Backpropagation

Lesson 2

COMP6252 (Deep Learning Technologies)

ECS, University of Southampton

Computing the gradient

- An essential part of Deep Learning is computing the gradient of some loss function
- In most situations one cannot compute the gradient analytically
- PyTorch computes the gradient using three concepts
  1. Computational Graph
  2. Maintain a list of the derivatives of **primitive operations**
  3. Use the chain rule from calculus

Chain rule

- The chain rule allows us to compute the derivative of a composite function. Consider the following example

$$h = g(f(x))$$

- To compute $\frac{\partial h}{\partial x}$, the chain rule gives

$$\frac{\partial h}{\partial x} = \frac{\partial h}{\partial g}\frac{\partial g}{\partial f}\frac{\partial f}{\partial x}$$

- The crucial point in the above is that if we know each individual derivative then the result could be computed as the product.

Example

Let $f(x) = x^2$, $g(f) = \log(f)$,$h = g + 1$ with $x = 3$. We have:

$$\frac{\partial f}{\partial x} = 2x = 6$$
$$\frac{\partial g}{\partial f} = \frac{1}{f} = \frac{1}{9}$$
$$\frac{\partial h}{\partial g} = 1$$

Therefore

$$\frac{\partial h}{\partial x} = 1 \times \frac{1}{9} \times 6 = \frac{2}{3}$$

An important part of the above is that we know the derivative of **primitive operations/functions**: even the most complicated of expressions can be broken down into a sequence of primitive operations.

How does PyTorch use the chain rule?

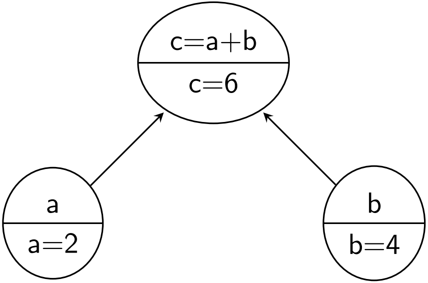
- Now that we know about the chain rule, how does PyTorch use it to compute the gradient?
- It constructs a graph where each primitive operation is represented by a node
- For each such node, it attaches auxillary nodes (actually functions) to compute its derivative
- As an example, let us see how PyTorch computes the following

$$
\begin{aligned}
a &= 2 \\
b &= 4 \\
c &= a + b \\
d &= \log(a) * \log(b) \text{ //not a primitive op. More later} \\
e &= c * d
\end{aligned}
$$

Computational Graph

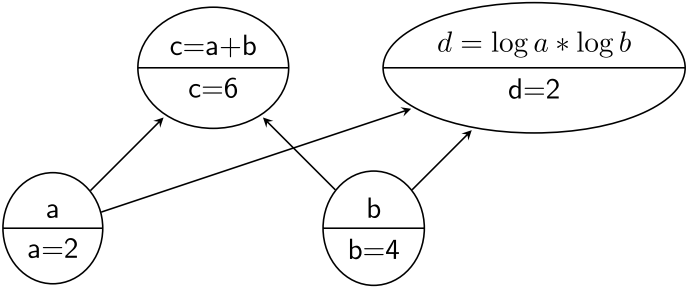
$$a = 2$$
$$b = 4$$

Computational Graph



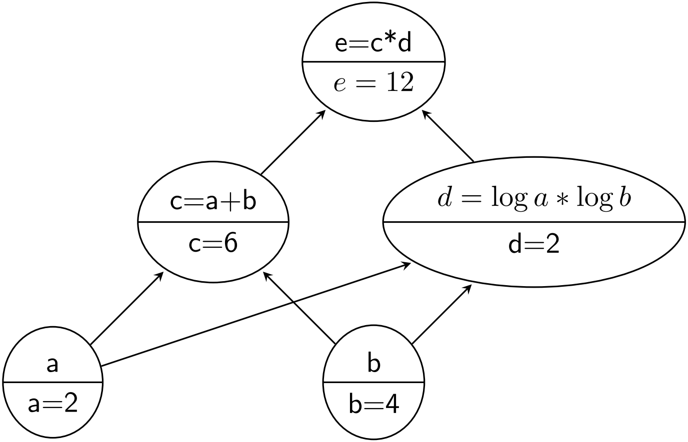
$$a = 2$$
$$b = 4$$
$$c = a + b$$

Computational Graph



$$a = 2$$
$$b = 4$$
$$c = a + b$$
$$d = \log(a) * \log(b)$$

Computational Graph



$a = 2$

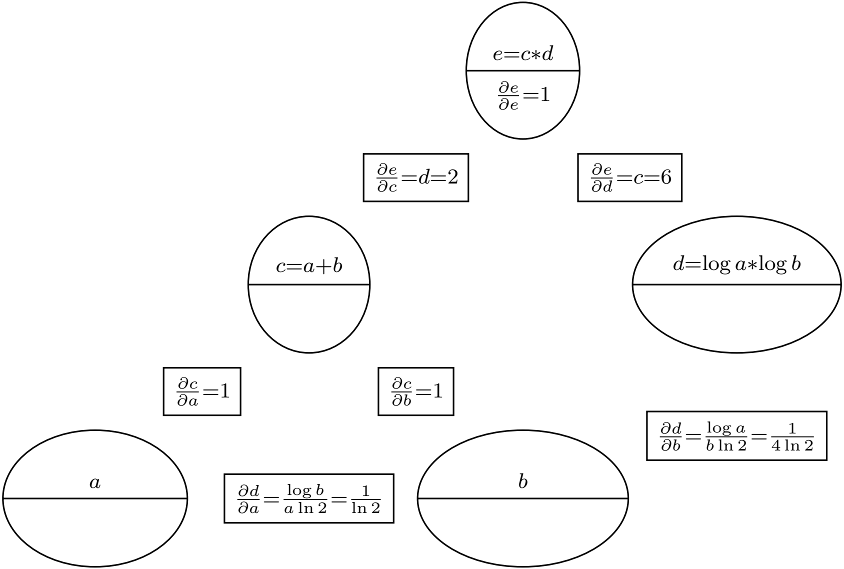
$b = 4$

$c = a + b$

$d = \log(a) * \log(b)$

$e = c * d$

Backward pass



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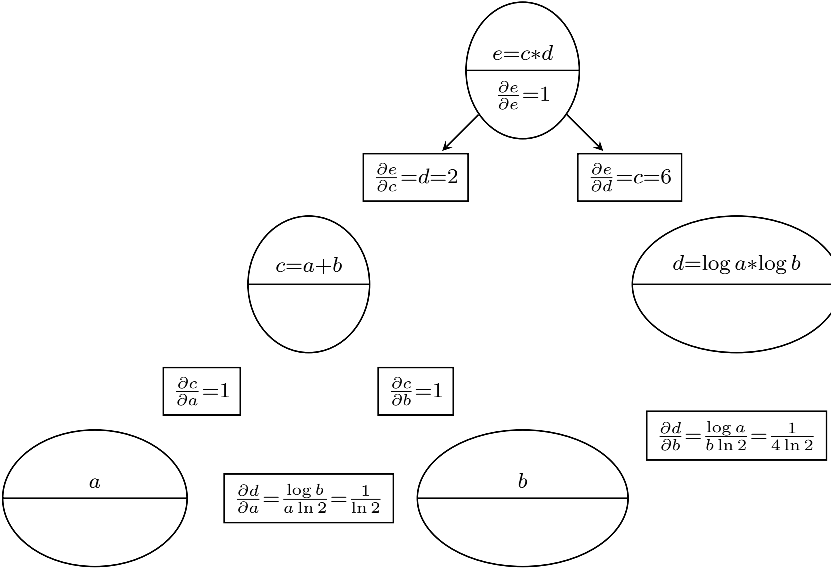

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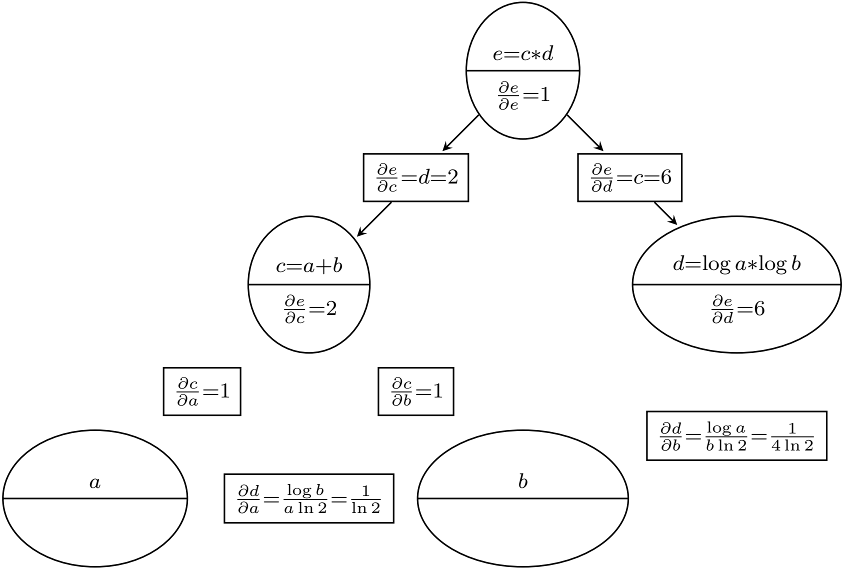

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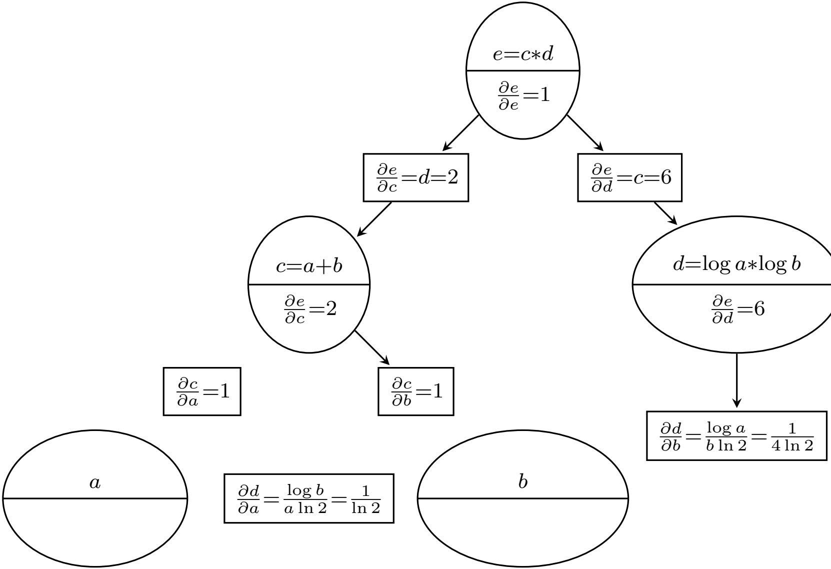

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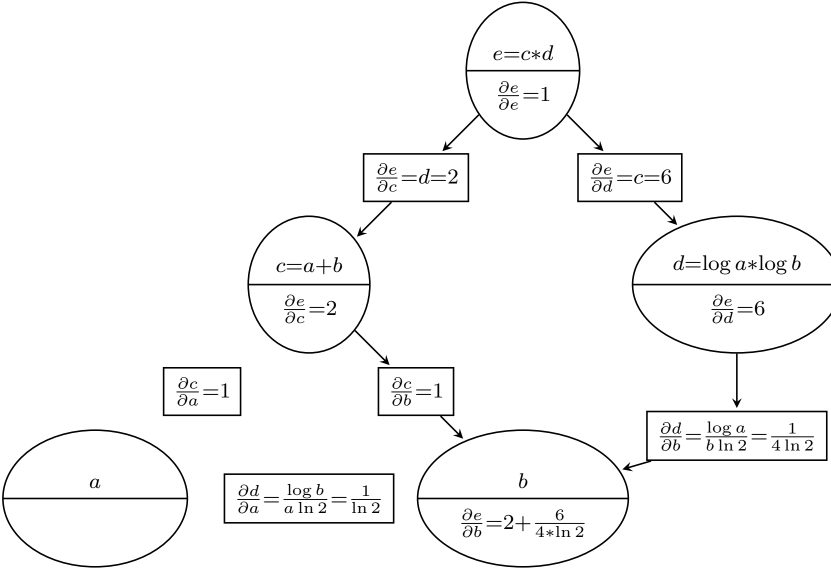

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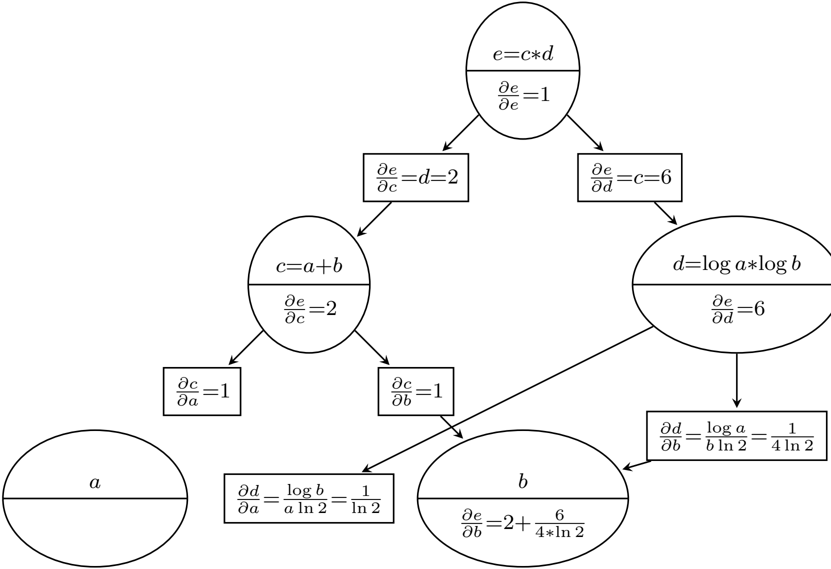

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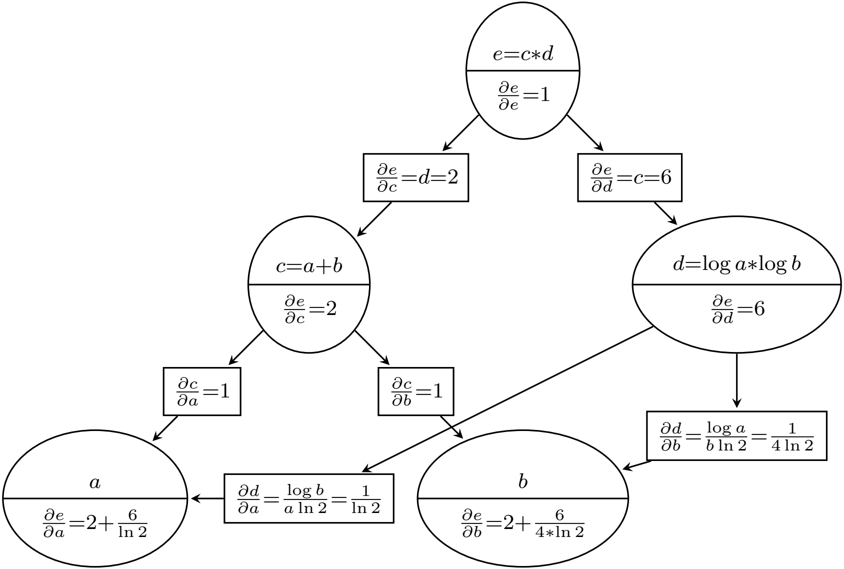

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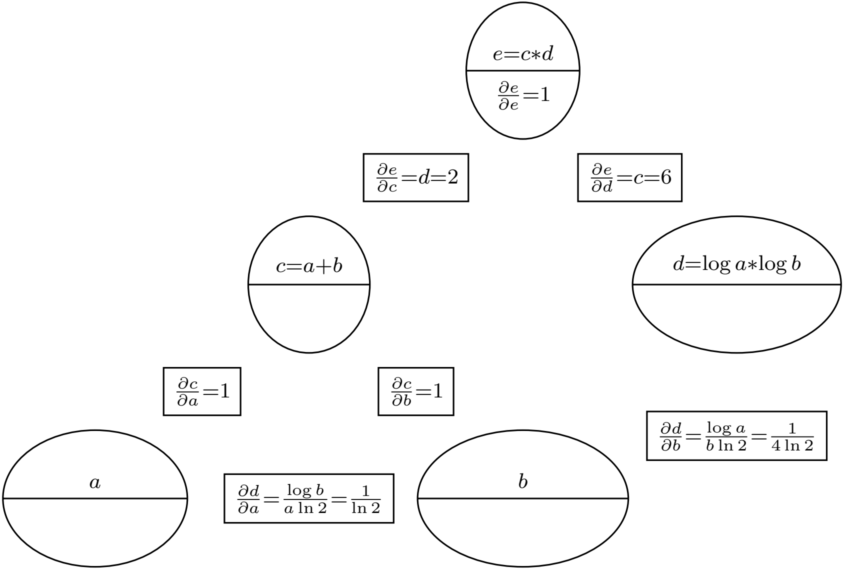

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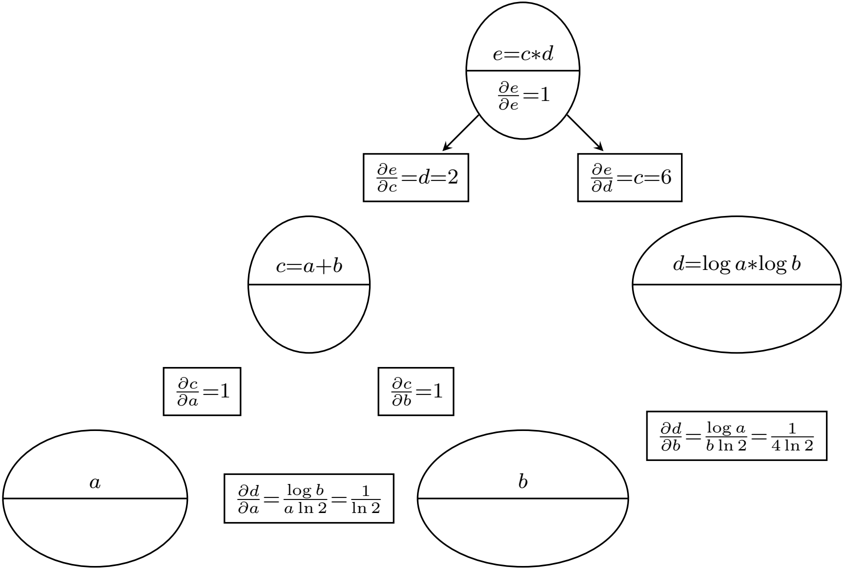

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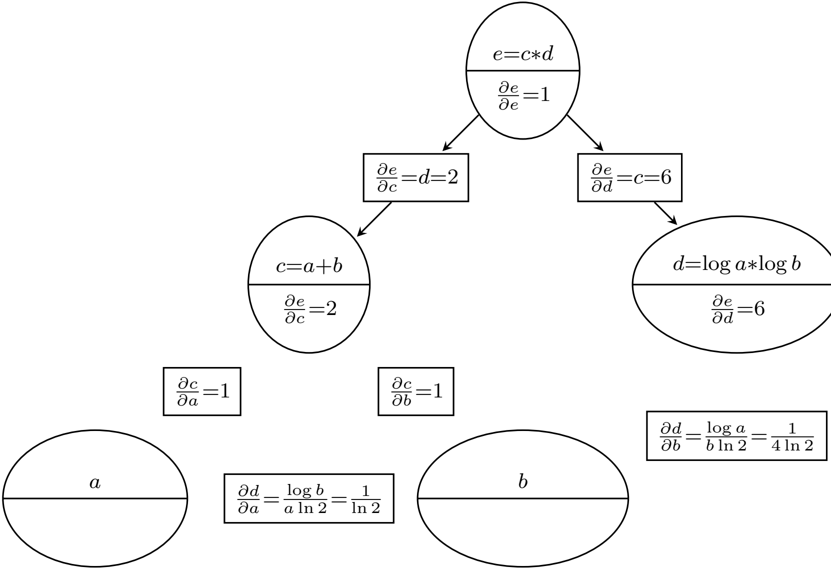

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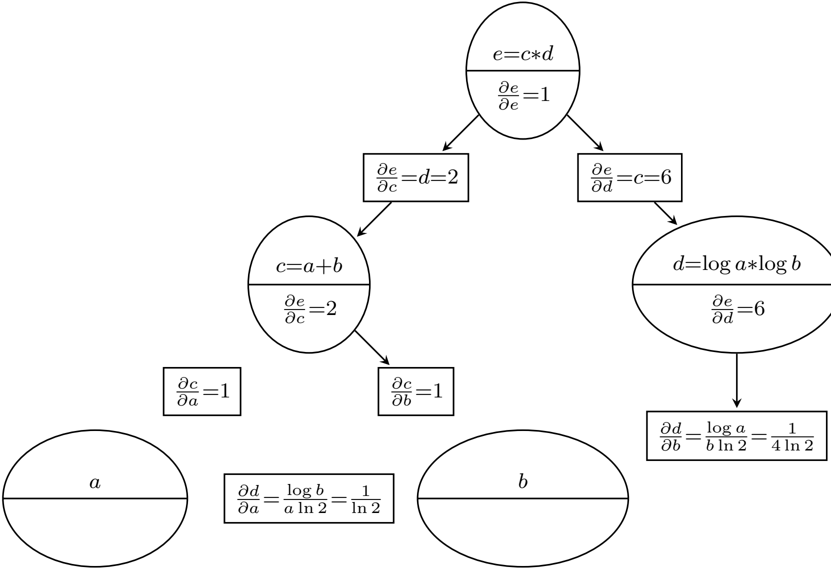

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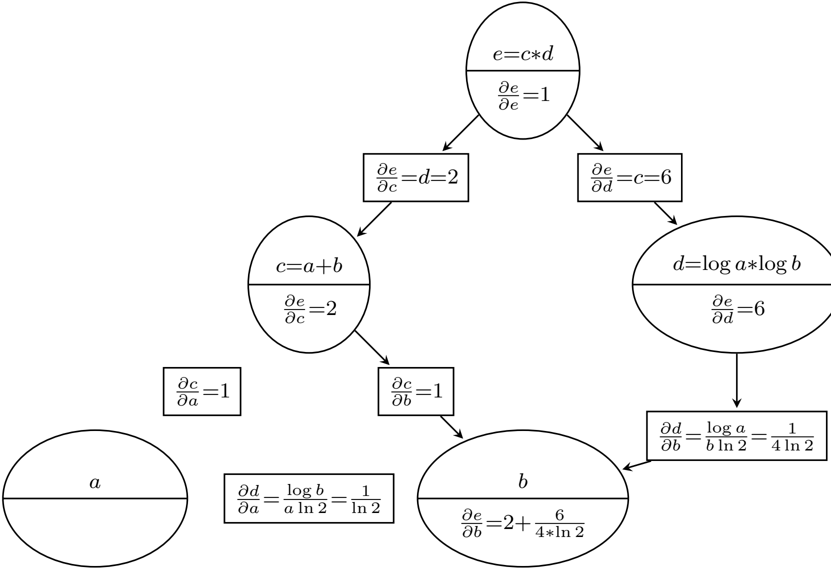

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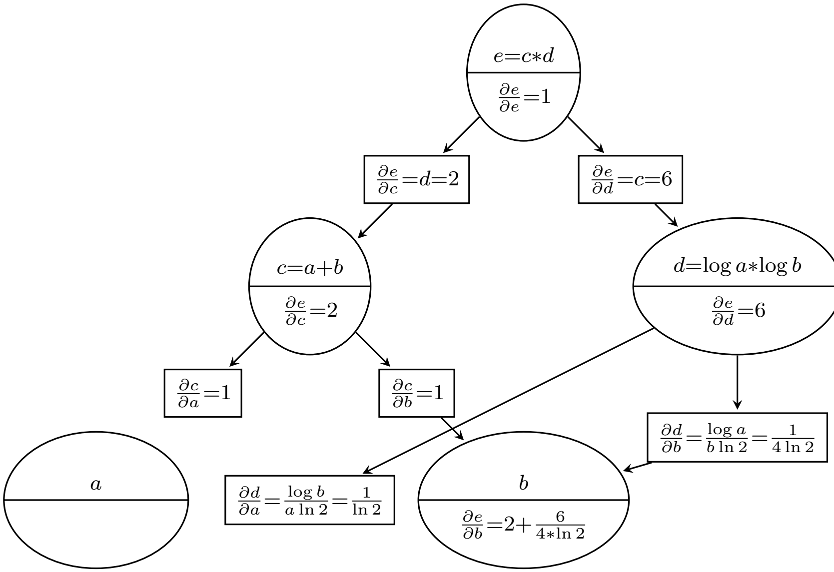

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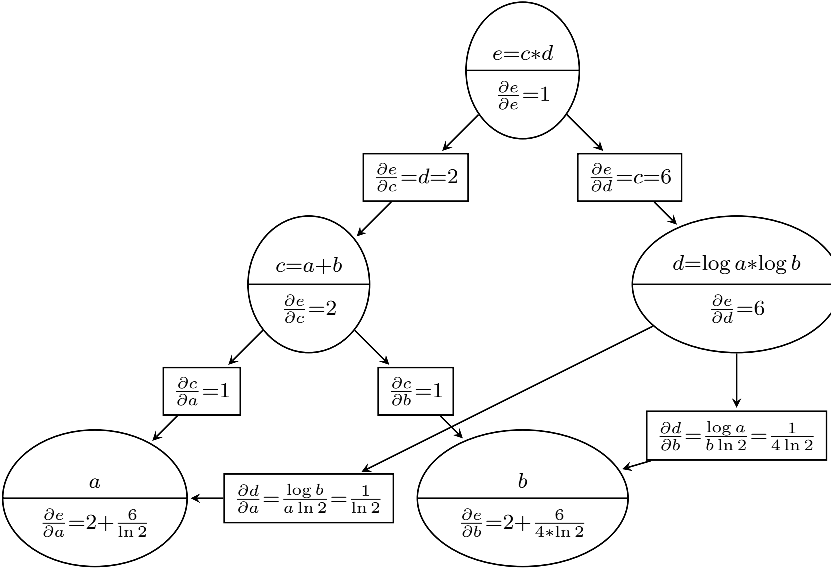
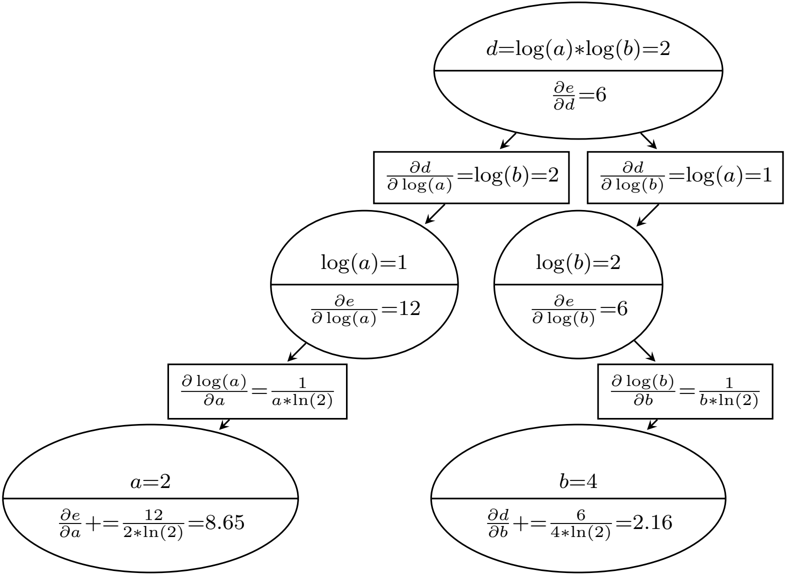


Details for node d



PyTorch Details

- PyTorch implements the above using a graph of gradient functions
- We can map our graph to PyTorch implementation as follows
  1. The oval nodes represent the gradient functions
  2. The rectangular nodes represent the outputs of those functions
- The starting point is `e.grad_fn` with input 1. The output of `e.grad_fn(1.)` is `[2,6]` as expected.
- The output `[2,6]` is used as input to the functions `e.grad_fn.next_functions`
- The code for the whole graph is shown on the corresponding notebook