

# Theano

Frédéric Bastien

Département d'Informatique et de Recherche Opérationnelle

Université de Montréal

Montréal, Canada

`bastienf@iro.umontreal.ca`

TODO: Presentation prepared with Pierre Luc Carrier and Arnaud  
Bergeron TODO: lab.zip

**MILA**

Institut de Montréal des algorithmes d'apprentissage

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## Slides

PDF of the slides: <http://goo.gl/bcBeBV>

## Introduction

### Theano

- Compiling/Running

- Modifying expressions

- GPU

- Debugging

- Scan

### Exercices

## High level

Python <- {NumPy/SciPy/libgpuarray} <- Theano <- Pylearn2

- ▶ 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
- ▶ Pylearn2: machine learning framework for researchers

# Python

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

## NumPy/SciPy

- ▶ Python floats are full-fledged objects on the heap
  - ▶ Not suitable for high-performance computing!
- ▶ 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

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- 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
  - ▶ No subroutines -> global optimization
  - ▶ Strongly typed -> compiles to C
  - ▶ Array oriented -> easy parallelism
  - ▶ Support for looping and branching in expressions
- ▶ Automatic speed and stability optimizations
- ▶ Can reuse other technologies for best performance.
  - ▶ BLAS, SciPy, Cython, Numba, PyCUDA, CUDA, ...
- ▶ Automatic differentiation and R op
- ▶ Sparse matrices (CPU only)
- ▶ Extensive unit-testing and self-verification
- ▶ 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 lab
- ▶ Core technology for a few Silicon-Valley start-ups
- ▶ Many contributors (some from outside our lab)
- ▶ Used to teach many university classes
- ▶ Has been used for research at big companies

Theano: [deeplearning.net/software/theano/](http://deeplearning.net/software/theano/)

Deep Learning Tutorials: [deeplearning.net/tutorial/](http://deeplearning.net/tutorial/)

## Simple example

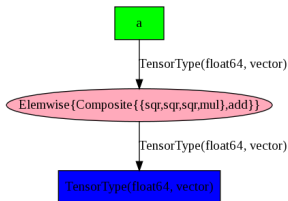
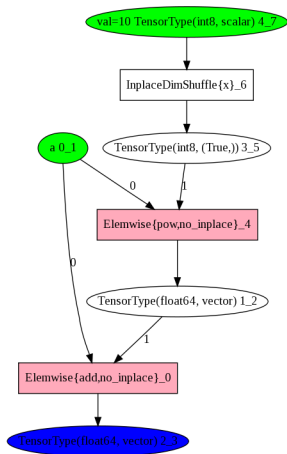
```
import theano
# declare symbolic variable
a = theano.tensor.vector("a")

# 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

- ▶ 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)
- ▶ Extensible

## 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
- ▶ TODO: optimizations

## 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

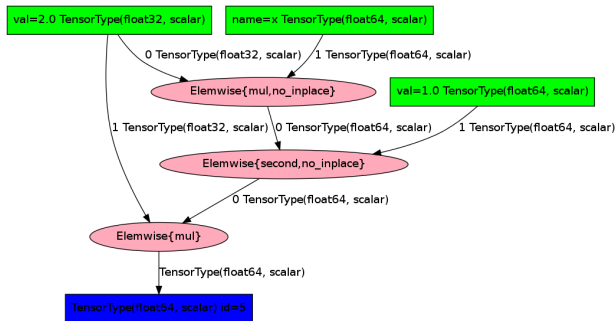
- ▶ `FAST_RUN`: default. Fastest execution, slowest compilation
- ▶ `FAST_COMPILE`: Fastest compilation, slowest execution. No C code.
- ▶ `DEBUG_MODE`: Adds lots of checks. Raises error messages in situations other modes regard as fine.
- ▶ `optimizer=fast_compile`: as `mode=FAST_COMPILE`, but with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



## 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
- ▶ `T.fscalar`, `T.fvector`, `T.fmatrix` are all 32 bit
- ▶ `T.scalar`, `T.vector`, `T.matrix` resolve to 32 bit or 64 bit depending on theano's `floatX` flag
- ▶ `floatX` is `float64` by default, set it to `float32`
- ▶ Set device flag to `gpu` (or a specific `gpu`, like `gpu0`)
- ▶ Flag: `warn_float64='ignore', 'warn', 'raise', 'pdb'`



## CuDNN

- ▶ R1 and R2 is supported.
- ▶ It is enabled automatically if available.
- ▶ Theano flag to get 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: exception\_\_verbosity=high

Debugprint of the apply node:

```
Elemwise{add,no_inplace} [@A] <TensorType(float64, vector)> ''  
|<TensorType(float64, vector)> [@B] <TensorType(float64, vector)>  
|<TensorType(float64, vector)> [@C] <TensorType(float64, vector)>  
|<TensorType(float64, vector)> [@C] <TensorType(float64, vector)>
```

## 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



## 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!

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# Questions?