Deep learning

5.3. PyTorch optimizers

François Fleuret
https://fleuret.org/dlc/
The PyTorch package `torch.optim` provides many optimizers.

An optimizer has an internal state to keep quantities such as moving averages, and operates on an iterator over `Parameters`.

- Values specific to the optimizer can be specified to its constructor, and
- its `step` method updates the internal state according to the `grad` attributes of the `Parameters`, and updates the latter according to the internal state.
We implemented the standard SGD as follows

```python
for e in range(nb_epochs):
    for b in range(0, train_input.size(0), batch_size):
        output = model(train_input[b:b+batch_size])
        loss = criterion(output, train_target[b:b+batch_size])
        model.zero_grad()
        loss.backward()
        with torch.no_grad():
            for p in model.parameters(): p -= eta * p.grad
```

which can be re-written with the `torch.optim` package as

```python
optimizer = torch.optim.SGD(model.parameters(), lr = eta)
for e in range(nb_epochs):
    for b in range(0, train_input.size(0), batch_size):
        output = model(train_input[b:b+batch_size])
        loss = criterion(output, train_target[b:b+batch_size])
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```
We have at our disposal many variants of the SGD:

- `torch.optim.SGD` (momentum, and Nesterov’s algorithm),
- `torch.optim.Adam`
- `torch.optim.Adadelta`
- `torch.optim.Adagrad`
- `torch.optim.RMSprop`
- `torch.optim.LBFGS`
- ...

An optimizer can also operate on several iterators, each corresponding to a group of `Parameters` that should be handled similarly. For instance, different layers may have different learning rates or momentums.
So to use Adam, with its default setting, we just have to replace in our example

\[
\text{optimizer} = \text{optim.SGD(model.parameters(), lr = eta)}
\]

with

\[
\text{optimizer} = \text{optim.Adam(model.parameters(), lr = eta)}
\]

⚠️ The learning rate may have to be different if the functional was not properly scaled.

Notes

In particular, Adam is often more tolerant to a higher learning rate than standard SGD, and it is good practice to try several values of learning rates.
An example putting all this together
We now have the tools to build and train a deep network:

- fully connected layers,
- convolutional layers,
- pooling layers,
- ReLU.

And we have the tools to optimize it:

- Loss,
- back-propagation,
- stochastic gradient descent.

The only piece missing is the policy to initialize the parameters.

PyTorch initializes parameters with default rules when modules are created. They normalize weights according to the layer sizes (Glorot and Bengio, 2010) and behave usually very well. We will come back to this.
We re-use our model from 4.6. “Writing a PyTorch module”.

class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 32, kernel_size = 5)
        self.conv2 = nn.Conv2d(32, 64, kernel_size = 5)
        self.fc1 = nn.Linear(256, 200)
        self.fc2 = nn.Linear(200, 10)

    def forward(self, x):
        x = F.relu(F.max_pool2d(self.conv1(x), kernel_size = 3))
        x = F.relu(F.max_pool2d(self.conv2(x), kernel_size = 2))
        x = x.view(x.size(0), -1)
        x = F.relu(self.fc1(x))
        x = self.fc2(x)
        return x
train_set = torchvision.datasets.MNIST(root = data_dir,
    train = True, download = True)
train_input = train_set.data.view(-1, 1, 28, 28).float()
train_targets = train_set.targets

lr, nb_epochs, batch_size = 1e-1, 10, 100

model = Net()

optimizer = torch.optim.SGD(model.parameters(), lr = lr)
criterion = nn.CrossEntropyLoss()

model.to(device)
criterion.to(device)
train_input, train_targets = train_input.to(device), train_targets.to(device)

mu, std = train_input.mean(), train_input.std()
train_input.sub_(mu).div_(std)

for e in range(nb_epochs):
    for input, targets in zip(train_input.split(batch_size),
        train_targets.split(batch_size)):
        output = model(input)
        loss = criterion(output, targets)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

Notes

This is the sketch of any deep learning training procedure. As we will see in 8.5. “DataLoader
and neuro-surgery”, the data is usually accessed via a torch.utils.data.DataLoader.
References