Introduction to PyTorch

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Why PyTorch?

- Relatively new (Aug. 2016?) Python toolkit based on Torch
- Overwhelmingly positive reception by the deep learning community. See e.g. `http://www.fast.ai/2017/09/08/introducing-pytorch-for-fastai/`
- *Dynamic* computation graphs:
  - *"process complex inputs and outputs, without worrying to convert every batch of input into a big fat tensor"*
    E.g. sequences with different length
  - Control structures, sampling
- Flexibility to implement low-level and high-level functionality.
- Modularization uses object orientation.

Tensors

- Tensors hold data
- Similar to numpy arrays

```
# 'Unitialized' Tensor with values from  memory:
x = torch.Tensor(5, 3)
# Randomly initialized Tensor (values in [0..1]):
y = torch.rand(5, 3)
print(x + y)
```

Output:

```
0.9404  1.0569  1.1124
 0.3283  1.1417  0.6956
 0.4977  1.7874  0.2514
 0.9630  0.7120  1.0820
 1.8417  1.1237  0.1738
[torch.FloatTensor of size 5x3]
```

- In-place operations can increase efficiency: `y.add_(x)`
- 100+ Tensor operations: `http://pytorch.org/docs/master/torch.html`

Tensors ↔ NumPy

```
import torch
a = torch.ones(5)
b = a.numpy()
print(b)
```

Output:

```
[ 1.  1.  1.  1.  1.]
```

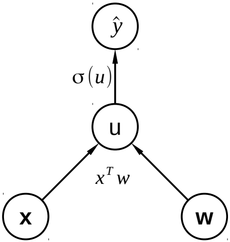
```
import numpy as np
a = np.ones(3)
b = torch.from_numpy(a)
print(b)
```

Output:

```
 1
 1
 1
[torch.DoubleTensor of size 3]
```

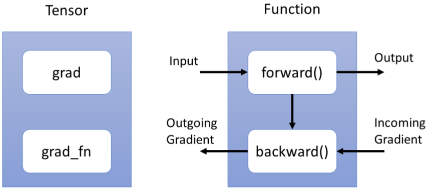
Automatic differentiation

- Central concept: `Tensor` class
- a Tensor corresponds to a node in a function graph
- If you set `my_tensor.requires_grad=True`, all operations are tracked, and gradients can be computed automatically



Functional composition

- If a Tensor was created by functional composition (`x = a + b`), then `my_function = x.grad_fn` references the function
  (For example, `ThAddBackward` corresponds to Tensor addition)
- `x.backward()` computes the gradient for the tensor (and, recursively, for all input tensors). The values of the gradient computation are then stored in `a.grad`, `b.grad` and `x.grad`
- `my_function.forward()` method:
  Computes (Tensor) output value from input Tensors
- `my_function.backward()` method:
  Provides the gradient for the function. It is used in the recursive gradient computation (`x.backward()`) via the chain rule.



Automatic differentiation: Example

```
# Set requires_grad=True, if gradient is to be computed
x = Variable(3 * torch.ones(1), requires_grad=True)
y = x + 2*x**2
y.backward()
```

Value of `x.grad`?

Defining a neural network

- A self-defined neural net should inherit from `nn.Module`
- `torch.nn` contains predefined layers:
  - `nn.Linear(input_size, output_size)`, `nn.Conv2d(in_channels, out_channels, kernel_size)`, ...
  - Set layers as class attributes:
  - All parameter Tensors get automatically registered with the neural net (can be accessed by `net.parameters()`)
- Functions without learnable paramters (`torch.nn.functional`) do not have to be registered as class attributes:
  - `relu(...)`, `tanh(...)`, ...
- Prediction needs to be implemened in `net.forward(...)`

```
class Net(nn.Module):
    def __init__(self, num_features, hidden_size):
        super(Net, self).__init__()
        # self.learnable_layer = ...

    def forward(self, x):
        return # do prediction
```

Linear Regression

- What is layer and learnable parameters?
- How to do prediction?

Linear Regression

```
import torch.nn as nn

class LinearRegression(nn.Module):
    def __init__(self, num_features):
        super(LinearRegression, self).__init__()
        self.linear_layer = nn.Linear(num_features, 1)

    def forward(self, x):
        return self.linear_layer(x)
```

Linear Regression: prediction for one instance (with untrained model)

- `x_instance`: features, torch.FloatTensor of size 10 (`num_features`)
- `y_instance`: label, torch.FloatTensor of size 1
- Type of `y_predicted`?

```
num_features = 10
lr_model = LinearRegression(num_features)
y_predicted = lr_model.forward(x_tensor)
```

Linear Regression: training the model

- Loss function: Define yourself or pre-defined.
  - `loss=(y_var-y_predicted)**2`
  - ```
    criterion = nn.MSELoss()
    loss = criterion(y_var, y_predicted)
    ```
- Training update: Define yourself or pre-defined.
  - ```
    loss.backward()
    for w in lr_model.parameters():
      w.sub_(f.grad.data * 0.0001) # subtract gradient
    ```
  - ```
    optimizer = optim.SGD(lr_model.parameters(), lr=0.0001)
    ...
    loss.backward()
    optimizer.step()
    ```
- Note:
  - Gradients are accumulated (added) in the Tensors for each call of `.backward()`
  - need to be set to zero for next gradient update
  - `optimizer.zero_grad()` sets gradients of all network Variables to zero
    ```

Linear Regression: training the model

```
lr_model = LinearRegression(num_features)
optimizer = optim.SGD(lr_model.parameters(), lr=0.0001)
criterion = nn.MSELoss()
for epoch in range(num_epochs):
    for x_instance, y_instance in data:
        y_pred = lr_model.forward(x_instance)
        optimizer.zero_grad()
        loss = criterion(y_pred, y_instance)
        loss.backward()
        optimizer.step()
```

Comments:

- Here, we are using only 1 example at a time for our updates.
- Instead of using plain SGD, there are better learning methods that can adapt their learning rate per parameter (e.g. *Adam*)
- Question: `step()` does not take any arguments. How does it know which parameters to update?

Materials

- http://pytorch.org/tutorials/beginner/deep_learning_60min_blitz.html
- http://pytorch.org/tutorials/beginner/pytorch_with_examples.html
- http://pytorch.org/tutorials/beginner/deep_learning_nlp_tutorial.html

Homework

- Learn regression models for predicting house prices.
- Derivation of gradient for logistic regression.

Homework: Boston house prices prediction

- Dataset:
  - Harrison & Rubinfeld, 1978
  - Predict median house price (in 1000USD) per district/town.
  - 506 instances, 13 features
- Features:
  - CRIM per capita crime rate by town
  - ZN proportion of residential land zoned for lots over 25,000 sq.ft.
  - INDUS proportion of non-retail business acres per town
  - CHAS Charles River dummy variable ($= 1$ if tract bounds river; 0 otherwise)
  - NOX nitric oxides concentration (parts per 10 million)
  - RM average number of rooms per dwelling
  - AGE proportion of owner-occupied units built prior to 1940
  - DIS weighted distances to five Boston employment centres
  - RAD index of accessibility to radial highways
  - TAX full-value property-tax rate per $10,000$ USD
  - PTRATIO pupil-teacher ratio by town B $1000(Bk - 0.63)^2$ where Bk is the proportion of blacks by town
  - LSTAT % lower status of the population

Homework: Boston houses prediction

- Linear regression:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x} + \mathbf{b}$$

- Neural network regression (one hidden layer, ReLu activation):

$$\hat{\mathbf{y}} = \mathbf{W}_B max(\mathbf{0}, \mathbf{W}_A\mathbf{x} + \mathbf{b}_A) + \mathbf{b}_B$$