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Artificial Intelligence Research

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Autograd & Modules

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Deep Learning DIY
ENS ULM

PyTorch

- **Autograd**
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  - Visualizing the Computation Graph
- **Modules**
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  - Forward and Backward Hooks
  - Buffers
  - Extending Autograd & Grad-checking
  - CUDA API, float API, train/eval API
- **Autograd Tips & Tricks**
  - Execution Time
  - Pointers & Nodes

Refresher – Training Loop

```
import torch
import torch.nn as nn
```

```
# define network structure
net = nn.Sequential(nn.Linear(3 * 32 * 32, 1000), nn.ReLU(), nn.Linear(1000, 10))
criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.SGD(net.parameters(), lr = 0.01, momentum=0.9, weight_decay=1e-4)
```

<-- Magic! nn.Module

```
# load data
train_set = torchvision.datasets.CIFAR10(root='.', train=True, transform=transform_list)
train_loader = torch.utils.data.DataLoader(train_set, batch_size=64)
```

```
# training loop
for (batch, target) in train_loader:

    output = net(batch)
    loss = criterion(output, targets)

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

<-- Magic!   Autograd

Autograd in a Nutshell

- Autograd = Automatic Differentiation
- Idea: use the chain rule on a graph of operations with *leaves* and *nodes*

- Dynamic vs. Static graph
- Computation graph is created *during* each forward call

- Back in the time (until v4.0), use of Variables encapsulating Tensors
- Now only Tensors with data and grad attributes

Hands on!

- Autograd handles well almost every basic tensor operation you could think of!

```
# don't hit enter before to guessed the answer!
x = torch.Tensor(4, 10)
x.requires_grad=True
loss = x[:, :4].sum()
loss.backward()
x.grad
```

Hands on!

- Autograd handles well almost every basic tensor operation you could think of!

```
# don't hit enter before to guessed the answer!
x = torch.Tensor(4, 10)
x.requires_grad=True
loss = x[:, :4].sum()
loss.backward()
x.grad
```

```
tensor([[1., 1., 1., 1., 0., 0., 0., 0., 0., 0.],
        [1., 1., 1., 1., 0., 0., 0., 0., 0., 0.],
        [1., 1., 1., 1., 0., 0., 0., 0., 0., 0.],
        [1., 1., 1., 1., 0., 0., 0., 0., 0., 0.]])
```

Hands on!

- Autograd handles well almost every basic tensor operation you could think of!

```
# don't hit enter before to guessed the answer!
x = torch.Tensor(2, 3)
x.requires_grad=True
y = torch.Tensor([[1, 2], [3, 4]])
loss = y.mm(x).sum()
loss.backward()
x.grad
```

Hands on!

- Autograd handles well almost every basic tensor operation you could think of!

```
# don't hit enter before to guessed the answer!
x = torch.Tensor(2, 3)
x.requires_grad=True
y = torch.Tensor([[1, 2], [3, 4]])
loss = y.mm(x).sum()
loss.backward()
x.grad
```

```
tensor([[4., 4., 4.],
        [6., 6., 6.]])
```

Hands on!

- Autograd handles well almost every basic tensor operation you could think of!
- **Bonus exercise**: what about second order gradients?

```
# don't hit enter before to guessed the answer!
x = torch.Tensor([[1, 2, 3, 4]])
x.requires_grad=True
y = 2 * x
y.backward(torch.Tensor([[1, 0, 0, 0]]))
x.grad
```

Hands on!

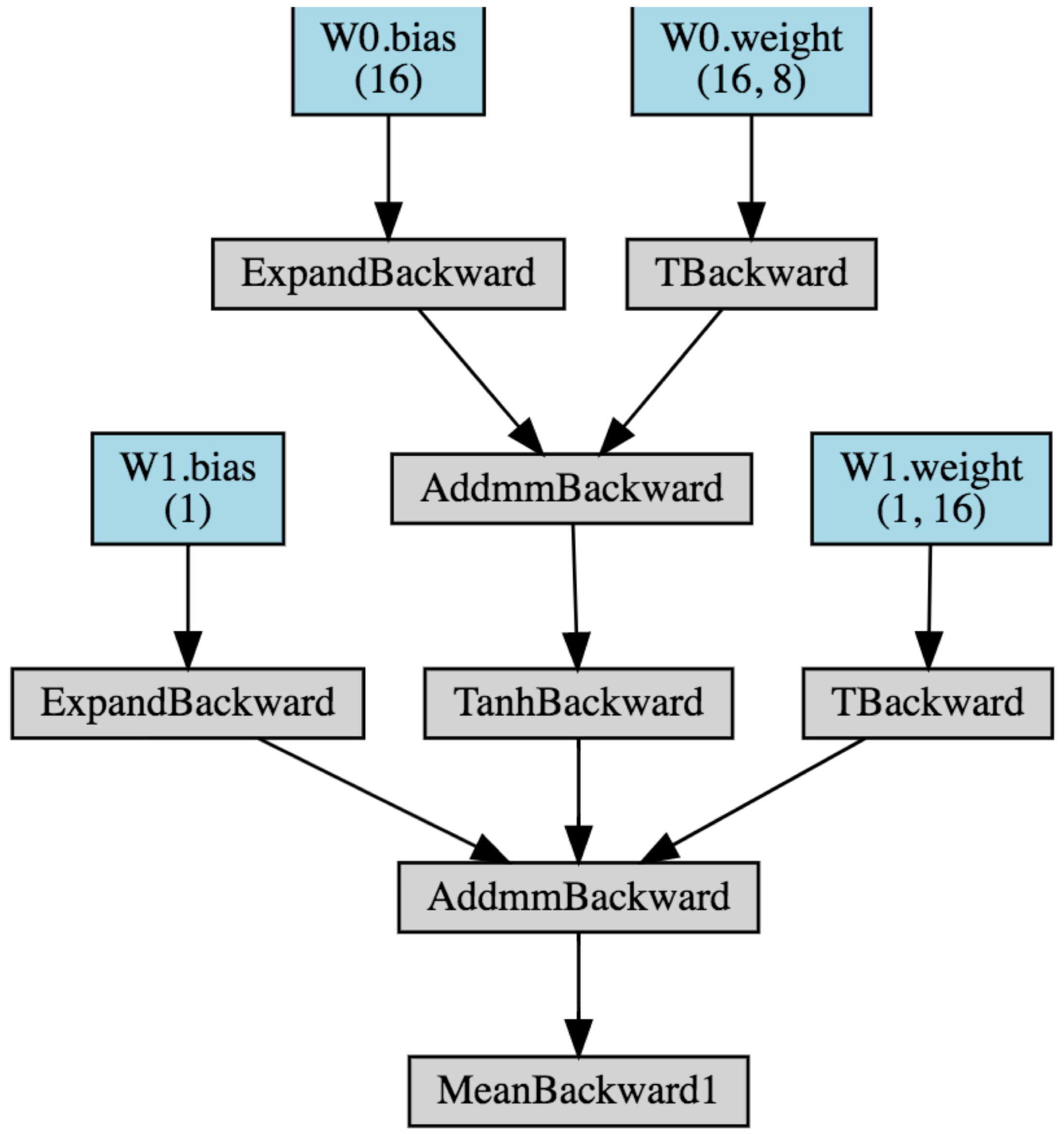
- Autograd handles well almost every basic tensor operation you could think of!
- **Bonus exercise**: what about second order gradients?

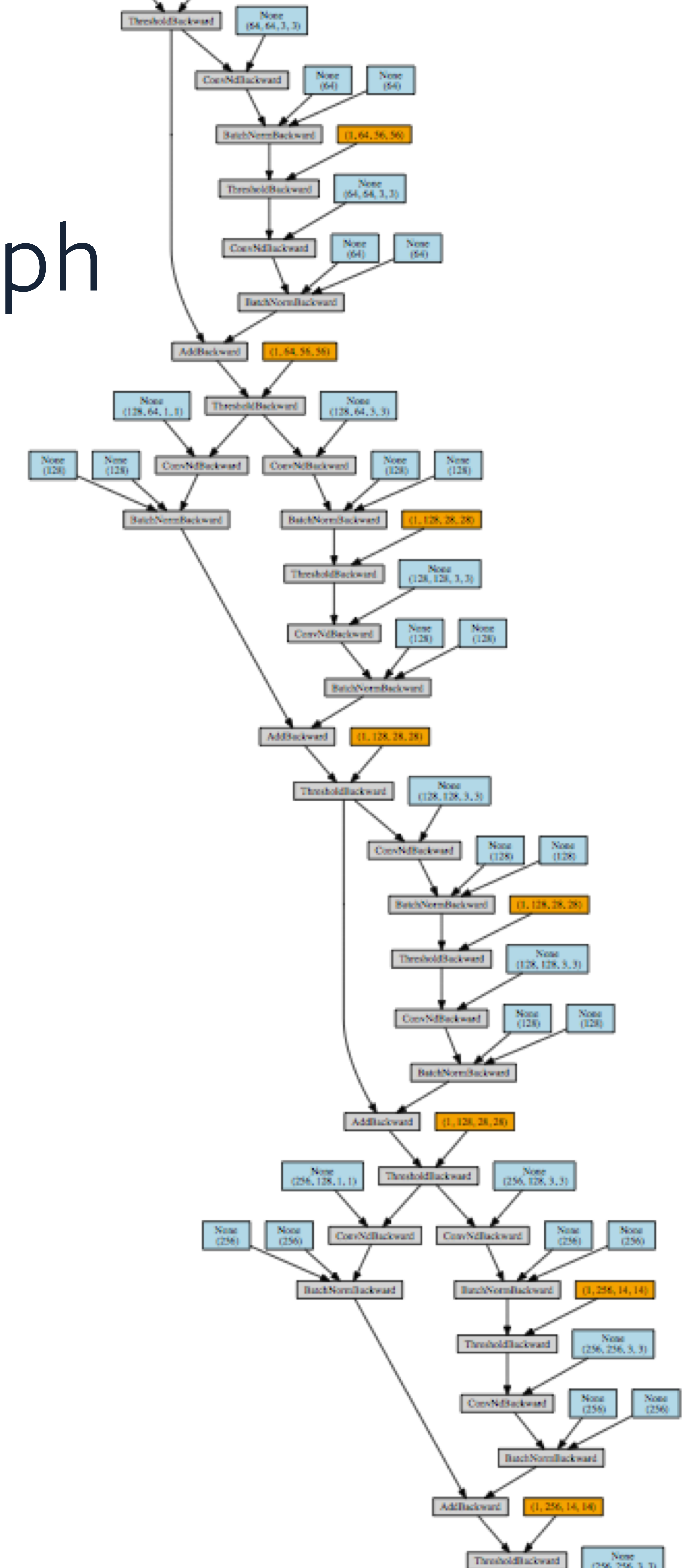
```
# don't hit enter before to guessed the answer!
x = torch.Tensor([[1, 2, 3, 4]])
x.requires_grad=True
y = 2 * x
y.backward(torch.Tensor([[1, 0, 0, 0]]))
x.grad
```

```
tensor([[2., 0., 0., 0.]])
```

Visualizing the Computation Graph

- Autograd handles well almost every basic tensor operation you could think of!
- **Bonus exercise**: clone and test https://github.com/szagoruyko/pytorchviz





Volatile mode

- Volatile mode, why does it exist?

```
net = nn.Linear(10, 5)
print('Data: ', net.weight.data)  # <--- some data
print('Grad: ', net.weight.grad)  # <--- None
```

```
# normal mode
x = torch.rand(2, 10)
y = net(x).sum()
y.backward()
print('Data: ', net.weight.data) # <--- some data
print('Grad: ', net.weight.grad) # <--- some data
```

```
# volatile mode
with torch.no_grad():
    x = torch.rand(2, 10)
    y = net(x).sum()
    y.backward()
    print('Data: ', net.weight.data)  # <--- some data
    print('Grad: ', net.weight.grad)  # <--- this will raise an error
```

Build your own module

```
class Linear(nn.Module):
    """
    This is a docstring.
    This must be filled by you.
    This is important.
    """

    def __init__(self, in_features, out_features):
        super(Linear, self).__init__()
        self.in_features = in_features
        self.out_features = out_features
        self.weight = Parameter(torch.Tensor(out_features, in_features))
        self.reset_parameters()

    def reset_parameters(self):
        stdv = 1. / math.sqrt(self.weight.size(1))
        torch.nn.init.uniform_(self.weight.data, -stdv, stdv)

    def forward(self, input):
        return F.linear(input, self.weight, self.bias)

    def extra_repr(self):
        return 'in_features={}, out_features={}, bias={}'.format(
            self.in_features, self.out_features, self.bias is not None
        )
```

Parameter

Initialization, important!

Backend

Just to look nicer

Build your own module

- Permute the features of an input (input = batch x features).
- How to test it?
- Wait, is this module even useful?
- **Bonus exercise**: how do you write the backprop by hand?

```
class Permutation(nn.Module):

    def __init__(self, input_features, axis=1):
        super(Permutation, self).__init__()
        self.input_features = input_features
        self.axis = axis
        self.perm = # ... (use torch.randperm)

    def forward(self, input):
        return # ... (use torch.index_select(axis, perm))
```

Forward and Backward Hooks

- Print/plot the activations norms in a “deep” FC network. What do you observe?
- **Bonus exercise**: how about storing the activation norms when you want during training?

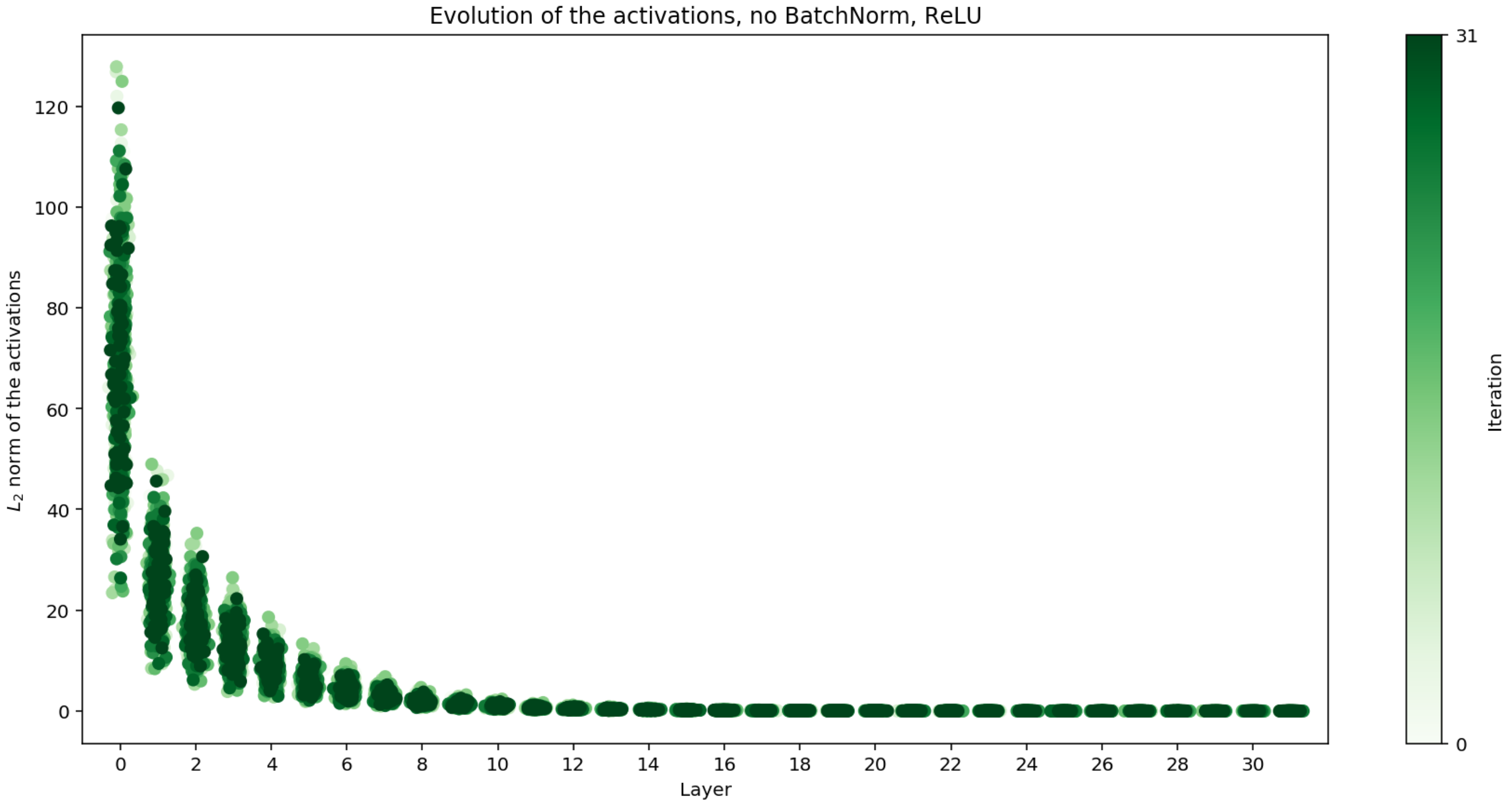
```
def deep_net(n_layers, features=1000):
    # returns a FC network with n_layers of size features
    # use: nn.Sequential(*layers)


def forward_hook(module, input, output):
    # provides, for module, input and output activations
    # use: .norm()

def register_forward_hooks(net, forward_hook):
    # resister hooks for every layer in net
    # use: net.children() to get the layers
    # use: layer.register_forward_hook(forward_hook) for every layer
    # ...
```

Forward and Backward Hooks

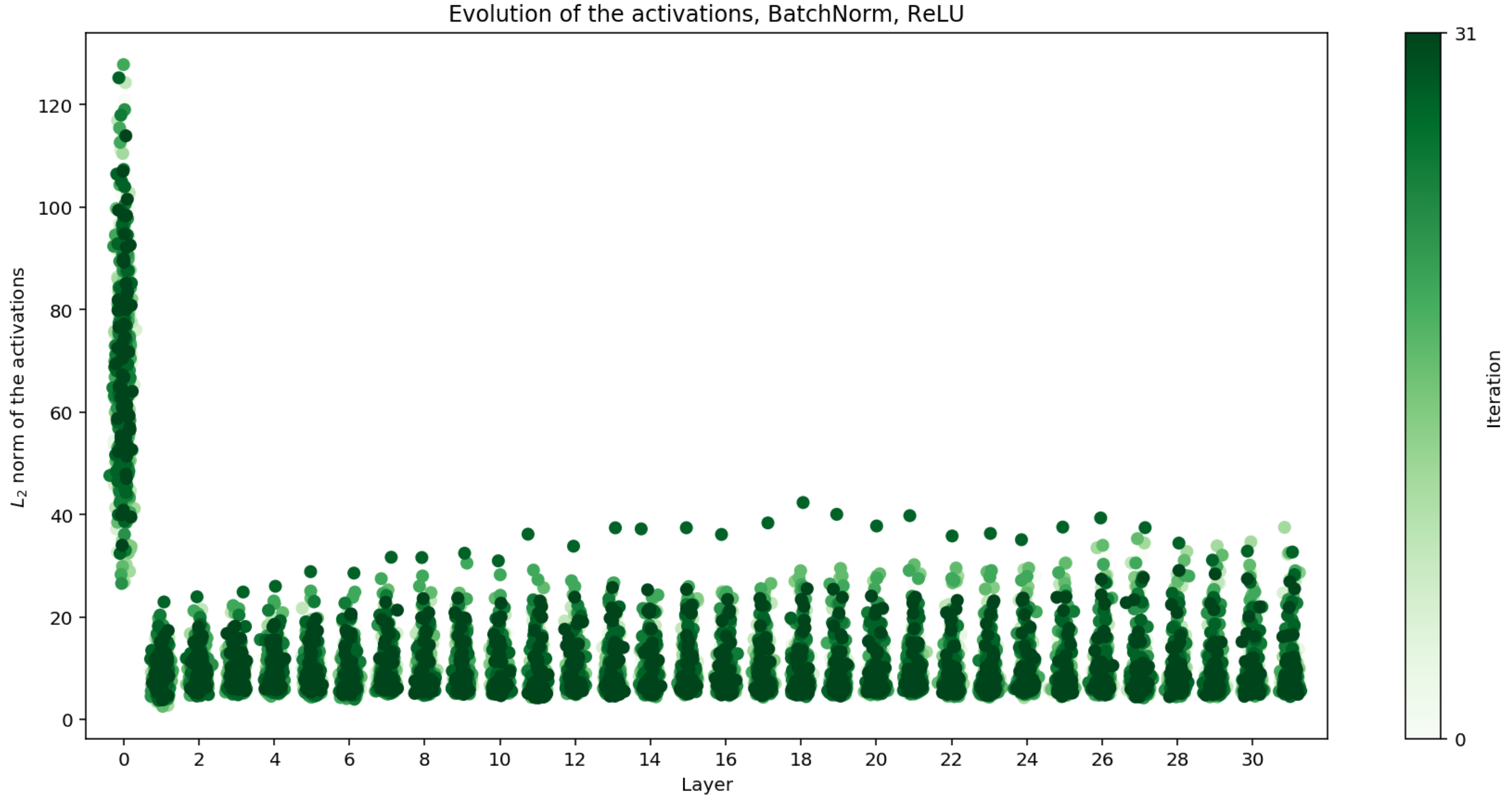
- Importance of a good normalization!
- Vanishing/exploding gradients (search the web for it…)



Bad

Forward and Backward Hooks

- Importance of a good normalization!
- Vanishing/exploding gradients (search the web for it...)



Good

Forward and Backward Hooks

- Print the backpropagated gradient sizes
- Does this match with the gradients wrt the weights?
- **Bonus exercise**: use grad_output and input to recover weight.grad

```python
# print  sizes
def backward_hook(module, grad_input, grad_output):
    # use: .size()

# register hook for every layer
def register_backward_hooks(net, backward_hook):
    # guess how to register a backward hook
    # ...
```

Buffers

- You want a stateful part of your model that is not a parameter, appears in state_dict()
- Normalize each batch channel by its current mean
- Accumulate an exponential moving average of the means over the iterations (why?)
- How to test it?
- **Bonus exercise**: what about dividing by the std? Numerical stability?

```
class Normalize(nn.Module):

    def __init__(self, num_features, momentum=0.1):
        # you know what to write here
        # use: self.register_buffer('running_mean, torch.Tensor(...))
        #...

    def reset_parameters(self):
        # ...
```

Buffers

- You want a stateful part of your model that is not a parameter, appears in state_dict()
- Normalize each batch channel by its current mean
- Accumulate an exponential moving average of the means over the iterations (why?)
- How to test it?
- **Bonus exercise**: what about dividing by the std? Numerical stability?

```
def forward(self, input):
    # training mode: use batch statistics and update running statistics
    if self.training:
        # ...

    # eval mode: use running statistics
    else:
        #...

    # return output
    return #...
```

CUDA API

- cuda(), why, where to use it? Don't forget the cpu()

```
# define network structure
net = nn.Sequential(nn.Linear(3 * 32 * 32, 1000), nn.ReLU(), nn.Linear(1000, 10)).cuda()
criterion = nn.CrossEntropyLoss().cuda()
optimizer = torch.optim.SGD(net.parameters(), lr = 0.01, momentum=0.9, weight_decay=1e-4)
```

```
# load data
train_set = torchvision.datasets.CIFAR10(root='.', train=True, transform=transform_list)
train_loader = torch.utils.data.DataLoader(train_set, batch_size=64)
```

```
# training loop
for (batch, target) in train_loader:
    batch = batch.cuda()
    target = target.cuda()
    output = net(batch)
    loss = criterion(output, targets)

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

Float API

- double(), half() why, where to use it?

```
# define network structure
net = nn.Sequential(nn.Linear(3 * 32 * 32, 1000), nn.ReLU(), nn.Linear(1000, 10)).half()
criterion = nn.CrossEntropyLoss().half()
optimizer = torch.optim.SGD(net.parameters(), lr = 0.01, momentum=0.9, weight_decay=1e-4)
```

```
# load data
train_set = torchvision.datasets.CIFAR10(root='.', train=True, transform=transform_list)
train_loader = torch.utils.data.DataLoader(train_set, batch_size=64)
```

```
# training loop
for (batch, target) in train_loader:    batch = batch.half()
                                        target = target.half()
    output = net(batch)
    loss = criterion(output, targets)

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

Other important APIs

- APIsTrain/eval mode. Why is it useful?

```
net = nn.Linear(2, 2)

print(net.training)  # True, default behavior
net.eval()           # eval mode
print(net.training)  # False
```

- Dataparallell

```
net = torch.nn.DataParallel(nn.Linear(3, 3))
```

Gradchecking

- Idea: finite differences to check the analytic gradient computed by autograd / defined by you
- Why gradcheck when I rely on autograd?

```
x = torch.rand(256, 2, requires_grad=True).double()
y = torch.randint(0, 10, (256, ), requires_grad=True).double()
custom_op = nn.Linear(2, 10).double()
res = torch.autograd.gradcheck(custom_op, (x, ))
print(res)
```

Autograd tips & Tricks

- Pointers are everywhere. Don't forget to clone()

```
net = nn.Linear(2, 2)
w = net.weight.clone()
print(w)

x = torch.rand(1, 2)
y = net(x).sum()
y.backward()
net.weight.data -= 0.01 * net.weight.grad # <--- What is this?
print(w)
```

Autograd tips & Tricks

- Weight sharing. Why use it?

```
net = nn.Sequential(nn.Linear(2, 2), nn.Linear(2, 2))
net[0].weight = net[1].weight  # weight sharing

x = torch.rand(1, 2)
y = net(x).sum()
y.backward()
print(net[0].weight.grad)
print(net[1].weight.grad)
```

Autograd tips & Tricks

- Execution time for complicated layers.

Useful Ressources

- The Notebook on the course website: https://www.di.ens.fr/~lelarge/dldiy/
- PyTorch repo: https://github.com/pytorch/pytorch. Explore it! (typing ‘t’ will prompt a search by filename), in particular torch.nn, torch.optim.
- More about Autograd: https://openreview.net/pdf?id=BJJsrmfCZ
- PyTorch Tutorials: https://pytorch.org/tutorials/