions** and our **labels**.

Our code looks like this now:

```
torch.manual_seed(42)
a = torch.randn(1, requires_grad=True, dtype=torch.flo
b = torch.randn(1, requires_grad=True, dtype=torch.flo
print(a, b)

lr = 1e-1
n_epochs = 1000

# Defines a MSE loss function
loss_fn = nn.MSELoss(reduction='mean')

optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor

    # No more manual loss!
```

PyTorch's loss in action — no more manual loss computation!

At this point, there's only one piece of code left to change: the **predictions**. It is then time to introduce PyTorch's way of implementing a...

Model

In PyTorch, a **model** is represented by a regular **Python class** that inherits from the **Module** class.

The most fundamental methods it needs to implement are:

- `__init__(self)` : **it defines the parts that make up the model** —in our case, two *parameters*, **a** and **b**.

> *You are **not** limited to defining **parameters**, though... **models can contain other models (or layers) as its attributes** as well, so you can easily nest them. We'll see an example of this shortly as well.*

- `forward(self, x)` : it performs the **actual computation**, that is, it **outputs a prediction**, given the input **x**.

> *You should* ***NOT call the*** `forward(x)` *method, though. You should* ***call the whole model itself****, as in* `model(x)` *to perform a forward pass and output predictions.*

Let’s build a proper (yet simple) model for our regression task. It should look like this:

```
class ManualLinearRegression(nn.Module):
    def __init__(self):
        super().__init__()
        # To make "a" and "b" real parameters of the m
        self.a = nn.Parameter(torch.randn(1, requires_
        self.b = nn.Parameter(torch.randn(1, requires_

    def forward(self, x):
```

Building our “Manual” model, creating parameter by parameter!

In the `__init__` method, we define our **two parameters**, **a** and **b**, using the `Parameter()` class, to tell PyTorch these **tensors should be considered parameters of the model they are an attribute of**.

Why should we care about that? By doing so, we can use our model’s `parameters()` method to retrieve **an iterator over all model’s parameters**, **even** those parameters of **nested models**, that we can use to feed our optimizer (instead of building a list of parameters ourselves!).

Moreover, we can get the **current values for all parameters** using our model’s `state_dict()` method.

> ***IMPORTANT****: we need to* ***send our model to the same device where the data is****. If our data is made of GPU tensors, our model must “live” inside the GPU as well.*

We can use all these handy methods to change our code, which should be looking like this:

```python
torch.manual_seed(42)

# Now we can create a model and send it at once to the
model = ManualLinearRegression().to(device)
# We can also inspect its parameters using its state_d
print(model.state_dict())

lr = 1e-1
n_epochs = 1000

loss_fn = nn.MSELoss(reduction='mean')
optimizer = optim.SGD(model.parameters(), lr=lr)

for epoch in range(n_epochs):
    # What is this?!?
    model.train()

    # No more manual prediction!
```

PyTorch's model in action — no more manual prediction/forward step!

Now, the printed statements will look like this—final values for parameters **a** and **b** are still the same, so everything is ok :-)

```
OrderedDict([('a', tensor([0.3367], device='cuda:0')),
('b', tensor([0.1288], device='cuda:0'))])
OrderedDict([('a', tensor([1.0235], device='cuda:0')),
('b', tensor([1.9690], device='cuda:0'))])
```

I hope you noticed one particular statement in the code, to which I assigned a comment **"What is this?!?"**— `model.train()` .

> *In PyTorch, models have a* `train()` *method which, somewhat disappointingly,* ***does NOT perform a training step****. Its only purpose is to* ***set the model to training mode****. Why is this important? Some models may use mechanisms like* ***Dropout****, for instance, which have* ***distinct behaviors in training and evaluation*** *phases.*

Nested Models

In our model, we manually created two parameters to perform a linear regression. Let’s use PyTorch’s **Linear** model as an attribute of our own, thus creating a nested model.

Even though this clearly is a contrived example, as we are pretty much wrapping the underlying model without adding anything useful (or, at all!) to it, it illustrates well the concept.

In the `__init__` method, we created an **attribute** that contains our **nested** `Linear` **model**.

In the `forward()` method, we **call the nested model itself** to perform the forward pass (*notice, we are **not** calling* `self.linear.forward(x)` *!*).

```
class LayerLinearRegression(nn.Module):
    def __init__(self):
        super().__init__()
        # Instead of our custom parameters, we use a Li
        self.linear = nn.Linear(1, 1)

    def forward(self, x):
```

Building a model using PyTorch’s Linear layer

Now, if we call the `parameters()` method of this model, **PyTorch will figure the parameters of its attributes in a recursive way**. You can try it yourself using something like: `[*LayerLinearRegression().parameters()]` to get a list of all parameters. You can also add new `Linear` attributes and, even if you don’t use them at all in the forward pass, they will **still** be listed under `parameters()` .

Sequential Models

Our model was simple enough… You may be thinking: *“why even bother to build a class for it?!”* Well, you have a point…

For **straightforward models**, that use **run-of-the-mill layers**, where the output of a layer is sequentially fed as an input to the next, we can use a, er… **Sequential** model :-)

In our case, we would build a Sequential model with a single argument, that is, the `Linear` layer we used to train our linear regression. The model would look like this:

```
# Alternatively, you can use a Sequential model
model = nn.Sequential(nn.Linear(1, 1)).to(device)
```

Simple enough, right?

Training Step

So far, we've defined an **optimizer**, a **loss function** and a **model**. Scroll up a bit and take a quick look at the code *inside the loop*. Would it **change** if we were using a **different optimizer**, or **loss**, or even **model**? If not, how can we make it **more generic**?

Well, I guess we could say all these lines of code **perform a training step**, given those **three elements** (*optimizer, loss and model*),the **features** and the **labels**.

So, how about **writing a function that takes those three elements** and **returns another function that performs a training step**, taking a set of features and labels as arguments and returning the corresponding loss?

Then we can use this general-purpose function to build a **`train_step()`** function to be called inside our training loop. Now our code should look like this… see how **tiny** the training loop is now?

```python
def make_train_step(model, loss_fn, optimizer):
    # Builds function that performs a step in the trai
    def train_step(x, y):
        # Sets model to TRAIN mode
        model.train()
        # Makes predictions
        yhat = model(x)
        # Computes loss
        loss = loss_fn(y, yhat)
        # Computes gradients
        loss.backward()
        # Updates parameters and zeroes gradients
        optimizer.step()
        optimizer.zero_grad()
        # Returns the loss
        return loss.item()

    # Returns the function that will be called inside
    return train_step

# Creates the train_step function for our model, loss
```

Building a function to perform one step of training!

Let's give our training loop a rest and focus on our **data** for a while… so far, we've simply used our *Numpy arrays* turned **PyTorch tensors**. But we can do better, we can build a…

Dataset

In PyTorch, a **dataset** is represented by a regular **Python class** that inherits from the **Dataset** class. You can think of it as a kind of a Python **list of tuples**, each tuple corresponding to **one point (features, label)**.

The most fundamental methods it needs to implement are:

- `__init__(self)` : it takes **whatever arguments** needed to build a **list of tuples**—it may be the name of a CSV file that will be loaded and processed; it may be *two tensors*, one for features, another one for labels; or anything else, depending on the task at hand.

> *There is **no need to load the whole dataset in the constructor method** (`__init__`). If your **dataset is big** (tens of thousands of image files, for instance), loading it at once would not be memory efficient. It is recommended to **load them on demand** (whenever `__get_item__` is called).*

- **`__get_item__(self, index)`** : it allows the dataset to be **indexed**, so it can work **like a list** (`dataset[i]`)—it must **return a tuple (features, label)** corresponding to the requested data point. We can either return the **corresponding slices** of our **pre-loaded** dataset or tensors or, as mentioned above, **load them on demand** (like in this example).
- **`__len__(self)`** : it should simply return the **size** of the whole dataset so, whenever it is sampled, its indexing is limited to the actual size.

Let's build a simple custom dataset that takes two tensors as arguments: one for the features, one for the labels. For any given index, our dataset class will return the corresponding slice of each of those tensors. It should look like this:

```
from torch.utils.data import Dataset, TensorDataset

class CustomDataset(Dataset):
    def __init__(self, x_tensor, y_tensor):
        self.x = x_tensor
        self.y = y_tensor

    def __getitem__(self, index):
        return (self.x[index], self.y[index])

    def __len__(self):
        return len(self.x)

# Wait, is this a CPU tensor now? Why? Where is .to(de
x_train_tensor = torch.from_numpy(x_train).float()
```

Creating datasets using train tensors

Once again, you may be thinking "*why go through all this trouble to wrap a couple of tensors in a class?*". And, once again, you do have a point… if a dataset is nothing else but a **couple of tensors**, we can use PyTorch's **TensorDataset** class, which will do pretty much what we did in our custom dataset above.

> *Did you notice we built our **training tensors** out of Numpy arrays but we **did not send them to a device**? So, they are **CPU** tensors now! **Why**?*

> *We **don't want our whole training data to be loaded into GPU tensors**, as we have been doing in our example so far, because **it takes up space** in our precious **graphics card's RAM.***

OK, fine, but then again, **why** are we building a dataset anyway? We're doing it because we want to use a…

DataLoader

Until now, we have used the **whole training data** at every training step. It has been **batch gradient descent** all along. This is fine for our *ridiculously small dataset*, sure, but if we want to go serious about all this, we **must** use **mini-batch** gradient descent. Thus, we need mini-batches. Thus, we need to **slice** our dataset accordingly. Do you want to do it *manually*?! Me neither!

So we use PyTorch's **DataLoader** class for this job. We tell it which **dataset** to use (the one we just built in the previous section), the desired **mini-batch size** and if we'd like to **shuffle** it or not. That's it!

Our **loader** will behave like an **iterator**, so we can **loop over it** and **fetch a different mini-batch** every time.

```
from torch.utils.data import DataLoader

train_loader = DataLoader(dataset=train_data, batch_siz
```

Building a data loader for our training data

To retrieve a sample mini-batch, one can simply run the command below—it will return a list containing two tensors, one for the features, another one for the labels.

```
next(iter(train_loader))
```

How does this change our training loop? Let's check it out!

```
losses = []
train_step = make_train_step(model, loss_fn, optimizer

for epoch in range(n_epochs):
    for x_batch, y_batch in train_loader:
        # the dataset "lives" in the CPU, so do our mi
        # therefore, we need to send those mini-batche
        # device where the model "lives"
        x_batch = x_batch.to(device)
        y_batch = y_batch.to(device)
```

Using mini-batch gradient descent!

Two things are different now: not only we have an *inner loop* to load each and every *mini-batch* from our `DataLoader` but, more importantly, we are now **sending only one mini-batch to the device**.

> *For bigger datasets,* ***loading data sample by sample*** *(into a* ***CPU*** *tensor) using* ***Dataset's*** `__get_item__` *and then* ***sending all samples*** *that belong to the same* ***mini-batch at once to your GPU*** *(device) is the way to go in order to make the* ***best use of your graphics card's RAM****.*

> *Moreover, if you have* ***many GPUs*** *to train your model on, it is best to keep your dataset "agnostic" and assign the batches to different GPUs during training.*

So far, we've focused on the **training data** only. We built a *dataset* and a *data loader* for it. We could do the same for the **validation** data, using the **split** we performed at the beginning of this post… or we could use `random_split` instead.

Random Split

PyTorch's **`random_split()`** method is an easy and familiar way of performing a **training-validation split**. Just keep in mind that, in our example, we need to apply it to the **whole dataset** (*not the training dataset* we built in two sections ago).

Then, for each subset of data, we build a corresponding `DataLoader`, so our code looks like this:

```python
from torch.utils.data.dataset import random_split

x_tensor = torch.from_numpy(x).float()
y_tensor = torch.from_numpy(y).float()

dataset = TensorDataset(x_tensor, y_tensor)

train_dataset, val_dataset = random_split(dataset, [80
```

Splitting the dataset into training and validation sets, the PyTorch way!

Now we have a **data loader** for our **validation set**, so, it makes sense to use it for the…

Evaluation

This is the **last** part of our journey—we need to change the training loop to include the **evaluation of our model**, that is, computing the **validation loss**. The first step is to include another inner loop to handle the *mini-batches* that come from the *validation loader* , sending them to the same *device* as our model. Next, we make **predictions** using our model (line 23) and compute the corresponding **loss** (line 24).

That's pretty much it, but there are **two small**, **yet important**, things to consider:

- `torch.no_grad()` : even though it won't make a difference in our simple model, it is a **good practice** to **wrap the validation** inner loop with this **context manager to disable any gradient calculation** that you may inadvertently trigger —**gradients belong in training**, not in validation steps;
- `eval()` : the only thing it does is **setting the model to evaluation mode** (just like its `train()` counterpart did), so the model can adjust its behavior regarding some operations, like **Dropout**.

Now, our training loop should look like this:

```
losses = []
val_losses = []
train_step = make_train_step(model, loss_fn, optimizer

for epoch in range(n_epochs):
    for x_batch, y_batch in train_loader:
        x_batch = x_batch.to(device)
        y_batch = y_batch.to(device)

        loss = train_step(x_batch, y_batch)
        losses.append(loss)

    with torch.no_grad():
        for x_val, y_val in val_loader:
            x_val = x_val.to(device)
            y_val = y_val.to(device)
```

Computing validation loss

Is there **anything else** we can improve or change? Sure, there is **always something else** to add to your model—using a **learning rate scheduler**, for instance. But this post is already *waaaay too long*, so I will stop right here.

"*Where is the full working code with all bells and whistles?*", you ask? You can find it **here**.

Final Thoughts

Although this post was *much longer* than I anticipated when I started writing it, I wouldn't make it any different—I believe it has **most of the necessary steps** one needs go to trough in order to **learn**, in a **structured** and **incremental** way, how to **develop Deep Learning models using PyTorch**.

Hopefully, after finishing working through all code in this post, you'll be able to better appreciate and more easily work your way through PyTorch's official tutorials.

If you have any thoughts, comments or questions, please leave a comment below or contact me on Twitter.