Deep learning

4.3. PyTorch modules and batch processing

François Fleuret

https://fleuret.org/dlc/
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Usually \texttt{torch.nn.functional} is imported as \texttt{F}, and \texttt{torch.nn} as \texttt{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.
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>>> 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)
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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

`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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```python
>>> 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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```

The first parameter of a loss is traditionally called the \textbf{input} and the second the \textbf{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`.

```python
>>> 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:

<table>
<thead>
<tr>
<th>Batch size</th>
<th>Time per epoch</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4h22min</td>
</tr>
<tr>
<td>64</td>
<td>4min50s</td>
</tr>
</tbody>
</table>

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.

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**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.
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Processing samples one by one:

- Copying the \( x_n \)s to cache memory
- Copying the \( f_d \)s’ parameters to cache memory
- Computing a \( f_d(.) \)
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and we want to compute \( f(x_1), f(x_2), f(x_3) \).
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.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.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

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

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

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

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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

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which gives a tensorial expression for the full batch

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

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

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

and

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