AMMI – Introduction to Deep Learning

4.3. PyTorch modules and batch processing

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Elements from `torch.nn.functional` are autograd-compliant functions which compute a result from provided arguments alone. This is usually imported as `F`. 
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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()`.
Functions and modules from torch.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.
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            [ 0.0557, 0.6046, 0.0864, -0.5929, 1.2606]])
>>> F.relu(x)
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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.
The module

```
torch.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 produce a tensor of size \( N \times D \).
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>>> 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.empty(523, 10).normal_()
>>> y = f(x)
>>> y.size()
torch.Size([523, 4])
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⚠️ The weights and biases are automatically randomized at creation. We will come back to that later.
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>>> y = torch.tensor([[ 0. ]])
>>> f(x, y)
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The first parameter of a loss is traditionally called the \texttt{input} and the second the \texttt{target}. These two quantities may be of different dimensions or even types for some losses (\textit{e.g.} for classification).
Criteria do not accept a tensor with `requires_grad` to `True` for target.

```python
>>> import torch
>>> f = torch.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 `torch.nn` process samples by batches. This is motivated by the computational speed-up it induces.

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 parameter have to be copied there every time it is used.
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It also cuts down the use of Python loops, which are awfully slow.
Consider a model composed of three modules

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Copying the \( x_n \)s to cache memory

Copying the \( f_d \)s’ parameters to cache memory

Computing a \( f_d(x_n) \)

Processing samples one by one:
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Processing samples one by one:

Batch processing:
def timing(x, w, batch = False, nb = 101):
    t = torch.zeros(nb)
    for u in range(0, t.size(0)):
        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.empty(2500, 1000).normal_()
w = torch.empty(1500, 1000).normal_()
print('Batch-processing speed-up on CPU %.1f' %
     (timing(x, w, batch = False) / timing(x, w, batch = True)))

x, w = x.cuda(), w.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

\[ \forall l, n, \ w^{(l)} \in \mathbb{R}^{d_l \times d_{l-1}}, \ x^{(l-1)}_n \in \mathbb{R}^{d_{l-1}}, \ s^{(l)}_n = w^{(l)} \cdot x^{(l-1)}_n. \]
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$$\forall l, n, \ w^{(l)} \in \mathbb{R}^{d_l \times d_{l-1}}, \ x_{n}^{(l-1)} \in \mathbb{R}^{d_{l-1}}, \ s_{n}^{(l)} = w^{(l)} x_{n}^{(l-1)}.$$ 

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.

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

which is an element of $$\mathbb{R}^{N \times D}.$$
To make all sample row vectors and apply a linear operator, we want

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

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And in `torch/nn/functional.py`

```python
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

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

and

\[
\left[ \frac{\partial \mathcal{L}}{\partial x(l)} \right] = \left[ \frac{\partial \ell}{\partial x(l+1)} \right] w^{(l+1)}.
\]
The end