A brief introduction to PyTorch

IACV 2018

Computer
Vision
Lab

Prerequisites

Notion of multidimensional arrays (tensors)

NumPy basics

Perceptron (Fully-connected layer)

Convolution (Correlation filter)

PyTorch vs TensorFlow (as of 2018)

- Both are powerful tools
- A matter of preference

- **PyTorch** is gaining traction in ML community
- PyTorch is easier for toy and research projects
- Clear “pythonic” API

- **TensorFlow** is great for deploying models in production
- TensorFlow graph definition API may incur engineering debt
- More than one way to do things

PyTorch tensor conventions

Images: 4D tensors with shape `(batch, channels, height, width)`

Labels: 1D tensors with shape `(batch, )`

Calling conventions: `torch.sum(a)` vs `a.sum()`

torch.nn.Dataset

A base class to wrap any dataset.

Each split (**train**, **test**) must be wrapped separately.

Two methods to implement:

- `__len__`: return length of dataset
- `__getitem__`: return an item, in our case - a tuple (image, label)

```
class MyArrayDataset(Dataset):
    def __init__(self, X, y):
        self.X = X
        self.y = y

    def __len__(self):
        return self.X.shape[0]

    def __getitem__(self, index):
        return self.X[index],
               self.y[index]
```

torch.nn.DataLoader

A wrapper around a class, derived from **`Dataset`** class

- Performs synchronous shuffling of the dataset samples
- Assembles samples into minibatches

```
loader = DataLoader(dataset, batch_size, shuffle, drop_last)
```

- Batch size - how many samples will be returned in one iteration
- Shuffle - whether to randomize samples, or address dataset in order
- Drop last - whether to return incomplete batch upon reaching dataset end

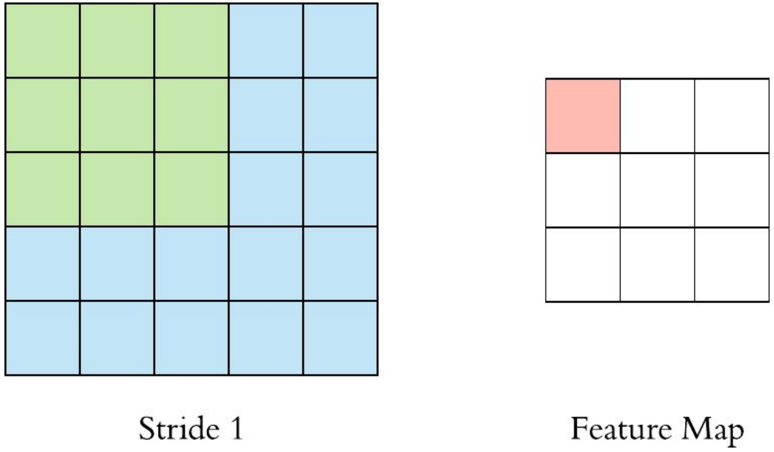
torch.nn.Module

- A parent class to all building blocks:
  - `torch.nn.Linear` - a fully connected layer
  - `torch.nn.Conv2d` - convolutional filter for 2D images
  - `torch.nn.MaxPool2d` - maximum pooling for 2D images (no learnable parameters)
  - `torch.nn.ReLU` - elementwise activation function (no learnable parameters)
- Also a parent class to compositions:
  - `torch.nn.Sequential(block1, block2, ...)` - chain of modules
- Also a parent class to your network:
  - Any building block with trainable parameters (convolution weights, batchnorm statistics) must be defined in class construction: `def __init__(self)`
  - Data flow goes in `def forward(self, *input)`
- `forward` function must compute everything using `torch.*` tensor ops
- **Backward** derivatives are computed automagically (*)

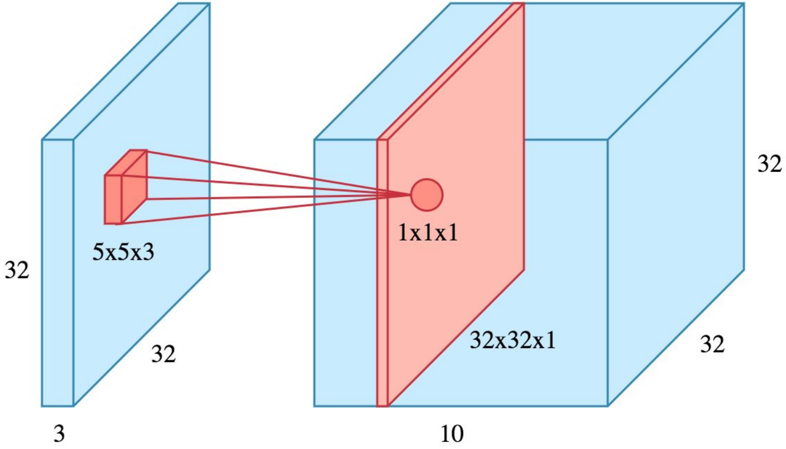
torch.nn.Conv2d

`nn.Conv2d: in_channels, out_channels, kernel_size, padding, bias`

in_channels=1, out_channels=1,
kernel_size=3, padding=0



in_channels=3, out_channels=10,
kernel_size=5, padding=2

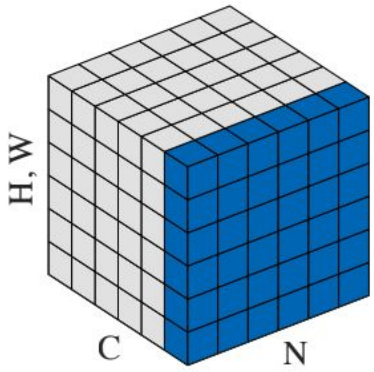


Images courtesy of [Arden Dertat](https://towardsdatascience.com/applied-deep-learning-part-4-convolutional-neural-networks-584bc134c1e2) https://towardsdatascience.com/applied-deep-learning-part-4-convolutional-neural-networks-584bc134c1e2

torch.nn.BatchNorm2d

nn.BatchNorm2d: `num_features`

- Mutually exclusive with bias in convolution
- Number of features must be same as the number of output features in preceding conv2d



Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

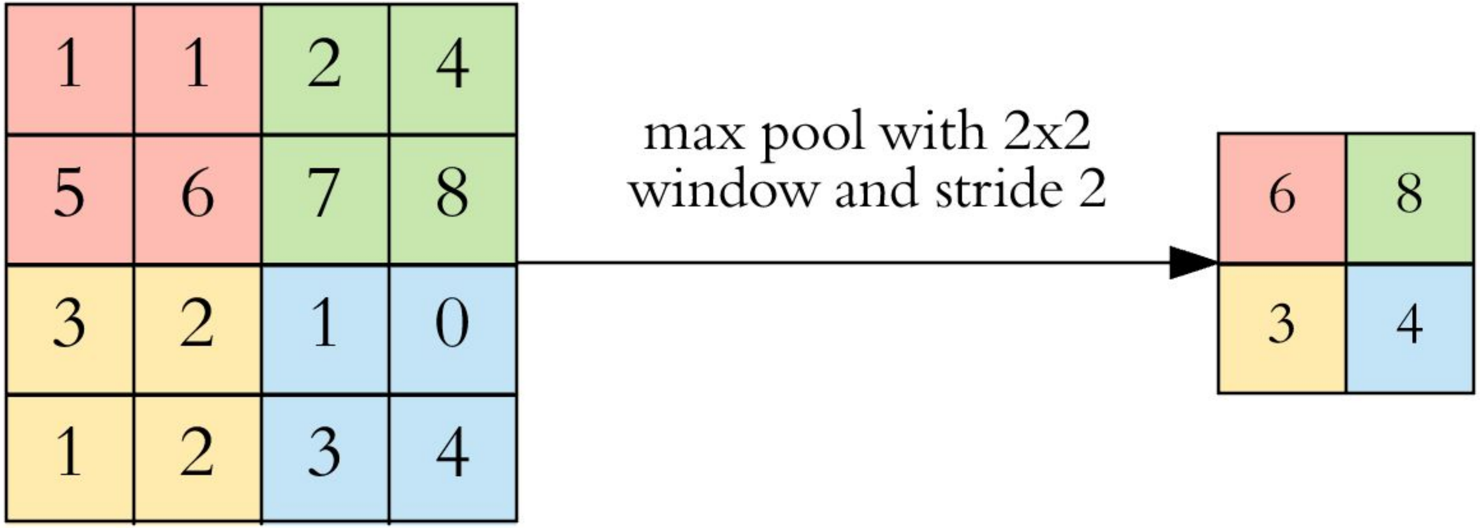
$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\boxed{\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}} \qquad \text{// normalize}$$

$$y_i \leftarrow \underline{\gamma\widehat{x}_i + \beta} \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

torch.nn.MaxPool2d

nn.MaxPool2d: `kernel_size, stride`



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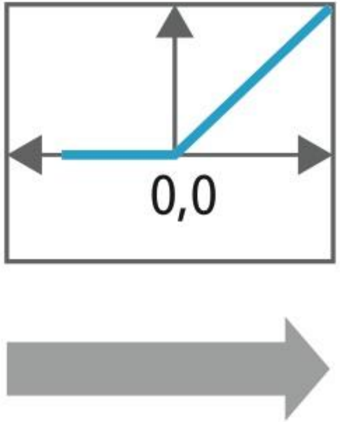
torch.nn.ReLU

`nn.ReLU`: no parameters

15	20	-10	35
18	-110	25	100
20	-15	25	-10
101	75	18	23



15	20	0	35
18	0	25	100
20	0	25	0
101	75	18	23

torch.nn.CrossEntropyLoss

`nn.CrossEntropyLoss: no parameters;  loss(y_hat, y)`

- Includes SoftMax activation for convenience
- Argument order matters!

$$\begin{bmatrix}1.2\\0.9\\0.4\end{bmatrix} \longrightarrow \boxed{\text{Softmax}} \longrightarrow \begin{bmatrix}0.46\\0.34\\0.20\end{bmatrix}$$

$$\hat{\mathbf{y}} \qquad\qquad\qquad\qquad\qquad \mathbf{y}$$

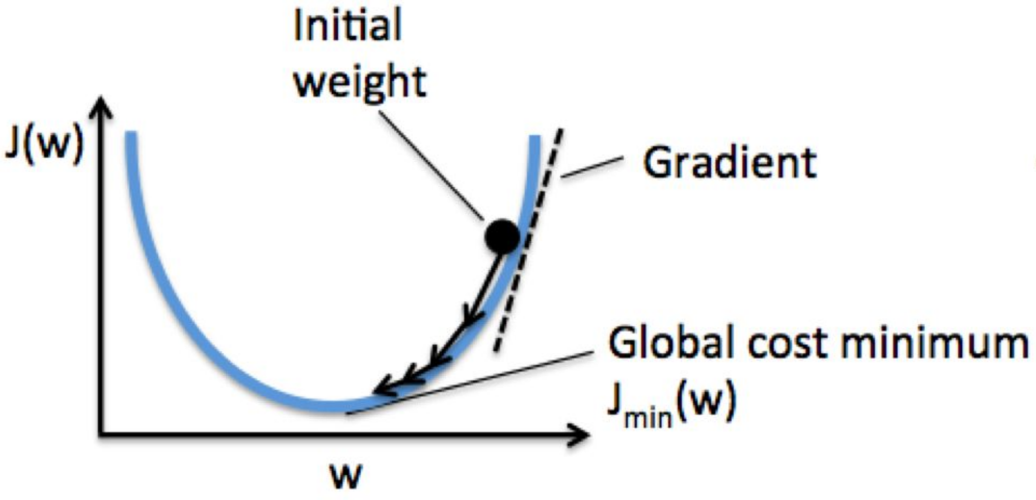
$$\begin{bmatrix}0.1\\0.5\\0.4\end{bmatrix} \quad D(\hat{\mathbf{y}}, \mathbf{y}) = -\sum_j y_j \ln \hat{y}_j \quad \begin{bmatrix}0\\1\\0\end{bmatrix}$$

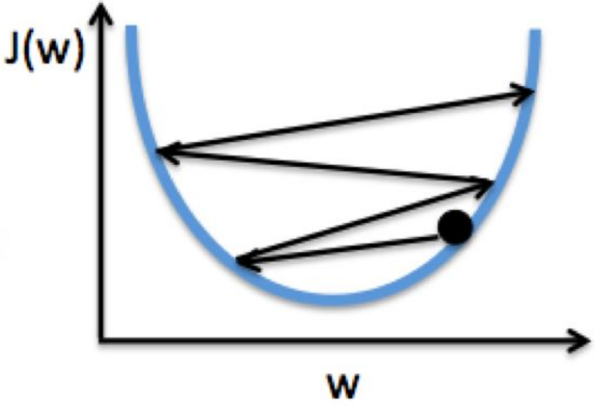
$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} \qquad \text{for } j = 1, \ldots, K$$

$$CE = -\sum_x p(x) \log q(x)$$

torch.nn.Optimizer

optim.SGD: `weights, lr`





CNN Model with one convolutional layer

```python
class CNN(nn.Module):
    def __init__(self, num_out_classes):
        super(CNN, self).__init__()
        self.op_conv = nn.Conv2d(
            in_channels=3, out_channels=20, \
            kernel_size=3, padding=1, bias=False)
        self.op_batchnorm = nn.BatchNorm2d(num_features=20)
        self.op_activation = nn.ReLU()

   def forward(self, x):
       x = self.op_conv(x)
       x = self.op_batchnorm(x)
       x = self.op_activation(x)
       return x
```

Typical PyTorch training loop

```
for epoch in range(num_epochs):
    for batch in loader_train:
        X_batch, y_batch = batch
        optimizer.zero_grad()       # zero the gradients
        y_hat_batch = cnn(X_batch) # forward pass
        loss = criterion(y_hat_batch, y_batch)
        loss.backward()             # backward pass
        optimizer.step()            # update parameters
```

Keep in mind

- Create separate cells to print tensors content (also from different cells)
- When in doubt, `print(tensor.shape)`
- Tensor operations can be invoked two ways: `tensor.sum()` `torch.sum(tensor)`
- Construct network from building blocks: `torch.nn.[Linear, Conv2d, MaxPool2d, ReLU, Linear]`
- Before running jupyter notebook, activate ex3 conda environment: `> source activate ex3`
- Comprehensive reference: https://pytorch.org/docs/stable/torch.html