Make a forward pass before the backward pass

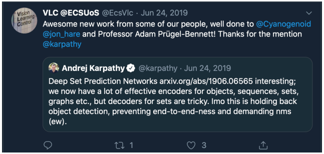
VLC = ∭ Vision Learning Control dVdLdC

Backpropagation: Understanding the implications of the chain rule

Jonathon Hare

Vision, Learning and Control
University of Southampton

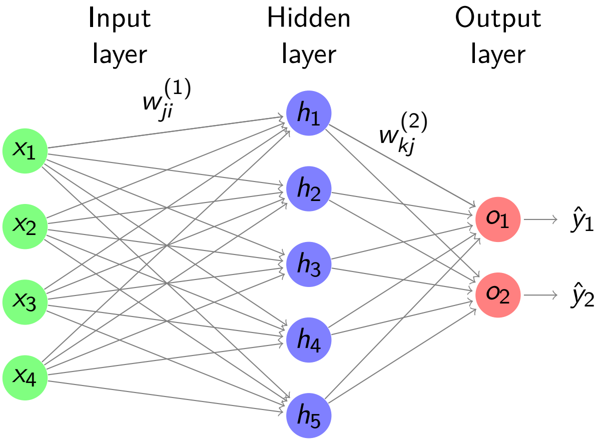
A lot of the ideas in this lecture come from Andrej Karpathy's blog post on backprop (https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b) and his CS231n Lecture Notes (http://cs231n.github.io/optimization-2/)



Topics

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

The unbiased Multilayer Perceptron (again)...



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

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

where f and g are activation functions.

Gradients of our simple unbiased MLP

- Let's assume MSE Loss

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

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?

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

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

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

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!)

Let's go back to a simpler expression

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

Let's go back to a simpler expression

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

Clearly the partial derivatives of the subexpressions are trivial:

$$
\begin{aligned}
\partial f / \partial z &= q \qquad & \partial f / \partial q &= z \\
\partial q / \partial x &= 1 \qquad & \partial q / \partial y &= 1
\end{aligned}
$$

Let's go back to a simpler expression

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

Clearly the partial derivatives of the subexpressions are trivial:

$$
\begin{aligned}
\partial f / \partial z &= q & \partial f / \partial q &= z \\
\partial q / \partial x &= 1 & \partial q / \partial y &= 1
\end{aligned}
$$

and the chain rule tells us how to combine these:

$$
\begin{aligned}
\partial f / \partial x &= \partial f / \partial q \cdot \partial q / \partial x = z \\
\partial f / \partial y &= \partial f / \partial q \cdot \partial q / \partial y = z
\end{aligned}
$$

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:

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

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

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'...

Unintuitive effects I: Multiplication

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

Unintuitive effects I: Multiplication

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

Unintuitive effects I: Multiplication

- 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)

Unintuitive effects I: Multiplication

- 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.

Unintuitive effects I: Multiplication

- 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 ($\boldsymbol{w}^\top \boldsymbol{x}_i$) where you perform many multiplications

Unintuitive effects I: Multiplication

- 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 ($\boldsymbol{w}^\top \boldsymbol{x}_i$) where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data

Unintuitive effects I: Multiplication

- 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 ($\boldsymbol{w}^\top \boldsymbol{x}_i$) where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data
  - multiply $\boldsymbol{x}_i$ by 1000, and the gradients also increase by 1000

Unintuitive effects I: Multiplication

- 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 ($\boldsymbol{w}^\top \boldsymbol{x}_i$) where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data
  - multiply $\boldsymbol{x}_i$ by 1000, and the gradients also increase by 1000
  - if you don't lower the learning rate to compensate your model might not learn

Unintuitive effects I: Multiplication

- 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 ($\boldsymbol{w}^\top \boldsymbol{x}_i$) where you perform many multiplications
  - the magnitude of the gradient is directly proportional to the magnitude of the data
  - multiply $\boldsymbol{x}_i$ 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!**

Unintuitive effects II: vanishing gradients of the sigmoid

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

Unintuitive effects II: vanishing gradients of the sigmoid

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

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?

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 $x = 0 \quad (\sigma(x) = 0.5,\ dx = 0.25)$

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 $x = 0 \quad (\sigma(x) = 0.5,\ dx = 0.25)$
  - This means that the maximum gradient that can flow out of a sigmoid will be a quarter of the input gradient

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 $x = 0 \quad (\sigma(x) = 0.5,\ dx = 0.25)$
  - 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?

Unintuitive effects III: dying ReLUs

- Modern networks tend to use ReLUs

Unintuitive effects III: dying ReLUs

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

Unintuitive effects III: dying ReLUs

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

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 $\boldsymbol{w}$ is initialised badly?
  - What happens if $\boldsymbol{w}$ receives an update that means that $\boldsymbol{w}^\top \boldsymbol{x} < 0 \; \forall \; \boldsymbol{x}$?
- 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
  - if they're appearing during training, maybe λ is too big?

Unintuitive effects IV: Exploding gradients in recurrent networks

- Recurrent networks apply a function recursively for some number of timesteps

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...

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 $z = a \prod_{n}^{\infty} b$

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 $z = a \prod_n^\infty b$
  - $z \to 0 \ if \ |b| < 1$

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 $z = a \prod_n^\infty b$
  - $z \to 0$ *if* $|b| < 1$
  - $z \to \infty$ *if* $|b| > 1$

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 $z = a \prod_n^\infty b$
  - $z \to 0$ *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)