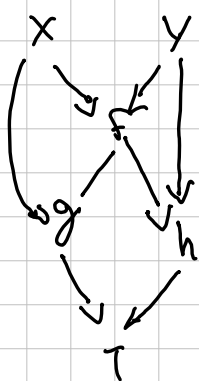


Take a computational graph and transform it to a graph in topological order. Example



→



$$T(x, y) =$$

$$T[g(x, f(z, y)), h(f(x, y), y)]$$

Now it is easier to traverse the tree (going from x to T or from T to x).

So, taking the derivative (eg $\frac{dT}{dy}$) is simple, since you can just look one node at a time.

To compute the derivatives, we traverse the graph in reverse topological order, and accumulate derivatives. Add possible derivatives, start at zero.

$$\frac{\partial T}{\partial V} = D_V = 0 \quad \forall V \in [T, h, g, f, x, y]$$

Then, we set $\underline{D_T = 1} = \frac{\partial T}{\partial T}$

Then, we go through the input nodes of T , and we start accumulating derivatives.

In this example, we accumulate the derivatives wrt g and h : $\frac{\partial T}{\partial g}$

$$D_g = \frac{\partial T}{\partial g} \times D_T, \quad D_h = \frac{\partial T}{\partial h} \times D_T$$

Then, we go to the next node in reverse topological order, h . Here we look at its inputs and accumulate

$$D_f = \frac{\partial h}{\partial f} \times D_h = \frac{\partial h}{\partial f} \frac{\partial T}{\partial h}$$

$$D_x = \frac{\partial h}{\partial x} D_h = \frac{\partial h}{\partial x} \frac{\partial T}{\partial h}$$

$\left\{ \begin{array}{l} \frac{\partial h}{\partial y} \text{ is "local derivative"} \\ \text{so, } D_y \neq \frac{\partial T}{\partial y}. \text{ We} \\ \text{need to get other} \\ \text{contributions} \end{array} \right.$

After h , we go to g , and compute

$$D_x = \frac{\partial g}{\partial x} \times D_g$$

$$D_f = D_f + \frac{\partial g}{\partial f} \times D_g = \frac{\partial h}{\partial f} \frac{\partial T}{\partial h} + \frac{\partial g}{\partial f} \frac{\partial T}{\partial g} = \frac{\partial T}{\partial f}.$$

Notice that we encounter a node as an input to another node for multiple times, we update its D_v , by adding the previous and new contribution. The reason is simple; if a node is an input in multiple nodes, then the function is of the form.

$$T(h(f, \dots), g(f, \dots), \dots)$$

So in order to correctly capture the (partial) derivative wrt f , we do (schematically)

$$\frac{\partial T}{\partial f} = \frac{\partial T}{\partial h} \frac{\partial h}{\partial f} + \frac{\partial T}{\partial g} \frac{\partial g}{\partial f}$$

So, we add all the contributions coming from the nodes h and g .

After g , we go to f and do

$$D_x = D_x + \frac{\partial f}{\partial x} D_f = \frac{\partial h}{\partial x} \frac{\partial T}{\partial h} + \frac{\partial g}{\partial x} \frac{\partial T}{\partial g} = \frac{\partial T}{\partial x}.$$

$$D_y = D_y + \frac{\partial f}{\partial y} D_f = \frac{\partial h}{\partial y} \frac{\partial T}{\partial h} + \frac{\partial g}{\partial y} \frac{\partial T}{\partial g} = \frac{\partial T}{\partial y}.$$