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.

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 $\mathbb{R}^C \to \mathbb{R}^D$ 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. We come back to this in a second.

Notes

For instance, given that a sample from the MNIST data-set is a 28×28 grayscale image, a minibatch of 64 samples would be stored in a tensor of size $64 \times 1 \times 28 \times 28$ and this is the type of tensors that a LeNet5 expects as input.

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 $\mathbb{R}^C \to \mathbb{R}^D$ 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**.

```
>>> 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.

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.

Notes

Let $f_1, \ldots, f_d$ be some modules of a model, and $x_1, \ldots, x_N$ be samples.
Evaluating

$$f_D(f_{D-1}(\ldots f_2(f_1(x_n)))), \quad n = 1, \ldots, N.$$

by batches is motivated by

1. an $f(x)$ can be computed only if the parameters of f and x are in the cache memory,
2. moving data into the cache memory is slower than the computation *per se*,
3. the [parameters of the] f_ds cannot all fit in the cache memory at the same time,
4. several x_n can [usually] fit in the cache memory at the same time.

Peak performance is achieved when there is no delay due to copying data to the memories. Optimizing the way copies are made to the memory is the bottleneck.
Note that this is a rough explanation of the issues related to cache memory and batch processing. There are actually multiple levels of cache, sharing between computational cores etc. Properly using highly parallel processing devics such as GPUs is a very difficult task which explains in particular the complexity of drivers and libraries such as NVIDIA's cudnn.

Consider a model composed of three modules

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

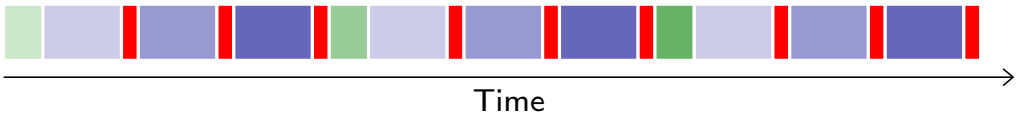
and we want to compute $f(x_1), f(x_2), f(x_3)$.

Copying the x_ns to cache memory

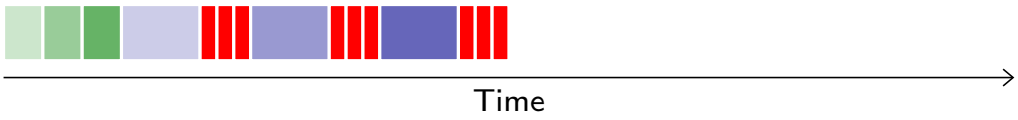
Copying the f_ds' parameters to cache memory

Computing a $f_d(.)$

Processing samples one by one:



Batch processing:



Notes

Each colored block represents and operation that takes time. Processing the samples one by one requires:

- copy sample x_1 to memory (first green),
- copy the parameters of f_1 to memory (first blue),
- compute $f_1(x_1)$ (first red),
- copy the parameters of f_2 to memory (second blue),
- apply f_2 on the previous result still in memory (second red),
- etc.

Processing the samples in the same batch, assuming that the three samples can be held in memory all together alongside the parameters of one function make the economy of copying again and again the parameters of the f_ds.
The goal of batch processing is to reuse as much as possible elements which are already in the cache memory.

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()
```


Notes

Here is an example where we compute a simple vector-matrix product. `w` are the function parameters and `x` the samples, and depending on the argument `batch` the computation is done one row at a time or in one shot, allowing the speed-up of the batch computation.

```
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

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

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.

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

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

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

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
```

Notes

$$\underbrace{\begin{bmatrix} — & s_1^{(l)} & — \\ & \vdots & \\ — & s_N^{(l)} & — \end{bmatrix}}_{s^{(l)} \in \mathbb{R}^{N \times d_l}} = \underbrace{\begin{bmatrix} — & x_1^{(l-1)} & — \\ & \vdots & \\ — & x_N^{(l-1)} & — \end{bmatrix}}_{x^{(l-1)} \in \mathbb{R}^{N \times d_{l-1}}} \underbrace{\begin{bmatrix} | & & | \\ w_1^{(l)} & \dots & w_{d_l}^{(l)} \\ | & & | \end{bmatrix}}_{w^{(l)} \in \mathbb{R}^{d_{l-1} \times d_l}}$$

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

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