

Theano

Frédéric Bastien

Département d'Informatique et de Recherche Opérationnelle

Université de Montréal

Montréal, Canada

`bastienf@iro.umontreal.ca`

Presentation prepared with Pierre Luc Carrier and Arnaud Bergeron

MILA

Institut de Montréal des algorithmes d'apprentissage

GTC 2015

Université 
de Montréal

Slides

- ▶ PDF of the slides: <http://goo.gl/bcBeBV>
- ▶ github repo of this presentation
<https://github.com/nouiz/gtc2015/>

Introduction

Theano

Compiling/Running

Modifying expressions

GPU

Debugging

Scan

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

- ▶ Pylearn2
- ▶ blocks
- ▶ PyMC 3
- ▶ lasagne
- ▶ sklearn-theano: Easy deep learning by combining Theano and sklearn.
- ▶ 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
- ▶ Auto-encoder
- ▶ Alex Net's
- ▶ GoogleLeNet
- ▶ Overfeat
- ▶ Generative Adversarial Nets
- ▶ SVM
- ▶ **many variations of above models**

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



Introduction

Theano

- Compiling/Running
- Modifying expressions
- GPU
- Debugging
- Scan

Exercices

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
- ▶ 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 operation as needed)
- ▶ Works on Linux, OS X and Windows

Project status?

- ▶ Mature: Theano has been developed and used since January 2008 (7 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

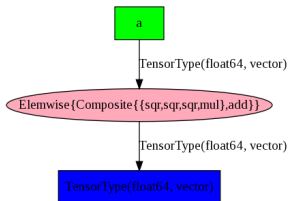
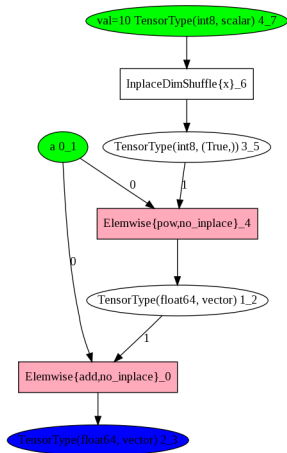
```
import theano
# declare symbolic variable
a = theano.tensor.vector("a")

# 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 Language

Mostly all of NumPy and more!

- ▶ Operations on scalar, vector, matrix, tensor, and sparse variables
- ▶ Linear algebra
- ▶ Element-wise nonlinearities
- ▶ Convolution
- ▶ Indexing, slicing and advanced indexing.
- ▶ Reduction
- ▶ Dimshuffle (n-dim transpose)

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) on 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 all slices, 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
- ▶ Modify outside 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 = 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
```

Which dict?

- ▶ Use `theano.compat.python2x.OrderedDict`
- ▶ Not `collections.OrderedDict`
 - ▶ This isn't available in older versions of python
- ▶ Not `{}` aka dict
 - ▶ The iteration order of this built-in class is not deterministic (thanks, Python!) so if Theano accepted this, the same script could compile different C programs each time you run it

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

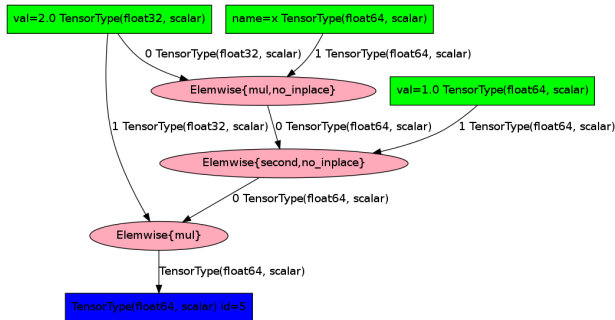
- ▶ `FAST_RUN`: default. Fastest execution, slowest compilation
- ▶ `FAST_COMPILE`: Fastest compilation, slowest execution. No C code.
- ▶ `DEBUG_MODE`: Adds lots of checks. Raises error messages in situations other modes regard as fine.
- ▶ `optimizer=fast_compile`: as `mode=FAST_COMPILE`, but with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

Modifying expressions

- ▶ The grad method
- ▶ Others

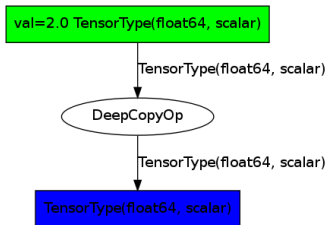
The grad method

```
>>> 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)  
>>> f = theano.function([x], g)  
# Print the optimized graph  
>>> theano.printing.pydotprint(f)
```



Others

- ▶ R_op, L_op for hessian free
- ▶ hessian
- ▶ jacobian
- ▶ you can navigate the graph if you need (go from the result of computation to its input, recursively)

Enabling GPU

- ▶ Theano current back-end only supports 32 bit on GPU
- ▶ libgpuarray (new-backend) support all dtype
- ▶ CUDA supports 64 bit, but 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 mismatch.
      (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 scalar', 'not scalar', 'not 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`

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

Error message: optimizer=fast_compile

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

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()
```

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]
```

Scan

- ▶ Allows looping (for, map, while)
- ▶ Allows recursion (reduce)
- ▶ Allows recursion with dependency on many of the previous time steps
- ▶ Optimize some cases like moving computation outside of scan
- ▶ The Scan grad is done via Backpropagation Through Time(BPTT)

When not to use scan

- ▶ If you only need it for “vectorization” or “broadcasting”. tensor and numpy.ndarray support them natively. This will be much better for that use case.
- ▶ If you do a fixed number of iteration that is very small (2,3). You are probably better to just unroll the graph to do it.

Scan Example1: Computing $\tanh(v \cdot \text{dot}(W) + b) * d$ where b is binomial 1

```
import theano
import theano.tensor as T
import numpy as np

# define tensor variables
W = T.matrix("W")
X = T.matrix("X")
b_sym = T.vector("b_sym")

# define shared random stream
trng = T.shared_randomstreams.RandomStreams(1234)
d=trng.binomial(size=W[1].shape)
```

Scan Example1: Computing $\tanh(v \cdot W + b) * d$ where d is binomial (2)

```
results, updates = theano.scan(  
    lambda v: T.tanh(T.dot(v, W) + b_sym) * d,  
    sequences=X)  
f = theano.function(inputs=[X, W, b_sym],  
                    outputs=[results],  
                    updates=updates)  
x = np.eye(10, 2, dtype=theano.config.floatX)  
w = np.ones((2, 2), dtype=theano.config.floatX)  
b = np.ones((2), dtype=theano.config.floatX)  
  
print f(x, w, b)
```

Scan Example2: Computing $\text{pow}(A, k)$

```
import theano
import theano.tensor as T
theano.config.warn.subtensor_merge_bug = False

k = T.iscalar("k")
A = T.vector("A")

def inner_fct(prior_result, B):
    return prior_result * B
```

Scan Example2: Computing $\text{pow}(A, k)$ (2)

```
result, updates = theano.scan(  
    fn=inner_fct,  
    outputs_info=T.ones_like(A),  
    non_sequences=A, n_steps=k)
```

```
# Scan provide us with A ** 1 through A ** k.  
# Keep only the last value. Scan optimize memory.  
final = result[-1]
```

```
power = theano.function(inputs=[A, k], outputs=final,  
                        updates=updates)
```

```
print power(range(10), 2)
```

```
#[ 0.  1.  4.  9. 16. 25. 36. 49. 64.  
81.]
```

Scan signature

```
result, updates = theano.scan(  
    fn=inner_fct,  
    sequences=[],  
    outputs_info=[T.ones_like(A)],  
    non_sequences=A,  
    n_steps=k)
```

- ▶ Updates are needed if there are random numbers generated in the inner function
 - ▶ Pass them to the call `theano.function(..., updates=updates)`
- ▶ The inner function of scan takes arguments like this: scan: sequences, outputs_info, non sequences

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!

Acknowledgments

- ▶ All people working or having worked at the LISA lab/MILA institute
- ▶ All Theano users/contributors
- ▶ Compute Canada, RQCHP, NSERC, and Canada Research Chairs for providing funds or access to compute resources.

Questions?