EE-559 – Deep learning

4.3. PyTorch modules and batch processing

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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 $\mathbb{R}^C \to \mathbb{R}^D$ 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)
tensor([[ 0.8008,  0.0000,  0.5019,  0.0000,  0.0000],
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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

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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_()
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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 **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 tensor with `requires_grad` to `True` for target.

```
>>> 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.

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.

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

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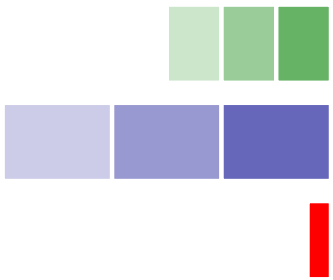
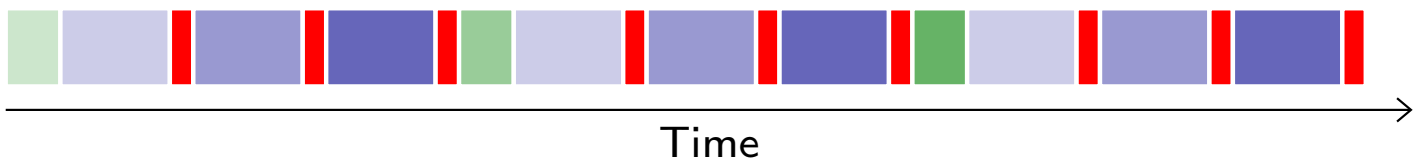


Copying the x_ns to cache memory

Copying the f_ds' parameters to cache memory

Computing a $f_d(.)$

Processing samples one by one:



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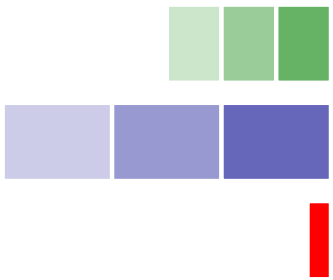

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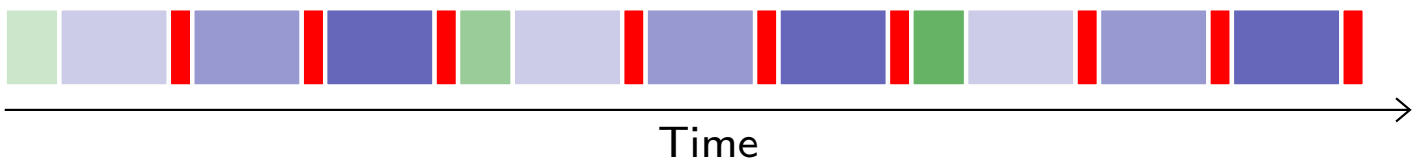

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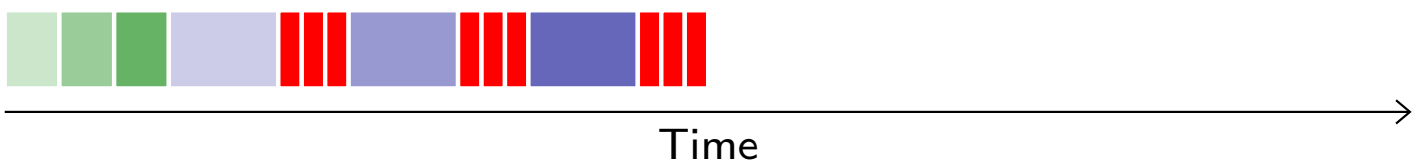

With

```
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

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

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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.

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

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

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

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

which gives a tensorial expression for the full batch

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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

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

and

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

The end