Deep learning

5.3. PyTorch optimizers

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Nov 2, 2020
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 moments.
So to use Adam, with its default setting, we just have to replace in our example

```python
optimizer = optim.SGD(model.parameters(), lr = eta)
```

with

```python
optimizer = optim.Adam(model.parameters(), lr = eta)
```

⚠️ The learning rate may have to be different if the functional was not properly scaled.
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.
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__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()
References