CSC2541: Neural Net Training Dynamics

Tutorial 1 - Backpropagation & Automatic Differentiation

University of Toronto, Winter 2022

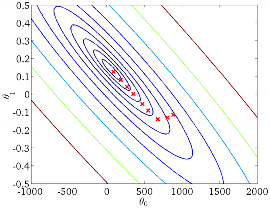
Slides adapted from CSC421

Overview

- Backpropagation is the central algorithm in training neural networks.
  - It's is an algorithm for computing gradients.
  - Really it's an instance of reverse mode automatic differentiation, which is much more broadly applicable than just neural networks.
    - This is "just" a clever and efficient use of the Chain Rule for derivatives.
    - We'll see how to implement an automatic differentiation system in this tutorial.

Recap: Gradient Descent

- **Recall:** Gradient descent moves opposite the gradient (the direction of steepest descent)



- We want to compute the cost gradient $\mathrm{d}\mathcal{J}/\mathrm{d}\mathbf{w}$, which is the vector of partial derivatives.
  - This is the average of $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$ over all the training examples, so in this lecture we focus on computing $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$.

Univariate Chain Rule

- **Recall**: if $f(x)$ and $x(t)$ are univariate functions, then

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t)) = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}t}.$$

Univariate Chain Rule

Recall: Univariate logistic least squares model

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

Let's compute the loss derivatives.

Univariate Chain Rule

How you would have done it in calculus class

$$
\begin{aligned}
\mathcal{L} &= \frac{1}{2}(\sigma(wx+b)-t)^2 \\
\frac{\partial \mathcal{L}}{\partial w} &= \frac{\partial}{\partial w}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial w}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial w}(\sigma(wx+b)-t) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)\frac{\partial}{\partial w}(wx+b) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)x
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial b} &= \frac{\partial}{\partial b}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial b}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial b}(\sigma(wx+b)-t) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)\frac{\partial}{\partial b}(wx+b) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)
\end{aligned}
$$

What are the disadvantages of this approach?

A more structured way to do it

Computing the loss:

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

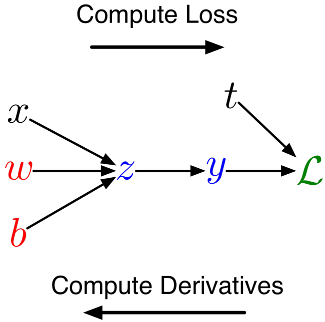
Computing the derivatives:

$$
\begin{aligned}
\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} &= y - t \\
\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\,\sigma'(z) \\
\frac{\partial\mathcal{L}}{\partial w} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}\,x \\
\frac{\partial\mathcal{L}}{\partial b} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}
\end{aligned}
$$

Remember, the goal isn't to obtain closed-form solutions, but to be able to write a program that efficiently computes the derivatives.

Univariate Chain Rule

- We can diagram out the computations using a computation graph.
- The nodes represent all the inputs and computed quantities, and the edges represent which nodes are computed directly as a function of which other nodes.



A slightly more convenient notation:

- Use $\overline{y}$ to denote the derivative $\mathrm{d}\mathcal{L}/\mathrm{d}y$, sometimes called the error signal.
- This emphasizes that the error signals are just values our program is computing (rather than a mathematical operation).
- This is not a standard notation, but I couldn't find another one that I liked.

Computing the loss:

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

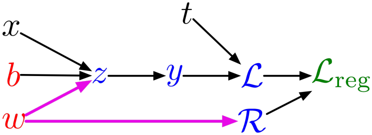
Computing the derivatives:

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

Multivariate Chain Rule

Problem: What if the computation graph has fan-out > 1?
This requires the multivariate Chain Rule!

L_2-Regularized regression



$$z = wx + b$$

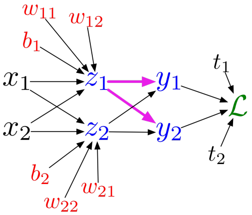
$$y = \sigma(z)$$

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

$$\mathcal{R} = \frac{1}{2}w^2$$

$$\mathcal{L}_{\text{reg}} = \mathcal{L} + \lambda\mathcal{R}$$

Multiclass logistic regression



$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$

$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$

$$\mathcal{L} = -\sum_k t_k \log y_k$$

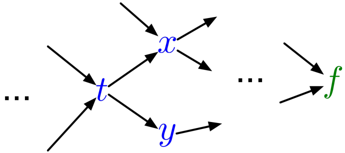
Multivariable Chain Rule

- In the context of backpropagation:

Mathematical expressions to be evaluated

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

Values already computed by our program



- In our notation:

$$\bar{t} = \bar{x}\,\frac{\mathrm{d}x}{\mathrm{d}t} + \bar{y}\,\frac{\mathrm{d}y}{\mathrm{d}t}$$

Backpropagation

Full backpropagation algorithm:

Let $v_1, \ldots, v_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

v_N denotes the variable we're trying to compute derivatives of (e.g. loss).

forward pass

For $i = 1, \ldots, N$

Compute v_i as a function of $\mathrm{Pa}(v_i)$

backward pass

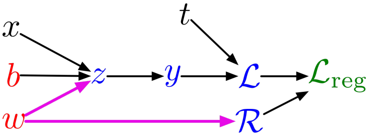
$\overline{v_N} = 1$

For $i = N-1, \ldots, 1$

$\overline{v_i} = \sum_{j \in \mathrm{Ch}(v_i)} \overline{v_j} \frac{\partial v_j}{\partial v_i}$

Backpropagation

Example: univariate logistic least squares regression



Forward pass:

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

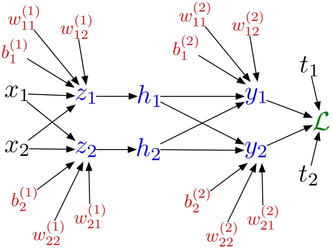
Backward pass:

$$
\begin{aligned}
\overline{\mathcal{L}_{\text{reg}}} &= 1 \\
\overline{\mathcal{R}} &= \overline{\mathcal{L}_{\text{reg}}}\, \frac{\mathrm{d}\mathcal{L}_{\text{reg}}}{\mathrm{d}\mathcal{R}} \\
&= \overline{\mathcal{L}_{\text{reg}}}\, \lambda \\
\overline{\mathcal{L}} &= \overline{\mathcal{L}_{\text{reg}}}\, \frac{\mathrm{d}\mathcal{L}_{\text{reg}}}{\mathrm{d}\mathcal{L}} \\
&= \overline{\mathcal{L}_{\text{reg}}} \\
\overline{y} &= \overline{\mathcal{L}}\, \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} \\
&= \overline{\mathcal{L}}\, (y - t)
\end{aligned}
$$

$$
\begin{aligned}
\overline{z} &= \overline{y}\, \frac{\mathrm{d}y}{\mathrm{d}z} \\
&= \overline{y}\, \sigma'(z) \\
\overline{w} &= \overline{z}\, \frac{\partial z}{\partial w} + \overline{\mathcal{R}}\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}w} \\
&= \overline{z}\, x + \overline{\mathcal{R}}\, w \\
\overline{b} &= \overline{z}\, \frac{\partial z}{\partial b} \\
&= \overline{z}
\end{aligned}
$$

Backpropagation

Multilayer Perceptron (multiple outputs):



Forward pass:

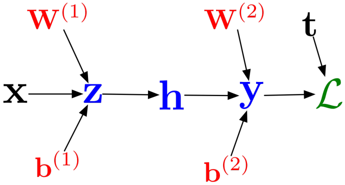
$$
\begin{aligned}
z_i &= \sum_j w_{ij}^{(1)} x_j + b_i^{(1)} \\
h_i &= \sigma(z_i) \\
y_k &= \sum_i w_{ki}^{(2)} h_i + b_k^{(2)} \\
\mathcal{L} &= \frac{1}{2} \sum_k (y_k - t_k)^2
\end{aligned}
$$

Backward pass:

$$
\begin{aligned}
\overline{\mathcal{L}} &= 1 \\
\overline{y_k} &= \overline{\mathcal{L}}\,(y_k - t_k) \\
\overline{w_{ki}^{(2)}} &= \overline{y_k}\, h_i \\
\overline{b_k^{(2)}} &= \overline{y_k} \\
\overline{h_i} &= \sum_k \overline{y_k} w_{ki}^{(2)} \\
\overline{z_i} &= \overline{h_i}\, \sigma'(z_i) \\
\overline{w_{ij}^{(1)}} &= \overline{z_i}\, x_j \\
\overline{b_i^{(1)}} &= \overline{z_i}
\end{aligned}
$$

Vector Form

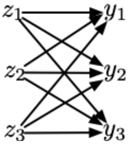
- Computation graphs showing individual units are cumbersome.
- As you might have guessed, we typically draw graphs over the vectorized variables.

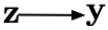


- We pass messages back analogous to the ones for scalar-valued nodes.

Vector Form

- Consider this computation graph:





- Backprop rules:

$$\overline{z_j} = \sum_k \overline{y_k} \frac{\partial y_k}{\partial z_j} \qquad \overline{\mathbf{z}} = \frac{\partial \mathbf{y}}{\partial \mathbf{z}}^\top \overline{\mathbf{y}},$$

where $\partial \mathbf{y} / \partial \mathbf{z}$ is the Jacobian matrix:

$$\frac{\partial \mathbf{y}}{\partial \mathbf{z}} = \begin{pmatrix} \frac{\partial y_1}{\partial z_1} & \cdots & \frac{\partial y_1}{\partial z_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial z_1} & \cdots & \frac{\partial y_m}{\partial z_n} \end{pmatrix}$$

Vector Form

Examples

- Matrix-vector product

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

- Elementwise operations

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

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

Vector Form

Full backpropagation algorithm (vector form):

Let $\mathbf{v}_1, \dots, \mathbf{v}_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

$\mathbf{v}_N$ denotes the variable we're trying to compute derivatives of (e.g. loss).
It's a scalar, which we can treat as a 1-D vector.

forward pass

For $i = 1, \dots, N$

  Compute $\mathbf{v}_i$ as a function of $\mathrm{Pa}(\mathbf{v}_i)$

backward pass

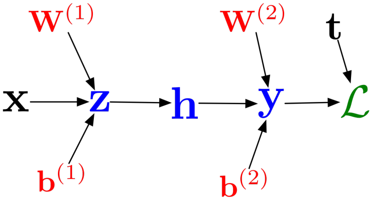
$\overline{\mathbf{v}_N} = 1$

For $i = N-1, \dots, 1$

$$\overline{\mathbf{v}_i} = \sum_{j \in \mathrm{Ch}(\mathbf{v}_i)} \frac{\partial \mathbf{v}_j}{\partial \mathbf{v}_i}^\top \overline{\mathbf{v}_j}$$

Vector Form

MLP example in vectorized form:



Forward pass:

$$\mathbf{z} = \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}$$
$$\mathbf{h} = \sigma(\mathbf{z})$$
$$\mathbf{y} = \mathbf{W}^{(2)}\mathbf{h} + \mathbf{b}^{(2)}$$
$$\mathcal{L} = \frac{1}{2}\|\mathbf{t} - \mathbf{y}\|^2$$

Backward pass:

$$\overline{\mathcal{L}} = 1$$
$$\overline{\mathbf{y}} = \overline{\mathcal{L}}\,(\mathbf{y} - \mathbf{t})$$
$$\overline{\mathbf{W}^{(2)}} = \overline{\mathbf{y}}\mathbf{h}^\top$$
$$\overline{\mathbf{b}^{(2)}} = \overline{\mathbf{y}}$$
$$\overline{\mathbf{h}} = \mathbf{W}^{(2)\top}\overline{\mathbf{y}}$$
$$\overline{\mathbf{z}} = \overline{\mathbf{h}} \circ \sigma'(\mathbf{z})$$
$$\overline{\mathbf{W}^{(1)}} = \overline{\mathbf{z}}\mathbf{x}^\top$$
$$\overline{\mathbf{b}^{(1)}} = \overline{\mathbf{z}}$$

Some Thoughts

- Backprop is used to train the overwhelming majority of neural nets today.
  - Even optimization algorithms much fancier than gradient descent (e.g. second-order methods) use backprop to compute the gradients.
- Despite its practical success, backprop is believed to be neurally implausible.
  - No evidence for biological signals analogous to error derivatives.
  - All the biologically plausible alternatives we know about learn much more slowly (on computers).
  - So how on earth does the brain learn?

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.
  - Today, 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”

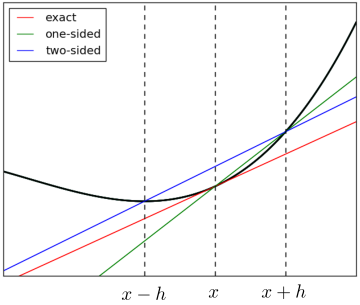
What Autodiff Is Not: Finite Differences

- We often use finite differences to check our gradient calculations.
- One-sided version:

$$\frac{\partial}{\partial x_i} f(x_1, \dots, x_N) \approx \frac{f(x_1, \dots, x_i + h, \dots, x_N) - f(x_1, \dots, x_i, \dots, x_N)}{h}$$

- Two-sided version:

$$\frac{\partial}{\partial x_i} f(x_1, \dots, x_N) \approx \frac{f(x_1, \dots, x_i + h, \dots, x_N) - f(x_1, \dots, x_i - h, \dots, x_N)}{2h}$$



Autodiff Is Not: Finite Differences

- 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.

Autodiff Is Not: Symbolic Differentiation

- 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.

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 (ops) 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:

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

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) …

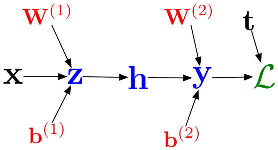
```python
# Define a function that returns gradients of training loss using Autograd.
training_gradient_fun = grad(training_loss)

# 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 tutorial 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!

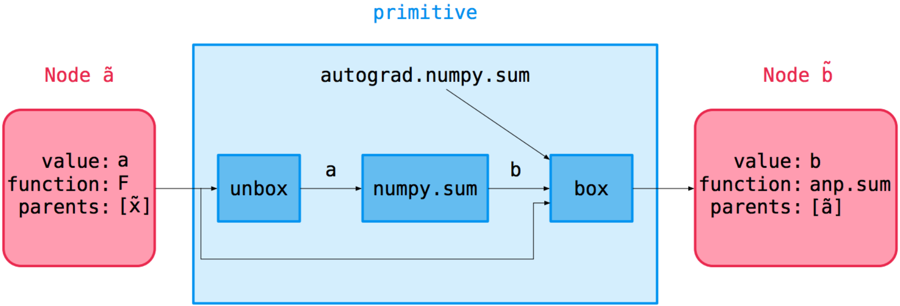
Building the Computation Graph



- 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

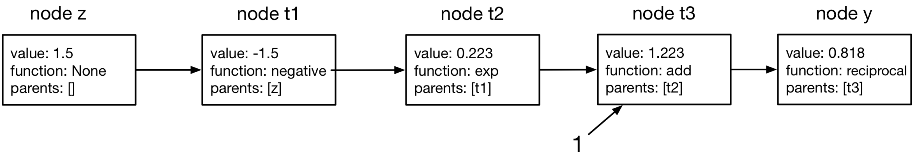
- Autograd's fake NumPy module provides primitive ops which look and feel like NumPy functions, but secretly build the computation graph.
- They wrap around NumPy functions:



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)
```



Recap: Vector-Jacobian Products

- Recall: 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):

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

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

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

Recap: Vector-Jacobian Products

Examples

- Matrix-vector product

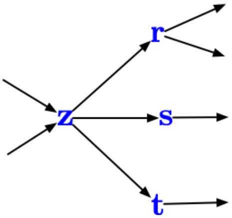
$$\mathbf{z} = \mathbf{W}\mathbf{x} \qquad \mathbf{J} = \mathbf{W} \qquad \overline{\mathbf{x}} = \mathbf{W}^\top \overline{\mathbf{z}}$$

- 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.

Backprop as Message Passing

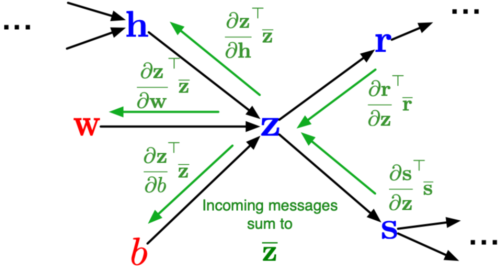


- Consider a naïve backprop implementation where the $\mathbf{z}$ module needs to compute $\overline{\mathbf{z}}$ using the formula:

$$\overline{\mathbf{z}} = \frac{\partial \mathbf{r}}{\partial \mathbf{z}}\overline{\mathbf{r}} + \frac{\partial \mathbf{s}}{\partial \mathbf{z}}\overline{\mathbf{s}} + \frac{\partial \mathbf{t}}{\partial \mathbf{z}}\overline{\mathbf{t}}$$

- This breaks modularity, since $\mathbf{z}$ needs to know how it's used in the network in order to compute partial derivatives of $\mathbf{r}$, $\mathbf{s}$, and $\mathbf{t}$.

Backprop as message passing:



- Each node receives a bunch of messages from its children, which it aggregates to get its error signal. It then passes messages to its parents.
- Each of these messages is a VJP.
- This formulation provides modularity: each node needs to know how to compute its outgoing messages, i.e. the VJPs corresponding to each of its parents (arguments to the function).
- The implementation of $\mathbf{z}$ doesn't need to know where $\overline{\mathbf{z}}$ came from.

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

- 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`