Machine Learning
Brendan Shillingford
July 6, 2016

nngraph

Today we'll do a simple introduction to `nngraph`.

We'll be working purely interactively today. Start as follows:

```
 ______                __    |  Torch7
/_  __/__  ________/ /   |  Scientific computing for Lua.
 / / / _ \/ __/ __/ _ \  |
/_/  \___/_/  \__/_//_/  |  https://github.com/torch
                         |  http://torch.ch

th> require 'nngraph'
true
```

If you get `true` as the return value of the `require`, then nngraph is installed. If it is not installed, install it by running `luarocks install nngraph`.

Start by reading over the first few sections in the README file: https://github.com/torch/nngraph/.

This practical's files can be found here: https://github.com/oxford-cs-ml-2015/practical5. Read `README.md` for setup instructions for the lab machine. The first practical's installer will have automatically installed `nngraph`.

Introduction

In lecture, we discussed the expressibility of neural network models by the variety of ways they can be combined together. A simple example is a feed-forward network, like the type encountered in the last few practicals. The `nn.Sequential` module is a container for other modules, so we had a recursive structure. The layers we've seen in Torch so far all have the same input and output types, though.

```
--          input object --v
output = model:forward(input)
-- ^-- output object
```

In the `nn.Linear`, `nn.Sigmoid`, `nn.Tanh`, `nn.LogSoftMax`, and most other layers, the type of `input` and `output` were always `Tensors`.

But what if a module needs to produce more than one output, or to take more than one input? In Torch's `nn` module, several modules do this, such as `nn.CAddTable` which performs an element-wise addition. Its input is a Lua `table` of `Tensors` that are all the same size, and its output is another `Tensor` of the same size. We can try it out:

```
+th> add = nn.CAddTable()
+th> t1 = torch.Tensor{1,2,3}
+th> t2 = torch.Tensor{3,4,10}
+th> add:forward({t1, t2})
  4
  6
 13
[torch.DoubleTensor of dimension 3]
```

Since this layer takes an arbitrary number of inputs, it is useful for combining other pieces of networks together.

A slight digression: Suppose `input` to `nn.CAddTable` is of type/shape `{ Tensor, Tensor }` (a table of tensors) and `output` is of type `Tensor`. The type/shape of the backward messages matches these: `gradInput` ($\frac{\partial loss}{\partial input}$) matches that of `input`, and `gradOutput` ($\frac{\partial loss}{\partial output}$) matches that of `output`. *Optional exercise:* verify this for yourself in code, or reading its source.

An example

Say we want to create a module that computes $\mathbf{z} = \text{sigmoid}(\text{linear}_w(\mathbf{x})) + \mathbf{x}$, where linear signifies a linear transformation plus a bias term like the `nn.Linear` class. This is easy to draw as a graph, but expressing it in the sequential format is, although possible, very cumbersome. (For the curious, it involves a module called `nn.ParallelTable` that contains multiple modules that get evaluated on each entry of their input table.)

It is easy to write a forward pass manually, but we probably don't want to do that because then we need to write the backward pass manually as well. We'll see that this is sometimes a reasonable approach though, when you have a model with many steps. This will be the case for the LSTM code that we will look at next week.

This is our motivation for `nngraph`.

Playing with `nngraph`

Suppose we want to compute

$$\mathbf{z} = \mathbf{x}_1 + \mathbf{x}_2 \odot \text{linear}(\mathbf{x}_3) \qquad (*)$$

($\odot$ is element-wise multiplication), as a `nn.Module` so we can integrate it into a large network. In `nngraph` this could be done easier.

`nngraph` overloads the call operator (i.e. the `()` operator used for function calls) on all `nn.Module` objects. When the call operator is invoked, it returns a node wrapping the `nn.Module`. The call operator takes the parents of the node as arguments, which specify which modules will feed into this one during a forward pass.

To specify the module's inputs, we create dummy input nodes that perform the identity operation, then use these as parents for nodes that do computation. Here is the same addition example:

```
+th> x1 = nn.Identity()()
+th> x2 = nn.Identity()()
+th> a = nn.CAddTable()({x1, x2})
+th> m = nn.gModule({x1, x2}, {a})
```

Now `m` is a `nn.Module` that performs exactly the same computation as `nn.CAddTable` if you give either one a table with two Tensors.

To make sure we understand what is going on, note the types of each part of this line of code:

$$\underbrace{\texttt{a}}_{\text{graph node}} = \overbrace{\underbrace{\texttt{nn.CAddTable}()}_{\text{graph node}}(\{\texttt{x1}, \texttt{x2}\})}^{\texttt{nn.Module}}$$

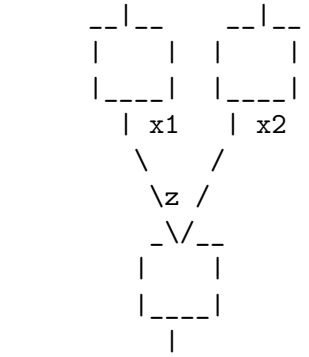
and `x1` and `x2` are graph nodes as well, *not* `nn.Module`'s. Similarly, note that `nn.Identity()` is a `nn.Module` instance but `nn.Identity()()` is a graph node.

As you can see, once we finish describing the graph, we create an `nn.gModule` (which is nngraph's `nn.Module` implementation wrapping the graph) performing the graph's computation as follows:

$$\underbrace{\texttt{m}}_{\texttt{nn.Module}} = \texttt{nn.gModule}(\overbrace{\{\texttt{x1}, \texttt{x2}\}}^{\texttt{table of input nodes}}, \underbrace{\{\texttt{a}\}}_{\texttt{table of output nodes}})$$

If there are any modules that have parameters, `nn.gModule` will automatically combine all these parameters.

Remember what we discussed in class: if you have a structure of the following shape:



During the forward pass, z is computed and used for both of the subsequent modules that depend on this value. The backward messages $\frac{\partial loss}{\partial x_1}$ and $\frac{\partial loss}{\partial x_2}$ both get *summed* as they are sent

backwards to the common node. This is a consequence of the multivariate chain rule. This is done internally in the background by `nngraph`.

Handin: create an instance of `nngraph`'s `nn.gModule` class that computes the expression marked $(*)$ from above. You can make up values for the sizes of the $\mathbf{x}_i$'s, as you need to specify sizes for the `nn.Linear` class. Feel free to look at the `nngraph` README linked to above for hints.

Call its `forward` function to verify that it works, and compare this result to something computed by hand.

Handin

See the one bolded "**Handin:**" part above.

If you finish early

Challenge 1: LSTMs

Try implementing an LSTM cell, using the equations in http://arxiv.org/abs/1308.0850 as reference, equations (7-11) on page 5. But **omit** the term in the sum input to the gates that refers to c_{t-1}. That is, create a module that takes as input c_{t-1}, h_{t-1}, x_t, and produces as output c_t, h_t.

If you attempt and want to see a solution, see the `lstm` function here: https://github.com/wojciechz/learning_to_execute/blob/master/main.lua#L23.

Challenge 2: computation graphs

The graph that we describe to nngraph is a computation graph, illustrating the dependencies between computations in a forward pass. By flipping the directions of the edges in this graph, we get the backwards graph.

Given a computation graph, which is always a directed acyclic graph (DAG), state an algorithm that gives a valid sequence of computations as a list specifying an evaluation order for the nodes. (Hint: this DAG is a dependency graph.) Note that once we have an order for this forward pass, we can just reverse this list to get an execution order for the backward pass.