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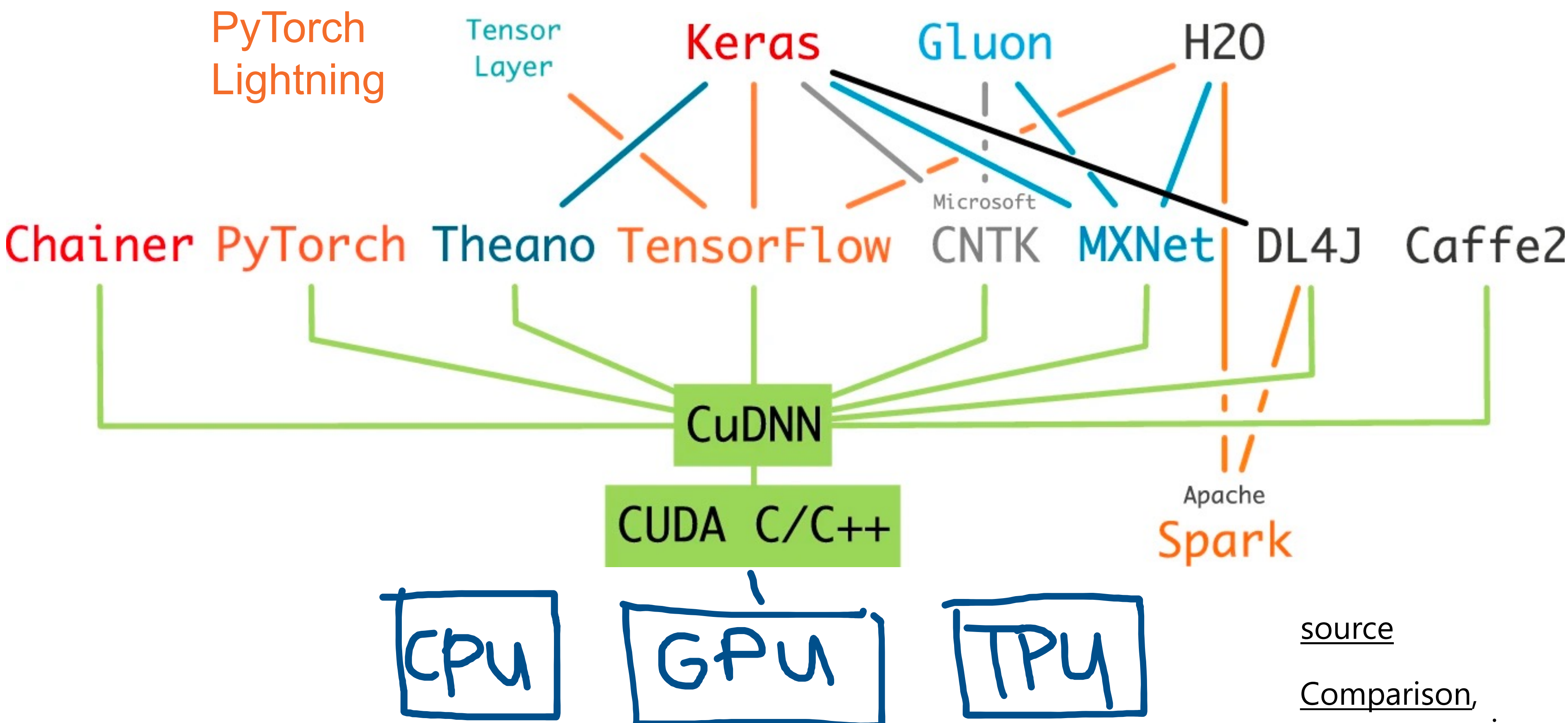
PyTorch.Next

Auto differentiation, data handling and code disentanglement

2021

Deep Learning Frameworks



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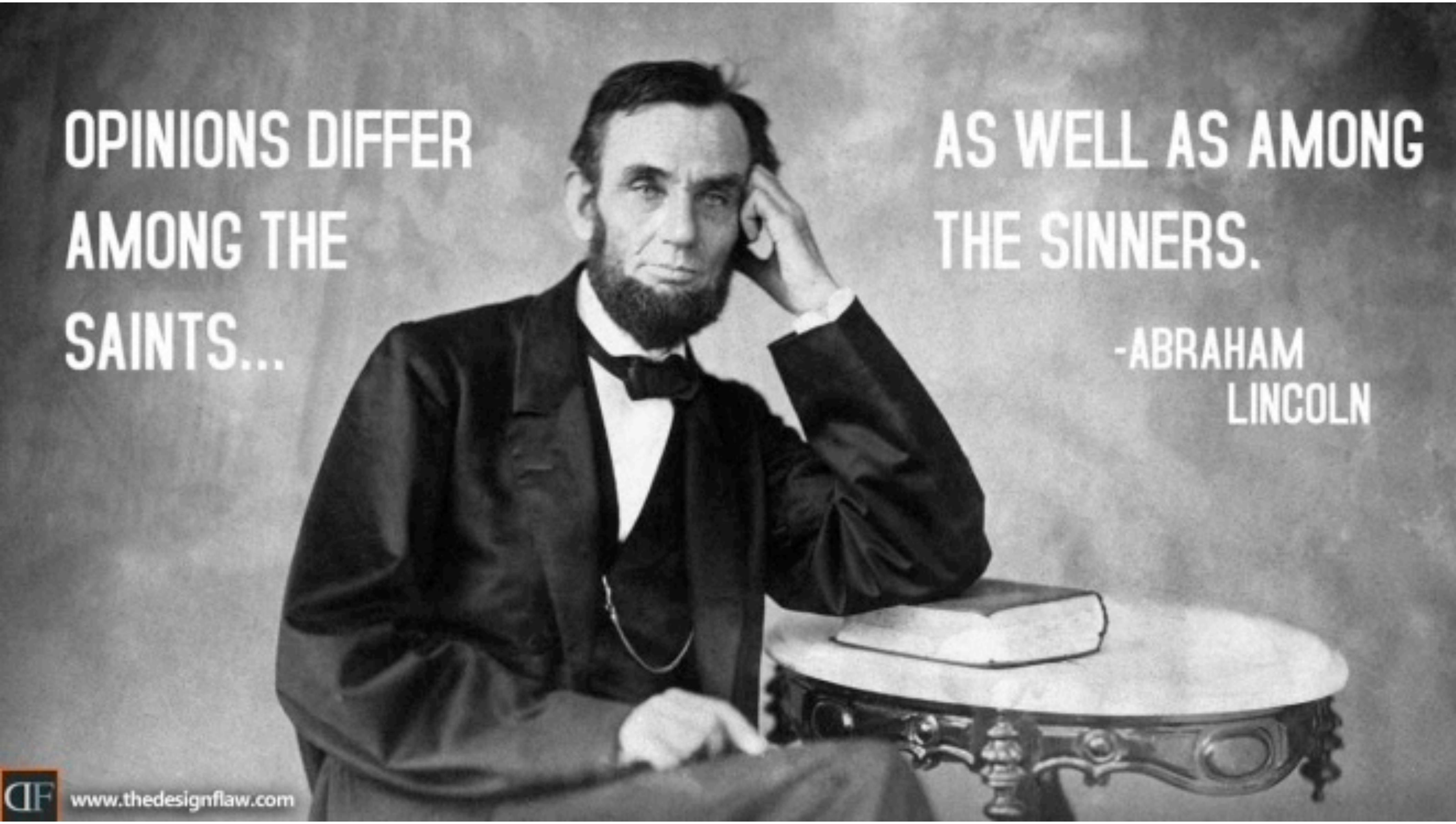
Comparison,
moar comparison

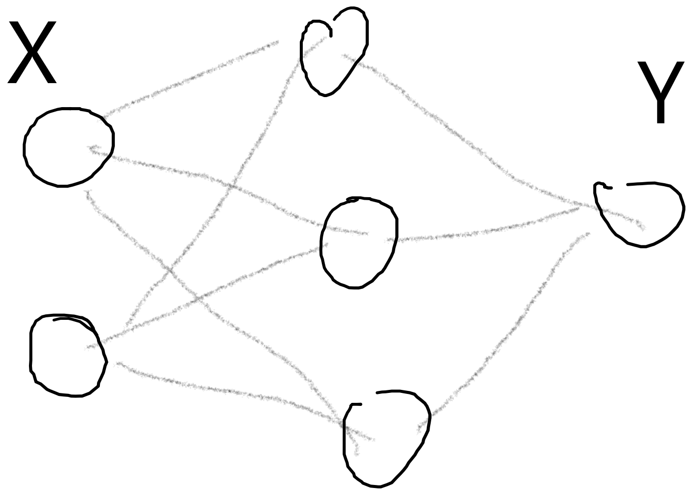

OPINIONS DIFFER
AMONG THE
SAINTS...
AS WELL AS AMONG
THE SINNERS.
-ABRAHAM
LINCOLN
www.thedesignflaw.com

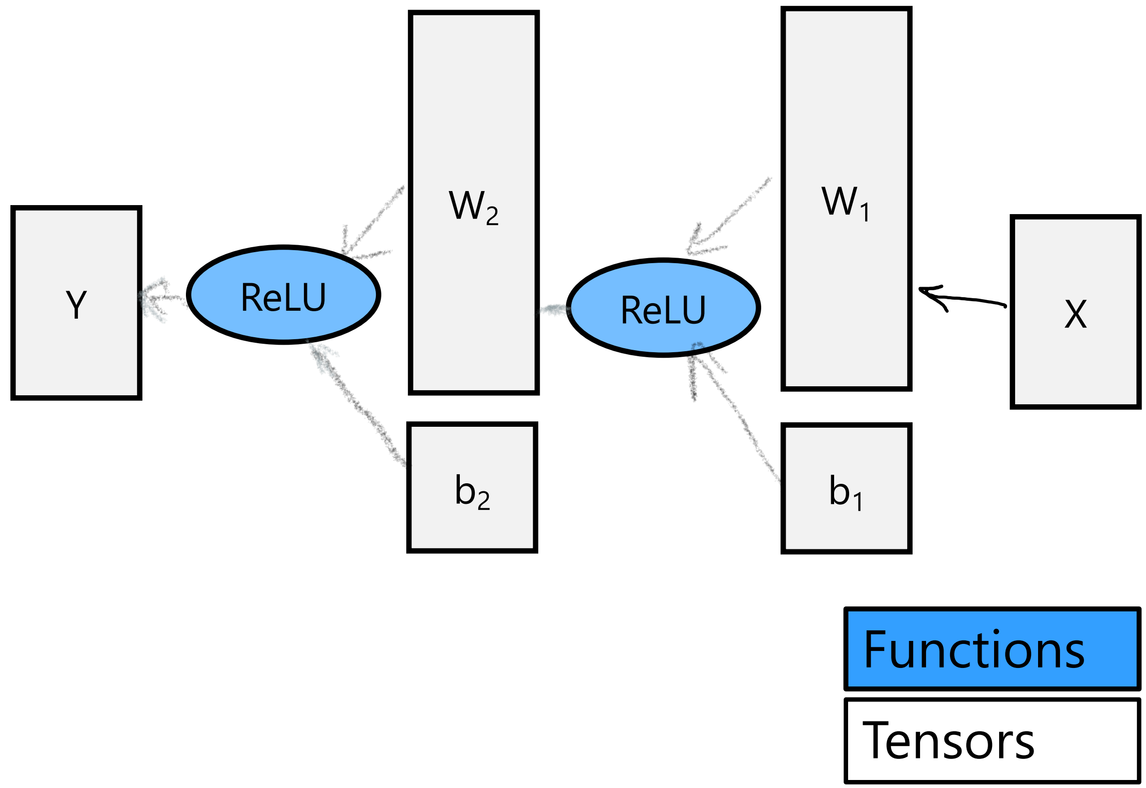
PyTorch highlights

- Simple, transparent development/ debugging
- Rich Ecosystem:
  - Plenty of pretrained models
  - NLP, Vision, ...
  - Interpretation
  - Hyper-optimization
- Production Ready (C++, ONNX, Services)
- Distributed Training, declarative data parallelism
- Cloud Deployment support
- Choice of many industry leaders and researchers

facebook Artificial Intelligence

Neural network representation





$$Y = \mathrm{relu}(W_2 \times \mathrm{relu}(W_1 X + b_1) + b_2)$$

Building blocks, tensors

```
torch.randn(*size)              # tensor with independent N(0,1) entries
torch.[ones|zeros](*size)       # tensor with all 1's [or 0's]
torch.Tensor(L)                 # create tensor from [nested] list or ndarray L
x.clone()                       # clone of x
with torch.no_grad():           # code wrap that stops autograd from tracking tensor history
requires_grad=True              # arg, when set to True, tracks computation
                                # history for future derivative calculations
```

```
x.size()                        # return tuple-like object of dimensions
torch.cat(tensor_seq, dim=0)    # concatenates tensors along dim
x.view(a,b,...)                 # reshapes x into size (a,b,...)
x.view(-1,a)                    # reshapes x into size (b,a) for some b
x.transpose(a,b)                # swaps dimensions a and b
x.permute(*dims)                # permutes dimensions
x.unsqueeze(dim)                # tensor with added axis
x.unsqueeze(dim=2)              # (a,b,c) tensor -> (a,b,1,c) tensor
```

Tensor creation and placement

```
>>> torch.zeros([2, 4], dtype=torch.int32)
tensor([[ 0,  0,  0,  0],
        [ 0,  0,  0,  0]], dtype=torch.int32)
>>> cuda0 = torch.device('cuda:0')
>>> torch.ones([2, 4], dtype=torch.float64, device=cuda0)
tensor([[ 1.0000,  1.0000,  1.0000,  1.0000],
        [ 1.0000,  1.0000,  1.0000,  1.0000]], dtype=torch.float64,
device='cuda:0')
```

- Keep in mind occurrence of tensors on devices: CPU, GPU, TPU
- Operations can be performed only if its arguments are inhabiting the same device

GPU, TPU support

```
torch.cuda.is_available                                # check for cuda
x.cuda()                                               # move x's data from
                                                       # CPU to GPU and return new object

x.cpu()                                                # move x's data from GPU to CPU
                                                       # and return new object

if not args.disable_cuda and torch.cuda.is_available(): # device agnostic code
    args.device = torch.device('cuda')                 # and modularity
else:                                                  #
    args.device = torch.device('cpu')                  #

net.to(device)                                         # recursively convert their
                                                       # parameters and buffers to
                                                       # device specific tensors

mytensor.to(device)                                    # copy your tensors to a device
                                                       # (gpu, cpu)
```

- https://pytorch.org/docs/stable/cuda.html
- http://pytorch.org/xla/release/1.5/index.html

Building blocks, graph

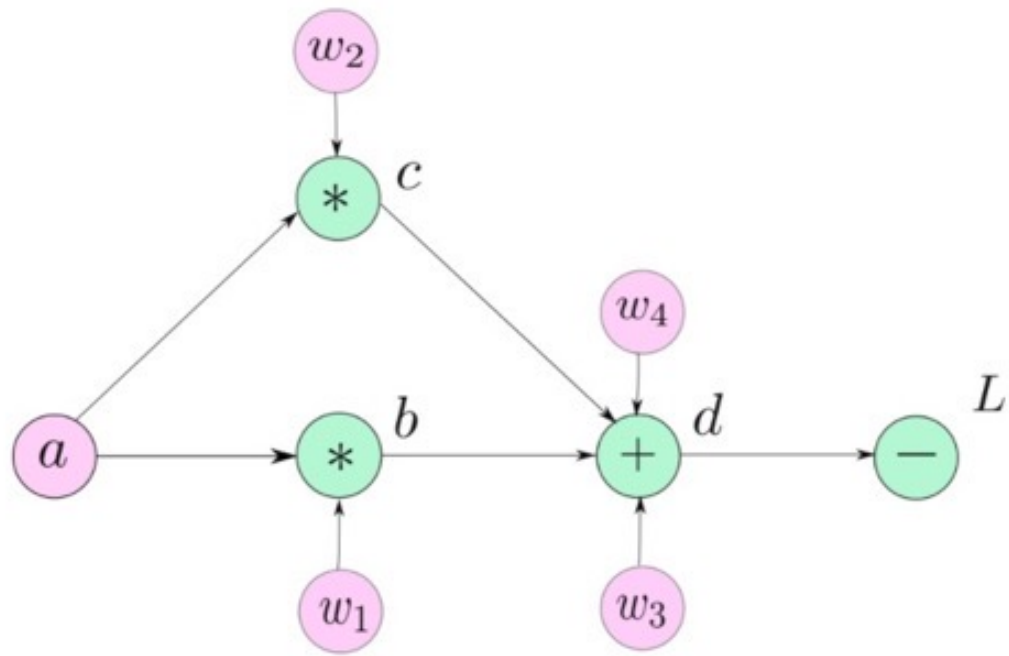
Toy example:

$$b = w_1 * a$$

$$c = w_2 * a$$

$$d = w_3 * b + w_4 * c$$

$$L = 10 - d$$



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Math operations

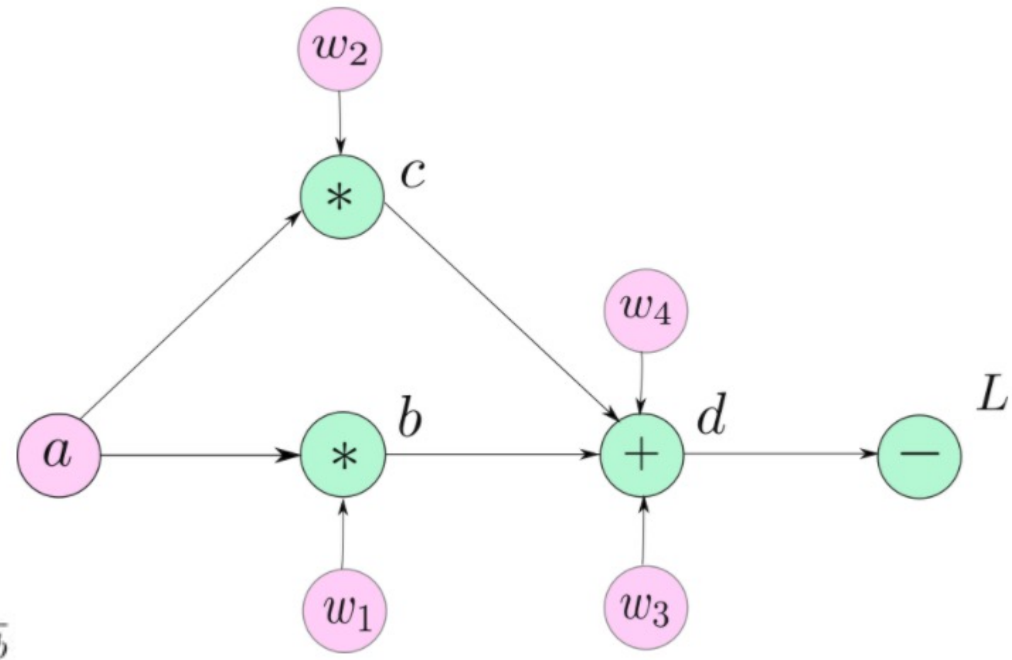
```
A.mm(B)       # matrix multiplication
A.mv(x)       # matrix-vector multiplication
x.t()         # matrix transpose
```

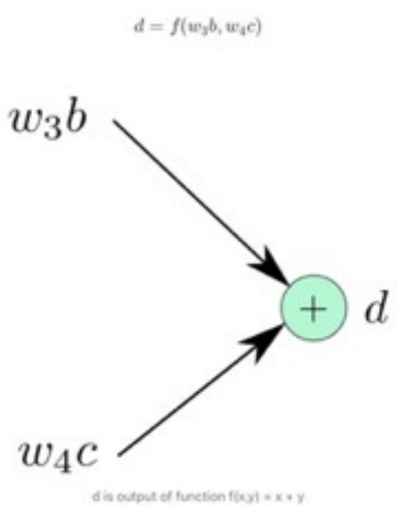
- https://pytorch.org/docs/stable/torch.html?highlight=mm#math-operations

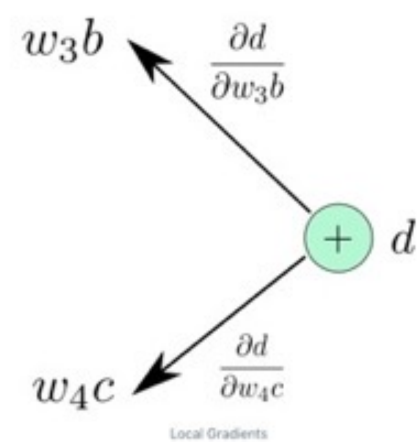
Computing backpropagation

$$b = w_1 * a$$
$$c = w_2 * a$$
$$d = w_3 * b + w_4 * c$$
$$L = 10 - d$$

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial d} * \frac{\partial d}{\partial b} * \frac{\partial b}{\partial w_1}$$







Computing gradient automatically

```
>> t1 = torch.randn((3,3), requires_grad = True)

>> t2 = torch.FloatTensor(3,3) # No way to specify requi
>> t2.requires_grad = True
```

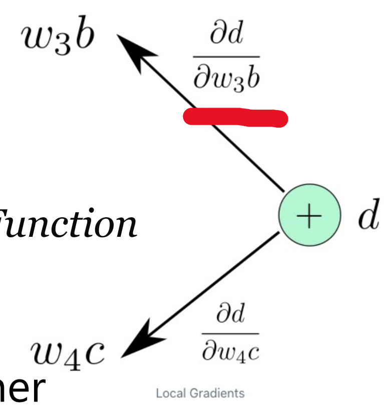
```
import torch

a = torch.randn((3,3), requires_grad = True)

w1 = torch.randn((3,3), requires_grad = True)
w2 = torch.randn((3,3), requires_grad = True)
w3 = torch.randn((3,3), requires_grad = True)
w4 = torch.randn((3,3), requires_grad = True)

b = w1*a
c = w2*a

d = w3*b + w4*c

L = 10 - d

print("The grad fn for a is", a.grad_fn)
print("The grad fn for d is", d.grad_fn)
```

Each **Tensor** has an attribute **grad_fn**, which refers to the mathematical operator that created it.

If **Tensor** is a leaf node (initialized by the user), then the **grad_fn** is **None**.

```
The grad fn for a is None
The grad fn for d is <AddBackward0 object at 0x1033afe48>
```

Functions



- All math steps represented by classes inherited from *torch.autograd.Function*
  - *forward*, computes node output and buffers it
  - *backward*, stores incoming gradient in **grad** and passes further

```
def backward (incoming_gradients):
        self.Tensor.grad = incoming_gradients

        for inp in self.inputs:
                if inp.grad_fn is not None:
                        new_incoming_gradients = //
                          incoming_gradient * local_grad(self.Tensor, inp)

                        inp.grad_fn.backward(new_incoming_gradients)
                else:
                        pass
```

Gradient descent

- Compute gradient for every tensor involved

```python
import torch

a = torch.randn((3,3), requires_grad = True)

w1 = torch.randn((3,3), requires_grad = True)
w2 = torch.randn((3,3), requires_grad = True)
w3 = torch.randn((3,3), requires_grad = True)
w4 = torch.randn((3,3), requires_grad = True)

b = w1*a
c = w2*a

d = w3*b + w4*c

# Replace L = (10 - d) by
L = (10 -d).sum()

L.backward()
```

- Make gradient descent step in the opposite direction:

```python
learning_rate = 0.5
w1 = w1 - learning_rate * w1.grad
```

Dynamic graph

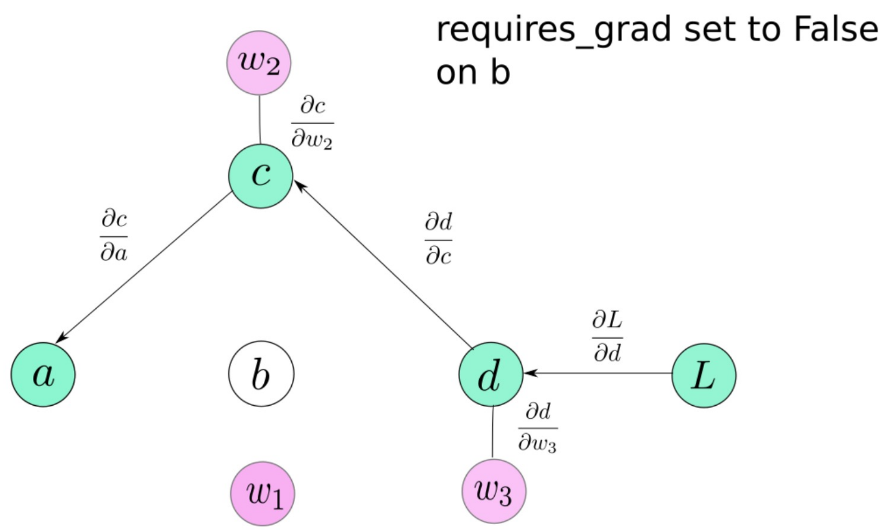
- Calling *forward* creates
  - graph with the intermediate node output values,
  - buffers for the non-leaf nodes,
  - buffers for intermediate gradient values.
- Calling *backward*
  - computes gradients and
  - frees the buffers and destroys the graph.
- Next time, calling *forward*
  - leaf node buffers from the previous run will be shared,
  - **non-leaf nodes buffers will be recreated**.

Gradient cleaning

- Due to the flexibility of the network architecture, it is not obvious when does iteration of a gradient descent stops, so *backward's* gradients are accumulated each time a variable (Tensor) occurs in the graph;
- It is usually desired for RNN cases;
- If you do not need to accumulate those, you must **clean previous gradient values** at the end of each iteration:
  - Either by x.data.zero_() for every model tensor x;
  - Or by optimizers's *zero_grad*() method, which is more preferable.

Freezing weights

- **Requires_grad** attribute of the *Tensor* class. By default, it's **False**. It comes handy when you must freeze some layers and stop them from updating parameters while training.
- Thus, no gradient would be propagated to them, or to those layers which depend upon these layers for gradient flow **requires_grad**.
- When set to **True**, **requires_grad** is contagious: even if one operand of an operation has **requires_grad** set to **True**, so will the result.



Pre-trained models' enhancement

```
model = torchvision.models.resnet18(pretrained=True)
for param in model.parameters():
    param.requires_grad = False
# Replace the last fully-connected layer
# Parameters of newly constructed modules have requires_grad=True by
default
model.fc = nn.Linear(512, 100)

# Optimize only the classifier
optimizer = optim.SGD(model.fc.parameters(), lr=1e-2, momentum=0.9)
```

Inference

- When we are computing gradients, we need to cache input values, and intermediate features as they maybe required to compute the gradient later. The gradient of **b=w1*a** w.r.t it's inputs **w1** and **a** is **a** and **w1,** respectively.
- We need to store these values for gradient computation during the backward pass. This affects the memory footprint of the network.
- While, we are performing inference, we don't compute gradients

```
with torch.no_grad:
        inference code goes here
```

- Even better and recent optimized context: `with torch.inference_mode` (link)

Neural Network class: torch.nn.Module

```python
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super(Model, self).__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Loss functions

```
nn.X                        # where X is BCELoss, CrossEntropyLoss,
                            # L1Loss, MSELoss, NLLLoss, SoftMarginLoss,
                            # MultiLabelSoftMarginLoss, CosineEmbeddingLoss,
                            # KLDivLoss, MarginRankingLoss, HingeEmbeddingLoss
                            # or CosineEmbeddingLoss
```

- https://pytorch.org/docs/stable/nn.html#loss-functions

Optimizers

```
opt = optim.x(model.parameters(), ...)      # create optimizer
opt.step()                                  # update weights
optim.X                                     # where X is SGD, Adadelta, Adagrad, Adam,
                                            # SparseAdam, Adamax, ASGD,
                                            # LBFGS, RMSProp or Rprop
```

- https://pytorch.org/docs/stable/optim.html

Data Utils

Datasets

```
Dataset                     # abstract class representing dataset
TensorDataset               # labelled dataset in the form of tensors
Concat Dataset              # concatenation of Datasets
```

- https://pytorch.org/docs/stable/data.html?highlight=dataset#torch.utils.data.Dataset

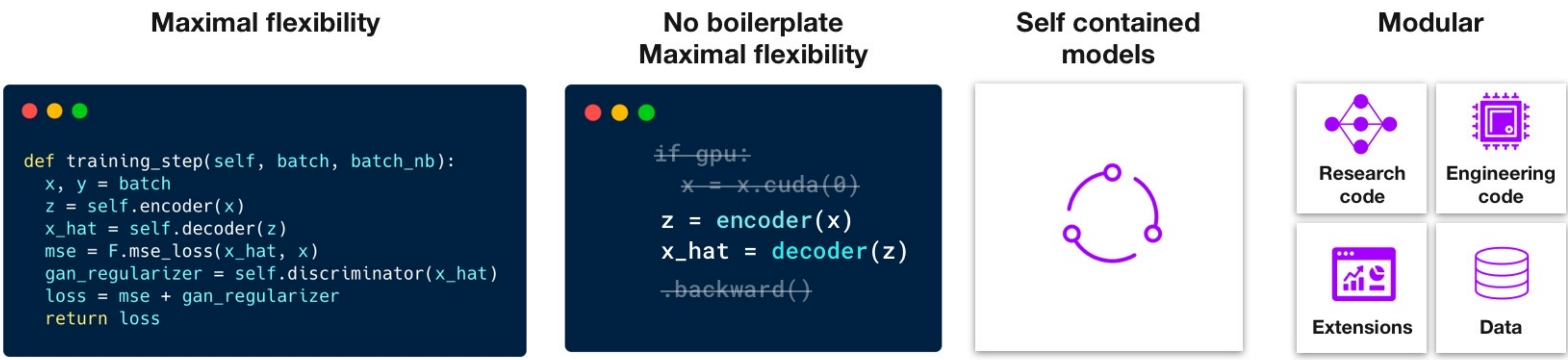
Dataloaders and DataSamplers

```
DataLoader(dataset, batch_size=1, ...)      # loads data batches agnostic
                                            # of structure of individual data points

sampler.Sampler(dataset,...)                # abstract class dealing with
                                            # ways to sample from dataset

sampler.XSampler where ...                  # Sequential, Random, Subset,
                                            # WeightedRandom or Distributed
```

- https://pytorch.org/docs/stable/data.html?highlight=dataloader#torch.utils.data.DataLoader

PyTorch Lightning

- The lightweight PyTorch wrapper for high-performance AI research.



https://github.com/PyTorchLightning/pytorch-lightning

PYTORCH

```python
# models
encoder = nn.Sequential(nn.Linear(28 * 28, 64), nn.ReLU(), nn.Linear(64, 3))
decoder = nn.Sequential(nn.Linear(3, 64), nn.ReLU(), nn.Linear(64, 28 * 28))

encoder.cuda(0)
decoder.cuda(0)

# download on rank 0 only
if global_rank == 0:
    mnist_train = MNIST(os.getcwd(), train=True, download=True)

# split dataset
transform=transforms.Compose([transforms.ToTensor(),
                              transforms.Normalize(0.5, 0.5)])
mnist_train = MNIST(os.getcwd(), train=True, download=True, transform=transform)

# train (55,000 images), val split (5,000 images)
mnist_train, mnist_val = random_split(mnist_train, [55000, 5000])

# The dataloaders handle shuffling, batching, etc...
mnist_train = DataLoader(mnist_train, batch_size=64)
mnist_val = DataLoader(mnist_val, batch_size=64)

# optimizer
params = [encoder.parameters(), decoder.parameters()]
optimizer = torch.optim.Adam(params, lr=1e-3)

# TRAIN LOOP
model.train()
num_epochs = 1
for epoch in range(num_epochs):
  for train_batch in mnist_train:
    x, y = train_batch
    x = x.cuda(0)
    x = x.view(x.size(0), -1)
    z = encoder(x)
    x_hat = decoder(z)
    loss = F.mse_loss(x_hat, x)
    print('train loss: ', loss.item())

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

# EVAL LOOP
model.eval()
with torch.no_grad():
  val_loss = []
  for val_batch in mnist_val:
    x, y = val_batch
    x = x.cuda(0)
    x = x.view(x.size(0), -1)
    z = encoder(x)
    x_hat = decoder(z)
    loss = F.mse_loss(x_hat, x)
    val_loss.append(loss)
  val_loss = torch.mean(torch.tensor(val_loss))
  model.train()
```

PYTORCH LIGHTNING

Turn PyTorch into Lightning

Lightning is just plain PyTorch

https://github.com/PyTorchLightning/pytorch-lightning

Ecosystem

- PyTorch lightning
- PyTorch geometric
- Hydra
- Horovod
- Skorch
- Captum
- And many others, see https://pytorch.org/ecosystem/

Moar stuff

- https://pytorch.org/docs/stable/index.html
- https://pytorch.org/tutorials/beginner/ptcheat.html
- http://neuralnetworksanddeeplearning.com/chap2.html
- https://www.khanacademy.org/math/differential-calculus/dc-chain
- https://blog.paperspace.com/pytorch-101-understanding-graphs-and-automatic-differentiation/

Conclusion

- PyTorch is a solid, flexible, production-ready foundation for real-life deep-learning applications
- Building blocks:
  - Tensors
  - Functions
- Dynamic graph automatic differentiation
  - CPU, GPU, TPU
- Rich ecosystem

Thank you!

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