CSC321 Lecture 10: Automatic Differentiation

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Overview

- Implementing backprop by hand is like programming in assembly language.
  - You'll probably never do it, but it's important for having a mental model of how everything works.
- Lecture 6 covered the math of backprop, which you are using to code it up for a particular network for Assignment 1
- This lecture: how to build an automatic differentiation (autodiff) library, so that you never have to write derivatives by hand
  - We'll cover a simplified version of Autograd, a lightweight autodiff tool.
  - PyTorch's autodiff feature is based on very similar principles.

Confusing Terminology

- Automatic differentiation (autodiff) refers to a general way of taking a program which computes a value, and automatically constructing a procedure for computing derivatives of that value.
  - In this lecture, we focus on reverse mode autodiff. There is also a forward mode, which is for computing directional derivatives.
- Backpropagation is the special case of autodiff applied to neural nets
  - But in machine learning, we often use backprop synonymously with autodiff
- Autograd is the name of a particular autodiff package.
  - But lots of people, including the PyTorch developers, got confused and started using "autograd" to mean "autodiff"

What Autodiff Is Not

- Autodiff is not finite differences.
  - Finite differences are expensive, since you need to do a forward pass for *each* derivative.
  - It also induces huge numerical error.
  - Normally, we only use it for testing.
- Autodiff is both efficient (linear in the cost of computing the value) and numerically stable.

What Autodiff Is Not

- Autodiff is not symbolic differentiation (e.g. Mathematica).
  - Symbolic differentiation can result in complex and redundant expressions.
  - Mathematica's derivatives for one layer of soft ReLU (univariate case):

```
D[Log[1 + Exp[w * x + b]], w]
```

$$\text{Out[11]=} \quad \frac{e^{b+w\,x}\,w}{1+e^{b+w\,x}}$$

  - Derivatives for two layers of soft ReLU:

```
In[19]:= D[Log[1 + Exp[w2 * Log[1 + Exp[w1 * x + b1]] + b2]], w1]
```

$$\text{Out[19]=} \quad \frac{e^{b1+b2+w1\,x+w2\,\mathrm{Log}\left[1+e^{b1+w1\,x}\right]}\,w2\,x}{\left(1+e^{b1+w1\,x}\right)\left(1+e^{b2+w2\,\mathrm{Log}\left[1+e^{b1+w1\,x}\right]}\right)}$$

  - There might not be a convenient formula for the derivatives.
- The goal of autodiff is not a formula, but a procedure for computing derivatives.

What Autodiff Is

Recall how we computed the derivatives of logistic least squares regression. An autodiff system should transform the left-hand side into the right-hand side.

Computing the loss:

$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2
\end{aligned}
$$

Computing the derivatives:

$$
\begin{aligned}
\overline{\mathcal{L}} &= 1 \\
\overline{y} &= y - t \\
\overline{z} &= \overline{y}\,\sigma'(z) \\
\overline{w} &= \overline{z}\,x \\
\overline{b} &= \overline{z}
\end{aligned}
$$

What Autodiff Is

- An autodiff system will convert the program into a sequence of primitive operations which have specified routines for computing derivatives.
- In this representation, backprop can be done in a completely mechanical way.

Original program:

$$z = wx + b$$

$$y = \frac{1}{1 + \exp(-z)}$$

$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

Sequence of primitive operations:

$$\begin{aligned}
t_1 &= wx \\
z &= t_1 + b \\
t_3 &= -z \\
t_4 &= \exp(t_3) \\
t_5 &= 1 + t_4 \\
y &= 1/t_5 \\
t_6 &= y - t \\
t_7 &= t_6^2 \\
\mathcal{L} &= t_7/2
\end{aligned}$$

What Autodiff Is

```python
import autograd.numpy as np
from autograd import grad

def sigmoid(x):
    return 0.5*(np.tanh(x) + 1)

def logistic_predictions(weights, inputs):
    # Outputs probability of a label being true according to logistic model.
    return sigmoid(np.dot(inputs, weights))

def training_loss(weights):
    # Training loss is the negative log-likelihood of the training labels.
    preds = logistic_predictions(weights, inputs)
    label_probabilities = preds * targets + (1 - preds) * (1 - targets)
    return -np.sum(np.log(label_probabilities))
```

very sneaky!

… (load the data) …

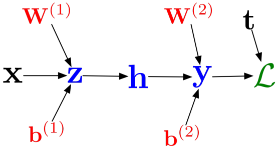
```python
# Define a function that returns gradients of training loss using Autograd.
training_gradient_fun = grad(training_loss)

# Optimize weights using gradient descent.
weights = np.array([0.0, 0.0, 0.0])
print "Initial loss:", training_loss(weights)
for i in xrange(100):
    weights -= training_gradient_fun(weights) * 0.01

print  "Trained loss:", training_loss(weights)
```

Autograd constructs a function for computing derivatives

Autograd

- The rest of this lecture covers how Autograd is implemented.
- Source code for the original Autograd package:
    - `https://github.com/HIPS/autograd`
- Autodidact, a pedagogical implementation of Autograd — you are encouraged to read the code.
    - `https://github.com/mattjj/autodidact`
    - Thanks to Matt Johnson for providing this!

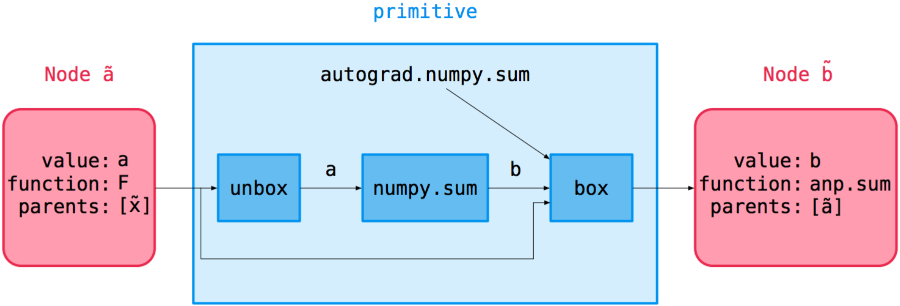
Building the Computation Graph



- Most autodiff systems, including Autograd, explicitly construct the computation graph.
  - Some frameworks like TensorFlow provide mini-languages for building computation graphs directly. Disadvantage: need to learn a totally new API.
  - Autograd instead builds them by tracing the forward pass computation, allowing for an interface nearly indistinguishable from NumPy.
- The `Node` class (defined in `tracer.py`) represents a node of the computation graph. It has attributes:
  - `value`, the actual value computed on a particular set of inputs
  - `fun`, the primitive operation defining the node
  - `args` and `kwargs`, the arguments the op was called with
  - `parents`, the parent `Node`s

Building the Computation Graph

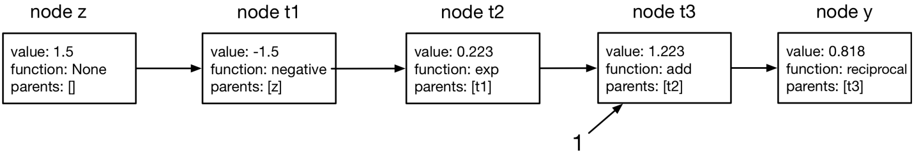
- Autograd's fake NumPy module provides primitive ops which look and feel like NumPy functions, but secretly build the computation graph.
- They wrap around NumPy functions:



Building the Computation Graph

Example:

```python
def logistic(z):
    return 1. / (1. + np.exp(-z))

# that is equivalent to:
def logistic2(z):
    return np.reciprocal(np.add(1, np.exp(np.negative(z))))

z = 1.5
y = logistic(z)
```



Vector-Jacobian Products

- Previously, I suggested deriving backprop equations in terms of sums and indices, and then vectorizing them. But we'd like to implement our primitive operations in vectorized form.
- The Jacobian is the matrix of partial derivatives:

$$\mathbf{J} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

- The backprop equation (single child node) can be written as a vector-Jacobian product (VJP):

$$\overline{x_j} = \sum_i \overline{y_i} \frac{\partial y_i}{\partial x_j} \qquad \overline{\mathbf{x}} = \overline{\mathbf{y}}^\top \mathbf{J}$$

- That gives a row vector. We can treat it as a column vector by taking

$$\overline{\mathbf{x}} = \mathbf{J}^\top \overline{\mathbf{y}}$$

Vector-Jacobian Products

Examples

- Matrix-vector product

$$\mathbf{z} = \mathbf{W}\mathbf{x} \qquad \mathbf{J} = \mathbf{W} \qquad \overline{\mathbf{x}} = \mathbf{W}^\top \overline{\mathbf{z}}$$

- Elementwise operations

$$\mathbf{y} = \exp(\mathbf{z}) \qquad \mathbf{J} = \begin{pmatrix} \exp(z_1) & & 0 \\ & \ddots & \\ 0 & & \exp(z_D) \end{pmatrix} \qquad \overline{\mathbf{z}} = \exp(\mathbf{z}) \circ \overline{\mathbf{y}}$$

- Note: we never explicitly construct the Jacobian. It's usually simpler and more efficient to compute the VJP directly.

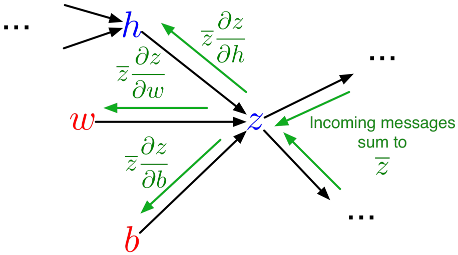
Vector-Jacobian Products

- For each primitive operation, we must specify VJPs for *each* of its arguments. Consider $y = \exp(x)$.
- This is a function which takes in the output gradient (i.e. $\overline{y}$), the answer (y), and the arguments (x), and returns the input gradient ($\overline{x}$)
- `defvjp` (defined in `core.py`) is a convenience routine for registering VJPs. It just adds them to a dict.
- Examples from `numpy/numpy_vjps.py`

```
defvjp(negative, lambda g, ans, x: -g)
defvjp(exp,      lambda g, ans, x: ans * g)
defvjp(log,      lambda g, ans, x: g / x)

defvjp(add,         lambda g, ans, x, y : g,
                    lambda g, ans, x, y : g)
defvjp(multiply,    lambda g, ans, x, y : y * g,
                    lambda g, ans, x, y : x * g)
defvjp(subtract,    lambda g, ans, x, y : g,
                    lambda g, ans, x, y : -g)
```

Backward Pass

- Recall that the backprop computations are more modular if we view them as message passing.



- This procedure can be implemented directly using the data structures we've introduced.

Backward Pass

- The backwards pass is defined in `core.py`.
- The argument g is the error signal for the end node; for us this is always $\overline{\mathcal{L}} = 1$.

```
def backward_pass(g, end_node):
    outgrads = {end_node: g}
    for node in toposort(end_node):
        outgrad = outgrads.pop(node)
        fun, value, args, kwargs, argnums = node.recipe
        for argnum, parent in zip(argnums, node.parents):
            vjp = primitive_vjps[fun][argnum]
            parent_grad = vjp(outgrad, value, *args, **kwargs)
            outgrads[parent] = add_outgrads(outgrads.get(parent), parent_grad)
    return outgrad

def add_outgrads(prev_g, g):
    if prev_g is None:
        return g
    return prev_g + g
```

Backward Pass

- grad (in differential_operators.py) is just a wrapper around make_vjp (in core.py) which builds the computation graph and feeds it to backward_pass.
- grad itself is viewed as a VJP, if we treat $\overline{\mathcal{L}}$ as the 1×1 matrix with entry 1.

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \frac{\partial \mathcal{L}}{\partial \mathbf{w}} \overline{\mathcal{L}}$$

```
def make_vjp(fun, x):
    """Trace the computation to build the computation graph, and return
    a function which implements the backward pass."""
    start_node = Node.new_root()
    end_value, end_node = trace(start_node, fun, x)
    def vjp(g):
        return backward_pass(g, end_node)
    return vjp, end_value

def grad(fun, argnum=0):
    def gradfun(*args, **kwargs):
        unary_fun = lambda x: fun(*subval(args, argnum, x), **kwargs)
        vjp, ans = make_vjp(unary_fun, args[argnum])
        return vjp(np.ones_like(ans))
    return gradfun
```

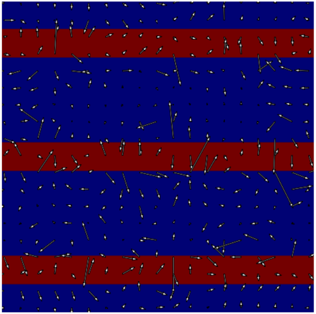
Recap

- We saw three main parts to the code:
  - tracing the forward pass to build the computation graph
  - vector-Jacobian products for primitive ops
  - the backwards pass
- Building the computation graph requires fancy NumPy gymnastics, but other two items are basically what I showed you.
- You're encouraged to read the full code ($<$ 200 lines!) at:

  `https://github.com/mattjj/autodidact/tree/master/autograd`

Differentiating through a Fluid Simulation

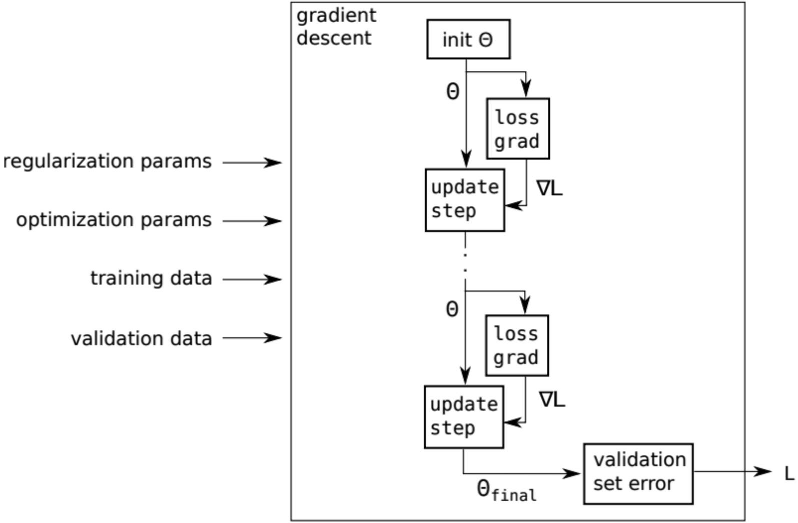
```python
def project(vx, vy):
    # Project the velocity field to be approximately mass-conserving,
    # using a few iterations of Gauss-Seidel.
    p = np.zeros(vx.shape)
    h = 1.0/vx.shape[0]
    div = -0.5 * h * (np.roll(vx, -1, axis=0) - np.roll(vx, 1, axis=0)
                    + np.roll(vy, -1, axis=1) - np.roll(vy, 1, axis=1))
    for k in range(10):
        p = (div + np.roll(p, 1, axis=0) + np.roll(p, -1, axis=0)
                 + np.roll(p, 1, axis=1) + np.roll(p, -1, axis=1))/4.0
    vx -= 0.5*(np.roll(p, -1, axis=0) - np.roll(p, 1, axis=0))/h
    vy -= 0.5*(np.roll(p, -1, axis=1) - np.roll(p, 1, axis=1))/h
    return vx, vy

def advect(f, vx, vy):
    # Move field f according to x and y velocities (u and v)
    # using an implicit Euler integrator.
    rows, cols = f.shape
    cell_ys, cell_xs = np.meshgrid(np.arange(rows),
                                   np.arange(cols))
    center_xs = (cell_xs - vx).ravel()
    center_ys = (cell_ys - vy).ravel()

    # Compute indices of source cells.
    left_ix = np.floor(center_xs).astype(int)
    top_ix  = np.floor(center_ys).astype(int)
    rw = center_xs - left_ix
    bw = center_ys - top_ix
    left_ix  = np.mod(left_ix,     rows)
    right_ix = np.mod(left_ix + 1, rows)
    top_ix   = np.mod(top_ix,      cols)
    bot_ix   = np.mod(top_ix  + 1, cols)

    flat_f = (1 - rw) * ((1 - bw)*f[left_ix,  top_ix] \
                          + bw*f[left_ix,  bot_ix]) \
                 + rw * ((1 - bw)*f[right_ix, top_ix] \
                          + bw*f[right_ix, bot_ix])
    return np.reshape(flat_f, (rows, cols))

def simulate(vx, vy, smoke, num_time_steps):
    for t in range(num_time_steps):
        vx_updated = advect(vx, vx, vy)
        vy_updated = advect(vy, vx, vy)
        vx, vy = project(vx_updated, vy_updated)
        smoke = advect(smoke, vx, vy)
    return smoke, frame_list
```



Differentiating through a Fluid Simulation

https://github.com/HIPS/autograd#end-to-end-examples

Gradient-Based Hyperparameter Optimization



Gradient-Based Hyperparameter Optimization