Make a forward pass before the backward pass



Backpropagation: Understanding the implications of the chain rule

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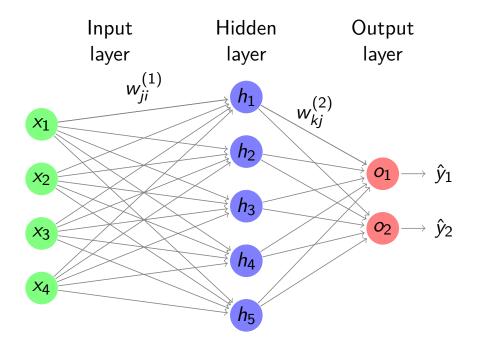
A lot of the ideas in this lecture come from Andrej Karpathy's blog post on backprop (https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b) and his CS231n Lecture Notes (http://cs231n.github.io/optimization-2/)



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

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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.

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Gradients of our simple unbiased MLP

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!)

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Let's go back to a simpler expression

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

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

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:

$$\partial f/\partial x = \partial f/\partial q \cdot \partial q/\partial x = z$$

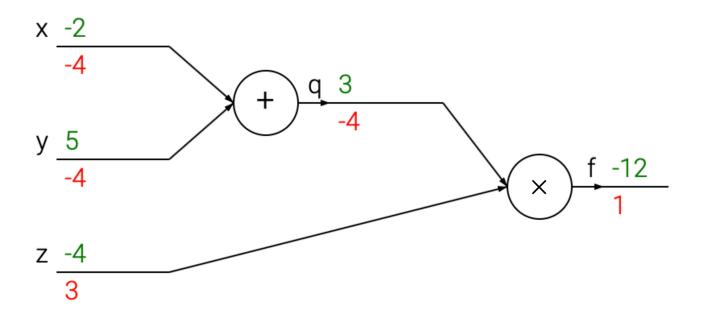
 $\partial f/\partial y = \partial f/\partial q \cdot \partial q/\partial y = z$

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

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A computational graph perspective

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



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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

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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'...

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Unintuitive effects I: Multiplication

- Consider the multiplication operation f(a, b) = a * 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!

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Unintuitive effects II: vanishing gradients of the sigmoid

- 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?

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Unintuitive effects III: dying ReLUs

- 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 η is too big?

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Unintuitive effects IV: Exploding gradients in recurrent networks

- 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 $z = a \prod_{n=0}^{\infty} b$
 - ullet z
 ightarrow 0 if |b| < 1
 - $z \to \infty$ 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)

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