Introduction to Theano

A Fast Python Library for Modelling and Training

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Objectives

Today: Introduction to Theano

- Theoretical part
- Small examples

Tomorrow, 16:30: Practical session

- Hands-on exercises on the basics of Theano
- Hands-on exercises on debugging in Theano
- Examples of basic deep models (ConvNets, RNNs)
- Bring a laptop with a browser (GPU instances on Amazon)

All the material is online at
`https://github.com/mila-udem/summerschool2016/`

Overview
- Motivation
- Basic Usage

Graph definition and Syntax
- Graph structure
- 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
- Debugging
- Extending Theano
- New features

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 (8 years 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
- PyMC 3
- sklearn-theano
- Platoon
- Theano-MPI
- ...

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

```python
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

```python
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)

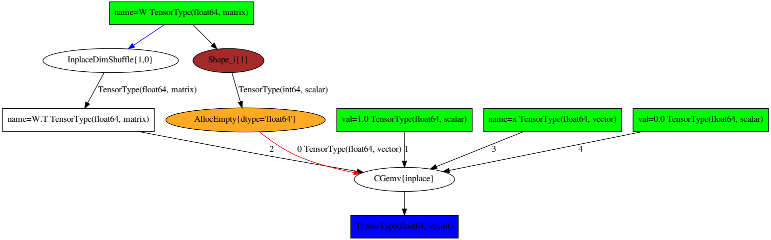
```
theano.printing.debugprint(f)
CGemv{inplace} [@A] ''   3
 |AllocEmpty{dtype='float64'} [@B] ''   2
 | |Shape_i{1} [@C] ''   1
 |   |W [@D]
 |TensorConstant{1.0} [@E]
 |InplaceDimShuffle{1,0} [@F] 'W.T'   0
 | |W [@D]
 |x [@G]
 |TensorConstant{0.0} [@H]

theano.printing.pydotprint(f)
```

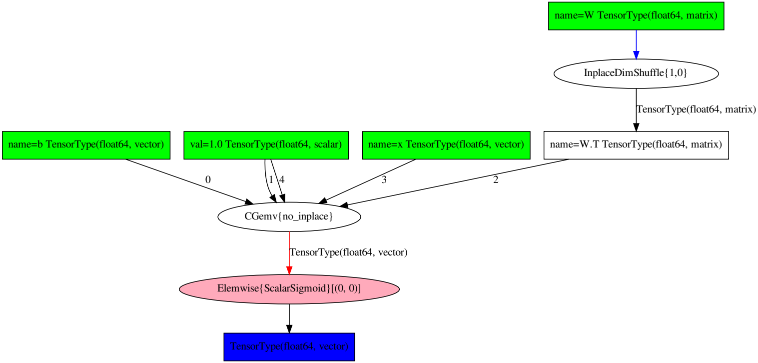
```
theano.printing.debugprint(g)
Elemwise{ScalarSigmoid}[(0, 0)] [@A] ''   2
 |CGemv{no_inplace} [@B] ''   1
   |b [@C]
   |TensorConstant{1.0} [@D]
   |InplaceDimShuffle{1,0} [@E] 'W.T'   0
   | |W [@F]
   |x [@G]
   |TensorConstant{1.0} [@D]

theano.printing.pydotprint(g)
```

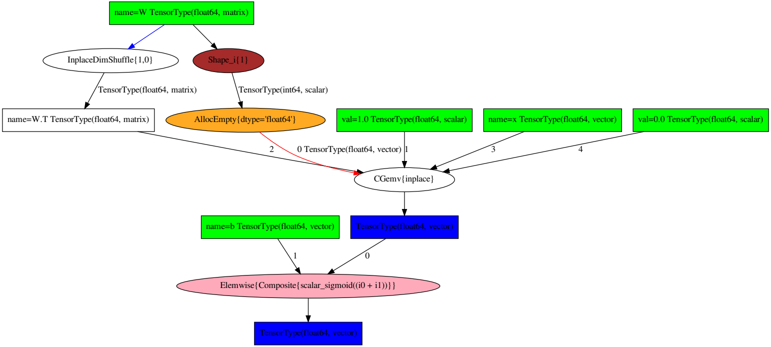
pydotprint(f)



pydotprint(g)



pydotprint(h)



d3viz

d3viz enables interactive visualization of graphs in a web browser

```python
from theano.d3viz import d3viz

d3viz(f, './d3viz_f.html')
d3viz(g, './d3viz_g.html')
d3viz(h, './d3viz_h.html')
```

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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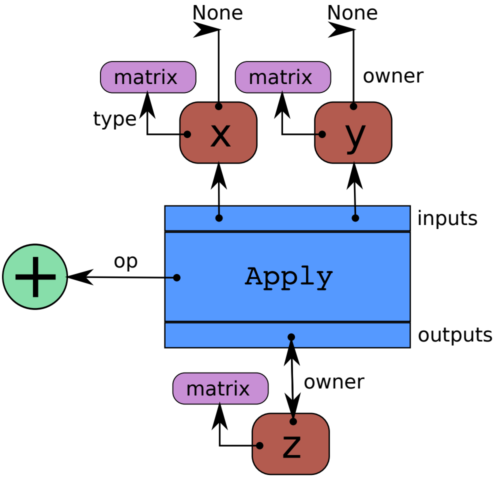
Graph structure

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

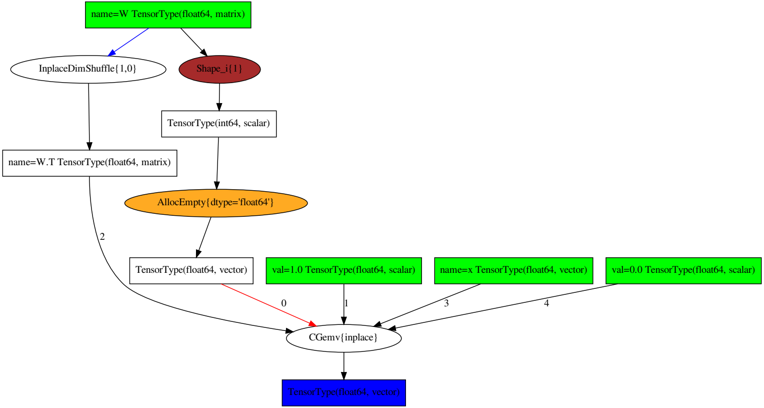
- `Variable` nodes, or variables, that represent *data*
- `Apply` nodes, that represent the application of *mathematical operations*

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


None
None
matrix
matrix
owner
type
x
y
inputs
op
Apply
outputs
matrix
owner
z

pydotprint(f, compact=False)



Strong typing

- All Theano variables have a type
- Different categories of types. Most used:
  - TensorType for NumPy ndarrays
  - GpuArrayType for CUDA arrays (CudaNdarrayType in the old back-end)
  - 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

```python
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

With the variables defined earlier:

```
x = T.vector('x')
W = T.matrix('W')
b = T.vector('b')
dot = T.dot(x, W)
out = T.nnet.sigmoid(dot + b)
```

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 $\mathbb{R}$.

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

The whole $M \times N$ Jacobian matrix $\frac{\partial g}{\partial x}\Big|_x$ is not needed.
We only need $\nabla g_x : \mathbb{R}^M \to \mathbb{R}^N, v \mapsto v \cdot \frac{\partial g}{\partial x}\Big|_x$

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

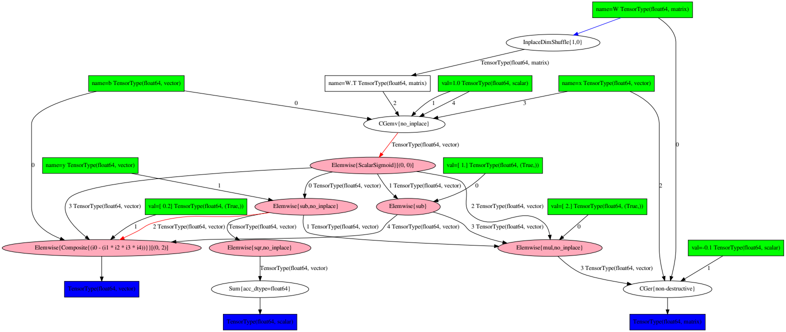
Using the gradients

- 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)
```


name=W TensorType(float64, matrix)
InplaceDimShuffle{1,0}
TensorType(float64, matrix)
name=b TensorType(float64, vector)
name=W.T TensorType(float64, matrix)
val=1.0 TensorType(float64, scalar)
name=x TensorType(float64, vector)
CGemv{no_inplace}
TensorType(float64, vector)
name=y TensorType(float64, vector)
Elemwise{ScalarSigmoid}[(0, 0)]
val=[1.] TensorType(float64, (True,))
0 TensorType(float64, vector)
1 TensorType(float64, vector)
3 TensorType(float64, vector)
val=[0.2] TensorType(float64, (True,))
Elemwise{sub,no_inplace}
Elemwise{sub}
2 TensorType(float64, vector)
val=[2.] TensorType(float64, (True,))
4 TensorType(float64, vector)
Elemwise{Composite{(i0 - (i1 * i2 * i3 * i4))}}[(0, 2)]
Elemwise{sqr,no_inplace}
Elemwise{mul,no_inplace}
val=-0.1 TensorType(float64, scalar)
Sum{acc_dtype=float64}
CGer{non-destructive}
TensorType(float64, vector)
TensorType(float64, scalar)
TensorType(float64, matrix)

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]
```

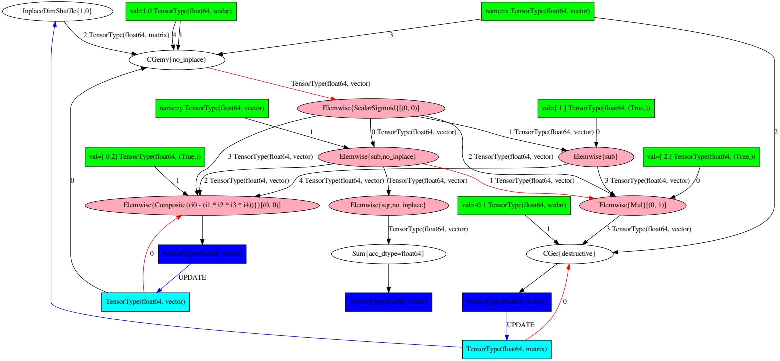
- Use `W.get_value()` and `W.set_value()` to access the value later

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


InplaceDimShuffle{1,0}
val=1.0 TensorType(float64, scalar)
name=x TensorType(float64, vector)
2 TensorType(float64, matrix)
4
1
3
CGemv{no_inplace}
TensorType(float64, vector)
name=y TensorType(float64, vector)
Elemwise{ScalarSigmoid}[(0, 0)]
val=[1.] TensorType(float64, (True,))
0 TensorType(float64, vector)
1 TensorType(float64, vector)
2
val=[0.2] TensorType(float64, (True,))
3 TensorType(float64, vector)
Elemwise{sub,no_inplace}
2 TensorType(float64, vector)
Elemwise{sub}
val=[2.] TensorType(float64, (True,))
4 TensorType(float64, vector)
Elemwise{Composite{(i0 - (i1 * i2 * i3 * i4))}}[(0, 0)]
Elemwise{sqr,no_inplace}
val=-0.1 TensorType(float64, scalar)
Elemwise{Mul}[(0, 1)]
TensorType(float64, vector)
Sum{acc_dtype=float64}
CGer{destructive}
TensorType(float64, scalar)
TensorType(float64, matrix)
UPDATE

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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 an 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 pre-defined modes govern the runtime and how much optimizations are applied

- `mode='FAST_RUN'`: default, make the runtime as fast as possible, launching overhead. Includes moving computation to GPU if a GPU was selected
- `mode='FAST_COMPILE'`: minimize launching overhead, around NumPy speed
- `optimizer='fast_compile'`: enables code generation and GPU use, but limits graph optimizations
- `mode='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 `ifelse` for instance)

Using the GPU

We want to make the use of GPUs as transparent as possible.
Theano features a new GPU back-end, with

- More dtypes, not only `float32`
- Easier interaction with GPU arrays from Python
- Multiple GPUs and multiple streams
- **In the development version only, not the 0.8.2 release**

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

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

You want to make sure to use float32 for speed

- `'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')`
- Experimental support for `'float16'` on some GPUs

Configuration flags

Configuration flags can be set in a couple of ways:

- `THEANO_FLAGS=device=cuda0,floatX=float32` in the shell
- In Python:

```
theano.config.device = 'cuda0'
theano.config.floatX = 'float32'
```

- In the `.theanorc` configuration file:

```
[global]
device = cuda0
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 transfered to GPU

Example: Loop with accumulation

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

# Symbolic description of the result
result, updates = theano.scan(fn=lambda prior_result, A: prior_result * A,
                              outputs_info=T.ones_like(A),
                              non_sequences=A,
                              n_steps=k)

# We only care about A**k, but scan has provided us with A**1 through A**k.
# Discard the values that we don't care about. Scan is smart enough to
# notice this and not waste memory saving them.
final_result = result[-1]

# compiled function that returns A**k
power = theano.function(inputs=[A, k], outputs=final_result, updates=updates)

print power(range(10), 2)
# [  0.   1.   4.   9.  16.  25.  36.  49.  64.  81.]
print power(range(10), 4)
# [  0.00000000e+00   1.00000000e+00   1.60000000e+01   8.10000000e+01
#    2.56000000e+02   6.25000000e+02   1.29600000e+03   2.40100000e+03
#    4.09600000e+03   6.56100000e+03]
```

Visualization, debugging, and diagnostic tools

The *definition* of a Theano function is separate from its *execution*. To help with this, we provide:

- Information in error messages
- Diagnostic tools

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.

Has been used to implement 3D convolution using FFT on GPU

The harder 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)
- Now easier: C code in a separate file

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

Features recently added to Theano

- New GPU back-end (dev branch), with:
  - Arrays of all dtypes, half-precision float (`float16`) for some operations
  - Support for multiple GPUs in the same function
  - Experimental support for OpenCL
- Performance improvements
  - Better interface and implementations for convolution and transposed convolution
  - Integration of CuDNN (now v5) for 2D/3D convolutions and pooling
  - CNMeM and a similar allocator
  - Data-parallelism with Platoon (https://github.com/mila-udem/platoon/)
- Faster compilation
  - Execution of un-optimized graph on GPU (quicker compile time)
  - Easier serialization/deserialization of optimized function graphs, GPU shared variables
  - Swapping/removing updates without recompiling
  - Partial evaluation of a compiled function
- Diagnostic tools
  - Interactive visualization (d3viz)
  - `PdbBreakPoint`
  - Creation stack trace (in progress)

What to expect in the future

- Better support for int operations on GPU (indexing, argmax)
- More CuDNN operations (basic RNNs, batch normalization)
- Simpler, faster optimization mode
- Data-parallelism across nodes in Platoon

Acknowledgements

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Thanks for your attention

Questions, comments, requests?

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- Slides: `theano/course/intro_theano.pdf`
- Notebook with the code examples: `theano/course/intro_theano.ipynb`

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More resources

- Documentation: `http://deeplearning.net/software/theano/`
- Code: `http://github.com/Theano/Theano/`
- Article: The Theano Development Team, "Theano: A Python framework for fast computation of mathematical expressions", `https://arxiv.org/abs/1605.02688`