THE DATA SCIENCE LAB

Neural Regression Using PyTorch: Model Accuracy

Dr. James McCaffrey of Microsoft Research explains how to evaluate, save and use a trained regression model, used to predict a single numeric value such as the annual revenue of a new restaurant based on variables such as menu prices, number of tables, location and so on.

By James McCaffrey 03/12/2021

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The goal of a regression problem is to predict a single numeric value, for example, predicting the annual revenue of a new restaurant based on variables such as menu prices, number of tables, location and so on. There are several classical statistics techniques for regression problems. Neural regression solves a regression problem using a neural network. This article is the fourth in a series of four articles that present a complete end-to-end production-quality example of neural regression using PyTorch. The recurring example problem is to predict the price of a house based on its area in square feet, air conditioning (yes or no), style ("art_deco," "bungalow," "colonial") and local school ("johnson," "kennedy," "lincoln").

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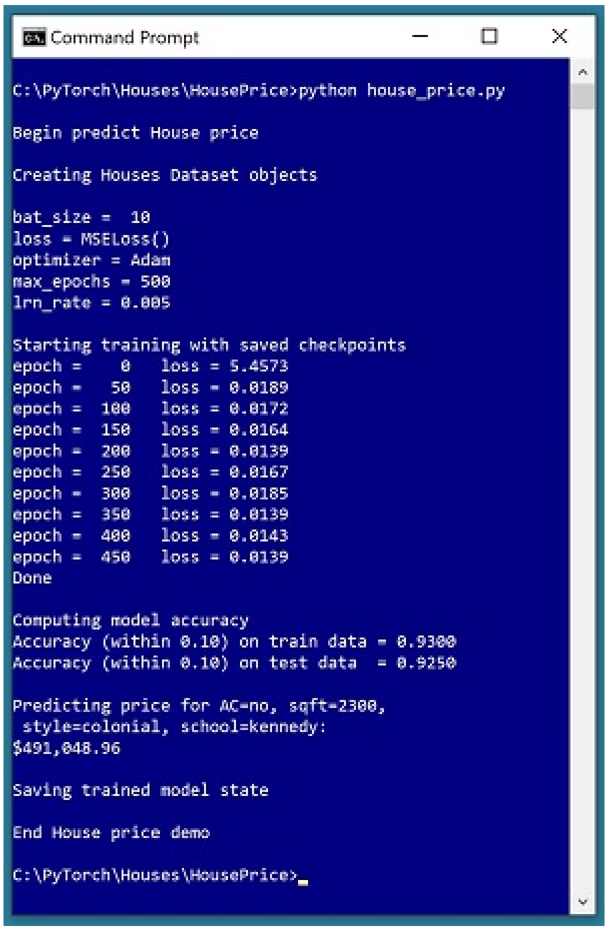
The process of creating a PyTorch neural network for regression consists of six steps:

1. Prepare the training and test data
2. Implement a Dataset object to serve up the data in batches
3. Design and implement a neural network
4. Write code to train the network
5. Write code to evaluate the model (the trained network)
6. Write code to save and use the model to make predictions for new, previously unseen data

Each of the six steps is complicated. And the six steps are tightly coupled which adds to the difficulty. This article covers the fifth and sixth steps -- evaluating, saving, and using a trained regression model.

A good way to see where this series of articles is headed is to take a look at the screenshot of the demo program in **Figure 1**. The demo begins by creating Dataset and DataLoader objects which have been designed to work with the house data. Next, the demo creates an 8-(10-10)-1 deep neural network. The demo prepares training by setting up a loss function (mean squared error), a training optimizer function (Adam) and parameters for training (learning rate and max epochs).



```
C:\PyTorch\Houses\HousePrice>python house_price.py

Begin predict House price

Creating Houses Dataset objects

bat_size =  10
loss = MSELoss()
optimizer = Adam
max_epochs = 500
lrn_rate = 0.005

Starting training with saved checkpoints
epoch =    0   loss = 5.4573
epoch =   50   loss = 0.0189
epoch =  100   loss = 0.0172
epoch =  150   loss = 0.0164
epoch =  200   loss = 0.0139
epoch =  250   loss = 0.0167
epoch =  300   loss = 0.0185
epoch =  350   loss = 0.0139
epoch =  400   loss = 0.0143
epoch =  450   loss = 0.0139
Done

Computing model accuracy
Accuracy (within 0.10) on train data = 0.9300
Accuracy (within 0.10) on test data  = 0.9250

Predicting price for AC=no, sqft=2300,
 style=colonial, school=kennedy:
$491,048.96

Saving trained model state

End House price demo

C:\PyTorch\Houses\HousePrice>_
```

[Click on image for larger view.]
Figure 1: Predicting the Price of a House Using Neural Regression

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The demo trains the neural network for 500 epochs in batches of 10 items. An epoch is one complete pass through the training data. The training data has 200 items, therefore, one training epoch consists of processing 20 batches of 10 training items.

During training, the demo computes and displays a measure of the current error (also called loss) every 50 epochs. Because error slowly decreases, it appears that training is succeeding. Behind the scenes, the demo program saves checkpoint information after every 50 epochs so that if the training machine crashes, training can be resumed without having to start over from the beginning.

After training the network, the demo program computes the prediction accuracy of the model based on whether or not the predicted house price is within 10 percent of the true house price. The accuracy on the training data is 93.00 percent (186 out of 200 correct) and the accuracy on the test data is 92.50 percent (37 out of 40 correct). Because the two accuracy values are similar, it is likely that model overfitting has not occurred.

Next, the demo uses the trained model to make a prediction on a new, previously unseen house. The raw input is (air conditioning = "no", square feet area = 2300, style = "colonial", school = "kennedy"). The raw input is normalized and encoded as (air conditioning = -1, area = 0.2300, style = 0,0,1, school = 0,1,0). The computed output price is 0.49104896 which is equivalent to $491,048.96 because the raw house prices were all normalized by dividing by 1,000,000.

The demo program concludes by saving the trained model using the state dictionary approach. This is the most common of three standard techniques.

This article assumes you have an intermediate or better familiarity with a C-family programming language, preferably Python, but doesn't assume you know very much about PyTorch. The complete source code for the demo program, and the two data files used, are available in the download that accompanies this article. All normal error checking code has been omitted to keep the main ideas as clear as possible.

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To run the demo program, you must have Python and PyTorch installed on your machine. The demo programs were developed on Windows 10 using the Anaconda 2020.02 64-bit distribution (which contains Python 3.7.6) and PyTorch version 1.7.0 for CPU installed via pip. You can find detailed step-by-step installation instructions for this configuration in my **blog post**.

The House Data

The raw House data is synthetic and was generated programmatically. There are a total of 240 data items, divided into a 200-item training dataset and a 40-item test dataset. The raw data looks like:

```
no    1275   bungalow   $318,000.00   lincoln
yes   1100   art_deco   $335,000.00   johnson
no    1375   colonial   $286,000.00   kennedy
yes   1975   bungalow   $512,000.00   lincoln
. . .
no    2725   art_deco   $626,000.00   kennedy
```

Each line of tab-delimited data represents one house. The value to predict, house price, is in 0-based column [3]. The predictors variables in columns [0], [1], [2] and [4] are air conditioning yes-no, area in square feet, architectural style and local school. For simplicity, there are just three house styles and three schools.

House area values were normalized by dividing by 10,000 and house prices were normalized by dividing by 1,000,000. Air conditioning was binary encoded as no = -1, yes = +1. Style was one-hot encoded as "art_deco" = (1,0,0), "bungalow" = (0,1,0), "colonial" = (0,0,1). School was one-hot encoded as "johnson" = (1,0,0), "kennedy" = (0,1,0), "lincoln" = (0,0,1). The resulting normalized and encoded data looks like:

```
-1   0.1275   0 1 0   0.3180   0 0 1
 1   0.1100   1 0 0   0.3350   1 0 0
-1   0.1375   0 0 1   0.2860   0 1 0
 1   0.1975   0 1 0   0.5120   0 0 1
. . .
-1   0.2725   1 0 0   0.6260   0 1 0
```

After the structure of the training and test files was established, I designed and coded a PyTorch Dataset class to read the house data into memory and serve the data up in batches using a PyTorch DataLoader object. A Dataset class definition for the normalized and encoded House data is shown in **Listing 1**.

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Listing 1: A Dataset Class for the Student Data

```
    tmp_x = all_xy[:,[0,1,2,3,4,6,7,8]]
    tmp_y = all_xy[:,5].reshape(-1,1)    # 2-D

    self.x_data = T.tensor(tmp_x, \
      dtype=T.float32).to(device)
    self.y_data = T.tensor(tmp_y, \
      dtype=T.float32).to(device)

  def __len__(self):
    return len(self.x_data)

  def __getitem__(self, idx):
    preds = self.x_data[idx,:]  # or just [idx]
    price = self.y_data[idx,:]
    return (preds, price)       # tuple of matrices
```

Preparing data and defining a PyTorch Dataset is not trivial. You can find the article that explains how to create Dataset objects and use them with DataLoader objects **here**.

The Neural Network Architecture

In the previous **article** in this series, I described how to design and implement a neural network for regression for the House data. One possible definition is presented in **Listing 2**. The code defines an 8-(10-10)-1 neural network with relu() activation on the hidden nodes.

Listing 2: A Neural Network for the Student Data

```
    self.hid1 = T.nn.Linear(8, 10)  # 8-(10-10)-1
    self.hid2 = T.nn.Linear(10, 10)
    self.oupt = T.nn.Linear(10, 1)

    T.nn.init.xavier_uniform_(self.hid1.weight)
    T.nn.init.zeros_(self.hid1.bias)
    T.nn.init.xavier_uniform_(self.hid2.weight)
    T.nn.init.zeros_(self.hid2.bias)
    T.nn.init.xavier_uniform_(self.oupt.weight)
    T.nn.init.zeros_(self.oupt.bias)

  def forward(self, x):
    z = T.relu(self.hid1(x))
    z = T.relu(self.hid2(z))
    z = self.oupt(z)  # no activation
    return z
```

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If you are new to PyTorch, the number of design decisions for a neural network can seem intimidating. But with every program you write, you learn which design decisions are important and which don't affect the final prediction model very much, and the pieces of the design puzzle eventually fall into place.

The Overall Program Structure

The overall structure of the PyTorch neural regression program, with a few minor edits to save space, is shown in **Listing 3**. I prefer to indent my Python programs using two spaces rather than the more common four spaces.

Listing 3: The Structure of the Demo Program

```
def main():
  # 0. get started
  print("Begin predict House price ")
  T.manual_seed(4)
  np.random.seed(4)

  # 1. create Dataset and DataLoader objects
  # 2. create neural network
  # 3. train network
  # 4. evaluate model
  # 5. make a prediction
  # 6. save model
  print("End House price demo ")

if __name__== "__main__":
  main()
```

It's important to document the versions of Python and PyTorch being used because both systems are under continuous development. Dealing with versioning incompatibilities is a significant headache when working with PyTorch and is something you should not underestimate.

I like to use "T" as the top-level alias for the torch package. Most of my colleagues don't use a top-level alias and spell out "torch" many of times per program. Also, I use the full form of sub-packages rather than supplying aliases such as "import torch.nn.functional as functional." In my opinion, using the full form is easier to understand and less error-prone than using many aliases.

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The demo program defines a program-scope CPU device object. I usually develop my PyTorch programs on a desktop CPU machine. After I get that version working, converting to a CUDA GPU system only requires changing the global device object to T.device("cuda") plus a minor amount of debugging.

The demo program defines just one helper method, accuracy(). All of the rest of the program control logic is contained in a single main() function. It is possible to define other helper functions such as train_net(), evaluate_model() and save_model(), but in my opinion this modularization approach unexpectedly makes the program more difficult to understand rather than easier to understand.

Saving Checkpoints

In almost all non-demo scenarios, it's a good idea to periodically save the state of the network during training so that if your training machine crashes, you can recover without having to start from scratch. The demo program shown running in **Figure 1** saves checkpoints using these statements:

```
if epoch % 50 == 0:
  dt = time.strftime("%Y_%m_%d-%H_%M_%S")
  fn = ".\\Log\\" + str(dt) + str("-") + \
   str(epoch) + "_checkpoint.pt"
  info_dict = {
    'epoch' : epoch,
    'net_state' : net.state_dict(),
    'optimizer_state' : optimizer.state_dict()
  }
  T.save(info_dict, fn)
```

A checkpoint is saved every 50 epochs. A file name that looks like "2021_03_25-10_32_57-700_checkpoint.pt" is created. The file name contains the date (March 25, 2021), time (10:32 and 57 seconds AM), and epoch (700). The network state information is stored in a Dictionary object. The code assumes that there is an existing directory named Log. You must save the network state and the optimizer state. You can optionally save other information such as the epoch, and the states of the NumPy and PyTorch random number generators.

If the training machine crashes, you can recover training with code like:

```
fn = ".\\Log\\2021_03_25-10_32_57-700_checkpoint.pt"
chkpt = T.load(fn)
net = Net().to(device)
net.load_state_dict(chkpt['net_state'])
optimizer.load_state_dict(chkpt['optimizer_state'])
  . . .
epoch_saved = chkpt['epoch'] + 1
for epoch in range(epoch_saved, max_epochs):
  T.manual_seed(1 + epoch)
  # resume training as usual
```

If you want to recover training exactly as it would be if your machine hadn't crashed, which is usually the case, you must set the PyTorch random number generator seed value on each training epoch. This is necessary because DataLoader uses the PyTorch random number generator to serve up training items in a random order, and as of PyTorch version 1.7, there is no built-in way to save the state of a DataLoader object. If you don't set the PyTorch random seed in each epoch, you can recover from a crash. But the resulting training will be slightly different than if your machine had not crashed because the DataLoader will start using a different batch of training items.

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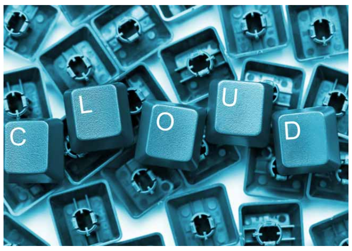

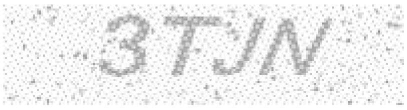

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