EE-559 – Deep learning

4b. PyTorch modules, batch processing

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- `torch.nn.Conv2d`
- `torch.nn.Linear`
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Subclasses of `torch.nn.Module` are losses and network components. The latter embed `torch.nn.Parameter`s to be optimized during training.

⚠ Since they are almost exclusively used with autograd, elements from `torch.nn` only process `Variable`s.

The term "tensor" is used for both `Tensor`s and `Variable`s in what follows.

⚠ Functions and modules from `torch.nn` process only batches of inputs stored in a tensor with an additional first dimension to index them, and produce a corresponding tensor with an additional dimension.

E.g. a fully connected layer $\mathbb{R}^C \to \mathbb{R}^D$ expects as input a tensor of size $N \times C$ and compute a tensor of size $N \times D$, where N is the number of samples.

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torch.nn.functional.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.

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>>> x = Variable(Tensor(2, 5).normal_())
>>> x
Variable containing:
-0.2066 -1.7997 -0.0653  0.6481  0.0253
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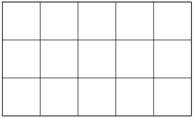
```

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

For what follows, note that pooling and convolution have two additional standard parameters:

- The **padding** specifies the size of a zeroed frame added around the input,
- the **stride** specifies a step size when moving the filter across the signal.

Here with $C \times 3 \times 5$ as input



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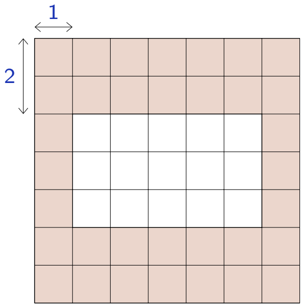
Here with $C \times 3 \times 5$ as input, a padding of $(2, 1)$



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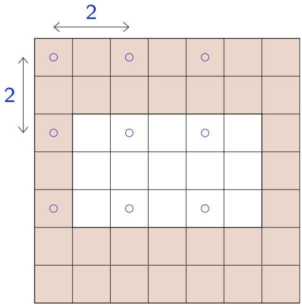

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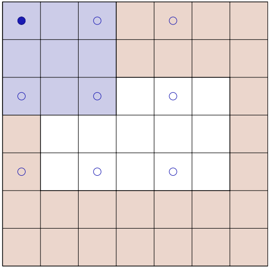
Here with $C \times 3 \times 5$ as input, a padding of $(2, 1)$, a stride of $(2, 2)$, and a kernel of size $C \times 3 \times 3$



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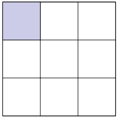

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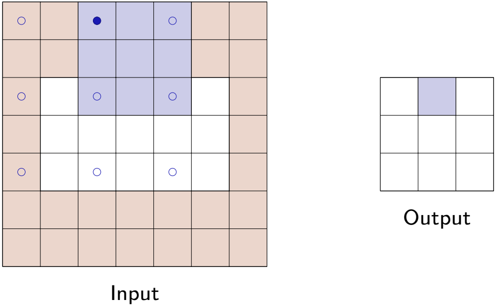

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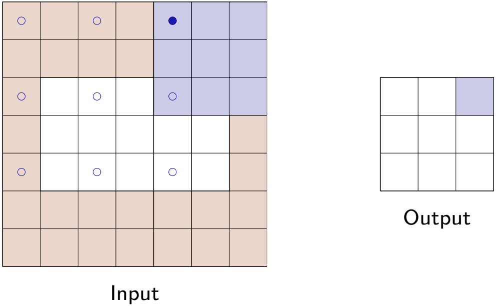

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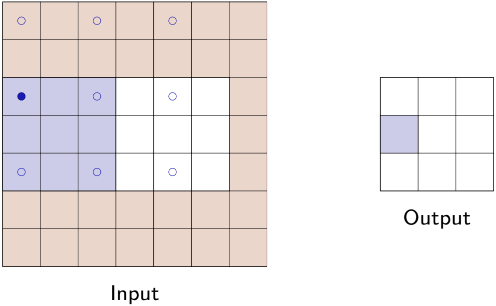

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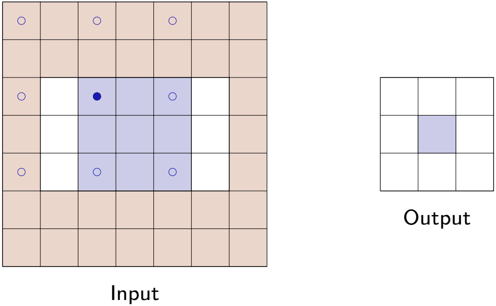

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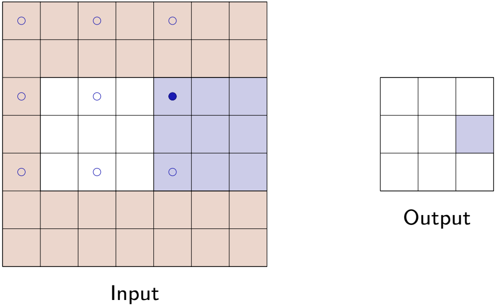

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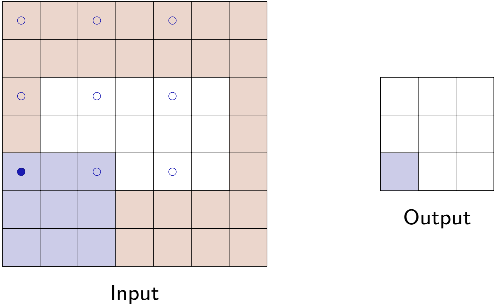

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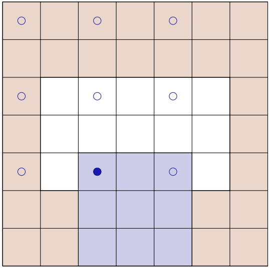

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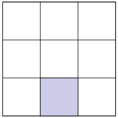

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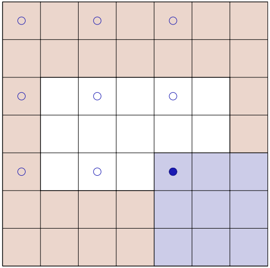
Here with $C \times 3 \times 5$ as input, a padding of $(2, 1)$, a stride of $(2, 2)$, and a kernel of size $C \times 3 \times 3$, the output is $1 \times 3 \times 3$.



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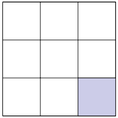

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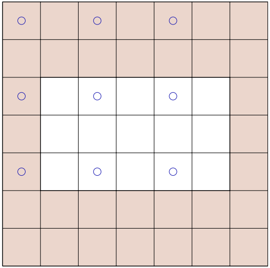

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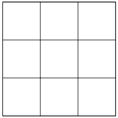

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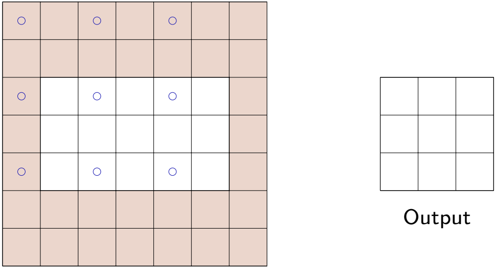

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Pooling operations have a default stride equal to their kernel size, and convolutions have a default stride of 1.

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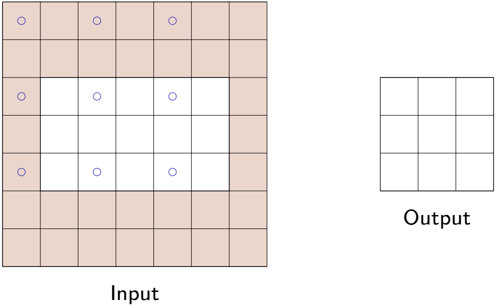

Pooling operations have a default stride equal to their kernel size, and convolutions have a default stride of 1. Padding is zero by default, and is useful for instance to generate an output of same size as the input.

```
torch.nn.functional.max_pool2d(input, kernel_size,
                               stride=None, padding=0, dilation=1,
                               ceil_mode=False, return_indices=False)
```

Takes as input a $N \times C \times H \times W$ tensor, and a kernel size (h, w) or k interpreted as (k, k), applies the max-pooling on each channel of each sample separately, and produce if the padding is 0 a $N \times C \times \lfloor H/h \rfloor \times \lfloor W/w \rfloor$ output.

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```
>>> x = Variable(Tensor(1, 2, 3, 6).random_(3))
>>> x
Variable containing:
(0 ,0 ,.,.) =
  1  2  0  1  1  0
  2  2  1  2  2  2
  0  2  0  1  1  0

(0 ,1 ,.,.) =
  1  0  0  2  0  2
  0  0  0  1  0  2
  1  1  1  1  1  0
[torch.FloatTensor of size 1x2x3x6]

>>> torch.nn.functional.max_pool2d(x, (1, 2))
Variable containing:
(0 ,0 ,.,.) =
  2  1  1
  2  2  2
  2  1  1

(0 ,1 ,.,.) =
  1  2  2
  0  1  2
  1  1  1
[torch.FloatTensor of size 1x2x3x3]
```

```
class torch.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 produce a tensor of size $N \times D$.

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```
>>> f = torch.nn.Linear(in_features = 10, out_features = 4)
>>> f.weight.size()
torch.Size([4, 10])
>>> f.bias.size()
torch.Size([4])
>>> x = Variable(Tensor(523, 10).normal_())
>>> y = f(x)
>>> y.size()
torch.Size([523, 4])
```

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torch.Size([523, 4])
```

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

```
torch.nn.Conv2d(in_channels, out_channels,
                kernel_size,
                stride=1, padding=0, dilation=1, groups=1, bias=True)
```

Implements a standard 2d convolutional layer. The kernel size is either a pair (h, w) or a single value k interpreted as (k, k).

It takes as input a $N \times C \times H \times W$ tensor and returns a tensor $N \times D \times (H - h + 1) \times (W - w + 1)$

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```
>>> l = torch.nn.Conv2d(in_channels = 4, out_channels = 5, kernel_size = (2, 3))
>>> l.weight.size()
torch.Size([5, 4, 2, 3])
>>> l.bias.size()
torch.Size([5])
>>> x = Variable(Tensor(117, 4, 10, 3).normal_())
>>> y = l(x)
>>> y.size()
torch.Size([117, 5, 9, 1])
```

As for the fully connected layer, weights and biases are randomized.

```
mnist_train = datasets.MNIST('./data/mnist/', train = True, download = True)

# Take the 13th example, shape it as a batch of a single one-channel image
x = mnist_train.train_data[12].float().view(1, 1, 28, 28)

f = torch.nn.Conv2d(1, 5, kernel_size=3)

f.bias.data.zero_()

f.weight.data[0] = Tensor([ [  0,  0,  0 ],
                            [  0,  1,  0 ],
                            [  0,  0,  0 ] ])

f.weight.data[1] = Tensor([ [  1,  1,  1 ],
                            [  1,  1,  1 ],
                            [  1,  1,  1 ] ])

f.weight.data[2] = Tensor([ [ -1,  0,  1 ],
                            [ -1,  0,  1 ],
                            [ -1,  0,  1 ] ])

f.weight.data[3] = Tensor([ [ -1, -1, -1 ],
                            [  0,  0,  0 ],
                            [  1,  1,  1 ] ])

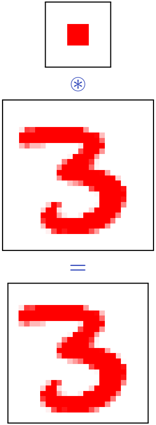
f.weight.data[4] = Tensor([ [  0, -1,  0 ],
                            [ -1,  4, -1 ],
                            [  0, -1,  0 ] ])

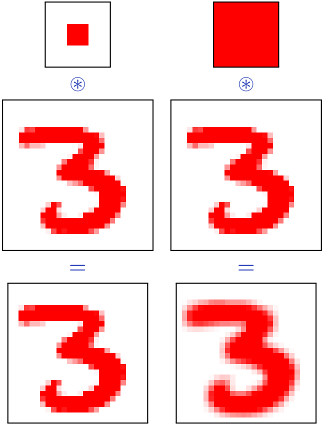
y = f(Variable(x)).data

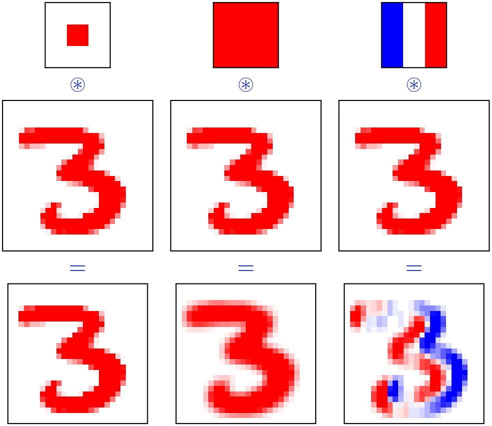
save_2d_tensor_as_image(f.weight.data[0], 'conv-filters-{:d}.png',
                        signed = True)

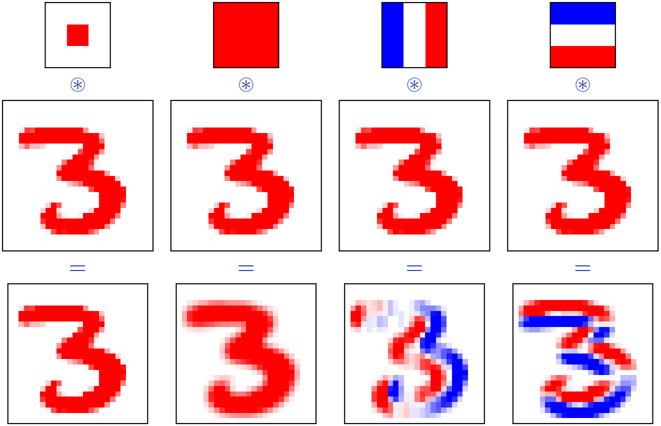
save_2d_tensor_as_image(x[0], 'conv-mnist-orig.png', signed = True)

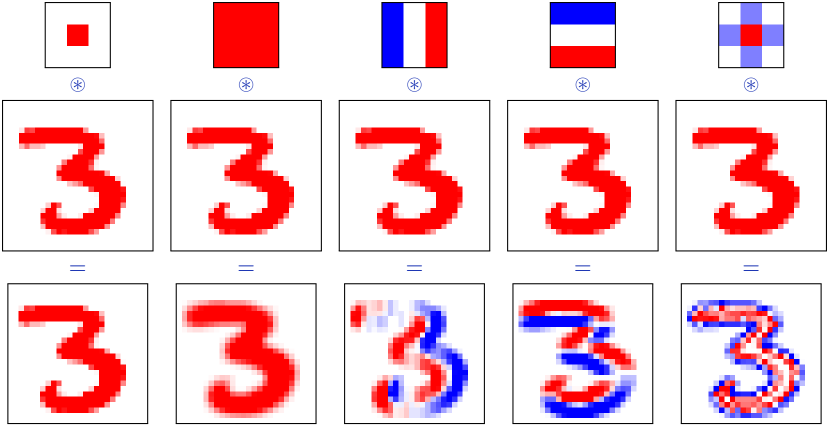
save_2d_tensor_as_image(y[0], 'conv-mnist-results-{:d}.png',
                        signed = True)
```











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>>> f = torch.nn.MSELoss()
>>> x = Variable(Tensor([[ 3 ]]))
>>> y = Variable(Tensor([[ 0 ]]))
>>> f(x, y)
Variable containing:
 9
[torch.FloatTensor of size 1]

>>> x = Variable(Tensor([[ 3, 0, 0, 0 ]]))
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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).

Remember that `Module`s' inputs and outputs are `Variable`s. Data `Tensor`s should be wrapped before forwarding them into a `Module`.

```
>>> import torchvision
>>> mnist = torchvision.datasets.MNIST('./data/mnist/')
>>> x = mnist.train_data.float()
>>> x = x.view(x.size(0), -1)
>>> l = nn.Linear(x.size(1), 10)
>>> y = l(x)
/.../
RuntimeError: addmm(): argument 'mat1' (position 1) must be Variable, not torch.
      FloatTensor
>>> x = torch.autograd.Variable(x)
>>> y = l(x)
```

Conversely, results are also `Variable`s, so to retrieve a loss as an actual standard python float, one has to do

```
>>> f = torch.nn.L1Loss()
>>> u = f(Variable(Tensor([1, 2, 3])), Variable(Tensor([1, 2, 9])))
>>> u
Variable containing:
 2
[torch.FloatTensor of size 1]

>>> u.data[0]
2.0
```

⚠ Criteria do not compute the gradient with respect to the target, and will not accept a `Variable` with `requires_grad` to `True` as the target.

```
>>> f = torch.nn.MSELoss()
>>> x = Variable(Tensor([ 3, 2 ]), requires_grad = True)
>>> y = Variable(Tensor([ 0, -2 ]), requires_grad = True)
>>> f(x, y)
/.../
AssertionError: nn criterions don't compute the gradient w.r.t. targets - please mark
      these variables as volatile or not requiring gradients
```

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To do so, given a training set

$$(x_n, y_n) \in \mathbb{R}^D \times \{1, \dots, C\}, \; n = 1, \dots, N,$$

we will consider an output with as many units as there are classes, and the target will be a tensor $z \in \mathbb{R}^{N \times C}$, with -1 everywhere but for the correct labels:

$$\forall n, \; z_{n,m} = \begin{cases} 1 & \text{if } \; m = y_n \\ -1 & \text{otherwise.} \end{cases}$$

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$$\begin{pmatrix} 2 \\ 1 \\ 1 \\ 3 \\ 2 \end{pmatrix} \Rightarrow \begin{pmatrix} -1 & 1 & -1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \end{pmatrix}.$$

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Although MSE is a regression loss, using it like this gives excellent results.

Both the convolutional and pooling layers take as input batches of samples, each one being itself a 3d tensor $C \times H \times W$.

The output has the same structure, and tensors have to be explicitly reshaped before being forwarded to a fully connected layer.

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```
>>> mnist = datasets.MNIST('./data/mnist/', train = True, download = True)
>>> d = mnist.train_data
>>> d.size()
torch.Size([60000, 28, 28])
>>> x = d.view(d.size(0), 1, d.size(1), d.size(2))
>>> x.size()
torch.Size([60000, 1, 28, 28])
>>> x = x.view(x.size(0), -1)
>>> x.size()
torch.Size([60000, 784])
```

We can now put all this together and define our first convolutional network for MNIST, with two convolutional layers, and two fully-connected layers:

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Total 105,506 parameters and 1,333,200 products for the forward pass.

Creating a module

To create a `Module`, one has to inherit from the base class and implement the constructor `__init__(self, ...)` and the forward pass `forward(self, x)`.

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class Net(nn.Module):
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        self.conv1 = nn.Conv2d(1, 32, kernel_size=5)
        self.conv2 = nn.Conv2d(32, 64, kernel_size=5)
        self.fc1 = nn.Linear(256, 200)
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    def forward(self, x):
        x = F.relu(F.max_pool2d(self.conv1(x), kernel_size=3, stride=3))
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        return x
```

As long as you use autograd-compliant operations, the backward pass is implemented automatically.

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for k in model.parameters():
    print(k.size())
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torch.Size([32, 1, 5, 5])
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class Buggy(nn.Module):
    def __init__(self):
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        self.conv = nn.Conv2d(1, 32, kernel_size=5)
        self.param = Parameter(Tensor(123, 456))
        self.ouch = {}
        self.ouch[0] = nn.Linear(543, 21)

model = Buggy()

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The proper policy then is to use `Module.add_module(name, module)`

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class NotBuggyAnymore(nn.Module):
    def __init__(self):
        super(NotBuggyAnymore, self).__init__()
        self.conv = nn.Conv2d(1, 32, kernel_size=5)
        self.param = Parameter(Tensor(123, 456))
        self.add_module('ahhh_0', nn.Linear(543, 21))

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`Module.register_parameter(name, parameter)` allows to similarly register `Parameter`s explicitly.

Another option is to add modules in a field of type `nn.ModuleList`, which is a list of modules properly dealt with by PyTorch's machinery.

```
class AnotherNotBuggy(nn.Module):
    def __init__(self):
        super(AnotherNotBuggy, self).__init__()
        self.conv = nn.Conv2d(1, 32, kernel_size=5)
        self.param = Parameter(Tensor(123, 456))
        self.other_stuff = nn.ModuleList()
        self.other_stuff.append(nn.Linear(50, 75))
        self.other_stuff.append(nn.Linear(125, 999))

model = AnotherNotBuggy()

for k in model.parameters():
    print(k.size())
```

prints

```
torch.Size([123, 456])
torch.Size([32, 1, 5, 5])
torch.Size([32])
torch.Size([75, 50])
torch.Size([75])
torch.Size([999, 125])
torch.Size([999])
```

Batch processing

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

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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.

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

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

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

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

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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

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

and

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

Batch processing allows to use efficient matrix product implementations, which in particular deal properly with cache memory

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```
import torch, time

def timing(x, w, nb = 51):
    t = torch.FloatTensor(nb)

    for u in range(t.size(0)):
        t0 = time.perf_counter()
        # Batch processing
        y = x.mm(w.t())
        y.is_cuda and torch.cuda.synchronize()
        t[u] = time.perf_counter() - t0
    tb = t.median()[0][0]

    for u in range(t.size(0)):
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        # Ugly loop
        for k in range(y.size(0)): y[k] = w.mv(x[k])
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    tl = t.median()[0][0]

    print('{:s} batch vs. loop speed ratio {:.01f}'
          .format((y.is_cuda and 'GPU') or 'CPU', tl / tb))

x = torch.FloatTensor(2500, 1000).normal_()
w = torch.FloatTensor(1500, 1000).normal_()
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Prints:

```
CPU batch vs. loop speed ratio 10.0
GPU batch vs. loop speed ratio 80.7
```

Practical session:

https://fleuret.org/dlc/dlc-practical-4.pdf

The end