PyTorch and Neural Nets

CS285 Deep RL

Instructor: Kyle Stachowicz

[Adapted from Marwa Abdulhai’s CS285 Fa22 Slides]

PyTorch Tutorial (Colab)

https://colab.research.google.com/drive/12nQiv6aZHXNuCfAAuTjJenDWKQbIt2Mz

http://bit.ly/cs285-pytorch-2023

Goal of this course

Train an agent to perform useful tasks

$\pi_\theta(a|s)$ $\quad$ $\hat{\Delta}_{t+1} = f_\theta(s_t, a_t)$

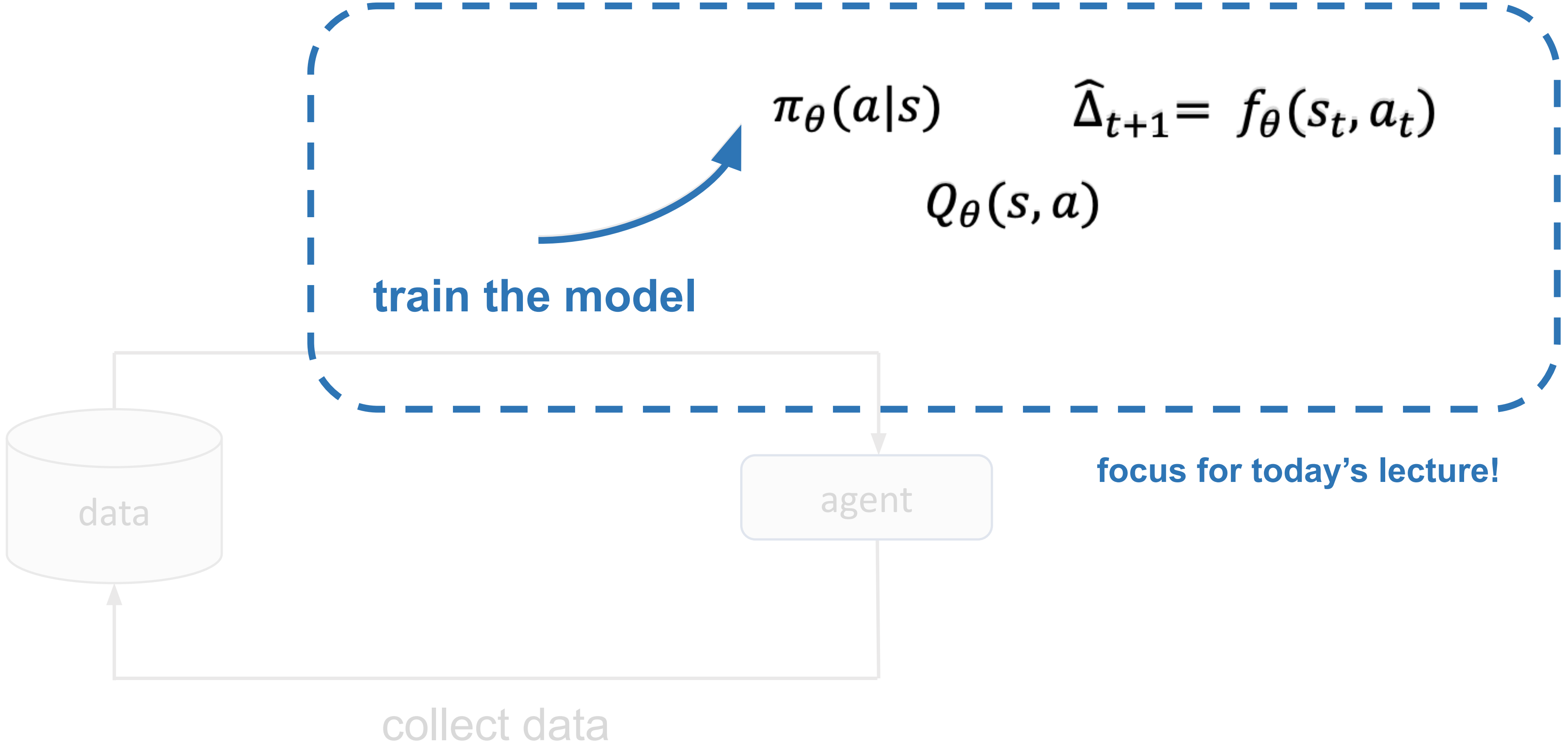
$Q_\theta(s, a)$

train the model

collect data

Goal of this course

Train an agent to perform useful tasks



How do train a model?

$$\theta^* = \arg\min_\theta \sum_{(x,y)\in D} \mathcal{L}(f_\theta(x), y)$$

gradient descent

dataset

loss

neural network

PyTorch does all of these!

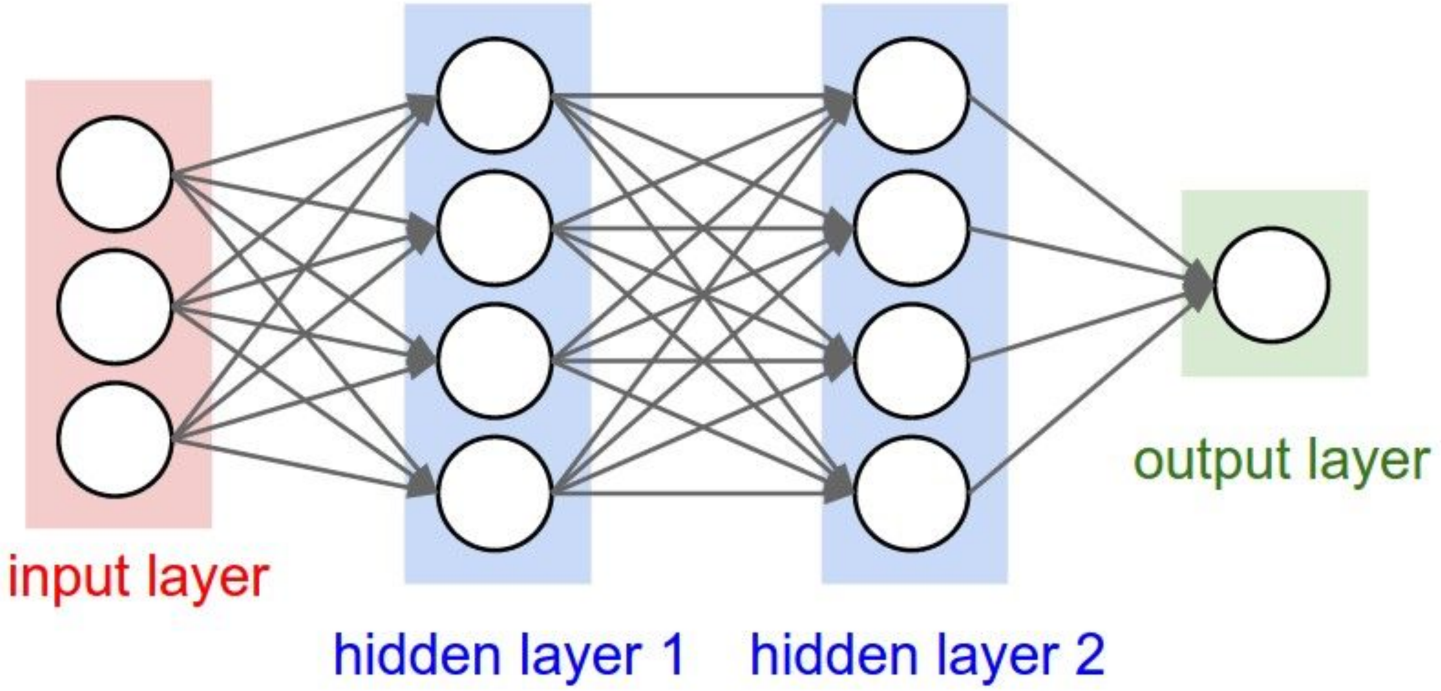
What is PyTorch?

Python library for:

- Defining neural networks
- Automating computing gradients
- And more! (datasets, optimizers, GPUs, etc.)

$$\theta^* = \underbrace{\arg\min_{\theta}}_{\text{gradient descent}} \sum_{(x,y)\in \underbrace{D}_{\text{dataset}}} \underbrace{\mathcal{L}}_{\text{loss}}(\underbrace{f_{\theta}}_{\text{neural network}}(x), y)$$

How does PyTorch work?



You define:	$h_1 = \sigma(W_1 x)$ $\quad h_2 = \sigma(W_2 h_1)$ $\quad y = \sigma(W_3 h_2)$
PyTorch computes:	$\frac{\partial y}{\partial W_1} = \frac{\partial y}{\partial h_2} \frac{\partial h_2}{\partial h_1} \frac{\partial h_1}{\partial W_1}$ $\quad \frac{\partial y}{\partial W_2} = \frac{\partial y}{\partial h_2} \frac{\partial h_2}{\partial W_1}$ $\quad \frac{\partial y}{\partial W_3}$

[picture from Stanford's CS231n]

NumPy

- Fast CPU implementations
- **CPU-only**
- **No autodiff**
- **Imperative**

PyTorch

- Fast CPU implementations
- **Allows GPU**
- **Supports autodiff**
- **Imperative**

Other features include:

- Datasets and dataloading
- Common neural network operations
- Built-in optimizers (Adam, SGD, …)

The Basics

python

```
arr_a = [1, 3, 4, 5, 9]
arr_b = [9, 5, 7, 2, 5]

# Element-wise operations
list_sum = [a + b for a, b in zip(list_a, list_b)]
list_prod = [a * b for a, b in zip(list_a, list_b)]
list_doubled = [2 * a for a in list_a]

# Indexing
value = list_a[3]
list_slice = list_a[2:3]

arr_idx = [3, 2, 1]
arr_indexed = [arr_a[i] for i in arr_idx]
```

NumPy

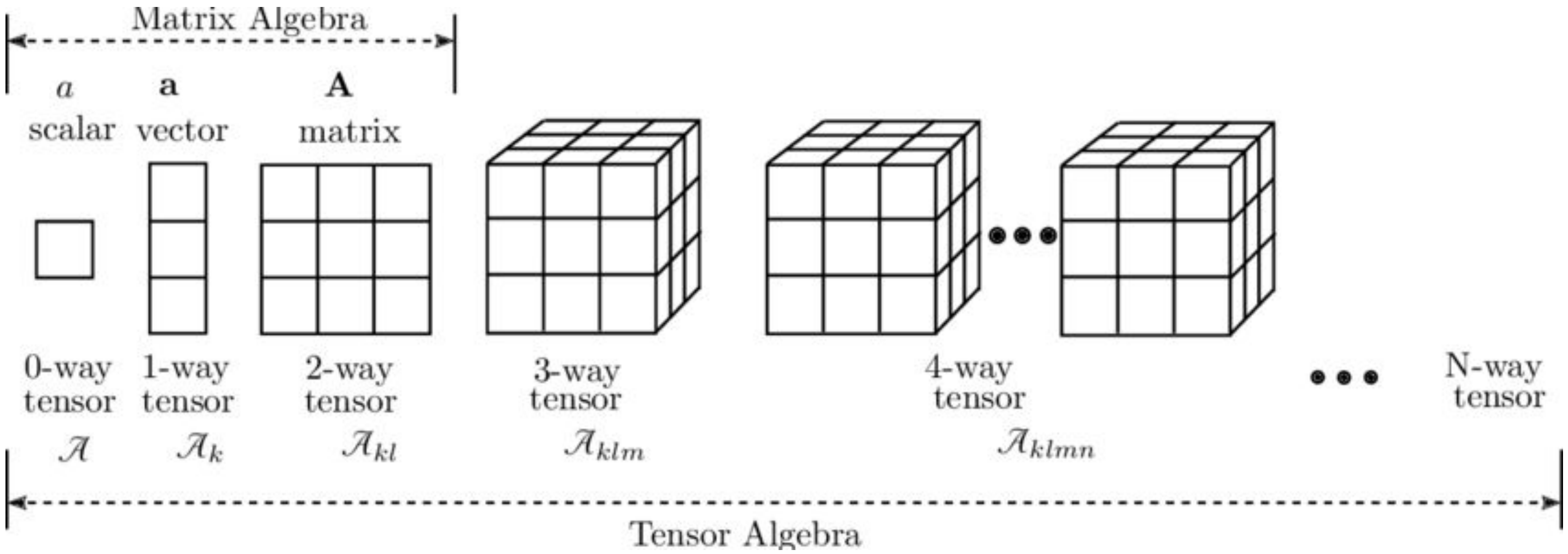
```
import numpy as np

arr_a = np.array([1, 3, 4, 5, 9])
arr_b = np.array([9, 5, 7, 2, 5])

# Element-wise operations
arr_sum = a + b
arr_prod = a * b
arr_doubled = 2 * a

# Indexing
value = arr_a[3]
arr_slice = arr_a[2:3]

arr_idx = np.array([3, 2, 1])
arr_indexed = arr_a[arr_idx]
```

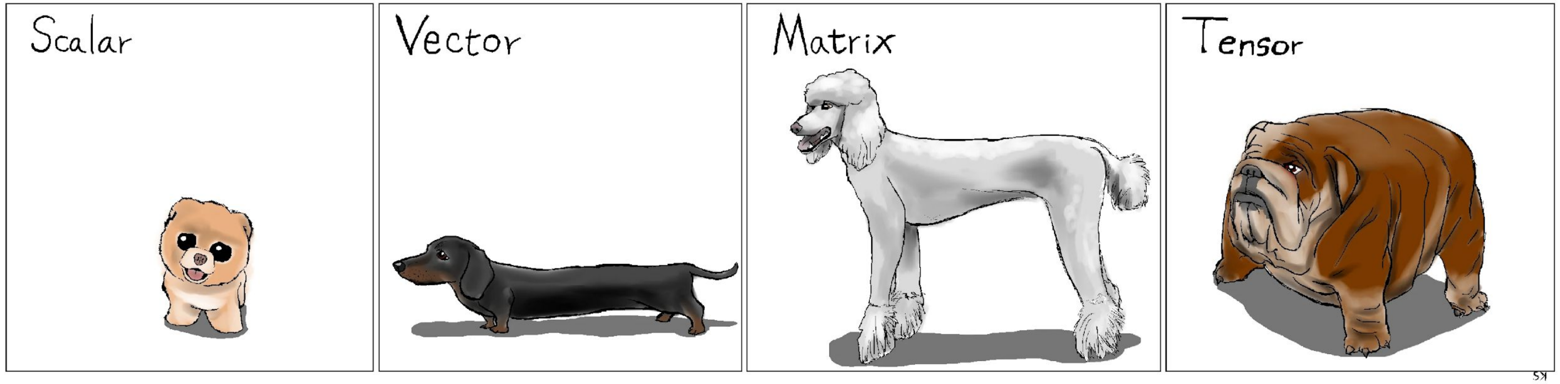
PyTorch

```
import torch

tensor_a = torch.tensor([1, 3, 4, 5, 9])
tensor_b = torch.tensor([9, 5, 7, 2, 5])

# Element-wise operations
tensor_sum = tensor_a + tensor_b
tensor_prod = tensor_a * tensor_b
tensor_doubled = 2 * tensor_a

# Indexing
value = tensor_a[3]
tensor_slice = tensor_a[2:3]

tensor_idx = torch.tensor([3, 2, 1])
tensor_indexed = tensor_a[tensor_idx]
```

100x faster!

Multidimensional Arrays





Multidimensional Indexing

PyTorch

NumPy

Axis 1

A

Axis 0

32	27	5	54	1
99	4	23	3	57
76	42	34	82	5

```
A.shape == (3, 5)
```

PyTorch

NumPy

Multidimensional Indexing

Axis 1

Axis 0

32	27	5	54	1
99	4	23	3	57
76	42	34	82	5

```
A[0, 3]
```

Multidimensional Indexing

PyTorch

NumPy

Axis 1

Axis 0

32	27	5	54	1
99	4	23	3	57
76	42	34	82	5

```
A[:, 3]
```

PyTorch

NumPy

Multidimensional Indexing

Axis 1

Axis 0

32	27	5	54	1
99	4	23	3	57
76	42	34	82	5

```
A[0, :]
```

Multidimensional Indexing

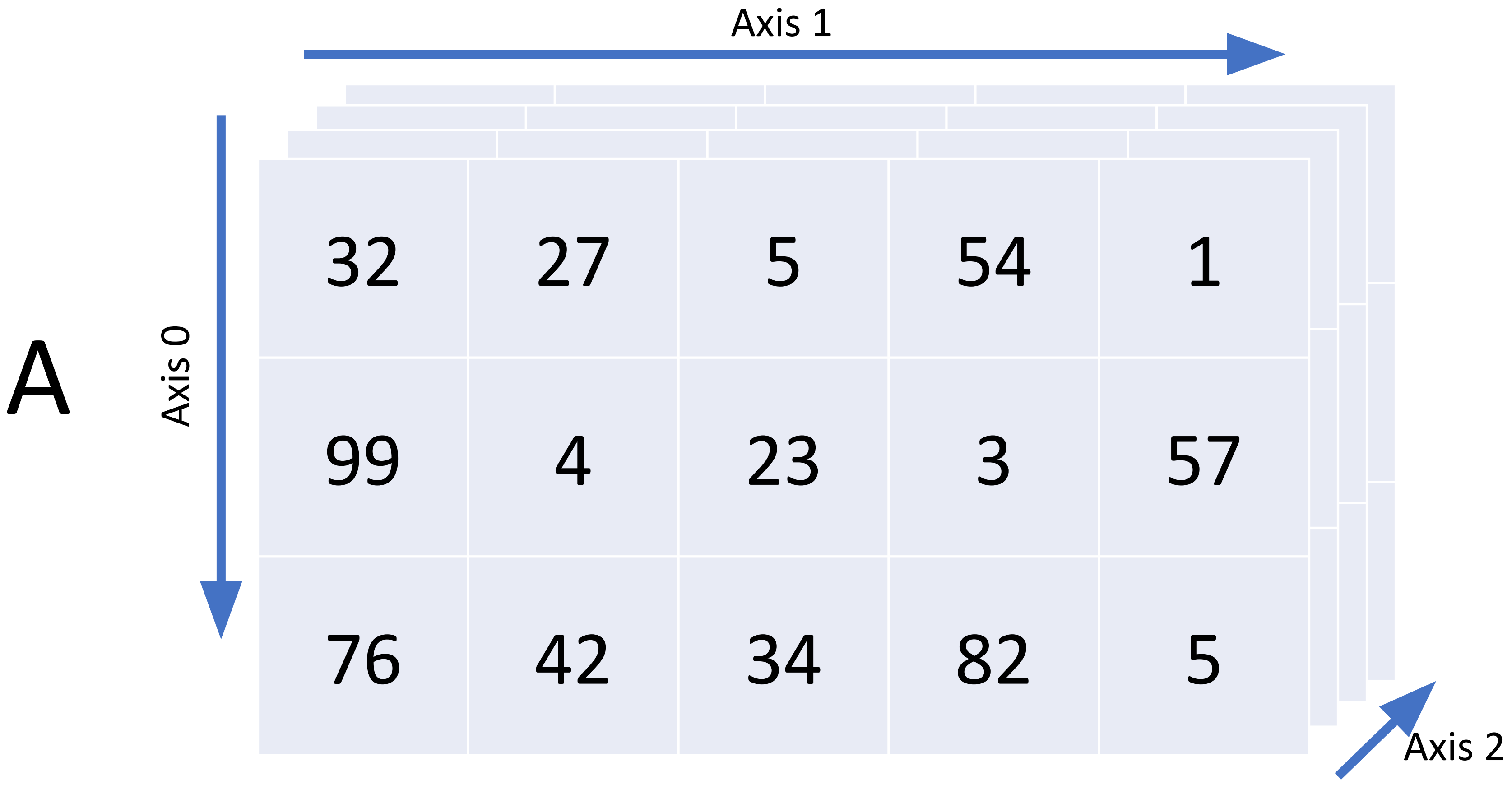
Axis 1

Axis 0

32	27	5	54	1
99	4	23	3	57
76	42	34	82	5

```
A[0, 2:4]
```

Multidimensional Indexing



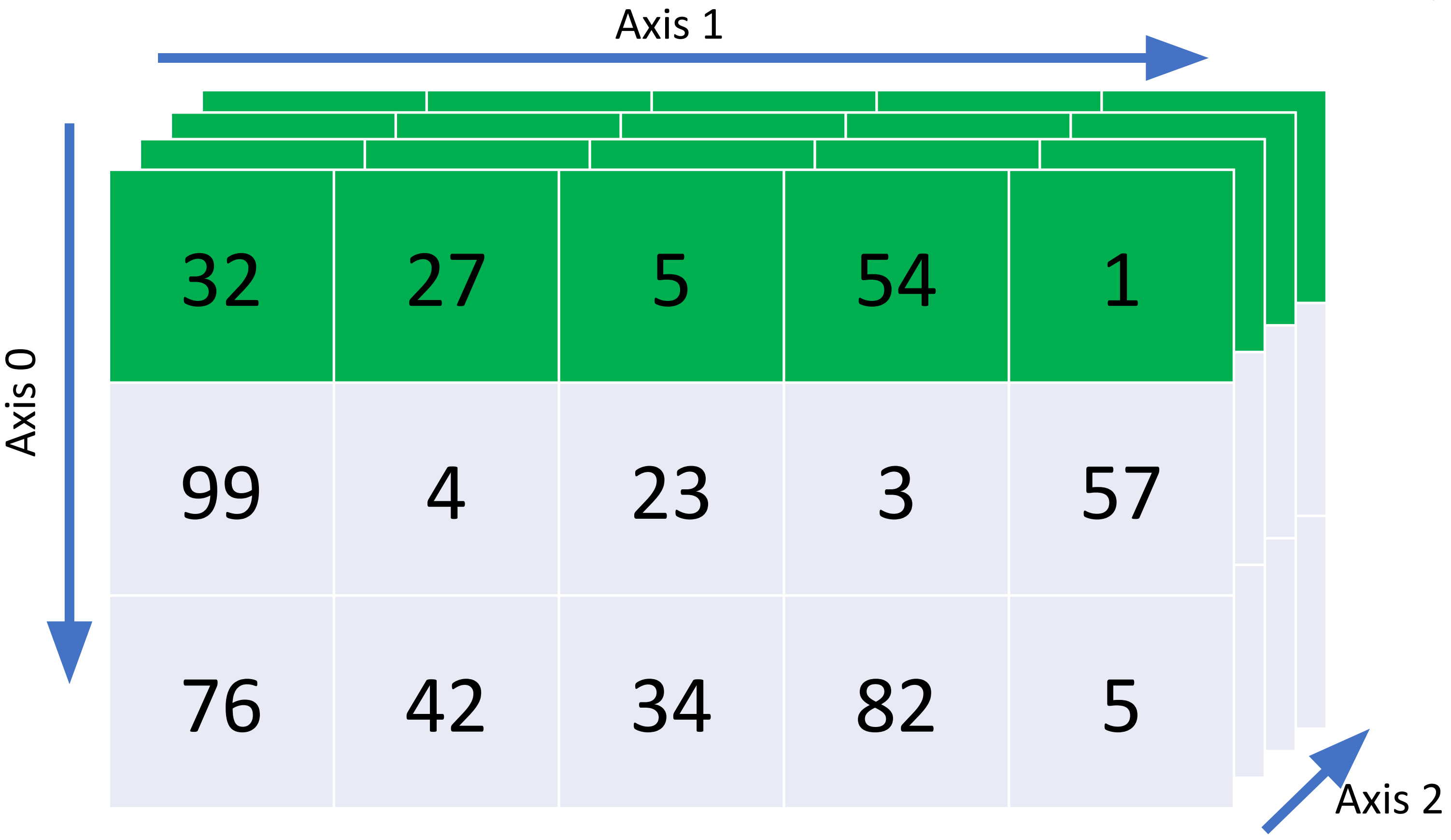

```
A.shape == (3, 5, 4)
```

Multidimensional Indexing

PyTorch

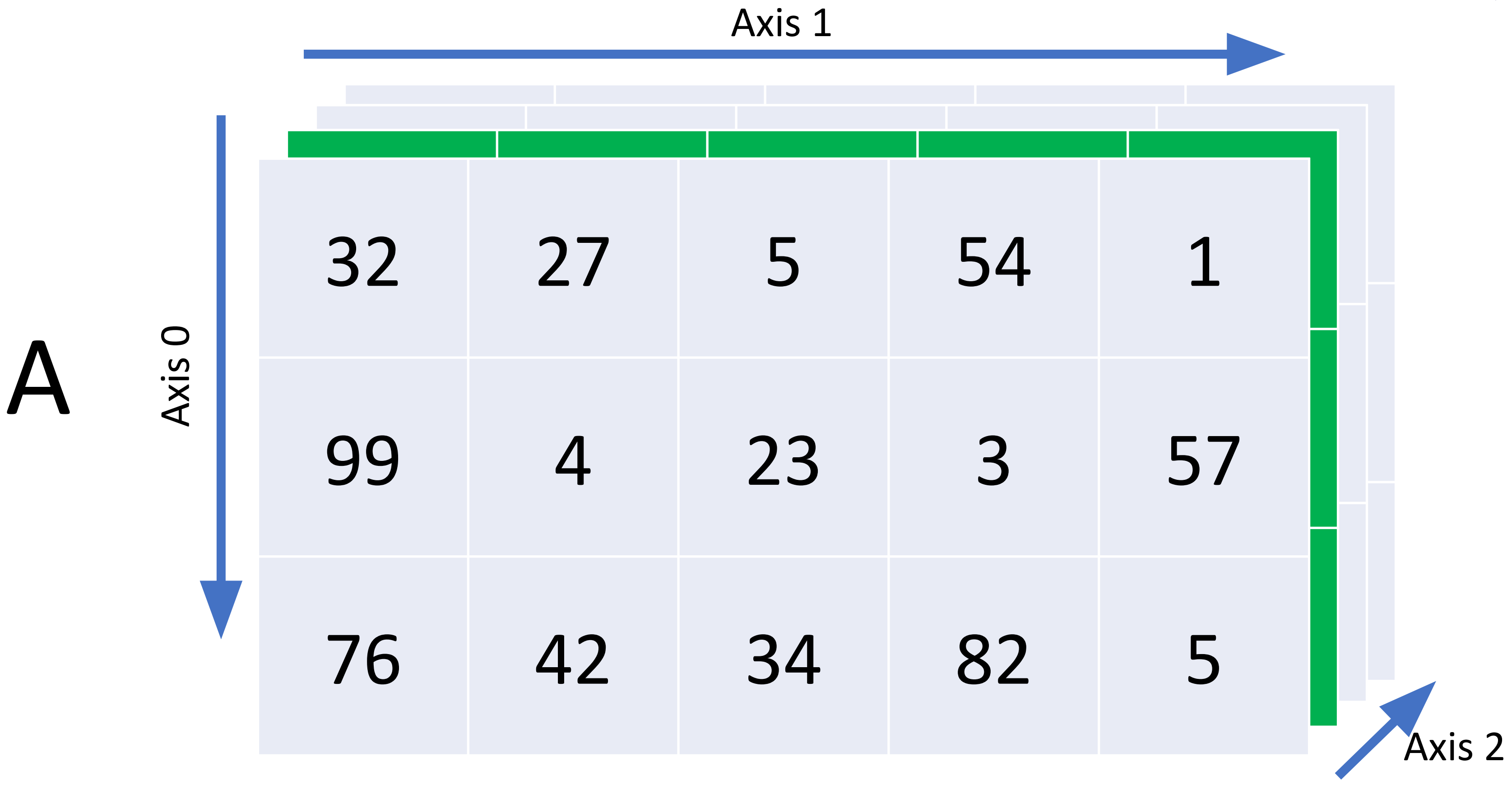
NumPy

A




```
A[0, ...]
```

Multidimensional Indexing

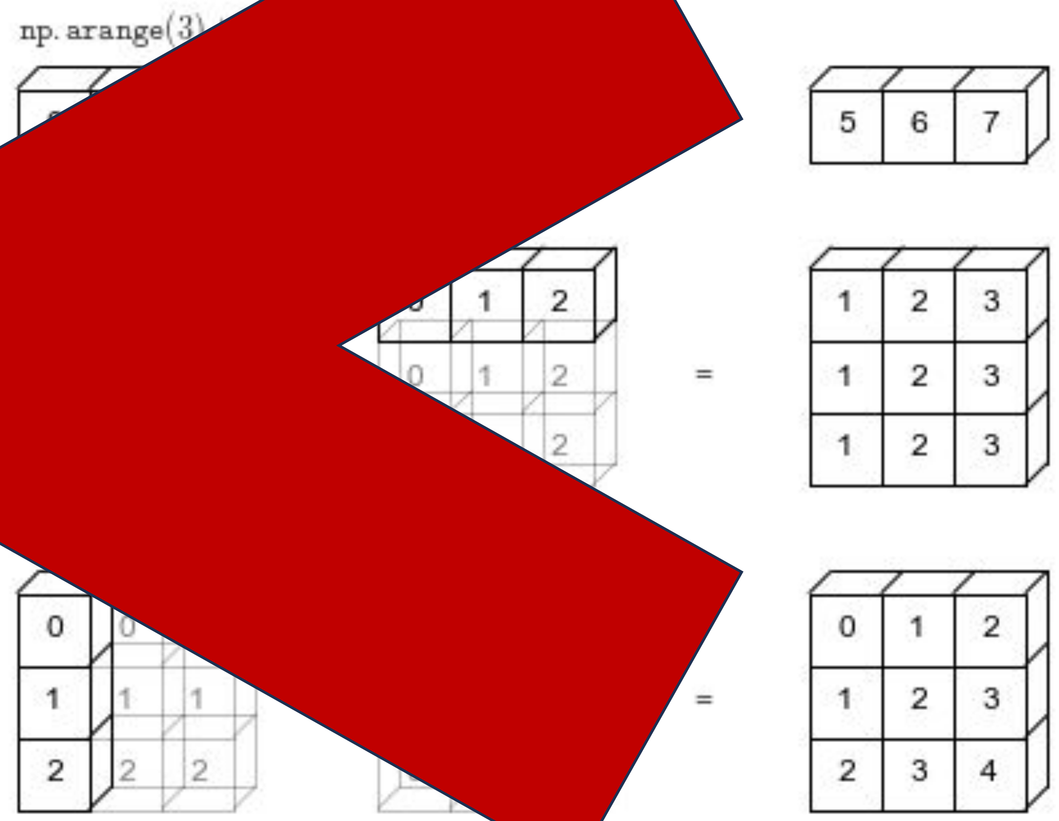


`A[..., 1]`

Broadcasting

TL;DR: Shap
like (6, 5, 4, 3,
to shape (6, 5, 4, 3,

(Trailing dimension
matched, arra
repeated alo
dimensions)



https://jakevdp.github.io/PythonDataScienceHandbook/02.05-computation-on-arrays-broadcasting.html

Shape Operations

NumPy

```python
A = np.random.normal(size=(10, 15))

# Indexing with newaxis/None
# adds an axis with size 1
A[np.newaxis] # -> shape (1, 10, 15)

# Squeeze removes a axis with size 1
A[np.newaxis].squeeze(0) # -> shape (10, 15)

# Transpose switches out axes.
A.transpose((1, 0)) # -> shape (15, 10)

# !!! BE CAREFUL WITH RESHAPE !!!
A.reshape(15, 10)     # -> shape (15, 10)
A.reshape(3, 25, -1) # -> shape (3, 25, 2)
```

PyTorch

```python
A = torch.randn((10, 15))

# Indexing with None
# adds an axis with size 1
A[None] # -> shape (1, 10, 15)

# Squeeze removes a axis with size 1
A[None].squeeze(0) # -> shape (10, 15)

# Permute switches out axes.
A.permute((1, 0)) # -> shape (15, 10)

# !!! BE CAREFUL WITH VIEW !!!
A.view(15, 10)     # -> shape (15, 10)
A.view(3, 25, -1) # -> shape (3, 25, 2)
```

Device Management

- Numpy: all arrays live on the CPU's RAM
- Torch: tensors can either live on CPU or GPU memory
  - Move to GPU with `.to("cuda")`/`.cuda()`
  - Move to CPU with `.to("cpu")`/`.cpu()`

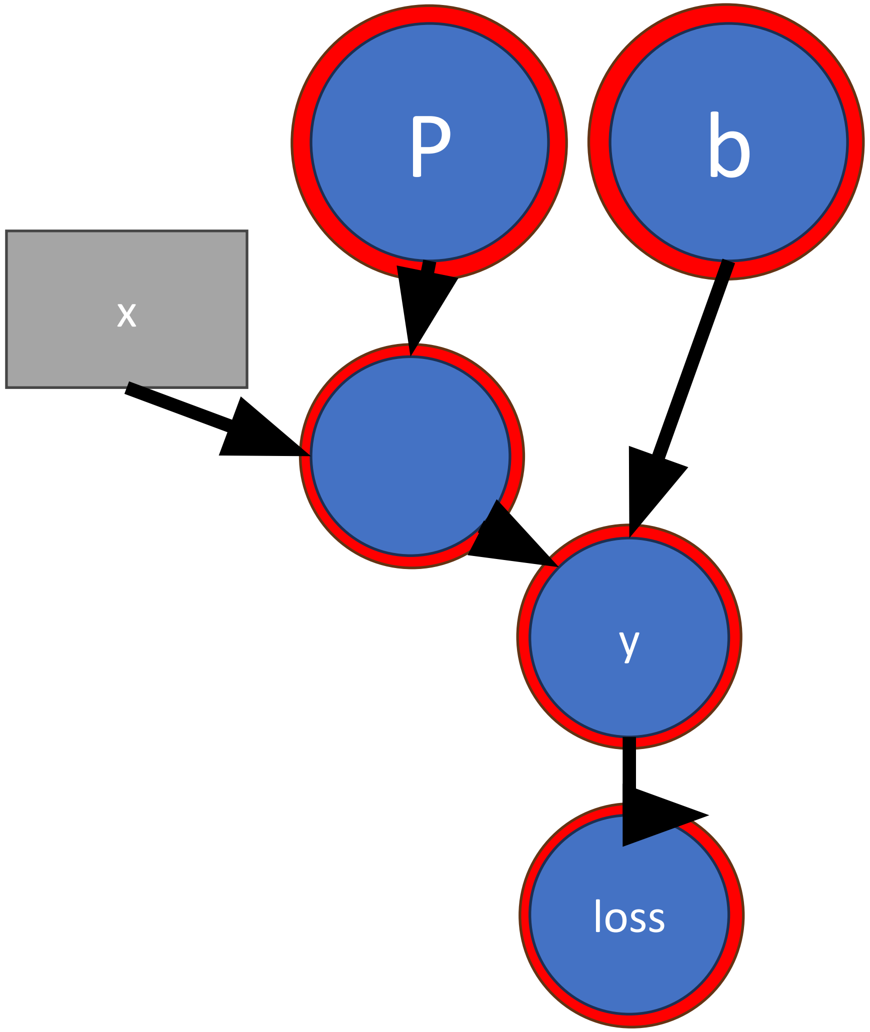
YOU CANNOT PERFORM OPERATIONS BETWEEN TENSORS ON DIFFERENT DEVICES!

```
[ ] device = torch.device("cuda")
    x = torch.zeros((2, 3))
    y = torch.ones((2, 3), device=device)
    z = x + y
```

```
---------------------------------------------------------------------------
RuntimeError                              Traceback (most recent call last)
<ipython-input-71-565d7b7035e6> in <module>
      2 x = torch.zeros((2, 3))
      3 y = torch.ones((2, 3), device=device)
----> 4 z = x + y

RuntimeError: Expected all tensors to be on the same device, but found at least two
devices, cuda:0 and cpu!
```

Computing Gradients

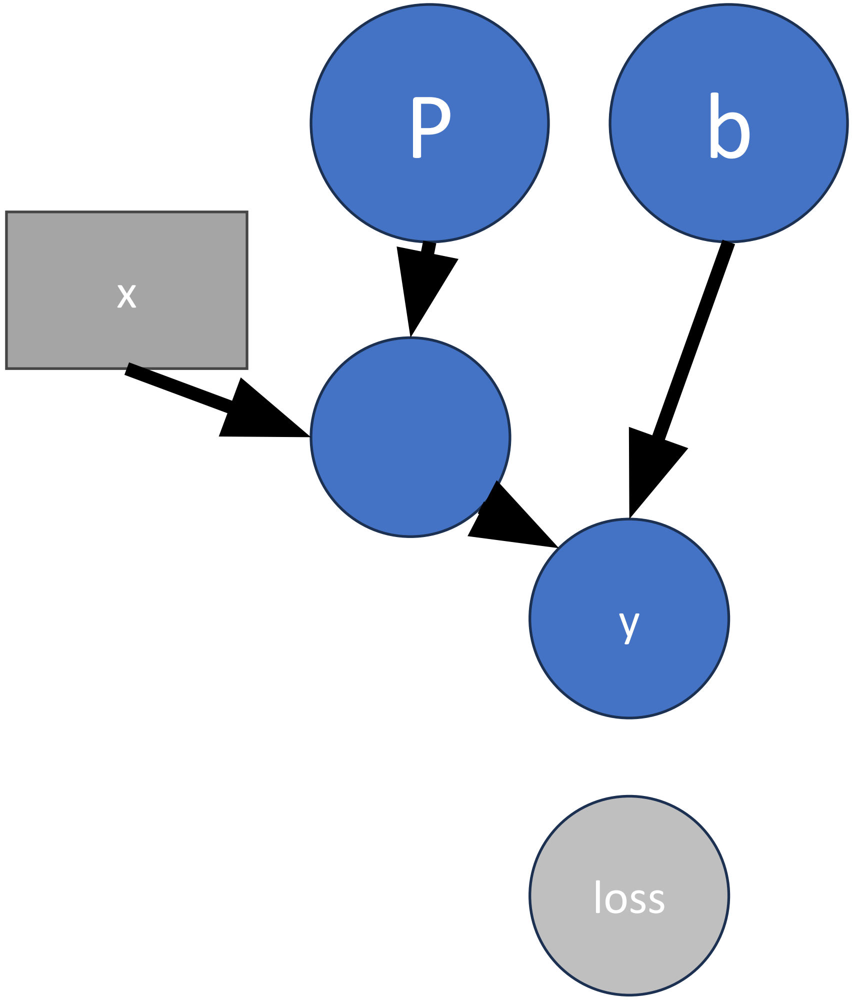
```
P = torch.randn((1024, 1024))
print(P.requires_grad) # -> False
P = torch.randn((1024, 1024), requires_grad=True)
b = torch.randn((1024,), requires_grad=True)
print(P.grad) # -> None
```



Computing Gradients

PyTorch

```
P = torch.randn((1024, 1024))
print(P.requires_grad) # -> False
P = torch.randn((1024, 1024), requires_grad=True)
b = torch.randn((1024,), requires_grad=True)
print(P.grad) # -> None

x = torch.randn((32, 1024))
y = torch.nn.relu(x @ P + b)

target = 3
loss = torch.mean((y - target) ** 2).detach()
```



Training Loop

PyTorch

```
net = (...).to("cuda")
dataset = ...
dataloader = ..
optimizer = ...
loss_ fn = ..
for epoch in range(num_epochs):
  # Training..
  net.train()
  for data, target in dataloader:
    data = torch.from_numpy(data).float().cuda()
    target = torch.from_numpy(data).float().cuda()

    prediction = net(data)
    loss = loss_fn(prediction, target)

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

  net.eval()
  # Do evaluation..
```

REMEMBER THIS!

Converting Numpy / PyTorch

Numpy -> PyTorch:

`torch.from_numpy(numpy_array).float()`

PyTorch -> Numpy:

- (If `requires_grad`) Get a copy without graph with `.detach()`
- (If on GPU) Move to CPU with `.to(“cpu”)/.cpu()`
- Convert to numpy with `.numpy`

All together:

`torch_tensor.detach().cpu().numpy()`

Custom networks

```python
import torch.nn as nn

class SingleLayerNetwork(nn.Module):
  def __init__(self, in_dim: int, out_dim: int, hidden_dim: int):
    super().__init__() # <- Don't forget this!
    self.net = nn.Sequential(
      nn.Module(in_dim, hidden_dim),
      nn.ReLU(),
      nn.Module(hidden_dim, out_dim),
    )

  def forward(self, x: torch.Tensor) -> torch.Tensor:
    return self.net(x)

batch_size = 256
my_net = SingleLayerNetwork(2, 32, 1).to("cuda")
output = my_net(torch.randn(size=(batch_size, 2)).cuda())
```

- Prefer `net()` over `net.forward()`
- Everything (network and its inputs) on the same device!!!

Torch Best Practices

- When in doubt, **`assert`** is your friend

```
assert x.shape == (B, N), \
       f"Expected shape ({B, N}) but got {x.shape}"
```

- Be extra careful with `.reshape/.view`
  - If you use it, assert before and after
  - Only use it to collapse/expand a single dim
  - In Torch, prefer `.flatten()/.permute()/.unflatten()`
- If you do some complicated operation, test it!
  - Compare to a pure Python implementation

Torch Best Practices (continued)

- Don’t mix numpy and Torch code
  - Understand the boundaries between the two
  - Make sure to cast 64-bit numpy arrays to 32 bits
  - `torch.Tensor` only in `nn.Module`!
- Training loop will always look the same
  - Load batch, compute loss
  - `.zero_grad()`, `.backward()`, `.step()`

PyTorch Tutorial (Colab)

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