Make a forward pass before the backward pass



### Backpropagation: Understanding the implications of the chain rule

#### Jonathon Hare

Vision, Learning and Control University of Southampton

A lot of the ideas in this lecture come from Andrej Karpathy's blog post on backprop (https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b) and his CS231n Lecture Notes (http://cs231n.github.io/optimization-2/)

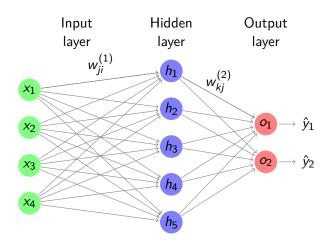


#### **Topics**

- A quick look at an MLP again
- The chain rule (again)
- Uninititive gradient effects
- A closer look at basic stochastic gradient descent algorithms

Jonathon Hare Backpropagation 3 / 13

### The unbiased Multilayer Perceptron (again)...



Without loss of generality, we can write the above as:

$$\hat{\mathbf{y}} = g(f(\mathbf{x}; \mathbf{W}^{(1)}); \mathbf{W}^{(2)}) = g(\mathbf{W}^{(2)}f(\mathbf{W}^{(1)}\mathbf{x}))$$

where f and g are activation functions.

Let's assume MSE Loss

$$\ell_{MSE}(\boldsymbol{\hat{y}}, \boldsymbol{y}) = \|\boldsymbol{\hat{y}} - \boldsymbol{y}\|_2^2$$

Let's assume MSE Loss

$$\ell_{MSE}(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2$$

• What are the gradients?

$$\nabla_{\boldsymbol{W}^*}\ell_{MSE}(g(\boldsymbol{W}^{(2)}f(\boldsymbol{W}^{(1)}\boldsymbol{x})),\boldsymbol{y})$$

Let's assume MSE Loss

$$\ell_{MSE}(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2$$

• What are the gradients?

$$\nabla_{\boldsymbol{W}^*}\ell_{MSE}(g(\boldsymbol{W}^{(2)}f(\boldsymbol{W}^{(1)}\boldsymbol{x})),\boldsymbol{y})$$

• Clearly we need to apply the chain rule (vector form) multiple times

Let's assume MSE Loss

$$\ell_{MSE}(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2$$

• What are the gradients?

$$\nabla_{\boldsymbol{W}^*}\ell_{MSE}(g(\boldsymbol{W}^{(2)}f(\boldsymbol{W}^{(1)}\boldsymbol{x})),\boldsymbol{y})$$

- Clearly we need to apply the chain rule (vector form) multiple times
- We could do this by hand

Let's assume MSE Loss

$$\ell_{MSE}(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2$$

• What are the gradients?

$$\nabla_{\boldsymbol{W}^*}\ell_{MSE}(g(\boldsymbol{W}^{(2)}f(\boldsymbol{W}^{(1)}\boldsymbol{x})),\boldsymbol{y})$$

- Clearly we need to apply the chain rule (vector form) multiple times
- We could do this by hand
- (But we're not that crazy!)

$$f(x, y, z) = (x + y)z$$
  
 $\equiv qz \text{ where } q = (x + y)$ 

$$f(x, y, z) = (x + y)z$$
  
 $\equiv qz \text{ where } q = (x + y)$ 

Clearly the partial derivatives of the subexpressions are trivial:

$$\partial f/\partial z = q$$
  $\partial f/\partial q = z$   $\partial q/\partial x = 1$   $\partial q/\partial y = 1$ 

$$f(x, y, z) = (x + y)z$$
  
 $\equiv qz \text{ where } q = (x + y)$ 

Clearly the partial derivatives of the subexpressions are trivial:

$$\partial f/\partial z = q$$
  $\partial f/\partial q = z$   
 $\partial q/\partial x = 1$   $\partial q/\partial y = 1$ 

and the chain rule tells us how to combine these:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \cdot \frac{\partial q}{\partial x} = z$$
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \cdot \frac{\partial q}{\partial y} = z$$

$$f(x, y, z) = (x + y)z$$
  
 $\equiv qz \text{ where } q = (x + y)$ 

Clearly the partial derivatives of the subexpressions are trivial:

$$\partial f/\partial z = q$$
  $\partial f/\partial q = z$   $\partial q/\partial x = 1$   $\partial q/\partial y = 1$ 

and the chain rule tells us how to combine these:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \cdot \frac{\partial q}{\partial x} = z$$
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \cdot \frac{\partial q}{\partial y} = z$$

so 
$$\nabla_{[x,y,z]}f = [z,z,q]$$

Jonathon Hare Backpropagation 6 / 13

### A computational graph perspective

$$f(x,y,z)=(x+y)z$$

#### An intuition of the chain rule

- Notice how every operation in the computational graph given its inputs can immediately compute two things:
  - 1 its output value
  - 2 the local gradient of its inputs with respect to its output value
- The chain rule tells us literally that each operation should take its local gradients and multiply them by the gradient that flows backwards into it

#### This is backpropagation

- The backprop algorithm is just the idea that you can perform the forward pass (computing and caching the local gradients as you go),
- and then perform a backward pass to compute the total gradient by applying the chain rule and re-utilising the cached local gradients

#### This is backpropagation

- The backprop algorithm is just the idea that you can perform the forward pass (computing and caching the local gradients as you go),
- and then perform a backward pass to compute the total gradient by applying the chain rule and re-utilising the cached local gradients
- Backprop is just another name for 'Reverse Mode Automatic Differentiation'...

• Consider the multiplication operation  $f(a, b) = a \times b$ .

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .
  - (in a computational graph these would be the local gradients w.r.t the inputs)

Jonathon Hare Backpropagation 10 / 13

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .
  - (in a computational graph these would be the local gradients w.r.t the inputs)
- If a is large and b is tiny the gradient assigned to b will be large, and the gradient to a small.

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .
  - (in a computational graph these would be the local gradients w.r.t the inputs)
- If a is large and b is tiny the gradient assigned to b will be large, and the gradient to a small.
- This has implications for e.g. linear classifiers  $(\mathbf{w}^{\top} \mathbf{x}_i)$  where you perform many multiplications

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .
  - (in a computational graph these would be the local gradients w.r.t the inputs)
- If a is large and b is tiny the gradient assigned to b will be large, and the gradient to a small.
- This has implications for e.g. linear classifiers  $(\mathbf{w}^{\top} \mathbf{x}_i)$  where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .
  - (in a computational graph these would be the local gradients w.r.t the inputs)
- If a is large and b is tiny the gradient assigned to b will be large, and the gradient to a small.
- This has implications for e.g. linear classifiers  $(\mathbf{w}^{\top} \mathbf{x}_i)$  where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data
  - multiply  $x_i$  by 1000, and the gradients also increase by 1000

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .
  - (in a computational graph these would be the local gradients w.r.t the inputs)
- If a is large and b is tiny the gradient assigned to b will be large, and the gradient to a small.
- This has implications for e.g. linear classifiers  $(\mathbf{w}^{\top} \mathbf{x}_i)$  where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data
  - multiply  $x_i$  by 1000, and the gradients also increase by 1000
  - if you don't lower the learning rate to compensate your model might not learn

Jonathon Hare Backpropagation 10 / 13

- Consider the multiplication operation  $f(a, b) = a \times b$ .
- The gradients are clearly  $\partial f/\partial b = a$  and  $\partial f/\partial a = b$ .
  - (in a computational graph these would be the local gradients w.r.t the inputs)
- If a is large and b is tiny the gradient assigned to b will be large, and the gradient to a small.
- This has implications for e.g. linear classifiers  $(\mathbf{w}^{\top} \mathbf{x}_i)$  where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data
  - multiply  $x_i$  by 1000, and the gradients also increase by 1000
  - if you don't lower the learning rate to compensate your model might not learn
  - Hence you need to always pay attention to data normalisation!

• It used to be popular to use sigmoids (or tanh) in the hidden layers...

Jonathon Hare Backpropagation 11 / 13

- It used to be popular to use sigmoids (or tanh) in the hidden layers...
- Gradient of  $\sigma(x) = \sigma(x)(1 \sigma(x))$

Jonathon Hare Backpropagation 11 / 13

- It used to be popular to use sigmoids (or tanh) in the hidden layers...
- Gradient of  $\sigma(x) = \sigma(x)(1 \sigma(x))$
- Thus as part of a larger network where this is the local gradient, if x
  is large (+ve or -ve), then all gradients backwards from this point will
  be zero due to multiplication of the chain rule
  - Why might x be large?

- It used to be popular to use sigmoids (or tanh) in the hidden layers...
- Gradient of  $\sigma(x) = \sigma(x)(1 \sigma(x))$
- Thus as part of a larger network where this is the local gradient, if x is large (+ve or -ve), then all gradients backwards from this point will be zero due to multiplication of the chain rule
  - Why might x be large?
- Maximum gradient is achieved when x = 0 ( $\sigma(x) = 0.5$ , dx = 0.25)

Backpropagation 11 / 13

- It used to be popular to use sigmoids (or tanh) in the hidden layers...
- Gradient of  $\sigma(x) = \sigma(x)(1 \sigma(x))$
- Thus as part of a larger network where this is the local gradient, if x is large (+ve or -ve), then all gradients backwards from this point will be zero due to multiplication of the chain rule
  - Why might x be large?
- Maximum gradient is achieved when x = 0  $(\sigma(x) = 0.5, dx = 0.25)$ 
  - This means that the maximum gradient that can flow out of a sigmoid will be a quarter of the input gradient

Backpropagation 11 / 13

- It used to be popular to use sigmoids (or tanh) in the hidden layers...
- Gradient of  $\sigma(x) = \sigma(x)(1 \sigma(x))$
- Thus as part of a larger network where this is the local gradient, if x is large (+ve or -ve), then all gradients backwards from this point will be zero due to multiplication of the chain rule
  - Why might x be large?
- Maximum gradient is achieved when x = 0  $(\sigma(x) = 0.5, dx = 0.25)$ 
  - This means that the maximum gradient that can flow out of a sigmoid will be a quarter of the input gradient
    - What's the implication of this in a deep network with sigmoid activations?

Backpropagation 11 / 13

Modern networks tend to use ReLUs

- Modern networks tend to use ReLUs
- Gradient is 1 for x > 0 and 0 otherwise

- Modern networks tend to use ReLUs
- Gradient is 1 for x > 0 and 0 otherwise
- Consider ReLU( $\boldsymbol{w}^{\top}\boldsymbol{x}$ )
  - What happens if w is initialised badly?
  - What happens if w receives an update that means that  $w^{\top}x < 0 \ \forall \ x$ ?

- Modern networks tend to use ReLUs
- Gradient is 1 for x > 0 and 0 otherwise
- Consider ReLU( $\boldsymbol{w}^{\top}\boldsymbol{x}$ )
  - What happens if w is initialised badly?
  - What happens if w receives an update that means that  $w^{\top}x < 0 \ \forall \ x$ ?
- These are dead ReLUs ones that never fire for all training data
  - Sometimes you can find that you have a large fraction of these
  - if you get them from the beginning, check weight initialisation and data normalisation
  - ullet if they're appearing during training, maybe  $\eta$  is too big?

 Recurrent networks apply a function recursively for some number of timesteps

- Recurrent networks apply a function recursively for some number of timesteps
- Often this recursion involves a multiplication at each timestep, the gradients of which are all multiplied together because of the chain rule...

- Recurrent networks apply a function recursively for some number of timesteps
- Often this recursion involves a multiplication at each timestep, the gradients of which are all multiplied together because of the chain rule...
- Consider  $z = a \prod_{n=1}^{\infty} b$

- Recurrent networks apply a function recursively for some number of timesteps
- Often this recursion involves a multiplication at each timestep, the gradients of which are all multiplied together because of the chain rule...
- Consider  $z = a \prod_{n=0}^{\infty} b$ 
  - $z \rightarrow 0$  if |b| < 1

- Recurrent networks apply a function recursively for some number of timesteps
- Often this recursion involves a multiplication at each timestep, the gradients of which are all multiplied together because of the chain rule...
- Consider  $z = a \prod_{n=1}^{\infty} b$ 
  - $z \to 0$  if |b| < 1
  - ullet  $z 
    ightarrow \infty$  if |b| > 1

- Recurrent networks apply a function recursively for some number of timesteps
- Often this recursion involves a multiplication at each timestep, the gradients of which are all multiplied together because of the chain rule...
- Consider  $z = a \prod_{n=1}^{\infty} b$ 
  - $z \rightarrow 0$  if |b| < 1
  - $z \rightarrow \infty$  if |b| > 1
- Same thing happens in the backward pass of an RNN (although with matrices rather than scalars, so the reasoning applies to the largest eigenvalue)