

Hands-on Lab: Deep Learning with the Theano Python Library

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MILA

Institut de Montréal des algorithmes d'apprentissage

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Slides

- ▶ PDF of the slides: <https://goo.gl/z0tynd>
- ▶ github repo of this presentation
<https://github.com/nouiz/gtc2016/>

Introduction

Theano

- Compiling/Running

- Modifying expressions

- GPU

- Debugging

Models

- Logistic Regression

- Convolution

Exercices

High level

Python <- {NumPy/SciPy/libgpuarray} <- Theano <- {...}

- ▶ Python: OO coding language
- ▶ Numpy: n -dimensional array object and scientific computing toolbox
- ▶ SciPy: sparse matrix objects and more scientific computing functionality
- ▶ libgpuarray: GPU n -dimensional array object in C for CUDA and OpenCL
- ▶ Theano: compiler/symbolic graph manipulation

High level (2)

Many [machine learning] library build on top of Theano

- ▶ Keras
- ▶ blocks
- ▶ lasagne
- ▶ sklearn-theano: Easy deep learning by combining Theano and sklearn.
- ▶ PyMC 3
- ▶ theano-rnn
- ▶ Morb
- ▶ ...

Some models build with Theano

Some models that have been build with Theano.

- ▶ Neural Networks
- ▶ Convolutional Neural Networks
- ▶ RNN, RNN CTC, LSTM
- ▶ NADE, RNADE
- ▶ Autoencoders
- ▶ Alex Net's
- ▶ GoogleLeNet
- ▶ Overfeat
- ▶ Generative Adversarial Nets
- ▶ SVMs
- ▶ **many variations of above models and more**

Python

- ▶ General-purpose high-level OO interpreted language
- ▶ Emphasizes code readability
- ▶ Comprehensive standard library
- ▶ Dynamic type and memory management
- ▶ Easily extensible with C
- ▶ Slow execution
- ▶ Popular in *web development* and *scientific communities*

NumPy/SciPy

- ▶ NumPy provides an n -dimensional numeric array in Python
 - ▶ Perfect for high-performance computing
 - ▶ Slices of arrays are views (no copying)
- ▶ NumPy provides
 - ▶ Elementwise computations
 - ▶ Linear algebra, Fourier transforms
 - ▶ Pseudorandom number generators (many distributions)
- ▶ SciPy provides lots more, including
 - ▶ Sparse matrices
 - ▶ More linear algebra
 - ▶ Solvers and optimization algorithms
 - ▶ Matlab-compatible I/O
 - ▶ I/O and signal processing for images and audio

What's missing?

- ▶ Non-lazy evaluation (required by Python) hurts performance
- ▶ Bound to the CPU
- ▶ Lacks symbolic or automatic differentiation
- ▶ No automatic speed and stability optimization

Goal of the stack

Fast to develop
Fast to run



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Exercises

Description

High-level domain-specific language for numeric computation.

- ▶ Syntax as close to NumPy as possible
- ▶ Compiles most common expressions to C for CPU and/or GPU
- ▶ Limited expressivity means more opportunities for optimizations
 - ▶ Strongly typed -> compiles to C
 - ▶ Array oriented -> easy parallelism
 - ▶ Support for looping and branching in expressions
 - ▶ No subroutines -> global optimization
- ▶ Automatic speed and numerical stability optimizations

Description (2)

- ▶ Automatic differentiation and R op (Hessian Free Optimization)
- ▶ Sparse matrices (CPU only)
- ▶ Can reuse other technologies for best performance
 - ▶ BLAS, SciPy, CUDA, PyCUDA, Cython, Numba, PyCUDA, ...
- ▶ Extensive unit-testing and self-verification
- ▶ Extensible (You can create new operations as needed)
- ▶ Works on Linux, OS X and Windows

Project status?

- ▶ Mature: Theano has been developed and used since January 2008 (8 yrs old)
- ▶ Driven hundreds research papers
- ▶ Good user documentation
- ▶ Active mailing list with participants from outside our institute
- ▶ Core technology for Silicon-Valley start-ups
- ▶ Many contributors (some from outside our institute)
- ▶ Used to teach many university classes
- ▶ Has been used for research at big companies

Theano: deeplearning.net/software/theano/

Deep Learning Tutorials: deeplearning.net/tutorial/

Simple example

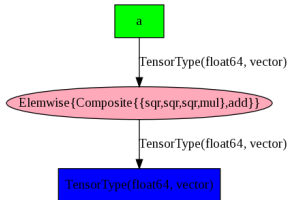
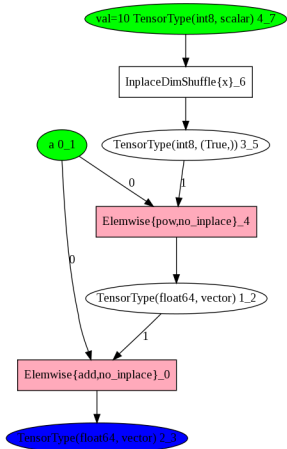
```
import theano
# declare symbolic variable
a = theano.tensor.vector("a")

# build symbolic expression
b = a + a ** 10

# compile function
f = theano.function([a], b)

# Execute with numerical value
print f([0, 1, 2])
# prints 'array([0, 2, 1026])'
```

Simple example



Overview of Library

Theano is many things

- ▶ Language
- ▶ Compiler
- ▶ Python library

Scalar math

Some example of scalar operations:

```
import theano
from theano import tensor as T
x = T.scalar()
y = T.scalar()
z = x + y
w = z * x
a = T.sqrt(w)
b = T.exp(a)
c = a ** b
d = T.log(c)
```

Vector math

```
from theano import tensor as T
x = T.vector()
y = T.vector()
# Scalar math applied elementwise
a = x * y
# Vector dot product
b = T.dot(x, y)
# Broadcasting (as NumPy, very powerful)
c = a + b
```

Matrix math

```
from theano import tensor as T
x = T.matrix()
y = T.matrix()
a = T.vector()
# Matrix-matrix product
b = T.dot(x, y)
# Matrix-vector product
c = T.dot(x, a)
```

Tensors

Using Theano:

- ▶ Dimensionality defined by length of “broadcastable” argument
- ▶ Can add (or do other elemwise op) two tensors with same dimensionality
- ▶ Duplicate tensors along broadcastable axes to make size match

```
from theano import tensor as T
tensor3 = T.TensorType(
    broadcastable=(False, False, False),
    dtype='float32')
x = T.tensor3()
```

Reductions

```
from theano import tensor as T
tensor3 = T.TensorType(
    broadcastable=(False, False, False),
    dtype='float32')
x = tensor3()

total = x.sum()
marginals = x.sum(axis=(0, 2))
mx = x.max(axis=1)
```

Dimshuffle

```
from theano import tensor as T
tensor3 = T.TensorType(
    broadcastable=(False, False, False))
x = tensor3()

y = x.dimshuffle((2, 1, 0))
a = T.matrix()

b = a.T
# Same as b
c = a.dimshuffle((0, 1))

# Adding to larger tensor
d = a.dimshuffle((0, 1, 'x'))
e = a + d
```

Indexing

As NumPy! This mean slices and index selection return view

return views, supported on GPU

`a_tensor[int]`

`a_tensor[int, int]`

`a_tensor[start:stop:step, start:stop:step]`

`a_tensor[::-1]` *# reverse the first dimension*

Advanced indexing, return copy

`a_tensor[an_index_vector]` *# Supported on GPU*

`a_tensor[an_index_vector, an_index_vector]`

`a_tensor[int, an_index_vector]`

`a_tensor[an_index_tensor, ...]`

Compiling and running expression

- ▶ `theano.function`
- ▶ shared variables and updates
- ▶ compilation modes

theano.function

```
>>> from theano import tensor as T
>>> x = T.scalar()
>>> y = T.scalar()
>>> from theano import function
>>> # first arg is list of SYMBOLIC inputs
>>> # second arg is SYMBOLIC output
>>> f = function([x, y], x + y)
>>> # Call it with NUMERICAL values
>>> # Get a NUMERICAL output
>>> f(1., 2.)
array(3.0)
```

Shared variables

- ▶ It's hard to do much with purely functional programming
- ▶ “shared variables” add just a little bit of imperative programming
- ▶ A “shared variable” is a buffer that stores a numerical value for a Theano variable
- ▶ Can write to as many shared variables as you want, once each, at the end of the function
- ▶ Can modify value outside of Theano function with `get_value()` and `set_value()` methods.

Shared variable example

```
>>> from theano import shared
>>> x = shared(0.)
>>> from theano.compat.python2x import OrderedDict
>>> updates = [(x, x + 1)]
>>> f = function([], updates=updates)
>>> f()
>>> x.get_value()
1.0
>>> x.set_value(100.)
>>> f()
>>> x.get_value()
101.0
```

Compilation modes

- ▶ Can compile in different modes to get different kinds of programs
- ▶ Can specify these modes very precisely with arguments to `theano.function`
- ▶ Can use a few quick presets with environment variable flags

Example preset compilation modes

- ▶ `FAST_RUN`: default. Fastest execution, slowest compilation
- ▶ `FAST_COMPILE`: Fastest compilation, slowest execution. No C code.
- ▶ `DEBUG_MODE`: Adds lots of checks. Raises error messages in situations other modes regard as fine.
- ▶ `optimizer=fast_compile`: as `mode=FAST_COMPILE`, but with C code.
- ▶ `theano.function(..., mode="FAST_COMPILE")`
- ▶ `THEANO_FLAGS=mode=FAST_COMPILE python script.py`

Modifying expressions

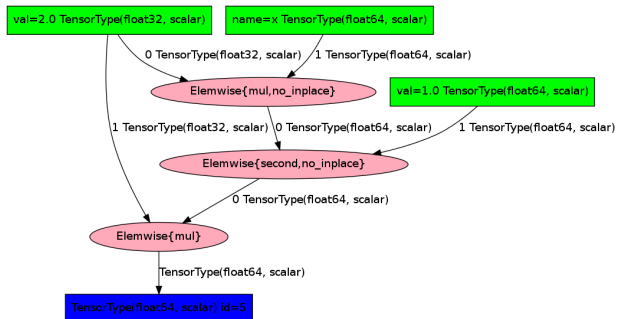
There are “macro” that automatically build bigger graph for you.

- ▶ theano.grad
- ▶ Others

Those functions can get called many times, for example to get the 2nd derivative.

The grad method

```
>>> x = T.scalar('x')
>>> y = 2. * x
>>> g = T.grad(y, x)
# Print the not optimized graph
>>> theano.printing.pydotprint(g)
```

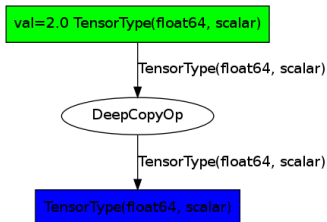


The grad method

```
>>> x = T.scalar('x')  
>>> y = 2. * x  
>>> g = T.grad(y, x)
```

Print the optimized graph

```
>>> f = theano.function([x], g)  
>>> theano.printing.pydotprint(f)
```



Others

- ▶ R_op, L_op for Hessian Free Optimization
- ▶ hessian
- ▶ jacobian
- ▶ clone the graph with replacement
- ▶ you can navigate the graph if you need (go from the result of computation to its input, recursively)

Enabling GPU

- ▶ Theano's current back-end only supports 32 bit on GPU
- ▶ libgpuarray (new-backend) supports all dtype
- ▶ CUDA supports 64 bit, but it is slow on gamer GPUs

GPU: Theano flags

Theano flags allow to configure Theano. Can be set via a configuration file or an environment variable.

To enable GPU:

- ▶ Set “device=gpu” (or a specific gpu, like “gpu0”)
- ▶ Set “floatX=float32”
- ▶ Optional: warn_float64={'ignore', 'warn', 'raise', 'pdb'}

floatX

Allow to change the dtype between float32 and float64.

- ▶ T.fscalar, T.fvector, T.fmatrix are all 32 bit
- ▶ T.dscalar, T.dvector, T.dmatrix are all 64 bit
- ▶ T.scalar, T.vector, T.matrix resolve to floatX
- ▶ floatX is float64 by default, set it to float32 for GPU

CuDNN

- ▶ R1 and R2 is supported.
- ▶ It is enabled automatically if available.
- ▶ Theano flag to get an error if can't be used:
"optimizer_including=cudnn"

Debugging

- ▶ `DEBUG_MODE`
- ▶ Error message
- ▶ `theano.printing.debugprint`

Error message: code

```
import numpy as np
import theano
import theano.tensor as T
x = T.vector()
y = T.vector()
z = x + x
z = z + y
f = theano.function([x, y], z)
f(np.ones((2,)), np.ones((3,)))
```


Error message: 1st part

```
Traceback (most recent call last):
```

```
[...]
```

```
ValueError: Input dimension mis-match.
```

```
    (input[0].shape[0] = 3, input[1].shape[0] = 2)
```

```
Apply node that caused the error:
```

```
    Elemwise{add,no_inplace}(<TensorType(float64, vector)>,
                             <TensorType(float64, vector)>,
                             <TensorType(float64, vector)>)
```

```
Inputs types: [TensorType(float64, vector),
               TensorType(float64, vector),
               TensorType(float64, vector)]
```

```
Inputs shapes: [(3,), (2,), (2,)]
```

```
Inputs strides: [(8,), (8,), (8,)]
```

```
Inputs scalar values: ['not_a_scalar', 'not_a_scalar', 'not_a_scalar']
```

Error message: 2st part

HINT: Re-running with most Theano optimization disabled could give you a back-traces when this node was created. This can be done with by setting the Theano flags “optimizer=fast_compile”. If that does not work, Theano optimizations can be disabled with “optimizer=None”.

HINT: Use the Theano flag “exception_verbosity=high” for a debugprint of this apply node.

Error message: Traceback

Traceback (most recent call last):

```
File "test.py", line 9, in <module>
```

```
    f(np.ones((2,)), np.ones((3,)))
```

```
File "/u/bastienf/repos/theano/compile/function_module.py",
```

```
    line 589, in __call__
```

```
        self.fn.thunks[self.fn.position_of_error])
```

```
File "/u/bastienf/repos/theano/compile/function_module.py",
```

```
    line 579, in __call__
```

```
    outputs = self.fn()
```

Error message: optimizer=fast_compile

Backtrace when the node is created:
File "test.py", line 7, in <module>
 z = z + y

debugprint

```
>>> from theano.printing import debugprint
>>> debugprint(a)
Elemwise{mul,no_inplace} [@A]  ' '
| TensorConstant{2.0} [@B]
| Elemwise{add,no_inplace} [@C]  ' z '
| <TensorType(float64, scalar)> [@D]
| <TensorType(float64, scalar)> [@E]
```

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Inputs

Load from disk and put in shared variable.

```
datasets = load_data(dataset)
train_set_x, train_set_y = datasets[0]
valid_set_x, valid_set_y = datasets[1]
```

allocate symbolic variables for the data
`index = T.lscalar()` *# index to a [mini]batch*

generate symbolic variables for input minibatch
`x = T.matrix('x')` *# data, 1 row per image*
`y = T.ivector('y')` *# labels*

Model

```
n_in = 28 * 28  
n_out = 10
```

```
# weights
```

```
W = theano.shared(  
    numpy.zeros((n_in, n_out),  
                dtype=theano.config.floatX))
```

```
# bias
```

```
b = theano.shared(  
    numpy.zeros((n_out, ),  
                dtype=theano.config.floatX))
```


Computation

the forward pass

```
p_y_given_x = T.nnet.softmax(T.dot(input, W) + b)
```

cost we minimize: the negative log likelihood

```
l = T.log(p_y_given_x)  
cost = -T.mean(l[T.arange(y.shape[0]), y])
```

the error

```
y_pred = T.argmax(p_y_given_x, axis=1)  
err = T.mean(T.neq(y_pred, y))
```

Gradient and Updates

compute the gradient of cost

```
g_W, g_b = T.grad(cost=cost, wrt=(W, b))
```

model parameters updates rules

```
updates = [(W, W - learning_rate * g_W),  
            (b, b - learning_rate * g_b)]
```

Training Function

```
# compile a Theano function that train the model
train_model = theano.function(
    inputs=[index], outputs=(cost, err),
    updates=updates,
    givens={
        x: train_set_x[index * batch_size:
                        (index + 1) * batch_size],
        y: train_set_y[index * batch_size:
                        (index + 1) * batch_size]
    }
)
```

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datasets = load_data(dataset)
train_set_x, train_set_y = datasets[0]
valid_set_x, valid_set_y = datasets[1]
```

allocate symbolic variables for the data
index = T.iscalar() *# index to a [mini]batch*

```
x = T.matrix('x') # the data, 1 row per image
y = T.ivector('y') # labels
```

Reshape matrix of rasterized images of shape (batch_size, 1, 28, 28)
to a 4D tensor, compatible for convolution
layer0_input = x.reshape((batch_size, 1, 28, 28))

Model

```
image_shape=(batch_size, 1, 28, 28),  
filter_shape=(nkerns[0], 1, 5, 5),
```

```
W_bound = ...  
W = theano.shared(  
    numpy.asarray(  
        rng.uniform(low=-W_bound, high=W_bound,  
                    size=filter_shape),  
        dtype=theano.config.floatX),  
)
```

the bias is a 1D tensor — one bias per output feature

```
b_values = numpy.zeros((filter_shape[0],), dtype=...  
b = theano.shared(b_values)
```

Computation

```
# convolve input feature maps with filters  
conv_out = conv.conv2d(input=x, filters=W)
```

```
# downsample each feature map individually, using max pooling  
pooled_out = downsample.max_pool_2d(  
    input=conv_out,  
    ds=(2, 2), // poolsize  
    ignore_border=True)
```

```
output = T.tanh(pooled_out +  
                 b.dimshuffle('x', 0, 'x', 'x'))
```

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Exercices

ipython notebook

- ▶ Introduction
- ▶ Exercices (Theano only exercices)
- ▶ lenet (small CNN model to quickly try it)

Connection instructions

- ▶ Navigate to `nvlabs.qwiklab.com`
- ▶ Login or create a new account
- ▶ Select the “Instructor-Led Hands-on Labs” class
- ▶ Find the lab called “Theano” and click Start
- ▶ After a short wait, lab instance connection information will be shown
- ▶ Please ask Lab Assistants for help!

Questions, Acknowledgments

Questions? Acknowledgments

- ▶ All people working or having worked at the LISA lab/MILA institute
- ▶ All Theano users/contributors
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