# Deep learning

## 4.3. PyTorch modules and batch processing

François Fleuret

https://fleuret.org/dlc/

UNIVERSITÉ DE GENÈVE

Elements from `torch.nn.functional` are autograd-compliant functions which compute a result from provided arguments alone.

Elements from `torch.nn.functional` are autograd-compliant functions which compute a result from provided arguments alone.

Subclasses of `torch.nn.Module` are losses and network components. The latter embed parameters to be optimized during training.

Parameters are of the type `torch.nn.Parameter` which is a `Tensor` with `requires_grad` to `True`, and known to be a model parameter by various utility functions, in particular `torch.nn.Module.parameters()`.

Elements from `torch.nn.functional` are autograd-compliant functions which compute a result from provided arguments alone.

Subclasses of `torch.nn.Module` are losses and network components. The latter embed parameters to be optimized during training.

Parameters are of the type `torch.nn.Parameter` which is a `Tensor` with `requires_grad` to `True`, and known to be a model parameter by various utility functions, in particular `torch.nn.Module.parameters()`.

Usually `torch.nn.functional` is imported as `F`, and `torch.nn` as `nn`.

⚠ Functions and modules from `nn` process **batches** of inputs stored in a tensor whose first dimension indexes them, and produce a corresponding tensor with the same additional dimension.

E.g. a fully connected layer $\mathbb{R}^C \rightarrow \mathbb{R}^D$ expects as input a tensor of size $N \times C$ and computes a tensor of size $N \times D$, where $N$ is the number of samples and can vary from a call to another. We come back to this in a second.

The autograd-compliant function

```
F.relu(input, inplace=False)
```

takes a tensor of any size as input, applies ReLU on each value to produce a result tensor of same size.

The autograd-compliant function

```
F.relu(input, inplace=False)
```

takes a tensor of any size as input, applies ReLU on each value to produce a result tensor of same size.

```
>>> x
tensor([[ 0.8008, -0.2586,  0.5019, -0.2002, -0.7416],
        [ 0.0557,  0.6046,  0.0864, -0.5929,  1.2606]])
>>> F.relu(x)
tensor([[ 0.8008,  0.0000,  0.5019,  0.0000,  0.0000],
        [ 0.0557,  0.6046,  0.0864,  0.0000,  1.2606]])
```

The autograd-compliant function

```
F.relu(input, inplace=False)
```

takes a tensor of any size as input, applies ReLU on each value to produce a result tensor of same size.

```
>>> x
tensor([[ 0.8008, -0.2586,  0.5019, -0.2002, -0.7416],
        [ 0.0557,  0.6046,  0.0864, -0.5929,  1.2606]])
>>> F.relu(x)
tensor([[ 0.8008,  0.0000,  0.5019,  0.0000,  0.0000],
        [ 0.0557,  0.6046,  0.0864,  0.0000,  1.2606]])
```

`inplace` indicates if the operation should modify the argument itself. This may be desirable to reduce the memory footprint of the processing.

The module

```
nn.Linear(in_features, out_features, bias=True)
```

implements a $\mathbb{R}^C \rightarrow \mathbb{R}^D$ fully-connected layer. It takes as input a tensor of size $N \times C$ and produces a tensor of size $N \times D$.

The module

```
nn.Linear(in_features, out_features, bias=True)
```

implements a $\mathbb{R}^C \to \mathbb{R}^D$ fully-connected layer. It takes as input a tensor of size $N \times C$ and produces a tensor of size $N \times D$.

```
>>> f = nn.Linear(in_features = 10, out_features = 4)
>>> for n, p in f.named_parameters(): print(n, p.size())
...
weight torch.Size([4, 10])
bias torch.Size([4])
>>> x = torch.randn(523, 10)
>>> y = f(x)
>>> y.size()
torch.Size([523, 4])
```

The module

```
nn.Linear(in_features, out_features, bias=True)
```

implements a $\mathbb{R}^C \to \mathbb{R}^D$ fully-connected layer. It takes as input a tensor of size $N \times C$ and produces a tensor of size $N \times D$.

```
>>> f = nn.Linear(in_features = 10, out_features = 4)
>>> for n, p in f.named_parameters(): print(n, p.size())
...
weight torch.Size([4, 10])
bias torch.Size([4])
>>> x = torch.randn(523, 10)
>>> y = f(x)
>>> y.size()
torch.Size([523, 4])
```

The weights and biases are automatically randomized at creation. We will come back to that later.

The module

```
nn.MSELoss()
```

implements the Mean Square Error loss: the sum of the component-wise squared differences, **divided by the total number of components in the tensors**.

The module

```
nn.MSELoss()
```

implements the Mean Square Error loss: the sum of the component-wise squared differences, **divided by the total number of components in the tensors**.

```
>>> f = nn.MSELoss()
>>> x = torch.tensor([[ 3. ]])
>>> y = torch.tensor([[ 0. ]])
>>> f(x, y)
tensor(9.)
>>> x = torch.tensor([[ 3., 0., 0., 0. ]])
>>> y = torch.tensor([[ 0., 0., 0., 0. ]])
>>> f(x, y)
tensor(2.2500)
```

The module

```
nn.MSELoss()
```

implements the Mean Square Error loss: the sum of the component-wise squared differences, **divided by the total number of components in the tensors**.

```
>>> f = nn.MSELoss()
>>> x = torch.tensor([[ 3. ]])
>>> y = torch.tensor([[ 0. ]])
>>> f(x, y)
tensor(9.)
>>> x = torch.tensor([[ 3., 0., 0., 0. ]])
>>> y = torch.tensor([[ 0., 0., 0., 0. ]])
>>> f(x, y)
tensor(2.2500)
```

The first parameter of a loss is traditionally called the **input** and the second the **target**.

The module

```
nn.MSELoss()
```

implements the Mean Square Error loss: the sum of the component-wise squared differences, **divided by the total number of components in the tensors**.

```
>>> f = nn.MSELoss()
>>> x = torch.tensor([[ 3. ]])
>>> y = torch.tensor([[ 0. ]])
>>> f(x, y)
tensor(9.)
>>> x = torch.tensor([[ 3., 0., 0., 0. ]])
>>> y = torch.tensor([[ 0., 0., 0., 0. ]])
>>> f(x, y)
tensor(2.2500)
```

The first parameter of a loss is traditionally called the **input** and the second the **target**. These two quantities may be of different dimensions or even types for some losses (e.g. for classification).

⚠ Criteria do not accept a target with `requires_grad` to `True`.

```
>>> import torch
>>> f = nn.MSELoss()
>>> x = torch.tensor([ 3., 2. ]).requires_grad_()
>>> y = torch.tensor([ 0., -2. ]).requires_grad_()
>>> f(x, y)
Traceback (most recent call last):
/.../
AssertionError: nn criterions don't compute the gradient w.r.t.
targets - please mark these tensors as not requiring gradients
```

## Batch processing

Functions and modules from `nn` process samples by batches. This is motivated by the computational speed-up it induces.

Training a large network on CIFAR10:

| Batch size | Time per epoch |
|---|---|
| 1 | 4h22min |
| 64 | 4min50s |

speed up of $\times$54.

To evaluate a module on a sample, both the module's parameters and the sample have to be first copied into **cache memory**, which is fast but small.

For any model of reasonable size, only a fraction of its parameters can be kept in cache, so a module's parameters have to be copied there every time they are used.

To evaluate a module on a sample, both the module's parameters and the sample have to be first copied into **cache memory**, which is fast but small.

For any model of reasonable size, only a fraction of its parameters can be kept in cache, so a module's parameters have to be copied there every time they are used.

**Memory transfers are slower than computation. Batch processing cuts down to one copy of the parameters to the cache per batch.**

To evaluate a module on a sample, both the module's parameters and the sample have to be first copied into **cache memory**, which is fast but small.

For any model of reasonable size, only a fraction of its parameters can be kept in cache, so a module's parameters have to be copied there every time they are used.

**Memory transfers are slower than computation. Batch processing cuts down to one copy of the parameters to the cache per batch.**

It also cuts down the use of Python loops, which are awfully slow.

Consider a model composed of three modules

$$f = f_3 \circ f_2 \circ f_1,$$

and we want to compute $f(x_1), f(x_2), f(x_3)$.

Consider a model composed of three modules

$$f = f_3 \circ f_2 \circ f_1,$$

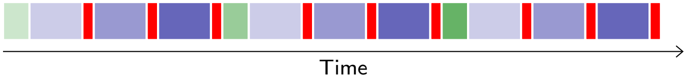
and we want to compute $f(x_1), f(x_2), f(x_3)$.

🟩🟩🟩 Copying the $x_n$s to cache memory

🟦🟦🟦 Copying the $f_d$s' parameters to cache memory

🟥 Computing a $f_d(.)$

Processing samples one by one:



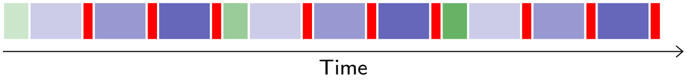
Consider a model composed of three modules

$$f = f_3 \circ f_2 \circ f_1,$$

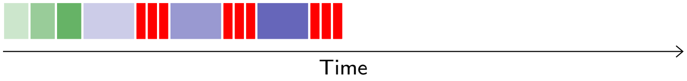
and we want to compute $f(x_1), f(x_2), f(x_3)$.

| | |
|---|---|
| 🟩🟩🟩 | Copying the $x_n$s to cache memory |
| 🟦🟦🟦 | Copying the $f_d$s' parameters to cache memory |
| 🟥 | Computing a $f_d(.)$ |

Processing samples one by one:



Batch processing:



With

```
def timing(x, w, batch = False, nb = 101):
    t = torch.zeros(nb)

    for u in range(nb):
        t0 = time.perf_counter()
        if batch:
            y = x.mm(w.t())
        else:
            y = torch.empty(x.size(0), w.size(0))
            for k in range(y.size(0)): y[k] = w.mv(x[k])
        y.is_cuda and torch.cuda.synchronize()
        t[u] = time.perf_counter() - t0

    return t.median().item()
```

```
x = torch.randn(2500, 1000)
w = torch.randn(1500, 1000)
print('Batch-processing speed-up on CPU %.1f' %
      (timing(x, w, batch = False) / timing(x, w, batch = True)))

x, w = x.to('cuda'), w.to('cuda')
print('Batch-processing speed-up on GPU %.1f' %
      (timing(x, w, batch = False) / timing(x, w, batch = True)))
```

prints

```
Batch-processing speed-up on CPU 4.6
Batch-processing speed-up on GPU 144.4
```

Formally, we have to revisit a bit some expressions we saw previously for fully connected layers. We had

$$\forall l, n,\ \ w^{(l)} \in \mathbb{R}^{d_l \times d_{l-1}},\ \ x_n^{(l-1)} \in \mathbb{R}^{d_{l-1}},\ \ \ s_n^{(l)} = w^{(l)}\, x_n^{(l-1)}.$$

Formally, we have to revisit a bit some expressions we saw previously for fully connected layers. We had

$$\forall l, n,\ w^{(l)} \in \mathbb{R}^{d_l \times d_{l-1}},\ x_n^{(l-1)} \in \mathbb{R}^{d_{l-1}},\ \ s_n^{(l)} = w^{(l)}\, x_n^{(l-1)}.$$

From now on, we will use row vectors, so that we can represent a series of samples as a 2d array with the first index being the sample's index.

$$x = \begin{pmatrix} x_{1,1} & \dots & x_{1,D} \\ \vdots & \ddots & \vdots \\ x_{N,1} & \dots & x_{N,D} \end{pmatrix} = \begin{pmatrix} (x_1)^\top \\ \vdots \\ (x_N)^\top \end{pmatrix},$$

which is an element of $\mathbb{R}^{N \times D}$.

To make all sample row vectors and apply a linear operator, we want

$$\forall n,\ s_n^{(l)} = \left(w^{(l)} \left(x_n^{(l-1)}\right)^\top\right)^\top = x_n^{(l-1)} \left(w^{(l)}\right)^\top$$

which gives a tensorial expression for the full batch

$$s^{(l)} = x^{(l-1)} \left(w^{(l)}\right)^\top.$$

To make all sample row vectors and apply a linear operator, we want

$$\forall n,\ s_n^{(l)} = \left(w^{(l)} \left(x_n^{(l-1)}\right)^\top\right)^\top = x_n^{(l-1)} \left(w^{(l)}\right)^\top$$

which gives a tensorial expression for the full batch

$$s^{(l)} = x^{(l-1)} \left(w^{(l)}\right)^\top.$$

And in `torch/nn/functional.py`

```
def linear(input, weight, bias=None):
    if input.dim() == 2 and bias is not None:
        # fused op is marginally faster
        return torch.addmm(bias, input, weight.t())

    output = input.matmul(weight.t())
    if bias is not None:
        output += bias
    return output
```

Similarly for the backward pass of a linear layer we get

$$\left[\!\left[\frac{\partial \mathscr{L}}{\partial w^{(l)}}\right]\!\right] = \left[\!\left[\frac{\partial \mathscr{L}}{\partial s^{(l)}}\right]\!\right]^{\top} x^{(l-1)},$$

and

$$\left[\!\left[\frac{\partial \mathscr{L}}{\partial x^{(l)}}\right]\!\right] = \left[\!\left[\frac{\partial \ell}{\partial s^{(l+1)}}\right]\!\right] w^{(l+1)}.$$

The End