Introduction to Theano

A Fast Python Library for Modelling and Training

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Objectives

This session will have 4 parts:

- Introduction to Theano
- Hands-on example: Logistic regression
- Hands-on example: ConvNet
- Hands-on example: LSTM

All the material is online at `github.com/lamblin/bayareadlschool/`

Theano vision

Mathematical symbolic expression compiler

- Easy to define expressions
  - Expressions mimic NumPy's syntax and semantics
  - Support for elementary operations (not only neural layers)
- 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: developed and used since January 2008 (8 years old)
- Good user documentation
- Active mailing list with participants worldwide
- Many contributors from different places
- Driven hundreds of research papers
- Used to teach university classes
- Core technology for Silicon Valley start-ups
- 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
- ...

Overview

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

Symbolic inputs

Symbolic, strongly-typed inputs

```
import theano
from theano import tensor as T
x = T.vector('x')
y = T.vector('y')
```

- All Theano variables have a type
- For instance `ivector`, `fmatrix`, `dtensor4`
- ndim, dtype, broadcastable pattern, device are part of the type
- shape and memory layout (strides) are **not**

Shared variables

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

W = theano.shared(W_val)
b = theano.shared(b_val)
W.name = 'W'
b.name = 'b'
```

- Symbolic variables, with a **value** associated to them
- The value is **persistent** across function calls
- The value is **shared** among all functions
- The value can be **updated**

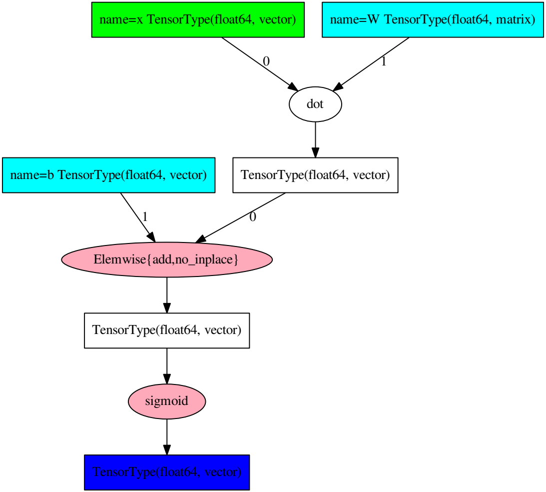
Build an expression

NumPy-like syntax

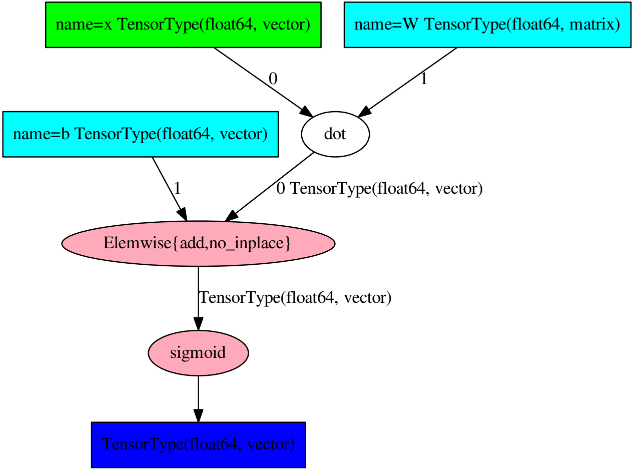
```
dot = T.dot(x, W)
out = T.nnet.sigmoid(dot + b)

C = ((out - y) ** 2).sum()
C.name = 'C'
```

- This creates new *variables*
- Outputs of mathematical operations
- Graph structure connecting them

pydotprint(out, compact=False)



pydotprint(out)



The back-propagation algorithm

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

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

The whole $M \times N$ Jacobian matrix $\left.\frac{\partial g}{\partial x}\right|_x$ is not needed.
We only need $\nabla g_x : \mathbb{R}^M \rightarrow \mathbb{R}^N, v \mapsto v \cdot \left.\frac{\partial g}{\partial x}\right|_x$
This is implemented for (almost) each mathematical operation in Theano.

Using theano.grad

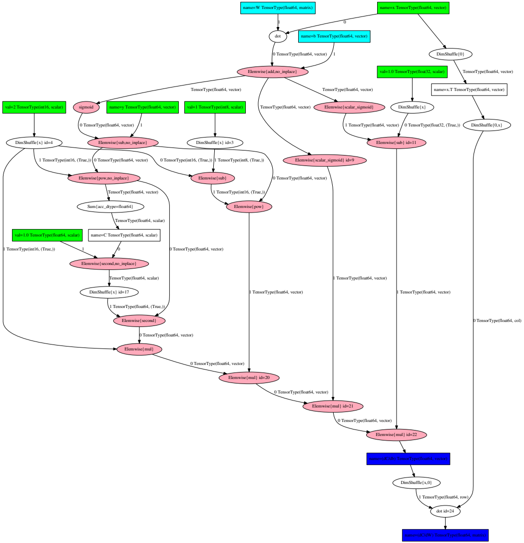
theano.grad traverses the graph, applying the chain rule.

```
dC_dW = theano.grad(C, W)
dC_db = theano.grad(C, b)
# or dC_dW, dC_db = theano.grad(C, [W, b])
```

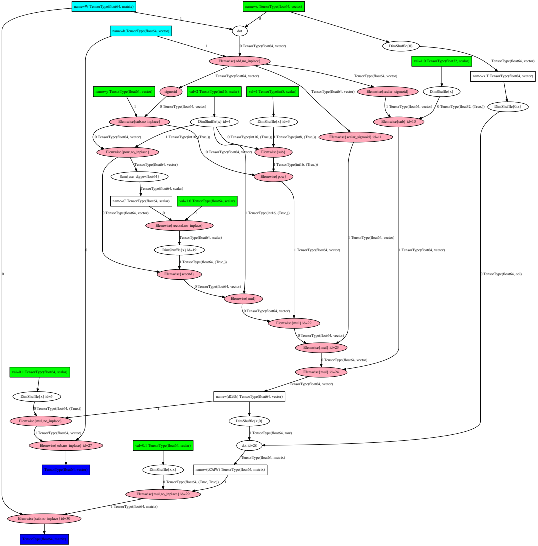
- dC_dW and dC_db are symbolic expressions, like W and b
- There are no numerical values at this point
- They are part of the same computation graph
- They can also be used to build new expressions

```
upd_W = W - 0.1 * dC_dW
upd_b = b - 0.1 * dC_db
```

pydotprint([dC_dW, dC_db])



pydotprint([upd_W, upd_b])



Computing values

Build a callable that compute outputs given inputs

- Shared variables are implicit inputs

```
predict = theano.function([x], out)
x_val = np.random.rand(4)
print(predict(x_val))
# -> array([ 0.9421594 ,  0.73722395,  0.67606977])

monitor = theano.function([x, y], [out, C])
y_val = np.random.uniform(size=3)
print(monitor(x_val, y_val))
# -> [array([ 0.9421594 ,  0.73722395,  0.67606977]),
#     array(0.6191236997823024)]

error = theano.function([out, y], C)
print(error([0.942, 0.737, 0.676], y_val))
# -> array(0.6002210054210885)
```

Updating shared variables

A function can compute new values for shared variables, and perform updates.

```
train = theano.function([x, y], C,
                        updates=[(W, upd_W),
                                 (b, upd_b)])
print(b.get_value())
# -> [ 1.  1.  1.]
train(x_val, y_val)
print(b.get_value())
# -> [ 0.9967082   0.99340064  0.97245715]
```

- 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

Graph optimizations

An optimization replaces a part of the graph with different nodes

- The types of the replaced nodes have to match
- The values should be equivalent

Different goals for optimizations:

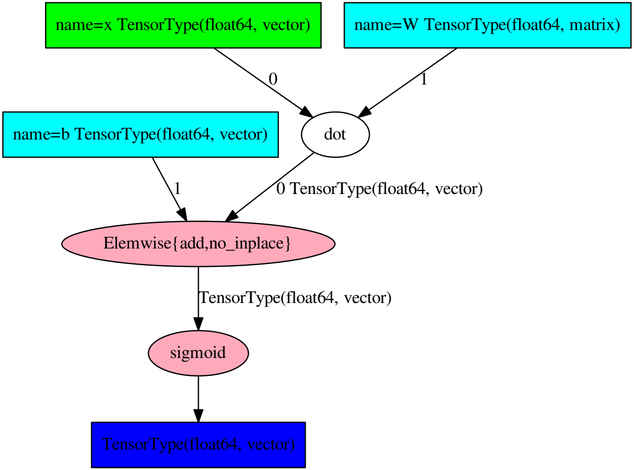
- Merge equivalent computations
- Simplify expressions: x/x becomes 1
- Numerical stability: "$\log(1+x)$" becomes "log1p(x)"
- Insert in-place an destructive versions of operations
- Use specialized, efficient versions (Elemwise loop fusion, BLAS, cuDNN)
- Shape inference
- Constant folding
- Transfer to GPU

Enabling/disabling optimizations

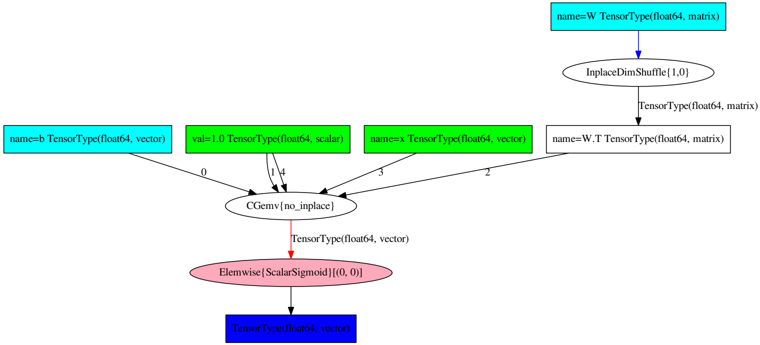
Trade-off between compilation speed, execution speed, error detection.
Different pre-defined modes govern the runtime and how much optimizations are applied

- `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

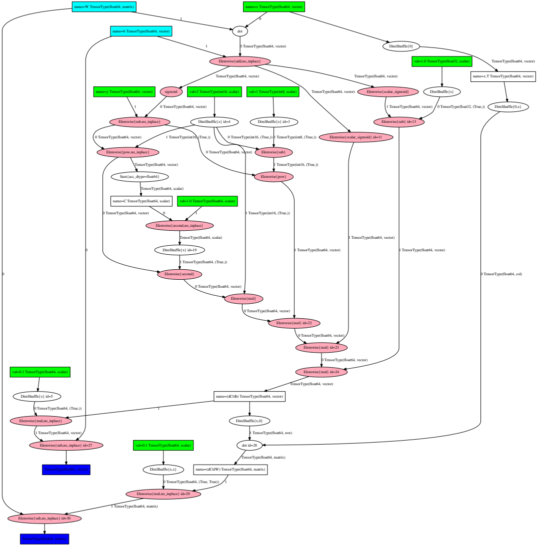
pydotprint(out)



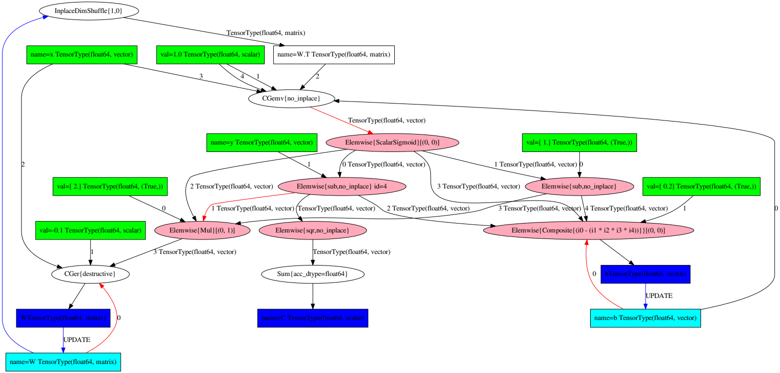
pydotprint(predict)



pydotprint([upd_W, upd_b])



pydotprint(train)



debugprint

```
debugprint(out)

sigmoid [id A] ''
 |Elemwise{add,no_inplace} [id B] ''
   |dot [id C] ''
   | |x [id D]
   | |W [id E]
   |b [id F]
```

```
debugprint(predict)

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

Code generation and execution

Code generation for Ops:

- Ops can define C++/CUDA code computing its output values
- Dynamic code generation is possible
  - For instance, loop fusion for arbitrary sequence of element-wise operations
- Code gets compiled into a Python module, cached, and imported
- Otherwise, fall back to a Python implementation

Code execution through a runtime environment, or VM:

- Calls the functions performing computation for the Ops
- Deals with ordering constraints, lazy execution
- A C++ implementation (CVM) to avoid context switches (in/out of the Python interpreter)

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`
- Experimental support for `'float16'` for storage
- Easier interaction with GPU arrays from Python
- Multiple GPUs and multiple streams
- **In the development version only, and future 0.9 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

Configuration flags

Configuration flags can be set in a couple of ways:

- In the `.theanorc` configuration file:

```
[global]
device = cuda0
floatX = float32
```

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

```python
theano.config.floatX = 'float32'
```

(`theano.config.device` cannot be set once Theano is imported)

Overview of scan

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

We will see a use of scan in the LSTM example.

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
- Get information at runtime
- Monitor NaN or large value
- Test values when building the graph
- Detect common sources of slowness
- Self-diagnostic tools

Extending Theano

Theano can be extended in a few different ways

- Creating an Op with Python code
  - Easy, using Python bindings for specialized libraries (PyCUDA, . . .)
  - Some runtime overhead is possible
  - Example: 3D convolution using FFT on GPU
- Creating an Op with C or CUDA code
  - Use the C-API of Python / NumPy / GpuArray, manage refcounts
  - No overhead of Python function calls, or from the interpreter
  - C code inline or in a separate file
  - Example: Caffe-style convolutions, using GEMM, on CPU and GPU
- Adding an optimization
  - Perform additional graph simplifications
  - Replace part of the graph by a new optimized Op

Features recently added to Theano

- New GPU back-end (dev branch), with:
  - Arrays of all dtypes, half-precision float (`float16`) for storage
  - Support for multiple GPUs in the same function
- 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 for GPU memory
  - Data-parallelism with Platoon (`github.com/mila-udem/platoon/`)
- Faster graph optimization phase
  - Execution of un-optimized graph on GPU (quicker compile time)
  - Various ways to avoid recompilation
- New diagnostic tools
  - Interactive visualization (d3viz)
  - `PdbBreakPoint`

What to expect in the near future

- Better support for int operations on GPU (indexing, argmax)
- More CuDNN operations (basic RNNs, batch normalization)
- Better support for 3D convolution / pooling
- Simpler, faster optimization mode
- Data-parallelism across nodes in Platoon

Acknowledgements

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- Stanford AI Lab and the organizers of the Deep Learning School

Thanks for your attention

Questions, comments, requests?

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`github.com/lamblin/bayareadlschool/`

- Slides: `intro_theano.pdf`
- Companion notebook: `intro_theano.ipynb`

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More resources

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

Examples

Tutorial repository on GitHub:
`github.com/lamblin/bayareadlschool/`

- Install the dependencies
- Clone the repository

  `git clone https://github.com/lamblin/bayareadlschool.git`
- Launch the notebook

  `jupyter notebook bayareadlschool`
- **Logistic regression:** Open `logistic_regression.ipynb`
- **ConvNet:** Navigate to `convnet`, then `lenet.ipynb`
- **LSTM:** Navigate to `lstm`, then `exercises.ipynb`