
PYTORCH

PYTORCH

A framework for fast, dynamic deep learning and scientific computing

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What is PyTorch?

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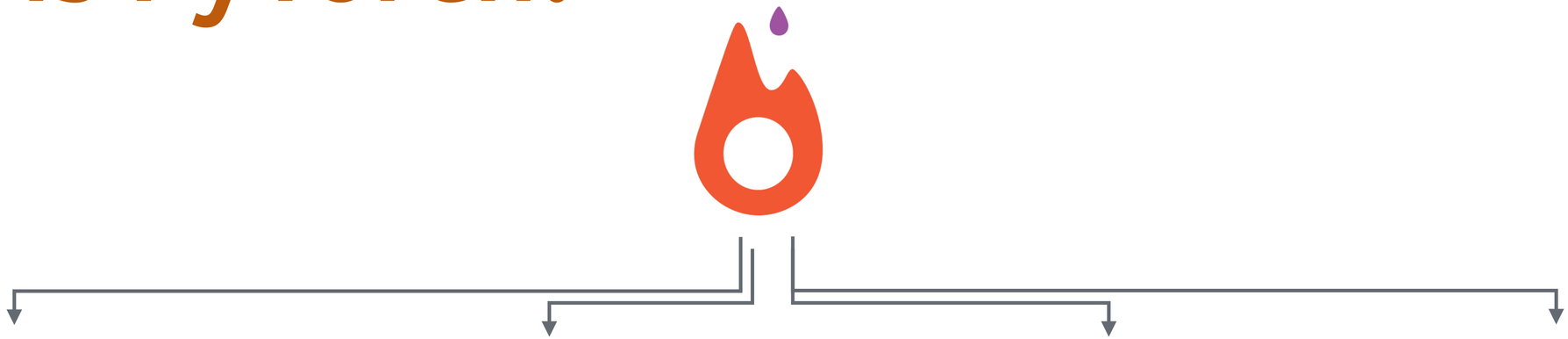


automatic differentiation engine

Ndarray library with GPU support

gradient based optimization package

Utilities (data loading, etc.)

Deep Learning

Reinforcement Learning

Numpy-alternative

ndarray library

- np.ndarray <-> torch.Tensor
- 200+ operations, similar to numpy
- very fast acceleration on NVIDIA GPUs

```numpy
# -*- coding: utf-8 -*-
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 = x.dot(w1)
    h_relu = np.maximum(h, 0)
    y_pred = h_relu.dot(w2)

    # Compute and print loss
    loss = np.square(y_pred - y).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 = h_relu.T.dot(grad_y_pred)
    grad_h_relu = grad_y_pred.dot(w2.T)
    grad_h = grad_h_relu.copy()
    grad_h[h < 0] = 0
    grad_w1 = x.T.dot(grad_h)

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

Numpy

```pytorch
import torch


dtype = torch.FloatTensor
# dtype = torch.cuda.FloatTensor # Uncomment this to run on GPU

# 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).type(dtype)
y = torch.randn(N, D_out).type(dtype)

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

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

    # Compute and print loss
    loss = (y_pred - y).pow(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 = h_relu.t().mm(grad_y_pred)
    grad_h_relu = grad_y_pred.mm(w2.t())
    grad_h = grad_h_relu.clone()
    grad_h[h < 0] = 0
    grad_w1 = x.t().mm(grad_h)

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

PyTorch

ndarray / Tensor library

Tensors are similar to numpy's ndarrays, with the addition being that Tensors can also be used on a GPU to accelerate computing.

```
from __future__ import print_function
import torch
```

Construct a 5x3 matrix, uninitialized:

```
x = torch.Tensor(5, 3)
print(x)
```

Out:

```
1.00000e-25 *
  0.4136  0.0000  0.0000
  0.0000  1.6519  0.0000
  1.6518  0.0000  1.6519
  0.0000  1.6518  0.0000
  1.6520  0.0000  1.6519
[torch.FloatTensor of size 5x3]
```

ndarray / Tensor library

Construct a randomly initialized matrix

```
x = torch.rand(5, 3)
print(x)
```

Out:

```
0.2598  0.7231  0.8534
 0.3928  0.1244  0.5110
 0.5476  0.2700  0.5856
 0.7288  0.9455  0.8749
 0.6663  0.8230  0.2713
[torch.FloatTensor of size 5x3]
```

Get its size

```
print(x.size())
```

Out:

```
torch.Size([5, 3])
```

ndarray / Tensor library

You can use standard numpy-like indexing with all bells and whistles!

```
print(x[:, 1])
```

Out:

```
0.7231
 0.1244
 0.2700
 0.9455
 0.8230
[torch.FloatTensor of size 5]
```

ndarray / Tensor library

```
y = torch.rand(5, 3)
print(x + y)
```

Out:

```
0.7931  1.1872  1.6143
 1.1946  0.4669  0.9639
 0.7576  0.8136  1.1897
 0.7431  1.8579  1.3400
 0.8188  1.1041  0.8914
[torch.FloatTensor of size 5x3]
```

NumPy bridge

Converting torch Tensor to numpy Array

```
a = torch.ones(5)
print(a)
```

Out:

```
1
 1
 1
 1
 1
[torch.FloatTensor of size 5]
```

```
b = a.numpy()
print(b)
```

Out:

```
[ 1.  1.  1.  1.  1.]
```

NumPy bridge

Converting torch Tensor to numpy Array

```
a = torch.ones(5)
print(a)
```

Out:

```
1
 1
 1
 1
 1
[torch.FloatTensor of size 5]
```

Zero memory-copy
very efficient

```
b = a.numpy()
print(b)
```

Out:

```
[ 1.  1.  1.  1.  1.]
```

NumPy bridge

See how the numpy array changed in value.

```
a.add_(1)
print(a)
print(b)
```

Out:

```
2
 2
 2
 2
 2
[torch.FloatTensor of size 5]

[ 2.  2.  2.  2.  2.]
```

NumPy bridge

Converting numpy Array to torch Tensor

See how changing the np array changed the torch Tensor automatically

```
import numpy as np
a = np.ones(5)
b = torch.from_numpy(a)
np.add(a, 1, out=a)
print(a)
print(b)
```

Out:

```
[ 2.  2.  2.  2.  2.]

 2
 2
 2
 2
 2
[torch.DoubleTensor of size 5]
```

All the Tensors on the CPU except a CharTensor support converting to NumPy and back.

Seamless GPU Tensors

CUDA Tensors

Tensors can be moved onto GPU using the `.cuda` function.

```
# let us run this cell only if CUDA is available
if torch.cuda.is_available():
    x = x.cuda()
    y = y.cuda()
    x + y
```

Deep Learning 101

a quick introduction

Types of typical operators

Convolution

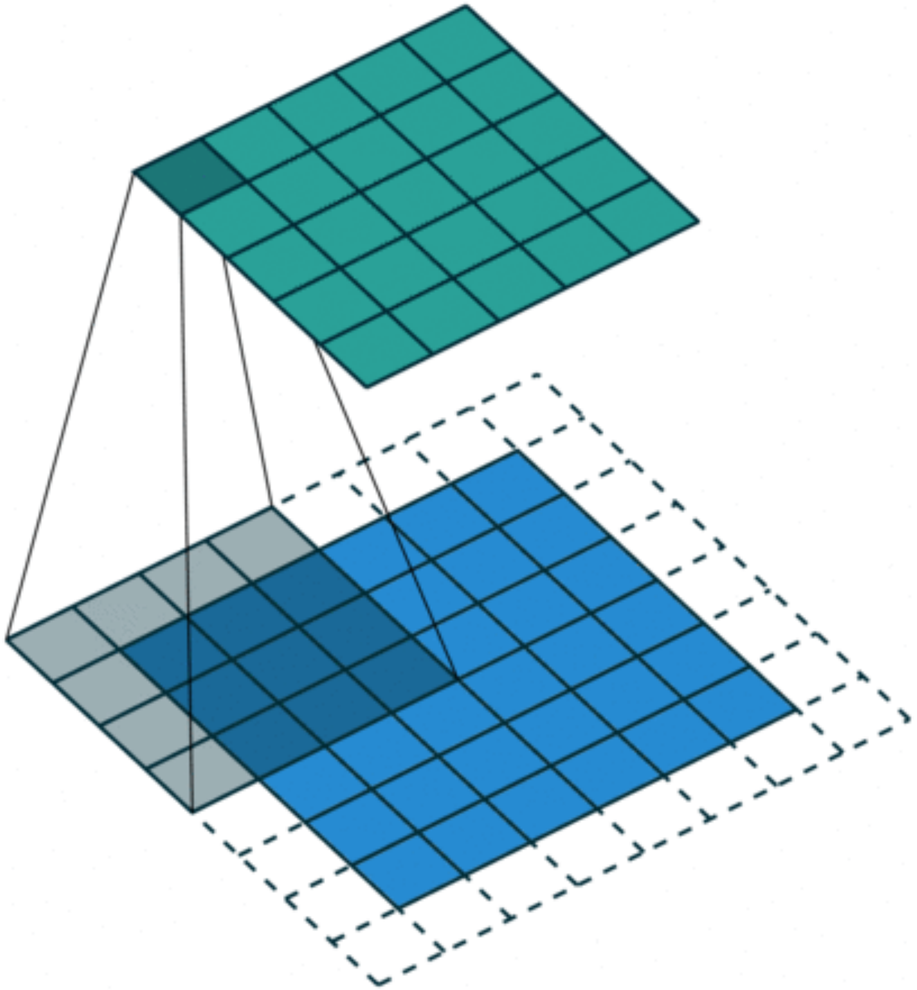
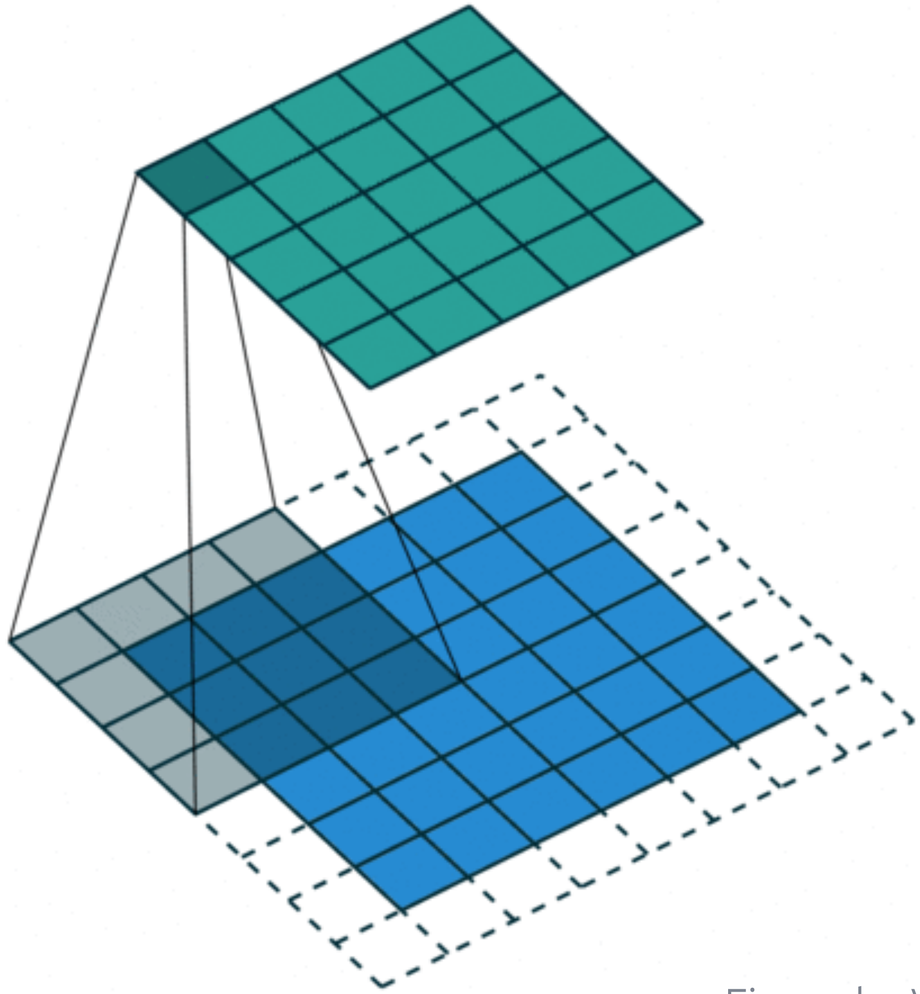
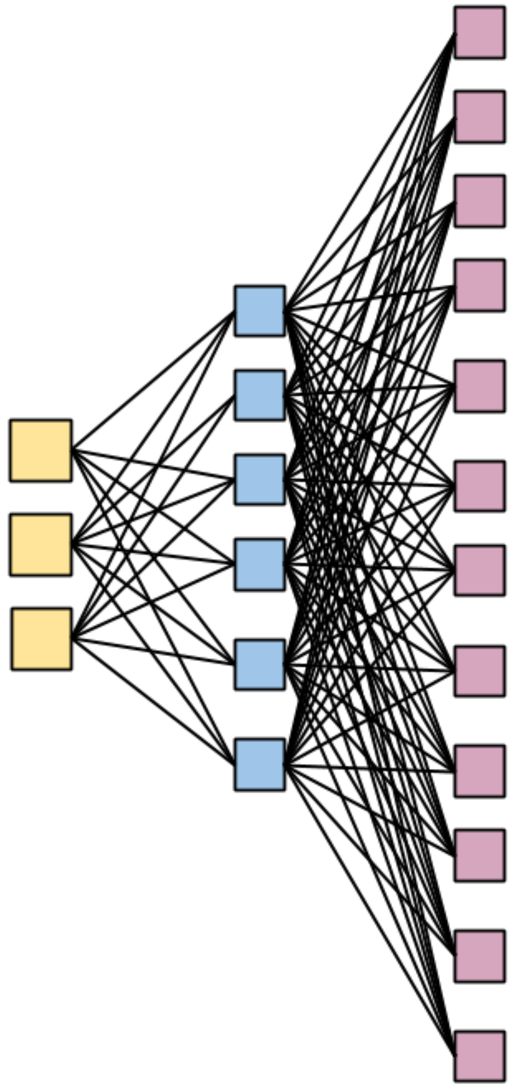


Figure by Vincent Dumolin: https://github.com/vdumoulin/conv_arithmetic

Types of typical operators

Convolution





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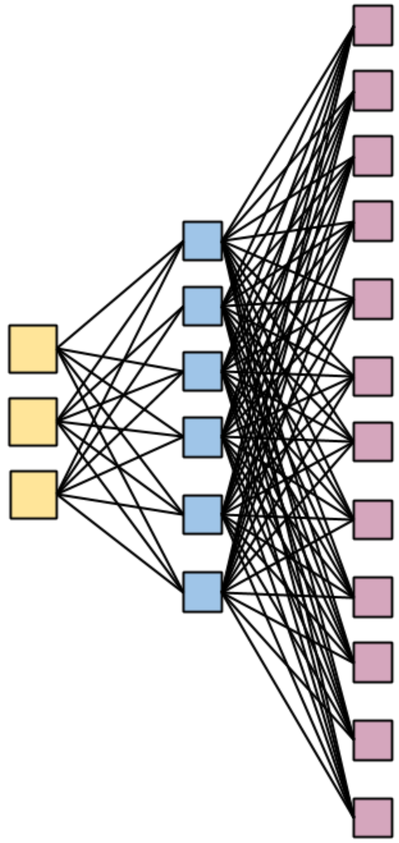
Types of typical operators

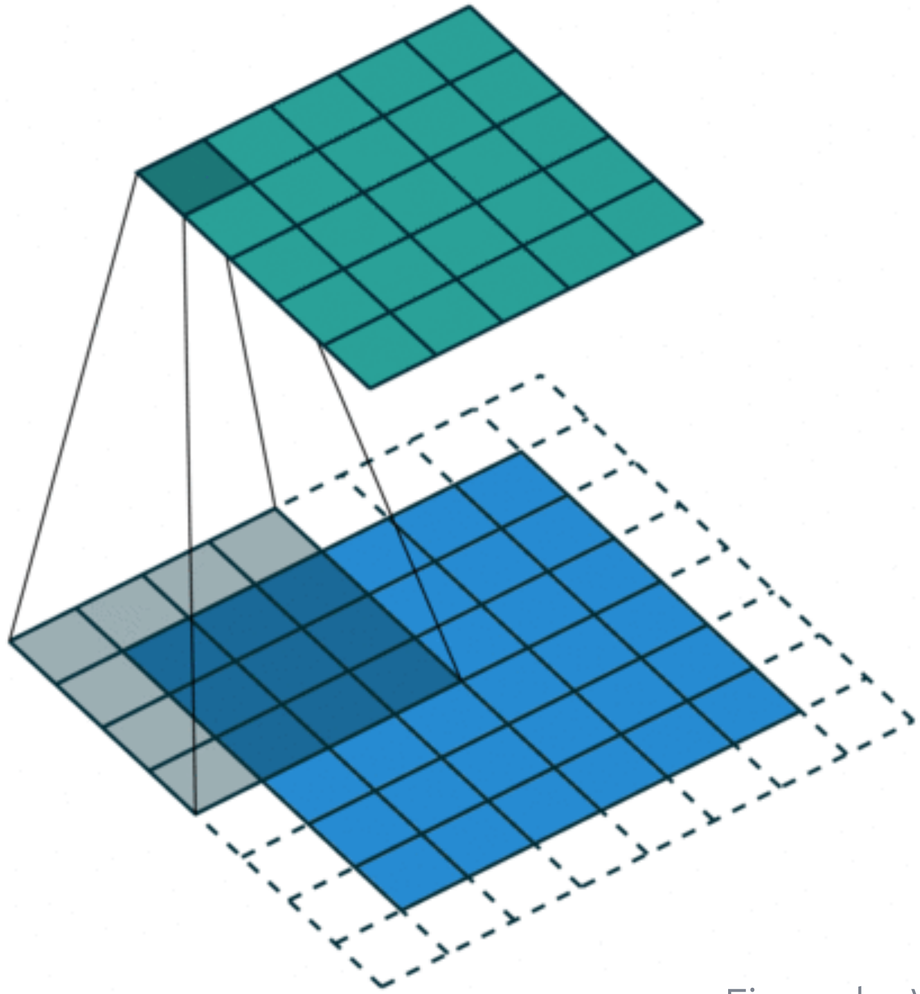
Convolution

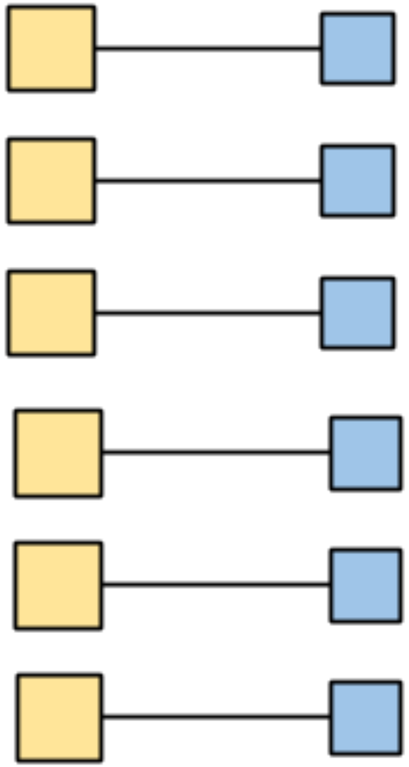


```
for oc in output_channel:
    for ic in input_channel:
        for h in output_height:
            for w in output_width:
                for kh in kernel_height:
                    for kw in kernel_width:
                        output_pixel += input_pixel * kernel_value
```

Figure by Vincent Dumolin: https://github.com/vdumoulin/conv_arithmetic

Types of typical operators





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Types of typical operators

Matrix Multiply

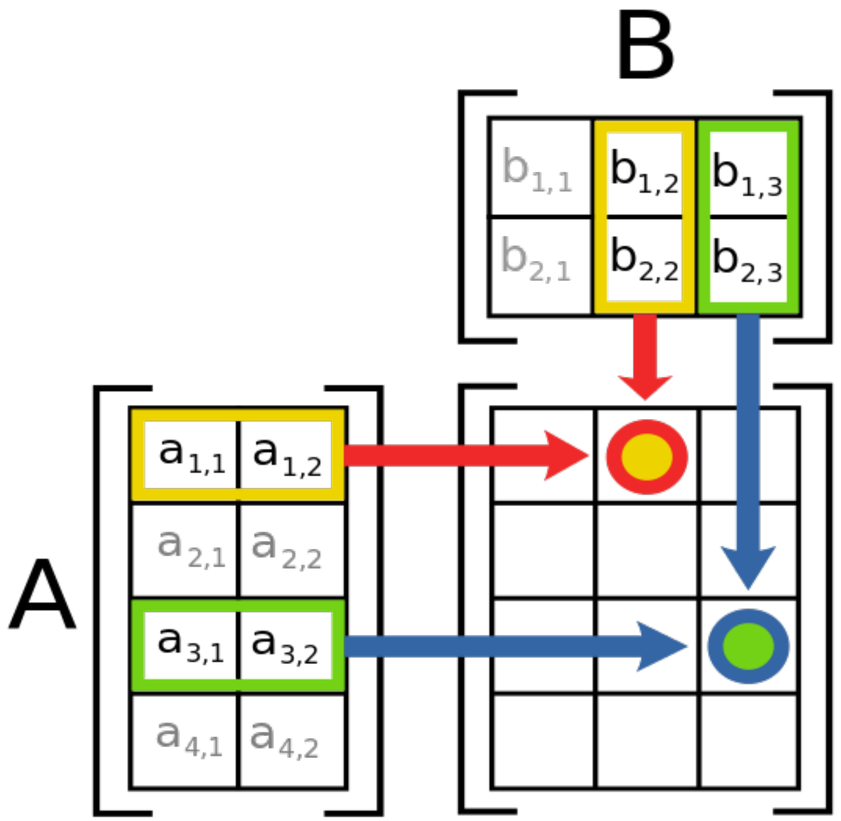


Figure by Wikipedia: https://en.wikipedia.org/wiki/Matrix_multiplication

Types of typical operators

Pointwise operations

```
for (i=0; i < data_length; i++) {
    output[i] = input1[i] + input2[i]
}
```

Figure by Wikipedia: https://en.wikipedia.org/wiki/Matrix_multiplication

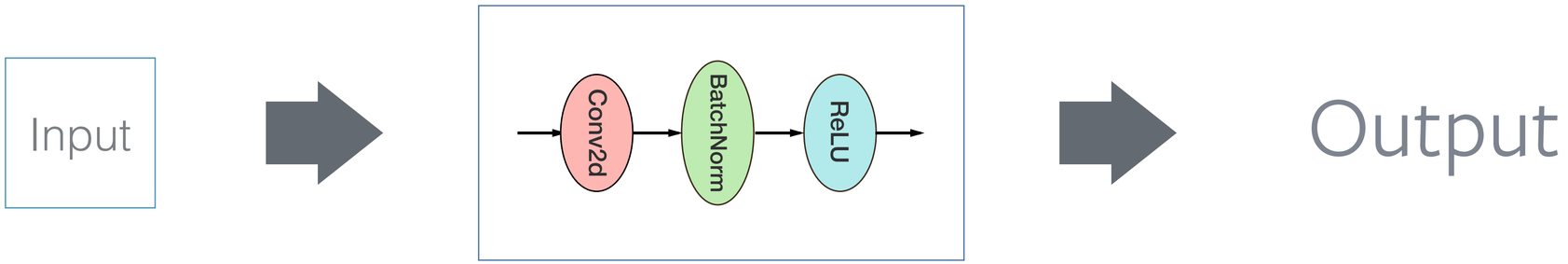
Types of typical operators

Reduction operations

```
double sum = 0.0;
for (i=0; i < data_length; i++) {
    sum += input[i];
}
```

Figure by Wikipedia: https://en.wikipedia.org/wiki/Matrix_multiplication

Chained Together



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Chained Together

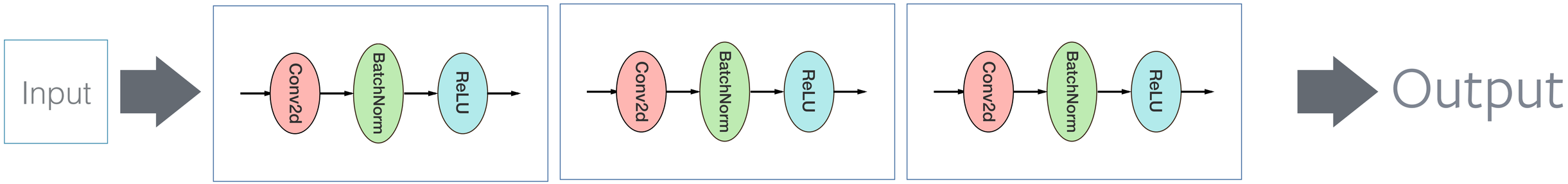
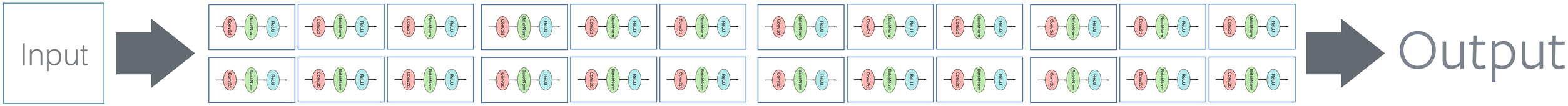


Figure by Wikipedia: https://en.wikipedia.org/wiki/Matrix_multiplication

Chained Together

"deep"



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Chained Together

"deep"

recurrent

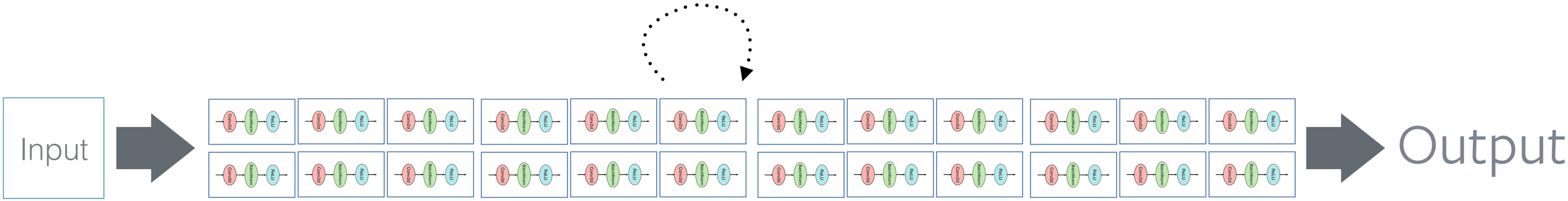
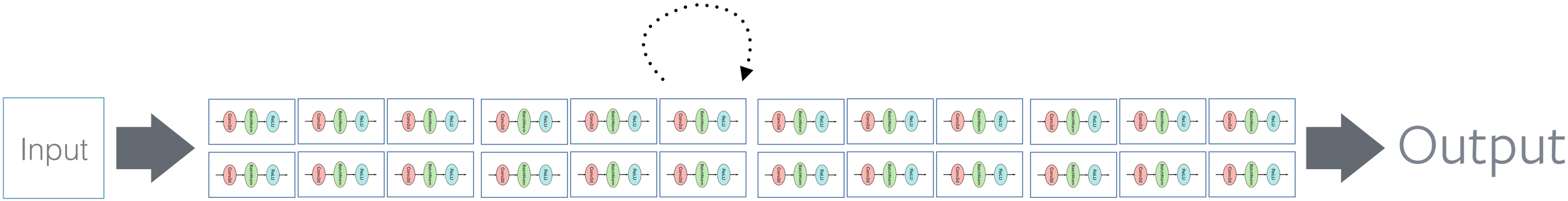


Figure by Wikipedia: https://en.wikipedia.org/wiki/Matrix_multiplication

Trained with Gradient Descent

"deep"

recurrent



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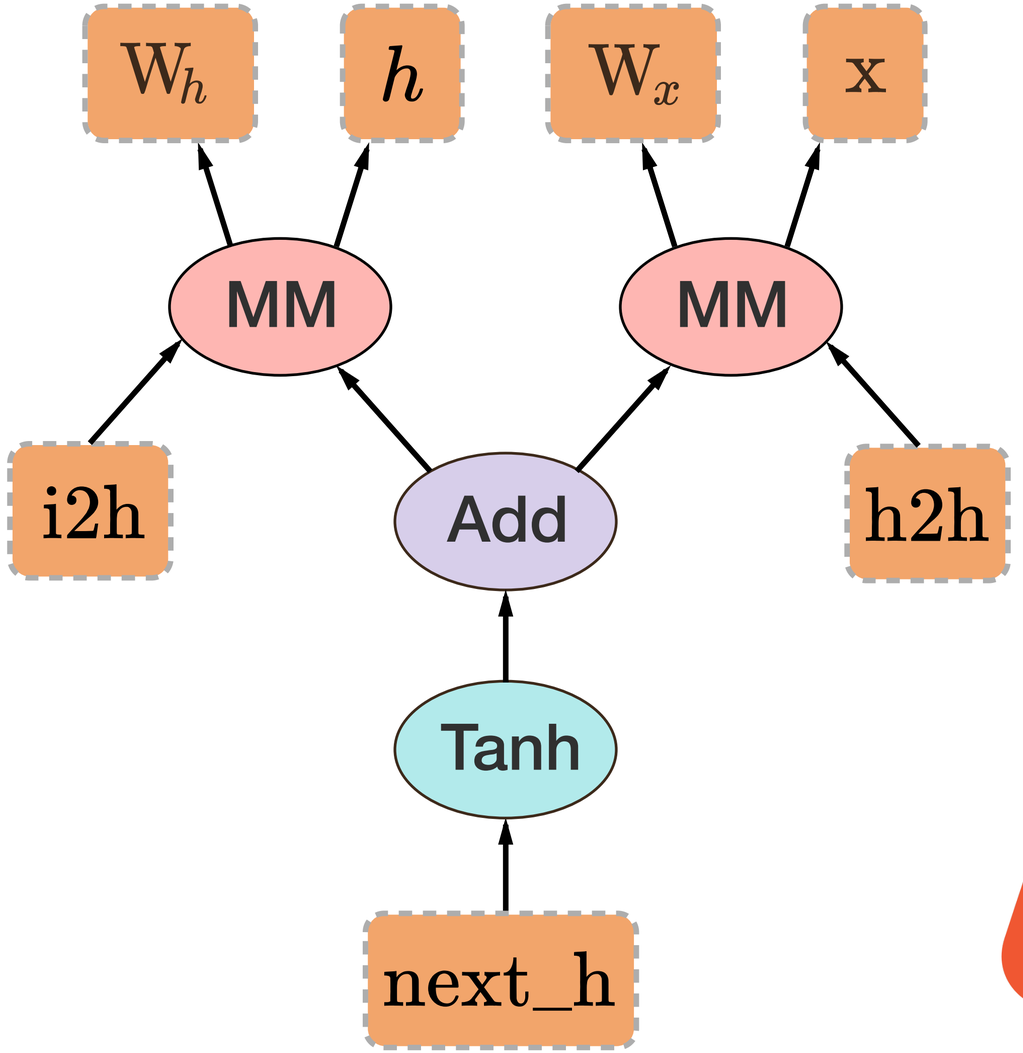
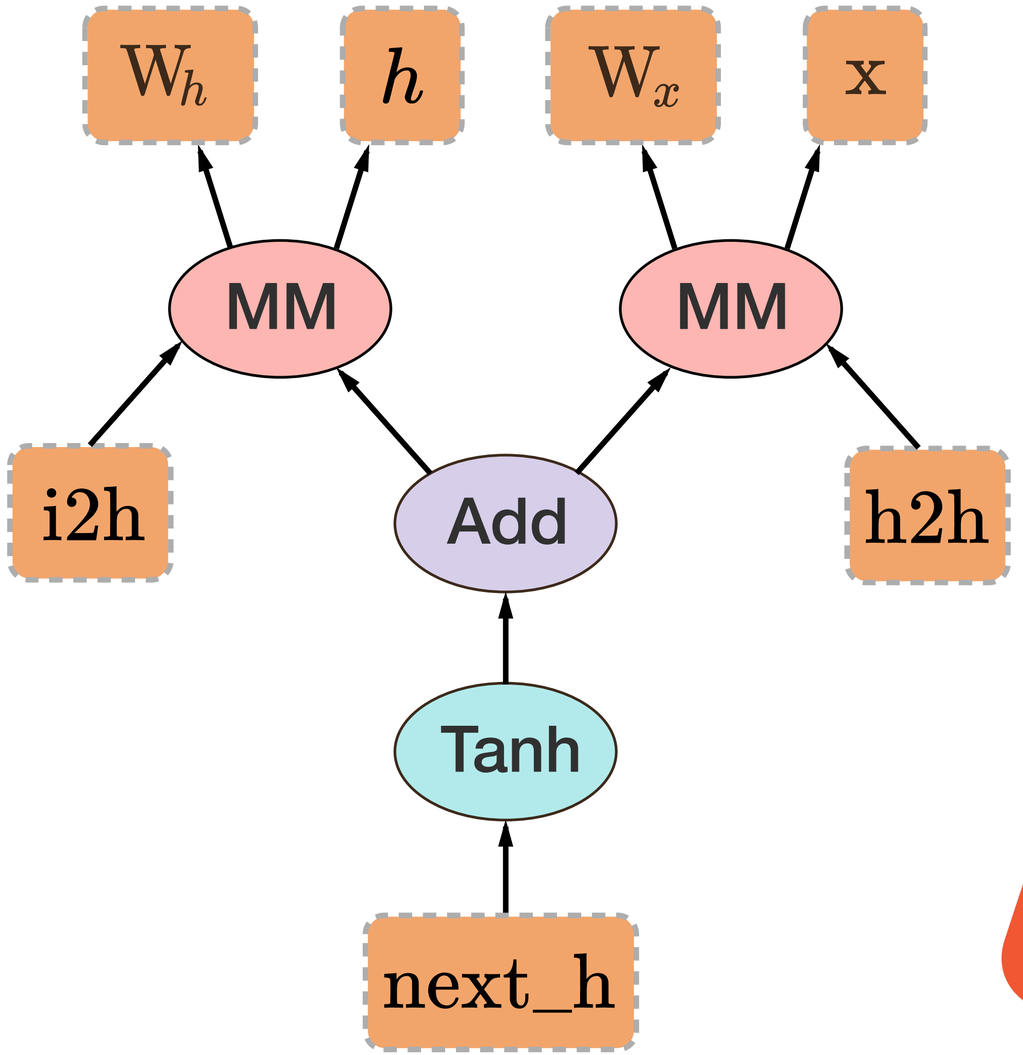
Trained with Gradient Descent

- Provide gradient computation
  - Gradient of one variable w.r.t. any variable in graph



Trained with Gradient Descent

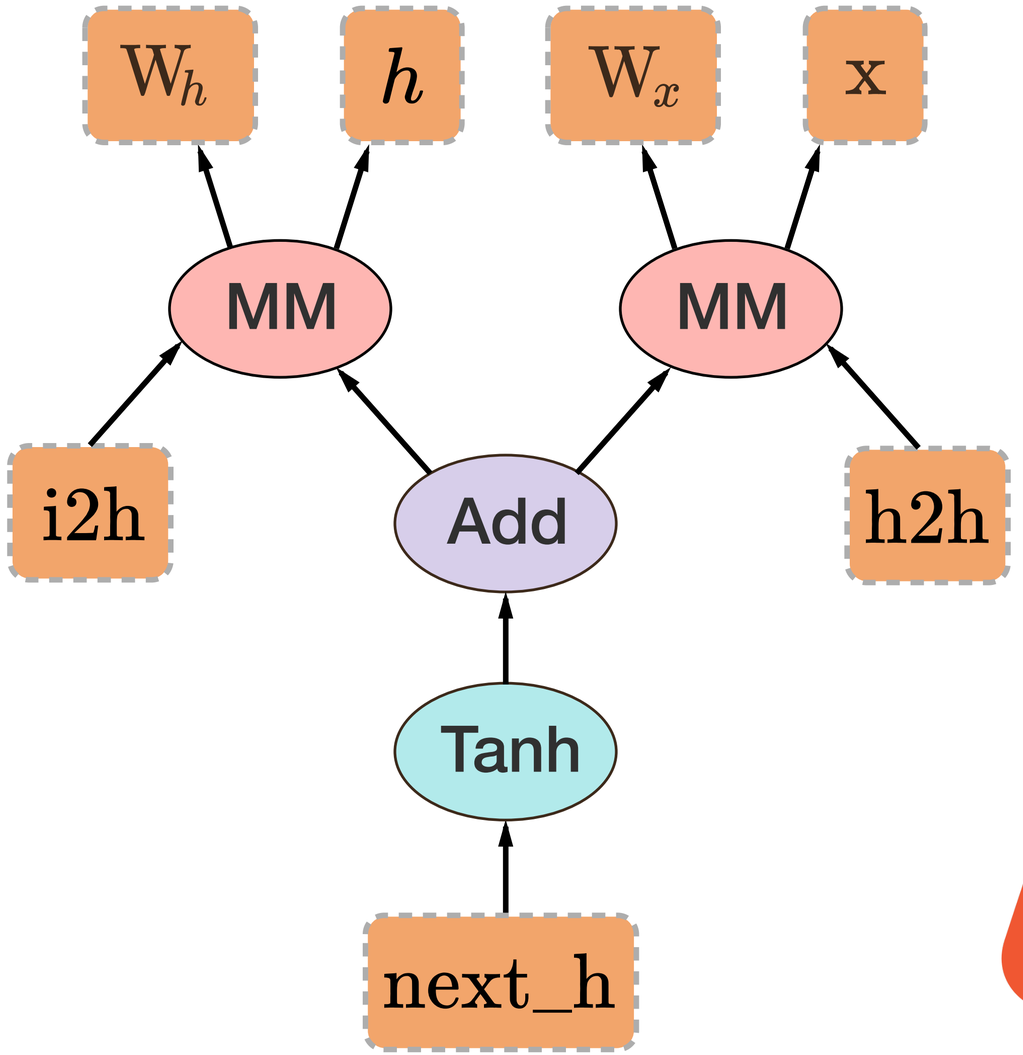
- Provide gradient computation
  - Gradient of one variable w.r.t. any variable in graph
  - For example, can compute: $\frac{dnext_h}{dW_h}$



Trained with Gradient Descent

- Provide gradient computation
  - Gradient of one variable w.r.t. any variable in graph
  - For example, can compute: $\frac{dnext_h}{dW_h}$
  - And then you usually do SGD step:

$$W_h = W_h - \alpha * \frac{dnext_h}{dW_h}$$



Computation Graph Toolkits

Computation Graph Toolkits

Declarative Toolkits

theano

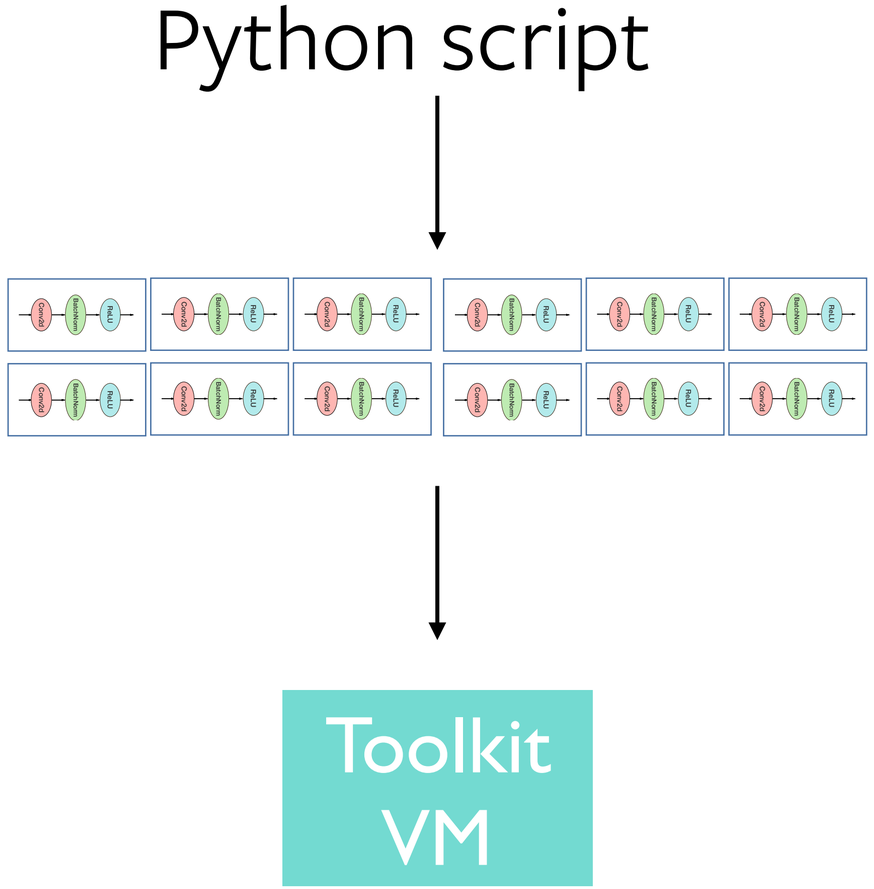
Caffe

Declarative Toolkits

1. Declare and compile a model

   typically in a high-level language like Python

2. Repeatedly execute the model in a VM



Computation Graph

Declarative Toolkits

- Declare a computation
  - with placeholder variables
- Compile it
- Run it in a Session

```
1  import tensorflow as tf
2  import numpy as np
3
4  trX = np.linspace(-1, 1, 101)
5  trY = 2 * trX + np.random.randn(*trX.shape) * 0.33
6
7  X = tf.placeholder("float")
8  Y = tf.placeholder("float")
9
10 def model(X, w):
11     return tf.multiply(X, w)
12
13 w = tf.Variable(0.0, name="weights")
14 y_model = model(X, w)
15
16 cost = tf.square(Y - y_model)
17
18 train_op = tf.train.GradientDescentOptimizer(0.01).minimize(cost)
19
20 with tf.Session() as sess:
21     tf.global_variables_initializer().run()
22
23     for i in range(100):
24         for (x, y) in zip(trX, trY):
25             sess.run(train_op, feed_dict={X: x, Y: y})
26
27     print(sess.run(w))
```

Input / output placeholders

Computation Graph

Declarative Toolkits

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```

Model definition

Computation Graph

Declarative Toolkits

- Declare a computation
  - with placeholder variables
- Compile it
- Run it in a Session

A separate turing-complete Virtual Machine

```
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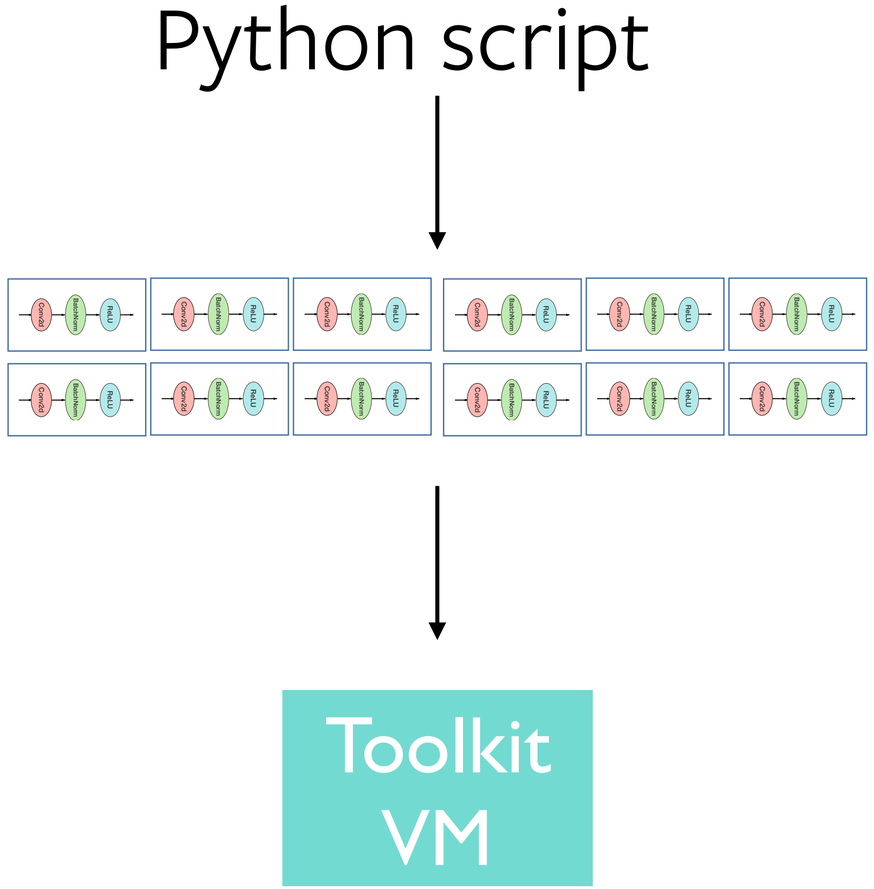

Imperative Toolkits

Imperative Toolkits

Run a computation

- computation is run

PYTORCH

HIPS Autograd

Dynet

Imperative Toolkits

- Run a computation
- computation is run!

```
1   import torch
2   from torch.autograd import Variable
3
4   trX = torch.linspace(-1, 1, 101)
5   trY = 2 * trX + torch.randn(*trX.size()) * 0.33
6
7   w = Variable(trX.new([0.0]), requires_grad=True)
8
9   for i in range(100):
10    for (x, y) in zip(trX, trY):
11      X = Variable(x)
12      Y = Variable(y)
13
14      y_model = X * w.expand_as(X)
15      cost = (Y - Y_model) ** 2
16      cost.backward(torch.ones(*cost.size()))
17
18      w.data = w.data + 0.01 * w.grad.data
19
20    print(w)
```

Imperative Toolkits

- Run a computation
- computation is run!
- no separate execution engine

```
1   import torch
2   from torch.autograd import Variable
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4   trX = torch.linspace(-1, 1, 101)
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17
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```

Imperative Toolkits

- Run a computation
- computation is run!
- no separate execution engine
- great for Dynamic Graphs!

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16      cost.backward(torch.ones(*cost.size()))
17
18      w.data = w.data + 0.01 * w.grad.data
19
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```

Imperative Toolkits

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- computation is run!
- no separate execution engine
- great for Dynamic Graphs!

About Dynamic Graphs……

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13
14      y_model = X * w.expand_as(X)
15      cost = (Y - Y_model) ** 2
16      cost.backward(torch.ones(*cost.size()))
17
18      w.data = w.data + 0.01 * w.grad.data
19
20    print(w)
```

Dynamic Graphs: a paradigm shift in AI Research

Today's AI → Active Research & Future AI → Tools for AI *keeping up with change*

PYTORCH

Chainer

mxnet

theano

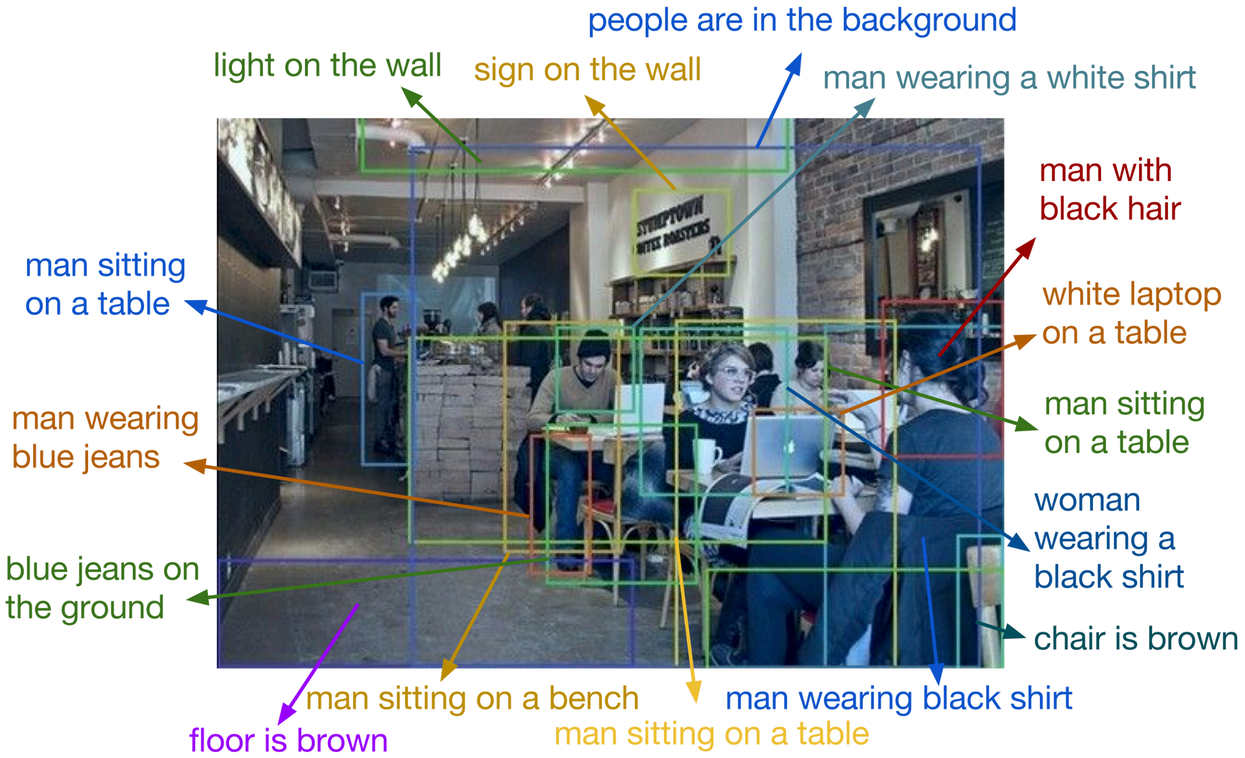
Caffe

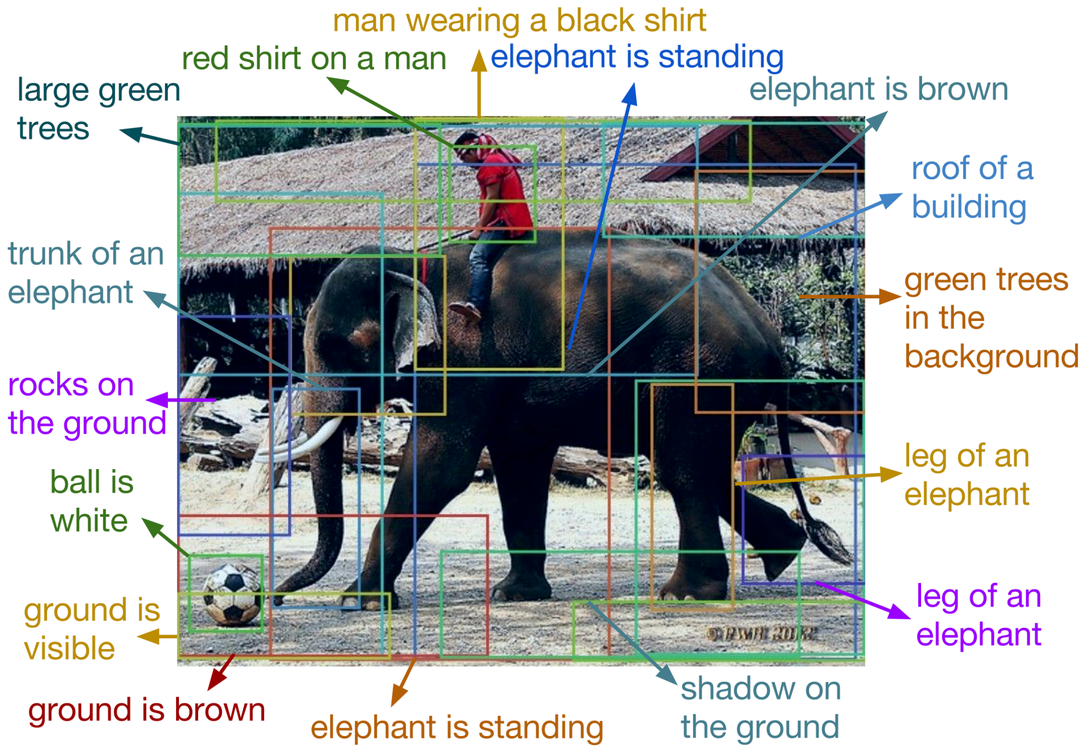
K

Today's AI

DenseCap by Justin Johnson & group

https://github.com/jcjohnson/densecap





Today's AI → Future AI → Tools for AI

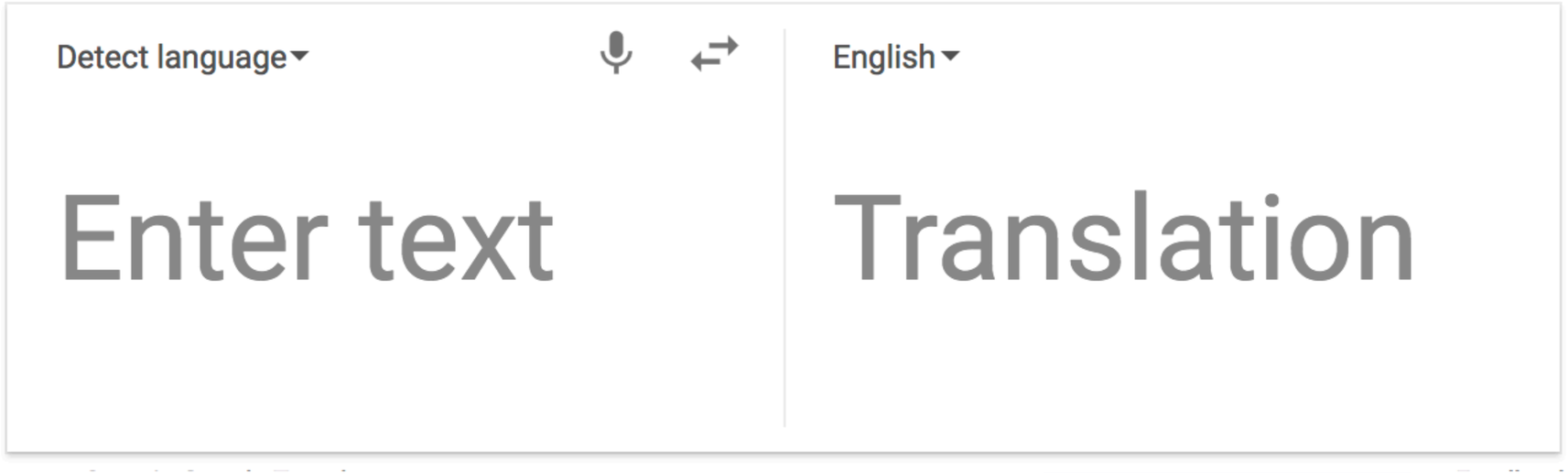
Today's AI

DeepMask by Pedro Pinhero & group

Today's AI → Future AI → Tools for AI

Today's AI

Machine Translation



Google Translate

BING TRANSLATOR

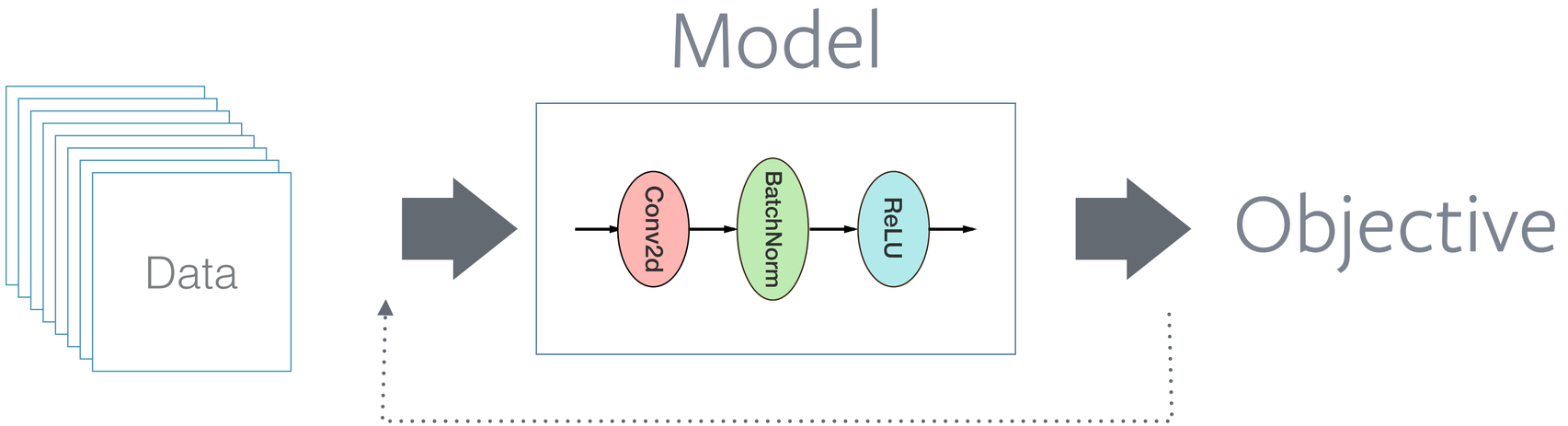
Today's AI → Future AI → Tools for AI

Today's AI

Text Classification (sentiment analysis etc.)
Text Embeddings
Graph embeddings
Machine Translation
Ads ranking

Today's AI

Train Model



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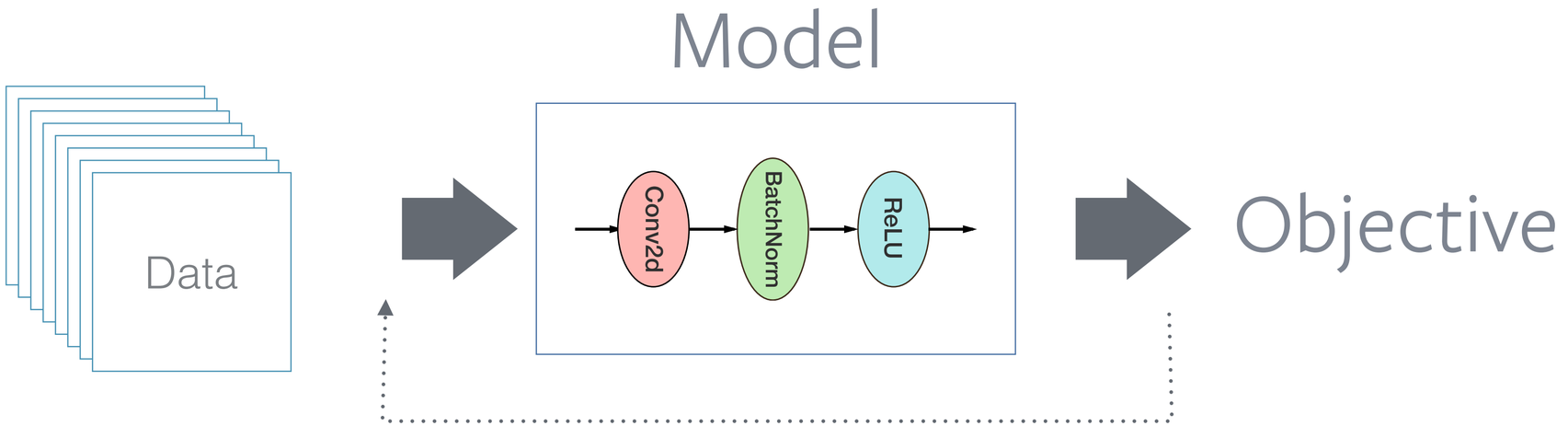
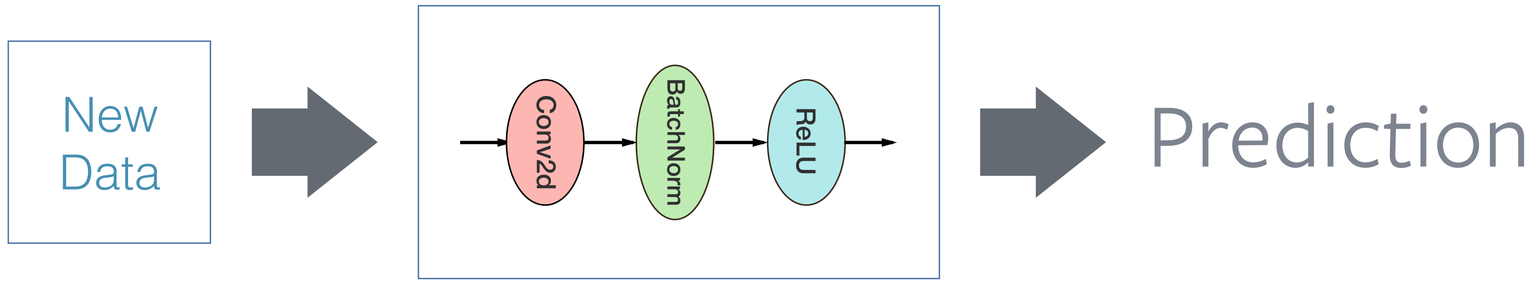
Today's AI

Train Model



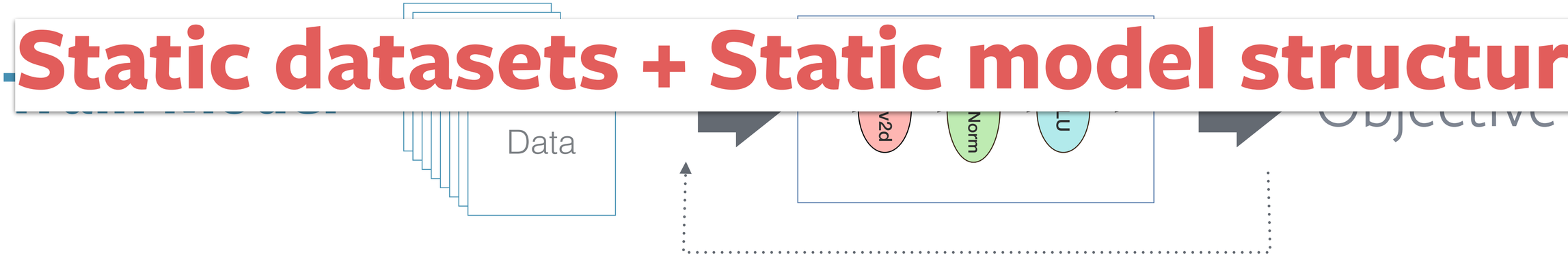
Deploy & Use



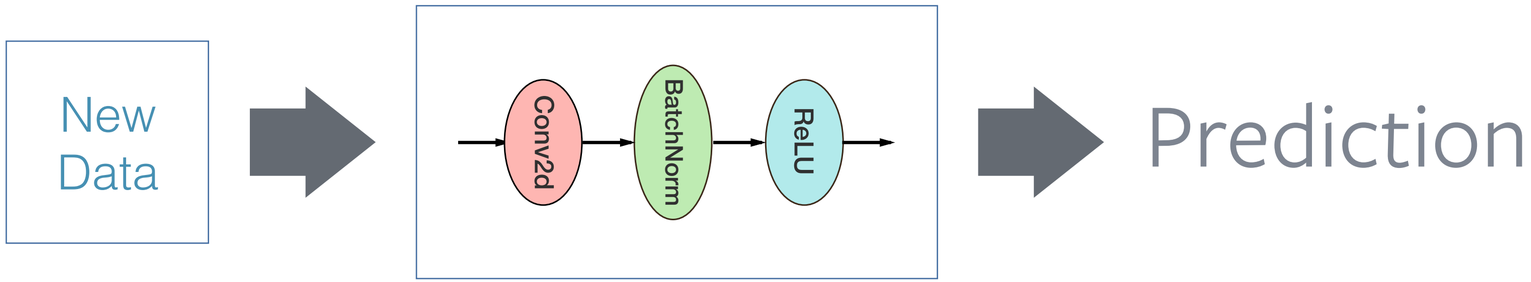
Today's AI → Future AI → Tools for AI

Today's AI

Static datasets + Static model structure



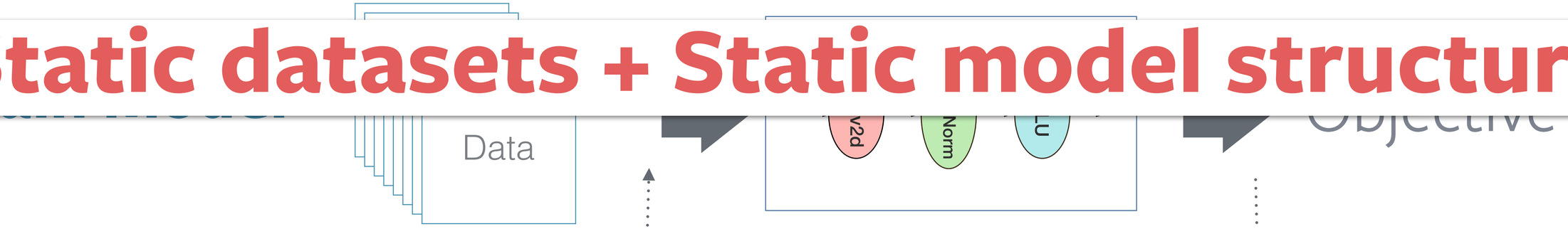
Deploy & Use



Today's AI → Future AI → Tools for AI

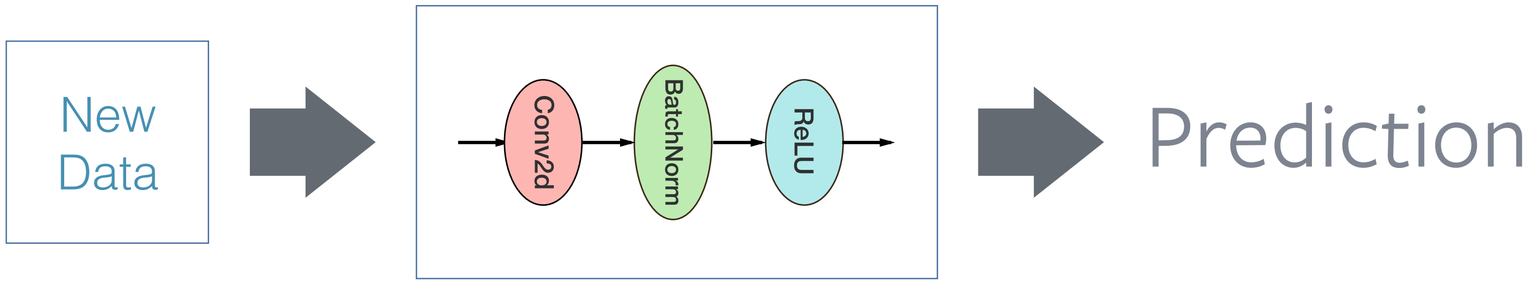
Today's AI

Static datasets + Static model structure



Offline Learning

Deploy & Use



Today's AI → Future AI → Tools for AI

Current AI Research / Future AI

Self-driving Cars

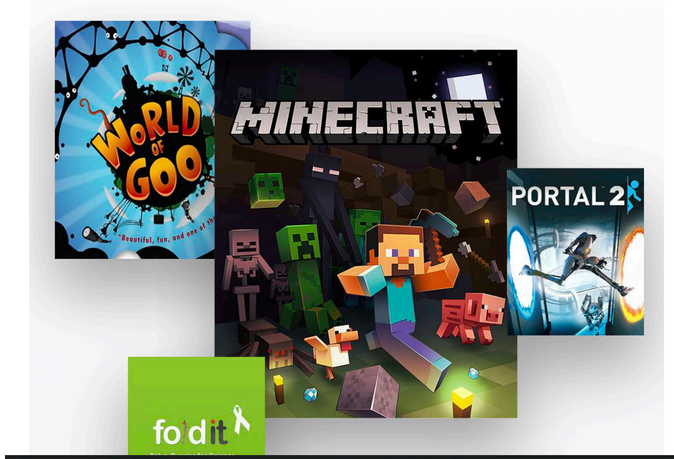
Today's AI → **Future AI** → Tools for AI

Current AI Research / Future AI

Agents trained in many environments

Cars

Video games



Internet

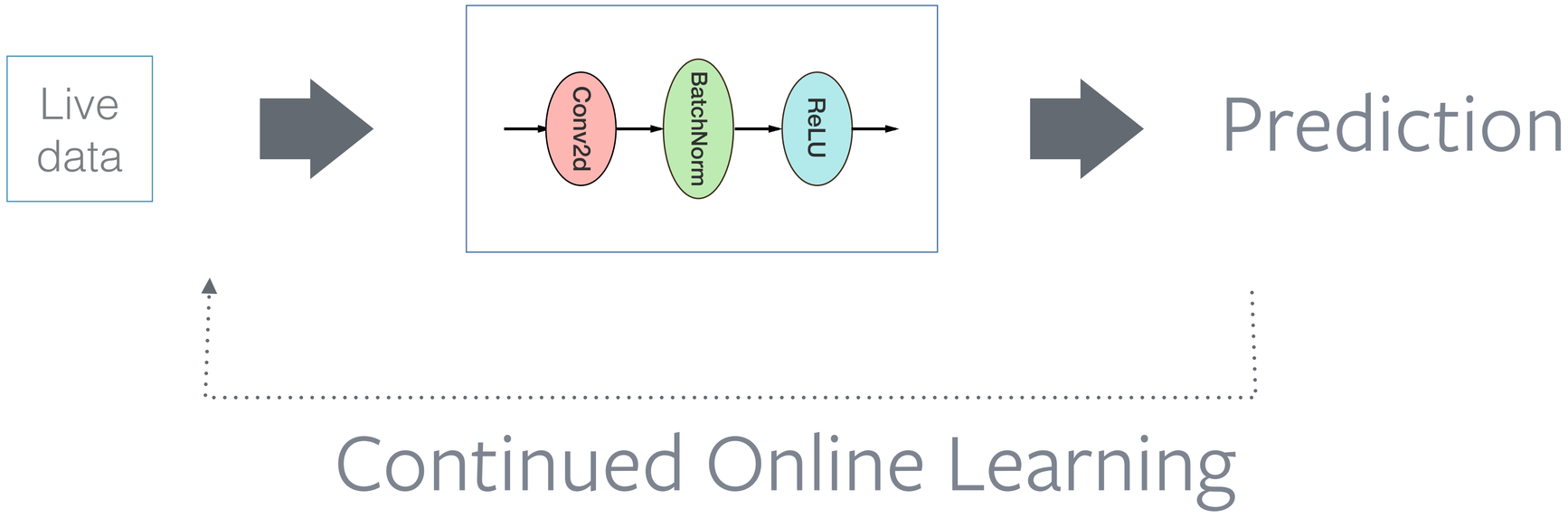
Today's AI → Future AI → Tools for AI

Current AI Research / Future AI

Dynamic Neural Networks

self-adding new memory or layers
changing evaluation path based on inputs

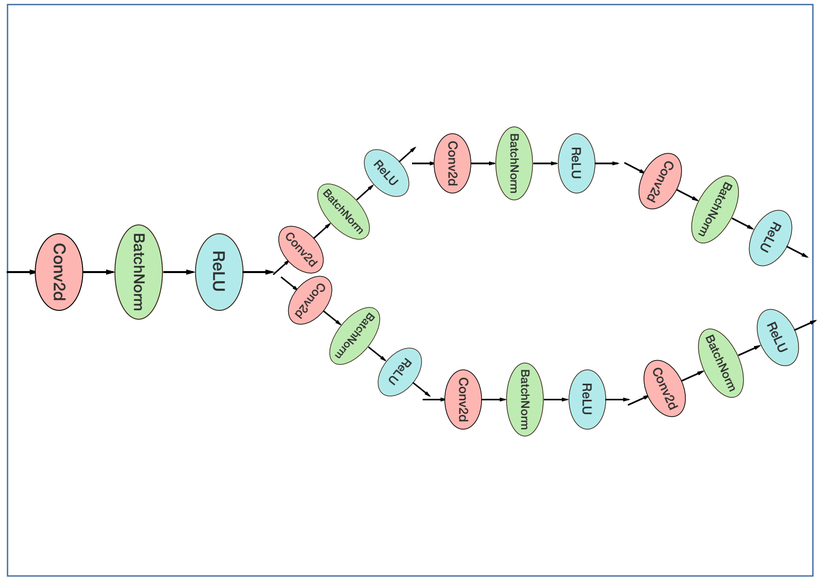
Current AI Research / Future AI



Today's AI → Future AI → Tools for AI

Current AI Research / Future AI

Sample-**1**



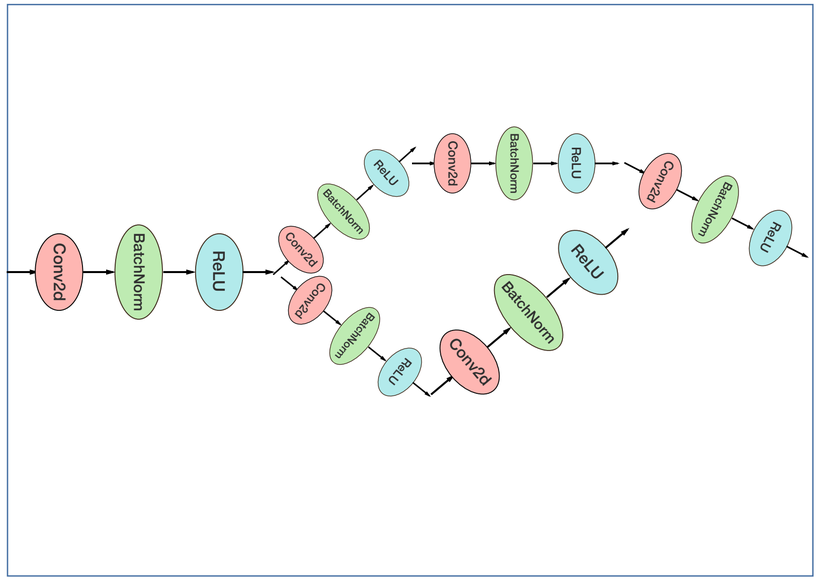
Prediction

Data-dependent change in model structure

Today's AI → **Future AI** → Tools for AI

Current AI Research / Future AI

Sample-**2**



Prediction

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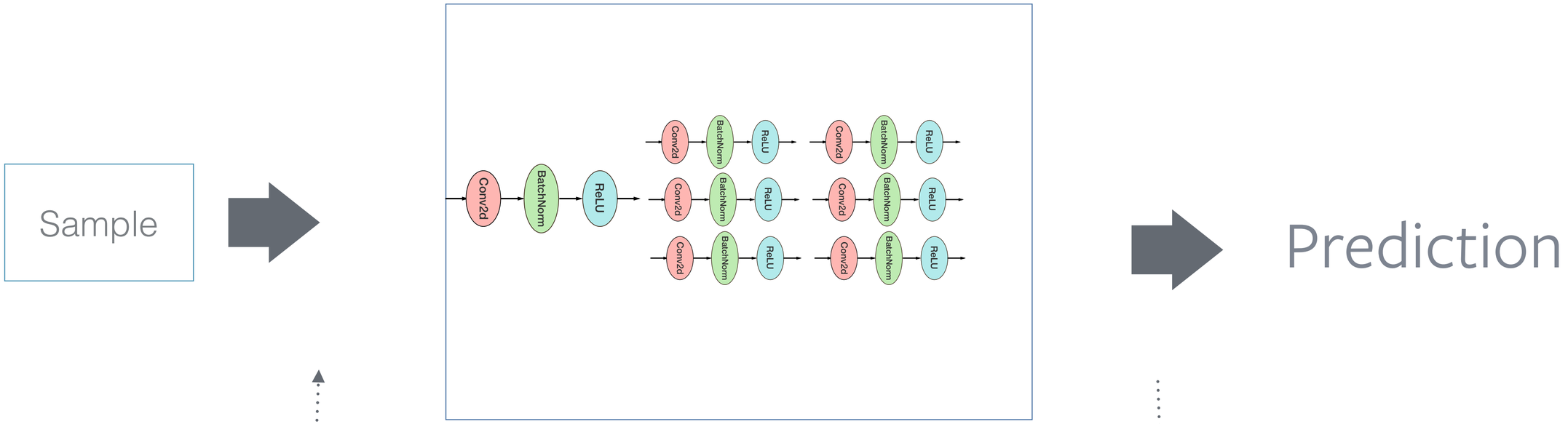
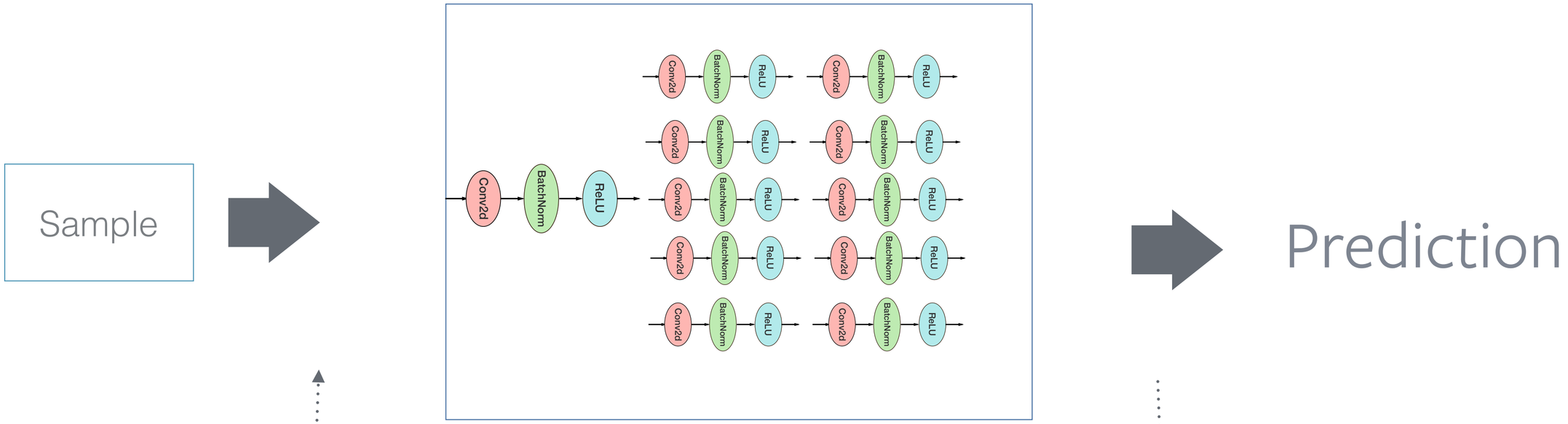
Today's AI → **Future AI** → Tools for AI

Current AI Research / Future AI



Today's AI → Future AI → Tools for AI

Current AI Research / Future AI



Today's AI → Future AI → Tools for AI

The need for a dynamic framework

- Interop with many dynamic environments
  - Connecting to car sensors should be as easy as training on a dataset
  - Connect to environments such as OpenAI Universe
- Dynamic Neural Networks
  - Change behavior and structure of neural network at runtime

Imperative Toolkits

- Run a computation
- computation is run!
- no separate execution engine
- great for Dynamic Graphs!

About Dynamic Graphs……

```
1   import torch
2   from torch.autograd import Variable
3
4   trX = torch.linspace(-1, 1, 101)
5   trY = 2 * trX + torch.randn(*trX.size()) * 0.33
6
7   w = Variable(trX.new([0.0]), requires_grad=True)
8
9   for i in range(100):
10    for (x, y) in zip(trX, trY):
11      X = Variable(x)
12      Y = Variable(y)
13
14      y_model = X * w.expand_as(X)
15      cost = (Y - Y_model) ** 2
16      cost.backward(torch.ones(*cost.size()))
17
18      w.data = w.data + 0.01 * w.grad.data
19
20    print(w)
```

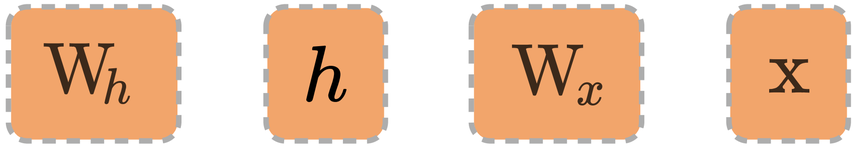
automatic differentiation engine

for deep learning and reinforcement learning

PyTorch Autograd

```
from torch.autograd import Variable
```

PyTorch Autograd




```
from torch.autograd import Variable

x = Variable(torch.randn(1, 10))
prev_h = Variable(torch.randn(1, 20))
W_h = Variable(torch.randn(20, 20))
W_x = Variable(torch.randn(20, 10))
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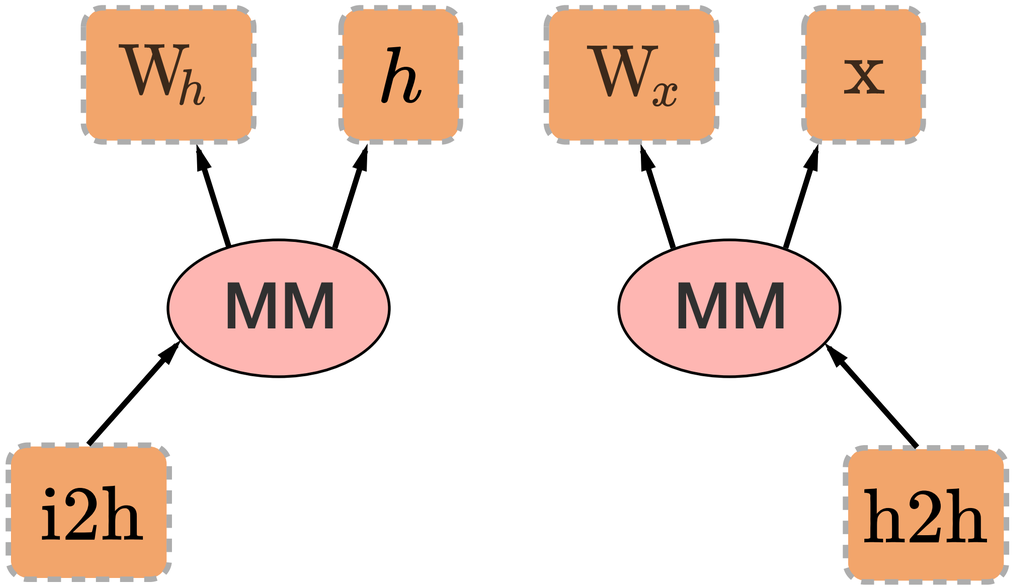
i2h = torch.mm(W_x, x.t())
h2h = torch.mm(W_h, prev_h.t())
```



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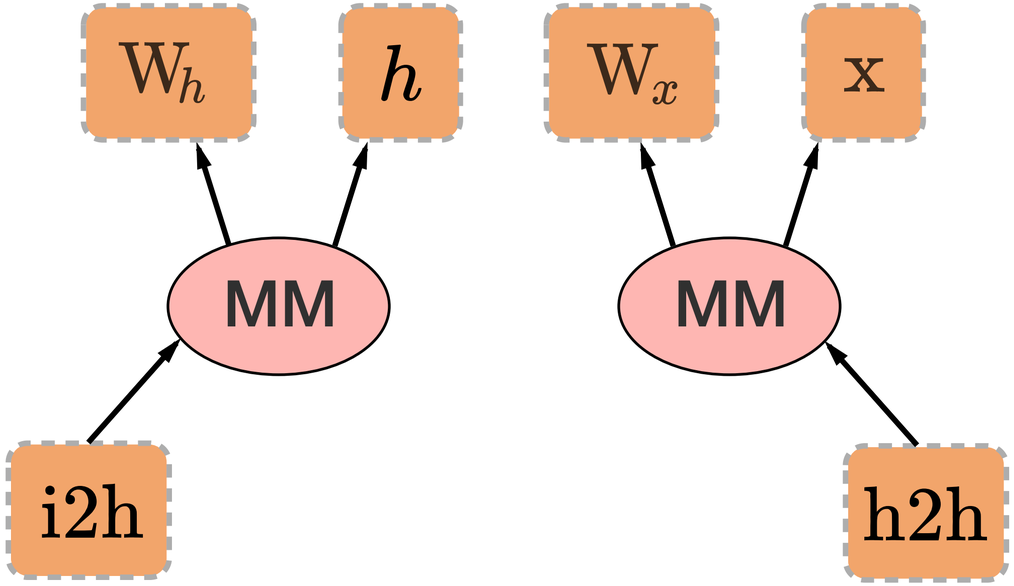
h2h = torch.mm(W_h, prev_h.t())
next_h = i2h + h2h
```



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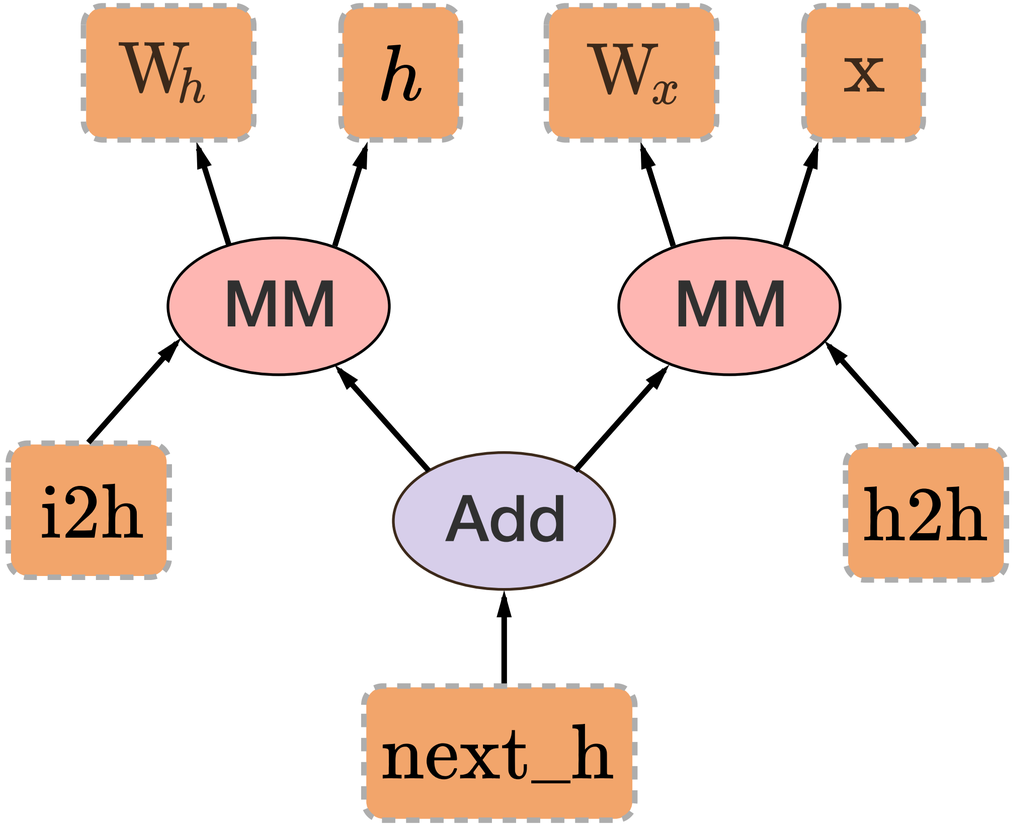

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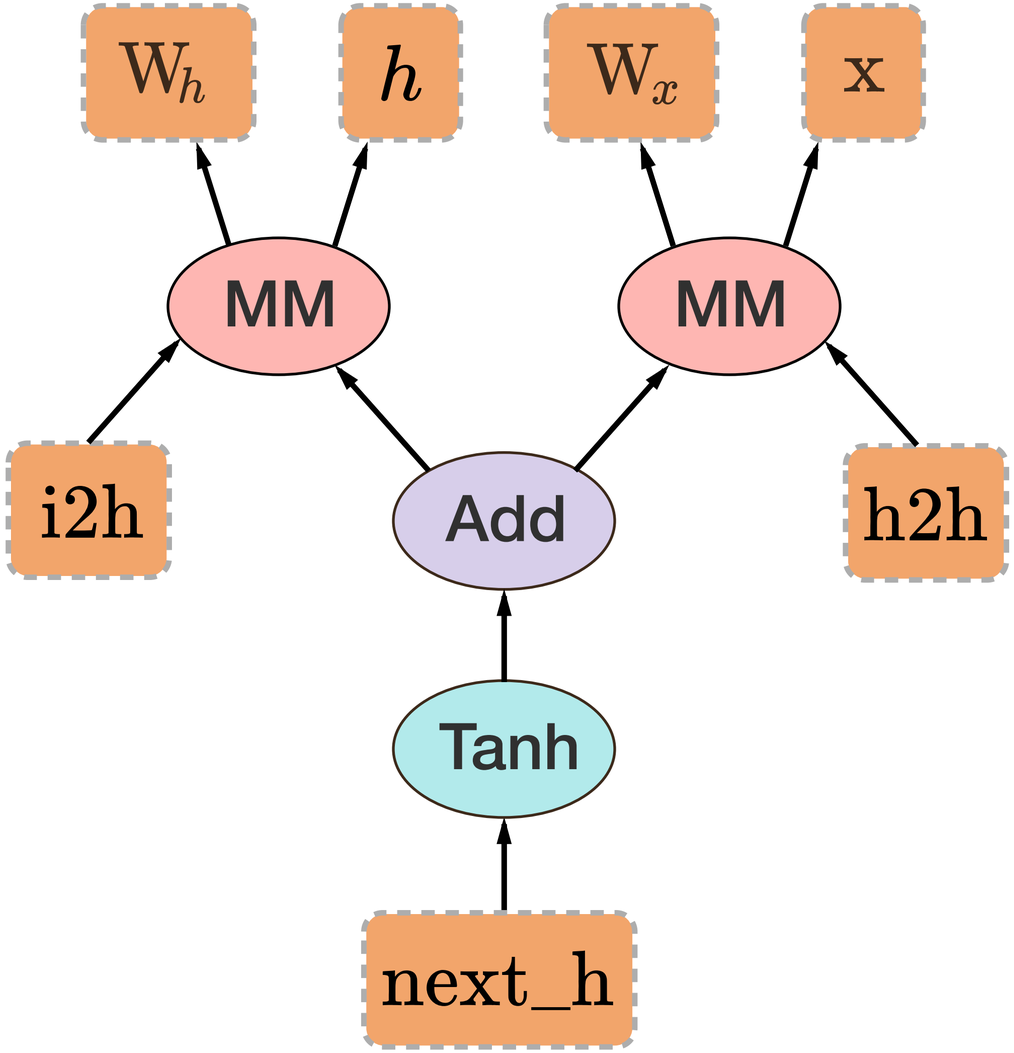
```



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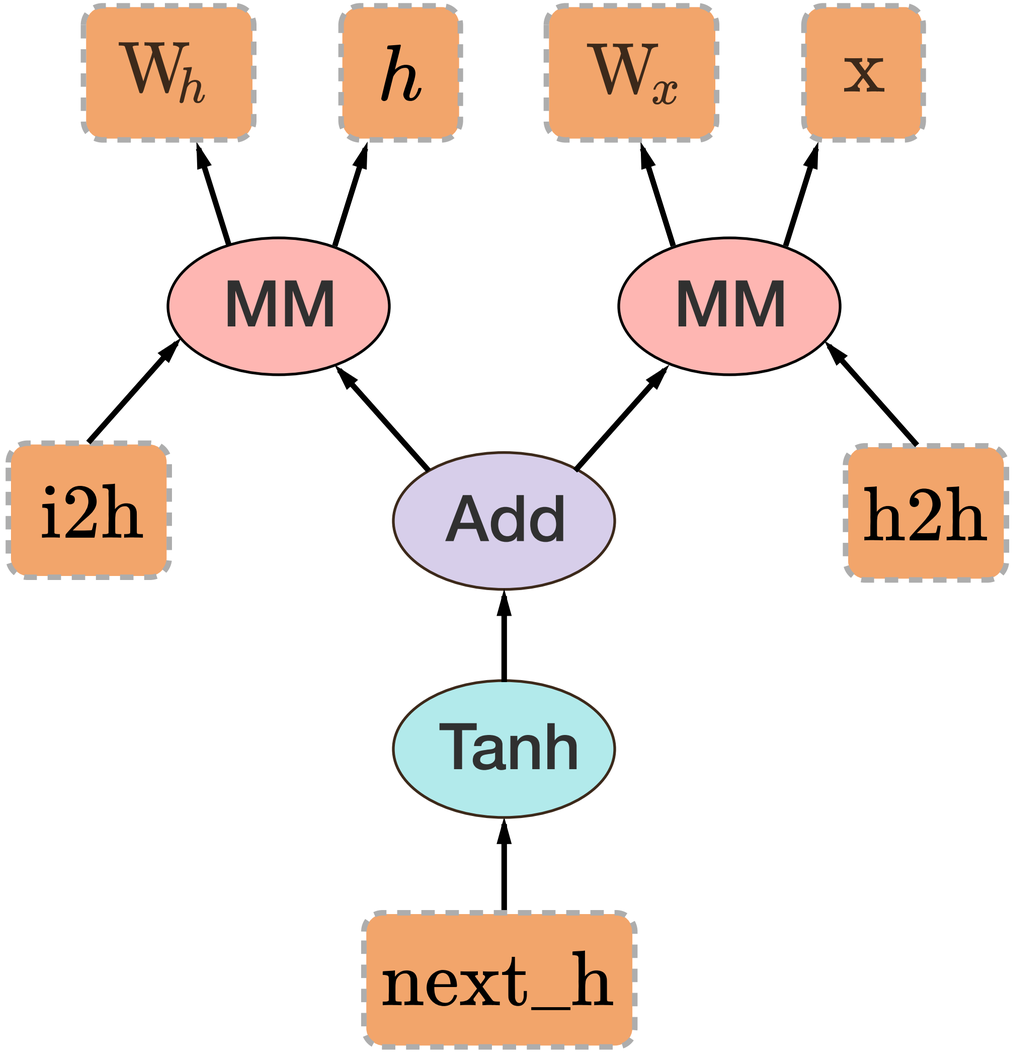
next_h = next_h.tanh()

next_h.backward(torch.ones(1, 20))
```



Neural Networks

```
1   class Net(nn.Module):
2       def __init__(self):
3           super(Net, self).__init__()
4           self.conv1 = nn.Conv2d(1, 10, kernel_size=5)
5           self.conv2 = nn.Conv2d(10, 20, kernel_size=5)
6           self.conv2_drop = nn.Dropout2d()
7           self.fc1 = nn.Linear(320, 50)
8           self.fc2 = nn.Linear(50, 10)
9
10      def forward(self, x):
11          x = F.relu(F.max_pool2d(self.conv1(x), 2))
12          x = F.relu(F.max_pool2d(self.conv2_drop(self.conv2(x)), 2))
13          x = x.view(-1, 320)
14          x = F.relu(self.fc1(x))
15          x = F.dropout(x, training=self.training)
16          x = self.fc2(x)
17          return F.log_softmax(x)
18
19  model = Net()
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Optimization package

SGD, Adagrad, RMSProp, LBFGS, etc.

```
net = Net()
optimizer = torch.optim.SGD(net.parameters(), lr=0.01, momentum=0.9)

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

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

Building models

Implementing Training loop

Checkpointing models

Python + PyTorch - an environment to do all of this

Interfacing with environments

Building optimizers

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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

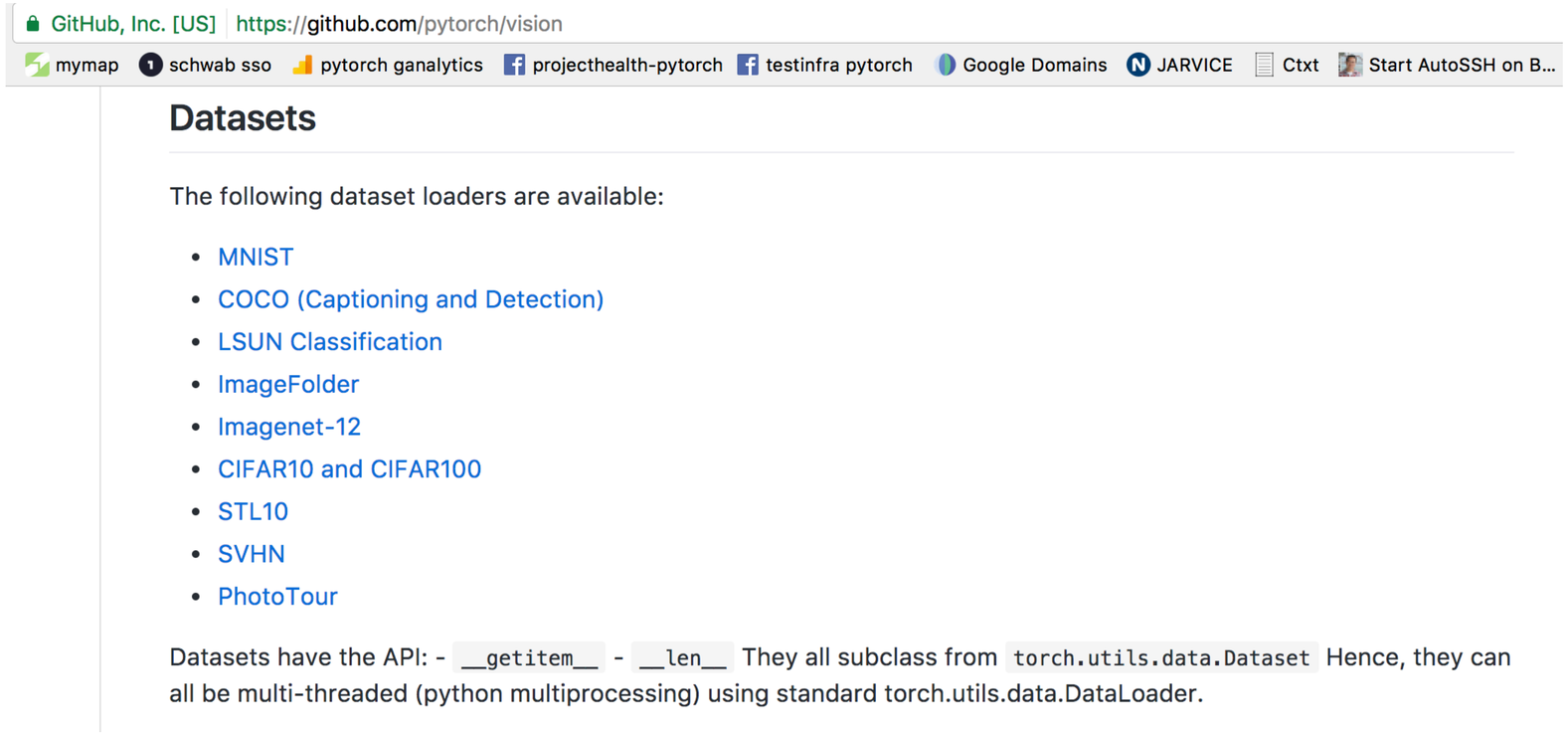
Writing Data Loaders

- 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

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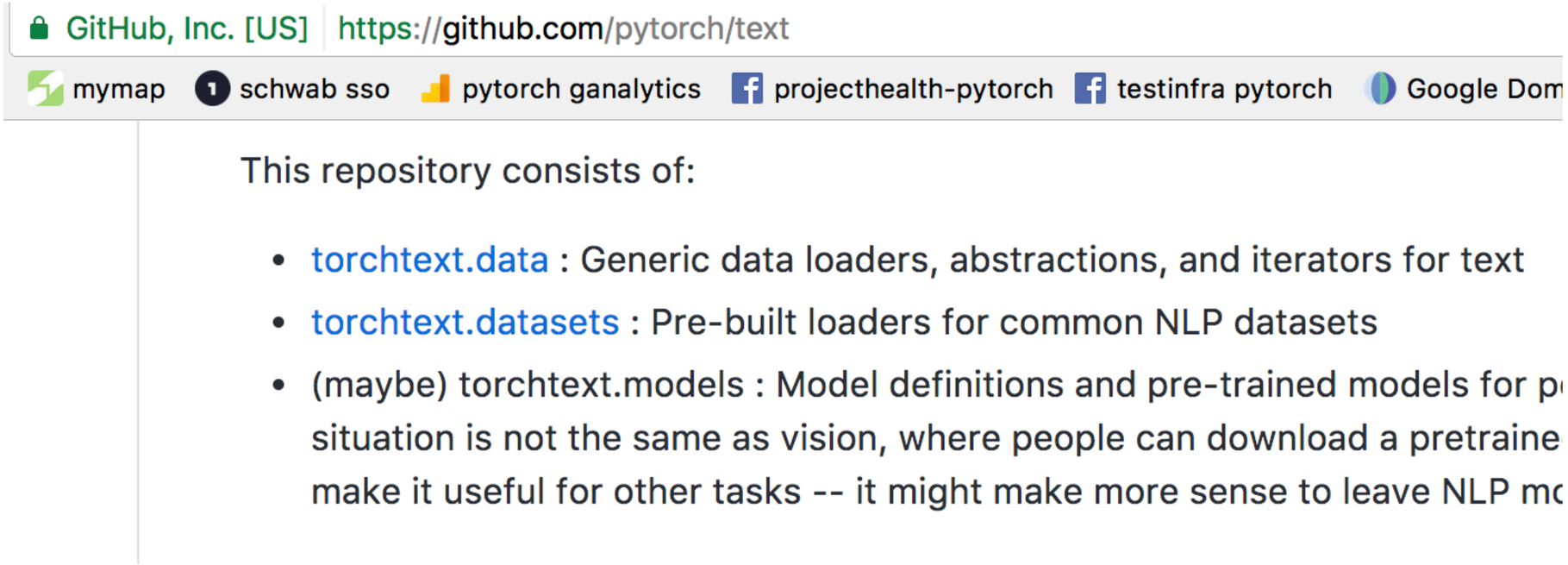

Writing Data Loaders

PyTorch solution:

- use regular Python to write Datasets:

  leverage existing Python code

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  Example: ParlAI

ParlAI

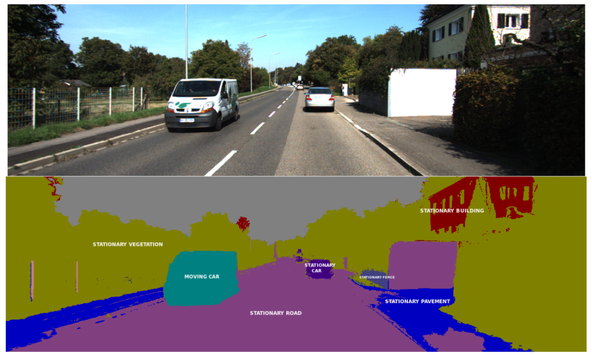
ParlAI (pronounced “par-lay”) is a framework for dialog AI research, implemented in Python.

Its goal is to provide researchers:

- a unified framework for training and testing dialog models
- multi-task training over many datasets at once
- seamless integration of Amazon Mechanical Turk for data collection and human evaluation

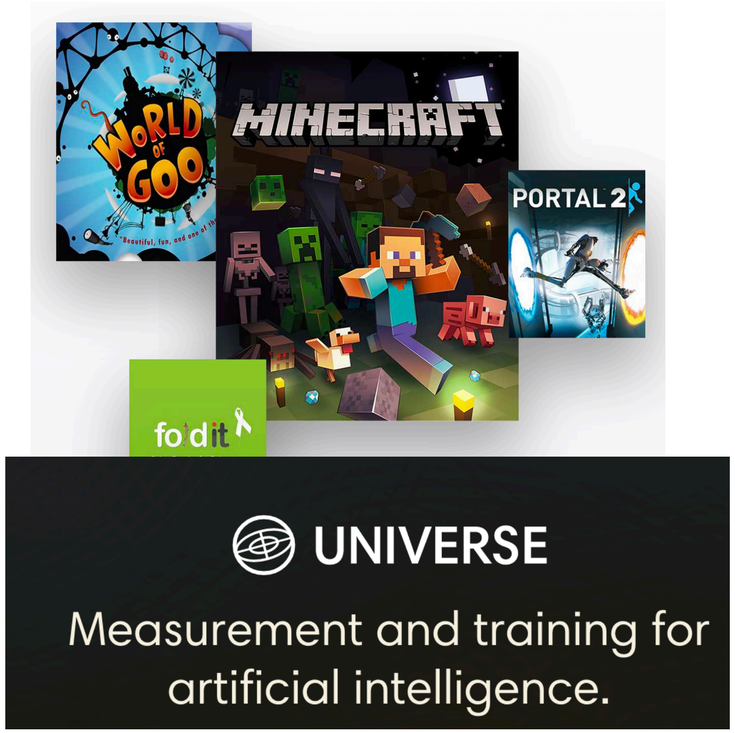
Over 20 tasks are supported in the first release, including popular datasets such as SQuAD, bAbI tasks, MCTest, WikiQA, WebQuestions, SimpleQuestions, WikiMovies, QACNN & QADailyMail, CBT, BookTest, bAbI Dialog tasks, Ubuntu Dialog, OpenSubtitles, Cornell Movie and VQA-COCO2014.

Interfacing with environments



Cars

Video games



Pretty much every environment provides a Python API

Debugging

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

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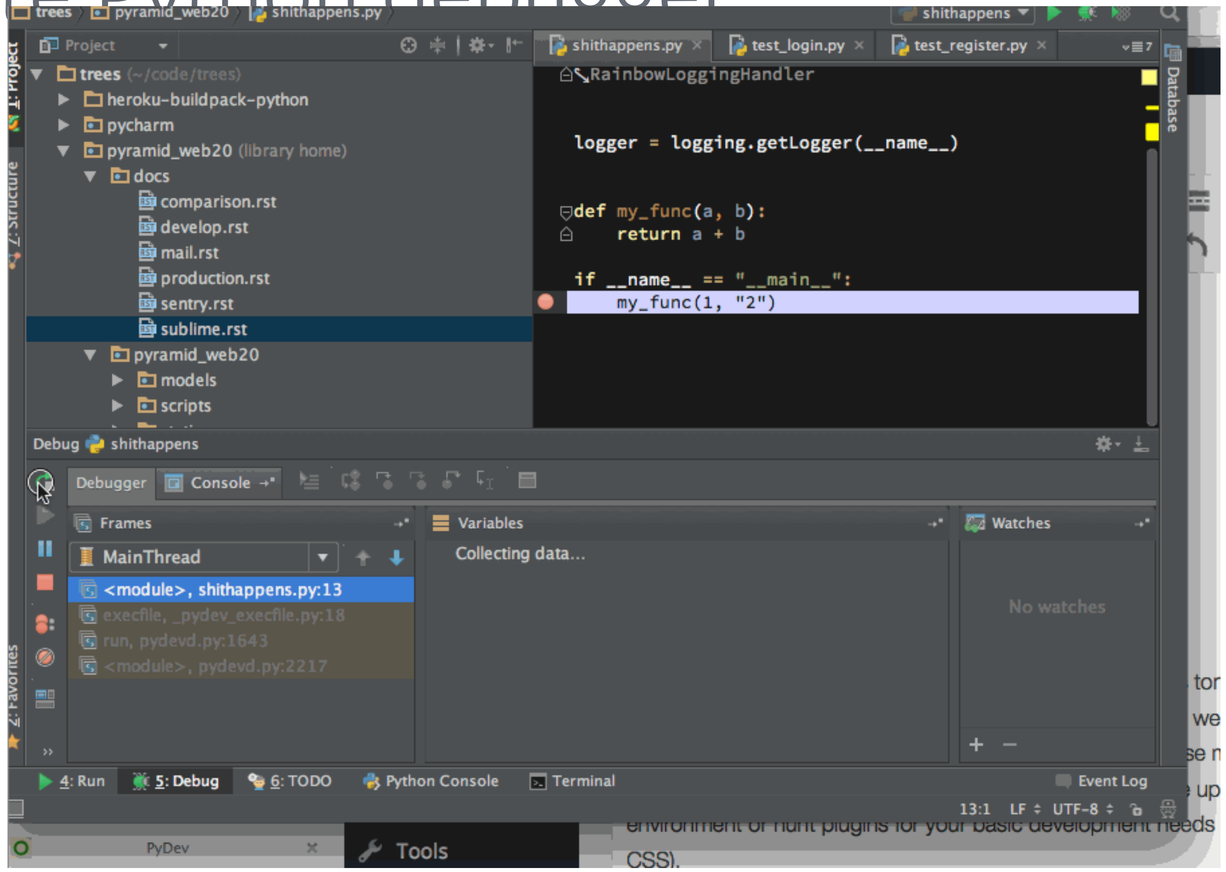


Ecosystem

- Use the entire Python ecosystem at your will
- Including SciPy, Scikit-Learn, etc.

Ecosyster

- Use the entire
- Including SciF

Brandon Amos @brandondamos · Jan 18

Why PyTorch's layer creation is powerful: Here's my layer that solves an optimization problem with a primal-dual interior point method.

```
def forward_single(input_i, Q, G, A, b, h, U_Q, U_S, R):
    nineq, nz = G.size()
    neq = A.size(0) if A.ndimension() > 0 else 0

    d = torch.ones(nineq).type_as(Q)
    nb = -b if b is not None else None
    factor_kkt(U_S, R, d, neq)
    x, s, z, y = solve_kkt(U_Q, d, G, A, U_S, input_i, torch.zeros(nineq).type_as(Q),
                           -h, nb, neq, nz)


    if torch.min(s) < 0:
        s -= torch.min(s) - 1
    if torch.min(z) < 0:
        z -= torch.min(z) - 1

    for i in range(20):
        rx = (torch.mv(A.t(),y) if neq > 0 else 0.) + \
             torch.mv(G.t(), z) + torch.mv(Q,x) + input_i
        rs = z
        ry = torch.mv(G,x) + s - h
        rz = torch.mv(A,x) - b if neq > 0 else torch.Tensor([0.])
        mu = torch.dot(s,z)/nineq
        pri_resid = torch.norm(ry) + torch.norm(rz)
        dual_resid = torch.norm(rx)
        d = z/s

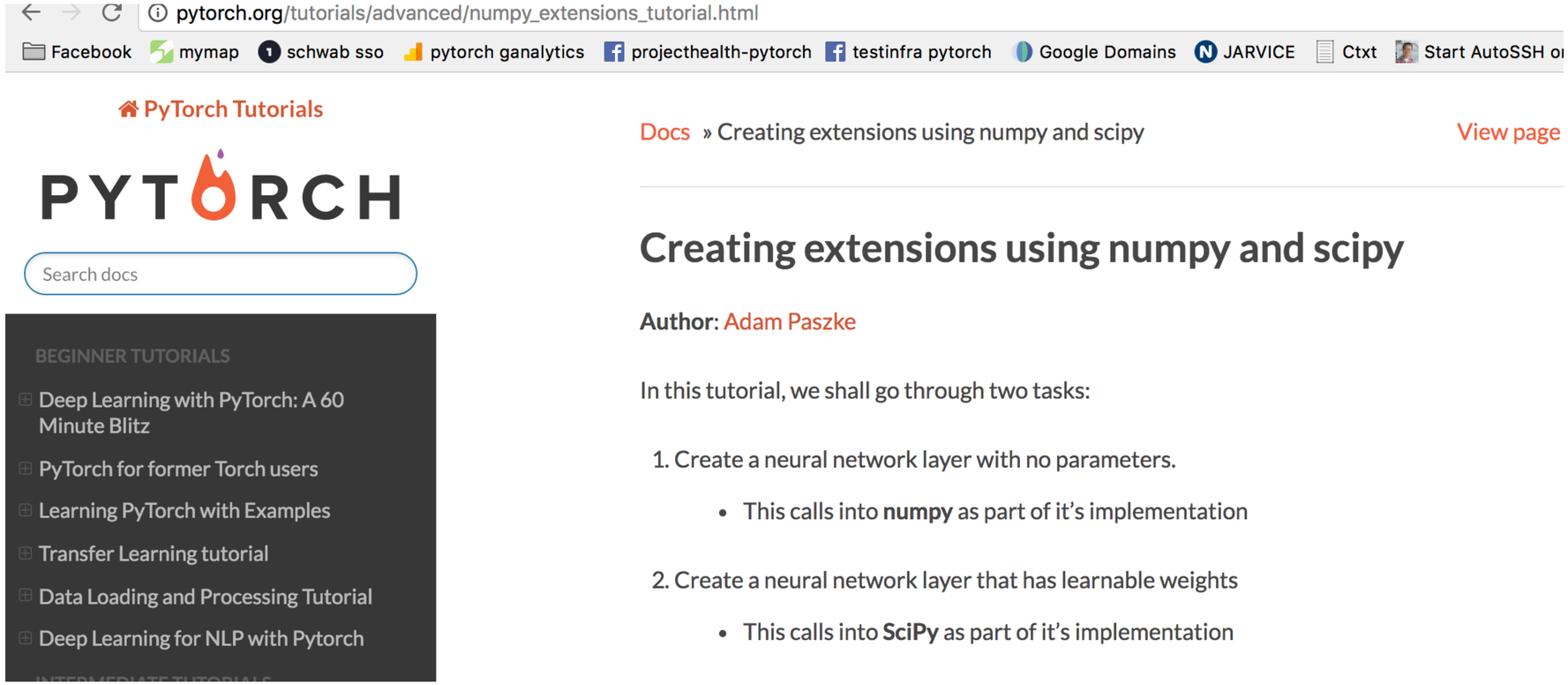
        factor_kkt(U_S, R, d, neq)
        dx_aff, ds_aff, dz_aff, dy_aff = solve_kkt(U_Q, d, G, A, U_S,
                                                   rx, rs, ry, rz, neq, nz)

        # compute centering directions
        alpha = min(min(get_step(z,dz_aff), get_step(s, ds_aff)), 1.0)
        sig = (torch.dot(s + alpha*ds_aff, z + alpha*dz_aff)/(torch.dot(s,z)))**3
        dx_cor, ds_cor, dz_cor, dy_cor = solve_kkt(
            U_Q, d, G, A, U_S, torch.zeros(nz).type_as(Q),
            (-mu*sig*torch.ones(nineq).type_as(Q) + ds_aff*dz_aff)/s,
            torch.zeros(nineq).type_as(Q), torch.zeros(neq).type_as(Q), neq, nz)

        dx = dx_aff + dx_cor
        ds = ds_aff + ds_cor
        dz = dz_aff + dz_cor
        dy = dy_aff + dy_cor if neq > 0 else None
```

Ecosystem

- Use the entire Python ecosystem at your will
- Including SciPy, Scikit-Learn, etc.



Ecosystem

- A shared model-zoo:

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

```
import torchvision.models as models
resnet18 = models.resnet18(pretrained=True)
alexnet = models.alexnet(pretrained=True)
```

Recent and Upcoming features

Distributed PyTorch

- MPI style distributed communication
- Broadcast Tensors to other nodes
- Reduce Tensors among nodes
  - for example: sum gradients among all nodes

Higher order derivatives

- grad(grad(grad(grad(grad(grad(grad(torch.norm(x))))))))

Higher order derivatives

- grad(grad(grad(grad(grad(grad(grad(torch.norm(x)))))))
- Useful to implement crazy ideas

Broadcasting and Advanced Indexing

- Numpy-style broadcasting
- Numpy-style indexing that covers advanced cases

JIT Compilation (upcoming)

- A full tracing JIT used to cache and compile subgraphs

A compiler for PyTorch

Add -> Mul

A simple use-case

```
d = (a + b) * c # , a, b, c, d are Tensors
```

```
for (i=0; i < data_length; i++) {
    out1[i] = a[i] + b[i];
}

for (i=0; i < data_length; i++) {
    d[i] = out1[i] * c[i];
}
```

Figure by Wikipedia: https://en.wikipedia.org/wiki/Matrix_multiplication

Add -> Mul

Fusion

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d = (a + b) * c # , a, b, c, d are Tensors
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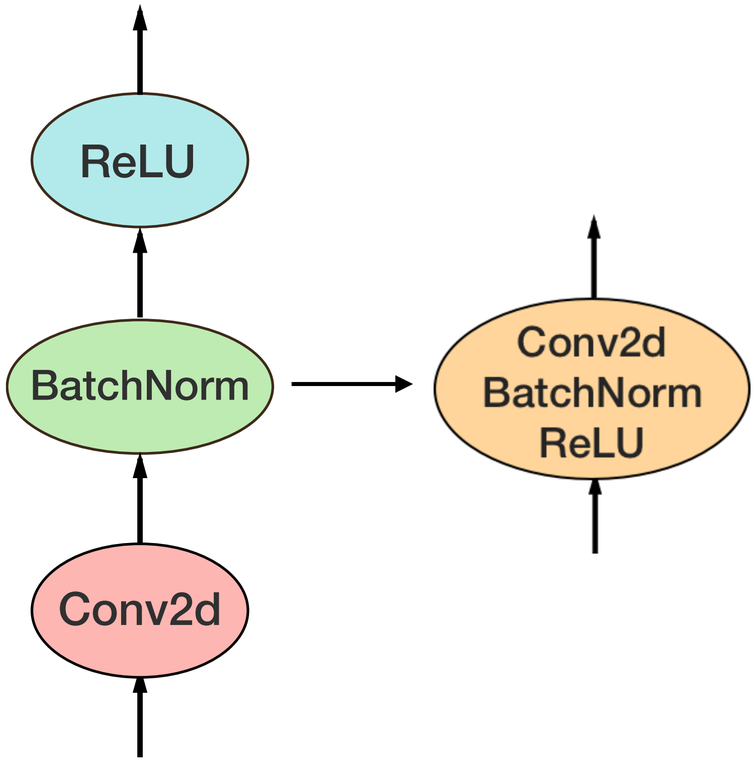
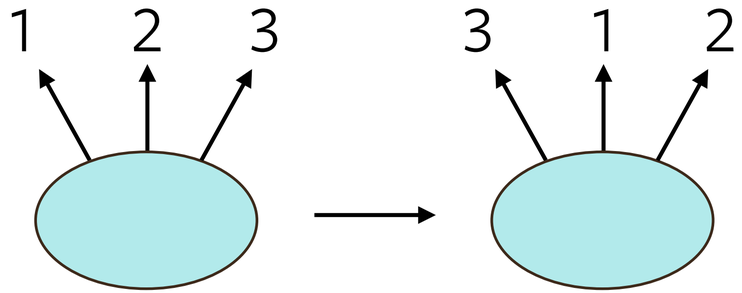
Compilation benefits

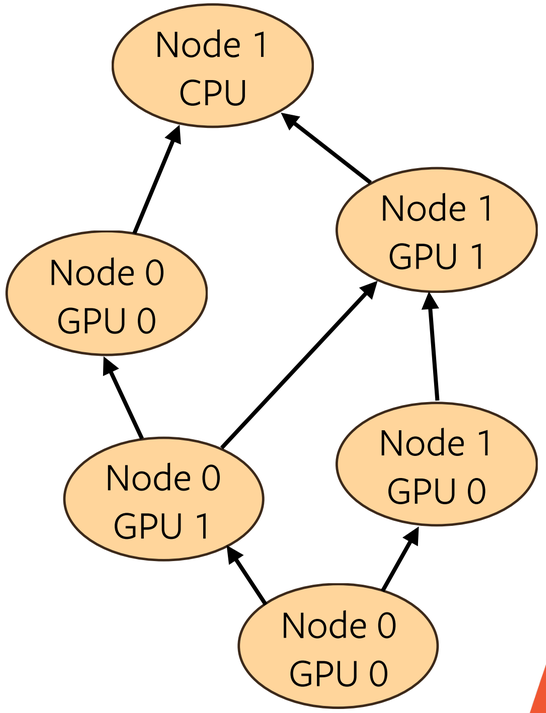
Kernel fusion



Out-of-order execution



Automatic work placement



Tracing JIT

```
def foo(x):
    y = x + 1
    z = y * 2
    return z

x = torch.Tensor([0, 1, 2, 3])

y  = foo(x)  # 2, 4, 6, 8
```

Tracing JIT

```
@torch.jit.trace
def foo(x):
    y = x + 1
    z = y * 2
    return z

x = torch.Tensor([0, 1, 2, 3])

y1  = foo(x)
y2  = foo(x)
```

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Trace

Add(x, 1) -> t1

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Trace

Add(x, 1) -> t1

Mul(t1, 2) -> retval

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Trace

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Add(x, 1) -> t1
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```

Tracing JIT

more details

- An IR with Tensors as first class types

Tracing JIT

more details

- An IR with Tensors as first class types
- optimized for reusable and cached traces
  - (unlike javascript tracers)

Tracing JIT

Gotcha: cannot handle control-flow yet

```
@torch.jit.trace
def foo(x):
    sum = x.sum().data[0]
    if sum < 5:
     return x + 1
    else:
     return x + 2

x = torch.Tensor([-1, 0, 1, 2])
x2 = torch.Tensor([1, 2, 3, 4])

y  = foo(x)  # 0, 1, 2, 3
y2 = foo(x2) # 2, 3, 4, 5
```

PYTORCH

With ❤ from

http://pytorch.org

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