PyTorch Tutorial

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Installing PyTorch

- 💻 On your own computer
  - Anaconda/Miniconda: `conda install pytorch -c pytorch`
  - Others via pip: `pip3 install torch`

- 🌐 On Princeton CS server (`ssh cycles.cs.princeton.edu`)
  - Non-CS students can request a *class account*.
  - Miniconda is highly recommended, because:
    - It lets you manage your own Python installation
    - It installs locally; no admin privileges required
    - It's lightweight and fits within your disk quota
  - Instructions:
    - `wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh`
    - `chmod u+x ./Miniconda3-latest-Linux-x86_64.sh`
    - `./Miniconda3-latest-Linux-x86_64.sh`
    - After Miniconda is installed: `conda install pytorch -c pytorch`

Writing code

- Up to you; feel free to use emacs, vim, PyCharm, etc. if you want.
- Our recommendations:

Jupyter Notebook

Also try Jupyter Lab!

- Install: `conda/pip3 install jupyter`
- 💻 Run on your computer
  - `jupyter notebook`
- 🌐 Run on Princeton CS server
  - Pick any 4-digit number, say 1234
  - 🌐 `hostname -s`
  - 🌐 `jupyter notebook --no-browser --port=1234`
  - 💻 `ssh -N -L 1234:localhost:1234 __@__.cs.princeton.edu`
  - First blank is username, second is hostname

VS Code

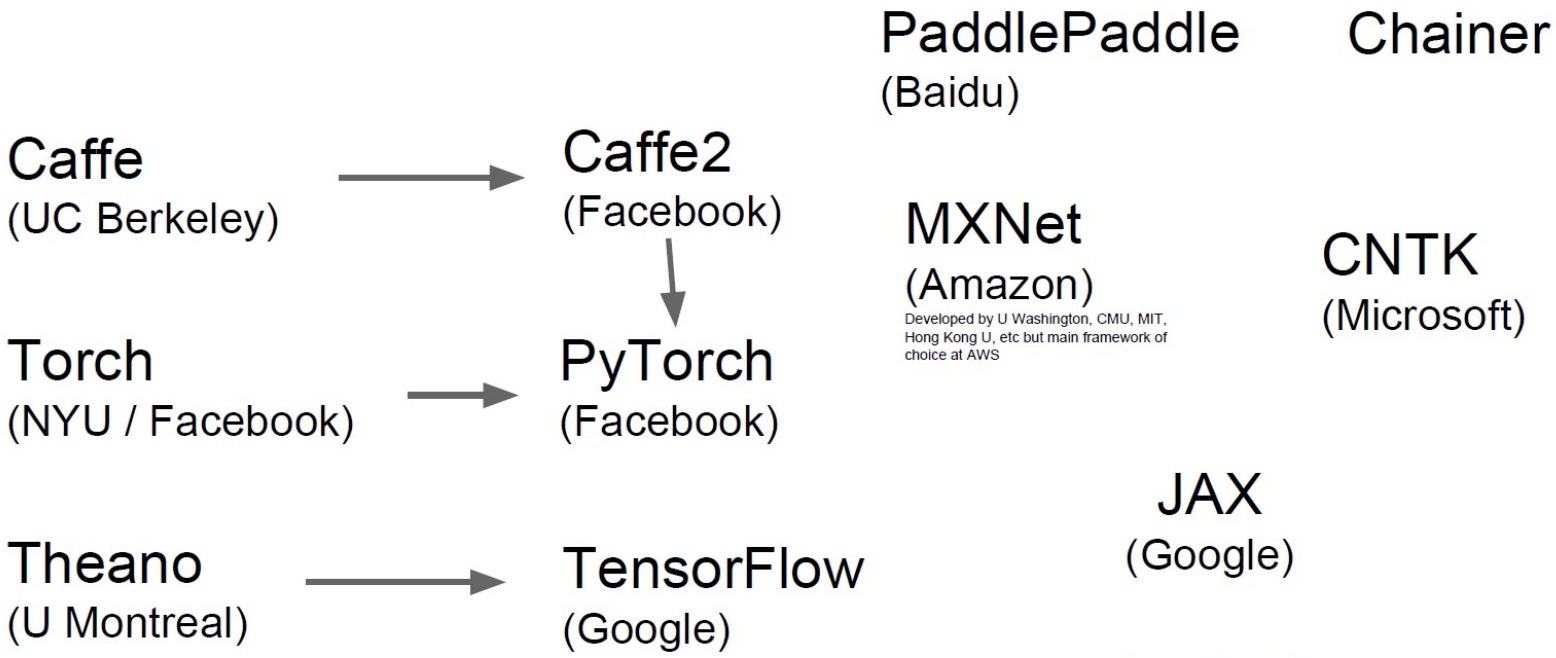
- Install the *Python* extension.
- 🌐 Install the *Remote Development* extension.
- Python files can be run like Jupyter notebooks by delimiting cells/sections with #%%
- Debugging PyTorch code is just like debugging any other Python code: see Piazza @108 for info.

Why talk about libraries?

- Advantage of various deep learning frameworks
  - Quick to develop and test new ideas
  - Automatically compute gradients
  - Run it all efficiently on GPU to speed up computation

Various Frameworks

- Various Deep Learning Frameworks



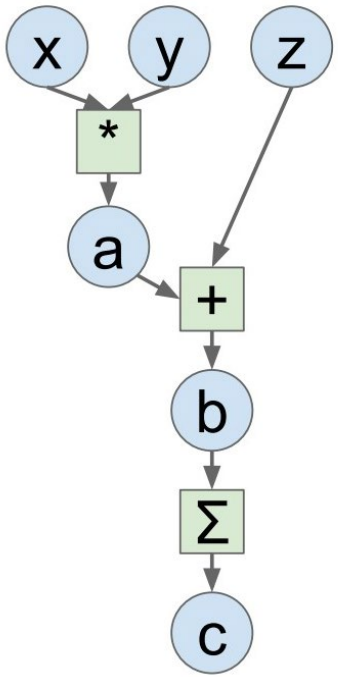
- Focus on PyTorch in this session.

Source: CS231n slides

Preview: (and advantages)

- Preview of Numpy & PyTorch & Tensorflow

Computation Graph



Numpy

```
import numpy as np
np.random.seed(0)

N, D = 3, 4

x = np.random.randn(N, D)
y = np.random.randn(N, D)
z = np.random.randn(N, D)

a = x * y
b = a + z
c = np.sum(b)

grad_c = 1.0
grad_b = grad_c * np.ones((N, D))
grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
grad_y = grad_a * x
```

Tensorflow

```
import numpy as np
np.random.seed(0)
import tensorflow as tf

N, D = 3, 4

with tf.device('/gpu:0'):
    x = tf.placeholder(tf.float32)
    y = tf.placeholder(tf.float32)
    z = tf.placeholder(tf.float32)

    a = x * y
    b = a + z
    c = tf.reduce_sum(b)

grad_x, grad_y, grad_z = tf.gradients(c, [x, y, z])

with tf.Session() as sess:
    values = {
        x: np.random.randn(N, D),
        y: np.random.randn(N, D),
        z: np.random.randn(N, D),
    }
    out = sess.run([c, grad_x, grad_y, grad_z],
                   feed_dict=values)
    c_val, grad_x_val, grad_y_val, grad_z_val = out
```

PyTorch

```
import torch

N, D = 3, 4

x = torch.rand((N, D),requires_grad=True)
y = torch.rand((N, D),requires_grad=True)
z = torch.rand((N, D),requires_grad=True)

a =x * y
b =a + z
c=torch.sum(b)

c.backward()
```

Advantages (continued)

- Which one do you think is better?

Advantages (continued)

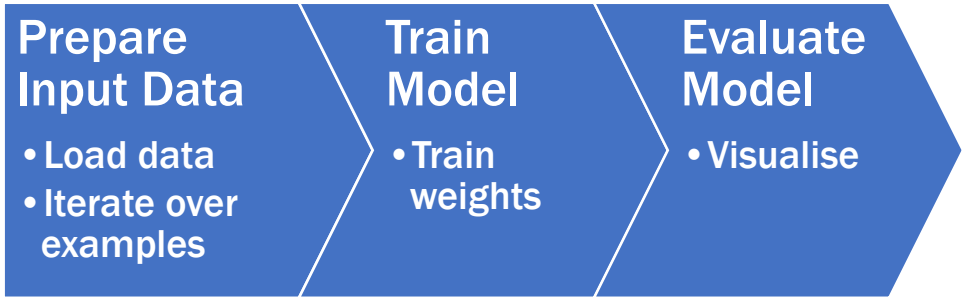
- Which one do you think is better?

PyTorch!

- **Easy Interface** – easy to use API. The code execution in this framework is quite easy. Also need a fewer lines to code in comparison.
  - It is easy to debug and understand the code.
- **Python usage** – This library is considered to be Pythonic which smoothly integrates with the Python data science stack.
  - It can be considered as NumPy extension to GPUs.
- **Computational graphs** – PyTorch provides an excellent platform which offers dynamic computational graphs. Thus a user can change them during runtime.
  - It includes many layers as Torch.
  - It includes lot of loss functions.
  - It allows building networks whose structure is dependent on computation itself.
  - **NLP**: account for variable length sentences. Instead of padding the sentence to a fixed length, we create graphs with different number of LSTM cells based on the sentence's length.

PyTorch

- Fundamental Concepts of PyTorch
  - Tensors
  - Autograd
  - Modular structure
    - Models / Layers
    - Datasets
    - Dataloader
  - Visualization Tools like
    - *TensorboardX* (monitor training)
    - *PyTorchViz* (visualise computation graph)
  - Various other functions
    - loss (MSE,CE etc..)
    - optimizers



Tensor

- **Tensor?**
- PyTorch Tensors are just like numpy arrays, but they can run on GPU.
- Examples:

```python
import numpy
# create a tensor
new_numpy = numpy.array([[1, 2], [3, 4]])
# create a 2 x 3 tensor with random values
empty_numpy = numpy.random.rand(2,3)
# create a 2 x 3 tensor with random values between -1 and 1
uniform_numpy = numpy.reshape(np.random.uniform(-1,1,6),[2,3])
# create a 2 x 3 tensor with random values from a uniform distribution on the interval [0, 1)
rand_numpy = numpy.random.rand(2, 3)
# create a 2 x 3 tensor of zeros
zero_numpy = numpy.zeros([2, 3])
```

```python
import torch
# create a tensor
new_tensor = torch.Tensor([[1, 2], [3, 4]])
# create a 2 x 3 tensor with random values
empty_tensor = torch.Tensor(2, 3)
# create a 2 x 3 tensor with random values between -1and 1
uniform_tensor = torch.Tensor(2, 3).uniform_(-1, 1)
# create a 2 x 3 tensor with random values from a uniform distribution on the interval [0, 1)
rand_tensor = torch.rand(2, 3)
# create a 2 x 3 tensor of zeros
zero_tensor = torch.zeros(2, 3)
```

And more operations like:

Indexing, slicing, reshape, transpose, cross product,
matrix product, element wise multiplication etc...

Tensor (continued)

- Attributes of a tensor *'t'*:
  - `t= torch.randn(1)`
- *`requires_grad` - making a trainable parameter*
  - *By default **False***
  - Turn on:
    - `t.requires_grad_()` or
    - `t= torch.randn(1,requires_grad=True)`
  - Accessing tensor value:
    - t.data
  - Accessing tensor gradient
    - t.grad
- *`grad_fn` – history of operations for autograd*
  - *t.grad_fn*

```python
import torch

N, D = 3, 4

x = torch.rand((N, D),requires_grad=True)
y = torch.rand((N, D),requires_grad=True)
z = torch.rand((N, D),requires_grad=True)

a = x * y
b = a + z
c=torch.sum(b)

c.backward()

print(c.grad_fn)
print(x.data)
print(x.grad)
```

```
<SumBackward0 object at 0x7fd0cb970cc0>
tensor([[0.4118, 0.2576, 0.3470, 0.0240],
        [0.7797, 0.1519, 0.7513, 0.7269],
        [0.8572, 0.1165, 0.8596, 0.2636]])
tensor([[0.6855, 0.9696, 0.4295, 0.4961],
        [0.3849, 0.0825, 0.7400, 0.0036],
        [0.8104, 0.8741, 0.9729, 0.3821]])
```

Loading Data, Devices and CUDA

- *Numpy arrays to PyTorch tensors*
  - **`torch.from_numpy(x_train)`**
  - **`Returns a cpu tensor!`**
- *PyTorch tensor to numpy*
  - **`t.numpy()`**
- *Using GPU acceleration*
  - **`t.to()`**
  - *Sends to whatever device (cuda or cpu)*
- *Fallback to cpu if gpu is unavailable:*
  - **`torch.cuda.is_available()`**
- Check cpu/gpu tensor OR numpy array ?
  - **`type(t)`** or **`t.type()`**
  - returns
    - numpy.ndarray
    - torch.Tensor
      - CPU - torch.cpu.FloatTensor
      - GPU - torch.cuda.FloatTensor

```
1  import torch
2  import torch.optim as optim
3  import torch.nn as nn
4  from torchviz import make_dot
5
6  device = 'cuda' if torch.cuda.is_available() else 'cpu'
7
8  # Our data was in Numpy arrays, but we need to transform them into PyTorch's Tensors
9  # and then we send them to the chosen device
10 x_train_tensor = torch.from_numpy(x_train).float().to(device)
11 y_train_tensor = torch.from_numpy(y_train).float().to(device)
12
13 # Here we can see the difference - notice that .type() is more useful
14 # since it also tells us WHERE the tensor is (device)
15 print(type(x_train), type(x_train_tensor), x_train_tensor.type())
```

*Assume *'t' is a tensor*

Autograd

- Autograd
  - *Automatic Differentiation Package*
  - *Don't need to worry about partial differentiation, chain rule etc..*
- backward() does that
  - `loss.backward()`
- Gradients are accumulated for each step by default:
  - Need to zero out gradients after each update
  - `t.grad.zero_()`

```
import torch

N, D = 3, 4

x = torch.rand((N, D),requires_grad=True)
y = torch.rand((N, D),requires_grad=True)
z = torch.rand((N, D),requires_grad=True)

a =x * y
b =a + z
c=torch.sum(b)

c.backward()
```

*Assume *'t' is a tensor*

Autograd (continued)

- Manual Weight Update - example

```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor
    error = y_train_tensor - yhat
    loss = (error ** 2).mean()

    loss.backward()

    with torch.no_grad():
        a -= lr * a.grad
        b -= lr * b.grad

    a.grad.zero_()
    b.grad.zero_()

print(a, b)
```

Optimizer

- Optimizers (*optim* package)
  - Adam, Adagrad, Adadelta, SGD etc..
  - Manually updating is ok if small number of weights
    - Imagine updating 100k parameters!
  - An optimizer takes the **parameters** we want to update, the **learning rate** we want to use (and possibly many other hyper-parameters as well!)
    and **performs the updates**

```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)


# Defines a SGD optimizer to update the parameters
optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor
    error = y_train_tensor - yhat
    loss = (error ** 2).mean()

    loss.backward()

    optimizer.step()

    optimizer.zero_grad()

print(a, b)
```

Loss

- Loss
  - Various predefined loss functions to choose from
  - L1, MSE, Cross Entropy ……

```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

# Defines a MSE loss function
loss_fn = nn.MSELoss(reduction='mean')

optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor

    loss = loss_fn(y_train_tensor, yhat)

    loss.backward()
    optimizer.step()
    optimizer.zero_grad()

print(a, b)
```

Model

- In PyTorch, a **model** is represented by a regular **Python class** that inherits from the Module class.
  - Two components
    - `__init__(self)`: **it defines the parts that make up the model** —in our case, two *parameters*, ***a*** and ***b***
    - `forward(self, x)`: it performs the **actual computation**, that is, it **outputs a prediction**, given the input **x**

Model (example)

- Example:

```
class ManualLinearRegression(nn.Module):
    def __init__(self):
        super().__init__()
        # To make "a" and "b" real parameters of the model, we need to wrap them with nn.Parameter
        self.a = nn.Parameter(torch.randn(1, requires_grad=True, dtype=torch.float))
        self.b = nn.Parameter(torch.randn(1, requires_grad=True, dtype=torch.float))

    def forward(self, x):
        # Computes the outputs / predictions
        return self.a + self.b * x
```

- Properties:
  - model = ManualLinearRegression()
    - model.state_dic() - returns a dictionary of trainable parameters with their current values
    - model.parameters() - returns a list of all trainable parameters in the model
    - model.train() or model.eval()

Putting things together

- Sample Code in practice

```
# Now we can create a model and send it at once to the device
model = ManualLinearRegression().to(device)
# We can also inspect its parameters using its state_dict
print(model.state_dict())

loss_fn = nn.MSELoss(reduction='mean')
optimizer = optim.SGD(model.parameters(), lr=lr)

for epoch in range(n_epochs):
    model.train()

    yhat = model(x_train_tensor)

    loss = loss_fn(y_train_tensor, yhat)
    loss.backward()
    optimizer.step()
    optimizer.zero_grad()

print(model.state_dict())
```

Complex Models

- Complex Model Class
- Predefined 'layer' modules

```
class LayerLinearRegression(nn.Module):
    def __init__(self):
        super().__init__()
        # Instead of our custom parameters, we use a Linear layer with single input and single output
        self.linear = nn.Linear(1, 1)

    def forward(self, x):
        # Now it only takes a call to the layer to make predictions
        return self.linear(x)
```

- 'Sequential' layer modules

```
class LayerLinearRegression(nn.Module):
    def __init__(self):
        super().__init__()
        # Instead of our custom parameters, we use a Linear layer with single input and single output
        self.seq_linear = nn.Sequential(nn.Linear(1, 2),nn.RELU(),nn.Linear(2,1))

    def forward(self, x):
        # Now it only takes a call to the layer to make predictions
        return self.seq_linear(x)
```

Dataset

- Dataset
  - In PyTorch, a **dataset** is represented by a regular **Python class** that inherits from the Dataset class. You can think of it as a kind of a Python **list of tuples**, each tuple corresponding to **one point (features, label)**
  - **3 components:**
    - __init__(self)
    - __get_item__(self, index)
    - __len__(self)
  - **Unless the dataset is huge (cannot fit in memory), you don't explictly need to define this class. Use `TensorDataset`**

```
from torch.utils.data import Dataset, TensorDataset

class CustomDataset(Dataset):
    def __init__(self, x_tensor, y_tensor):
        self.x = x_tensor
        self.y = y_tensor

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

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

x_train_tensor = torch.from_numpy(x_train).float()
y_train_tensor = torch.from_numpy(y_train).float()

train_data = CustomDataset(x_train_tensor, y_train_tensor)
print(train_data[0])

train_data = TensorDataset(x_train_tensor, y_train_tensor)
print(train_data[0])
```

Dataloader

- Dataloader
  - What happens if we have a huge dataset? Have to train in 'batches'
  - Use PyTorch's Dataloader class!
    - We tell it which **dataset** to use, the desired **mini-batch size** and if we'd like to **shuffle** it or not. That's it!
    - Our **loader** will behave like an **iterator**, so we can **loop over it** and **fetch a different mini-batch** every time.

```
from torch.utils.data import DataLoader

train_loader = DataLoader(dataset=train_data, batch_size=16, shuffle=True)
```

Dataloader (example)

- Sample Code in Practice:

```
losses = []

model = ManualLinearRegression().to(device)

loss_fn = nn.MSELoss(reduction='mean')
optimizer = optim.SGD(model.parameters(), lr=lr)

for epoch in range(n_epochs):
    for x_batch, y_batch in train_loader:
        model.train()

        x_batch = x_batch.to(device)
        y_batch = y_batch.to(device)
        yhat = model(x_train_tensor)

        loss = loss_fn(y_batch, yhat)
        loss.backward()
        optimizer.step()
        optimizer.zero_grad()

        losses.append(loss)

print(model.state_dict())
```

Split Data

- Random Split for Train, Val and Test Set
- [random_split()]

```
from torch.utils.data.dataset import random_split

x_tensor = torch.from_numpy(x).float()
y_tensor = torch.from_numpy(y).float()

dataset = TensorDataset(x_tensor, y_tensor)

train_dataset, val_dataset, test_dataset = random_split(dataset, [60, 20, 20])

train_loader = DataLoader(dataset=train_dataset, batch_size=16)
val_loader = DataLoader(dataset=val_dataset, batch_size=20)
test_loader = DataLoader(dataset=test_dataset, batch_size=20)
```

Saving / Loading Weights

Method 1

- Only inference/evaluation – save only state_dict
- Save:
  - torch.save(model.state_dict(), PATH)
- Load:
  - model = TheModelClass(*args, **kwargs)
  - model.load_state_dict(torch.load(PATH))
  - model.eval()

- CONVENTION IS TO SAVE MODELS USING EITHER A .PT OR A .PTH EXTENSION

https://pytorch.org/tutorials/beginner/saving_loading_models.html

Saving / Loading Weights (continued)

- Method 2
- Checkpoint – resume training / inference
  - Save:
    - torch.save({
      'epoch': epoch,
      'model_state_dict': model.state_dict(),
      'optimizer_state_dict': optimizer.state_dict(),
      'loss': loss,
      ...
      }, PATH)
  - Load:
    - model = TheModelClass(*args, **kwargs)
      optimizer = TheOptimizerClass(*args, **kwargs)

      checkpoint = torch.load(PATH)
      model.load_state_dict(checkpoint['model_state_dict'])
      optimizer.load_state_dict(checkpoint['optimizer_state_dict'])
      epoch = checkpoint['epoch']
      loss = checkpoint['loss']

      model.eval()
      # - or -
      model.train()

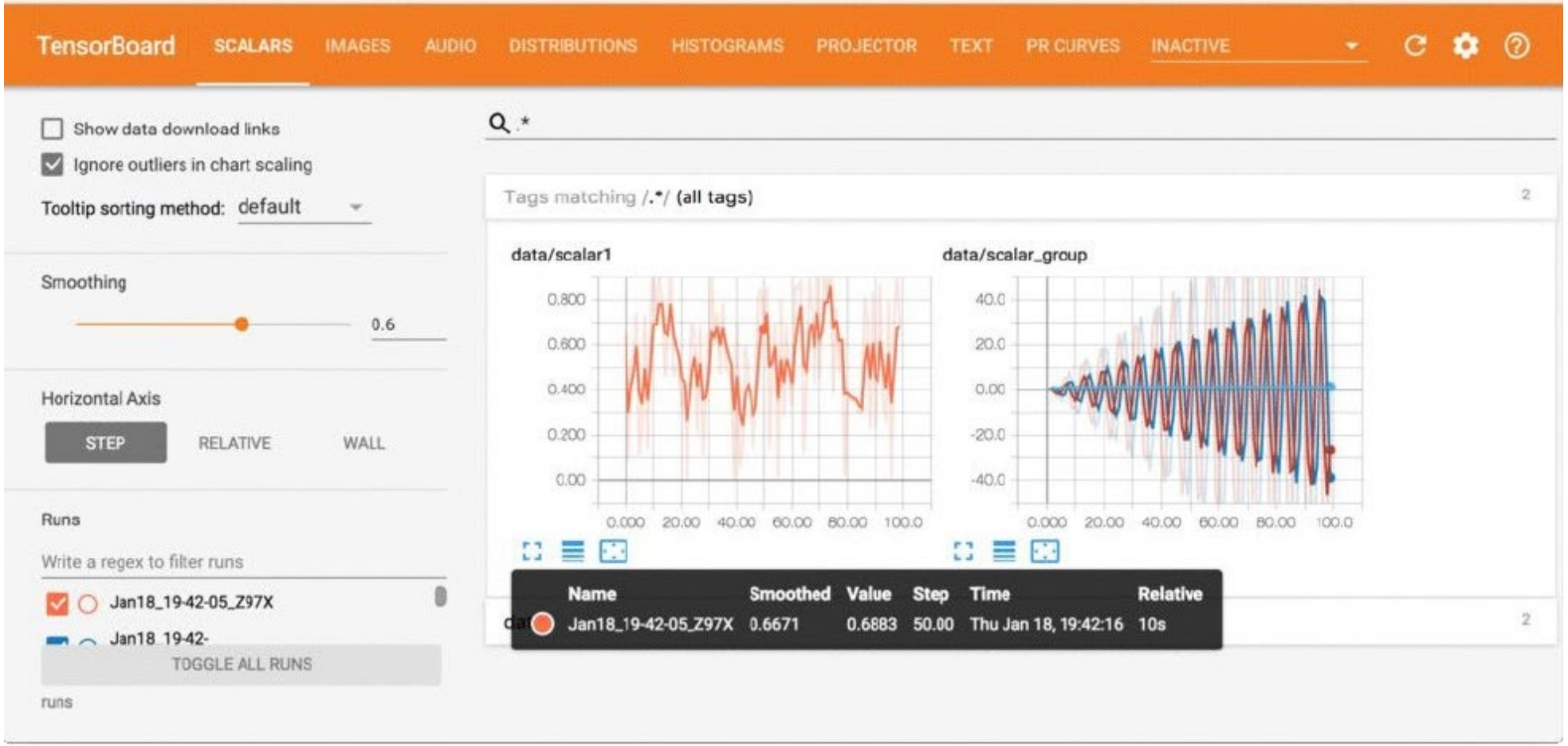
Evaluation

- Two important things:
  - torch.no_grad()
    - Don’t store the history of all computations
  - eval()
    - Tell compiler which mode to run on.

```
losses = []
val_losses = []
model = ManualLinearRegression().to(device)
loss_fn = nn.MSELoss(reduction='mean')
optimizer = optim.SGD(model.parameters(), lr=lr)

for epoch in range(n_epochs):
    for x_batch, y_batch in train_loader:
        model.train()

        x_batch = x_batch.to(device)
        y_batch = y_batch.to(device)
        yhat = model(x_train_tensor)

        loss = loss_fn(y_batch, yhat)
        loss.backward()
        optimizer.step()
        optimizer.zero_grad()

        losses.append(loss)

    with torch.no_grad():
        for x_val, y_val in val_loader:
            x_val = x_val.to(device)
            y_val = y_val.to(device)

            model.eval()

            yhat = model(x_val)
            val_loss = loss_fn(y_val, yhat)
            val_losses.append(val_loss.item())
```

Visualization

- TensorboardX (visualise training)
- PyTorchViz (visualise computation graph)

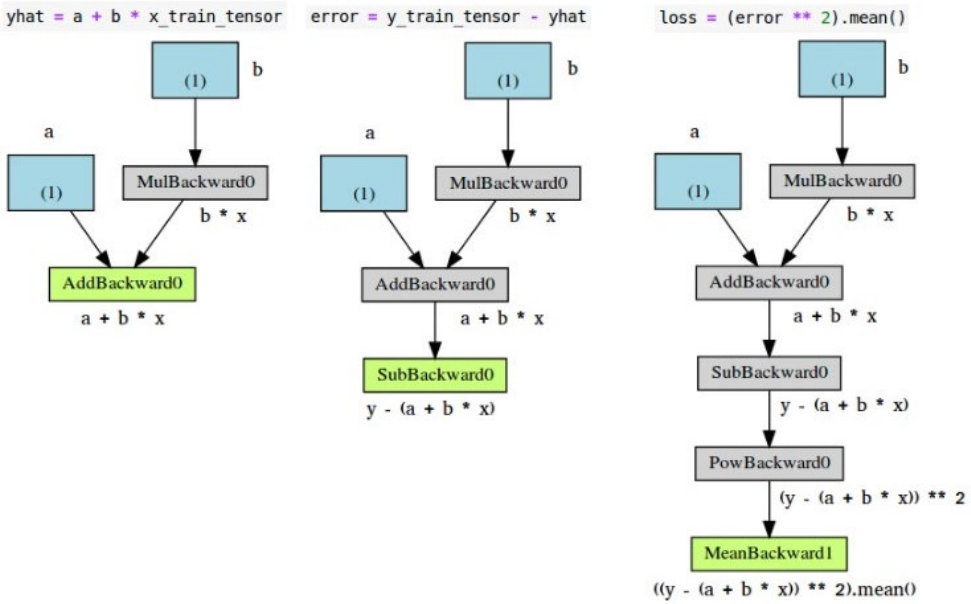


https://github.com/lanpa/tensorboardX/

Visualization (continued)

- PyTorchViz

```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)


# Defines a SGD optimizer to update the parameters
optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor
    error = y_train_tensor - yhat
    loss = (error ** 2).mean()

    loss.backward()

    optimizer.step()

    optimizer.zero_grad()

print(a, b)
```



https://github.com/szagoruyko/pytorchviz

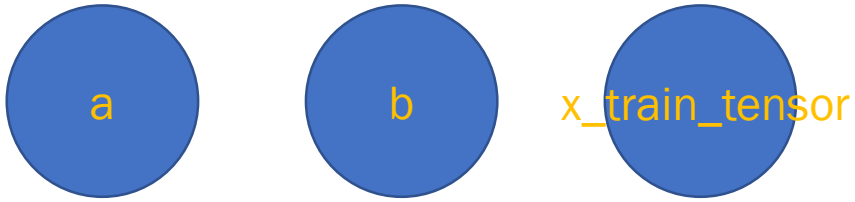
References

- Important References:
  - For setting up jupyter notebook on princeton ionic cluster
    - https://oncomputingwell.princeton.edu/2018/05/jupyter-on-the-cluster/
  - Best reference is PyTorch Documentation
    - https://pytorch.org/ and https://github.com/pytorch/pytorch
  - Good Blogs: (with examples and code)
    - https://lelon.io/blog/2018/02/08/pytorch-with-baby-steps
    - https://www.tutorialspoint.com/pytorch/index.htm
    - https://github.com/hunkim/PyTorchZeroToAll
  - Free GPU access for short time:
    - Google Colab provides free Tesla K80 **GPU** of about 12GB. You can run the session in an interactive **Colab** Notebook for 12 hours.
    - https://colab.research.google.com/

Misc

- Dynamic VS Static Computation Graph

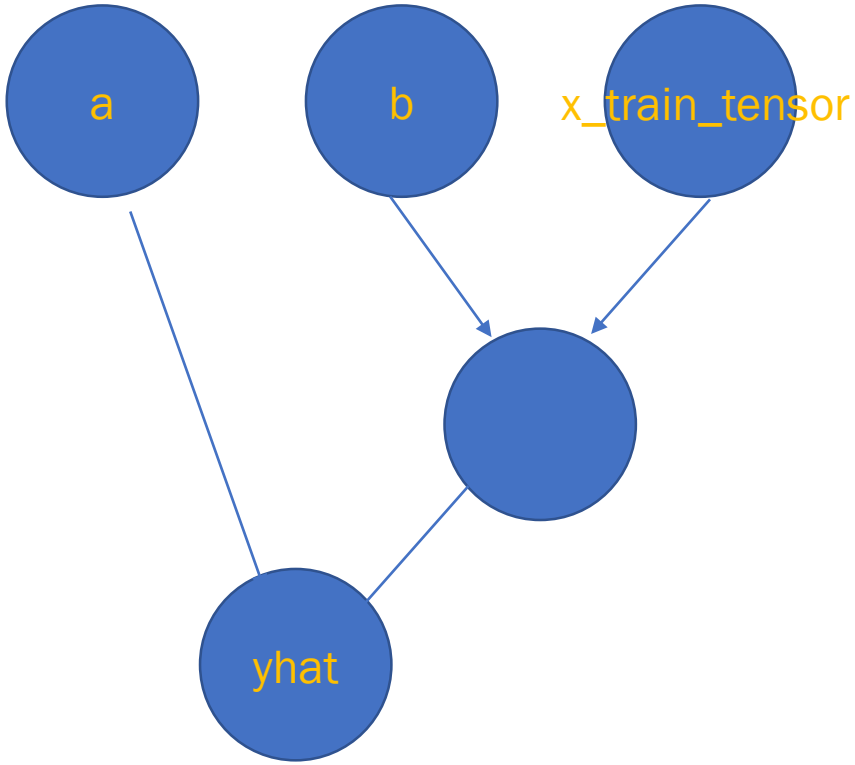
Epoch 1




```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

# Defines a MSE loss function
loss_fn = nn.MSELoss(reduction='mean')

optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor

    loss = loss_fn(y_train_tensor, yhat)

    loss.backward()
    optimizer.step()
    optimizer.zero_grad()

print(a, b)
```

Misc

- Dynamic VS Static Computation Graph




```
a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

# Defines a MSE loss function
loss_fn = nn.MSELoss(reduction='mean')

optimizer = optim.SGD([a, b], lr=lr)

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    optimizer.step()
    optimizer.zero_grad()

print(a, b)
```
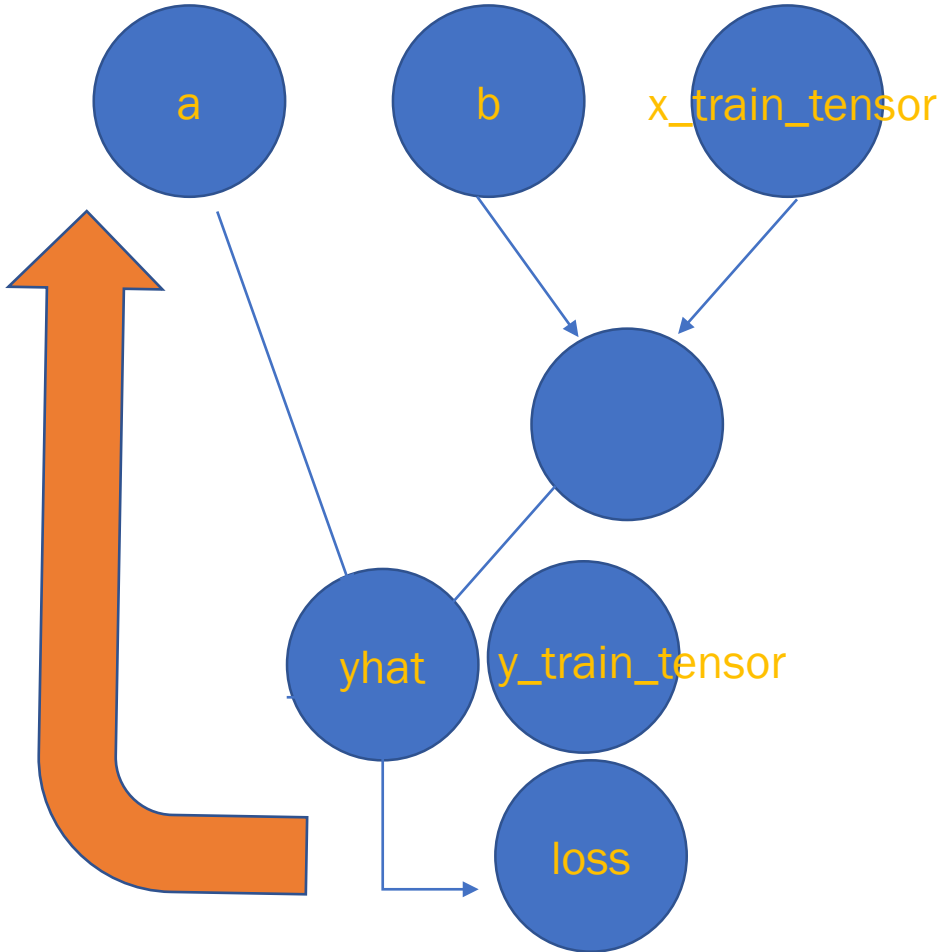

Misc

- Dynamic VS Static Computation Graph

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a = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)
b = torch.randn(1, requires_grad=True, dtype=torch.float, device=device)

# Defines a MSE loss function
loss_fn = nn.MSELoss(reduction='mean')

optimizer = optim.SGD([a, b], lr=lr)

for epoch in range(n_epochs):
    yhat = a + b * x_train_tensor

    loss = loss_fn(y_train_tensor, yhat)

    loss.backward()
    optimizer.step()
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print(a, b)
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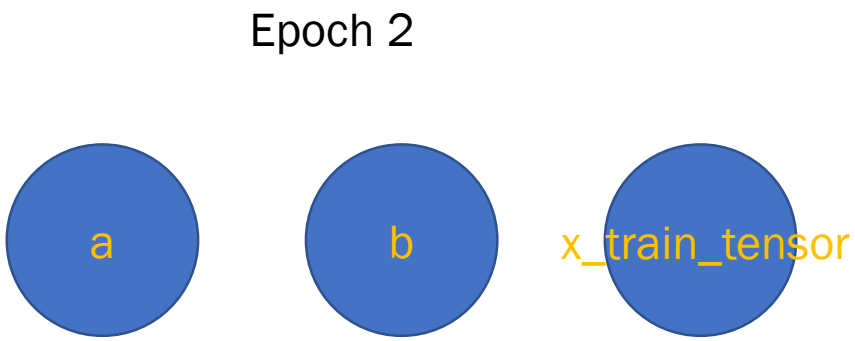


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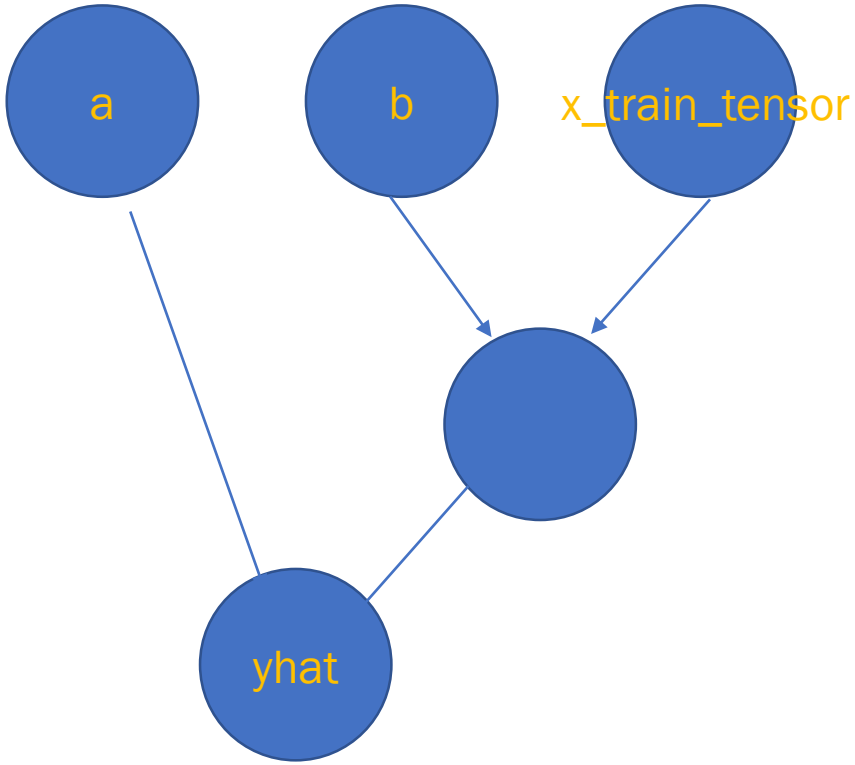


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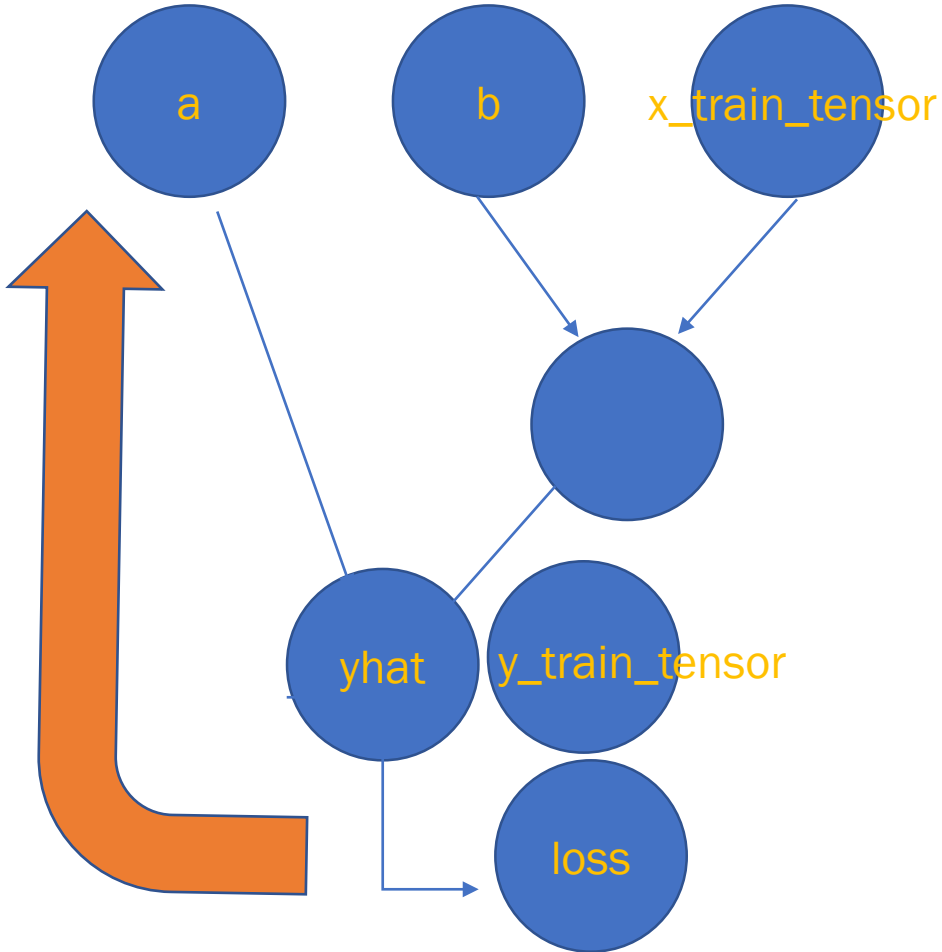


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Building the graph and computing the graph happen at the same time.

Seems inefficient, especially if we are building the same graph over and over again...

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Misc

- Alternative : Static Computation Graphs:

Alternative: Static graphs

Step 1: Build computational graph describing our computation (including finding paths for backprop)

Step 2: Reuse the same graph on every iteration

TensorFlow

```
import numpy as np
np.random.seed(0)
import tensorflow as tf

N, D = 3, 4

with tf.device('/gpu:0'):
    x = tf.placeholder(tf.float32)
    y = tf.placeholder(tf.float32)
    z = tf.placeholder(tf.float32)

    a = x * y
    b = a + z
    c = tf.reduce_sum(b)

grad_x, grad_y, grad_z = tf.gradients(c, [x, y, z])

with tf.Session() as sess:
    values = {
        x: np.random.randn(N, D),
        y: np.random.randn(N, D),
        z: np.random.randn(N, D),
    }
    out = sess.run([c, grad_x, grad_y, grad_z],
                   feed_dict=values)
    c_val, grad_x_val, grad_y_val, grad_z_val = out
```