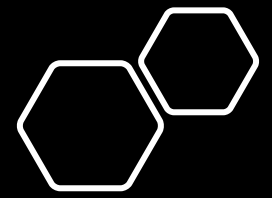
AIMS | African Institute for Mathematical Sciences RWANDA

AMMI Review sessions

Deep Learning Labs (3)

Autograd in Pytorch



13 Feb 2020

Autograd

- Autograd is now a core torch package for automatic differentiation

- In the forward phase, the autograd tape will remember all the operations it executed, and in the backward phase, it will replay the operations.

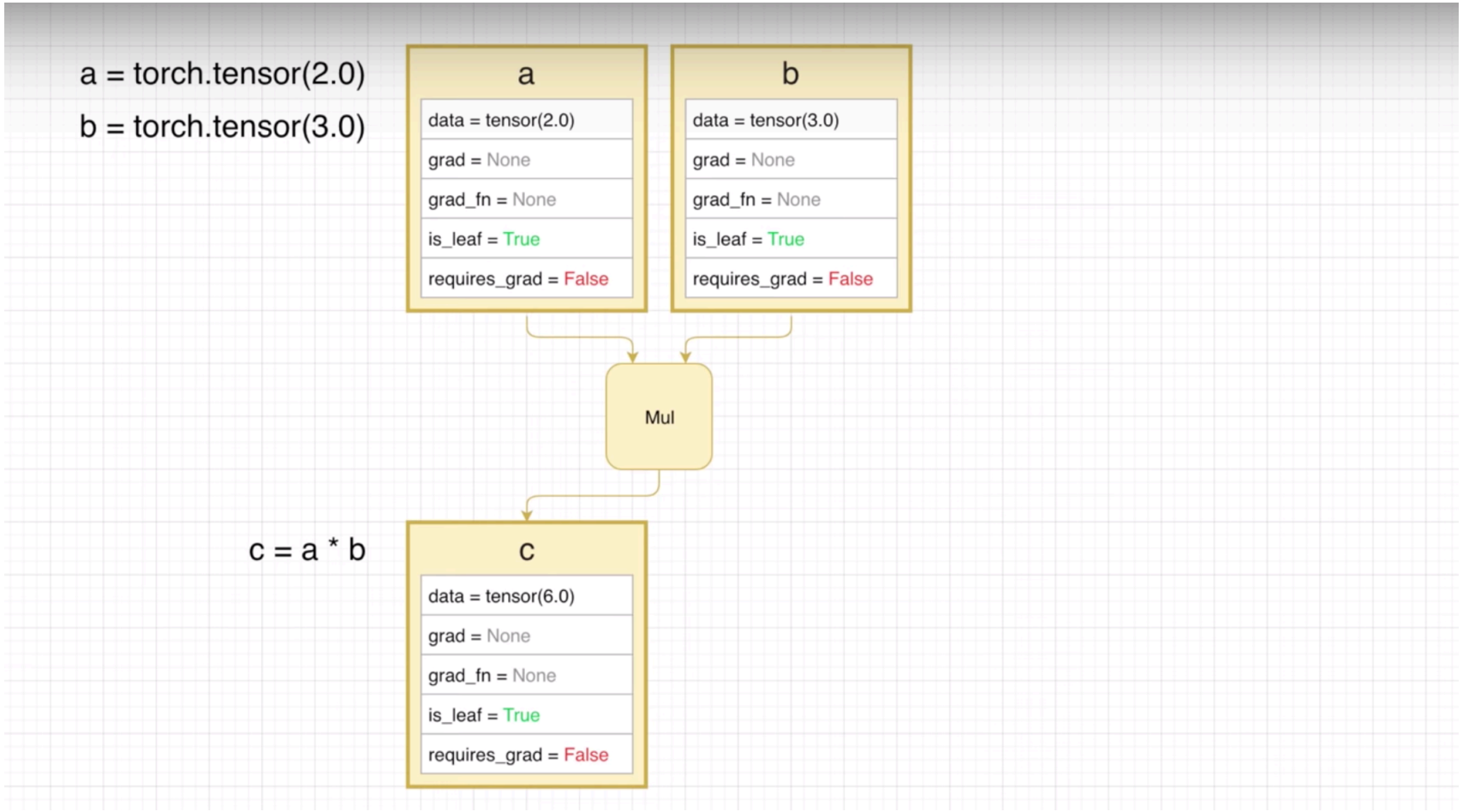
Tensors that track history

- if any input Tensor of an operation has requires_grad=True, the computation will be tracked. After computing the backward pass, a gradient w.r.t. this tensor is accumulated into .grad attribute.

- Each variable has a .grad_fn attribute that references a function that has created a function (except for Tensors created by the user - these have None as .grad_fn).

- If you want to compute the derivatives, you can call .backward() on a Tensor.

Tensors that track history



How Pytorch Backward() function works ?

The Gradient of scalar Loss function

- When we use gradient descent as learning algorithm of our model we need to compute the gradient of the loss w.r.t the model parameters.

- The loss term is usually a scalar value obtained by defining loss function (criterion) between the model prediction and and the true label — in a supervised learning problem setting — and usually we call loss.item() to get single python number out of the loss tensor.

The Gradient of scalar Loss function

- When we start propagating the gradients backward, we start by computing the derivative of this scalar loss (*L*) w.r.t to the direct previous hidden layer (*h*) which's a vector (group of weights)

- What would be the gradient in this case ?

- Simply it's a Jacobian vector (nx1) that contains the derivative of the loss with respect to all the hidden layer variables (h_1, h_2, h_3,… , h_n)

$$\text{for a function } l : \mathbf{R}^n \to \mathbf{R}$$

$$\mathbf{J_l} = \begin{bmatrix} \frac{\partial l}{\partial h_1} & \frac{\partial l}{\partial h_2} & \frac{\partial l}{\partial h_3} & \cdots & \frac{\partial l}{\partial h_n} \end{bmatrix}$$

The Gradient of vector loss function

- let say now we want to compute the gradient of a some loss vector (l) w.r.t to a hidden layer vector then we need to compute the full Jacobian

$$\text{for a function } l : \mathbf{R}^n \to \mathbf{R}^m$$

$$\mathbf{J_l} = \begin{bmatrix} \frac{\partial l_1}{\partial h_1} & \frac{\partial l_2}{\partial h_1} & \cdots & \frac{\partial l_m}{\partial h_1} \\ \frac{\partial l_1}{\partial h_2} & \frac{\partial l_2}{\partial h_2} & \cdots & \frac{\partial l_m}{\partial h_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial l_1}{\partial h_n} & \frac{\partial l_2}{\partial h_n} & \cdots & \frac{\partial l_m}{\partial h_n} \end{bmatrix}$$

- By looking into our gradient descent step

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} l(\theta)$$

- it’s obvious that we’re actually interested in the gradient vector rather than the full Jacobian

The Gradient of vector loss function

- The gradient thus can be obtained by summing the gradients of all variables in the loss vector w.r.t each variable in the hidden layer and would have the following formula:

$$\frac{l(\theta)}{dh} = \left[\frac{\partial l}{\partial h_1} \quad \frac{\partial l}{\partial h_2} \quad \cdots \quad \frac{\partial l}{\partial h_n}\right]^T$$

where

$$\frac{\partial l}{\partial h_i} = \frac{\partial l_1}{\partial h_i} + \frac{\partial l_2}{\partial h_i} + \cdots + \frac{\partial l_m}{\partial h_i}$$

The Jacobian-vector product

- We can easily show that we can obtain the gradient by multiplying the full Jacobian Matrix by a vector of ones as follows:

$$\frac{dl(\theta)}{dh} = \begin{bmatrix} \frac{\partial l_1}{\partial h_1} & \frac{\partial l_2}{\partial h_1} & \cdots & \frac{\partial l_m}{\partial h_1} \\ \frac{\partial l_1}{\partial h_2} & \frac{\partial l_2}{\partial h_2} & \cdots & \frac{\partial l_m}{\partial h_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial l_1}{\partial h_n} & \frac{\partial l_2}{\partial h_n} & \cdots & \frac{\partial l_m}{\partial h_n} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

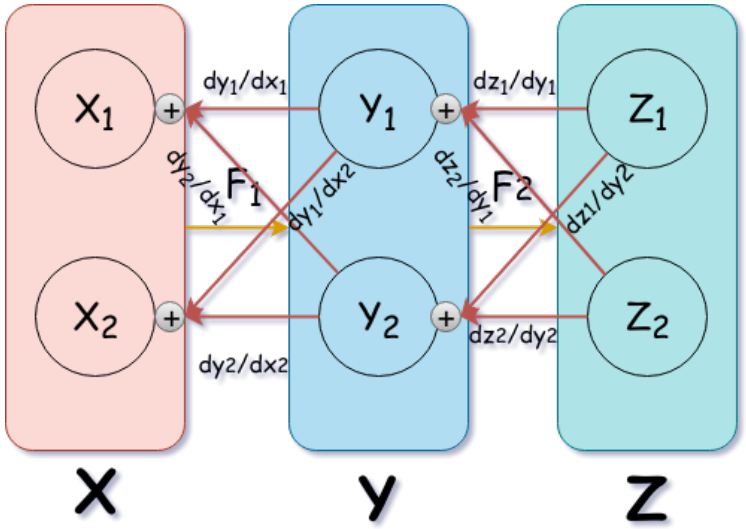
$$\ldots\ldots\ldots\ldots\ldots\ldots = \begin{bmatrix} \frac{\partial l_1}{\partial h_1} + \frac{\partial l_2}{\partial h_1} + \cdots + \frac{\partial l_m}{\partial h_1} \\ \frac{\partial l_1}{\partial h_2} + \frac{\partial l_2}{\partial h_2} + \cdots + \frac{\partial l_m}{\partial h_2} \\ \vdots \\ \frac{\partial l_1}{\partial h_n} + \frac{\partial l_2}{\partial h_n} + \cdots + \frac{\partial l_m}{\partial h_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial l}{\partial h_1} \\ \frac{\partial l}{\partial h_2} \\ \vdots \\ \frac{\partial l}{\partial h_n} \end{bmatrix}$$

- This ones vector is the argument that we pass to the Backward() function to compute the gradient, and this expression is called the Jacobian-vector product!

Jacobian-vector product in backpropagation

Let's take the following example:

- assume we have the following transformation functions f1 and f2 and x, y, z three vectors each of which is of 2 dimensions



- To use the chain rule to calculate $\frac{dz}{dx}$ we calculate $\frac{\mathrm{dz}}{dx} = \frac{dz}{dy} * \frac{dy}{dx}$

- Since z is a leaf node, we can directly compute the gradient $\frac{dz}{dy} = J_z \ @ \ \vec{1}$ using the Jacobian-vector product where J_z is the full Jacobian and $\vec{1}$ is vector of ones.

Jacobian-vector product in backpropagation

- Now if we want to compute $\frac{dz}{dx}$ we need to compute the full Jacobian J_y w.r.t x but **instead of multiplying it by ones vector we multiply it by the gradient vector** $\frac{dz}{dy}$ as follows

$$\frac{dz}{dx} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \frac{\partial y_2}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix} \begin{bmatrix} \frac{\partial z}{\partial y_1} \\ \frac{\partial z}{\partial y_2} \\ \vdots \\ \frac{\partial z}{\partial y_m} \end{bmatrix}$$

$$\ldots\ldots\ldots = \begin{bmatrix} \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x_1} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x_1} + \cdots + \frac{\partial z}{\partial y_m}\frac{\partial y_m}{\partial x_1} \\ \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x_2} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x_2} + \cdots + \frac{\partial z}{\partial y_m}\frac{\partial y_m}{\partial x_2} \\ \vdots \\ \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x_n} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x_n} + \cdots + \frac{\partial z}{\partial y_m}\frac{\partial y_m}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial z}{\partial x_1} \\ \frac{\partial z}{\partial x_2} \\ \vdots \\ \frac{\partial z}{\partial x_n} \end{bmatrix}$$

Jacobian-vector product in backpropagation

- As we propagate gradients backward keeping the full Jacobian Matrix is not memory friendly process specially if we are training a giant model where one full Jacobian Matrix could be of size bigger than100K parameters

- Instead **we only need to keep the most recent gradient which requires much less memory footprint.**

Why Pytorch uses Jacobian-vector product ?

- This way we can we can just keep multiplying the gradients vectors of descendent nodes in our computational graph with full — Jacobians of their ancestors backward to the leaf nodes.

- We can interpret the ones vector that we provide to the backward() function as **an external gradients from which the chain rule starts the multiplication process.**

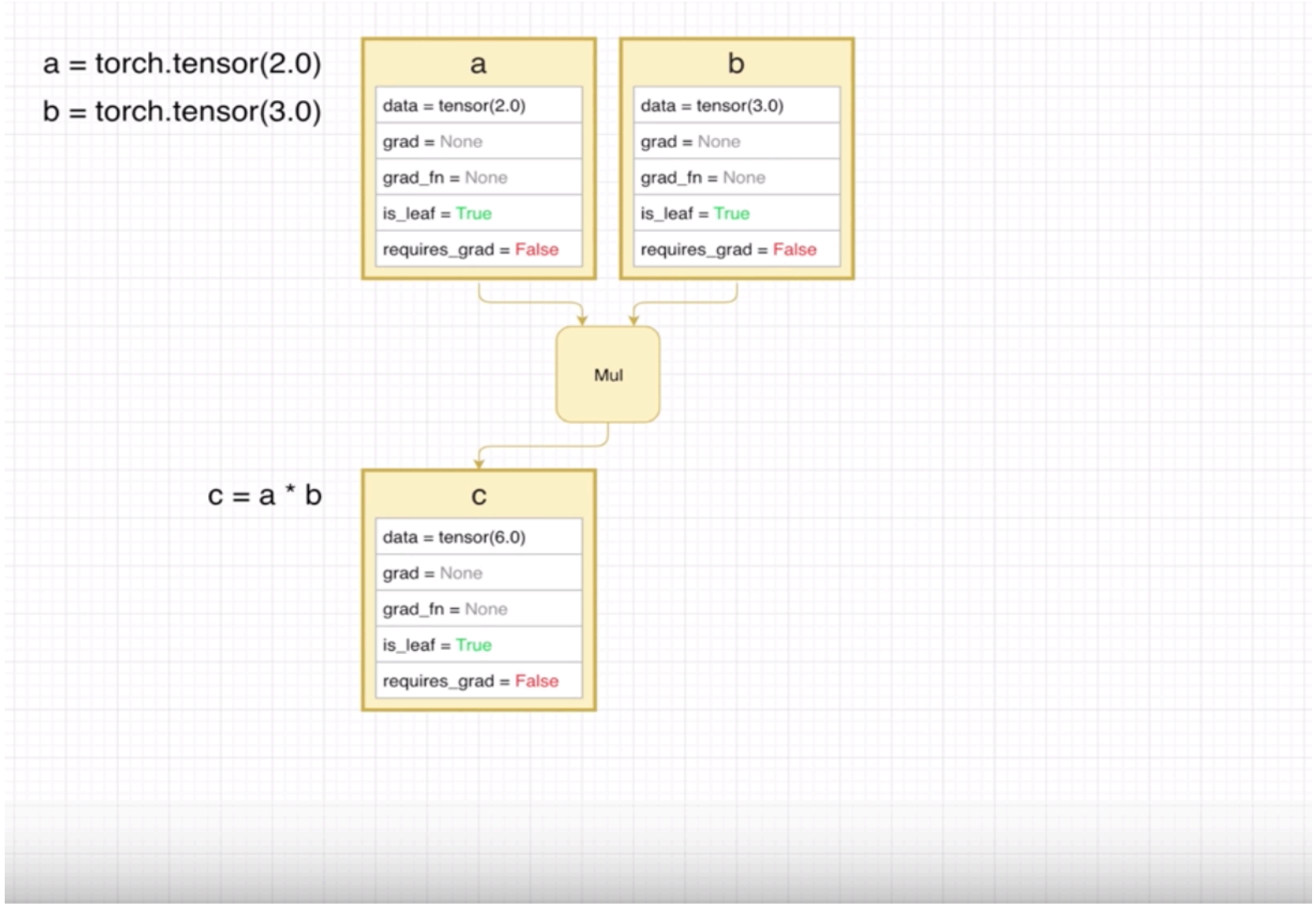
What if we submitted numbers other than ones in the external gradient vector (Backwad() argument) ?

- The values in the external gradient vector can serve like weights or **importances to each loss component**

- For example if we submit the vector [0.2 0.8] as parameter in the previous example, we get this

$$\frac{dz}{dy} = \begin{bmatrix} 0.2\frac{\partial z}{\partial y1} & 0.8\frac{\partial z}{\partial y2} \end{bmatrix}^T$$

How Computational graphs are constructed in Pytorch e.g (1)



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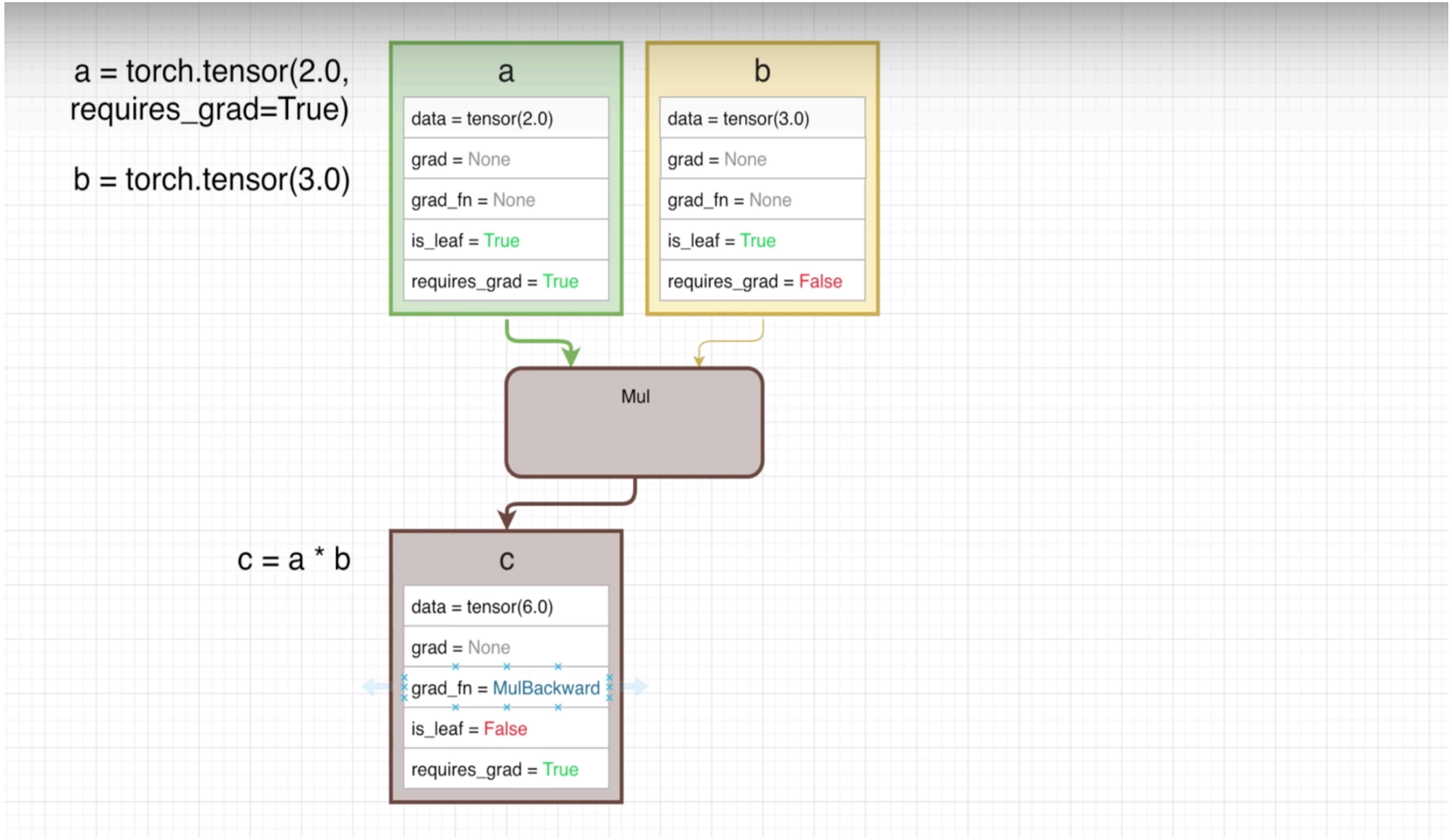

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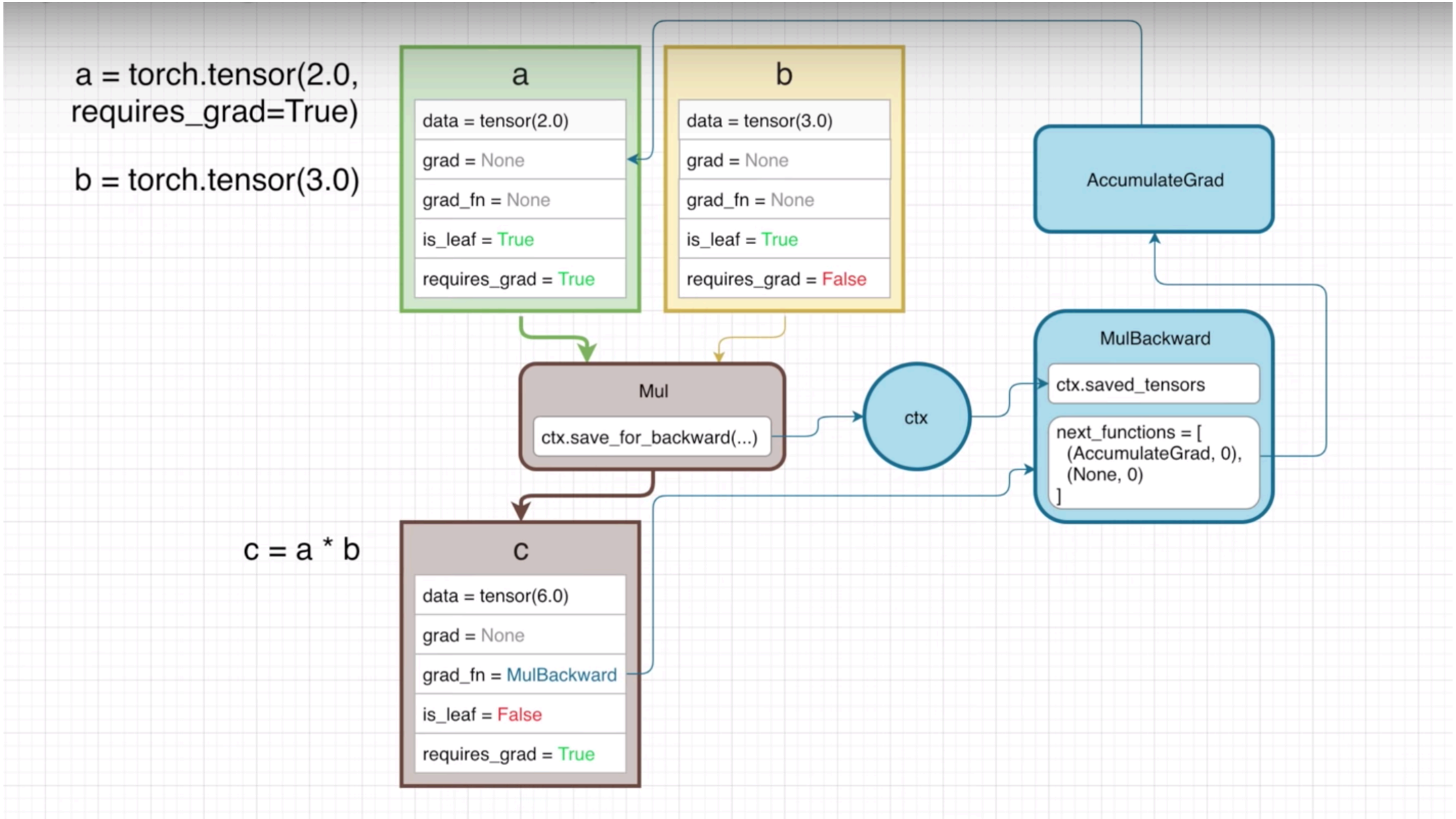

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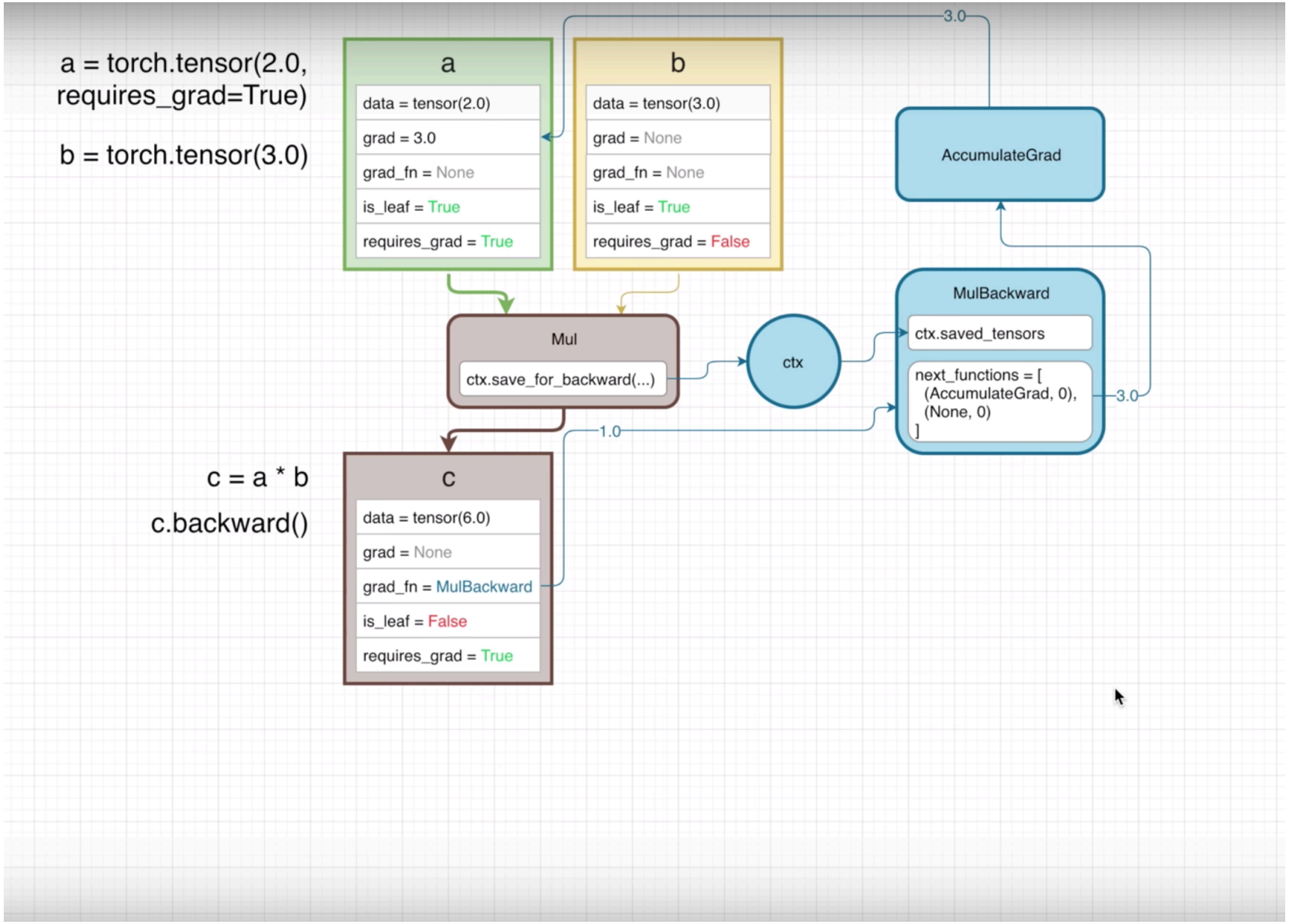
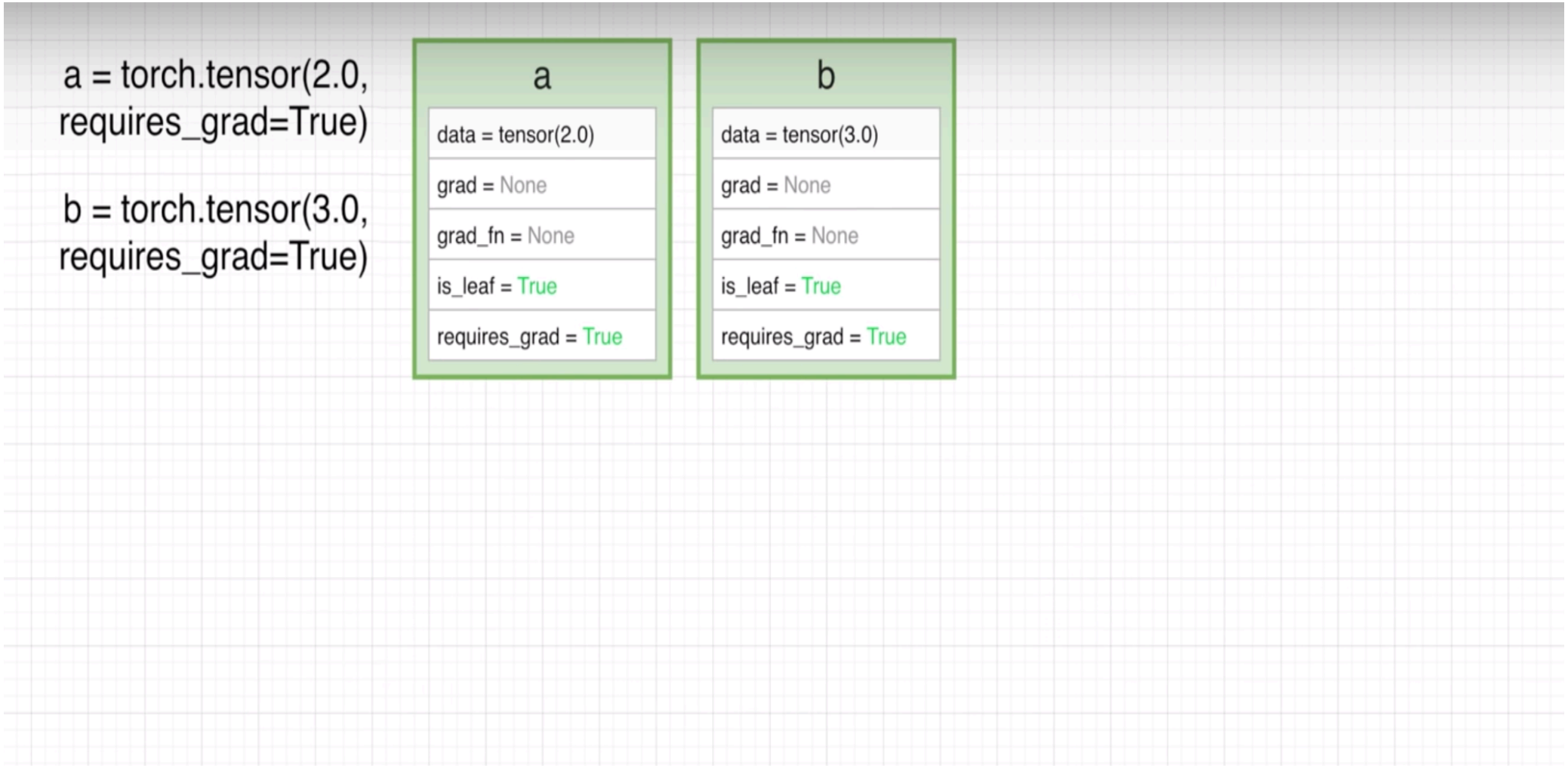


How Computational graphs are constructed in Pytorch e.g (2)



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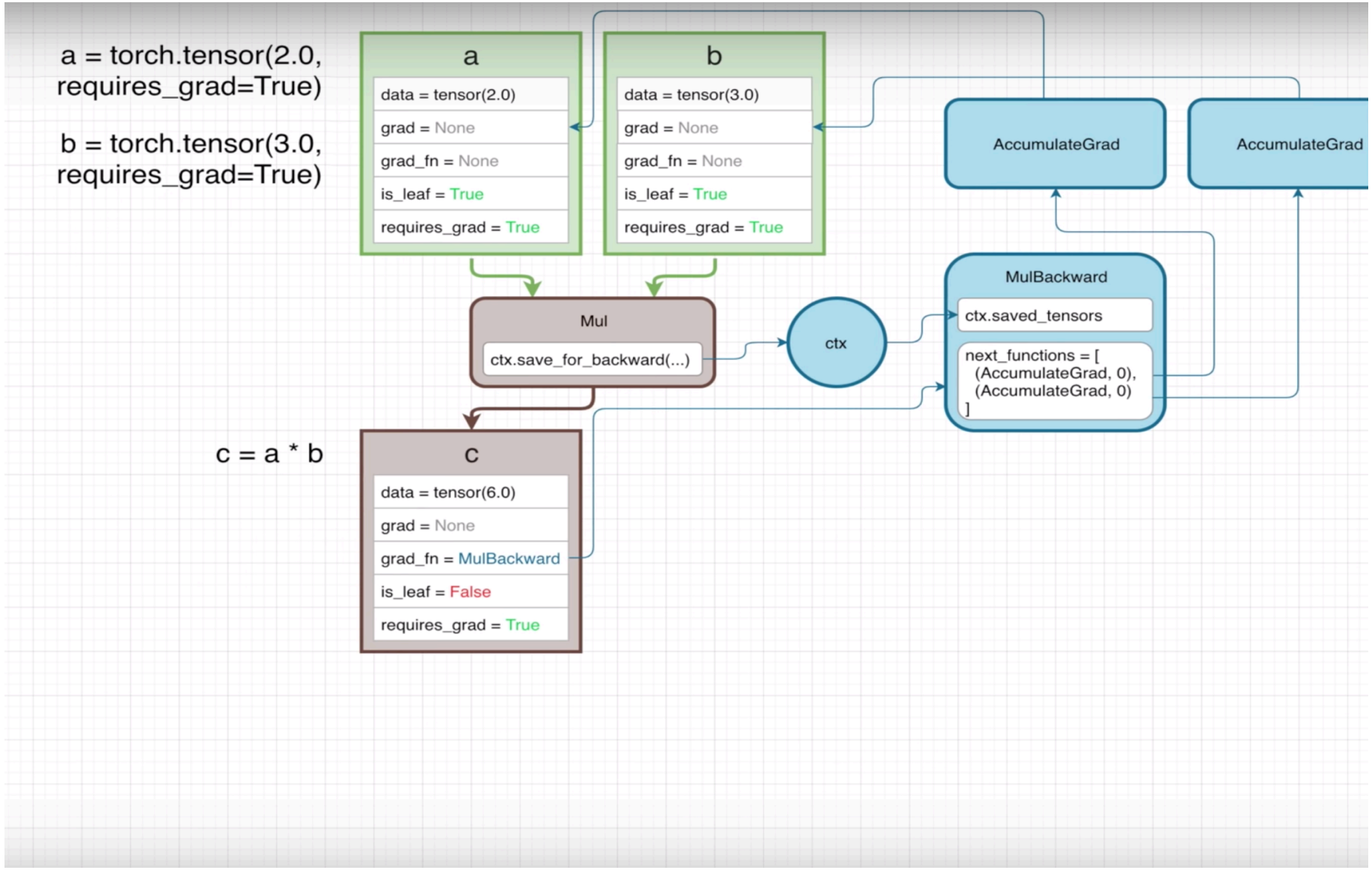

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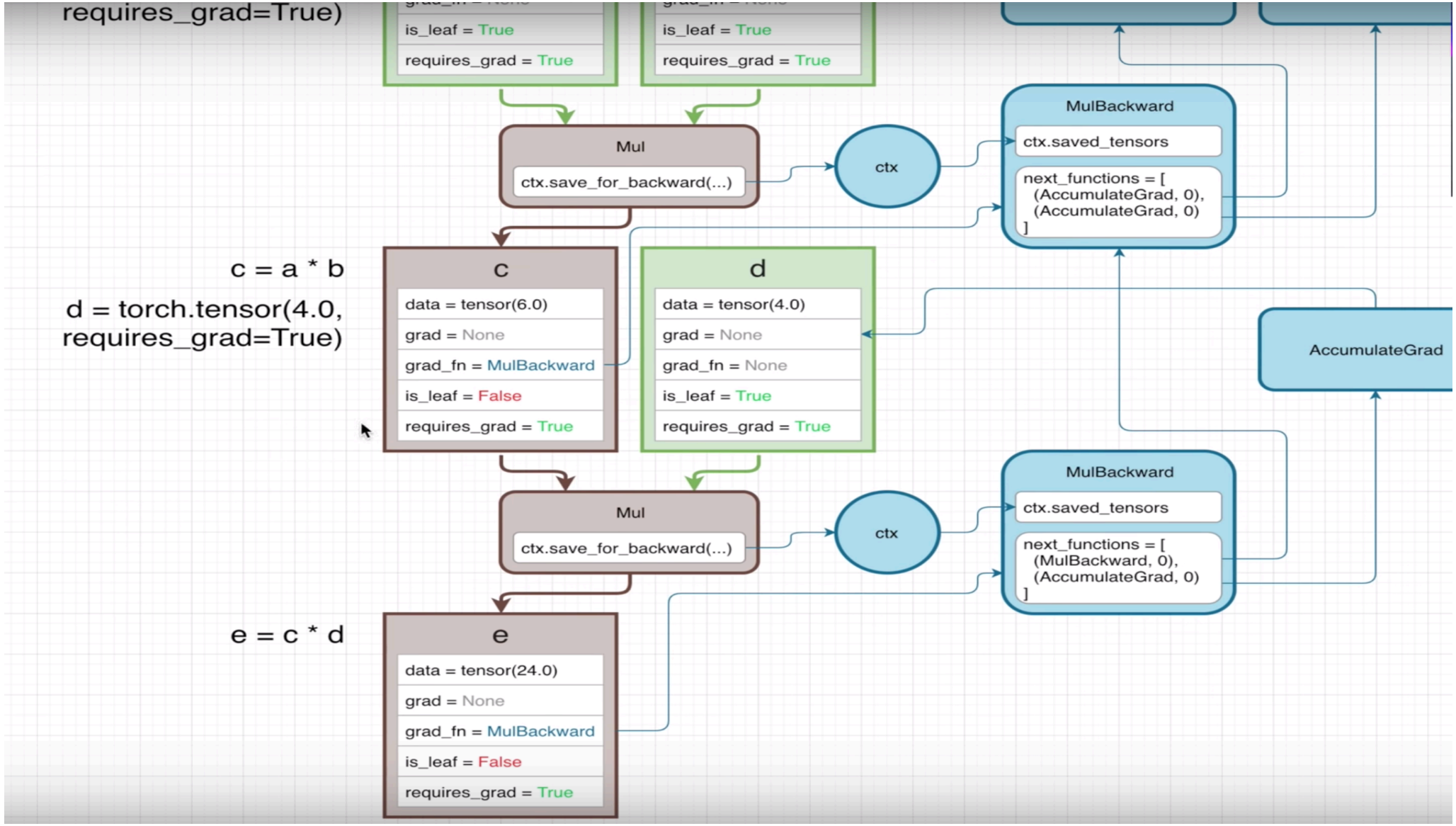

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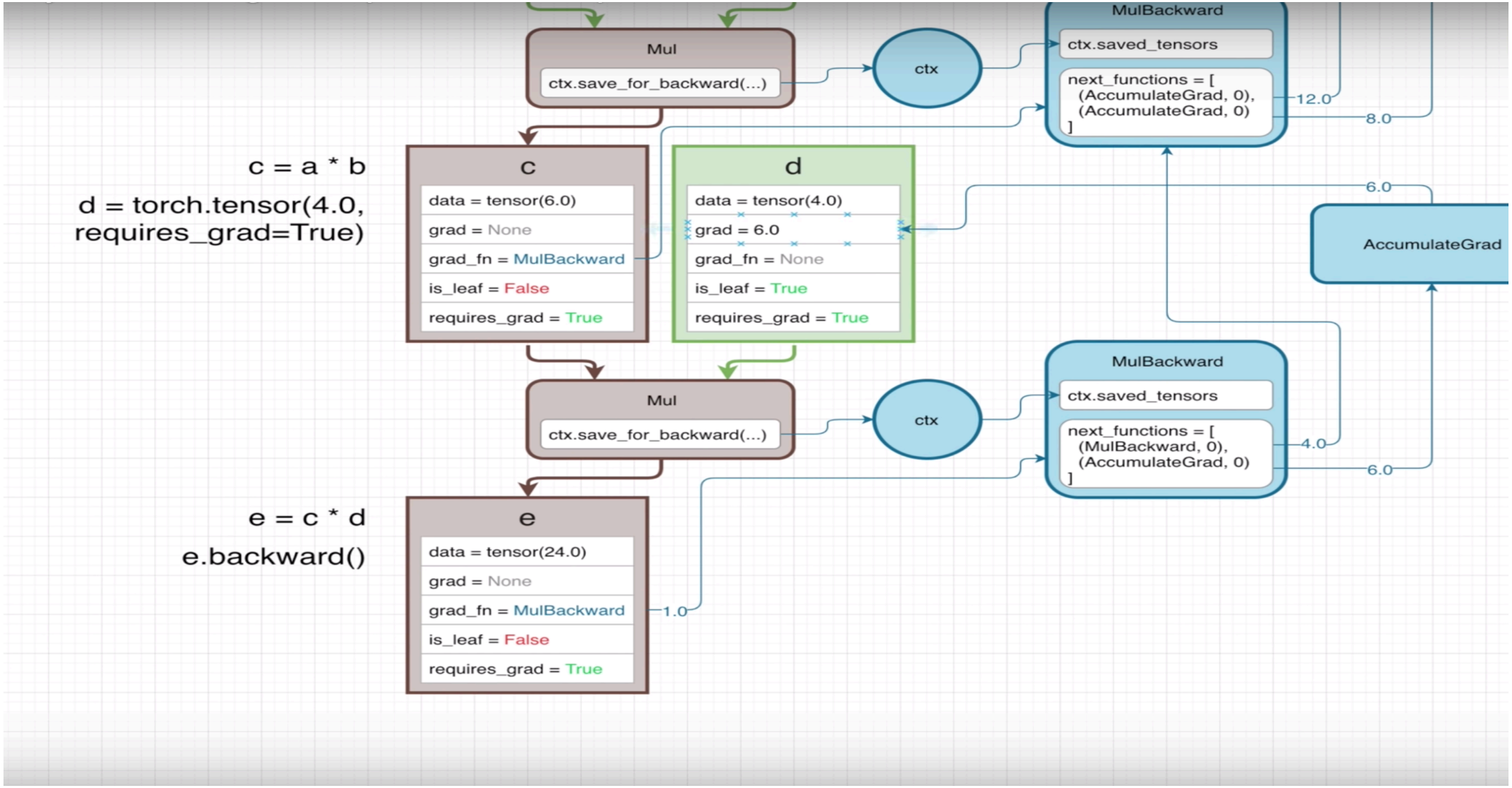

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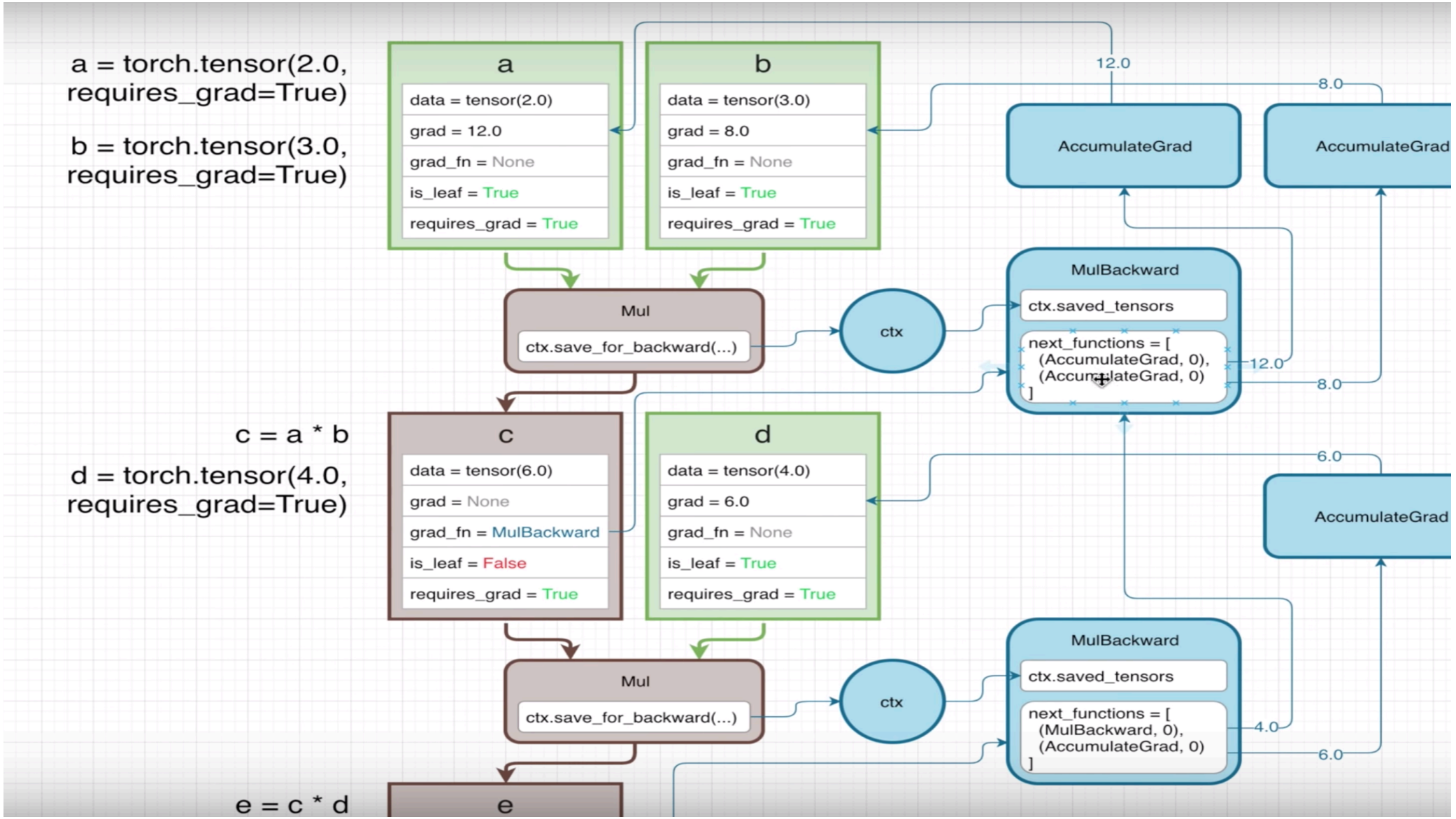

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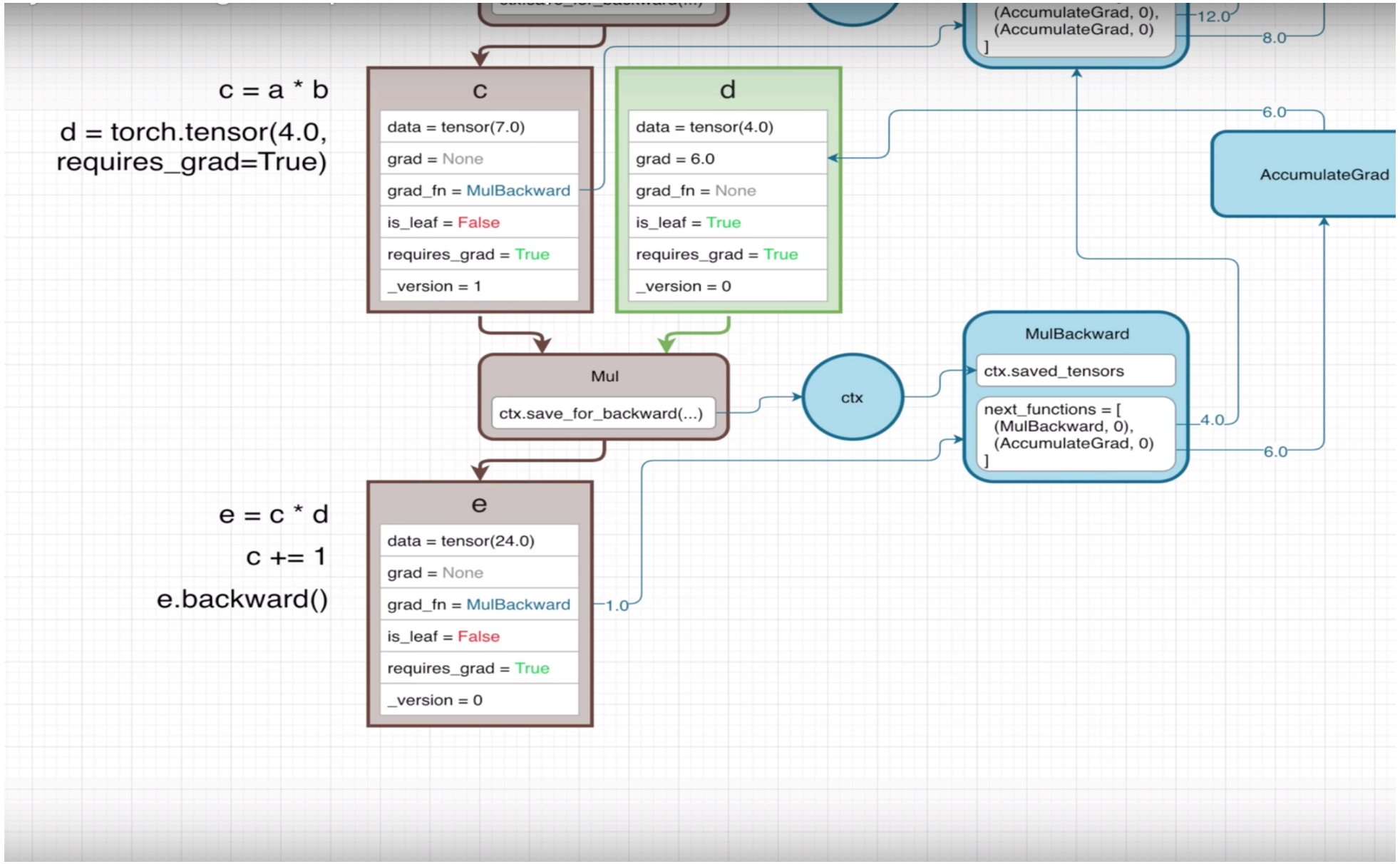
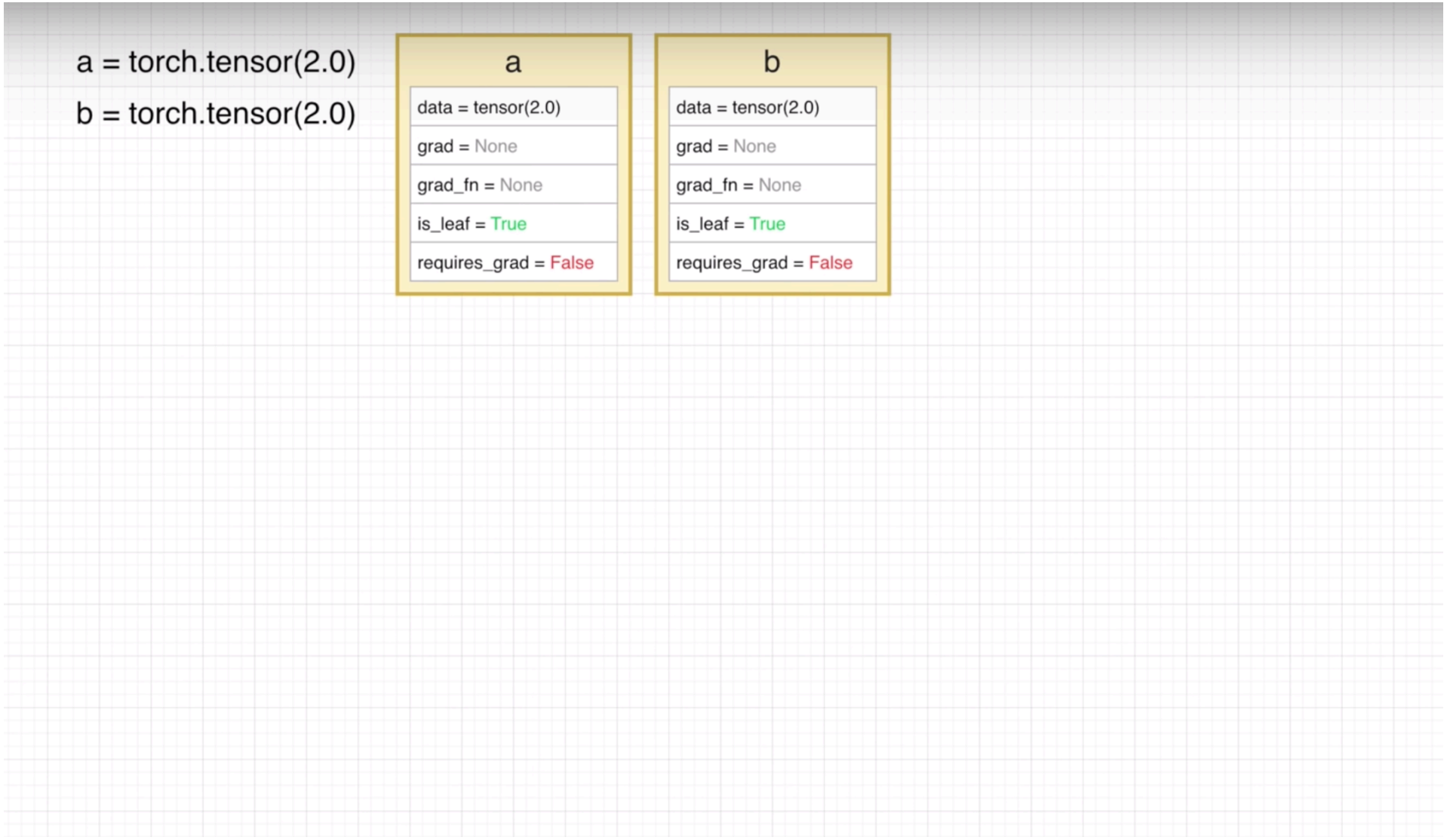


How Computational graphs are constructed in Pytorch e.g (3)



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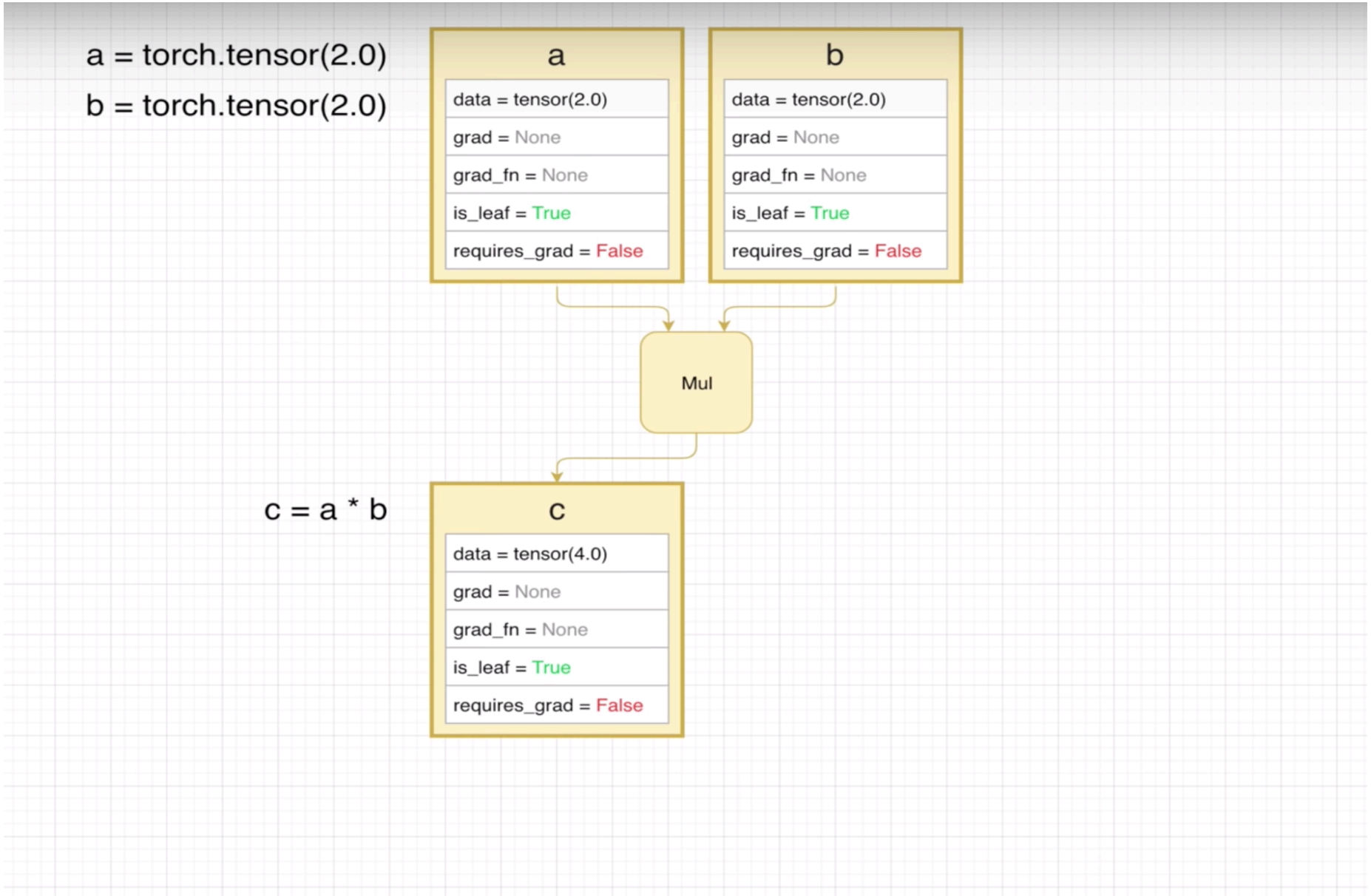

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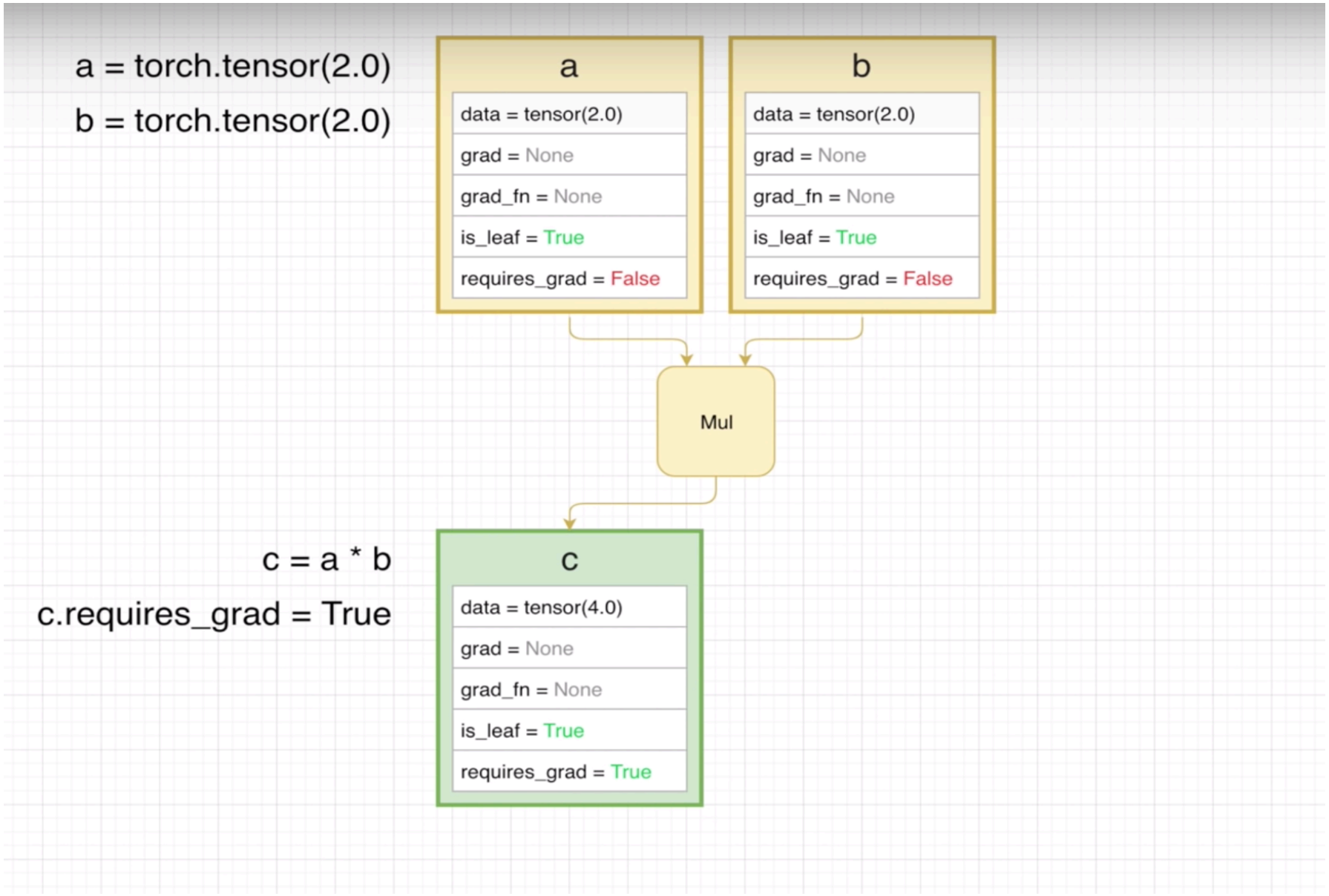

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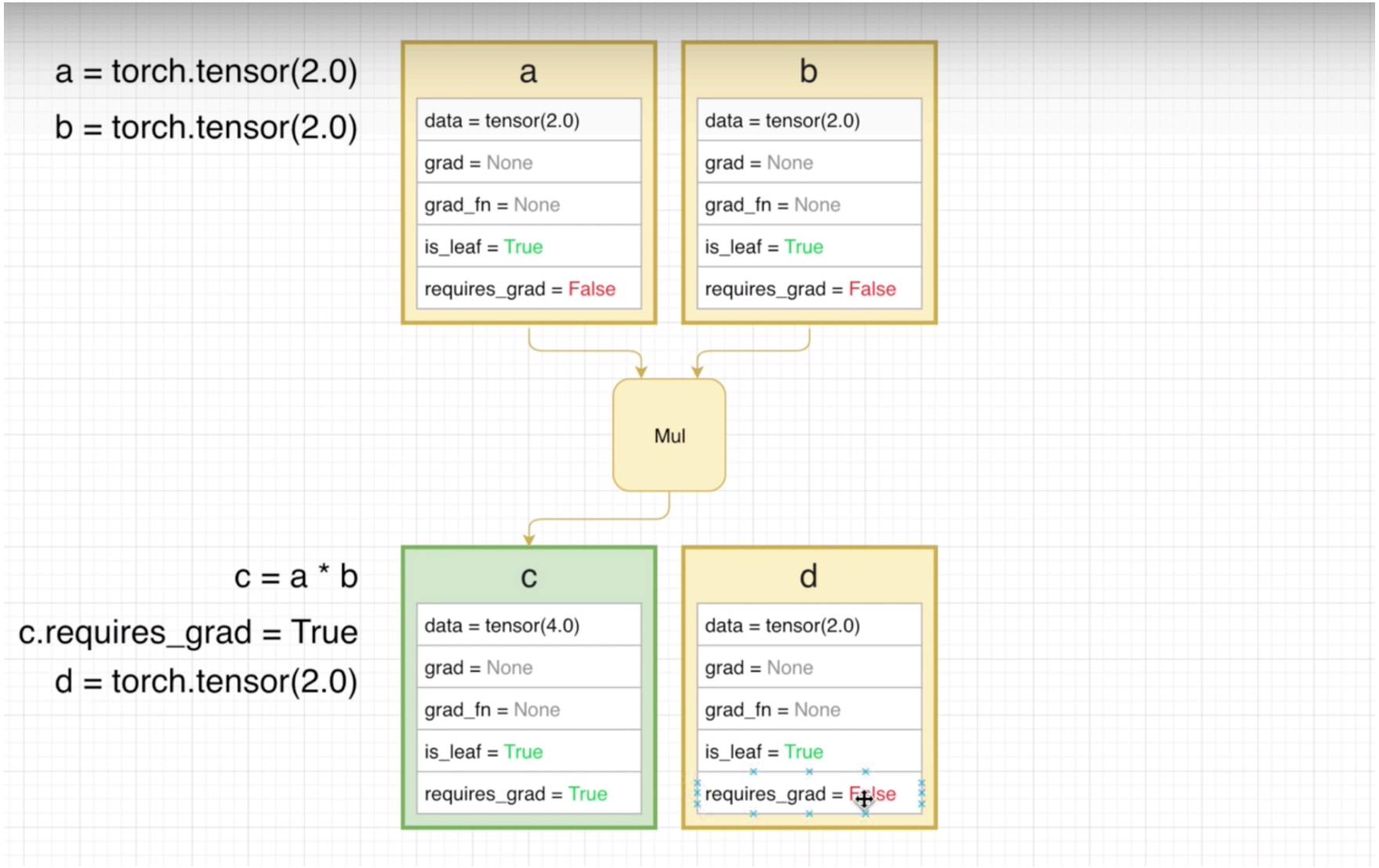

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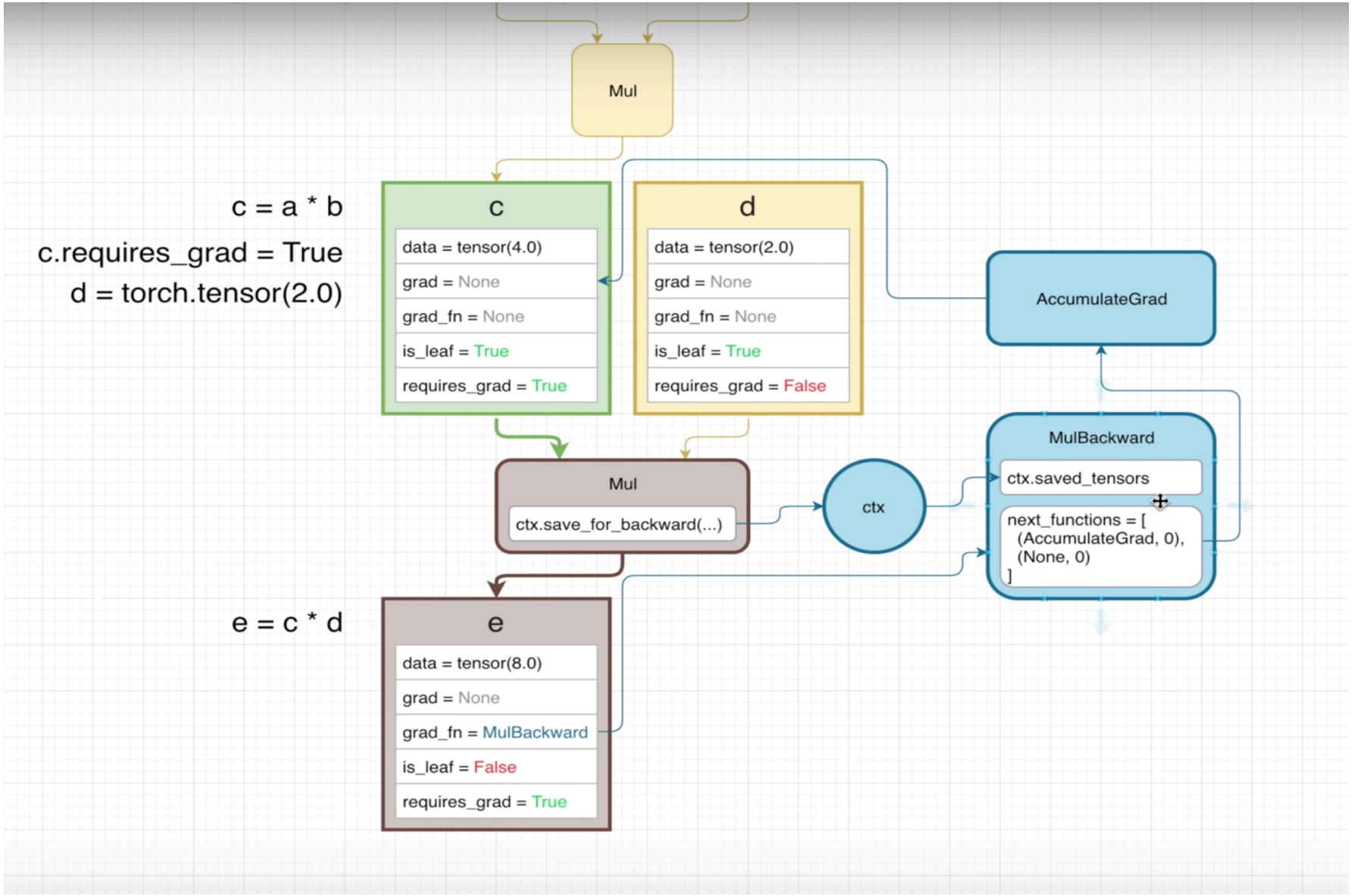

References

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- Mustafa Alghali, how-pytorch-backward-function-works
- Elliot Waite, PyTorch Autograd Explained - In-depth Tutorial