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

debugprint(out)
sigmoid [id A] ''
| Elemwise{add,no_inplace} [id B] ''
 | dot [id C] ''
 | | x [id D]
 | | W [id E]
 | b [id F]
Compiling a Theano function

Build a callable that compute outputs given inputs

```python
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)

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

theano.printing.pydotprint(f)
```

```python
theano.printing.debugprint(g)
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]

theano.printing.pydotprint(g)
```
pydotprint(f)
```
pydotprint(g)
```
pydotprint(h)
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

```python
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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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
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**Graph structure**
Strong typing
Differences from Python/NumPy

- **Apply**
  - `op`
  - `inputs`
  - `outputs`
  - `matrix`
  - `owner`

- **X**
  - `type`
  - `matrix`
  - `owner`

- **Y**
  - `matrix`
  - `owner`

- **Z**
  - `matrix`
  - `owner`
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]]))
# [[ 1.1  2.1  3.1]]
# [[ 1.2  2.2  3.2]]
```
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
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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With the variables defined earlier:

```python
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

```python
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])
```
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 $\mathbb{R}$.

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

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

```python
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
  ```python
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
  ```python
  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

\[
C_{\text{val}}, \; dC_{\text{dW\_val}}, \; dC_{\text{db\_val}} = \text{cost\_and\_grads}(x_{\text{val}}, \; W_{\text{val}}, \; b_{\text{val}}, \; y_{\text{val}})
\]
\[
W_{\text{val}} \leftarrow 0.1 \times dC_{\text{dW\_val}}
\]
\[
b_{\text{val}} \leftarrow 0.1 \times dC_{\text{db\_val}}
\]

\[
C_{\text{val}}, \; W_{\text{val}}, \; b_{\text{val}} = \text{cost\_and\_upd}(x_{\text{val}}, \; W_{\text{val}}, \; b_{\text{val}}, \; y_{\text{val}})
\]

- 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

```python
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
```
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
pydotprint(cost_and_perform_updates)
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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
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 \texttt{float32}
- Easier interaction with GPU arrays from Python
- Multiple GPUs and multiple streams
- \textbf{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 \texttt{shared} variables will be created in GPU memory
- Enables optimizations moving supported operations to GPU

You want to make sure to use \texttt{float32} for speed

- '\texttt{floatX}' is the default type of all tensors and sparse matrices.
- By default, aliased to '\texttt{float64}' for double precision on CPU
- Can be set to '\texttt{float32}' by a configuration flag
- You can always explicitly use \texttt{T.fmatrix()} or \texttt{T.matrix(dtype='float32')}
- Experimental support for '\texttt{float16}' on some GPUs
Configuration flags can be set in a couple of ways:

- **THEANO_FLAGS=device=cuda0,floatX=float32 in the shell**
- **In Python:**
  ```python
define_config(device='cuda0', floatX='float32', **kwargs):
    theano.config.device = device
    theano.config.floatX = floatX
```
- **In the .theanorc configuration file:**
  ```ini
  [global]
  device = cuda0
  floatX = float32
  ```
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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

\[
\begin{align*}
  k &= \text{T.iscalar}("k") \\
  A &= \text{T.vector}("A") \\

  \text{# Symbolic description of the result} \\
  \text{result, updates} &= \text{theano.scan}(\text{fn=\texttt{lambda} prior_result, A: prior_result} \times A, \\
  &\quad \text{outputs_info=\text{T.ones_like}(A),} \\
  &\quad \text{non_sequences=A,} \\
  &\quad \text{n_steps=k}) \\

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

  \text{# compiled function that returns } A^{**k} \\
  \text{power} &= \text{theano.function}(\text{inputs=[A, k]}, \text{outputs=final_result, updates=updates}) \\

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

See demo in Debug.ipynb.
The easy way: Python

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

```python
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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- The CRM and CIFAR for the organization.
Thanks for your attention

Questions, comments, requests?
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http://github.com/mila-udem/summerschool2016/

- Slides: theano/course/intro_theano.pdf
- Notebook with the code examples: theano/course/intro_theano.ipynb
Thanks for your attention

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More resources
  ▶ Documentation: http://deeplearning.net/software/theano/
  ▶ Code: http://github.com/Theano/Theano/