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Artificial Intelligence Research

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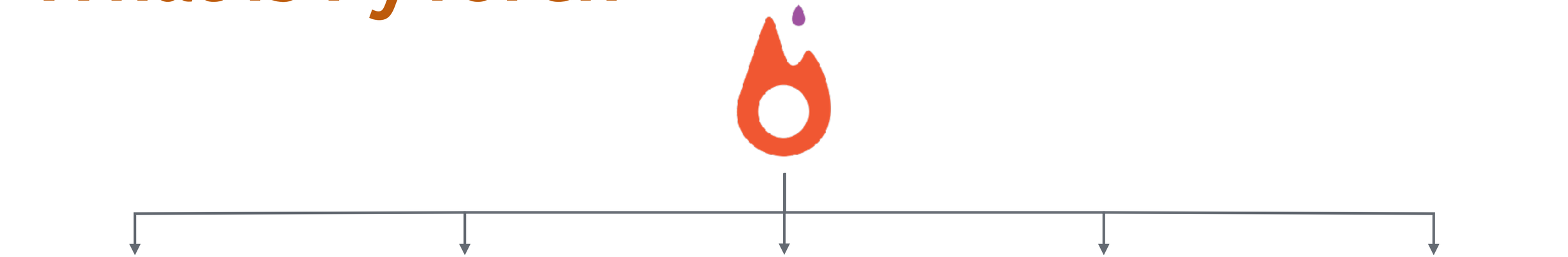
What is PyTorch?

What is PyTorch



efficient ndarray library with GPU support

automatic differentiation engine

machine learning primitives

gradient based optimization package

Machine Learning Ecosystem

CUDA

NumPy like interface

Probabilistic Modeling

Deep Learning

Reinforcement Learning

⋮

Data Loading

Visualization

Utility packages for image and text data

⋮

Tensor (ndarray) library

Tensor (ndarray) library

- NumPy-like API (np.ndarray <-> torch.Tensor)
- Very fast acceleration on NVIDIA GPUs

Tensor (ndarray) library

- NumPy-like API (np.ndarray <-> torch.Tensor)
  - Easy creation of Tensors with various dtypes and on different devices
  - Scientific computing methods (linear algebra, reduction, etc.)
  - Fast conversion from and to np.ndarray

Tensor (ndarray) library

- NumPy-like API (np.ndarray <-> torch.Tensor)

```
In [1]: import torch
        import numpy as np

In [2]: a = torch.rand(2, 2)  # a random Tensor
        a

Out[2]: tensor([[ 0.8836,  0.9006],
                [ 0.1145,  0.8328]])

In [3]: a + 1

Out[3]: tensor([[ 1.8836,  1.9006],
                [ 1.1145,  1.8328]])

In [4]: torch.svd(a)  # linear algebra operations! (SVD)

Out[4]: (tensor([[-0.8548, -0.5190],
                 [-0.5190,  0.8548]]),
         tensor([ 1.4521,  0.4358]),
         tensor([[-0.5611, -0.8278],
                 [-0.8278,  0.5611]]))

In [5]: a.numpy()  # convert to a NumPy ndarray

Out[5]: array([[ 0.88362992,  0.90055138],
               [ 0.11449063,  0.83281231]], dtype=float32)

In [6]: torch.from_numpy(np.zeros((2, 3)))  # convert a NumPy ndarray to a Tensor

Out[6]: tensor([[ 0.,  0.,  0.],
                [ 0.,  0.,  0.]], dtype=torch.float64)
```

Numpy

```
import numpy as np

# N is batch size: D_in is input dimension;
# H is hidden dimension; D_out is output dimension

N, D_in, H, D_out = 64, 1000, 100, 10

# Create random input and output data
x = np.random.randn(N, D_in)
y = np.random.randn(N, D_out)

# Randomly initialize weights
w1 = np.random.randn(D_in, H)
w2 = np.random.randn(H, D_out)

learning_rate = 1e-6
for t in range(500):
    # Forward pass: compute predicted y
    h = np.matmul(x, w1)
    h_relu = np.maximum(h, 0)
    y_pred = np.matmul(h_relu, w2)

    # Compute and print loss
    loss = ((y_pred - y) ** 2).sum()
    print(t, loss)

    # Backprop to compute gradients of w1 and
    # w2 with respect to loss
    grad_y_pred = 2.0 * (y_pred - y)
    grad_w2 = np.matmul(h_relu.T, grad_y_pred)
    grad_h_relu = np.matmul(grad_y_pred, w2.T)
    grad_h = grad_h_relu.copy()
    grad_h[h < 0] = 0
    grad_w1 = np.matmul(x.T, grad_h)

    # Update weights
    w1 -= learning_rate * grad_w1
    w2 -= learning_rate * grad_w2
```

PyTorch

```
import torch

# N is batch size: D_in is input dimension;
# H is hidden dimension; D_out is output dimension

N, D_in, H, D_out = 64, 1000, 100, 10

# Create random input and output data
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)

# Randomly initialize weights
w1 = torch.randn(D_in, H)
w2 = torch.randn(H, D_out)

learning_rate = 1e-6
for t in range(500):
    # Forward pass: compute predicted y
    h = torch.matmul(x, w1)
    h_relu = h.clamp(min=0)
    y_pred = torch.matmul(h_relu, w2)

    # Compute and print loss
    loss = ((y_pred - y) ** 2).sum()
    print(t, loss)

    # Backprop to compute gradients of w1 and
    # w2 with respect to loss
    grad_y_pred = 2.0 * (y_pred - y)
    grad_w2 = torch.matmul(h_relu.t(), grad_y_pred)
    grad_h_relu = torch.matmul(grad_y_pred, w2.t())
    grad_h = grad_h_relu.clone()
    grad_h[h < 0] = 0
    grad_w1 = torch.matmul(x.t(), grad_h)

    # Update weights
    w1 -= learning_rate * grad_w1
    w2 -= learning_rate * grad_w2
```

Tensor (ndarray) library

- Very fast acceleration on NVIDIA GPUs
  - Efficient scientific computing on GPU
  - Clean device management
  - Seamless conversion to and from CPU

Tensor (ndarray) library

- Very fast acceleration on NVIDIA GPUs

```
In [1]: import torch

In [2]: cuda = torch.device("cuda")  # cuda device object

In [3]: a = torch.rand(3, 3, device=cuda)  # create a random Tensor on GPU
        a

Out[3]: tensor([[ 0.7402,  0.1515,  0.7794],
                [ 0.3259,  0.3071,  0.4555],
                [ 0.3657,  0.1409,  0.5663]], device='cuda:0')

In [4]: a + 1  # operations also work on GPU

Out[4]: tensor([[ 1.7402,  1.1515,  1.7794],
                [ 1.3259,  1.3071,  1.4555],
                [ 1.3657,  1.1409,  1.5663]], device='cuda:0')

In [5]: a.svd()  # linear algebra operations on GPU! (SVD)

Out[5]: (tensor([[-0.7615,  0.5344, -0.3668],
                 [-0.4326, -0.8405, -0.3263],
                 [-0.4826, -0.0898,  0.8712]], device='cuda:0'),
         tensor([ 1.4171,  0.2102,  0.0898], device='cuda:0'),
         tensor([[-0.6218,  0.4226, -0.6594],
                 [-0.2232, -0.9026, -0.3681],
                 [-0.7507, -0.0817,  0.6555]], device='cuda:0'))

In [6]: cpu = torch.device("cpu")  # cpu device object
        a.to(cpu)  # convert to a CPU tensor

Out[6]: tensor([[ 0.7402,  0.1515,  0.7794],
                [ 0.3259,  0.3071,  0.4555],
                [ 0.3657,  0.1409,  0.5663]])
```

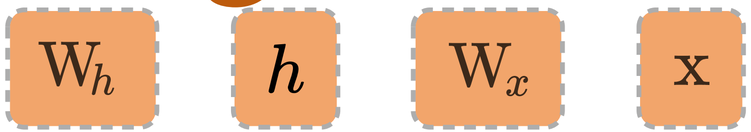
Automatic Differentiation Engine

Automatic Differentiation Engine

Computation as a graph built on-the-fly

Automatic Differentiation Engine

Computation as a graph built on-the-fly



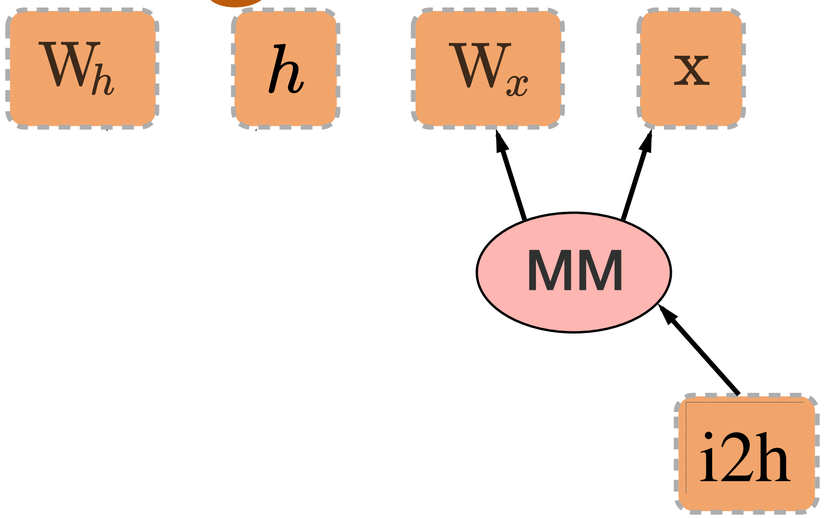

```
x = torch.randn(1, 10)
prev_h = torch.randn(1, 20)
W_h = torch.randn(20, 20)
W_x = torch.randn(20, 10)
```

Automatic Differentiation Engine

Computation as a graph built on-the-fly

```
x = torch.randn(1, 10)
prev_h = torch.randn(1, 20)
W_h = torch.randn(20, 20)
W_x = torch.randn(20, 10)

i2h = torch.mm(W_x, x.t())
```



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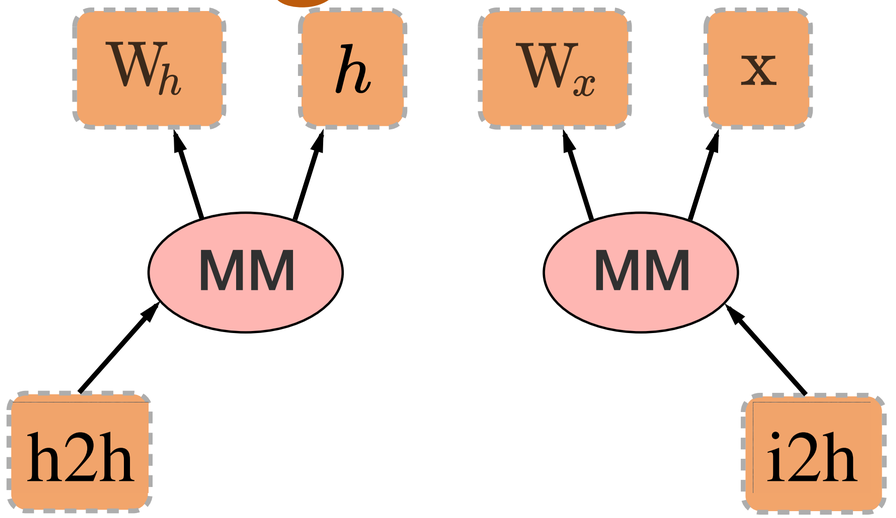
i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
```



Automatic Differentiation Engine

Computation as a graph built on-the-fly

```
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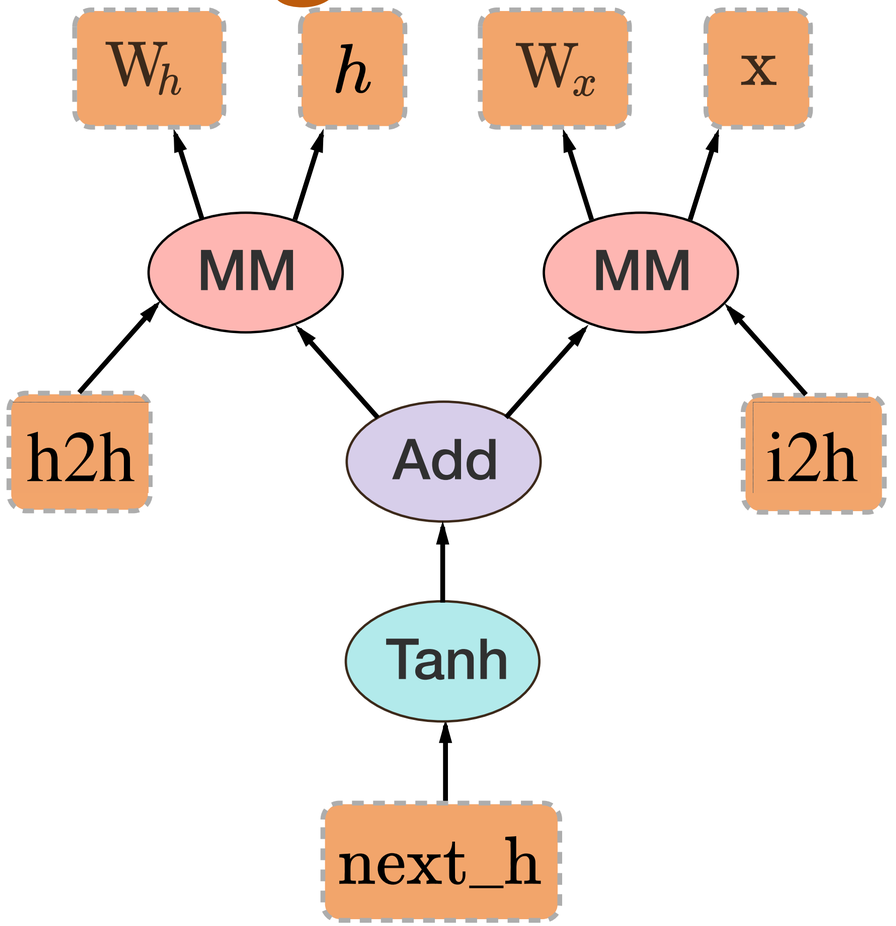
W_x = torch.randn(20, 10)

i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
next_h = next_h.tanh()
```



Automatic Differentiation Engine

Computation as a graph built on-the-fly

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i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
next_h = next_h.tanh()

loss = next_h.sum()
```

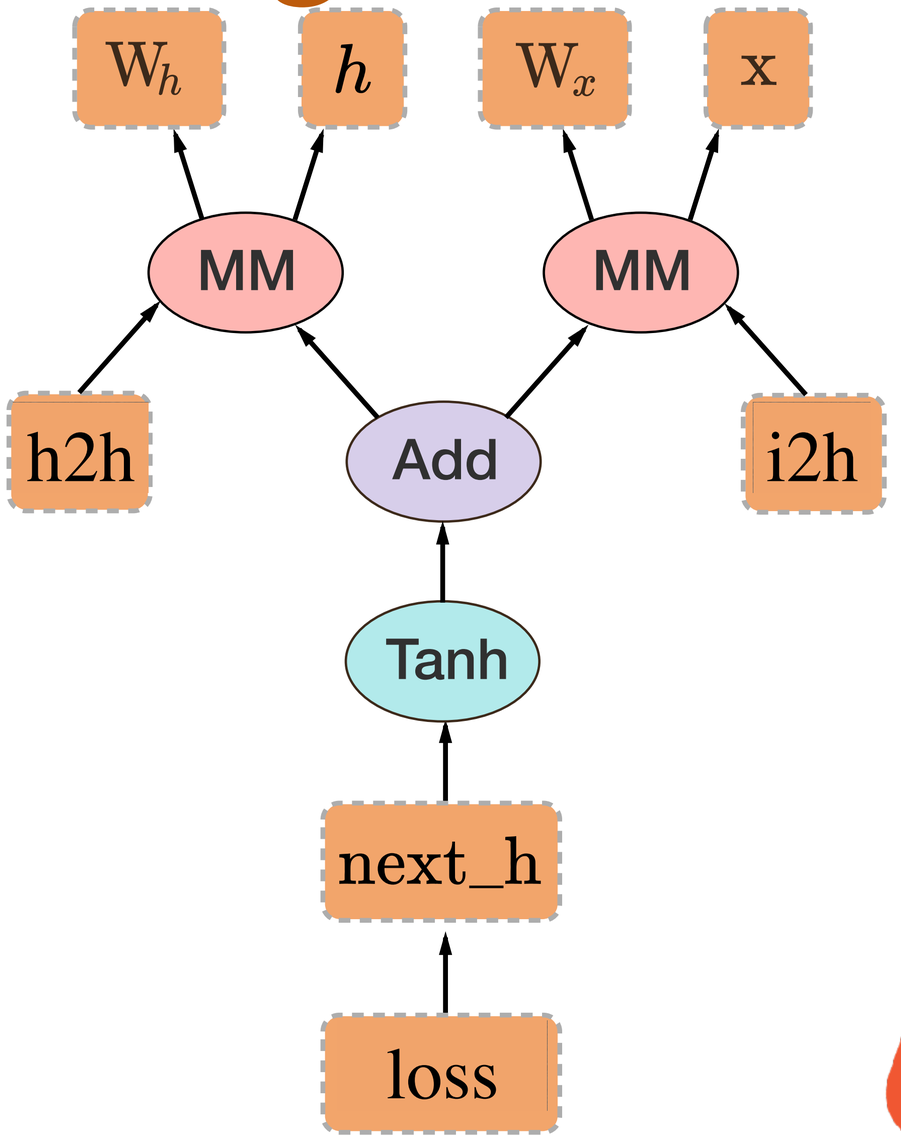

Automatic Differentiation Engine

Computation as a graph built on-the-fly

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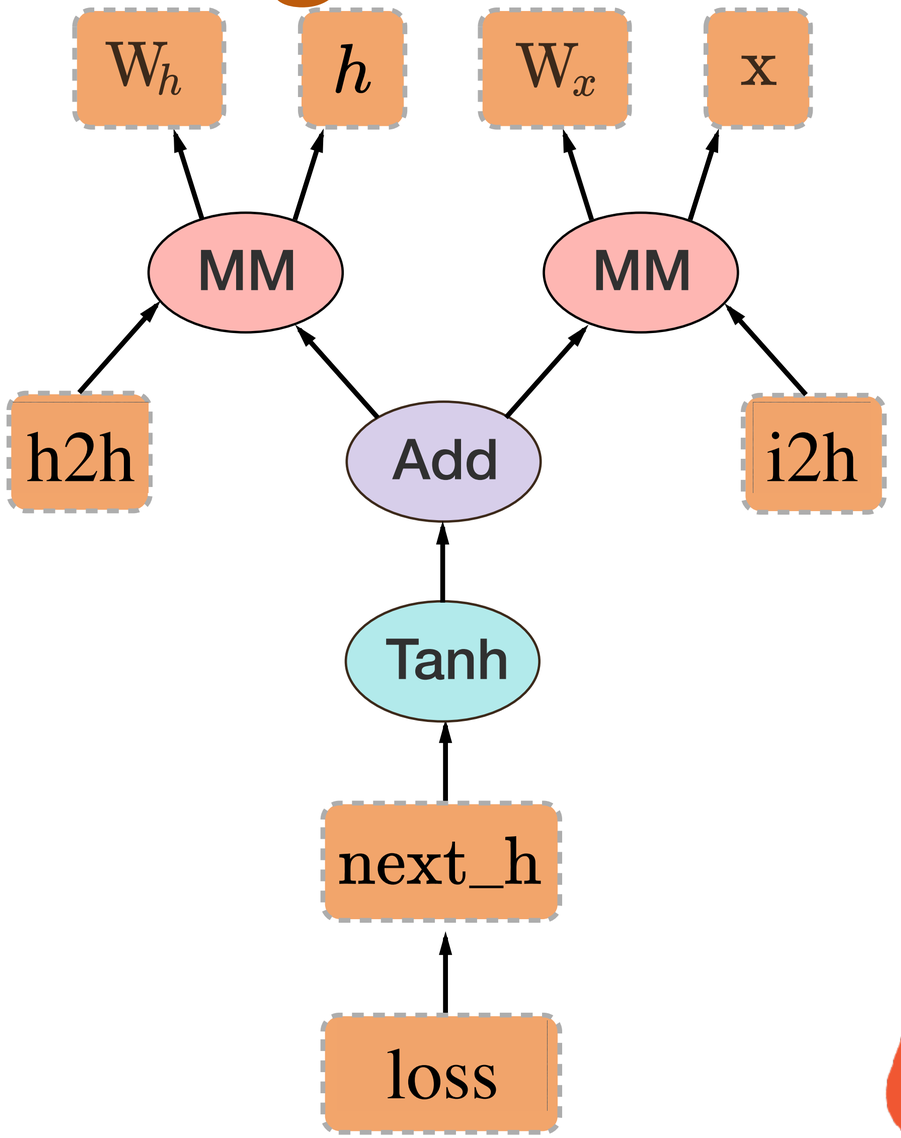
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
next_h = next_h.tanh()

loss = next_h.sum()
loss.backward()
```



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W_h = torch.randn(20, 20)
W_x = torch.randn(20, 10)

i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
next_h = next_h.tanh()

loss = next_h.sum()
loss.backward()  # compute gradients!
```
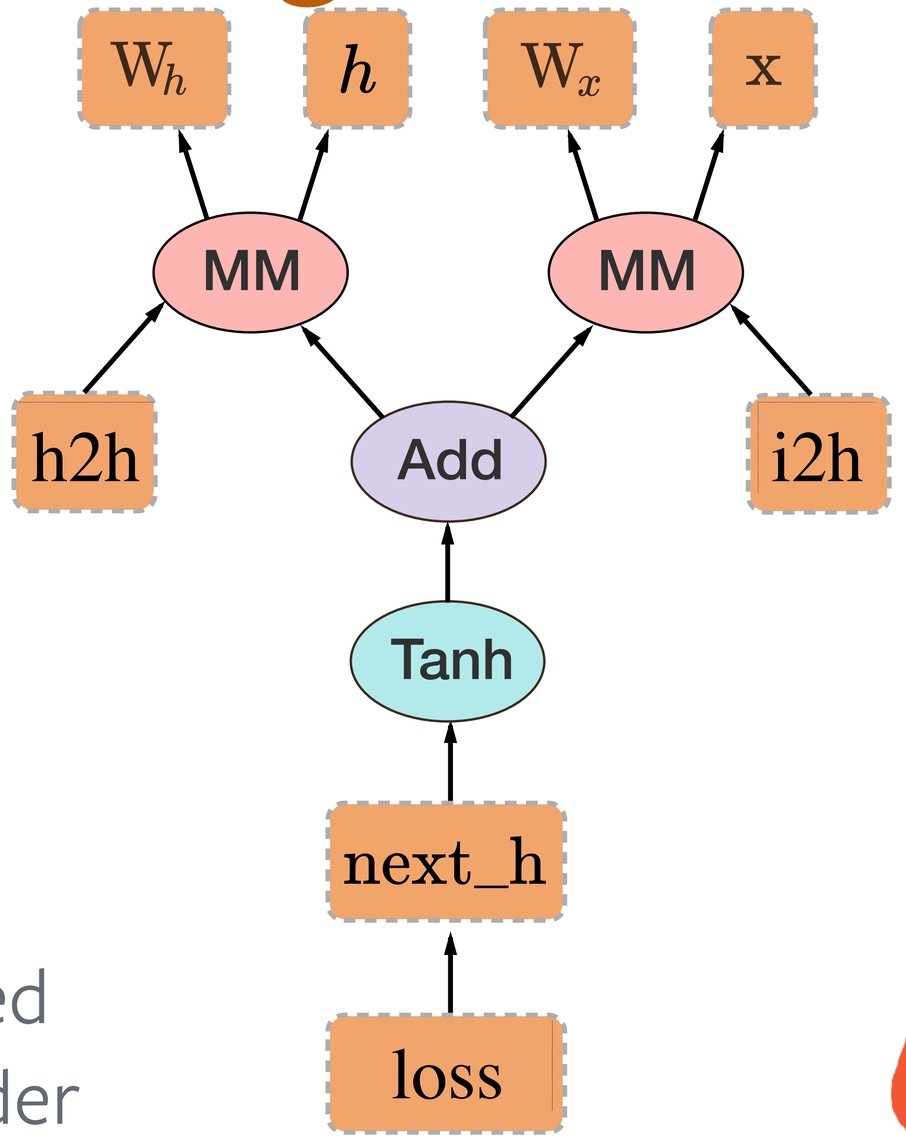



Gradient w.r.t. the input Tensors is computed step-by-step from `loss` to top in reverse order

Automatic Differentiation Engine

- Computation as a graph built on-the-fly
  - Can use Python primitives to build the graph (e.g. for-loop)
- Functions with efficient backward implementations
  - `torch.matmul`, `torch.fft`, `torch.svd`, `torch.trtrs`, etc.
- Gradients by automatic backpropagation through the graph
  - Higher-order gradients (backward traversal is also a graph)
  - Multi-device graphs

Efficient Machine Learning Primitives

Machine Learning primitives

- Deep Learning
  - torch.nn
- Reinforcement Learning, Probabilistic Modeling
  - torch.distributions
- and more...
  - scientific computing methods + autograd

Neural Networks

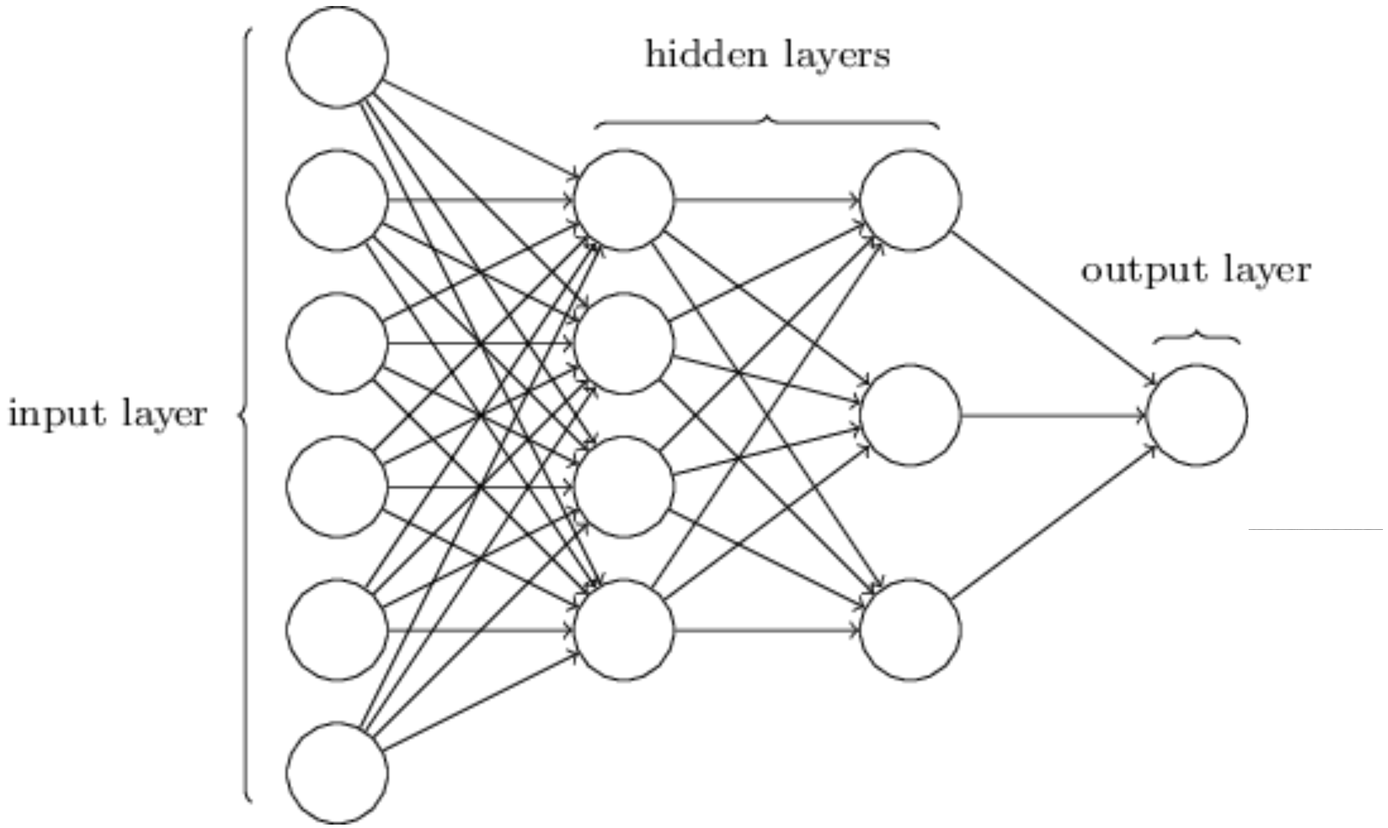
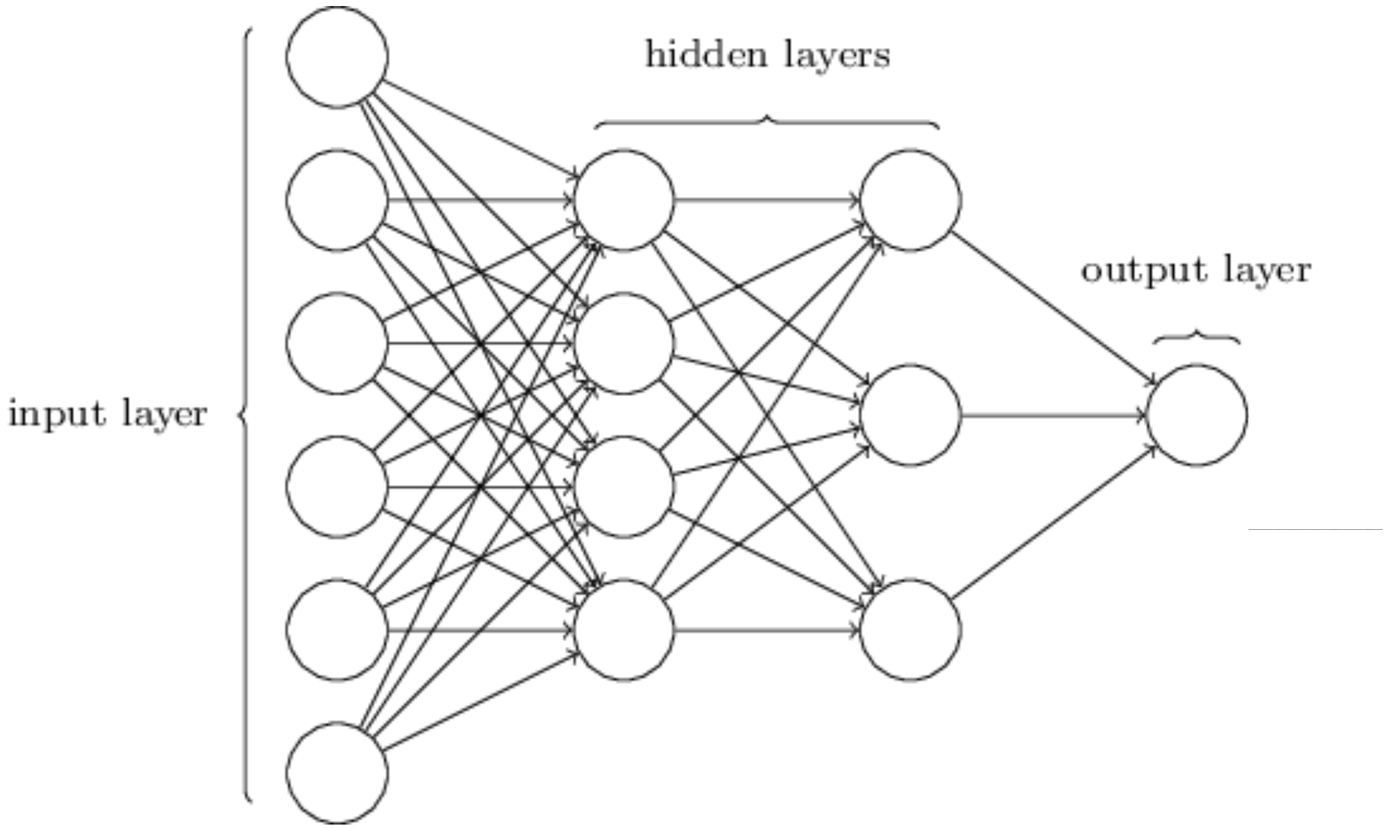


Figure by Md. Rezaul Karim

Neural Networks




```python
import torch.nn as nn

my_network = nn.Sequential(
    nn.Linear(6, 4),
    nn.Sigmoid(),
    nn.Linear(4, 3),
    nn.Sigmoid(),
    nn.Linear(3, 1),
)
```

Figure by Md. Rezaul Karim

Convolutional Neural Networks (CNN)

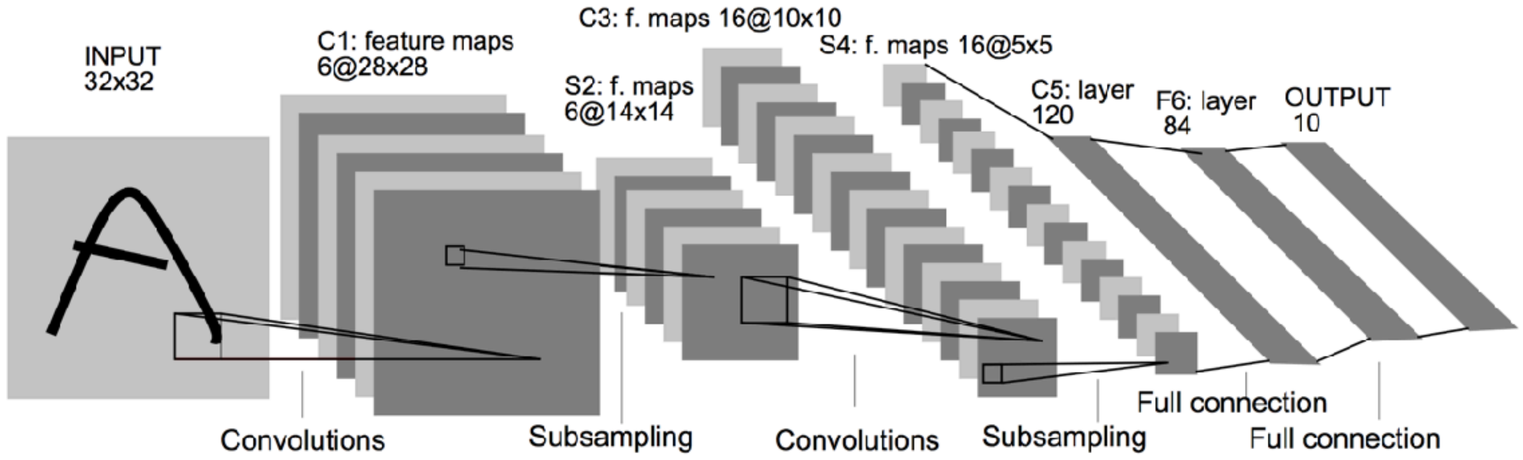
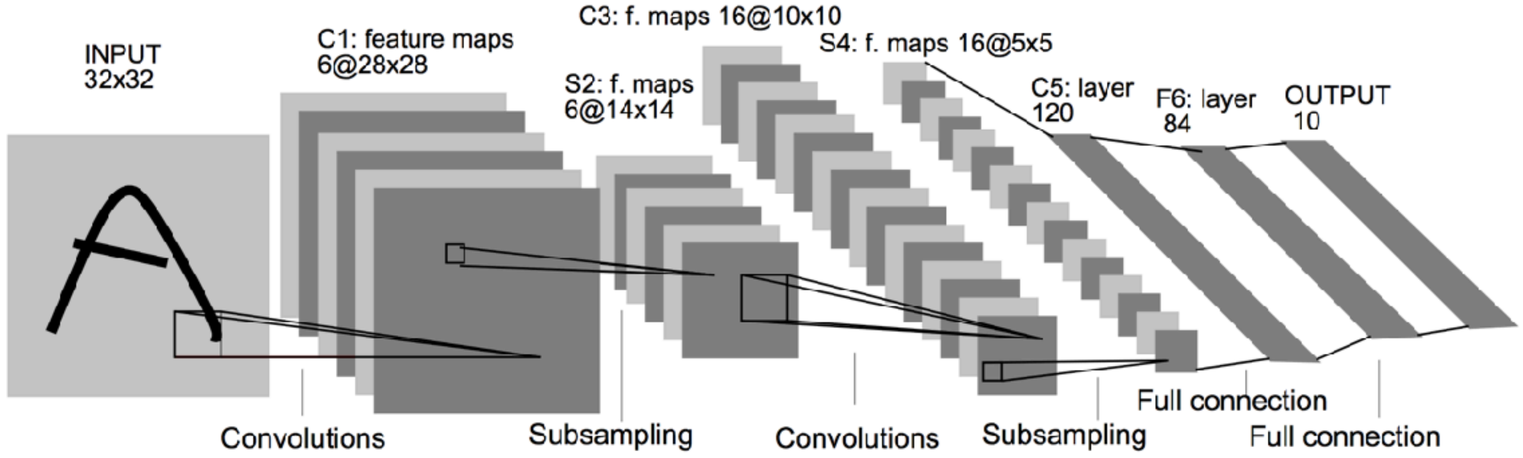


Figure by Yann LeCun et al.

Convolutional Neural Networks (CNN)




```python
import torch.nn as nn

class LeNet5(nn.Module):
    def __init__(self):
        super(LeNet5, self).__init__()
        self.feature = nn.Sequential(
            nn.Conv2d(1, 6, kernel_size=5),
            nn.Tanh(),
            nn.MaxPool2d(2),
            nn.Conv2d(6, 16, kernel_size=5),
            nn.Tanh(),
            nn.MaxPool2d(2),
        )
        self.fc = nn.Sequential(
            nn.Linear(400, 120),
            nn.Tanh(),
            nn.Linear(120, 84),
            nn.Tanh(),
            nn.Linear(84, 10),
        )

    def forward(self, input):
        features = self.feature(input)
        features = features.view(-1, 400)  # flatten
        return self.fc(features)

my_cnn = LeNet5()
```

Figure by Yann LeCun et al.

Recurrent Neural Networks (RNN)

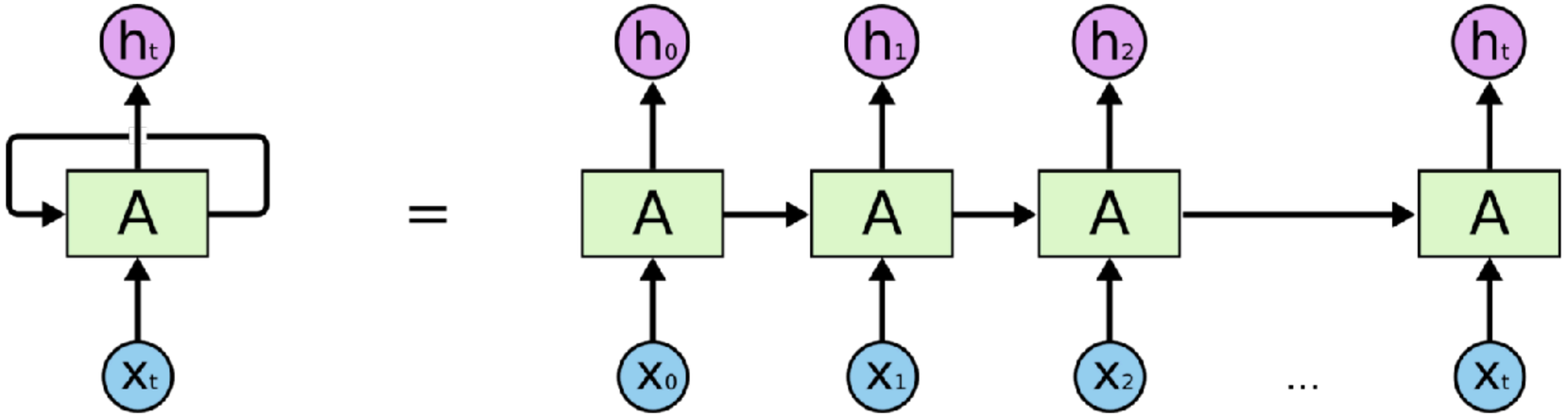
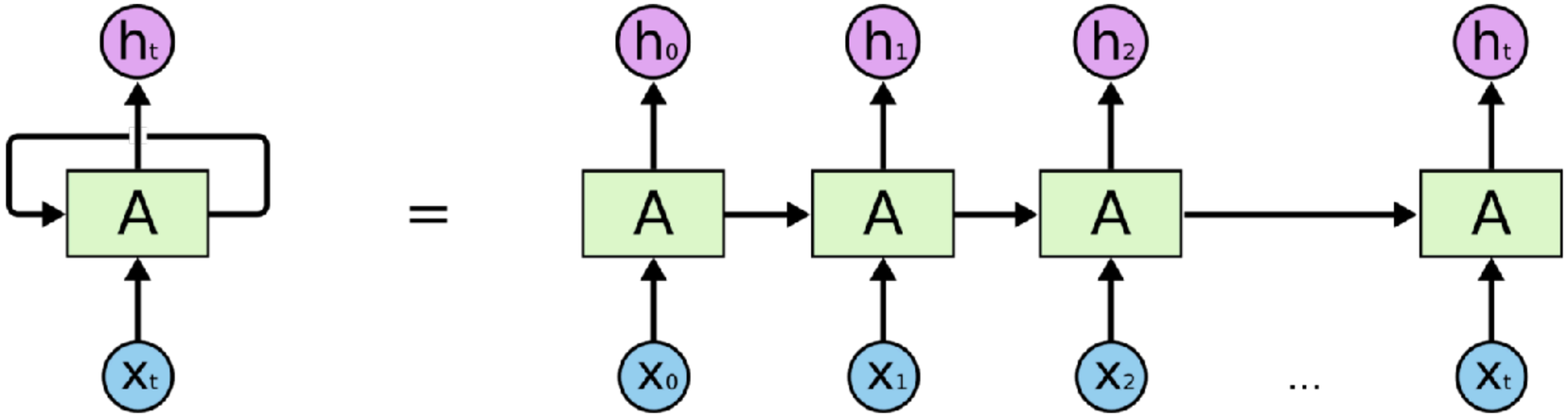


Figure by Pranoy Radhakrishnan

Recurrent Neural Networks (RNN)




```python
import torch.nn as nn

my_rnn = nn.LSTM(input_size=10, hidden_size=10)
```

Figure by Pranoy Radhakrishnan

Gradient based optimization package

Gradient based optimization package

- State-of-the-art optimization algorithms
  - `torch.optim.*`
  - SGD, Adam, RMSProp, L-BFGS, etc.
- Learning Rate scheduler
  - `torch.optim.lr_scheduler.*`
- Extensible API

```
optimizer = torch.optim.Adam(model.parameters())

for input, target in data:
    optimizer.zero_grad()
    output = model(input)
    loss = F.cross_entropy_loss(output, target)
    loss.backward()
    optimizer.step()
```

Machine Learning Ecosystem

Work items in practice

Writing Dataset loaders

Building models

Implementing Training loop

Checkpointing models

Interfacing with environments

Building optimizers

Dealing with GPUs

Building Baselines

Work items in practice

Writing Dataset loaders

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Python + PyTorch - an environment to do all of this

Interfacing with environments

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Writing Data Loaders

- every dataset is slightly differently formatted

Writing Data Loaders

- every dataset is slightly differently formatted
- have to be preprocessed and normalized differently

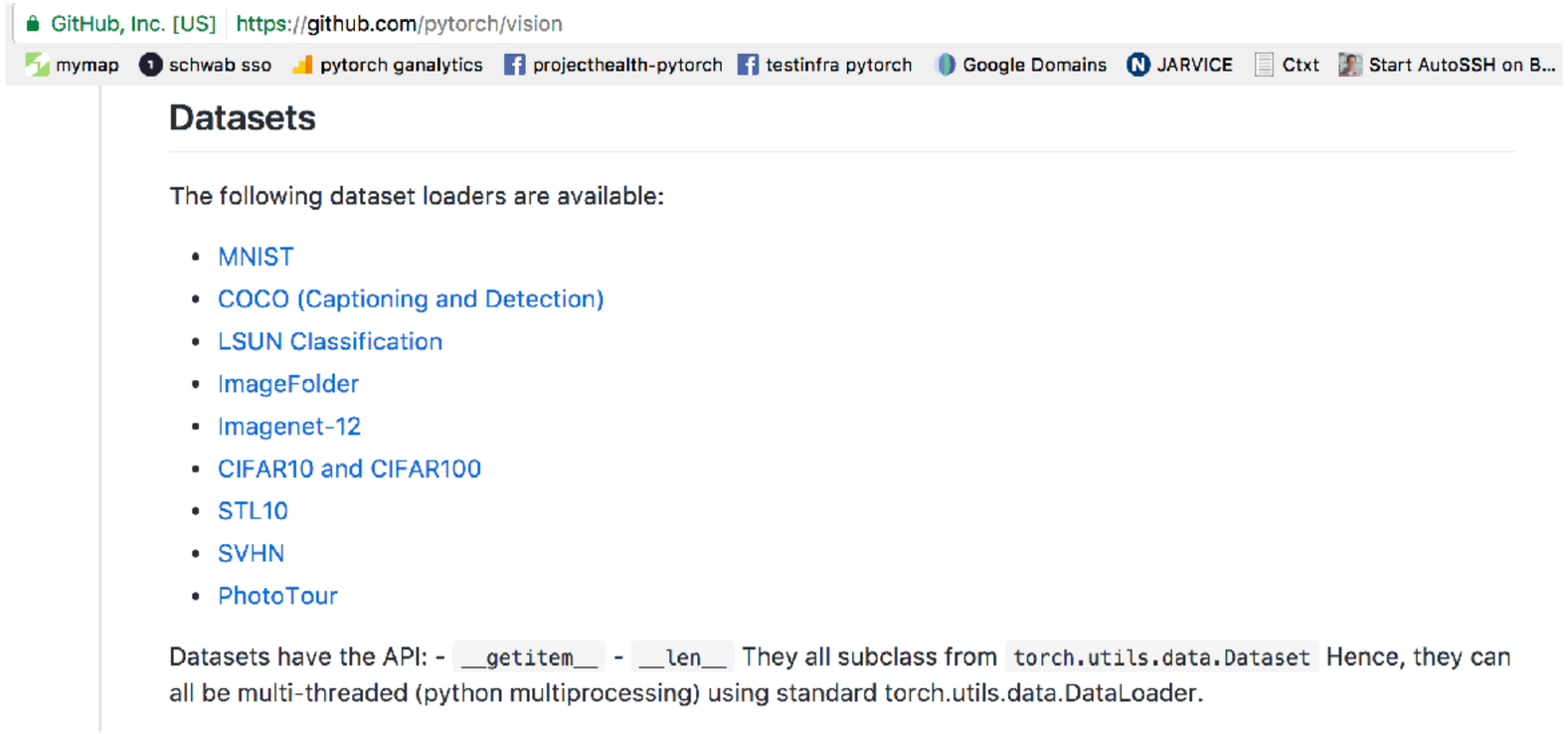
Writing Data Loaders

- every dataset is slightly differently formatted
- have to be preprocessed and normalized differently
- need a multithreaded Data loader to feed GPUs fast enough

Writing Data Loaders

PyTorch solution:

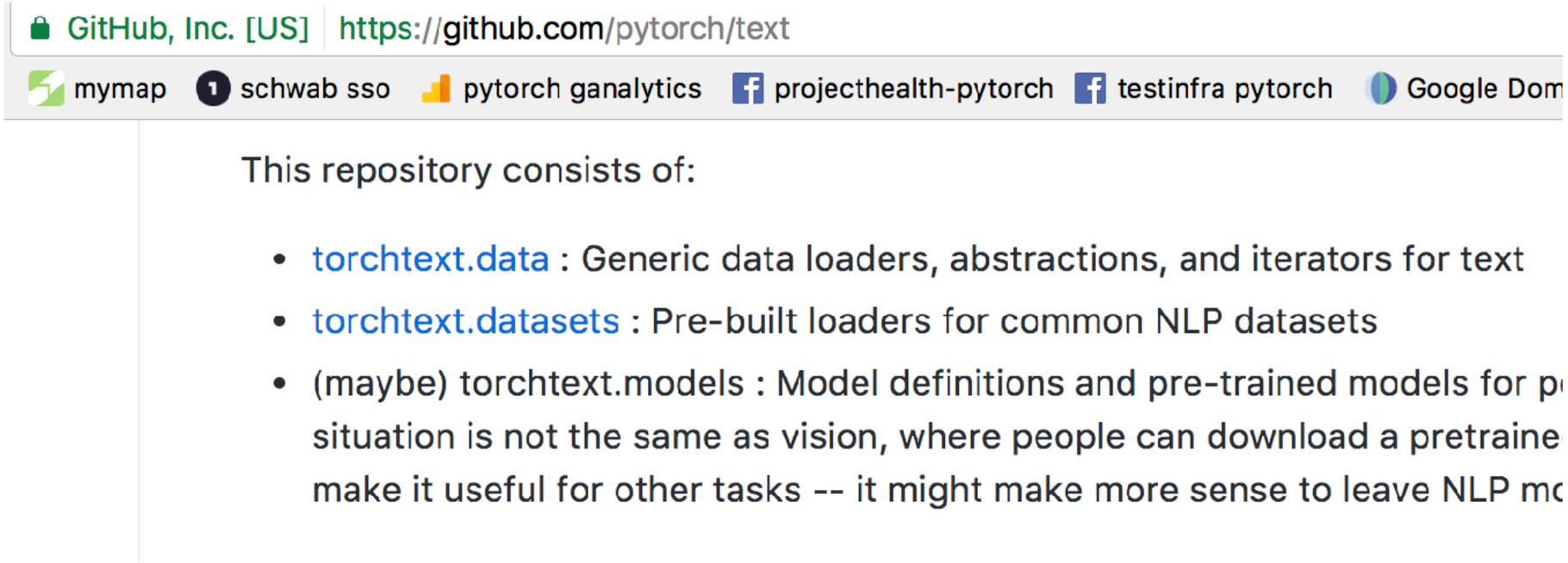
- share data loaders across the community!



Writing Data Loaders

PyTorch solution:

- share data loaders across the community!



Writing Data Loaders

PyTorch solution:

- use regular Python to write Datasets:

  leverage existing Python code

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PyTorch solution:

- use regular Python to write Datasets:

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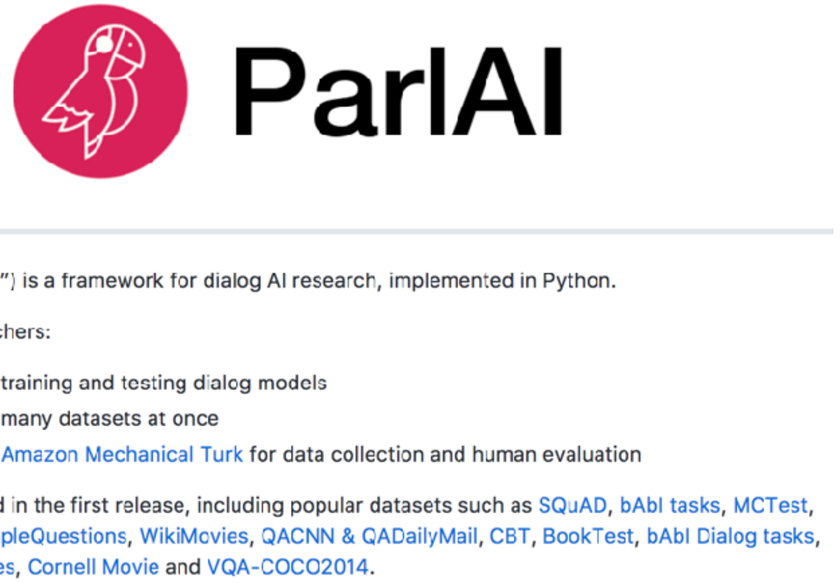
  Example: ParlAI



Writing Data Loaders

PyTorch solution:

- Code in practice

Writin

PyTorch

- Code in p

```
57  if opt.dataset in ['imagenet', 'folder', 'lfw']:
58      # folder dataset
59      dataset = dset.ImageFolder(root=opt.dataroot,
60                                 transform=transforms.Compose([
61                                     transforms.Scale(opt.imageSize),
62                                     transforms.CenterCrop(opt.imageSize),
63                                     transforms.ToTensor(),
64                                     transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5)),
65                                 ]))
66  elif opt.dataset == 'lsun':
67      dataset = dset.LSUN(db_path=opt.dataroot, classes=['bedroom_train'],
68                          transform=transforms.Compose([
69                              transforms.Scale(opt.imageSize),
70                              transforms.CenterCrop(opt.imageSize),
71                              transforms.ToTensor(),
72                              transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5)),
73                          ]))
74  elif opt.dataset == 'cifar10':
75      dataset = dset.CIFAR10(root=opt.dataroot, download=True,
76                             transform=transforms.Compose([
77                                 transforms.Scale(opt.imageSize),
78                                 transforms.ToTensor(),
79                                 transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5)),
80                             ])
81      )
82  assert dataset
83  dataloader = torch.utils.data.DataLoader(dataset, batch_size=opt.batchSize,
84                                           shuffle=True, num_workers=int(opt.workers))
```

Writing Da

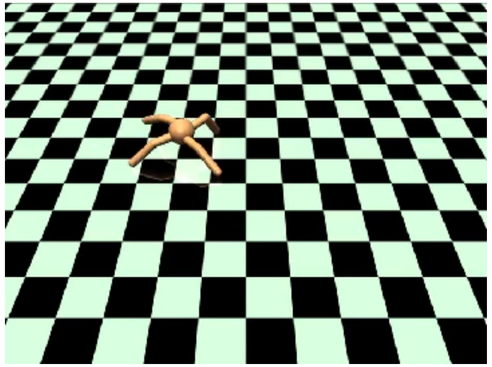
PyTorch soluti

- Code in practic

```
def __init__(self, root, annFile, transform=None, target_transform=None):
    from pycocotools.coco import COCO
    self.root = os.path.expanduser(root)
    self.coco = COCO(annFile)
    self.ids = list(self.coco.imgs.keys())
    self.transform = transform
    self.target_transform = target_transform

def __getitem__(self, index):
    """
    Args:
        index (int): Index

    Returns:
        tuple: Tuple (image, target). target is a list of captions for the image.
    """
    coco = self.coco
    img_id = self.ids[index]
    ann_ids = coco.getAnnIds(imgIds=img_id)
    anns = coco.loadAnns(ann_ids)
    target = [ann['caption'] for ann in anns]

    path = coco.loadImgs(img_id)[0]['file_name']

    img = Image.open(os.path.join(self.root, path)).convert('RGB')
    if self.transform is not None:
        img = self.transform(img)

    if self.target_transform is not None:
        target = self.target_transform(target)

    return img, target

def __len__(self):
    return len(self.ids)
```

Interfacing with environments

Cars



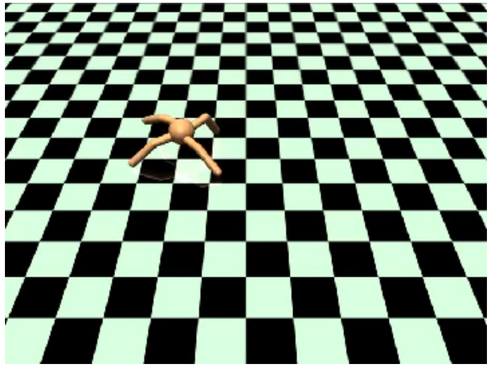
Simulations

Video games

Internet

Interfacing with environments

Cars



Simulations

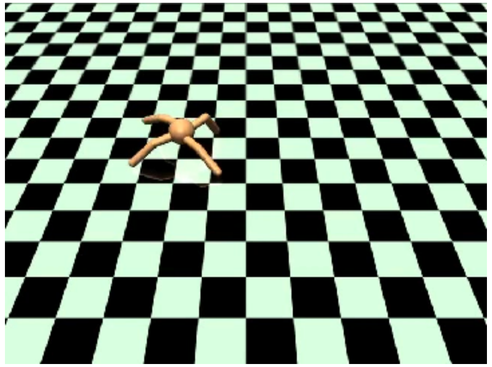
Video games

Internet

Pretty much every environment provides a Python API

Interfacing with environments

Cars



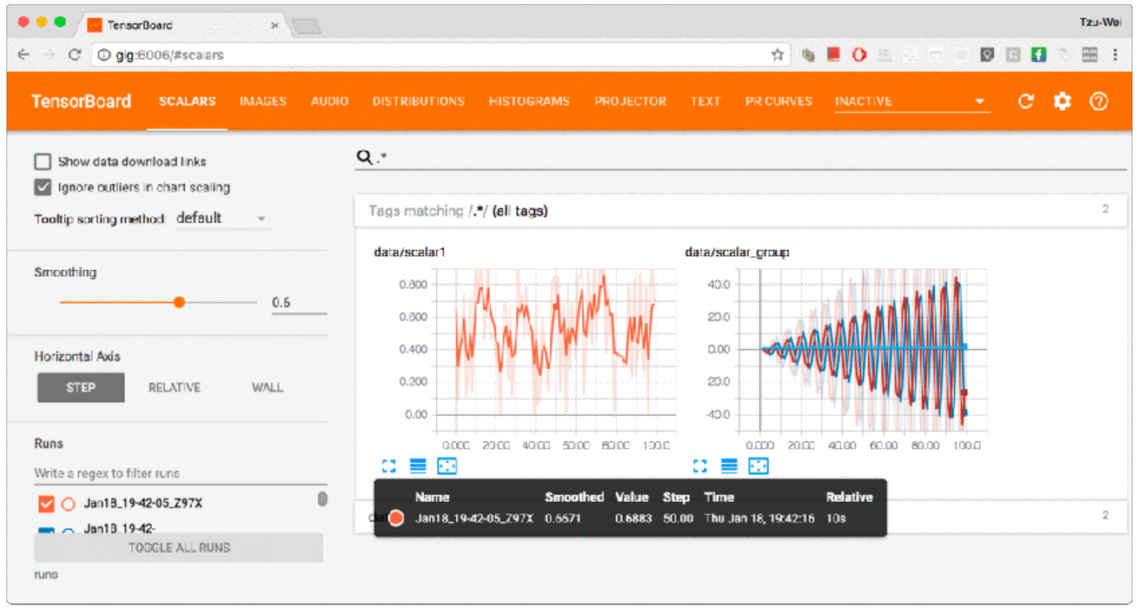
Simulations

Video games

Internet

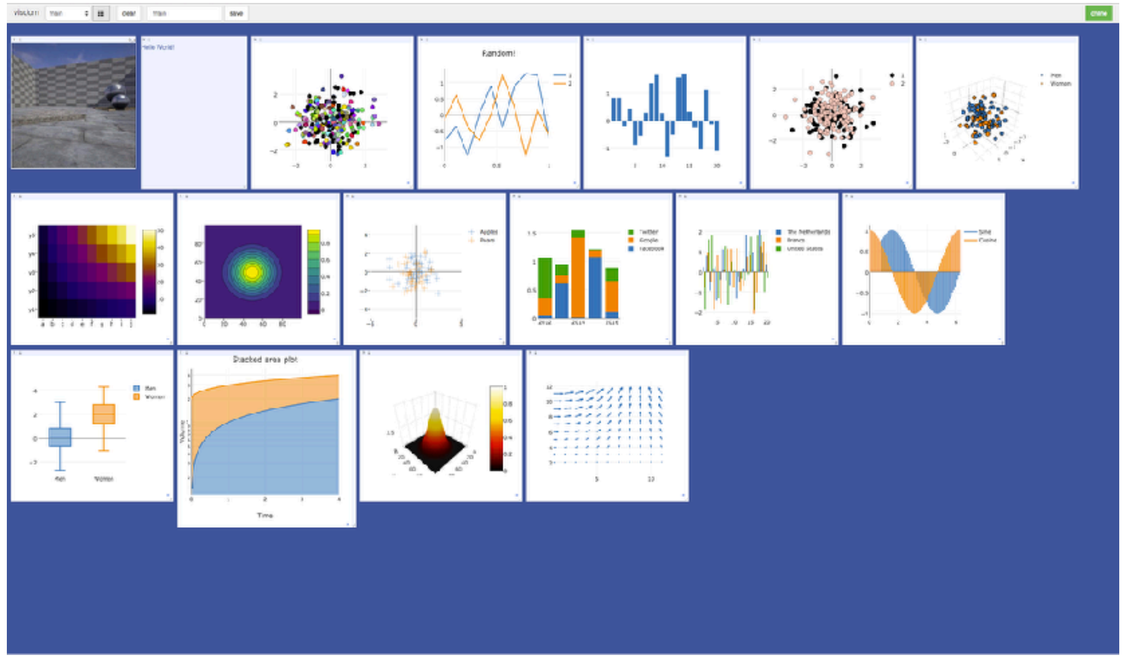
Natively interact with the environment directly

Visualization



Tensorboard-PyTorch

github.com/lanpa/tensorboard-pytorch



Visdom

github.com/facebookresearch/visdom

Debugging

- PyTorch is a Python extension

Debugging

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- Use your favorite Python debugger

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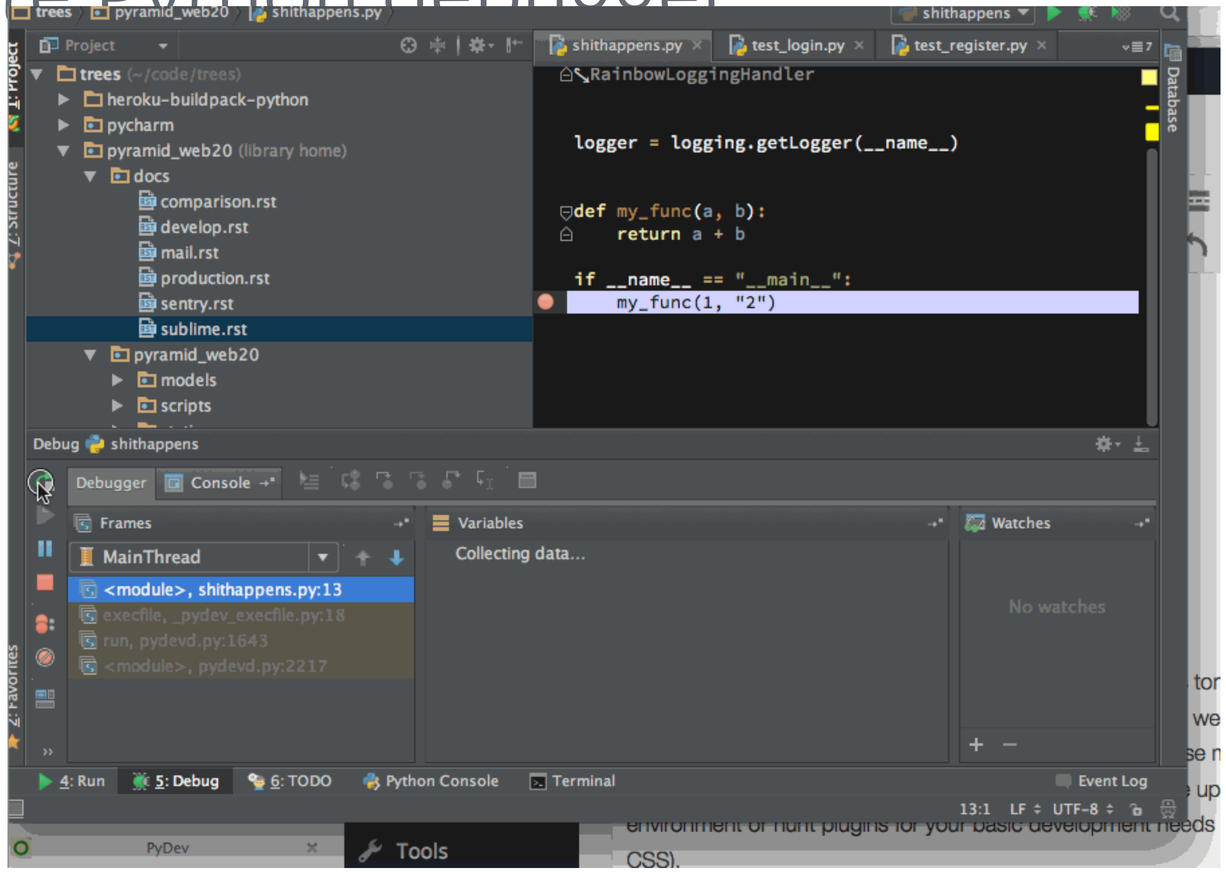


Debugging

- PyTorch is a Python extension
- Use your favorite Python debugger
- Use the most popular debugger:

Debugging

- PyTorch is a Python extension
- Use your favorite Python debugger
- Use the most popular debugger:

```
print(foo)
```

Identifying bottlenecks

- PyTorch is a Python extension
- Use your favorite Python profiler

SNAKEVIZ

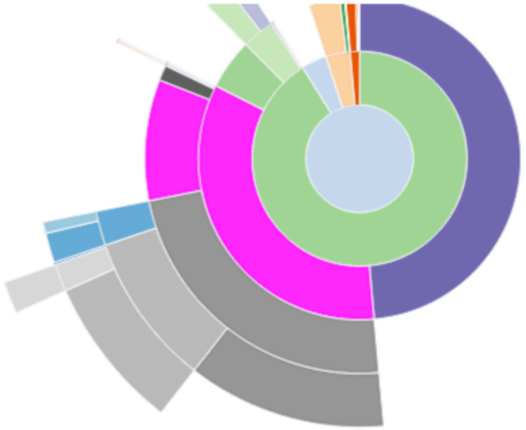
← PREVIOUS NEXT → G

SnakeViz
Installation
Starting SnakeViz
Generating Profiles
Interpreting Results
Controls
Notes
Contact

FUNCTION INFO

Placing your cursor over an arc will highlight that arc and any other visible instances of the same function call. It also display a list of information to the left of the sunburst.

Name:
filter
Cumulative Time:
0.000294 s (31.78 %)
File:
fnmatch.py
Line:
48
Directory:
/Users/jiffyclub/miniconda3/envs/snakevizdev/lib/python3.4/



Identifying bottlenecks

- PyTorch is a Python extension
- Use your favorite Python profiler: Line_Profiler

```
File: pystone.py
Function: Proc2 at line 149
Total time: 0.606656 s

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
   149                                           @profile
   150                                           def Proc2(IntParIO):
   151     50000        82003      1.6     13.5      IntLoc = IntParIO + 10
   152     50000        63162      1.3     10.4      while 1:
   153     50000        69065      1.4     11.4          if Char1Glob == 'A':
   154     50000        66354      1.3     10.9              IntLoc = IntLoc - 1
   155     50000        67263      1.3     11.1              IntParIO = IntLoc - IntGlob
   156     50000        65494      1.3     10.8              EnumLoc = Ident1
   157     50000        68001      1.4     11.2          if EnumLoc == Ident1:
   158     50000        63739      1.3     10.5              break
   159     50000        61575      1.2     10.1      return IntParIO
```

Compilation Time

- PyTorch is written for the impatient

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- PyTorch is written for the impatient
- Absolutely no compilation time when writing your scripts whatsoever

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- PyTorch is written for the impatient
- Absolutely no compilation time when writing your scripts whatsoever
- All core kernels are pre-compiled

Ecosystem

- Use the entire Python ecosystem at your will

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- Including SciPy, Scikit-Learn, etc.

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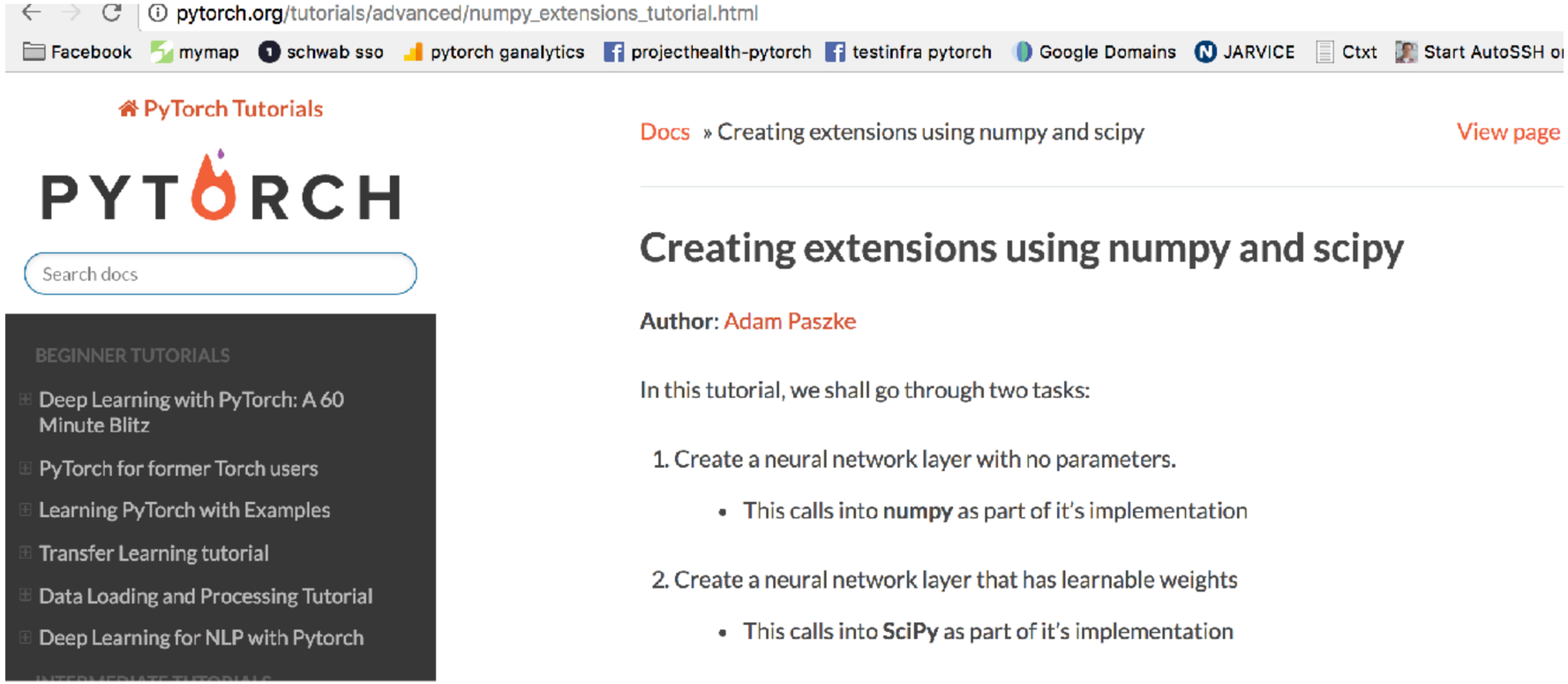


Machine Learning Ecosystem

Shared model zoo (pretrained models)

We provide pre-trained models, using the PyTorch `torch.utils.model_zoo`. These can be constructed by passing `pretrained=True`:

```
import torchvision.models as models
resnet18 = models.resnet18(pretrained=True)
alexnet = models.alexnet(pretrained=True)
squeezenet = models.squeezenet1_0(pretrained=True)
vgg16 = models.vgg16(pretrained=True)
densenet = models.densenet161(pretrained=True)
inception = models.inception_v3(pretrained=True)
```

torchvision

Machine Learning Ecosystem

Shared model zoo (pretrained models)

Top1 Accuracy

Model	32-float	12-bit	10-bit	8-bit	6-bit
MNIST	98.42	98.43	98.44	98.44	98.32
SVHN	96.03	96.03	96.04	96.02	95.46
CIFAR10	93.78	93.79	93.80	93.58	90.86
CIFAR100	74.27	74.21	74.19	73.70	66.32
STL10	77.59	77.65	77.70	77.59	73.40
AlexNet	55.70/78.42	55.66/78.41	55.54/78.39	54.17/77.29	18.19/36.25
VGG16	70.44/89.43	70.45/89.43	70.44/89.33	69.99/89.17	53.33/76.32
VGG19	71.36/89.94	71.35/89.93	71.34/89.88	70.88/89.62	56.00/78.62
ResNet18	68.63/88.31	68.62/88.33	68.49/88.25	66.80/87.20	19.14/36.49
ResNet34	72.50/90.86	72.46/90.82	72.45/90.85	71.47/90.00	32.25/55.71
ResNet50	74.98/92.17	74.94/92.12	74.91/92.09	72.54/90.44	2.43/5.36
ResNet101	76.69/93.30	76.66/93.25	76.22/92.90	65.69/79.54	1.41/1.18
ResNet152	77.55/93.59	77.51/93.62	77.40/93.54	74.95/92.46	9.29/16.75
SqueezeNetV0	56.73/79.39	56.75/79.40	56.70/79.27	53.93/77.04	14.21/29.74
SqueezeNetV1	56.52/79.13	56.52/79.15	56.24/79.03	54.56/77.33	17.10/32.46
InceptionV3	76.41/92.78	76.43/92.71	76.44/92.73	73.67/91.34	1.50/4.82

github.com/aaron-xichen/pytorch-playground

Machine Learning Ecosystem

Probabilistic programming

http://pyro.ai/

github.com/probtorch/probtorch

Machine Learning Ecosystem

Gaussian Processes

GPyTorch (Alpha Relase)

build passing

GPyTorch is a Gaussian Process library, implemented using PyTorch. It is designed for creating flexible and modular Gaussian Process models with ease, so that you don't have to be an expert to use GPs.

This package is currently under development, and is likely to change. Some things you can do right now:

- Simple GP regression (example here)
- Simple GP classification (example here)
- Multitask GP regression (example here)
- Scalable GP regression using kernel interpolation (example here)
- Scalable GP classification using kernel interpolation (example here)
- Deep kernel learning (example here)
- And (more!)

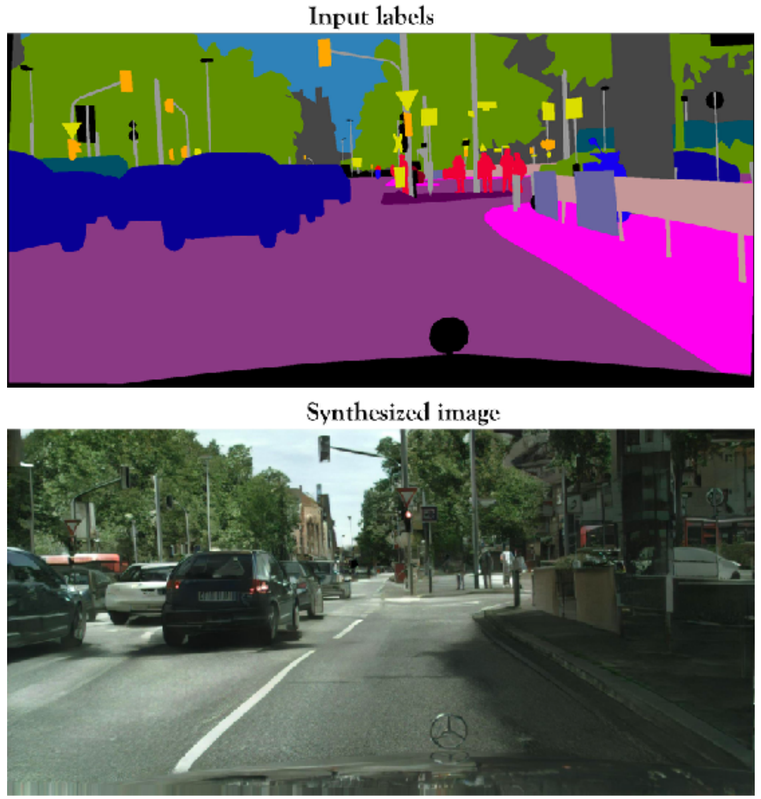
https://github.com/cornellius-gp/gpytorch

Machine Learning Ecosystem

Image-to-Image Translation

pix2pix & CycleGAN

github.com/junyanz/pytorch-CycleGAN-and-pix2pix

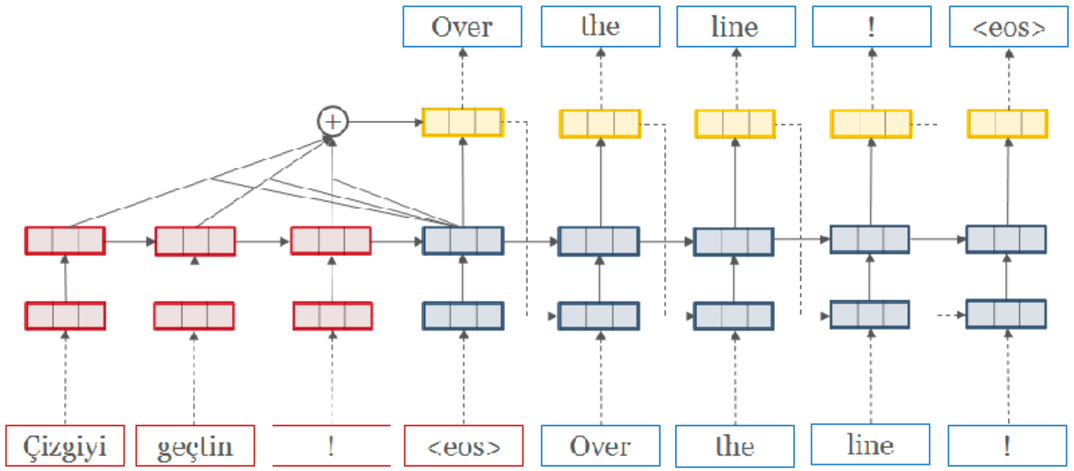


pix2pixHD

github.com/NVIDIA/pix2pixHD

Machine Learning Ecosystem

Machine Translation



OpenNMT-py: Open-Source Neural Machine Translation

github.com/OpenNMT/OpenNMT-py

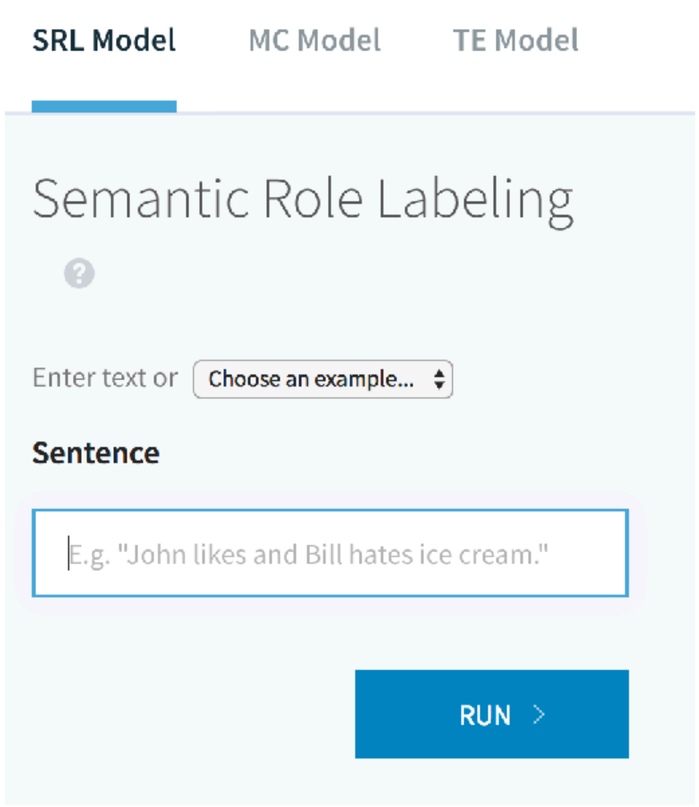
FAIR Sequence-to-Sequence Toolkit

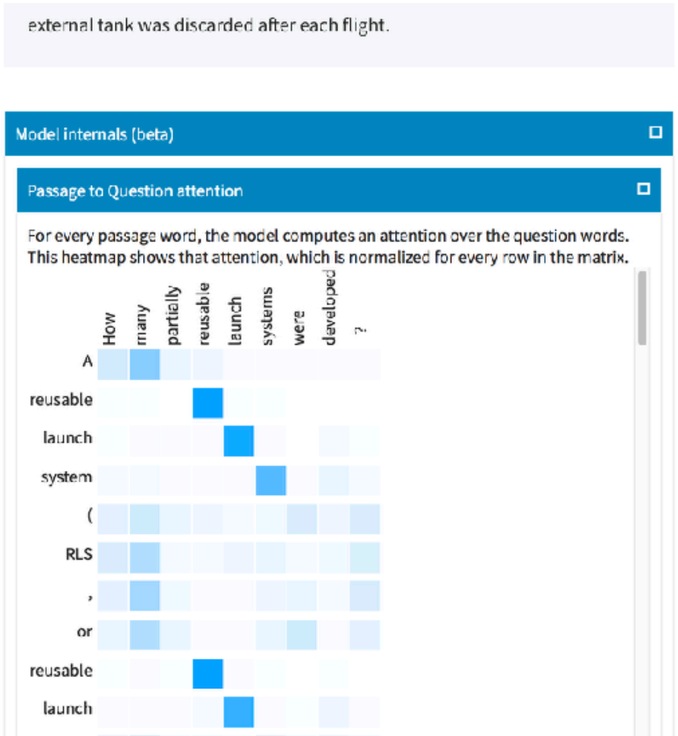
github.com/facebookresearch/fairseq-py

Machine Learning Ecosystem

General Linguistics Tasks

AllenNLP

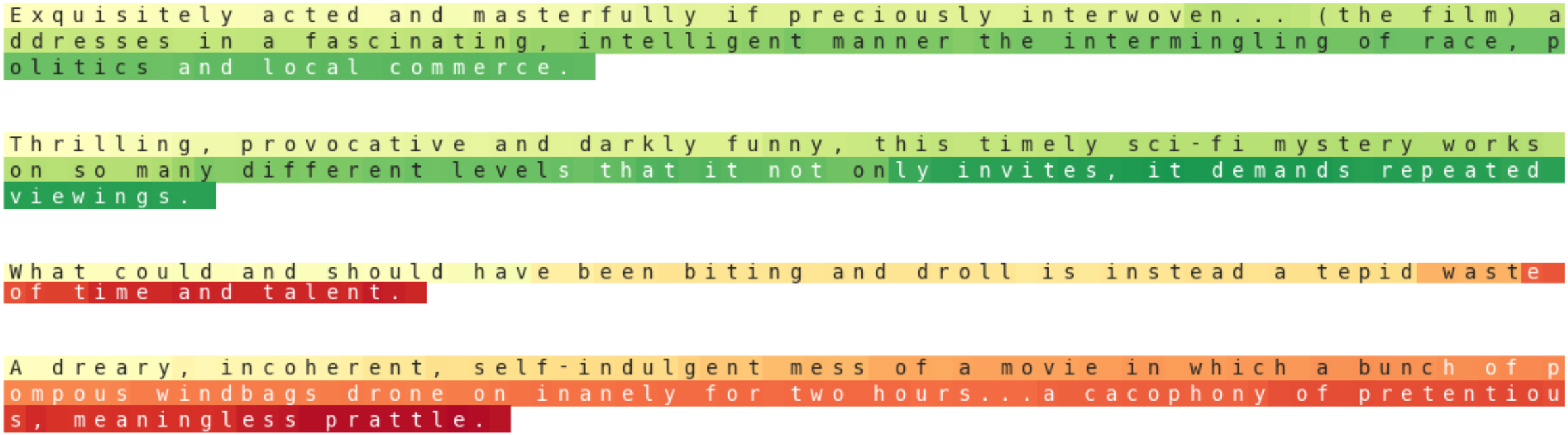




http://allennlp.org/

Machine Learning Ecosystem

Sentiment Discovery



https://github.com/NVIDIA/sentiment-discovery

Machine Learning Ecosystem

Optical Flow Estimation

FlowNet 2.0

github.com/NVIDIA/flownet2-pytorch

and many more...

- Distributed training
- Profiling
- Extending autograd
- C++ interface (ATen) and C++ extensions
- ONNX
- JIT
- ...

With ❤ from

http://pytorch.org

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