在CNN中的反向传播

1. 链式法则

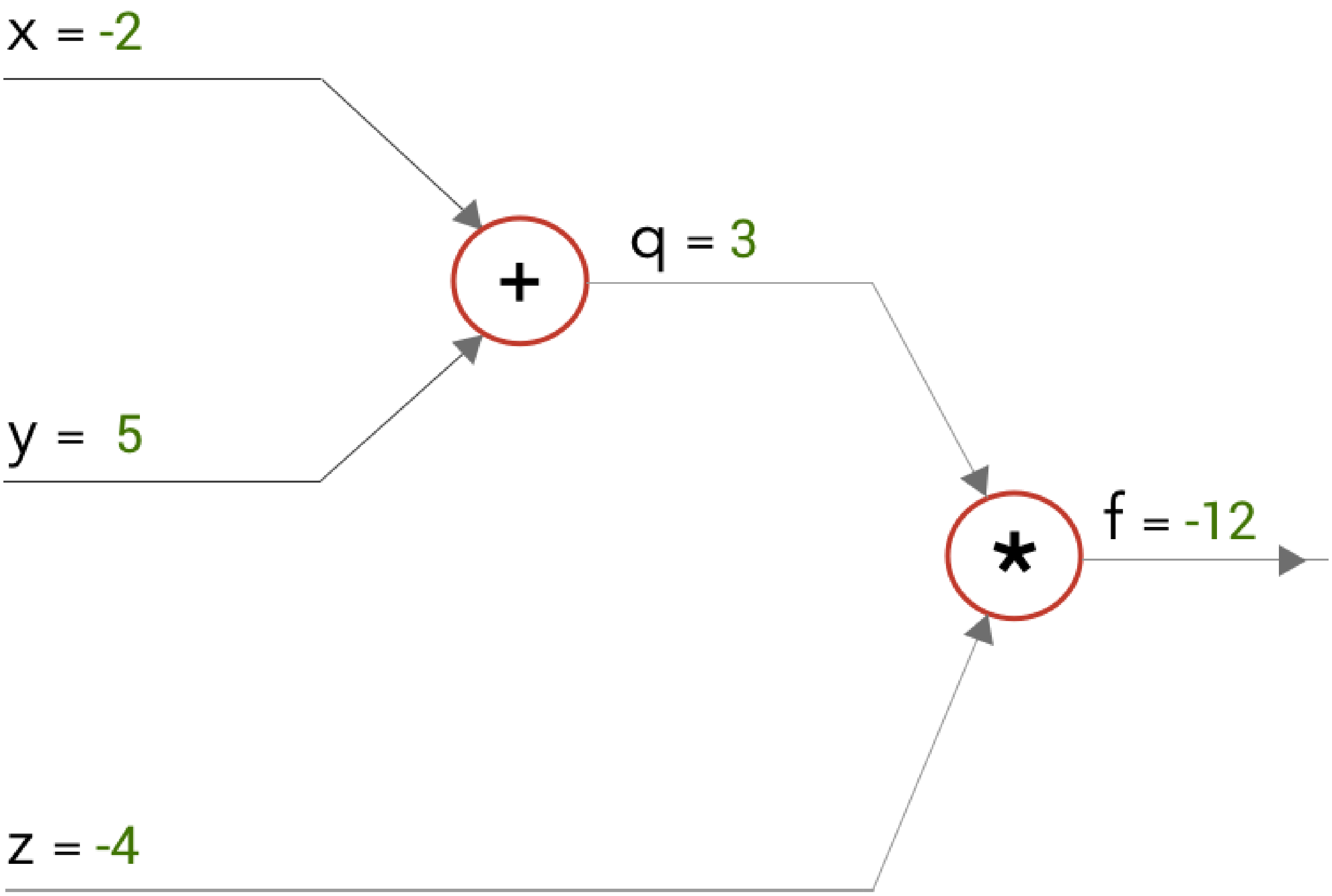
先理解一下在反向传播中的链式法则。
假设有下面这个等式：

$$f(x, y, z) = (x + y)z$$

我们可以把它划分成两个等式：

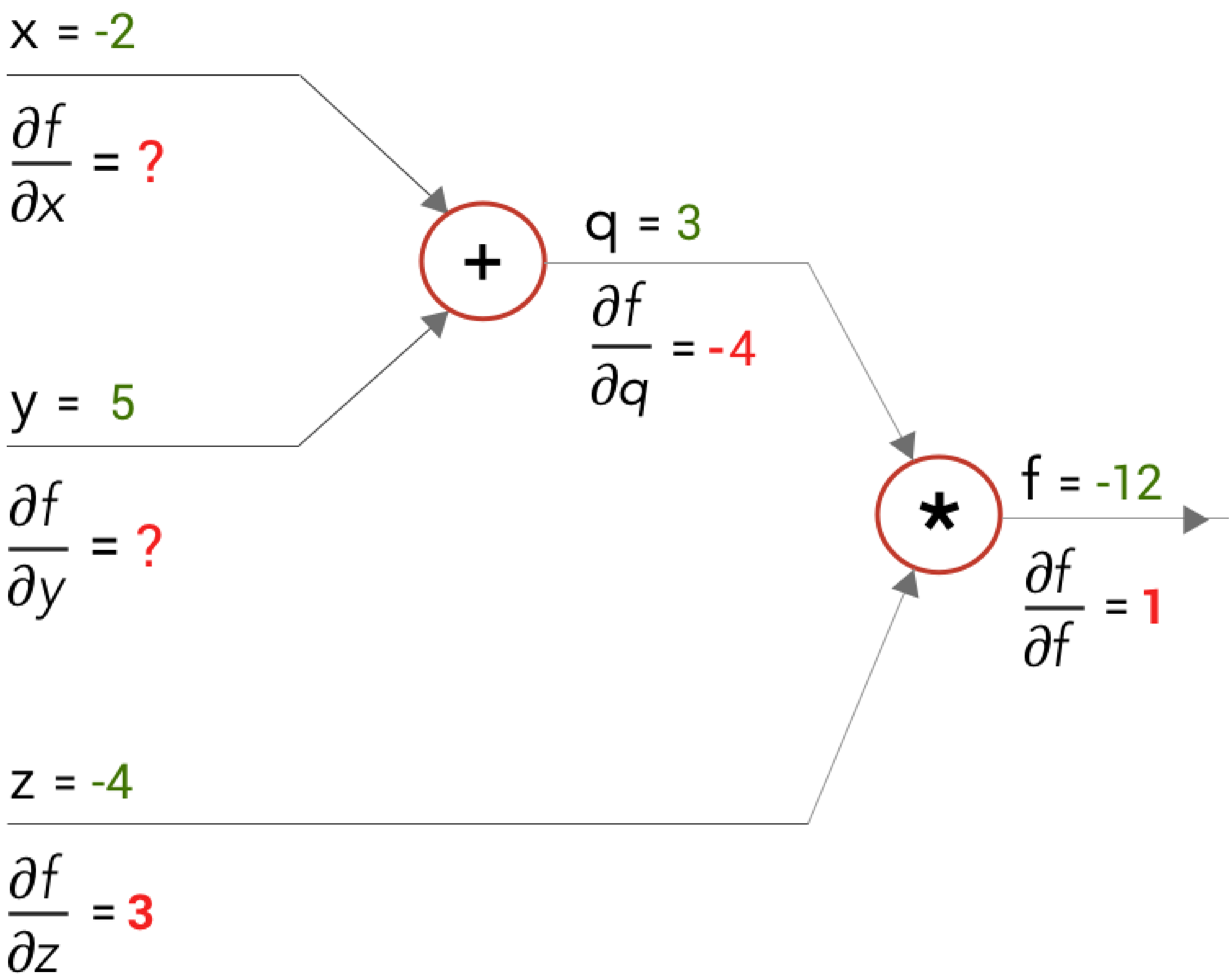
$$\begin{aligned} f(x, y, z) =& (x + y)z \\ q =& x + y \\ f =& q * z \end{aligned}$$

下面让我们画出关于x, y, z的计算图，其中$x = -2, y = 5, z = 4$：



当我们按照上图从左到右进行计算时（前向传播），可以得到$f = -12$。

现在让我们回到反向传播阶段。我们计算梯度从右往左，因此最后，我们可以得到关于我们的输入x, y, z的梯度：$\partial f / \partial x$、$\partial f / \partial y$和$\partial f / \partial z$。
在从右往左进行计算时，在乘积门，我们可以得到$\partial f / \partial q$和$\partial f / \partial z$，
在加和门我们可以得到$\partial q / \partial x$和$\partial q / \partial y$。



$$f = q * z \qquad\qquad q = x + y$$

$$\frac{\partial f}{\partial q} = z \mid z = -4 \qquad\qquad \frac{\partial q}{\partial x} = 1 \qquad \frac{\partial q}{\partial y} = 1$$

$$\frac{\partial f}{\partial z} = q \mid q = 3$$

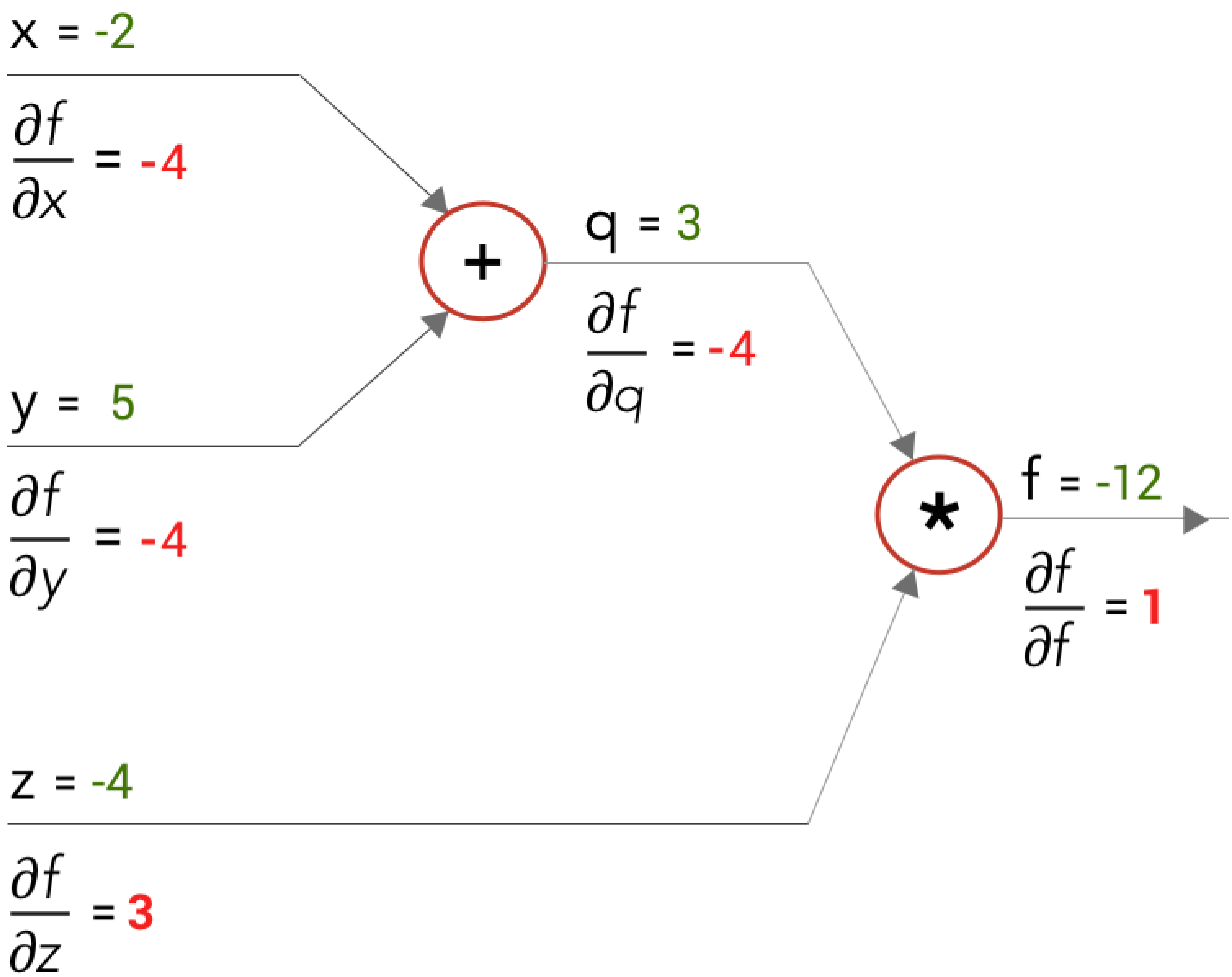
我们希望获得$\partial f/\partial x$和$\partial f/\partial y$，但是目前我们只获得了$\partial q/\partial x$和$\partial q/\partial y$，那么我们达到我们的目标

呢。
这里就可以使用链式法则来进行推导，通过链式法则，我们可以计算$\partial f/\partial x$：

Using chain rule:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} * \frac{\partial q}{\partial x}$$

那么我们可以计算得到$\partial f/\partial x$和$\partial f/\partial y$如下：

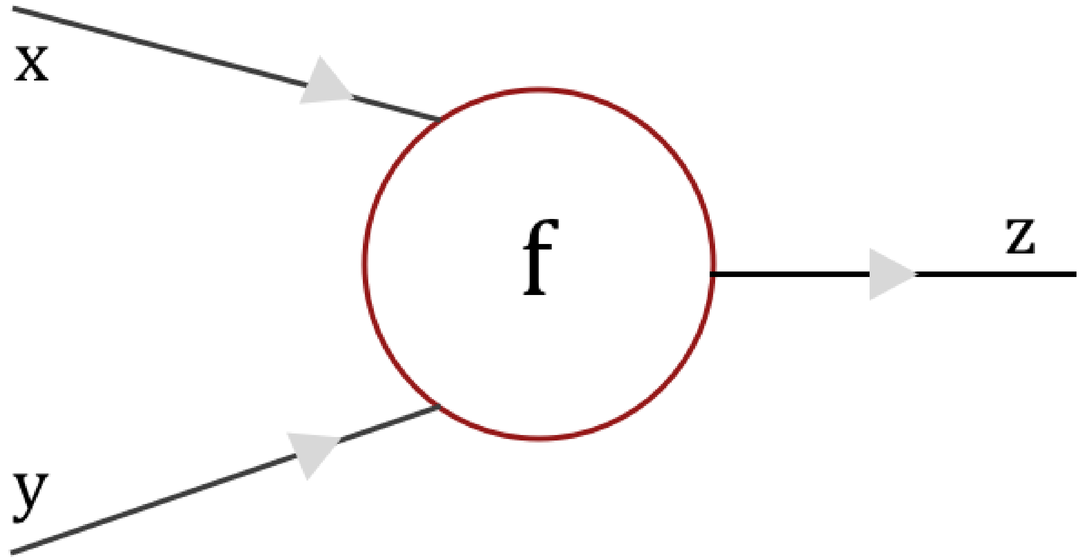


$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} * \frac{\partial q}{\partial x} = -4 * 1 = -4$$

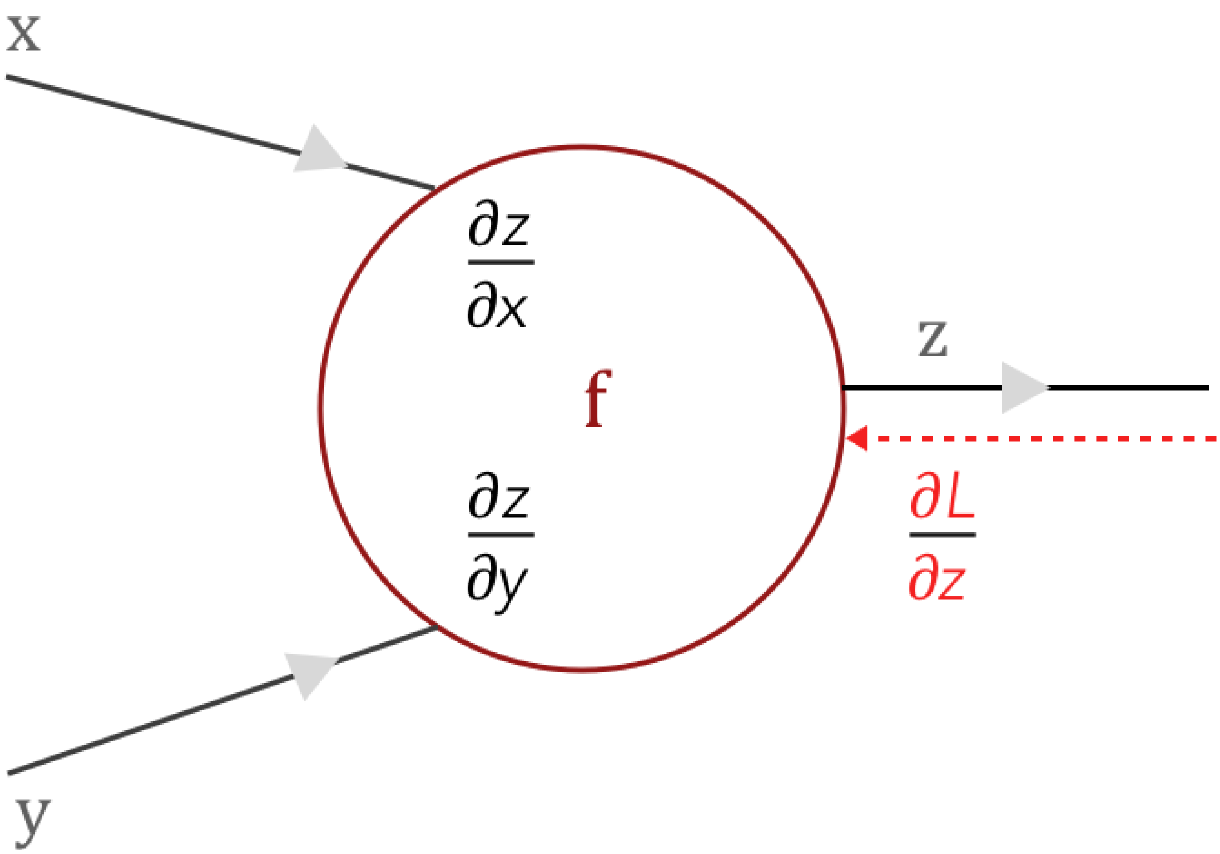
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} * \frac{\partial q}{\partial y} = -4 * 1 = -4$$

2. 在卷积层中的链式法则

如下所示，我们有一个门函数f，它的输入是x和y，输出是z：



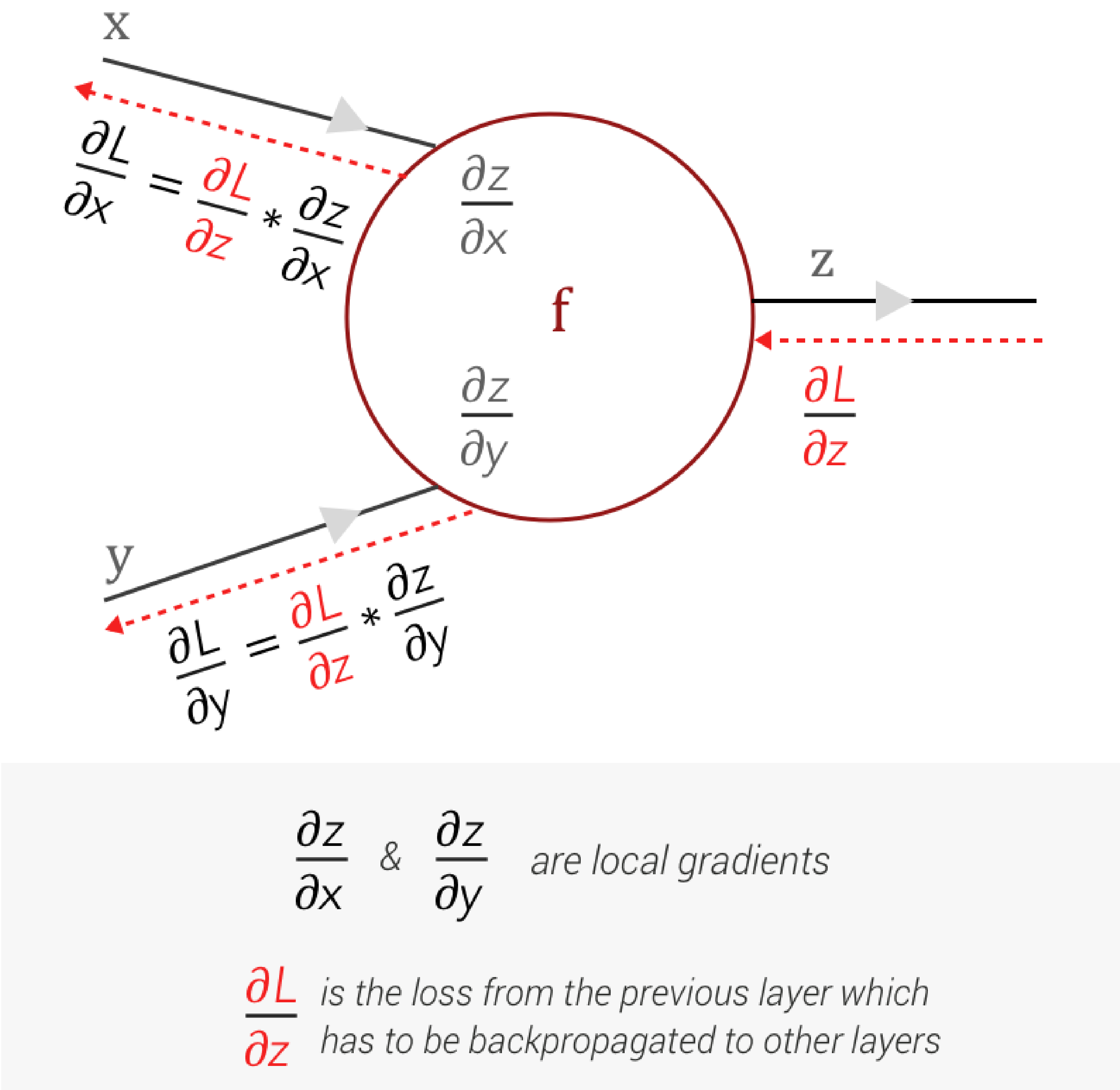
我们可以很容易的计算出局部梯度$\partial z/\partial x$ 和$\partial z/\partial y$。
对于前向传播阶段，我们可以通过一个CNN层，然后一直往后传，直到用损失函数计算出它的损失。
然后当我们计算损失反向传播时，一层一层的往前传，我们获得了对于z的梯度$\partial L/\partial z$。此时为了继续往前传，我们需要计算出$\partial L/\partial x$和$\partial L/\partial y$。



$\frac{\partial z}{\partial x}$ & $\frac{\partial z}{\partial y}$ *are local gradients*

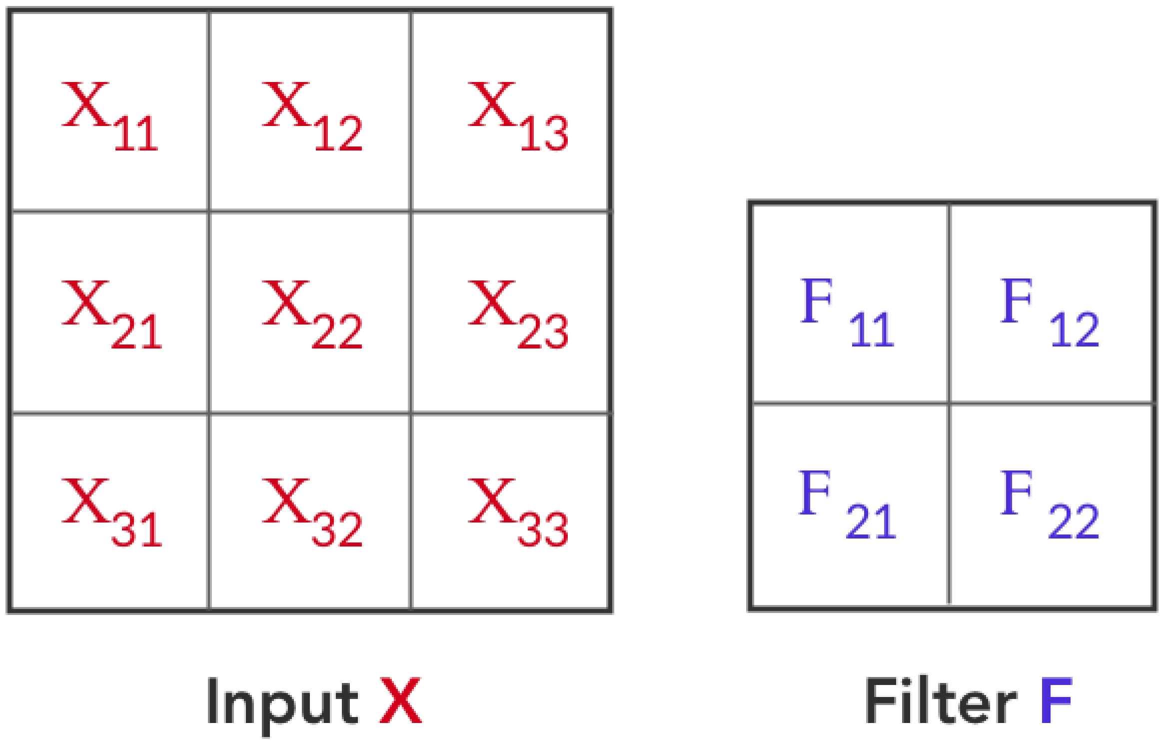
$\frac{\partial L}{\partial z}$ *is the loss from the previous layer which has to be backpropagated to other layers*

此时使用链式法则，我们可以计算出$\partial L / \partial x$和$\partial L / \partial y$:

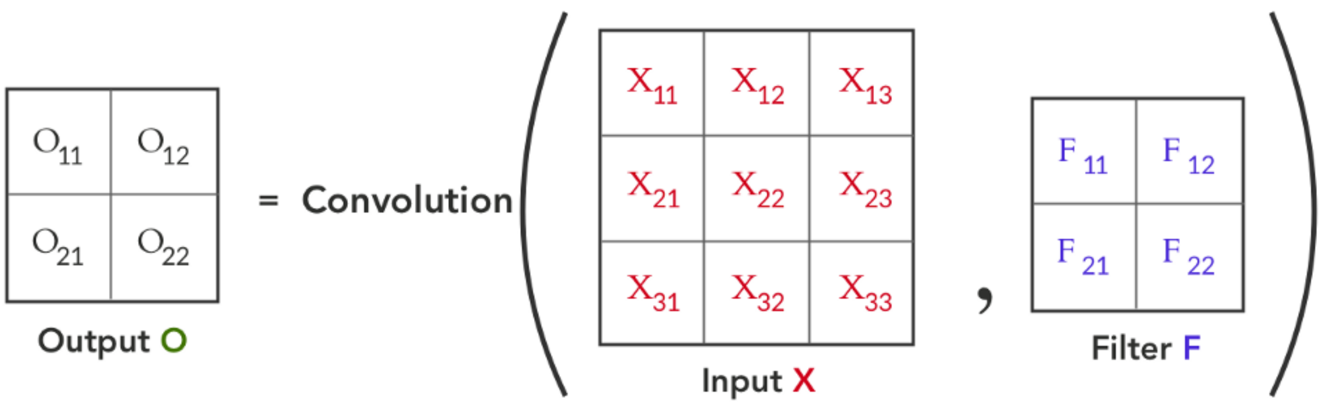


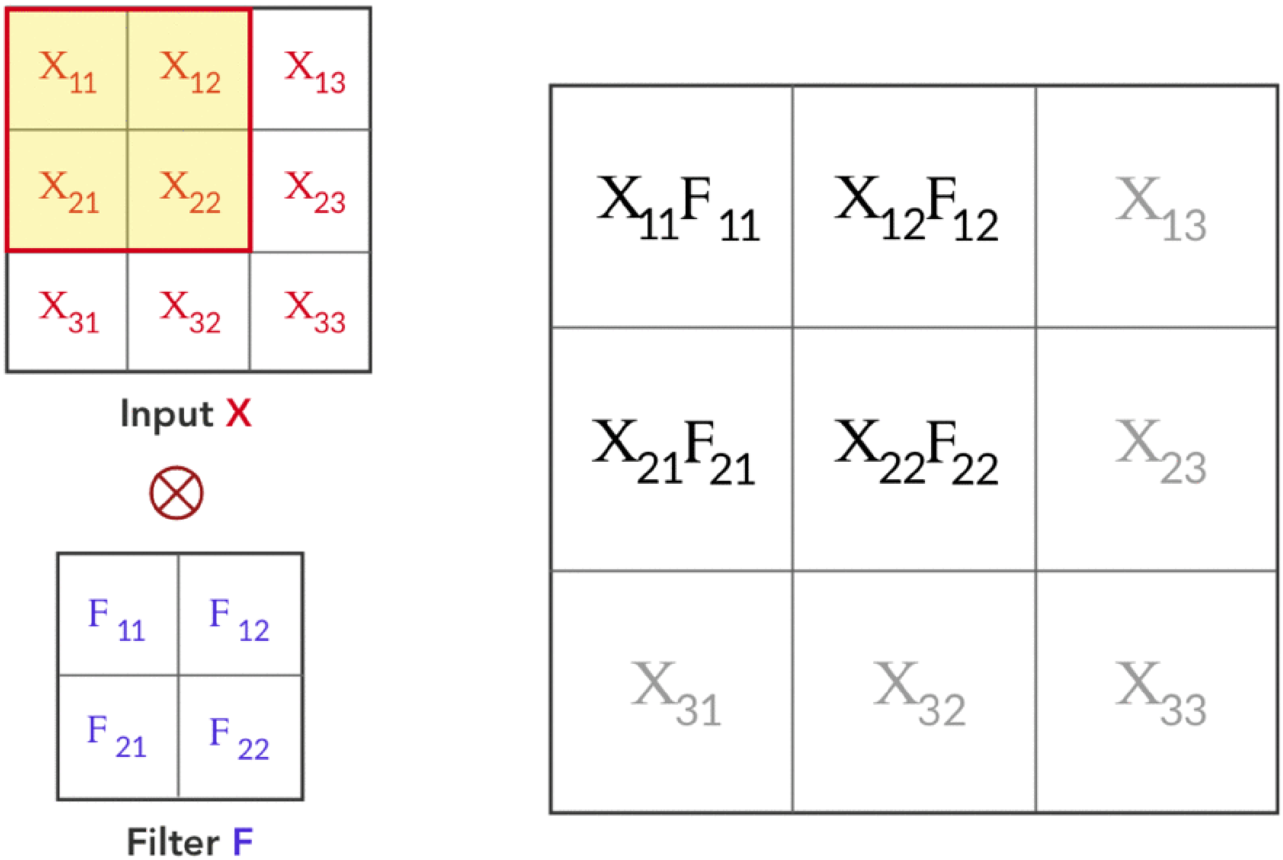
那么，具体的对于CNN中的卷积层是如何进行反向传播的呢?

现在，让我们假设f是一个卷积函数，对于输入X和卷积核F进行卷积计算，其中X是一个3×3的矩阵，而F是一个2×2的矩阵:



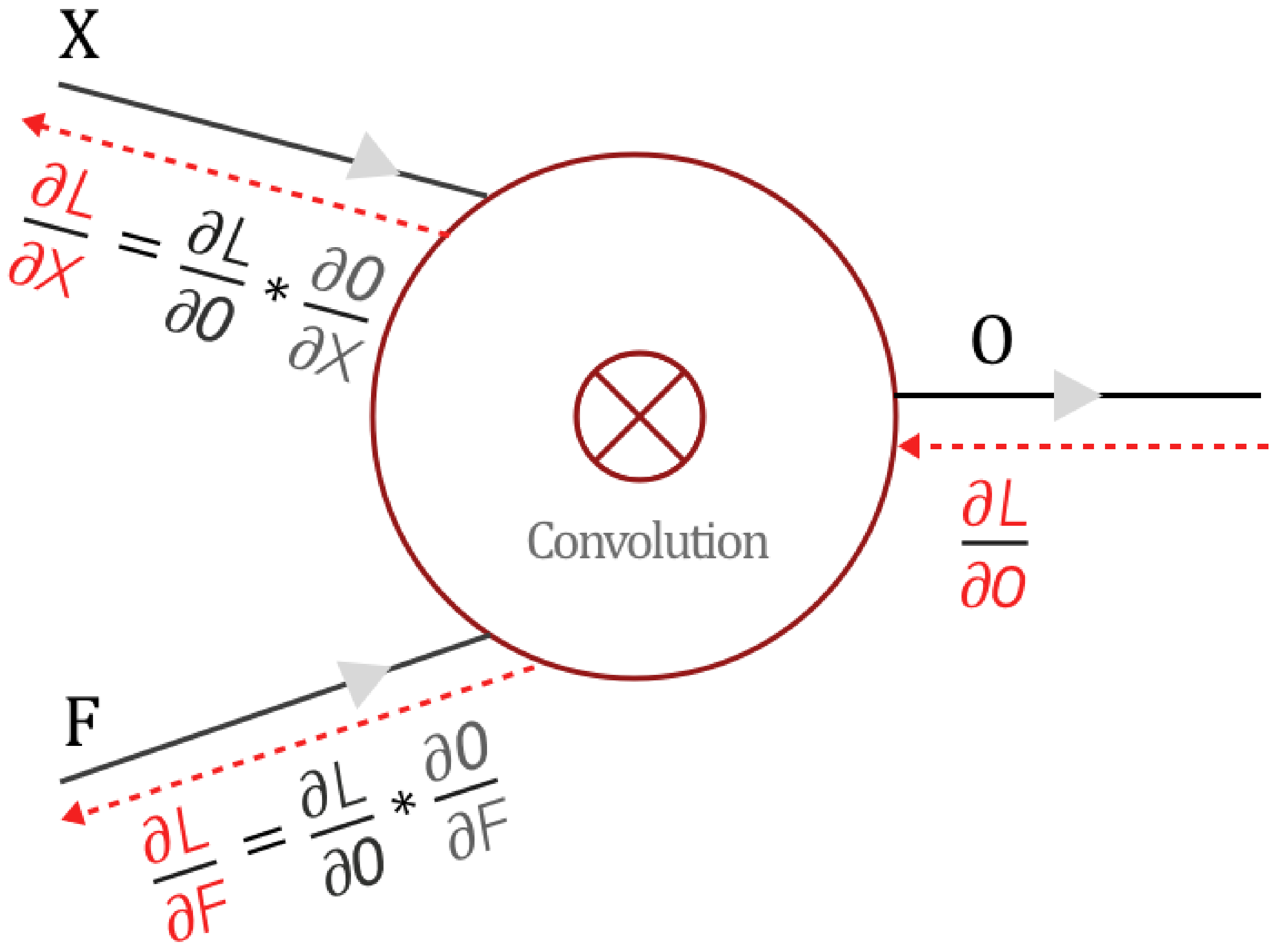
在X和F的卷积操作的输出为O，可以被表示为如下：

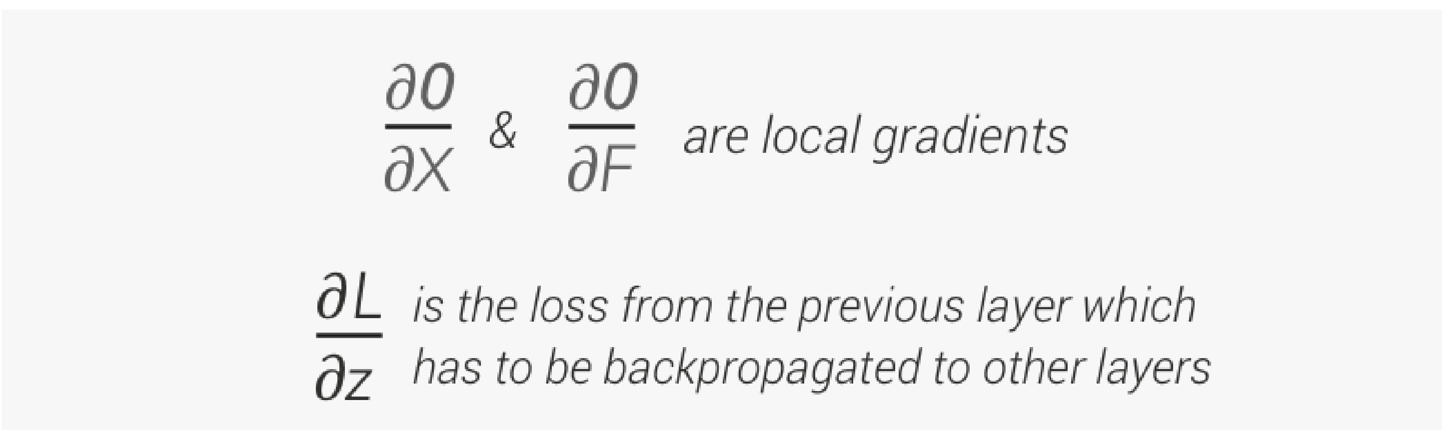




$$O_{11} = X_{11}F_{11} + X_{12}F_{12} + X_{21}F_{21} + X_{22}F_{22}$$

这就给了我们前向传播的过程，下面让我们来处理反向传播的过程。
正如上面提到的，我们已经获得了对当前输出O的梯度$\partial L/\partial O$，那么综合前面的链式法则和反向传播，我们可以得到：





3. 具体的计算梯度的方法

下面就让我们来计算$\partial L/\partial X$和$\partial L/\partial F$，

3.1 计算$\partial L/\partial F$

计算$\partial L/\partial F$主要通过如下两步：

- 找到局部梯度$\partial O/\partial F$
- 使用链式法则计算$\partial L/\partial F$

3.1.1 计算局部梯度$\partial O/\partial F$

这意味着我们需要计算输出矩阵O对于卷积核F的偏导，从卷积操作中，我们知道O^{11}与F^{11}、F^{12}、F^{21}、F^{22}均有关系：

Local Gradients → A

$$O_{11} = X_{11}F_{11} + X_{12}F_{12} + X_{21}F_{21} + X_{22}F_{22}$$

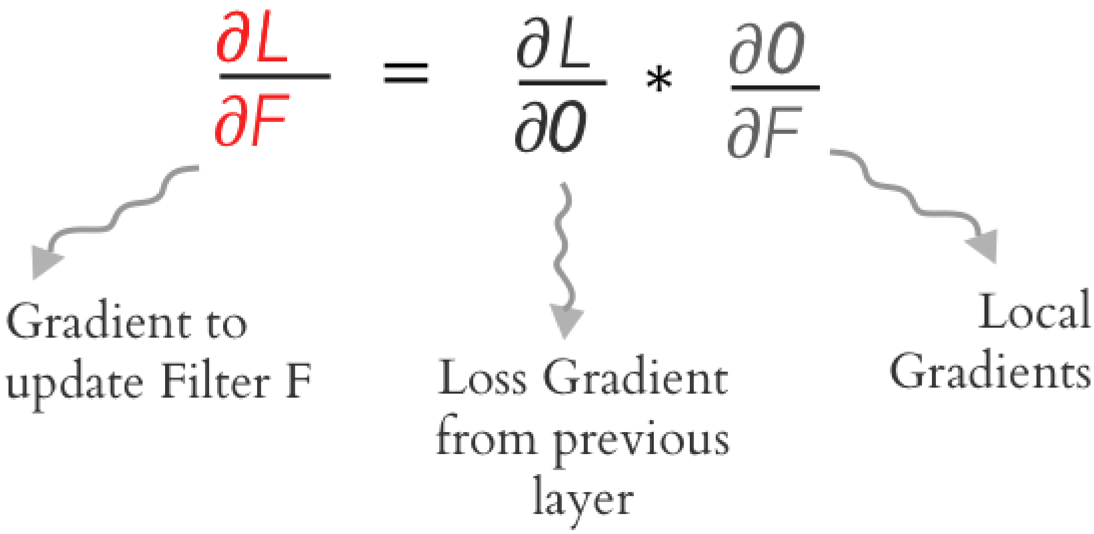
Finding derivatives with respect to F_{11} , F_{12} , F_{21} and F_{22}

$$\frac{\partial O_{11}}{\partial F_{11}} = X_{11} \quad \frac{\partial O_{11}}{\partial F_{12}} = X_{12} \quad \frac{\partial O_{11}}{\partial F_{21}} = X_{21} \quad \frac{\partial O_{11}}{\partial F_{22}} = X_{22}$$

Similarly, we can find the local gradients for O_{12} , O_{21} and O_{22}

3.1.2 使用链式法则

正如上面所描述的，我们按照下面的方法来计算$\partial L/\partial F$：



其中O和F都是矩阵，因此对于其中的每一个F_i的梯度，我们可以按照下面的方法来计算：

For every element of F

$$\frac{\partial L}{\partial F_i} = \sum_{k=1}^{M} \frac{\partial L}{\partial O_k} * \frac{\partial O_k}{\partial F_i}$$

扩展开来，我们可以得到：

$$\frac{\partial L}{\partial F_{11}} = \frac{\partial L}{\partial O_{11}} * \frac{\partial O_{11}}{\partial F_{11}} + \frac{\partial L}{\partial O_{12}} * \frac{\partial O_{12}}{\partial F_{11}} + \frac{\partial L}{\partial O_{21}} * \frac{\partial O_{21}}{\partial F_{11}} + \frac{\partial L}{\partial O_{22}} * \frac{\partial O_{22}}{\partial F_{11}}$$

$$\frac{\partial L}{\partial F_{12}} = \frac{\partial L}{\partial O_{11}} * \frac{\partial O_{11}}{\partial F_{12}} + \frac{\partial L}{\partial O_{12}} * \frac{\partial O_{12}}{\partial F_{12}} + \frac{\partial L}{\partial O_{21}} * \frac{\partial O_{21}}{\partial F_{12}} + \frac{\partial L}{\partial O_{22}} * \frac{\partial O_{22}}{\partial F_{12}}$$

$$\frac{\partial L}{\partial F_{21}} = \frac{\partial L}{\partial O_{11}} * \frac{\partial O_{11}}{\partial F_{21}} + \frac{\partial L}{\partial O_{12}} * \frac{\partial O_{12}}{\partial F_{21}} + \frac{\partial L}{\partial O_{21}} * \frac{\partial O_{21}}{\partial F_{21}} + \frac{\partial L}{\partial O_{22}} * \frac{\partial O_{22}}{\partial F_{21}}$$

$$\frac{\partial L}{\partial F_{22}} = \frac{\partial L}{\partial O_{11}} * \frac{\partial O_{11}}{\partial F_{22}} + \frac{\partial L}{\partial O_{12}} * \frac{\partial O_{12}}{\partial F_{22}} + \frac{\partial L}{\partial O_{21}} * \frac{\partial O_{21}}{\partial F_{22}} + \frac{\partial L}{\partial O_{22}} * \frac{\partial O_{22}}{\partial F_{22}}$$

将局部梯度$\partial O / \partial F$的结果导入可得：

$$\frac{\partial L}{\partial F_{11}} = \frac{\partial L}{\partial O_{11}} * X_{11} + \frac{\partial L}{\partial O_{12}} * X_{12} + \frac{\partial L}{\partial O_{21}} * X_{21} + \frac{\partial L}{\partial O_{22}} * X_{22}$$

$$\frac{\partial L}{\partial F_{12}} = \frac{\partial L}{\partial O_{11}} * X_{12} + \frac{\partial L}{\partial O_{12}} * X_{13} + \frac{\partial L}{\partial O_{21}} * X_{22} + \frac{\partial L}{\partial O_{22}} * X_{23}$$

$$\frac{\partial L}{\partial F_{21}} = \frac{\partial L}{\partial O_{11}} * X_{21} + \frac{\partial L}{\partial O_{12}} * X_{22} + \frac{\partial L}{\partial O_{21}} * X_{31} + \frac{\partial L}{\partial O_{22}} * X_{32}$$

$$\frac{\partial L}{\partial F_{22}} = \frac{\partial L}{\partial O_{11}} * X_{22} + \frac{\partial L}{\partial O_{12}} * X_{23} + \frac{\partial L}{\partial O_{21}} * X_{32} + \frac{\partial L}{\partial O_{22}} * X_{33}$$

对于上式，我们可以使用卷积的方式来表示：

$$\begin{bmatrix} \frac{\partial L}{\partial F_{11}} & \frac{\partial L}{\partial F_{12}} \\ \frac{\partial L}{\partial F_{21}} & \frac{\partial L}{\partial F_{22}} \end{bmatrix} = \text{Convolution}\left(\begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \\ X_{31} & X_{32} & X_{33} \end{bmatrix}, \begin{bmatrix} \frac{\partial L}{\partial O_{11}} & \frac{\partial L}{\partial O_{12}} \\ \frac{\partial L}{\partial O_{21}} & \frac{\partial L}{\partial O_{22}} \end{bmatrix} \right)$$

where

$$\begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \\ X_{31} & X_{32} & X_{33} \end{bmatrix} = \text{Input X} \qquad \begin{bmatrix} \frac{\partial L}{\partial O_{11}} & \frac{\partial L}{\partial O_{12}} \\ \frac{\partial L}{\partial O_{21}} & \frac{\partial L}{\partial O_{22}} \end{bmatrix} = \frac{\partial L}{\partial O} \ \text{Loss gradient from previous layer}$$

3.2 计算$\partial L/\partial X$

也是如上分两步走。

3.2.1 计算$\partial O/\partial X$

我们可以通过如下的方式计算得到$\partial O/\partial X$:

Local Gradients: $\longrightarrow$ B

$$O_{11} = X_{11}F_{11} + X_{12}F_{12} + X_{21}F_{21} + X_{22}F_{22}$$

Differentiating with respect to X_{11}, X_{12}, X_{21} *and* X_{22}

$$\frac{\partial O_{11}}{\partial X_{11}} = F_{11} \quad \frac{\partial O_{11}}{\partial X_{12}} = F_{12} \quad \frac{\partial O_{11}}{\partial X_{21}} = F_{21} \quad \frac{\partial O_{11}}{\partial X_{22}} = F_{22}$$

Similarly, we can find local gradients for O_{12}, O_{21} *and* O_{22}

3.2.2 使用链式法则

For every element of X_i

$$\frac{\partial L}{\partial X_i} = \sum_{k=1}^{M} \frac{\partial L}{\partial O_k} * \frac{\partial O_k}{\partial X_i}$$

对其进行扩展可得：

$$\frac{\partial L}{\partial X_{11}} = \frac{\partial L}{\partial O_{11}} * F_{11}$$

$$\frac{\partial L}{\partial X_{12}} = \frac{\partial L}{\partial O_{11}} * F_{12} + \frac{\partial L}{\partial O_{12}} * F_{11}$$

$$\frac{\partial L}{\partial X_{13}} = \frac{\partial L}{\partial O_{12}} * F_{12}$$

$$\frac{\partial L}{\partial X_{21}} = \frac{\partial L}{\partial O_{11}} * F_{21} + \frac{\partial L}{\partial O_{21}} * F_{11}$$

$$\frac{\partial L}{\partial X_{22}} = \frac{\partial L}{\partial O_{11}} * F_{22} + \frac{\partial L}{\partial O_{12}} * F_{21} + \frac{\partial L}{\partial O_{21}} * F_{12} + \frac{\partial L}{\partial O_{22}} * F_{11}$$

$$\frac{\partial L}{\partial X_{23}} = \frac{\partial L}{\partial O_{12}} * F_{22} + \frac{\partial L}{\partial O_{22}} * F_{12}$$

$$\frac{\partial L}{\partial X_{31}} = \frac{\partial L}{\partial O_{21}} * F_{21}$$

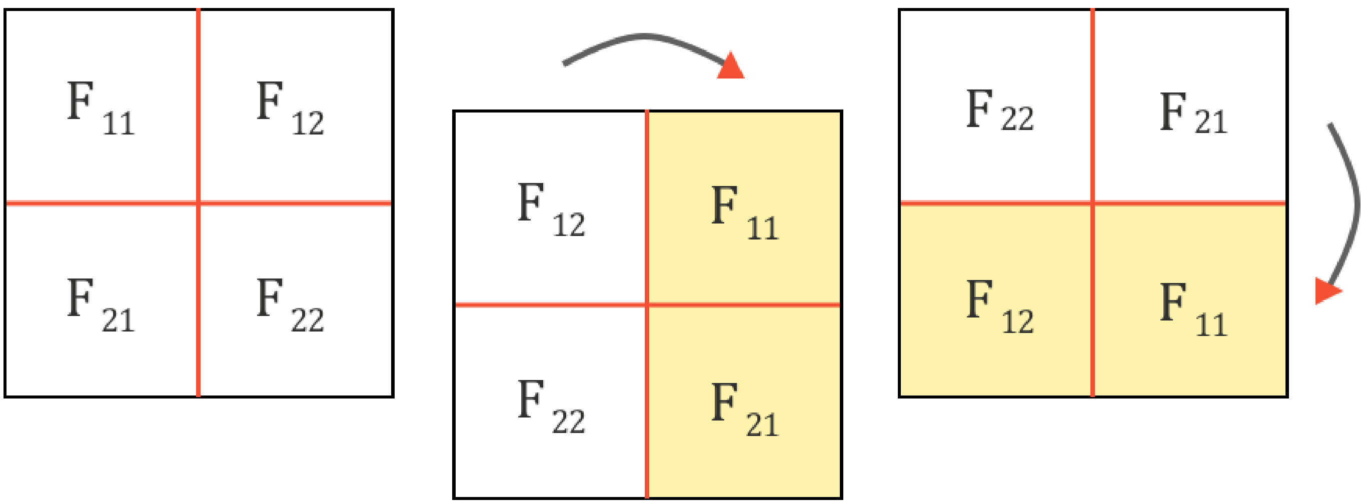
$$\frac{\partial L}{\partial X_{32}} = \frac{\partial L}{\partial O_{21}} * F_{22} + \frac{\partial L}{\partial O_{22}} * F_{21}$$

$$\frac{\partial L}{\partial X_{33}} = \frac{\partial L}{\partial O_{22}} * F_{22}$$

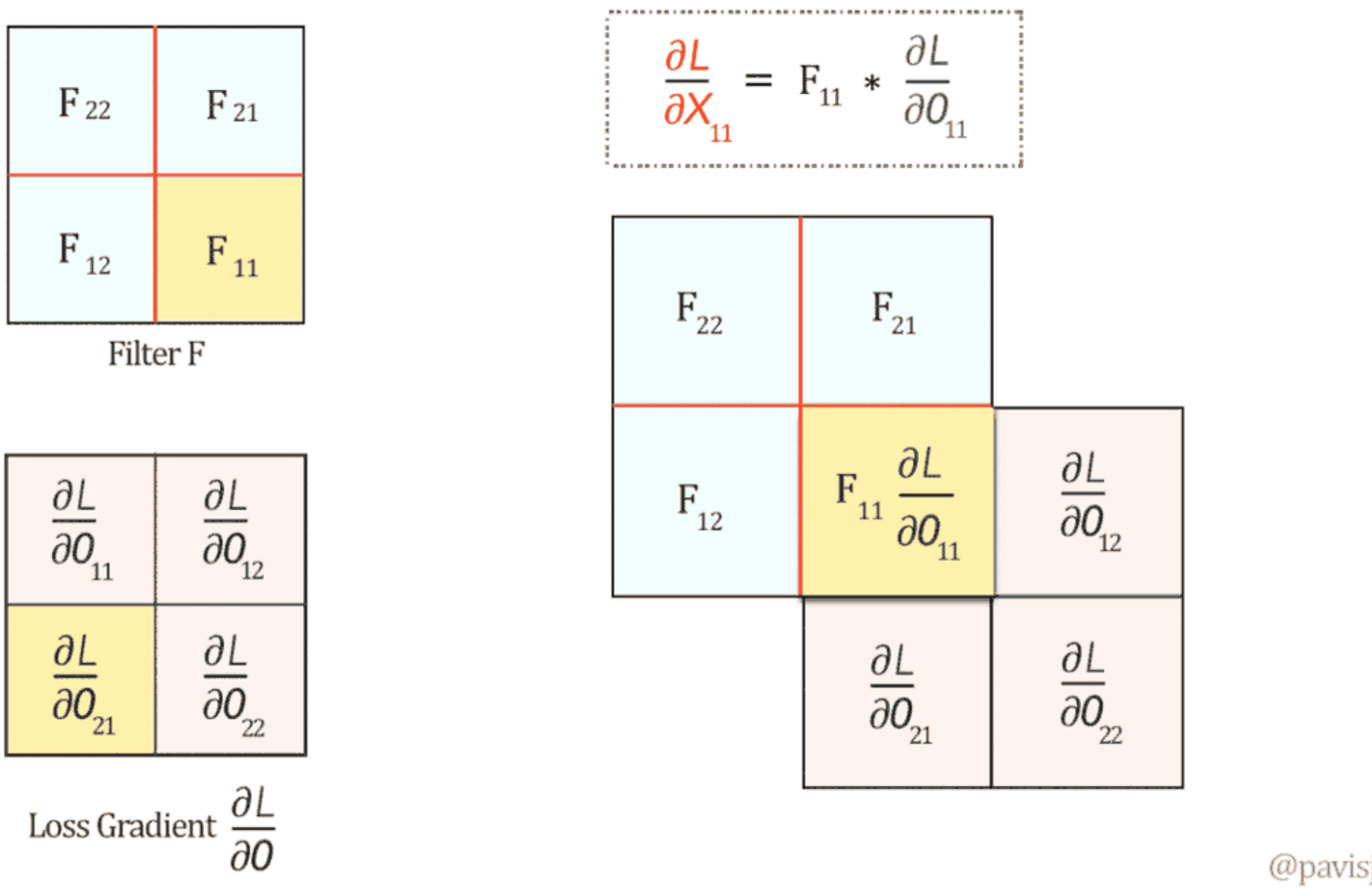
现在我们已经有了$\partial L/\partial X$。

其中$\partial L/\partial X$可以看做是将卷积核F旋转180度后，与梯度损失$\partial L/\partial O$的全卷积。

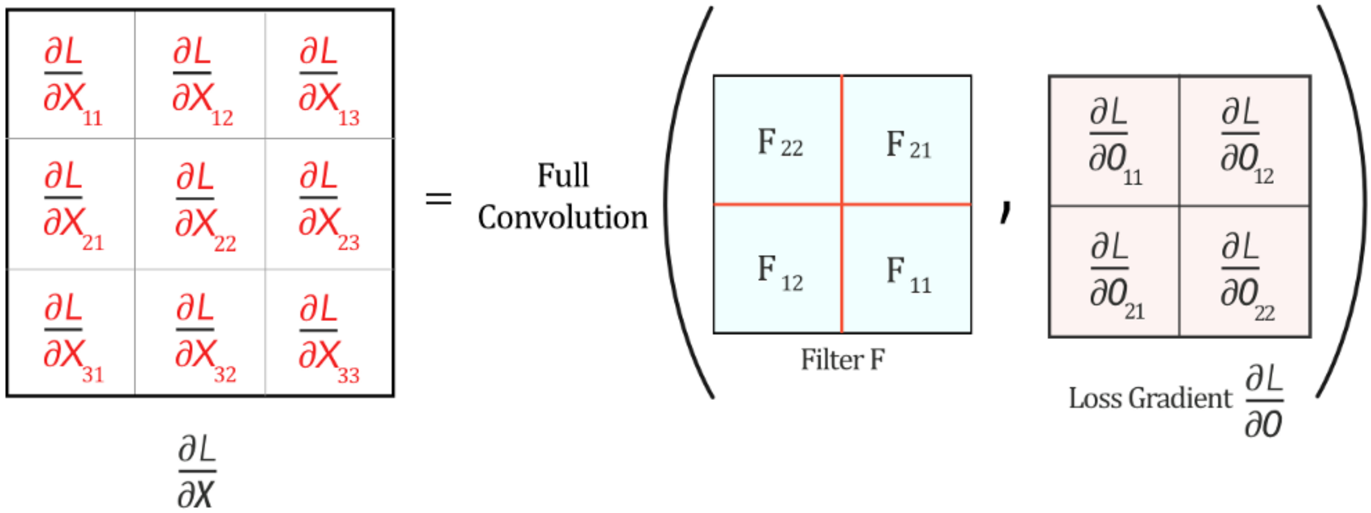
首先，我们将卷积核$F旋转180度



然后，我们可以在卷积核F和$\partial L/\partial O$之间做全卷积：



具体的数学表达如下：



4. 总结

在CNN中的反向传播其实也还是卷积操作：