Lecture 4: Backpropagation

CS4787/5777 — Principles of Large-Scale Machine Learning Systems

Continuing from last time: Forward Mode AD

- Fix one input variable x over $\mathbb{R}$.
- At each step of the computation, as we're computing some value y, also compute $\frac{\partial y}{\partial x}$.
- We can do this with a *dual numbers* approach: each number y is replaced with a pair $(y, \frac{\partial y}{\partial x})$.

Forward Mode AD Takeaways

- Each operation in the original program is replaced with two operations
  - one to compute the value y (same as original)
  - one to compute the derivative $\frac{\partial y}{\partial x}$
- The new operation has an analogous structure to the original one
  - since its the derivative
  - e.g. a matrix multiply would produce a new matrix multiply
- If the original operation had compute cost C, the new operation has cost $O(C)$.

Implementing Forward Mode AD

In Python, we can use operator overloading and dynamic typing. Suppose I write a function

In [4]:
```
def f(x):
    return x*x + 1.0
```

imagining that we will call it with `x` being a floating-point number.

- I can still call it with `x` being a dual number (because Python is not explicitly typed).
- When I do this, the operators `*` and `+` desugar to calls to my `__mul__` and `__add__` methods.
- I can do the differentiation in these methods.
- I can do this across the whole program to differentiate compositions of functions!

Benefits of Forward Mode AD

- Simple in-place operations

- Easy to extend to compute higher-order derivatives
- Only constant factor increase in memory use, since each $\frac{\partial y}{\partial x}$ object is the same size as y and is only *live* when y is

Problems with Forward Mode AD

- Differentiate with respect to **one** input
  - problematic for ML, where we usually want to compute gradients
  - If we are computing a gradient of $f : \mathbb{R}^d \to \mathbb{R}$, blow-up proportional to the dimension d

Reverse-Mode AD

- Fix one output ℓ over $\mathbb{R}$
- Compute partial derivatives $\frac{\partial \ell}{\partial y}$ for each value y
- Need to do this by going *backward* through the computation

Problem: can't just compute derivatives as-we-go like with forward mode AD.

Backpropagation: The usual type of Reverse-AD we use

Same as before: we replace each number/array y with a pair, except this time the pair is not $(y, \frac{\partial y}{\partial x})$ but instead $(y, \nabla_y \ell)$ where ℓ is one fixed output.

- I use ℓ here because usually in ML the output is a loss.
- Observe that $\nabla_y \ell$ always has the same shape as y.

Deriving Backprop from the Chain Rule

Suppose that the output ℓ can be written as

$$\ell = f(u),\ u = g(y).$$

Here, g represents the immediate next operation that consumes the intermediate value y (producing a new intermediate u), and f represents all the rest of the computation. Suppose all these expressions are scalars. By the chain rule,

$$\frac{\partial \ell}{\partial y} = g'(y) \cdot \frac{\partial \ell}{\partial u}.$$

That is, we can compute $\frac{\partial \ell}{\partial y}$ using only "local" information (information that's available in the program around where y is computed and used) and $\frac{\partial \ell}{\partial u}$.

Deriving Backprop from the Chain Rule

More generally, suppose that the output ℓ can be written as

$$\ell = F(u_1, u_2, \ldots, u_k),\ u_i = g_i(y).$$

Here, the $g_1, g_2, \ldots, g_k$ represent the immediate next operations that consume the intermediate value y (note that there may be many such g), the u_i are the arrays output by those operations, and F represents all the rest of the computation. By the multivariate chain rule,

$$\nabla_y \ell = \sum_{i=1}^{k} Dg_i(y)^T \nabla_{u_i} \ell.$$

Again, we see that we can compute $\frac{\partial \ell}{\partial y}$ using only "local" information and the gradients of the loss with respect to each array that immediately depends on y, i.e. $\nabla_{u_i} \ell$.

When can we compute the gradient with respect to y?

- Not immediately when we compute y.
- Not until **after** we've computed the gradient with respect to every other array/tensor that y was used to compute.

Idea: remember the order in which we computed all the intermediate arrays/tensors, and then compute their gradients in the reverse order.

When can we start computing the gradient with respect to y?

$$\nabla_y \ell = \sum_{i=1}^{k} Dg_i(y)^T \nabla_{u_i} \ell.$$

- The gradient with respect to y is a sum of a bunch of components, one for each array/tensor that immediately depends on y.
- We can compute each element of that sum as soon as we know the gradient with respect to the corresponding tensor.

High-level BP algorithm:

- For each array/tensor, initialize a gradient "accumulator" to 0. Set the gradient of ℓ with respect to itself to 1.
- For each array/tensor u **in reverse order of computation**, for each array/tensor y on which u depends, compute $D_y u^T \nabla_u \ell$ and add it to y's gradent accumulator.
    - Once this step is called for y, its gradient will be fully manifested in its gradient accumulator.

Suppose $u \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$. Then $D_y u \in \mathbb{R}^{n \times m}$ and $(D_y u)^T \in \mathbb{R}^{m \times n}$. And note that $\nabla_u \ell \in \mathbb{R}^n$

When can we start computing the gradient with respect to y?

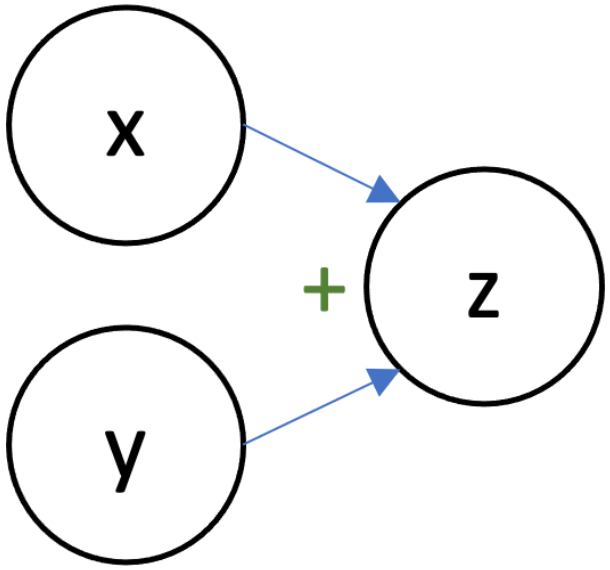
$$\underbrace{\nabla_y \ell}_{\text{this is used when we process y}} = \sum_{i=1}^{k} \underbrace{Dg_i(y)^T \nabla_{u_i} \ell}_{\text{this is computed when we process } u_i} .$$

- Since all the u_i were computed after y...
- ...because the u_i depend on y...
- ...if we process the gradients in the reverse order, this will work!

But how can we do this?

- Ordinary numbers in a program don't keep track of what they were computed "from"
- Ordinary numbers in a program don't keep track of the order in which they were computed

Computational Graphs



$$z = x + y$$

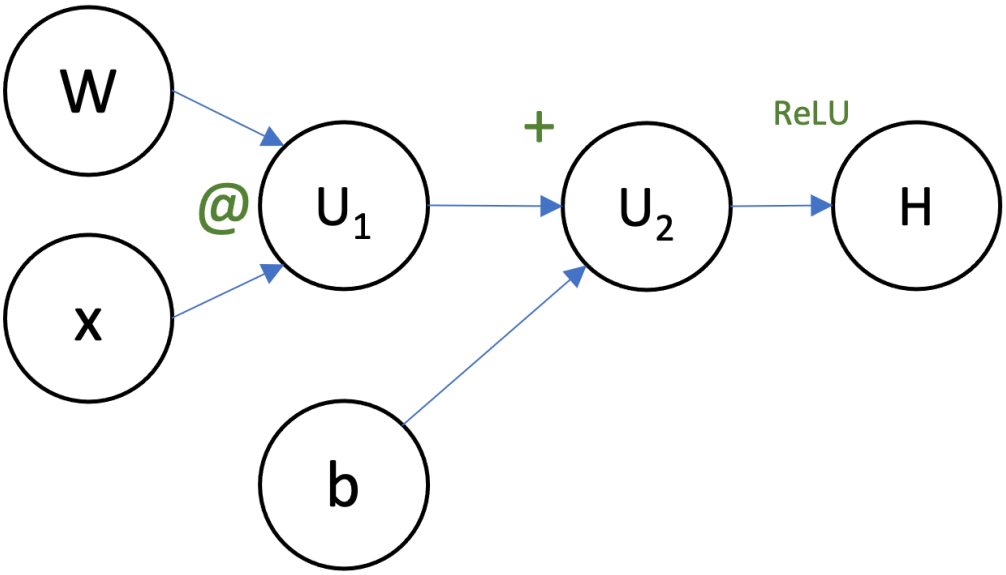
- Each node represents an scalar/vector/tensor/array.
- Edges represent dependencies.
  - $y \to u$ means that y was used to compute u

Exercise: Computational Graphs

Can you draw the computational graph for the function

$$H = \max(0, Wx + b)$$

for $W \in \mathbb{R}^{c \times d}$, $x \in \mathbb{R}^d$, and $b \in \mathbb{R}^c$?



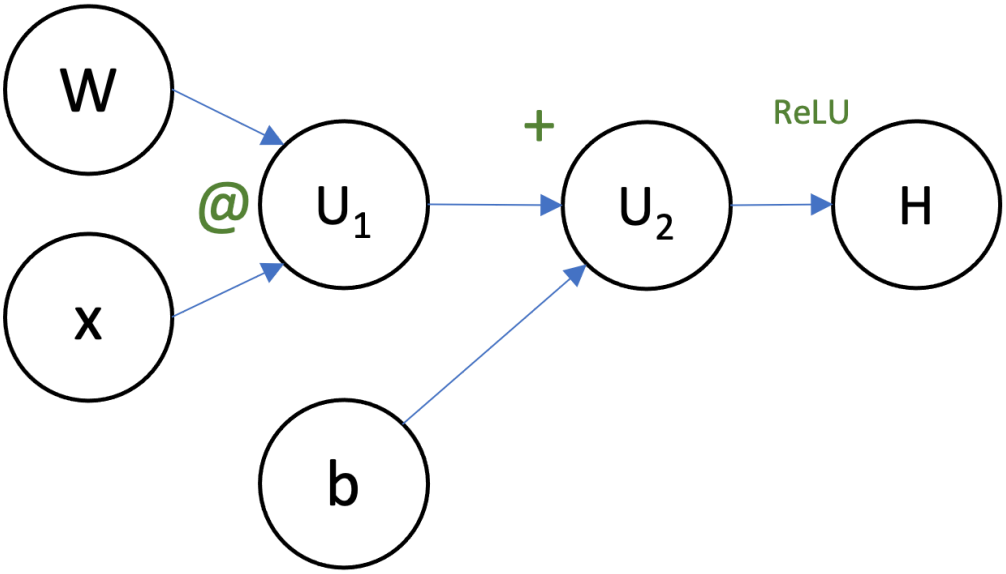
Backprop in Computational Graphs

To do backprop in a computation represented by a computational graph:

- we first move **forward** through the graph computing values (in the direction of the arrows),
- then we move **backward** through the graph accumulating gradients (opposite the direction of the arrows).

Exercise: Backprop

Using your computational graph, suppose that $W = 2$, $x = 3$, and $b = 1$. Write out (in order!) the steps that backprop would to to compute the gradients of H with respect to everything (W, x, and b).



- $U_1 = 2 \cdot 3 = 6$

- $U_2 = U_1 + b = 6 + 1 = 7$
- $H = \text{ReLU}(U_2) = \text{ReLU}(7) = 7$
- $\nabla_H H = \frac{\partial H}{\partial H} = 1$
- $\frac{\partial H}{\partial U_2} = \frac{\partial}{\partial U_2} H(\text{ReLU}(U_2)) = \text{ReLU}'(U_2) \cdot \frac{\partial H}{\partial H} = 1 \cdot 1 = 1$
- $\frac{\partial H}{\partial b} = \frac{\partial}{\partial b} H(U_2(b)) = H'(U_2(b)) \cdot U_2'(b) = \frac{\partial H}{\partial U_2} \cdot \frac{\partial U_2}{\partial b} = 1 \cdot 1 = 1$
- $\frac{\partial H}{\partial U_1} = \frac{\partial H}{\partial U_2} \cdot \frac{\partial U_2}{\partial U_1} = 1 \cdot 1 = 1$
- $\frac{\partial H}{\partial W} = \frac{\partial}{\partial W} H(Wx) = \frac{\partial H}{\partial U_1} \cdot x = 1 \cdot 3 = 3$
- $\frac{\partial H}{\partial x} = \frac{\partial}{\partial x} H(Wx) = \frac{\partial H}{\partial U_1} \cdot W = 1 \cdot 2 = 2$

Exercise 2: Backprop on a non-tree DAG

$$u = x + 1 \qquad y = xu = x(x+1)$$

$$x = 17$$

Note: $17 \cdot 18 = 306$ (according to ChatGPT)

- $\frac{dy}{dx} \leftarrow 0$
- $u = x + 1 = 17 + 1 = 18$
- $u.\text{grad} \leftarrow 0$
- $y = xu = 17 \cdot 18 = 306$
- $\frac{dy}{dy} \leftarrow 0$

- $\frac{dy}{dy} \leftarrow 1$
- $\frac{dy}{du} \leftarrow \frac{dy}{du} + \frac{dy}{dy} \cdot \frac{d}{du}(xu) = 0 + 1 \cdot x = 17$
- $\frac{dy}{dx} \leftarrow \frac{dy}{dx} + \frac{dy}{dy} \cdot u = 0 + 1 \cdot u = 18$
- $\frac{dy}{dx} \leftarrow \frac{dy}{dx} + \frac{dy}{du} \cdot \frac{d}{dx}(x+1) = 18 + 17 \cdot 1 = 35$

Advantages/Disadvantages of Backpropagation

$$F(u, v) = uv$$

$$\ell = F(x, x)$$

$$\frac{d\ell}{dx} = \frac{dF}{du} \cdot \frac{du}{dx} + \frac{dF}{dv} \cdot \frac{dv}{dx}$$

$$\frac{d\ell}{dx} = v \cdot 1 + u \cdot 1$$

$$\frac{d\ell}{dx} = v + u = x + x = 2x$$

Advantages:

- Compute gradients with little (constant-factor) overhead

Disadvantages:

- Memory!
  - Need to store a lot of derivatives
  - Need to manifest the whole compute graph
- Scheduling questions (how to order)

In [ ]: