

Introduction to Theano

A Fast Python Library for Modelling and Training

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August 4th, Deep Learning Summer School 2015, Montréal



Overview

Programming Tutorials

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Basic Usage

Graph definition and Syntax

Strong typing

Differences from Python/NumPy

Graph Transformations

Substitution and Cloning

Gradient

Shared variables

Make it fast!

Optimizations

Code Generation

GPU

Advanced Topics

Looping: the scan operation

Extending Theano

Recent Features

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Objectives

These tutorials should be the occasion for you to:

- ▶ Learn about software tools to implement deep learning algorithms
- ▶ Get some hand-on experience with these tools
- ▶ Play with simple implementation of existing algorithms
- ▶ Ask questions and get help from developers and researchers

<http://github.com/mila-udem/summerschool12015/>

Tutorials Schedule



Tuesday, August 4th (day 2)

- ▶ Introduction to Theano, Theano examples (Pascal Lamblin)

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NVIDIA®



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Wednesday, August 12th (day 10)

- ▶ Overflow session

Theano vision

Mathematical symbolic expression compiler

- ▶ Easy to define expressions
 - ▶ Expressions mimic NumPy's syntax and semantics
- ▶ Possible to manipulate those expressions
 - ▶ Substitutions
 - ▶ Gradient, R operator
 - ▶ Stability optimizations
- ▶ Fast to compute values for those expressions
 - ▶ Speed optimizations
 - ▶ Use fast back-ends (CUDA, BLAS, custom C code)
- ▶ Tools to inspect and check for correctness

Current status

- ▶ Mature: Theano has been developed and used since January 2008 (7 yrs old)
- ▶ Driven hundreds of research papers
- ▶ Good user documentation
- ▶ Active mailing list with participants worldwide
- ▶ Core technology for Silicon Valley start-ups
- ▶ Many contributors from different places
- ▶ Used to teach university classes
- ▶ Has been used for research at large companies

Theano: deeplearning.net/software/theano/

Deep Learning Tutorials: deeplearning.net/tutorial/

Related projects

Many libraries are built on top of Theano (mostly machine learning)

- ▶ Blocks
- ▶ Keras
- ▶ Lasagne
- ▶ Morb
- ▶ Pylearn2
- ▶ PyMC 3
- ▶ sklearn-theano
- ▶ theano-rnn
- ▶ ...

Basic usage

Theano defines a **language**, a **compiler**, and a **library**.

- ▶ Define a symbolic expression
- ▶ Compile a function that can compute values
- ▶ Execute that function on numeric values

Defining an expression

- Symbolic, strongly-typed inputs

```
import theano
from theano import tensor as T
x = T.vector('x')
W = T.matrix('W')
b = T.vector('b')
```

- NumPy-like syntax to build expressions

```
dot = T.dot(x, W)
out = T.nnet.sigmoid(dot + b)
```

Graph visualization (1)

```
debugprint(dot)
dot [@A] ''
  |x [@B]
  |W [@C]
```

```
debugprint(out)
sigmoid [@A] ''
  |Elemwise{add,no_inplace} [@B] ''
    |dot [@C] ''
      | |x [@D]
      | |W [@E]
      |b [@F]
```

Compiling a Theano function

Build a callable that compute outputs given inputs

```
f = theano.function(inputs=[x, W], outputs=dot)
g = theano.function([x, W, b], out)
h = theano.function([x, W, b], [dot, out])
i = theano.function([x, W, b], [dot + b, out])
```


Graph visualization (2)

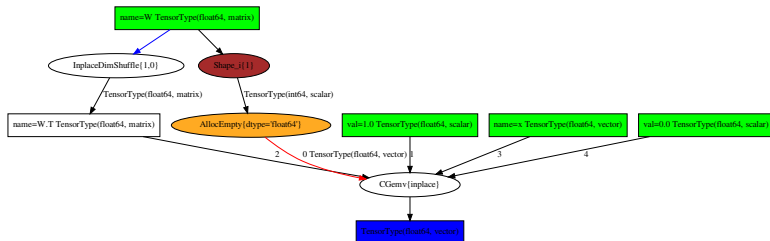
```
theano.printing.debugprint(f)
CGemv{inplace} [@A] '' 3
| Alloc [@B] '' 2
| | TensorConstant{0.0} [@C]
| | Shape_i{1} [@D] '' 1
| | | W [@E]
| TensorConstant{1.0} [@F]
| InplaceDimShuffle{1,0} [@G] 'W.T' 0
| | W [@E]
| x [@H]
| TensorConstant{0.0} [@C]

theano.printing.pydotprint(f)
```

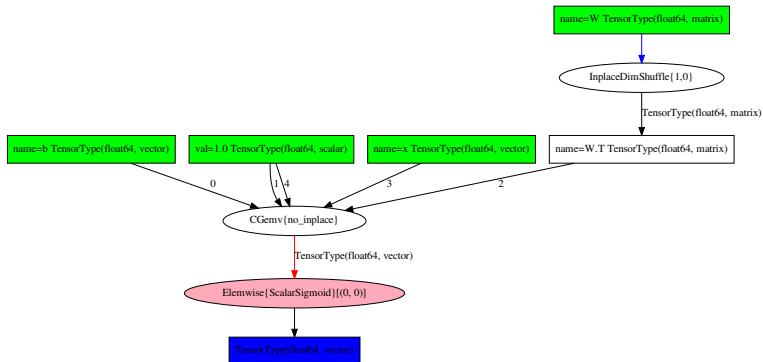
```
theano.printing.debugprint(g)
Elemwise{ScalarSigmoid}[(0, 0)] [@A] '' 2
| CGemv{no_inplace} [@B] '' 1
| | b [@C]
| | TensorConstant{1.0} [@D]
| | InplaceDimShuffle{1,0} [@E] 'W.T' 0
| | | W [@F]
| | x [@G]
| | TensorConstant{1.0} [@D]

theano.printing.pydotprint(g)
```

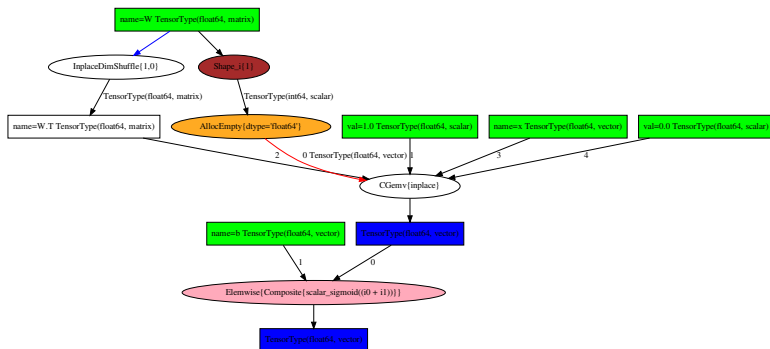
pydotprint(f)



pydotprint(g)



pydotprint(h)



Executing a Theano function

Call it with numeric values

```
import numpy as np
np.random.seed(42)
W_val = np.random.randn(4, 3)
x_val = np.random.rand(4)
b_val = np.ones(3)

f(x_val, W_val)
# -> array([ 1.79048354,  0.03158954, -0.26423186])

g(x_val, W_val, b_val)
# -> array([ 0.9421594 ,  0.73722395,  0.67606977])

h(x_val, W_val, b_val)
# -> [array([ 1.79048354,  0.03158954, -0.26423186]),
#      array([ 0.9421594 ,  0.73722395,  0.67606977])]

i(x_val, W_val, b_val)
# -> [array([ 2.79048354,  1.03158954,  0.73576814]),
#      array([ 0.9421594 ,  0.73722395,  0.67606977])]
```

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Graph structure

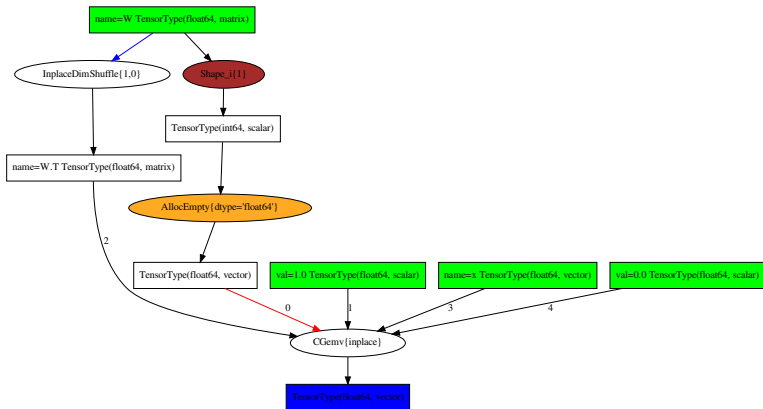
The graph that represents mathematical operations is **bipartite**, and has two sorts of nodes:

- ▶ Variable nodes, that represent *data*
- ▶ Apply nodes, that represent the application of *mathematical operations*

In practice:

- ▶ Variables are used for the graph inputs and outputs, and intermediate values
- ▶ Variables will hold data during the function execution phase
- ▶ An Apply node has inputs and outputs, which are Variables
- ▶ An Apply node represents the specific application of an Op on these input Variables
- ▶ The same Variable can be used as inputs by several Apply nodes

pydotprint(f, compact=False)



Strong typing

- ▶ All Theano variables have a type
- ▶ Different categories of types. Most used:
 - ▶ TensorType for NumPy ndarrays
 - ▶ CudaNdarrayType for CUDA arrays
 - ▶ Sparse for scipy.sparse matrices
- ▶ ndim, dtype, broadcastable pattern are part of the type
- ▶ shape and memory layout (strides) are **not**

Broadcasting tensors

- ▶ Implicit replication of arrays along broadcastable dimensions
- ▶ Broadcastable dimensions will **always** have length 1
- ▶ Such dimensions can be added to the left

```
r = T.row('r')
print(r.broadcastable)  # (True, False)
c = T.col('c')
print(c.broadcastable)  # (False, True)

f = theano.function([r, c], r + c)
print(f([[1, 2, 3]], [[.1], [.2]]))
```

No side effects

Create new variables, cannot *change* them

- ▶ `a += 1` works, returns new variable and re-assign
- ▶ `a[:] += 1`, or `a[:] = 0` do **not** work (the `__setitem__` method cannot return a new object)
- ▶ `a = T.inc_subtensor(a[:], 1)` or `a = T.set_subtensor(a[:], 0)`
- ▶ This will create a new variable, and re-assign `a` to it
- ▶ Theano will figure out later if it can use an in-place version

Exceptions:

- ▶ The `Print()` Op
- ▶ The `Assert()` Op
- ▶ You have to re-assign (or use the returned value)
- ▶ These can disrupt some optimizations

Python keywords

We cannot redefine Python's keywords: they affect the flow when building the graph, not when executing it.

- ▶ `if var:` will always evaluate to `True`. Use `theano.ifelse.ifelse(var, expr1, expr2)`
- ▶ `for i in var:` will not work if `var` is symbolic. If `var` is numeric: loop unrolling. You can use `theano.scan`.
- ▶ `len(var)` cannot return a symbolic shape, you can use `var.shape[0]`
- ▶ `print` will print an identifier for the symbolic variable, there is a `Print()` operation

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The givens keyword

Substitution at the last moment, when compiling a function

```
x_ = T.vector('x_')  
x_n = (x_ - x_.mean()) / x_.std()  
f_n = theano.function([x_, W], dot, givens={x: x_n})  
f_n(x_val, W_val)  
# -> array([ 1.90651511,  0.60431744, -0.64253361])
```

Cloning with replacement

Useful when building the expression graph

```
dot_n, out_n = theano.clone(  
    [dot, out],  
    replace={x: (x - x.mean()) / x.std()})  
f_n = theano.function([x, W], dot_n)  
f_n(x_val, W_val)  
# -> array([ 1.90651511,  0.60431744, -0.64253361])
```

The back-propagation algorithm

Application of the chain-rule for functions from \mathbb{R}^N to \mathbb{R} .

- ▶ $C : \mathbb{R}^N \rightarrow \mathbb{R}$
- ▶ $f : \mathbb{R}^M \rightarrow \mathbb{R}$
- ▶ $g : \mathbb{R}^N \rightarrow \mathbb{R}^M$
- ▶ $C(x) = f(g(x))$
- ▶ $\frac{\partial C}{\partial x} \Big|_x = \frac{\partial f}{\partial g} \Big|_{g(x)} \cdot \frac{\partial g}{\partial x} \Big|_x$

The whole $M \times N$ Jacobian matrix $\frac{\partial g}{\partial x} \Big|_x$ is not needed.

We only need $\nabla g_x : \mathbb{R}^M \rightarrow \mathbb{R}^N, v \mapsto v \cdot \frac{\partial g}{\partial x} \Big|_x$

Using theano.grad

```
y = T.vector('y')  
C = ((out - y) ** 2).sum()  
dC_dW = theano.grad(C, W)  
dC_db = theano.grad(C, b)  
# or dC_dW, dC_db = theano.grad(C, [W, b])
```

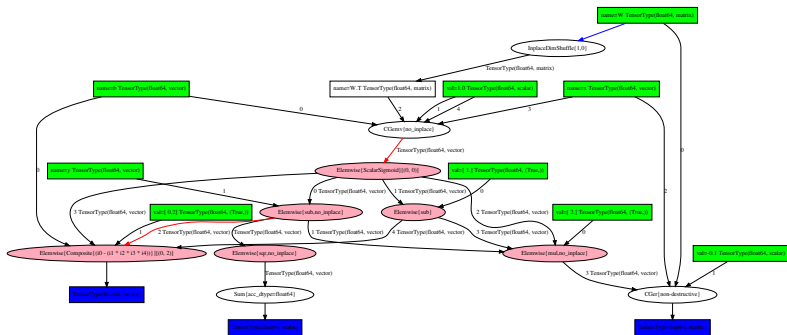
- ▶ `dC_dW` and `dC_db` are symbolic expressions, like `W` and `b`
- ▶ There are no numerical values at this point

Using the gradients

- ▶ The symbolic gradients can be used to build a Theano function

```
cost_and_grads = theano.function([x, W, b, y], [C, dC_dW, dC_db])
y_val = np.random.uniform(size=3)
print(cost_and_grads(x_val, W_val, b_val, y_val))
```
- ▶ They can also be used to build new expressions

```
upd_W = W - 0.1 * dC_dW
upd_b = b - 0.1 * dC_db
cost_and_upd = theano.function([x, W, b, y], [C, upd_W, upd_b])
print cost_and_upd(x_val, W_val, b_val, y_val)
```



Update values

Simple ways to update values

```
C_val, dC_dW_val, dC_db_val = cost_and_grads(x_val, W_val, b_val, y_val)
W_val -= 0.1 * dC_dW_val
b_val -= 0.1 * dC_db_val
```

```
C_val, W_val, b_val = cost_and_upd(x_val, W_val, b_val, y_val)
```

- ▶ Cumbersome
- ▶ Inefficient: memory, GPU transfers

Shared variables

- ▶ Symbolic variables, with a **value** associated to them
- ▶ The value is **persistent** across function calls
- ▶ The value is **shared** among all functions
- ▶ The variable has to be an **input variable**
- ▶ The variable is an **implicit input** to all functions using it

Using shared variables

```
x = T.vector('x')
y = T.vector('y')
W = theano.shared(W_val)
b = theano.shared(b_val)
dot = T.dot(x, W)
out = T.nnet.sigmoid(dot + b)
f = theano.function([x], dot)  # W is an implicit input
g = theano.function([x], out)  # W and b are implicit inputs
print(f(x_val))
# [ 1.79048354  0.03158954 -0.26423186]
print(g(x_val))
# [ 0.9421594  0.73722395  0.67606977]
```

- Use `W.get_value()` and `W.set_value()` to access the value later

Updating shared variables

```
C = ((out - y) ** 2).sum()
dC_dW, dC_db = theano.grad(C, [W, b])
upd_W = W - 0.1 * dC_dW
upd_b = b - 0.1 * dC_db
```

```
cost_and_perform_updates = theano.function(
    inputs=[x, y],
    outputs=C,
    updates=[(W, upd_W),
              (b, upd_b)])
```

- ▶ Variables W and b are **implicit inputs**
- ▶ Expressions upd_W and upd_b are **implicit outputs**
- ▶ All outputs, including the update expressions, are computed **before** the updates are performed



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Graph optimizations

An optimization replaces a part of the graph with different nodes

- ▶ The types of the replaced nodes have to match

Different goals for optimizations:

- ▶ Merge equivalent computations
- ▶ Simplify expressions: x/x becomes 1
- ▶ Numerical stability: Gives the right answer for “ $\log(1 + x)$ ” even if x is really tiny.
- ▶ Insert in-place and destructive versions of operations
- ▶ Use specialized, high-performance versions (Elemwise loop fusion, GEMV, GEMM)
- ▶ Shape inference
- ▶ Constant folding
- ▶ Transfer to GPU

Enabling/disabling optimizations

Trade-off between compilation speed, execution speed, error detection.

Different modes govern how much optimizations are applied

- ▶ 'FAST_RUN': default, make the runtime as fast as possible, launching overhead. Includes moving computation to GPU if a GPU was selected
- ▶ 'FAST_COMPILE': minimize launching overhead, around NumPy speed
- ▶ 'DEBUG_MODE': checks and double-checks everything, extremely slow
- ▶ Enable and disable particular optimizations or sets of optimizations
- ▶ Can be done globally, or for each function

C code for Ops

- ▶ Each operator can define C code computing the outputs given the inputs
- ▶ Otherwise, fall back to a Python implementation

How does this work?

- ▶ In Python, build a string representing the C code for a Python module
 - ▶ Stitching together code to extract data from Python structure,
 - ▶ Takes into account input and output types (ndim, dtype, ...)
 - ▶ String substitution for names of variables
- ▶ That module is compiled by g++
- ▶ The compiled module gets imported in Python
- ▶ Versioned cache of generated and compiled C code

For GPU code, same process, using CUDA and nvcc instead.

The C virtual machine (CVM)

A runtime environment, or VM, that calls the functions performing computation of different parts of the function (from inputs to outputs)

- ▶ Avoids context switching between C and Python
- ▶ Data structure containing
 - ▶ Addresses of inputs and outputs of all nodes (intermediate values)
 - ▶ Ordering constraints
 - ▶ Pointer to functions performing the computations
 - ▶ Information on what has been computed, and needs to be computed
- ▶ Set in advance from Python when compiling a function
- ▶ At runtime, if all operations have C code, calling the pointers will be fast
- ▶ Also enables lazy evaluation (for if/else for instance)

Using the GPU

We want to make the use of GPUs as transparent as possible, but

- ▶ Currently limited to float32 dtype
- ▶ Not easy to interact in Python with CudaNdarrays

Select GPU by setting the device flag to 'gpu' or 'gpu{0,1,2,...}'.

- ▶ All float32 **shared** variables will be created in GPU memory
- ▶ Enables optimizations moving supported operations to GPU

You want to make sure to use float32

- ▶ 'floatX' is the default type of all tensors and sparse matrices.
- ▶ By default, aliased to 'float64' for double precision on CPU
- ▶ Can be set to 'float32' by a configuration flag
- ▶ You can always explicitly use `T.fmatrix()` or `T.matrix(dtype='float32')`

Configuration flags

Configuration flags can be set in a couple of ways:

- ▶ `THEANO_FLAGS=device=gpu0,floatX=float32` in the shell

- ▶ In Python:

```
theano.config.device = 'gpu0'  
theano.config.floatX = 'float32'
```

- ▶ In the `.theanorc` configuration file:

```
[global]  
device = gpu0  
floatX = float32
```

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Symbolic looping

- ▶ Can perform map, reduce, reduce and accumulate, ...
- ▶ Can access outputs at previous time-step, or further back
- ▶ Symbolic number of steps
- ▶ Symbolic stopping condition (behaves as `do ... while`)
- ▶ Actually embeds a small Theano function
- ▶ Gradient through scan implements backprop through time
- ▶ Can be transferred to GPU

For more, come and see Philémon's presentation next Tuesday (Aug. 11th, day 9)

The easy way: Python

Easily wrap Python code, specialized library with Python bindings (PyCUDA, ...)

```
import theano
import numpy
from theano.compile.ops import as_op

def infer_shape_numpy_dot(node, input_shapes):
    ashp, bshp = input_shapes
    return [ashp[:-1] + bshp[-1:]]

@as_op(itypes=[theano.tensor.fmatrix, theano.tensor.fmatrix],
       otypes=[theano.tensor.fmatrix], infer_shape=infer_shape_numpy_dot)
def numpy_dot(a, b):
    return numpy.dot(a, b)
```

- ▶ Overhead of Python call could be slow
- ▶ To define the gradient, have to actually define a class deriving from Op, and define the grad method.

3D convolution using FFT on GPU was implemented that way last year

The hard way: C code

- ▶ Understand the C-API of Python / NumPy / CudaNdarray
- ▶ Handle arbitrary strides (or use GpuContiguous)
- ▶ Manage refcounts for Python
- ▶ No overhead of Python function calls, or from the interpreter (if garbage collection is disabled)

New contributors wrote Caffe-style convolutions, using GEMM, on CPU and GPU that way.

Features recently added to Theano

- ▶ Integration of CuDNN for 2D convolutions and pooling
- ▶ Execution of un-optimized graph on GPU (quicker compile time)
- ▶ Easier way of writing C code for Ops
- ▶ Serialize GPU shared variables as ndarrays, for loading on a machine with no GPU
- ▶ Easier serialization/deserialization of optimized function graphs
- ▶ Python 2 and 3 in a single code base

What to expect in the near future

- ▶ New GPU backend, with arrays of all dtypes, for CUDA and OpenCL
- ▶ Support for multiple GPUs in the same function
- ▶ GSoC project: manipulate functions without re-optimizing them
- ▶ GSoC project: faster optimization phase
- ▶ GSoC project: interactive visualization

Acknowledgements

- ▶ All people working or having worked at the MILA (previously LISA), especially Theano contributors
 - ▶ Frédéric Bastien, Yoshua Bengio, James Bergstra, Arnaud Bergeron, Olivier Breuleux, Pierre Luc Carrier, Ian Goodfellow, Razvan Pascanu, Joseph Turian, David Warde-Farley, and many more
- ▶ Compute Canada, Compute Québec, NSERC, the Canada Research Chairs, and CIFAR for providing funding or access to compute resources.

Thanks for your attention

Questions, comments, requests?

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<http://github.com/mila-udem/summerschool2015/>

- ▶ Slides: [intro_theano/intro_theano.pdf](#)
- ▶ Notebook with the code examples: [intro_theano/intro_theano.ipynb](#)

Exercises

Tutorial repository on GitHub:

<http://github.com/mila-udem/summerschool2015/>

- ▶ Install the dependencies
- ▶ Clone the repository
`git clone https://github.com/mila-udem/summerschool2015.git`
- ▶ Launch the notebook
`ipython notebook summerschool2015`
- ▶ Navigate to `intro_theano`, then `exercises.ipynb`