Theano
A Fast Python Library for Modelling and Training

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This tutorial will have 4 parts:

- Introduction to Theano – Motivation and design
- Walk-through example – LeNet on MNIST with Lasagne
- Exercises – Basics of Theano
- Hands-on example – Build your own classifier from VGG-16

All the material is online at github.com/mila-udem/summerschool2017

Hands-on examples
Go to http://mila.umontreal.ca/vmip

- Jupyter notebooks
- Executed on AWS instances with a GPU (K80)
Motivation and design

Goals
Design
Status

Symbolic expressions

Declaring inputs
Defining expressions
Deriving gradients

Function compilation

Compiling a Theano function
Graph optimizations
Graph visualization

Optimized execution

Code generation and execution
GPU

Advanced Topics

Looping: the scan operation
Debugging
Extending Theano
Development
Lasagne
Goals

Expressing models as mathematical expressions
- Not only a collection of standard layers or modules
- Not only regular gradient descent
- From an interpreted / scripting language

Automatically deriving gradients
- Define gradients for basic, elementary operations
- Treat those gradients as mathematical expressions as well
- Simplify automatically the resulting expression

Training the model efficiently
- Without having to write C / C++ / CUDA code
- Automatic simplification of the graph
- Automatic code generation
Theano: A mathematical symbolic expression compiler

Easy to define expressions
- Using Python
- 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)
- Inplace optimizations to reduce memory usage

Tools to inspect and check for correctness
Current status

- Mature: developed and used since January 2008 (9 years old)
- Theano 0.9 released in March 2017
- Driven > 1000 research papers
- Many contributors (123 for version 0.9)
- Active mailing list with participants worldwide
- 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
- rllab
- PyMC 3
- ...

For parallelism

- Platoon
- Theano-MPI
- Synkhronos
- Elephas (through Keras)
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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, strongly-typed inputs

import theano
from theano import tensor

\[
x = T.vector(\'x\')
\]
\[
y = T.vector(\'y\')
\]

All Theano variables have a type

\[
x = T.ivector(\'x\')
\]
\[
y = T.fmatrix(\'y\')
\]

\[
x = T.dtensor4(\'x\')
\]
\[
y = T.imatrix(\'y\')
\]

\[
x = T.dscalar(\'x\')
\]
\[
y = T.dvector(\'y\')
\]

\[
x = T.dmatrix(\'x\')
\]
\[
y = T.dthvector(\'y\')
\]

\[
x = T.dtensor3(\'x\')
\]
\[
y = T.dtensor2(\'y\')
\]

\[
x = T.dmatrix('x')
\]
\[
y = T.dmatrix('y')
\]

All Theano variables have a type

shape and memory layout (strides) are not

ndim, dtype, broadcastable pattern, device are part of the type
Shared variables

```python
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)
Declaring inputs
Defining expressions
Deriving gradients

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pydotprint(out)
The back-propagation algorithm

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

$\begin{align*}
&\text{C : } \mathbb{R}^N \to \mathbb{R} \\
&\text{f : } \mathbb{R}^M \to \mathbb{R} \\
&\text{g : } \mathbb{R}^N \to \mathbb{R}^M \\
&\text{C(x) = f(g(x))} \\
&\frac{\partial C}{\partial x} \bigg|_x = \frac{\partial f}{\partial g} \bigg|_{g(x)} \cdot \frac{\partial g}{\partial x} \bigg|_x
\end{align*}$

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

This is implemented for (almost) each mathematical operation in Theano.
Using \texttt{theano.grad}

\texttt{theano.grad} traverses the graph, applying the chain rule.

\begin{verbatim}
dC_dW = theano.grad(C, W)
dC_db = theano.grad(C, b)
# or dC_dW, dC_db = theano.grad(C, [W, b])
\end{verbatim}

- \( dC_dW \) and \( dC_db \) are symbolic expressions, like \( \text{out} \) and \( C \)
- 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

\begin{verbatim}
upd_W = W - 0.1 \times dC_dW
upd_b = b - 0.1 \times dC_db
\end{verbatim}
pydotprint([[dC_dW, dC_db]])
pydotprint([upd_W, upd_b])
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Computing values

Build a callable that compute outputs given inputs

- Shared variables are implicit inputs

```python
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(0.6137821438190066)]

error = theano.function([out, y], C)
print(error([0.942, 0.737, 0.676], y_val))
# -> array(0.613355628529845)
```
A function can compute new values for shared variables, and perform updates.

```python
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())
# -> [ 0.99639999  0.97684097  0.98318412]
```

- Variables $W$ and $b$ are **implicit inputs**
- Expressions $\text{upd}_W$ and $\text{upd}_b$ 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 and optimizers 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
- 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
Compiling a Theano function

Graph visualization

pydotprint(out)

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pydotprint(out)

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pydotprint(out)
pydotprint(predict)
pydotprint([upd_W, upd_b])
pydotprint(train)
debugprint(out)

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

dbgprint(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]
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  - Status

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  - Graph optimizations
  - Graph visualization

**Optimized execution**
  - Code generation and execution
  - GPU

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  - Debugging
  - Extending Theano
  - Development
  - Lasagne
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

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 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, but you can call `theano.gpuarray.use('cuda0')`
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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 transferred to GPU
Example: Loop with accumulation

```python
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
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
New features

- New GPU back-end, based on libgpuarray, with:
  - Arrays of all dtypes, half-precision float (float16) for storage
  - Better scheduling
  - Much simpler installation on Windows (conda package)

- Performance improvements
  - Integration of CuDNN (now v6) for 2D/3D convolutions and pooling, RNNs, batch normalization
  - Fast memory allocator on GPU
  - For memory: checkpointing in scan, gradients of long sequences
  - Data parallelism with Platoon (github.com/mila-udem/platoon/)

- Faster graph optimization phase
  - More optimization / compile time trade-offs (optimizer={o0,o1,...,o4})
  - Various ways to avoid recompilation

- Diagnostic tools
  - Interactive visualization (d3viz)
  - PdbBreakPoint
Current development

- Better support for int operations on GPU (indexing, argmax)
- Faster reductions on GPU
- Simpler, faster optimization mode
- Faster generation and loading of C++ / CUDA code
- More convolution variants: grouped, dilated, ... (GSoC)
- More linear algebra operations on GPU (GSoC)
- Data parallelism across nodes in Platoon
- OpFromGraph for re-defining gradients
Projects in our road map

- Constant shape inference when building the graph
- Better compilation cache for generated C++ code
- Continue refactoring graph optimization (for optimization speed)
- Optimize and re-use sub-graphs (like subroutines)
  - Improving OpFromGraph
  - Maybe cache them
- Deterministic mode
- Use CPU memory to offload intermediate results from GPU (maybe limited to Pascal GPUs)
What is Lasagne?

Lasagne is a thin framework/library on top of Theano. lasagne.readthedocs.org

- Does not hide Theano
- Builds Theano graphs easily by using layers
- Contains many preimplemented losses and optimizers
- Does not include a training loop
Acknowledgements

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Thanks for your attention

Questions, comments, requests?
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More resources
  ▶ Documentation: deeplearning.net/software/theano/
  ▶ Code: github.com/Theano/Theano/
  ▶ Deep Learning Tutorials: deeplearning.net/tutorial/
Examples

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