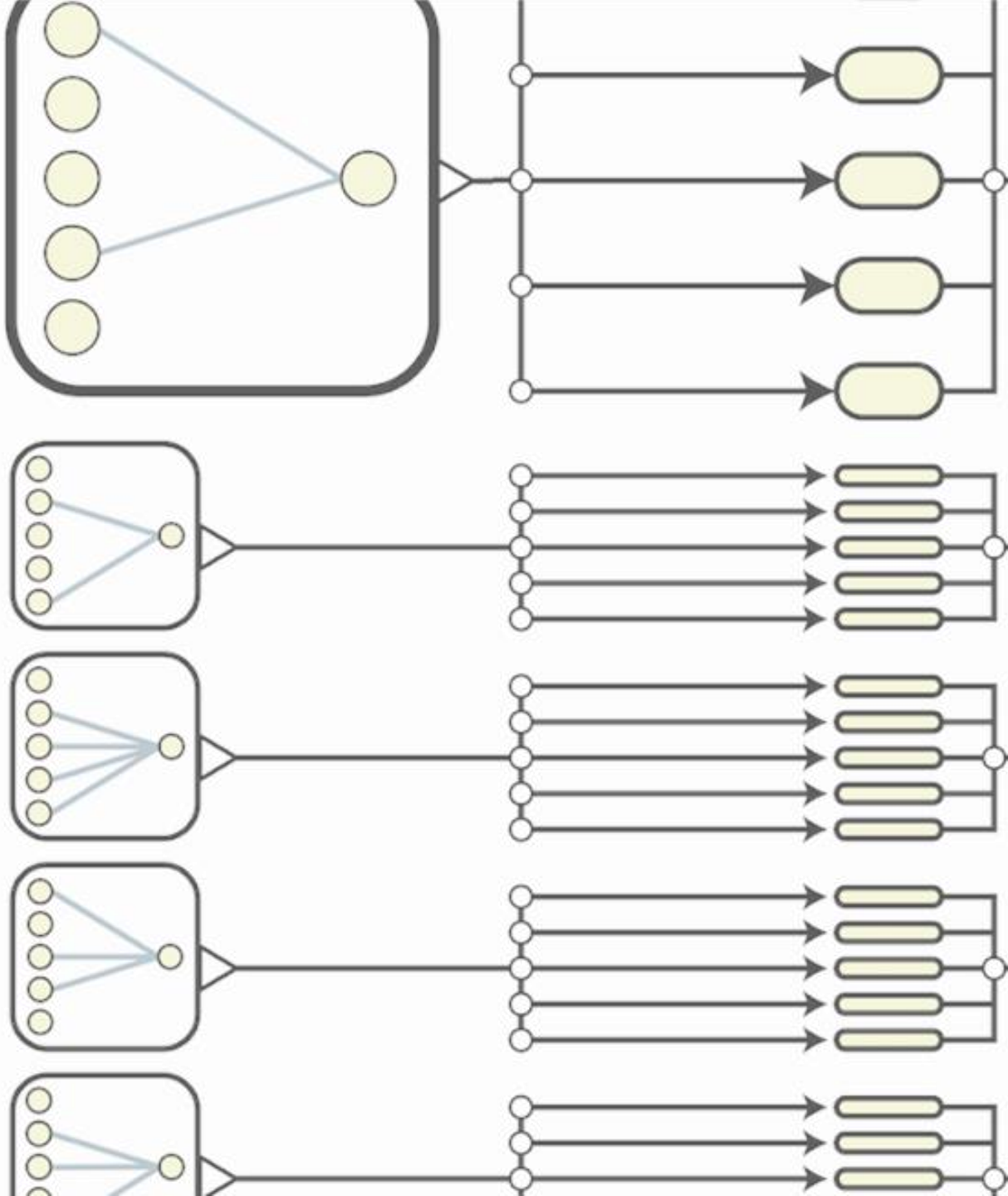


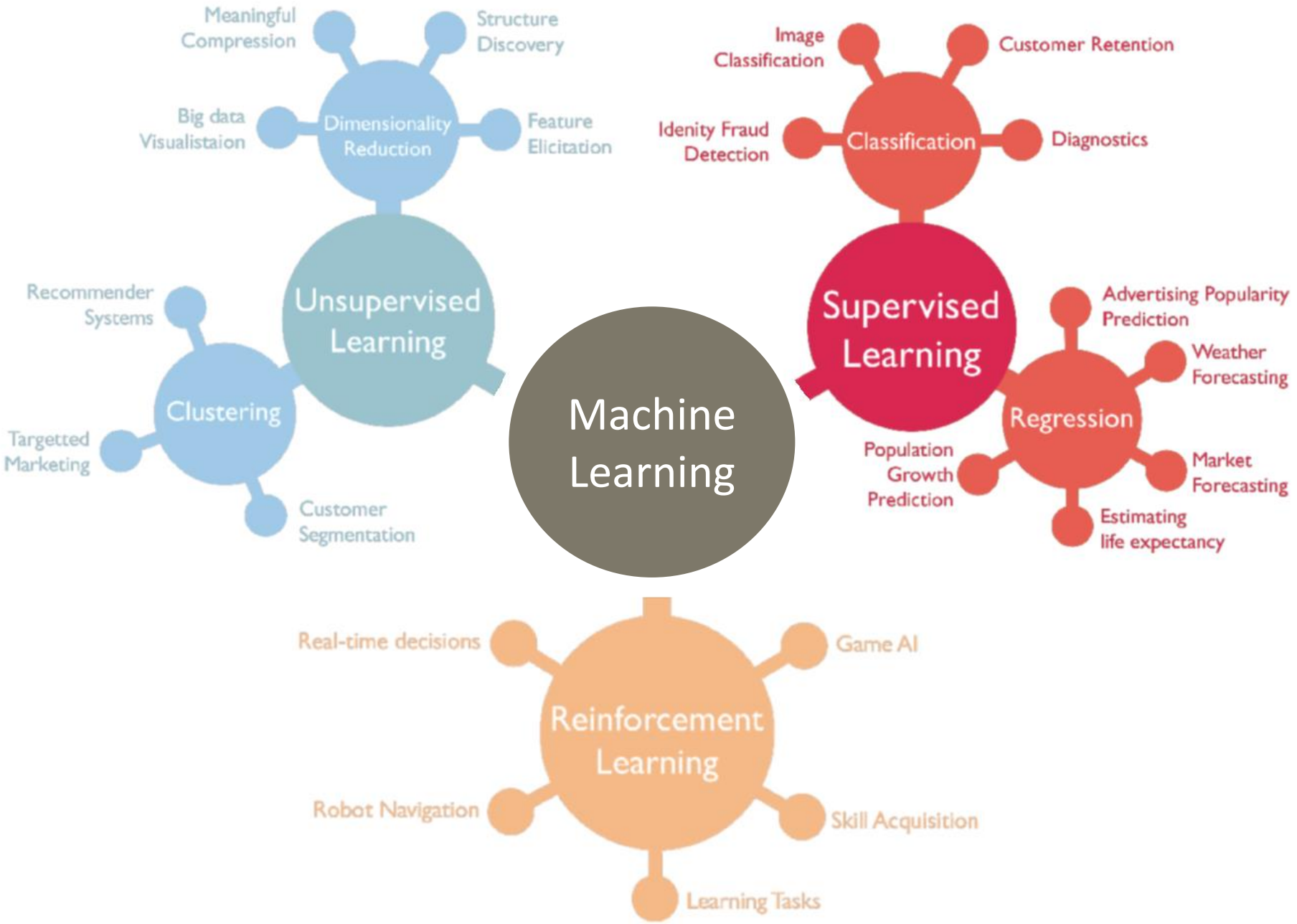
Wahlfach

Neuronale Netze - KI in der Medizin

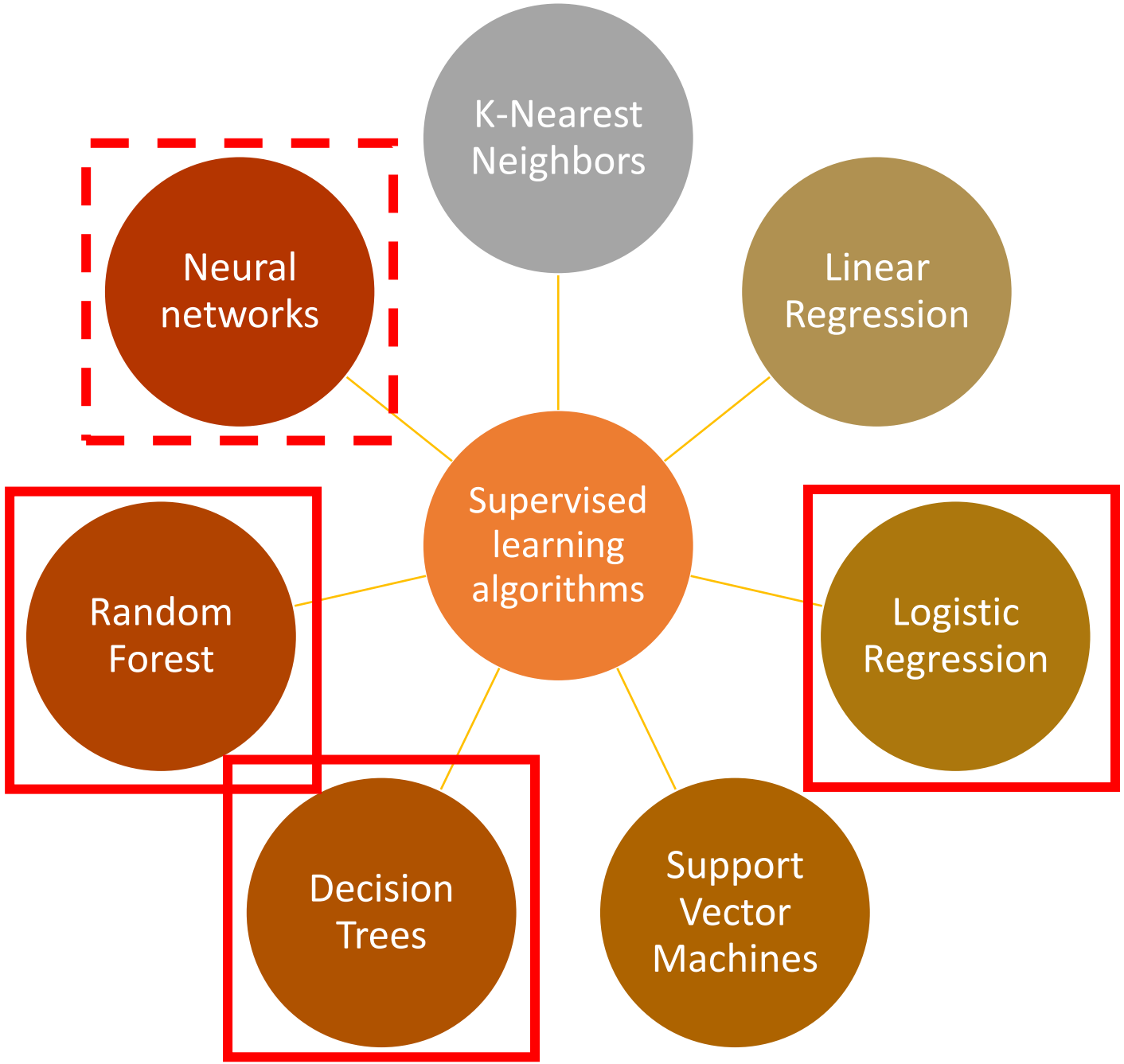
Themen des Wahlfachs

So., 10.12.2023	Crashkurs Python
Sa., 16.12.2023	Crashkurs Machine Learning
So., 17.12.2023	Crashkurs Deep Learning

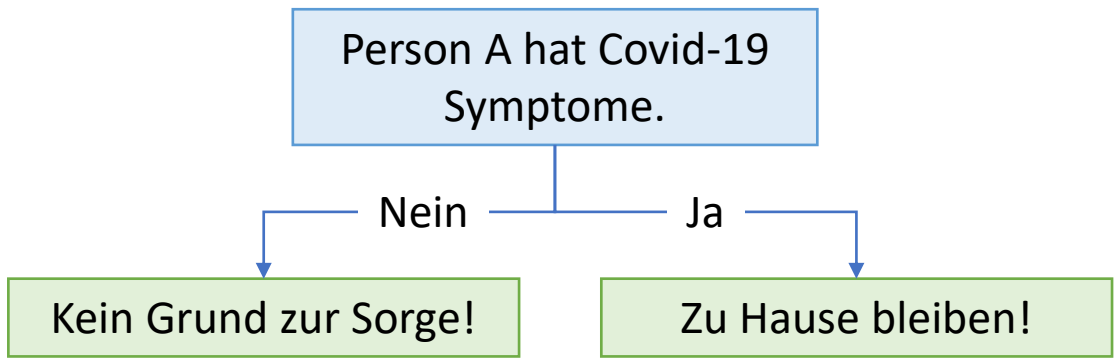
Welches Machine Learning System kommt am besten in Frage?

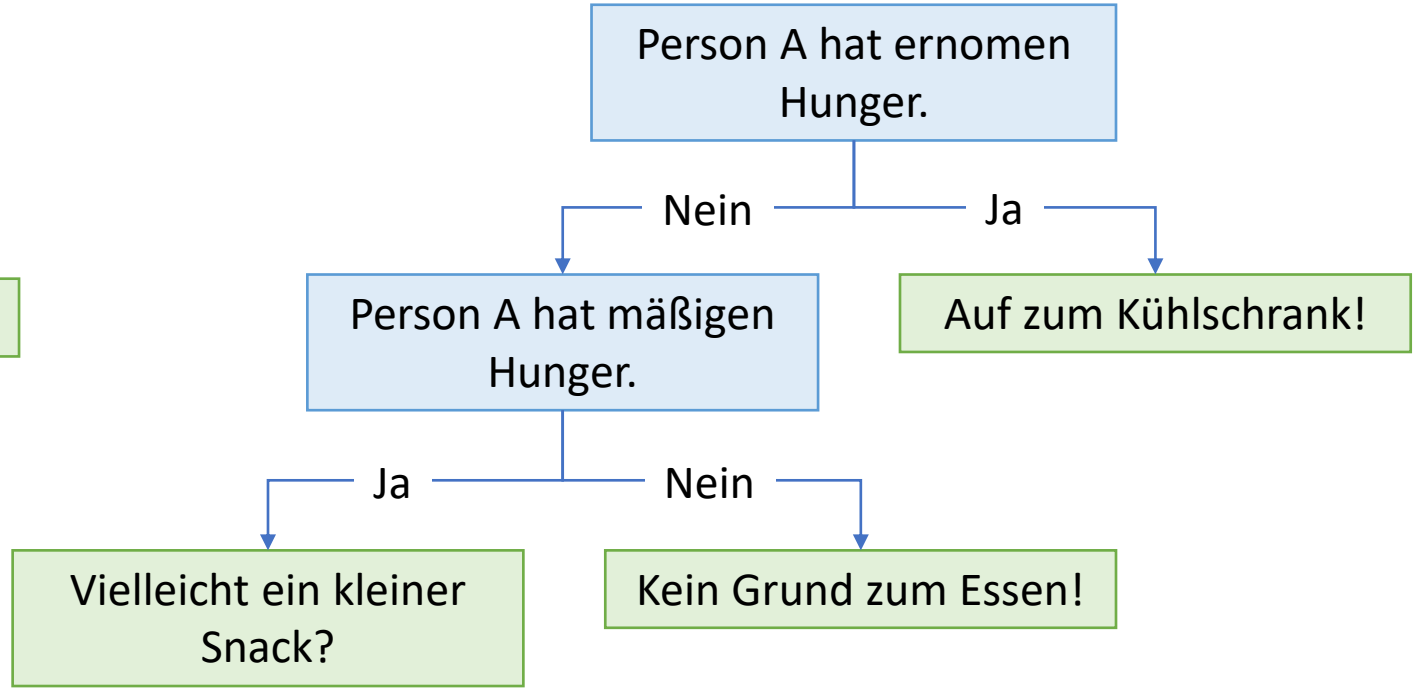


Die Qual der Wahl…

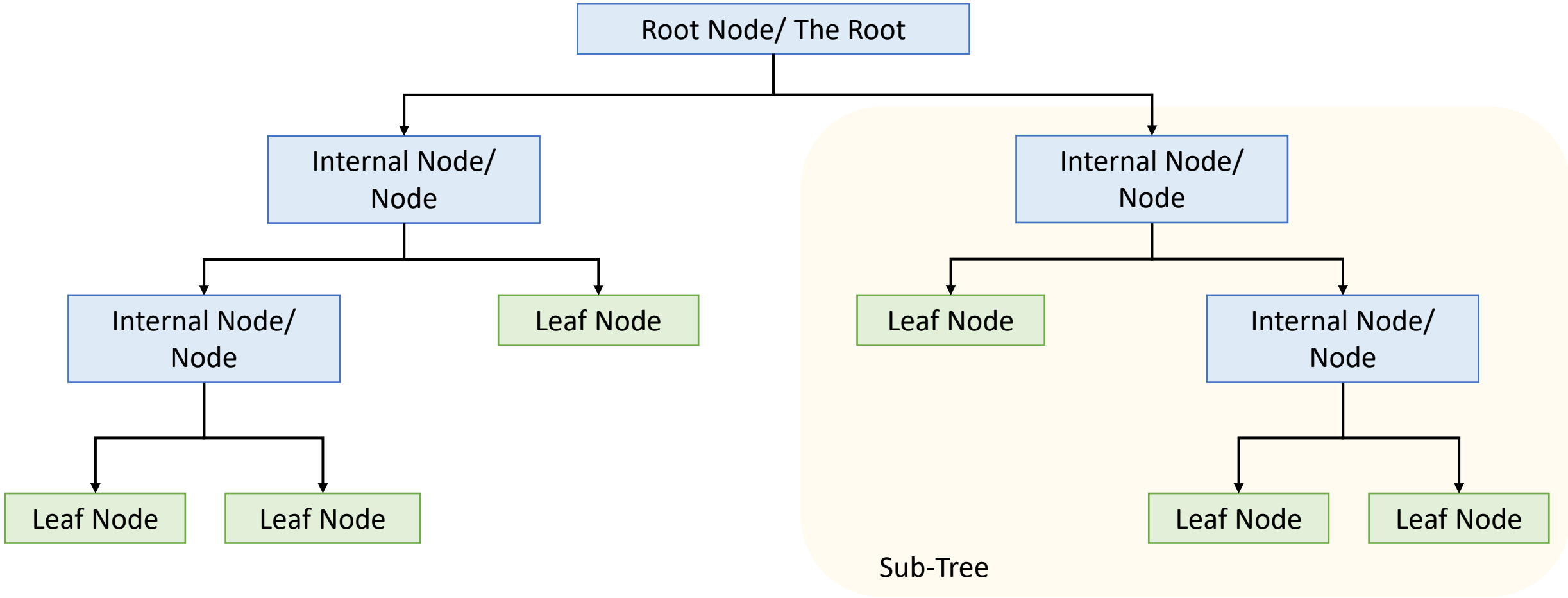


Im Auge des Sturms: Decision Trees



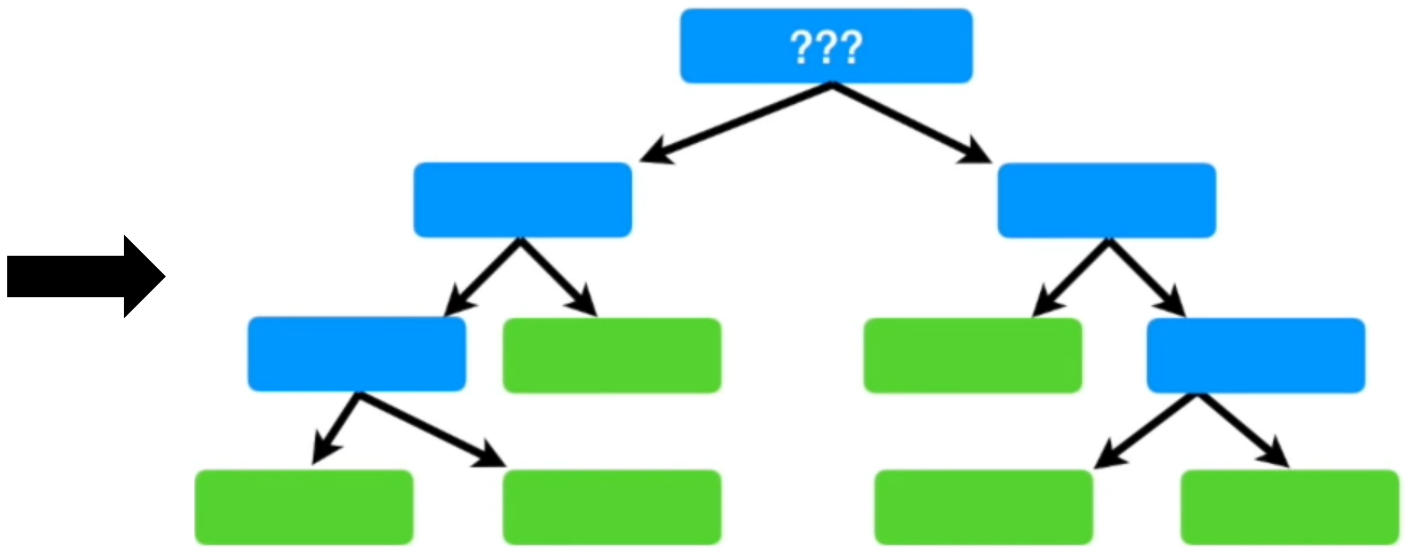


Im Auge des Sturms: Decision Trees



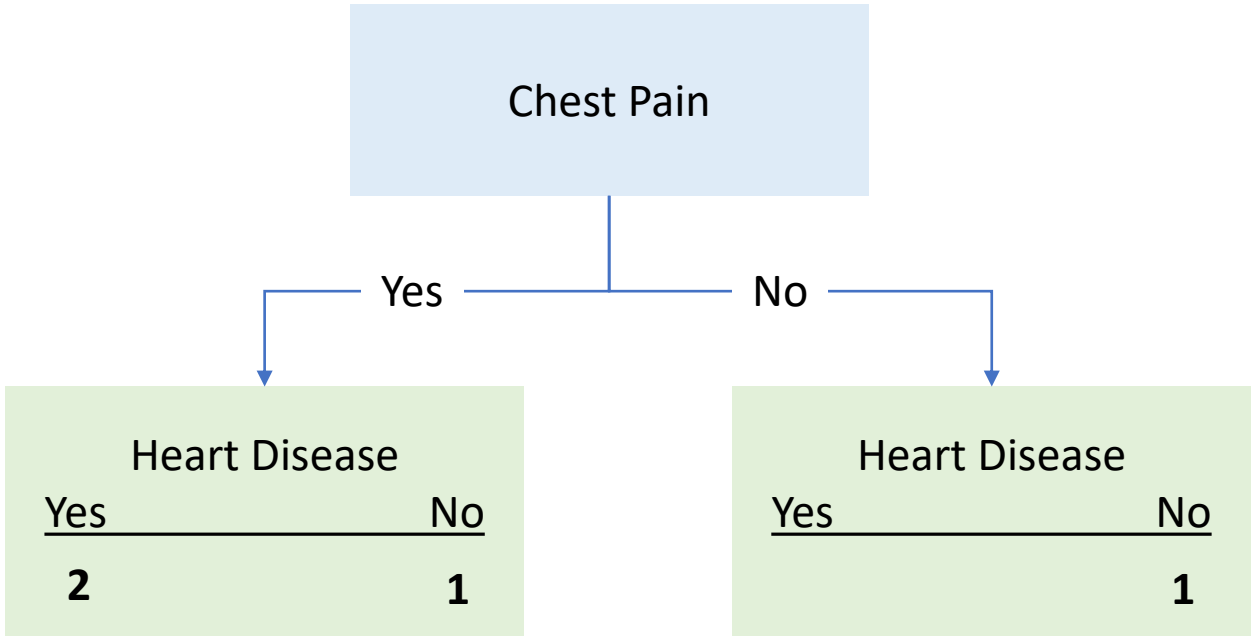
Im Auge des Sturms: Decision Trees

Chest Pain	Good Blood Circulation	Blocked Arteries	Heart Disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	??	Yes
…	…	…	…



Im Auge des Sturms: Decision Trees

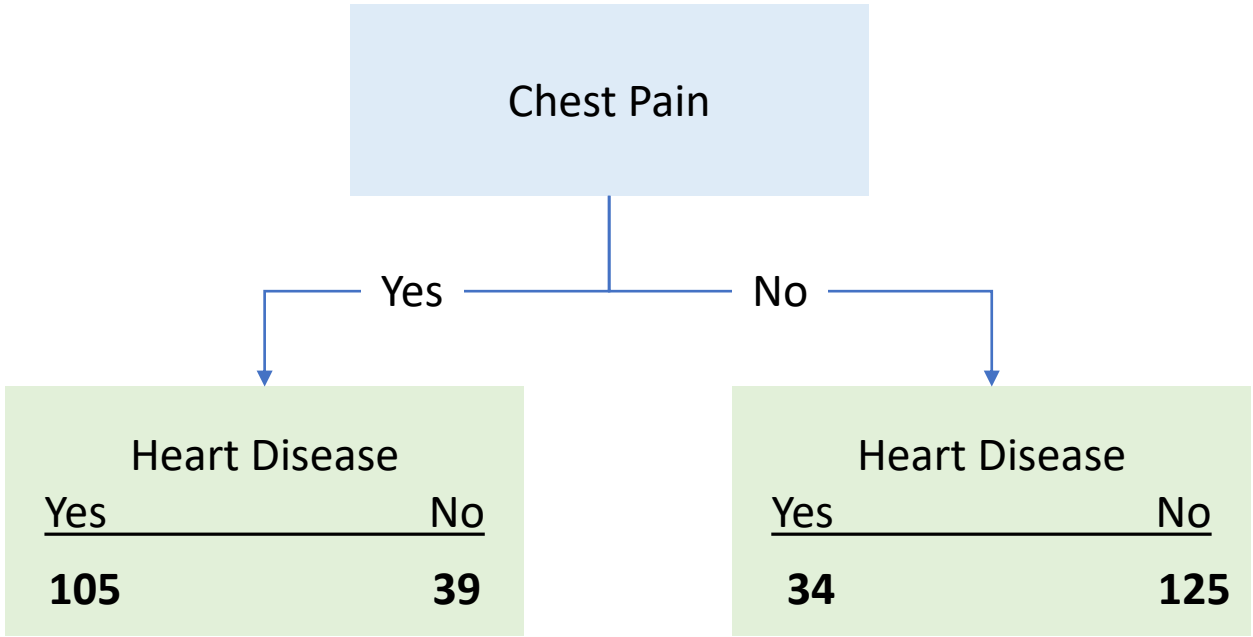
Chest Pain	Good Blood Circulation	Blocked Arteries	Heart Disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	??	Yes
…	…	…	…



Im Auge des Sturms: Decision Trees

Chest Pain	Good Blood Circulation	Blocked Arteries	Heart Disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	??	Yes
…	…	…	…

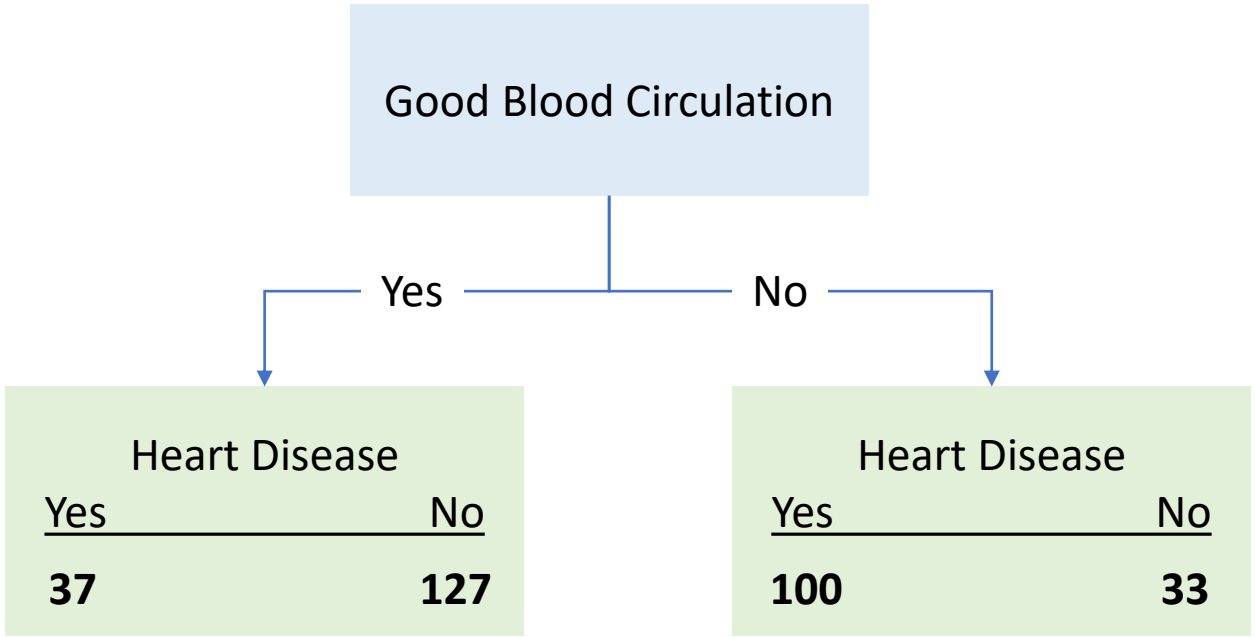
Total: 303 Patienten



Im Auge des Sturms: Decision Trees

Chest Pain	Good Blood Circulation	Blocked Arteries	Heart Disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	??	Yes
…	…	…	…

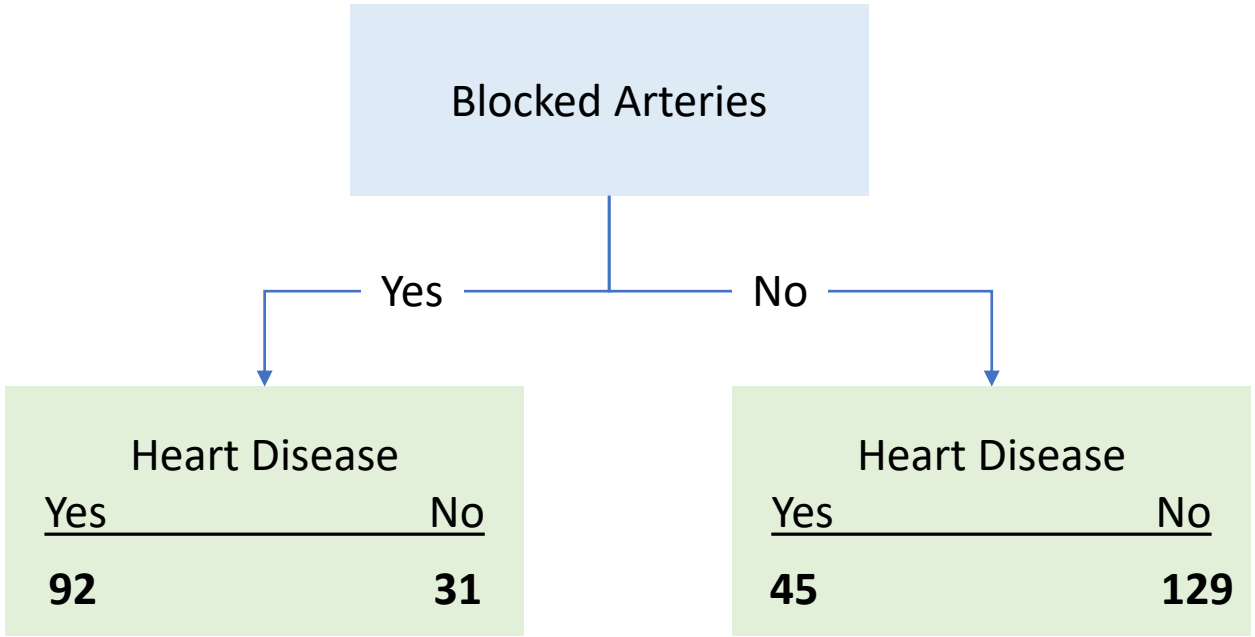
Total: 303 Patienten



Im Auge des Sturms: Decision Trees

Chest Pain	Good Blood Circulation	Blocked Arteries	Heart Disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	??	Yes
…	…	…	…

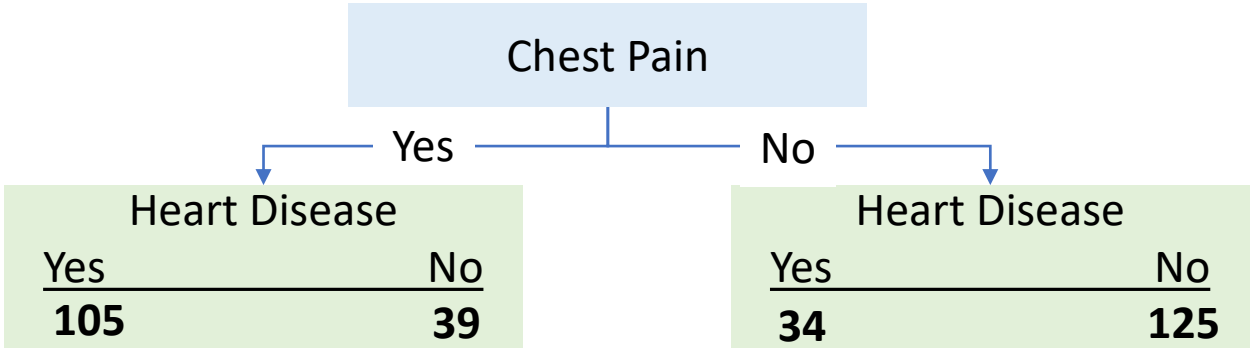
Total: 303 Patienten

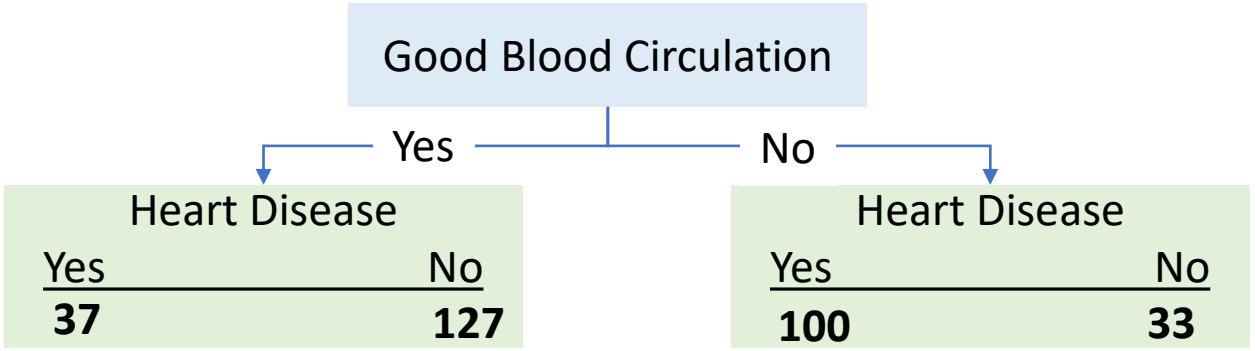


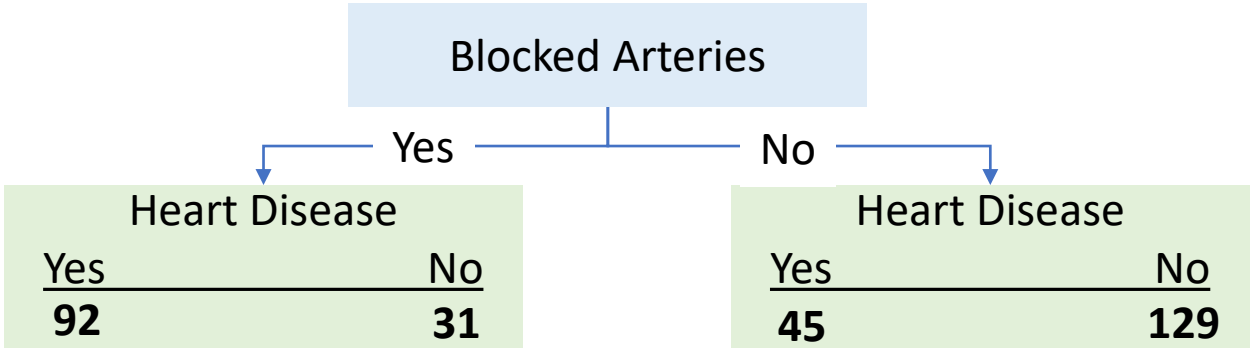
Im Auge des Sturms: Decision Trees

Chest Pain	Good Blood Circulation	Blocked Arteries	Heart Disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	??	Yes
…	…	…	…

Total: 303 Patienten







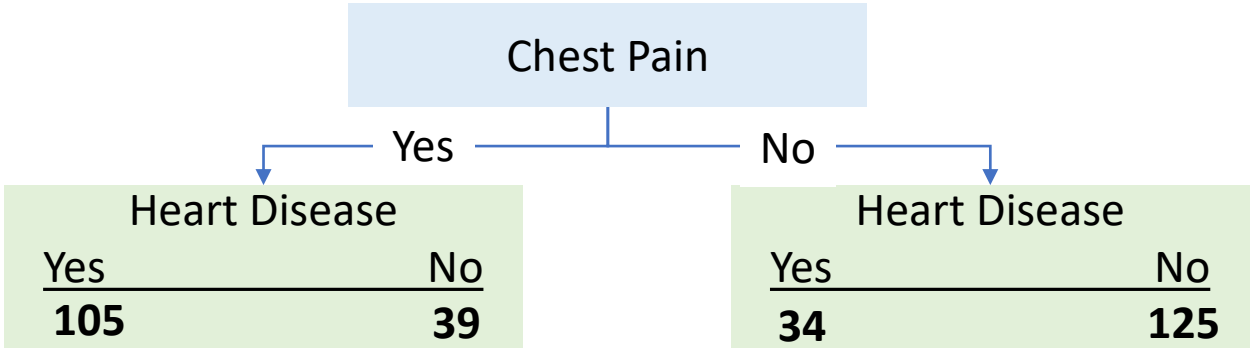
Wir sehen alle unserer Parameter erweisen sich als „impure“ (= unrein), d.h. keiner wäre als „Root Node“ perfekt geeignet.

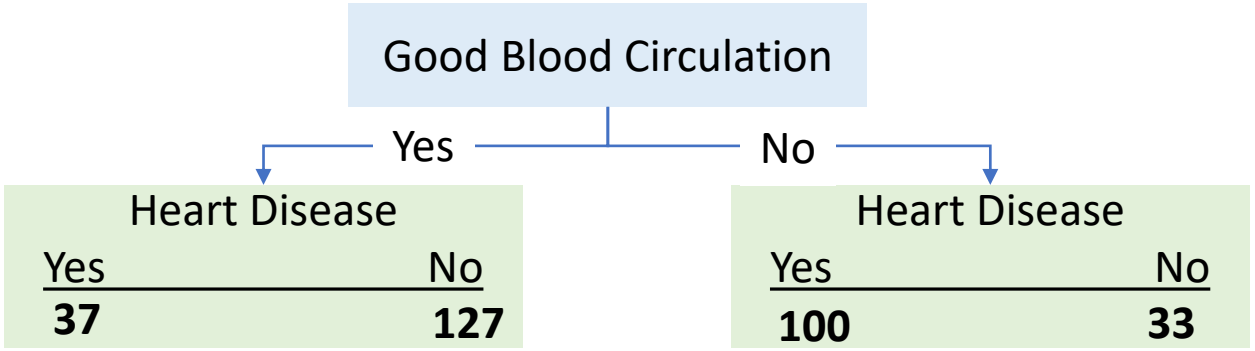
Wir machen einfach das Beste daraus und bestimmen den Reinsten aller Unreinen.

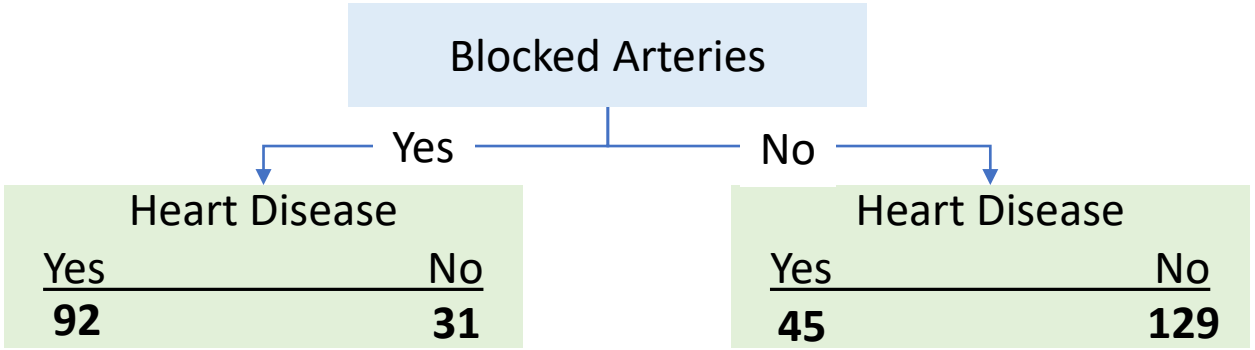
Aber wie misst man „**impurity**“?

Gini impurity =

$$1 - (\boldsymbol{probability\ of\ yes})^2 - (\boldsymbol{probability\ of\ no})^2$$







Gini-impurity des linken „Leaf“:

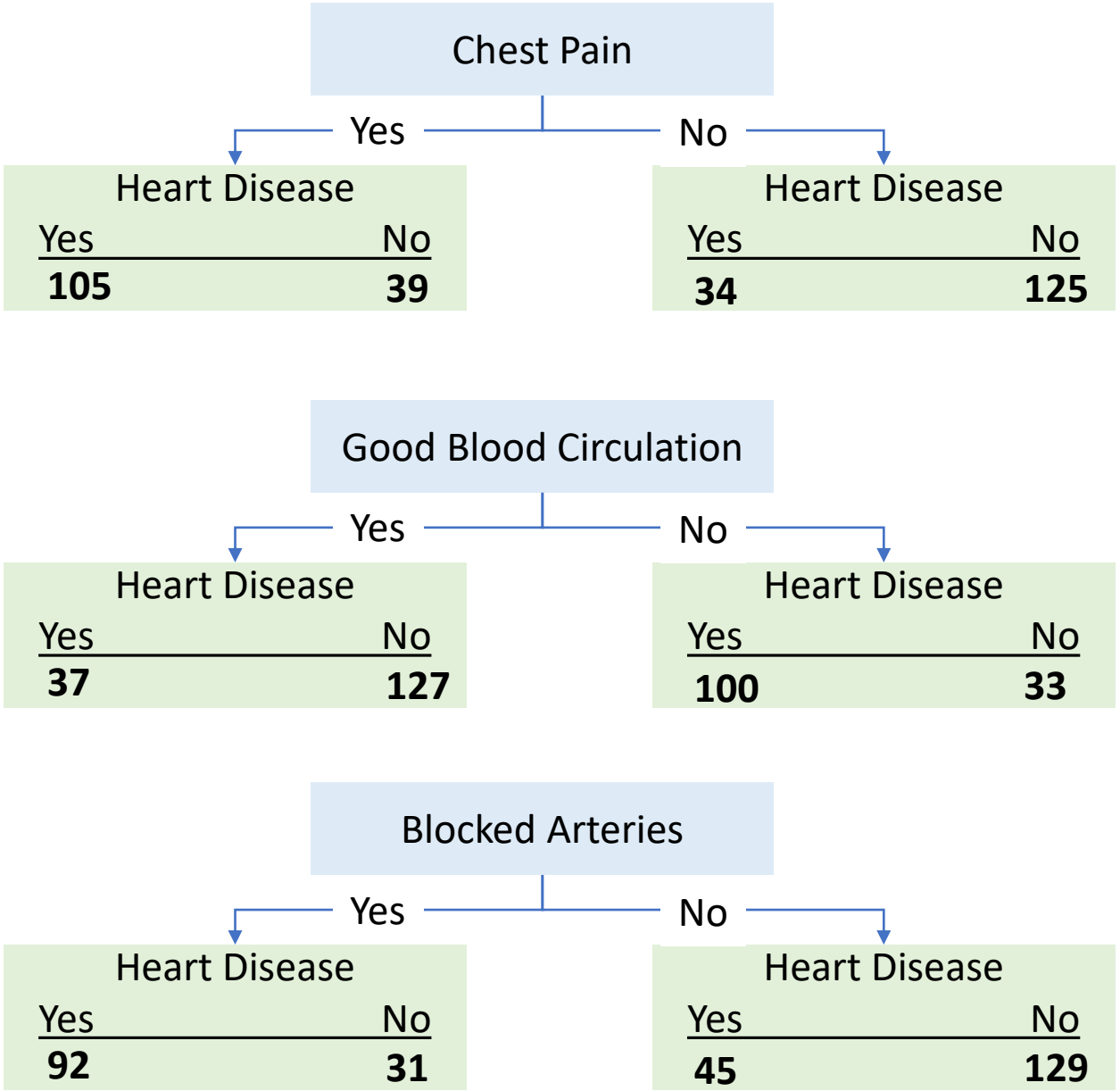
$$1 - \left(\frac{105}{105+39}\right)^2 - \left(\frac{39}{105+39}\right)^2 = 0.395$$

Gini-impurity des rechten „Leaf“:

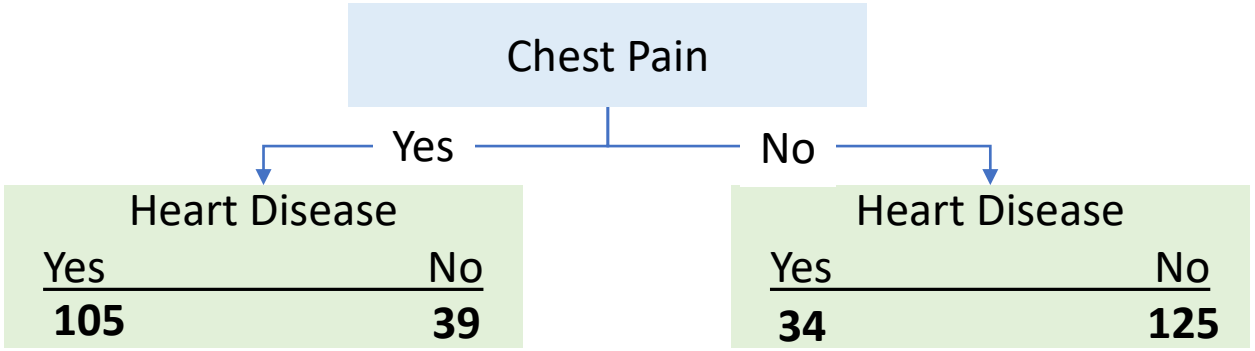
$$1 - \left(\frac{34}{34+125}\right)^2 - \left(\frac{125}{34+125}\right)^2 = 0.336$$

Gewichtete Gini-impurity für „Chest Pain“:

$$\left(\frac{144}{144+159}\right) * 0{,}395 + \left(\frac{159}{144+159}\right) * 0{,}336 = \mathbf{0,364}$$

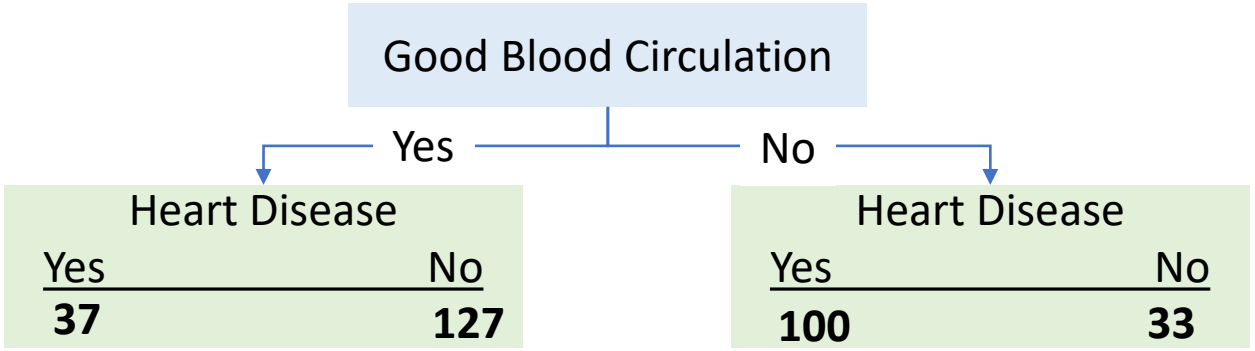


Gini-impurity für „Chest Pain“ = 0,364

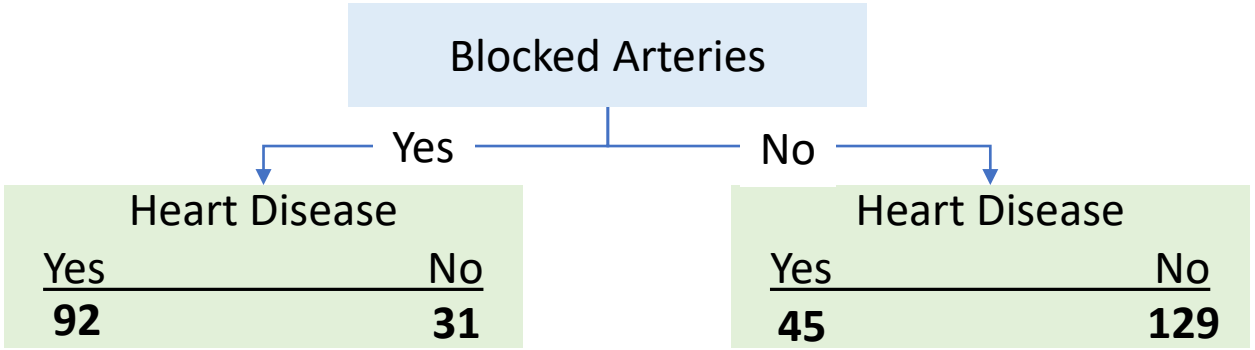


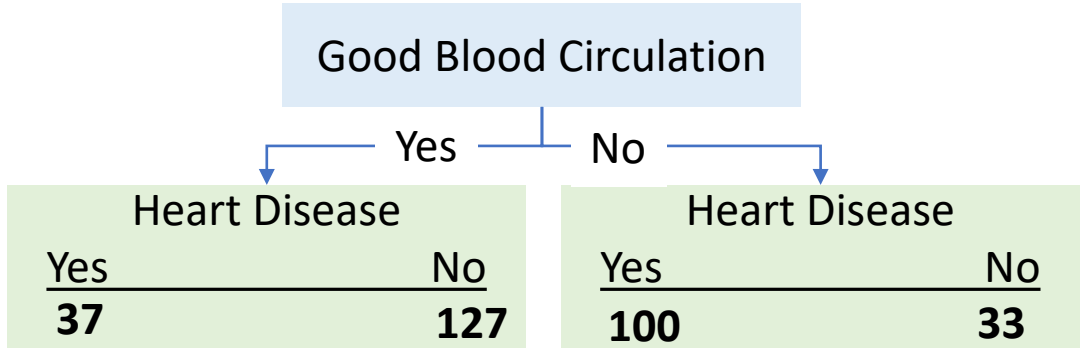
Gini-impurity für „Good Blood Circulation“ = 0,360

Good Blood Circulation hat folglich die geringste „impurity“, sodass es als bestmöglicher Root Node in Frage kommt!

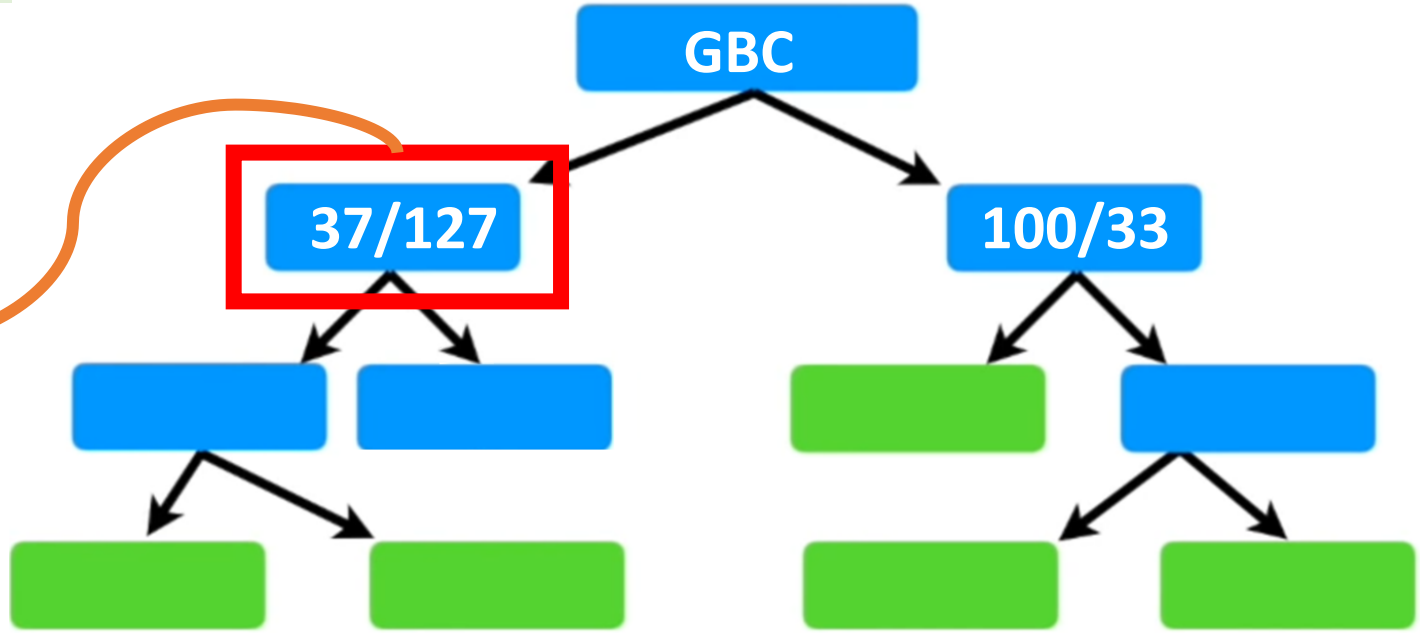


Gini-impurity für „Blocked Arteries“ = 0,381





Aber wie fahren wir mit diesen 164 Patientendaten fort?
Welchen Parameter nehmen wir als nächsten Internal Node?



Im Auge des Sturms: Decision Trees

Chest Pain

Yes | No

Heart Disease	
Yes	No
13	**98**

Heart Disease	
Yes	No
24	**29**

Gini impurity für Chest Pain = 0,3

164 Patienten

Blocked Arteries

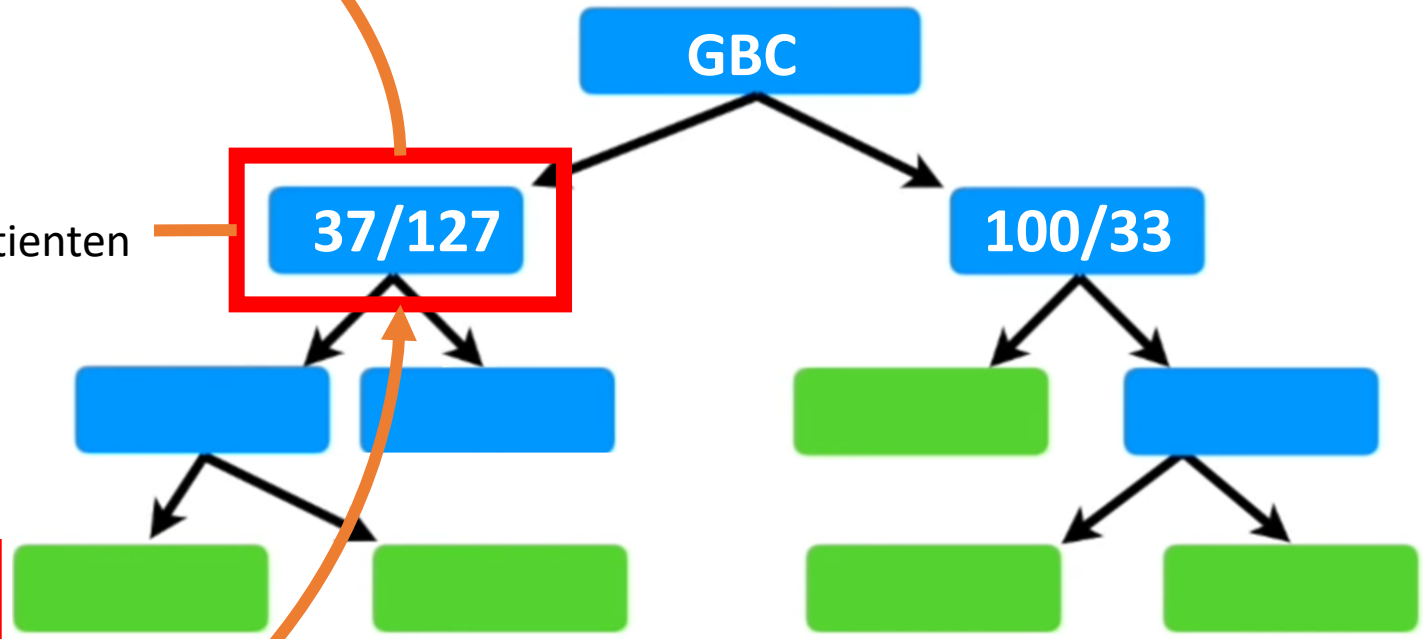
Yes | No

Heart Disease	
Yes	No
24	**25**

Heart Disease	
Yes	No
13	**102**

Gini impurity für Blocked Arteries = 0,290

164 Patienten



Blocked Arteries hat folglich die geringste „impurity“, sodass es als bestmöglicher Internal Node in Frage kommt!

Im Auge des Sturms: Decision Trees

Blocked Arteries

Yes | No

Heart Disease **24** | Heart Disease **25**

Gini impurity für Blocked Arteries = 0,520

Chest Pain

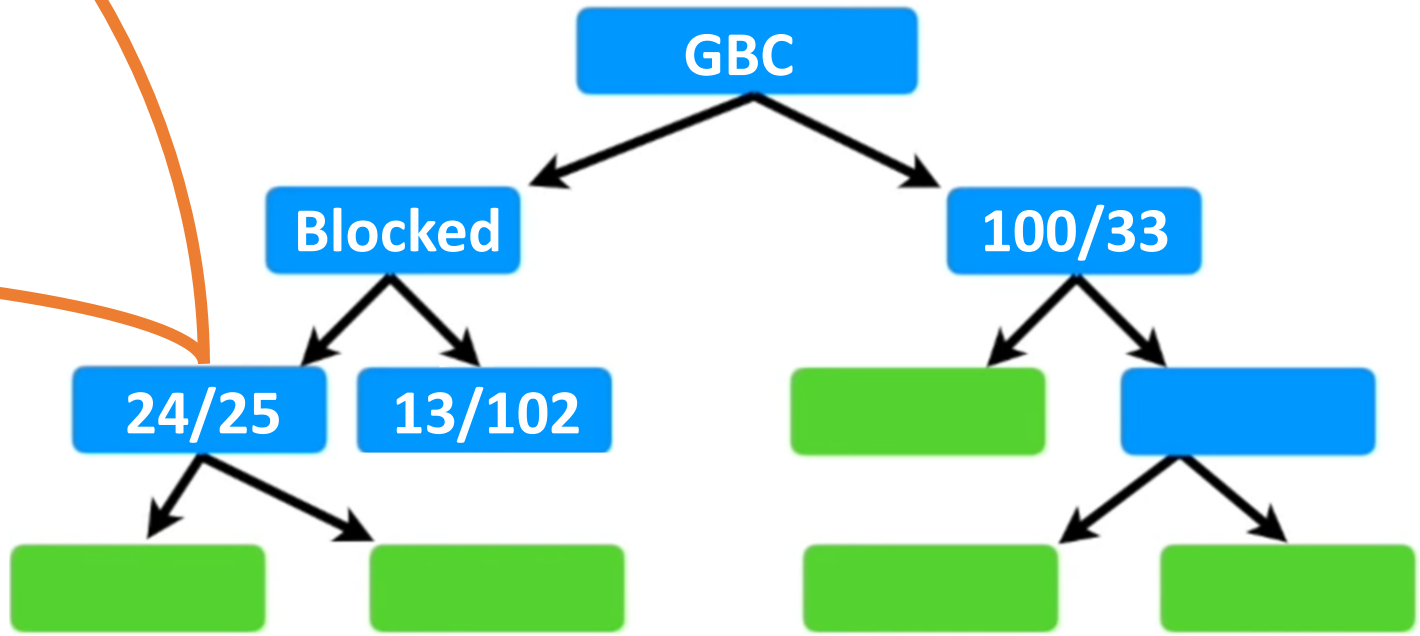
Yes | No

Heart Disease: Yes **17** / No **3**

Heart Disease: Yes **7** / No **22**

Gini impurity für Chest Pain = 0,218

Zwar nicht ganz perfekt, aber besser als wenn wir es beim letzten Internal Node gelassen hätten.



Im Auge des Sturms: Decision Trees

Blocked Arteries

Yes | No

Heart Disease	Heart Disease
12	**102**

Gini impurity für Blocked Arteries = 0,2

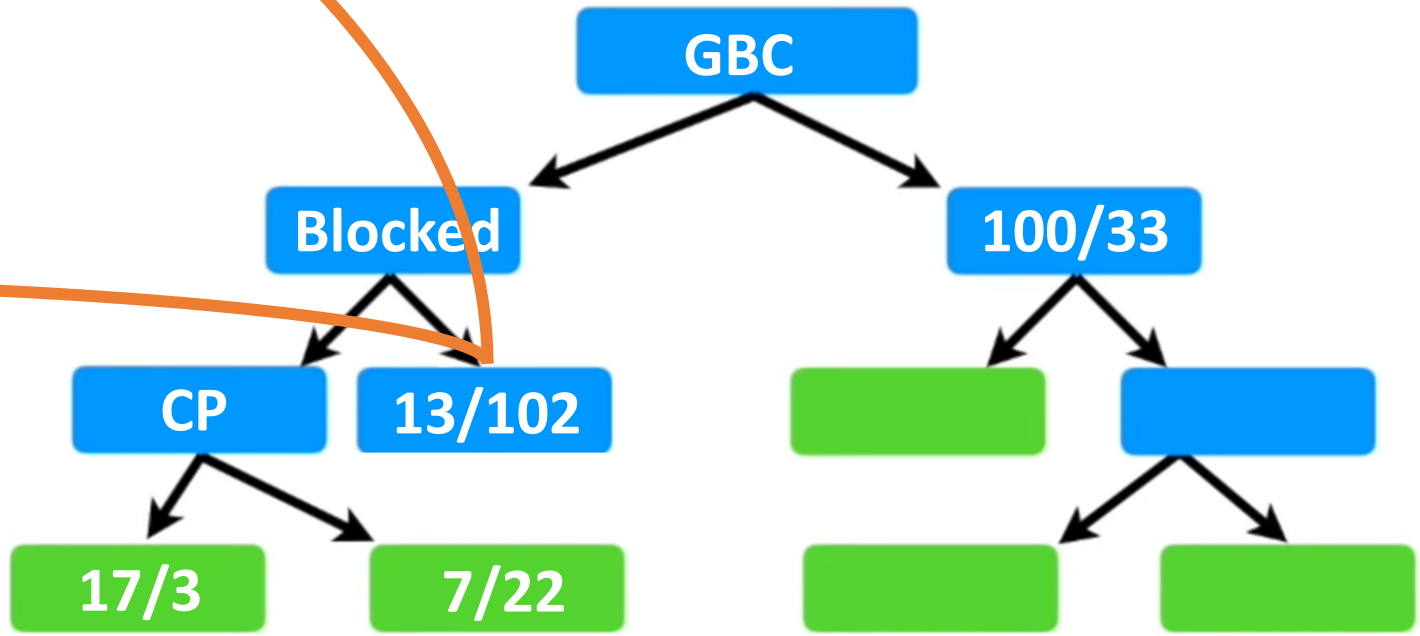
Chest Pain

Yes | No

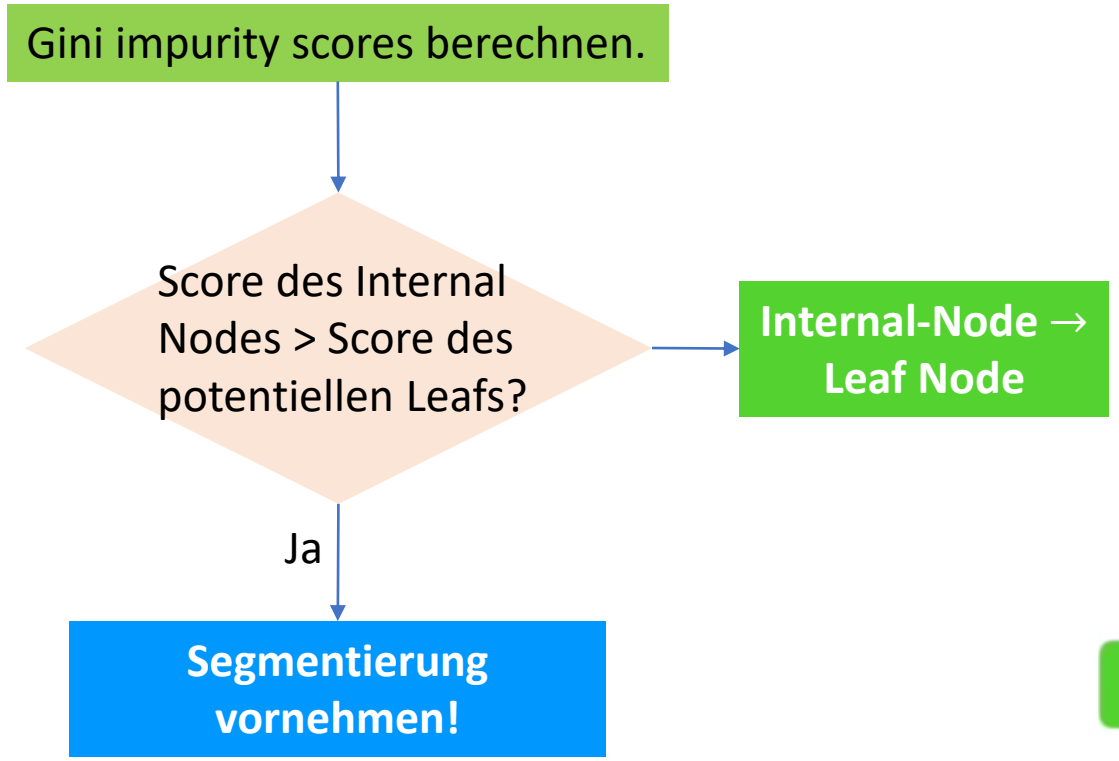
Heart Disease		Heart Disease	
Yes	No	Yes	No
7	**26**	**6**	**76**

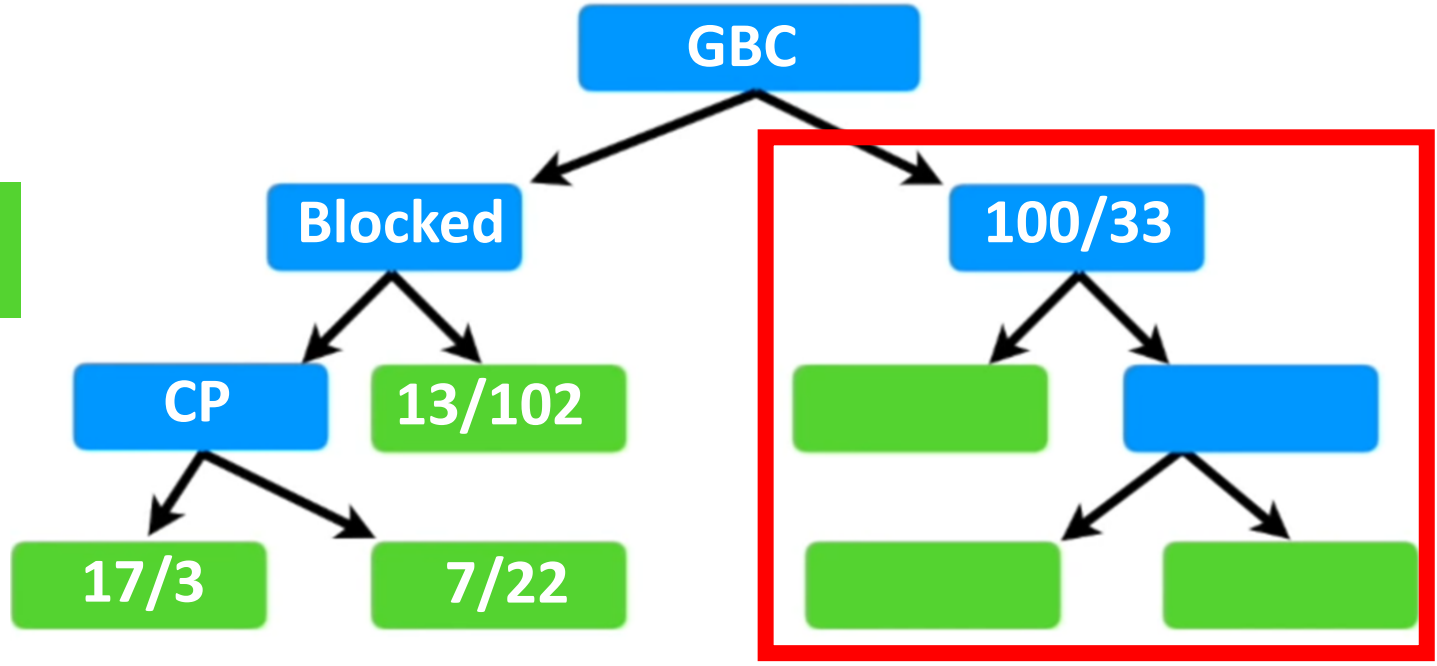
Gini impurity für Chest Pain = 0,29

Die Impurity wird schlechter, wenn wir Chest Pain miteinbeziehen. Wir fügen hier daher keinen neuen Node ein!



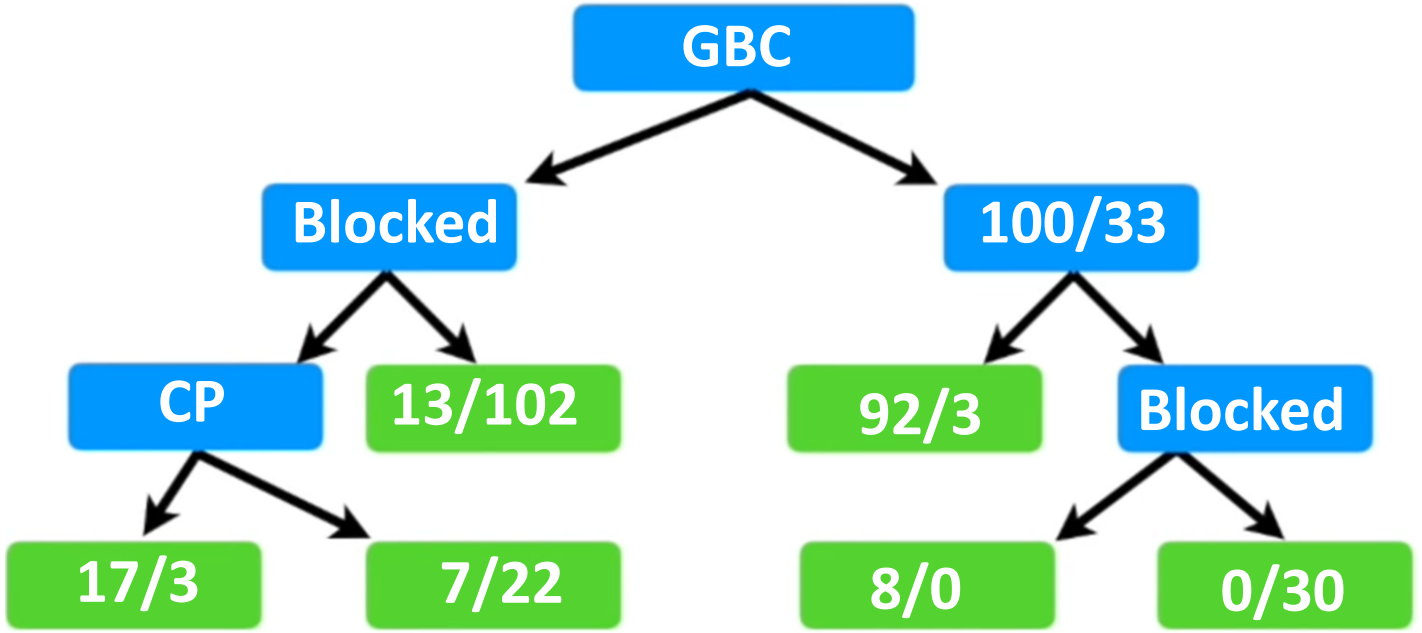
Nun fehlt nur noch die rechte Seite, wo wir nach dem gleichen Schma fortfahren:



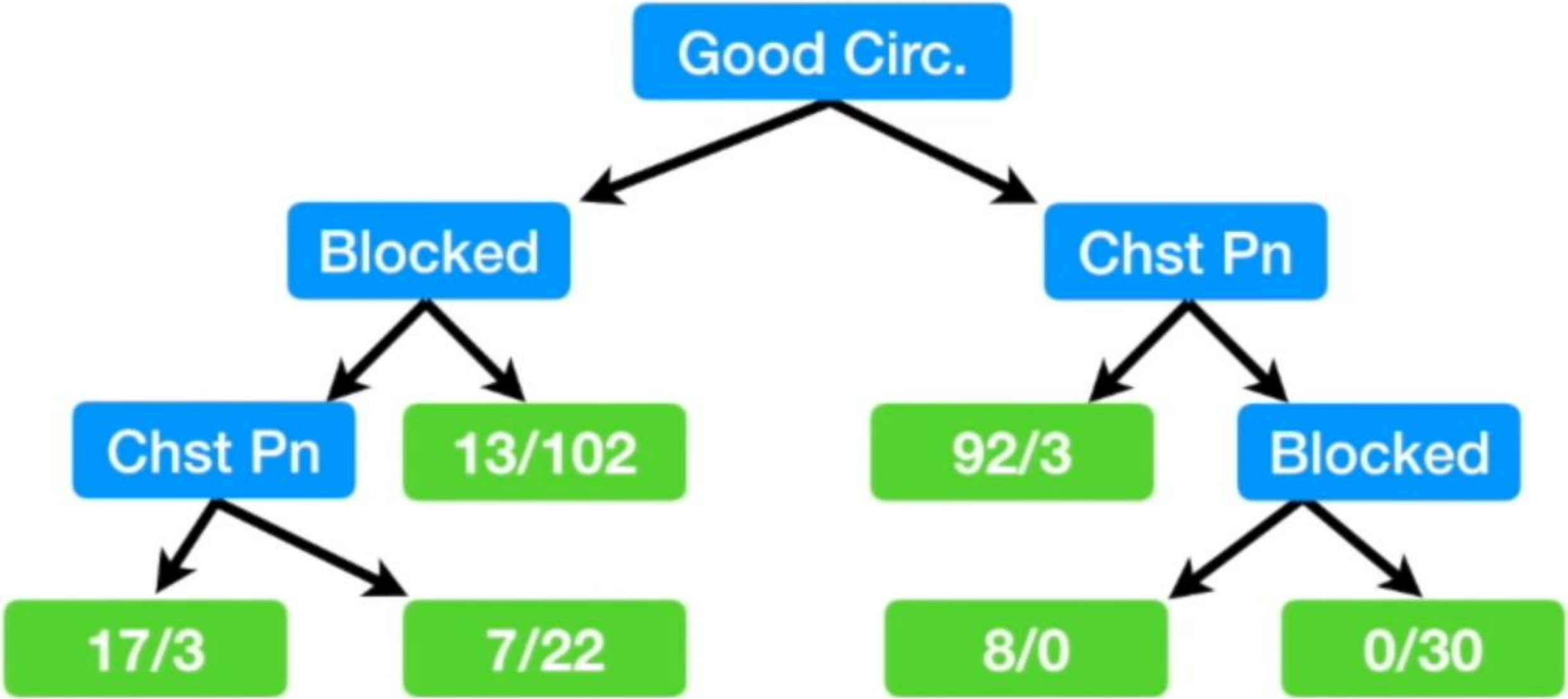


Im Auge des Sturms: Decision Trees

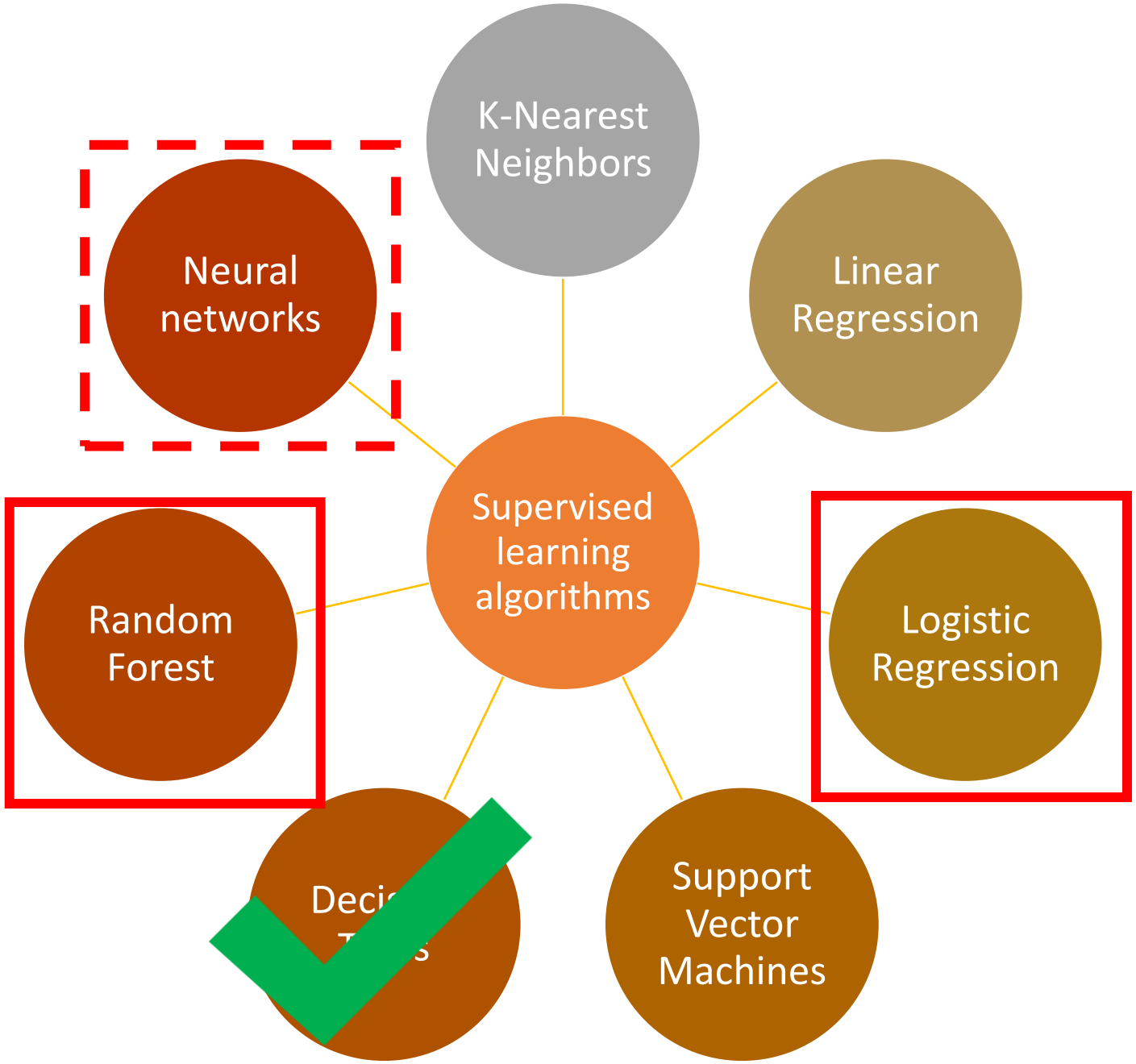
Chest Pain	Good Blood Circulation	Blocked Arteries	Heart Disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	??	Yes
…	…	…	…



Unsere Künstliche Intelligenz zur Klassifikation:



Die Qual der Wahl…



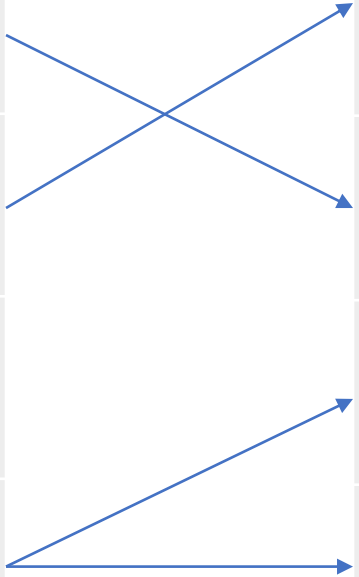
1 Decision Tree

1 Random Forest

Schritt 1: Wir kreieren einen „**bootstrapped dataset**“, indem wir

a) zufällig Zeilen vom originalen Dataset auswählen
b) dabei auch eine Zeile mehrmals nehmen dürfen -> random!

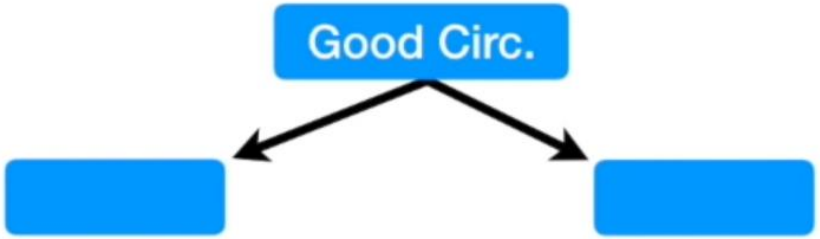
Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	No	Yes	167	Yes



Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	Yes	Yes	180	Yes
No	No	No	125	No
Yes	No	Yes	167	Yes
Yes	No	Yes	167	Yes

Schritt 2: Wir kreieren ein Decision Tree mit Hilfe unseres „bootstrapped“ Datensatzes. Dabei verwenden wir bei jedem Schritt aber nur zufällig ausgewählte Teile unseres gesamten Datensatzes, z.B. nur 2 Spalten.

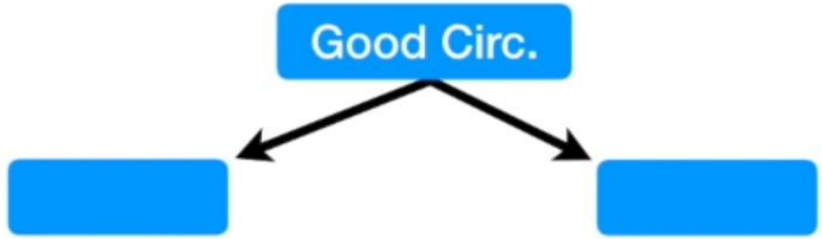
Schritt 2a: Um den Root Node zu bestimmen, nehmen wir mal zufällig nur GBC und Blocked Arteries in Betracht:



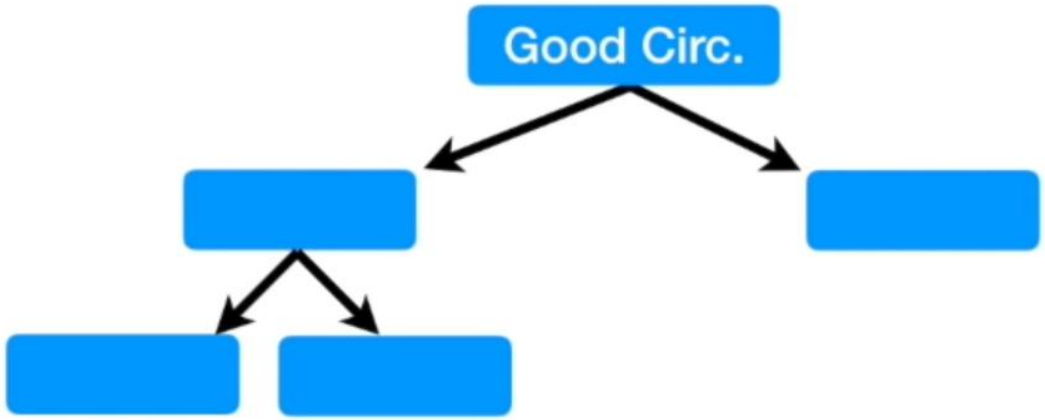
Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	Yes	Yes	180	Yes
No	No	No	125	No
Yes	No	Yes	167	Yes
Yes	No	Yes	167	Yes

Schritt 2: Wir kreieren ein Decision Tree mit Hilfe unsere „bootstrapped“ Datensatzes. Dabei verwenden wir bei jedem Schritt aber nur zufällig ausgewählte Teile unseres gesamten Datensatzes, z.B. nur 2 Spalten.

Schritt 2a: Um den Root Node zu bestimmen, nehmen wir mal zufällig nur GBC und Blocked Arteries in Betracht:



Schritt 2a: Um den nächsten Internal Node zu bestimmen, wählen wir 2 weitere Spalten zufällig aus.:



Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	Yes	Yes	180	Yes
No	No	No	125	No
Yes	No	Yes	167	Yes
Yes	No	Yes	167	Yes

Im Auge des Sturms: Random Forest

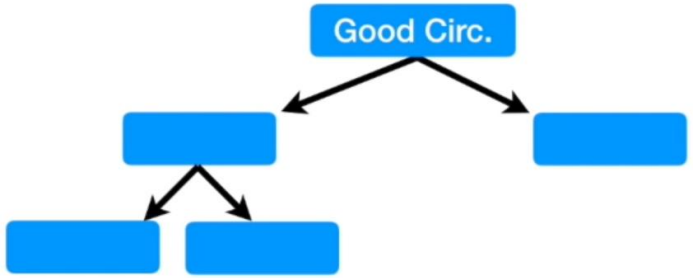
Schritt 1: Wir kreieren einen „**bootstrapped dataset**“, indem wir
a) zufällig Zeilen vom originalen Dataset auswählen
b) dabei auch eine Zeile mehrmals nehmen dürfen -> random!

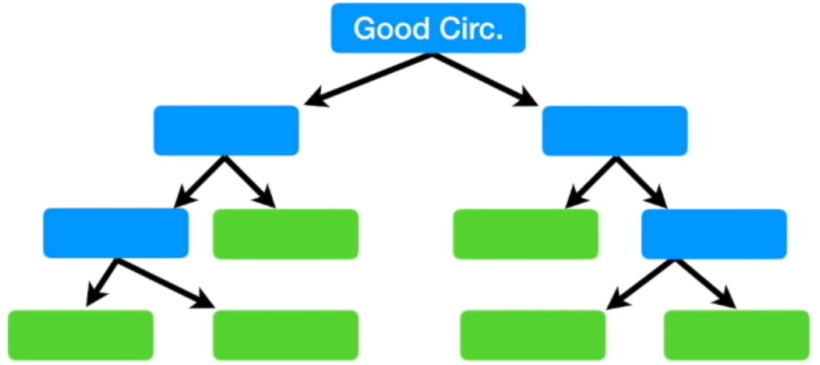
Schritt 2: Wir kreieren ein Decision Tree mit Hilfe unsere „bootstrapped“ Datensatzes. Dabei verwenden wir bei jedem Schritt aber nur zufällig ausgewählte Teile unseres gesamten Datensatzes, z.B. nur 2 Spalten.

Schritt 2a: Um den Root Node zu bestimmen, nehmen wir mal zufällig nur GBC und Blocked Arteries in Betracht:

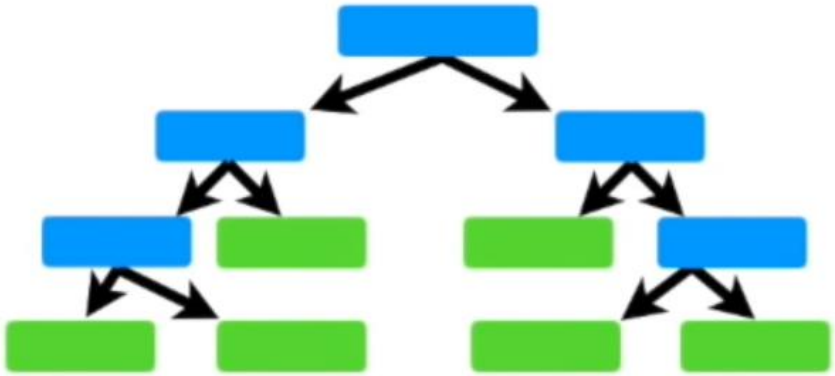
Schritt 2b: Um den nächsten Internal Node zu bestimmen, wählen wir 2 weitere Spalten zufällig aus.

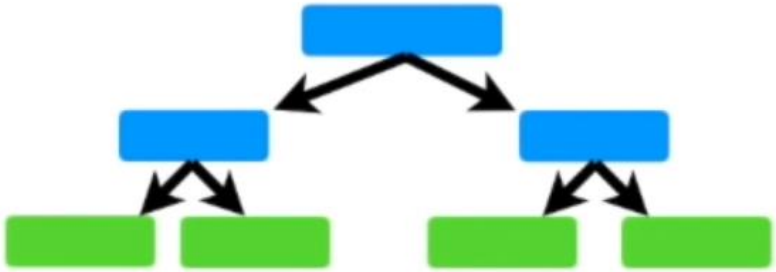
Schritt 2c: Dies führen wir fort, bis wir einen vollständigen Decision Tree erhalten.

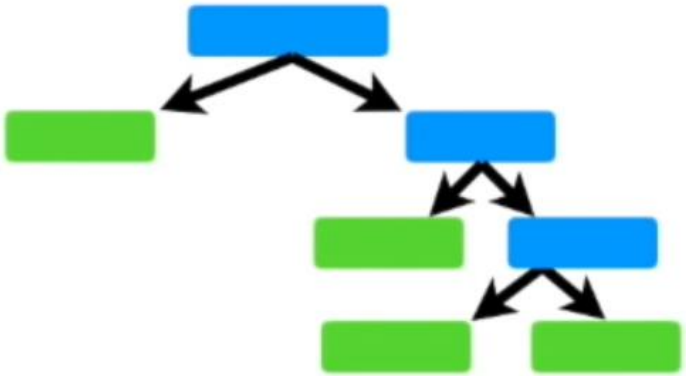




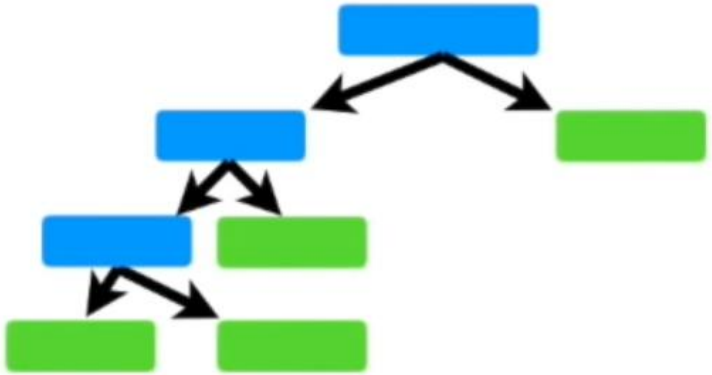
Diesen Prozess gehen wir also 100 male durch und kreieren hunderte verschiedenster Decision Trees, also einen Random Forest!

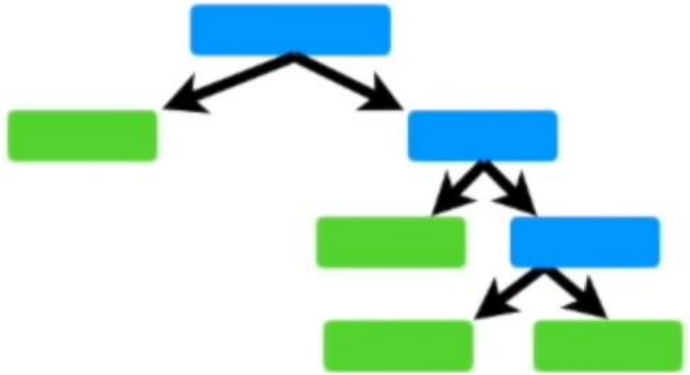


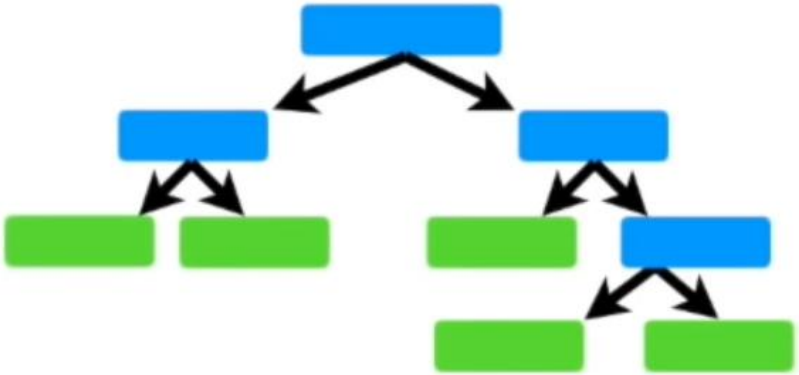




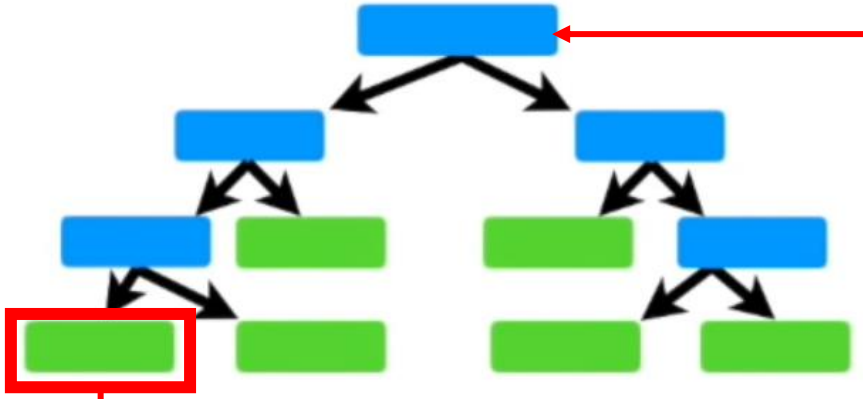
Aber was machen jetzt, wo wir „den Wald vor lauter Bäumen nicht sehen“?

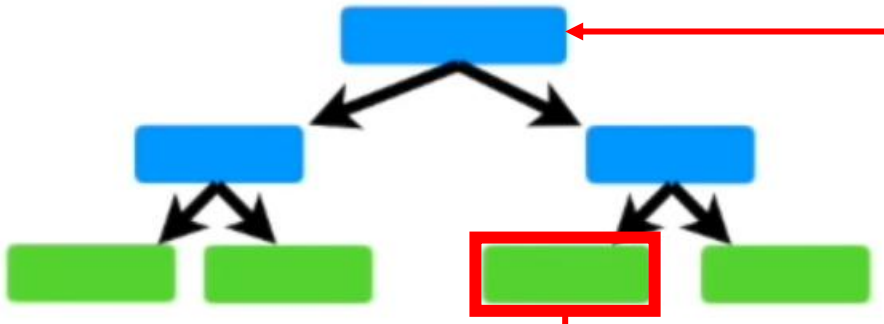






Im Auge des Sturms: Random Forest

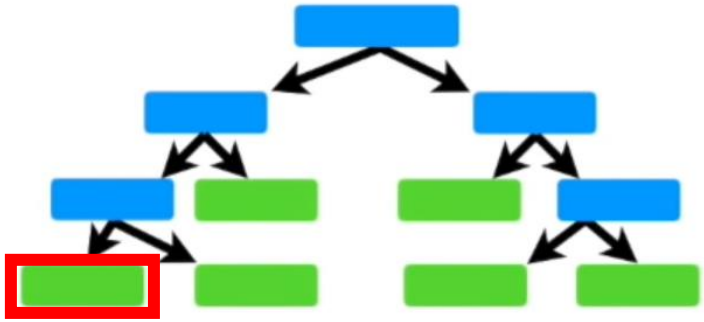


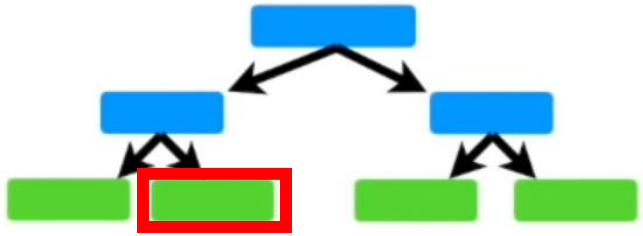


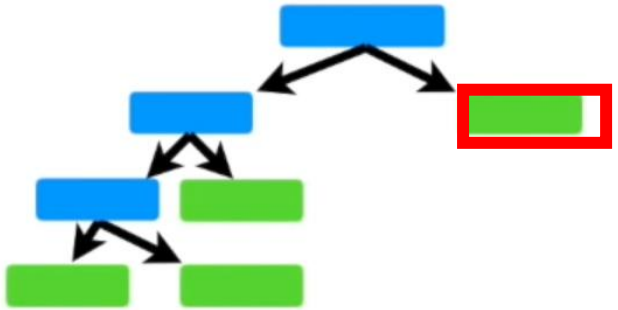
Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	No	No	168	???

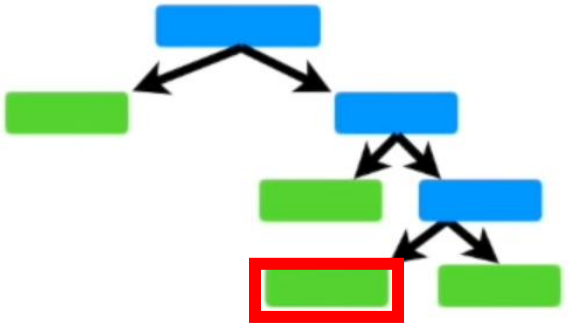
Heart Disease	
Yes	No
2	

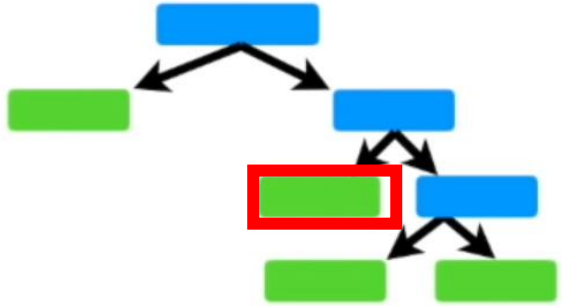
Im Auge des Sturms: Random Forest

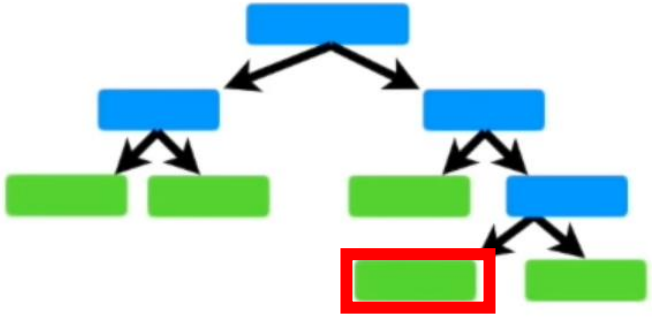








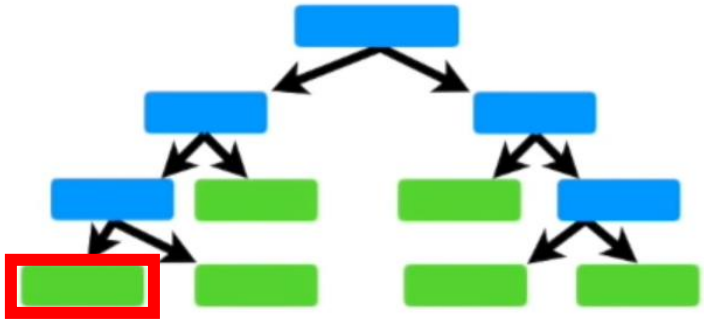


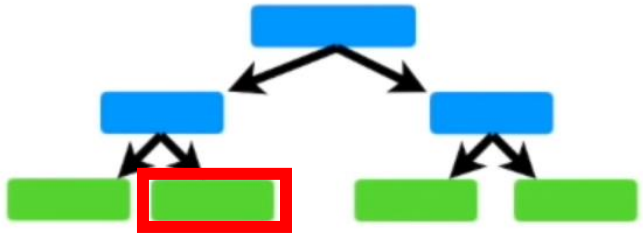


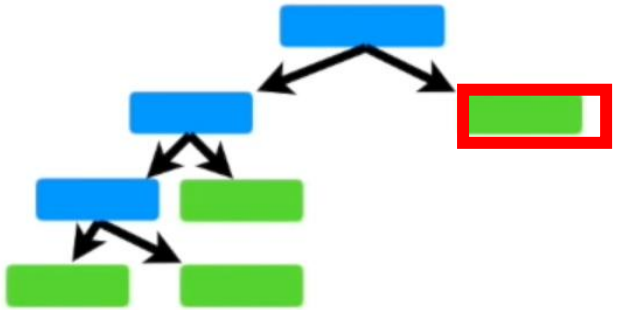
Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	No	No	168	???

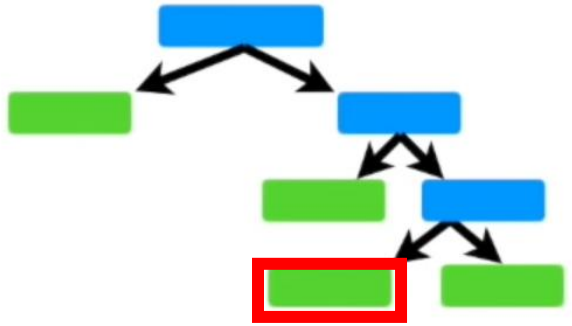
Heart Disease	
Yes	No
5	1

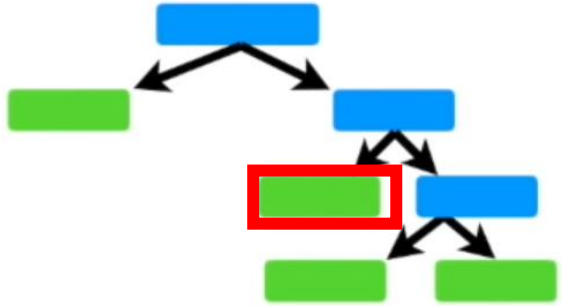
Wie geht Random Forest nun bei einem neuen Datensatz vor?

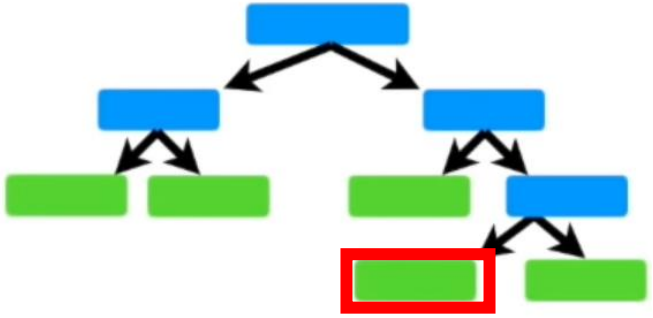












Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	No	No	168	**YES**

Heart Disease	
Yes	No
5	1

Bootstrapping

+

Aggregating

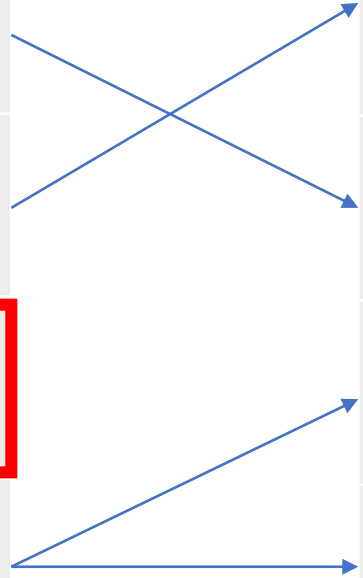
=

Bagging

Im Auge des Sturms: Random Forest

Woher weiß ich denn, dass mein Random Forest auch wirklich gut ist?

Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	No	Yes	167	Yes



Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	Yes	Yes	180	Yes
No	No	No	125	No
Yes	No	Yes	167	Yes
Yes	No	Yes	167	Yes

Woher weiß ich denn, dass mein Random Forest auch wirklich gut ist?

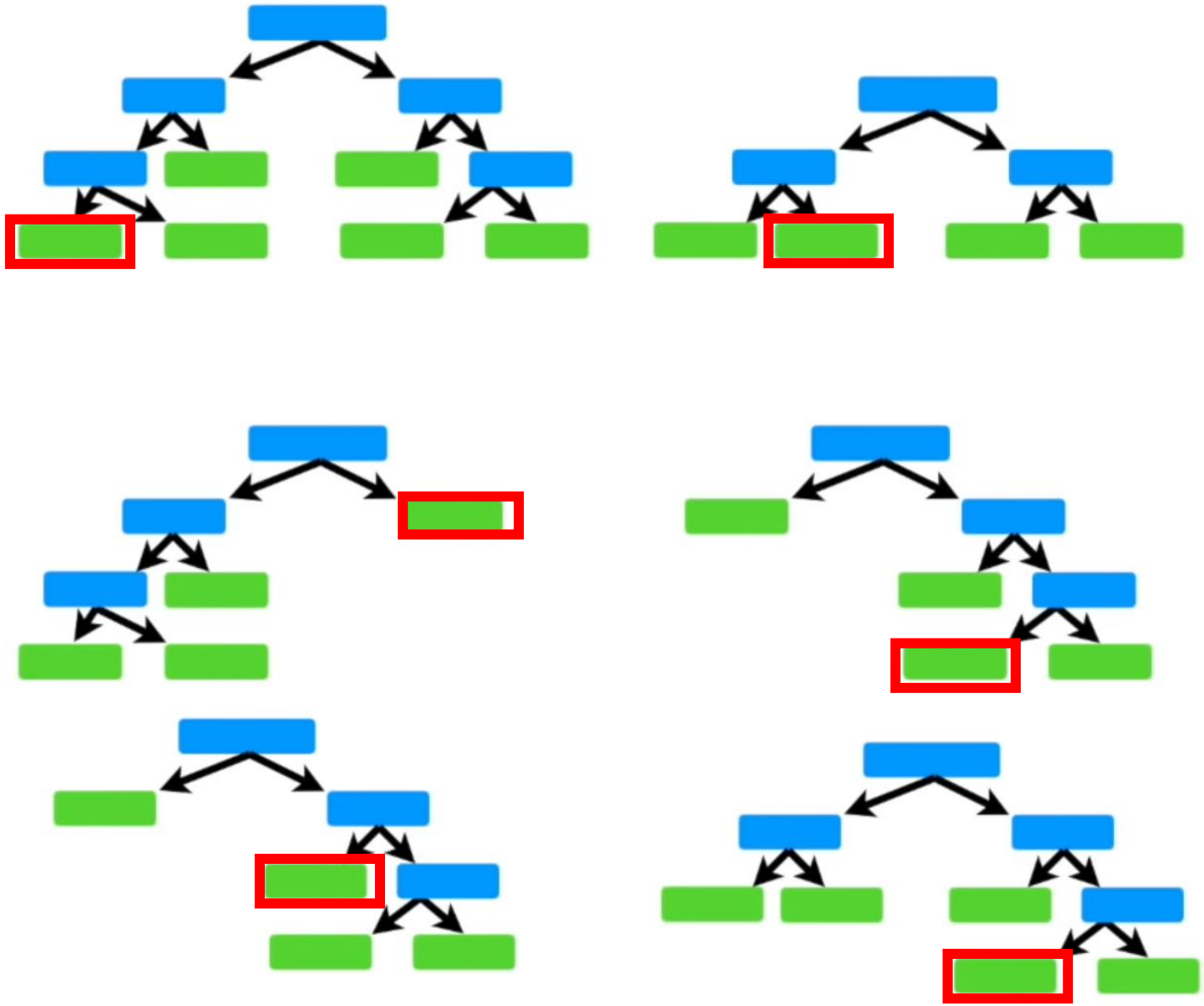
Wir erstellen ein „Out-Of-Bag-Dataset“!

Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	No	Yes	167	Yes

Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	Yes	No	210	No
…	…	…	…	…

Im Auge des Sturms: Random Forest

Woher weiß ich denn, dass mein Random Forest auch wirklich gut ist?



Wir erstellen ein „Out-Of-Bag-Dataset“!

Chest Pain	GBC	Blocked Arteries	Weight	Heart Disease
Yes	Yes	No	210	No

Heart Disease	
Yes	No
1	5

Die Genauigkeit unseres Random Forest kann mithilfe der korrekt klassifizierten „Out-Of-Bag“-Patienten bestimmt werden!

Falls ungenau: Neuer Random-Forest-Lauf!

1 Decision Tree

1 Random Forest

Classification-tree in scikit-learn

```
# Import DecisionTreeClassifier
from sklearn.tree import DecisionTreeClassifier
# Import train_test_split
from sklearn.model_selection import train_test_split
# Import accuracy_score
from sklearn.metrics import accuracy_score
# Split the dataset into 80% train, 20% test
X_train, X_test, y_train, y_test= train_test_split(X, y,
                                                   test_size=0.2,
                                                   stratify=y,
                                                   random_state=1)
# Instantiate dt
dt = DecisionTreeClassifier(max_depth=2, random_state=1)
```

```
# Fit dt to the training set
dt.fit(X_train,y_train)

# Predict the test set labels
y_pred = dt.predict(X_test)
# Evaluate the test-set accuracy
accuracy_score(y_test, y_pred)
```

```
0.903508771929824 59
```

Random Forests: Classification & Regression

Classification:

- Aggregates predictions by majority voting
- `RandomForestClassifier` in scikit-learn

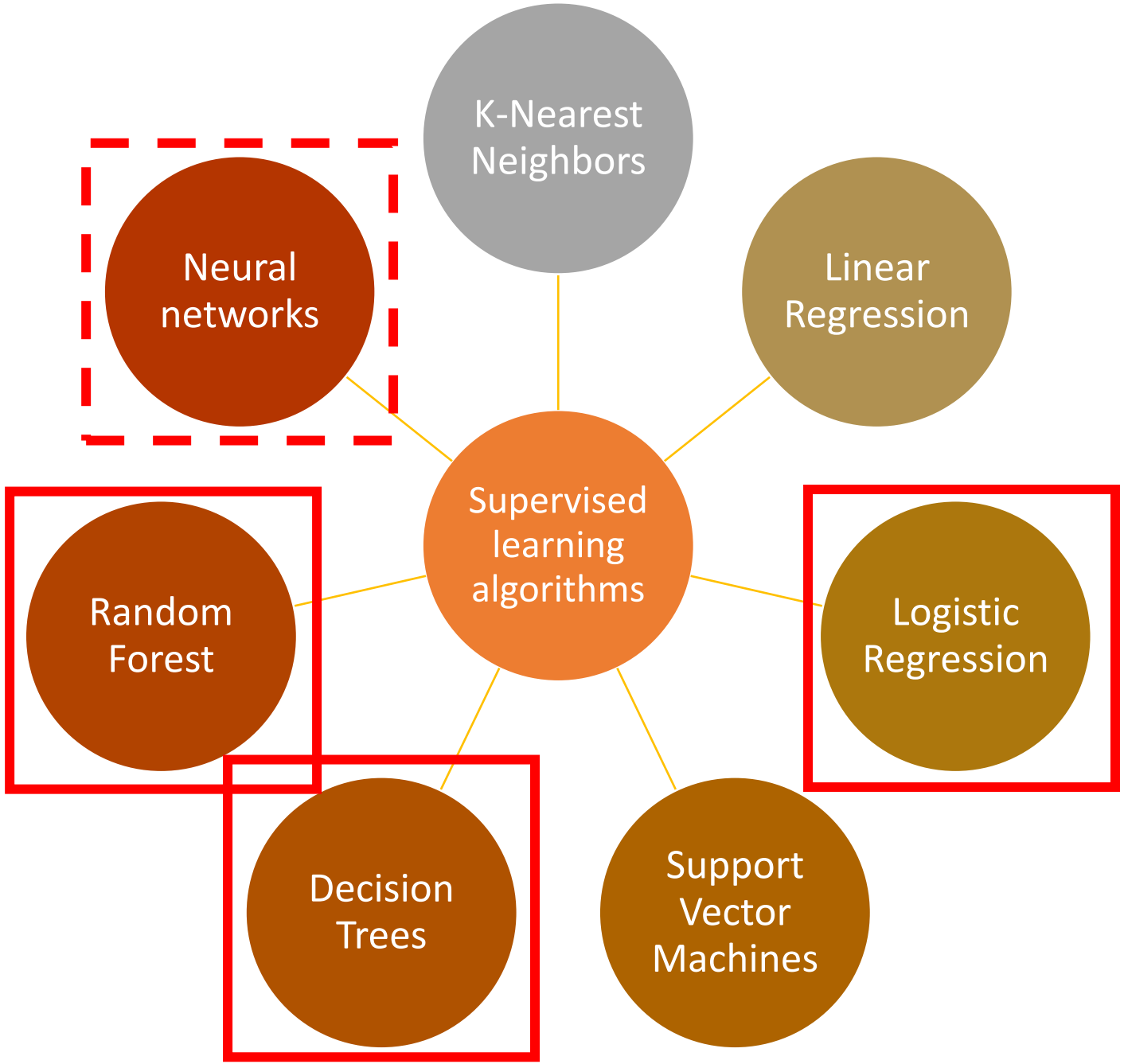
Regression:

- Aggregates predictions through averaging
- `RandomForestRegressor` in scikit-learn

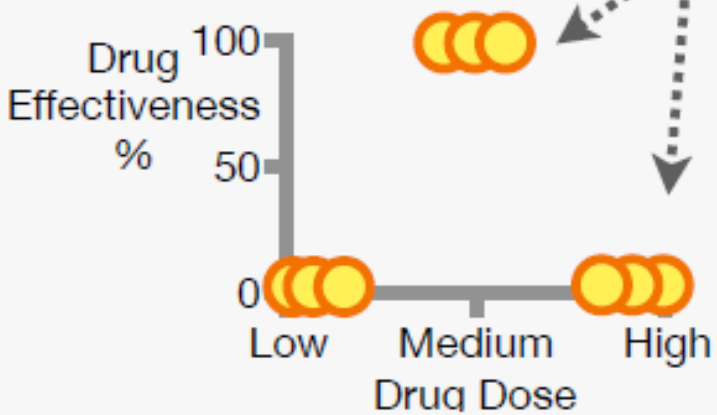
Auf zu Colab!

Supervised Learning with scikit-learn

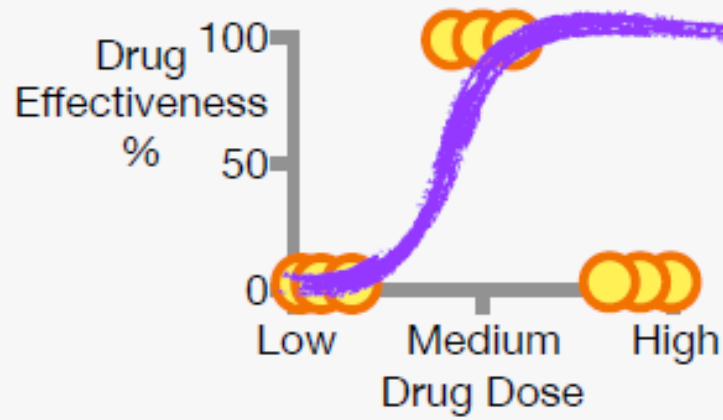
Die Qual der Wahl…



1 **The Problem:** We have data that show the Effectiveness of a drug for different Doses....



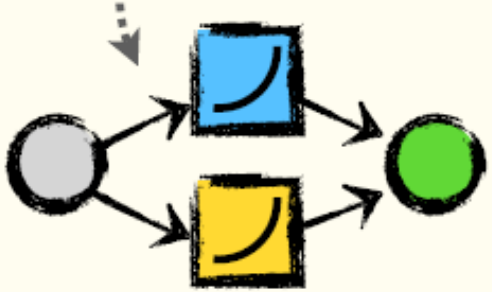
...and the **s-shaped squiggle** that **Logistic Regression** uses would not make a good fit. In this example, it would misclassify the high Doses.



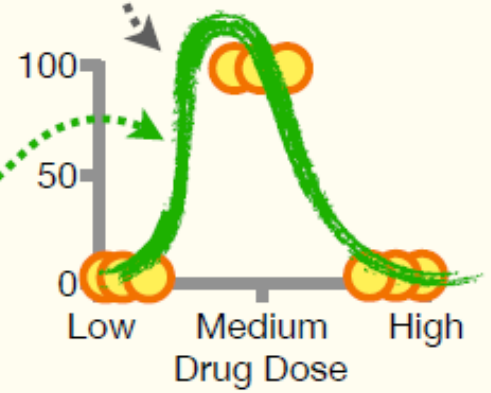
2

A Solution: Although they sound super intimidating, all **Neural Networks** do is fit **fancy squiggles** or **bent shapes** to data. And like **Decision Trees** and **SVMs**, **Neural Networks** do fine with any relationship among the variables.

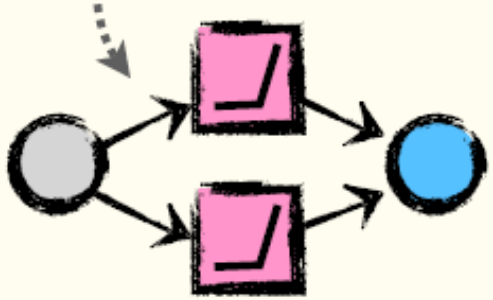
For example, we could get this **Neural Network**...



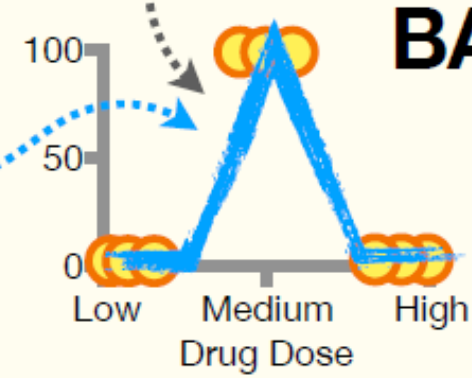
...to fit a **fancy squiggle** to the data...



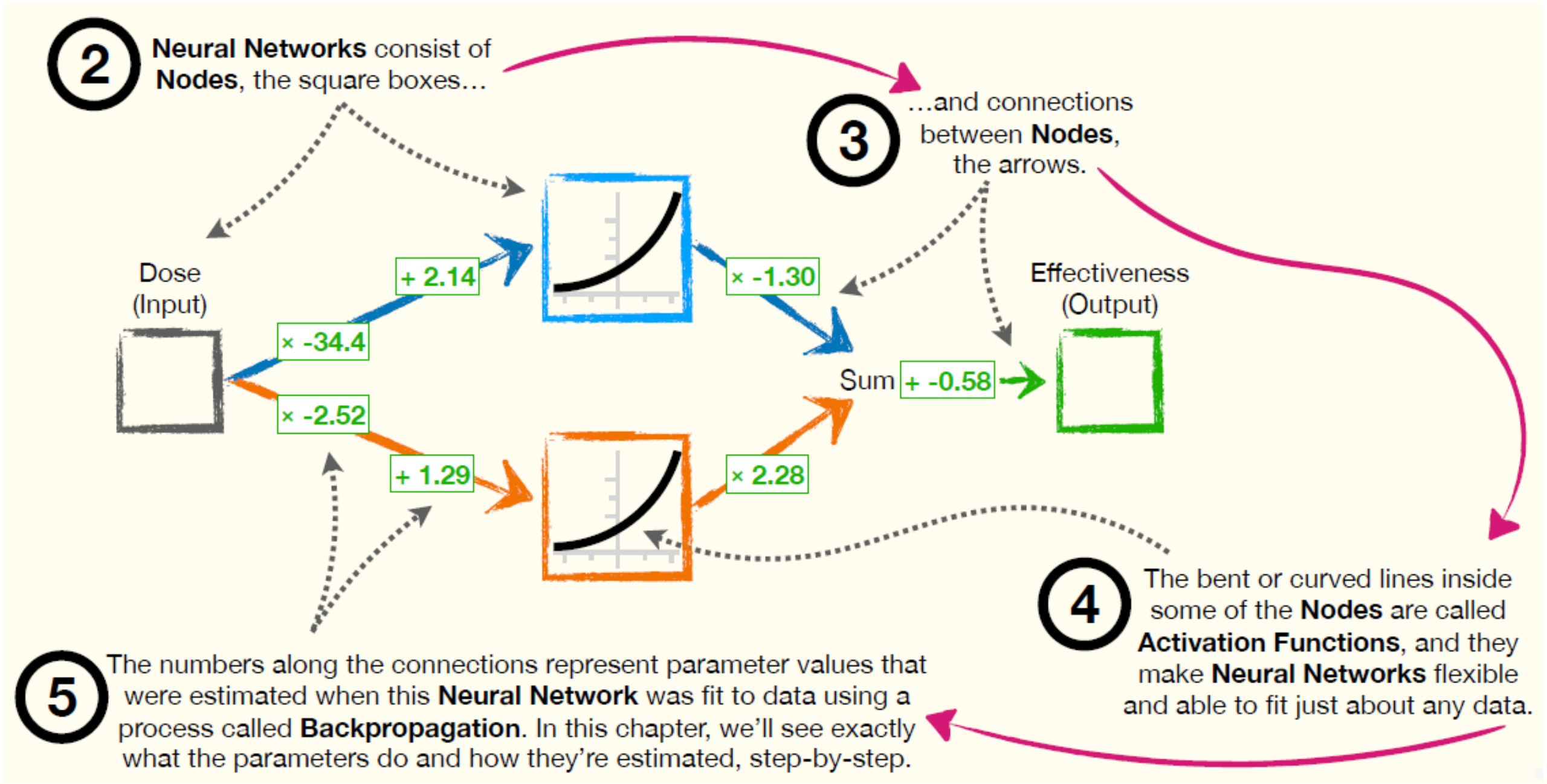
...or we could get this **Neural Network**...



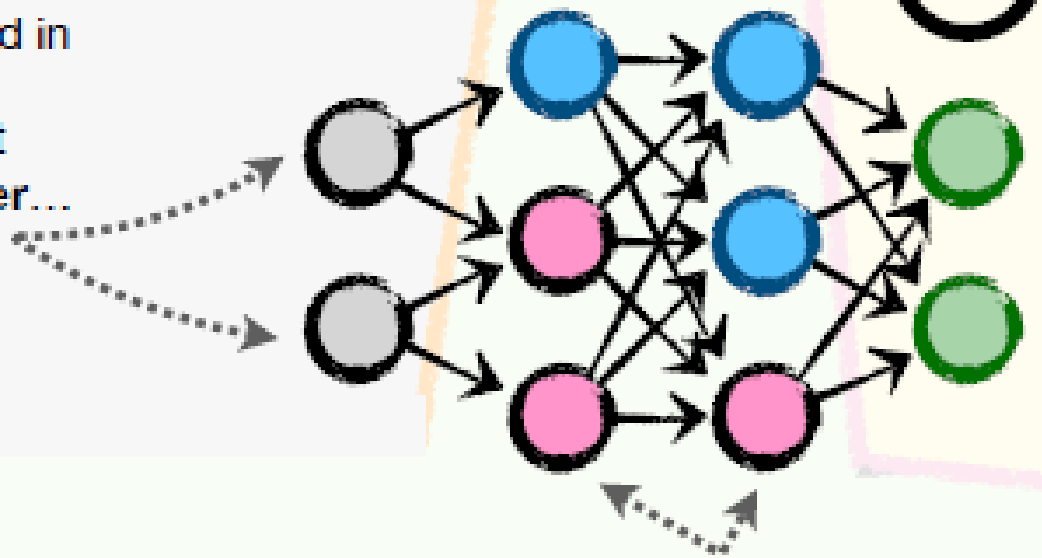
...to fit a **bent shape** to the data.



BAM!!!

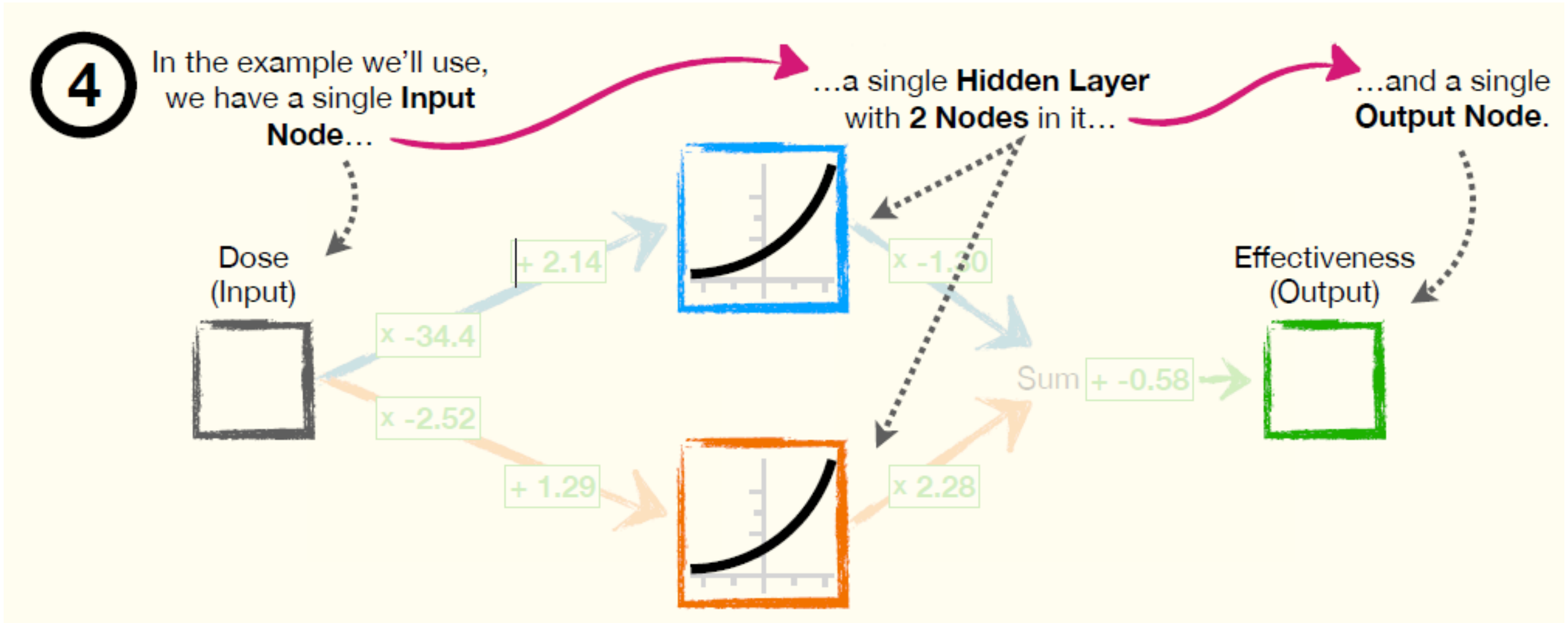

2
Neural Networks consist of Nodes, the square boxes…
3
…and connections between Nodes, the arrows.
Dose (Input)
+ 2.14
× -34.4
× -2.52
+ 1.29
× -1.30
× 2.28
Sum
+ -0.58
Effectiveness (Output)
4
The bent or curved lines inside some of the Nodes are called Activation Functions, and they make Neural Networks flexible and able to fit just about any data.
5
The numbers along the connections represent parameter values that were estimated when this Neural Network was fit to data using a process called Backpropagation. In this chapter, we'll see exactly what the parameters do and how they're estimated, step-by-step.

1 **Neural Networks** are organized in **Layers**. Usually, a **Neural Network** has multiple **Input Nodes** that form an **Input Layer**...



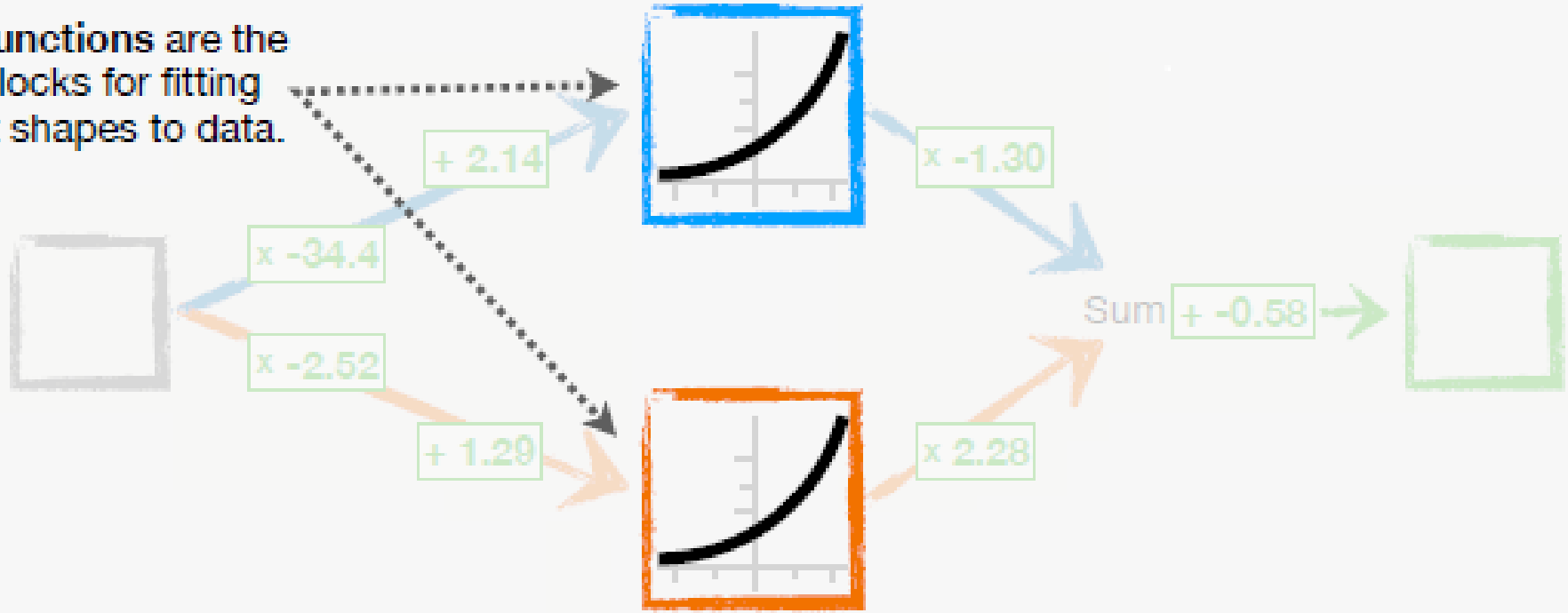
2 ...and usually there are multiple **Output Nodes** that form an **Output Layer**...

3 ...and the **Layers** of **Nodes** between the **Input** and **Output Layers** are called **Hidden Layers**. Part of the *art* of **Neural Networks** is deciding how many **Hidden Layers** to use and how many **Nodes** should be in each one. Generally speaking, the more **Layers** and **Nodes**, the more complicated the shape that can be fit to the data.


4
In the example we'll use, we have a single Input Node...
...a single Hidden Layer with 2 Nodes in it...
...and a single Output Node.
Dose (Input)
+ 2.14
x -34.4
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)

1

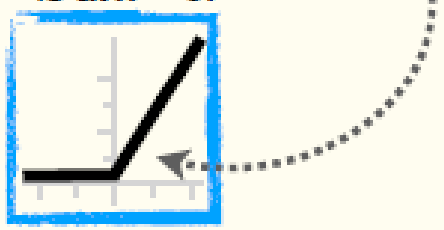
The **Activation Functions** are the basic building blocks for fitting squiggles or bent shapes to data.



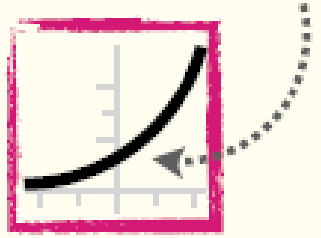
2

There are lots of different **Activation Functions**. Here are three that are commonly used:

ReLU, which is short for **Rectifled Linear Unit** and sounds like the name of a robot, is probably the most commonly used **Activation Function** with large **Neural Networks**. It's a **Bent Line**, and the bend is at $x = 0$.

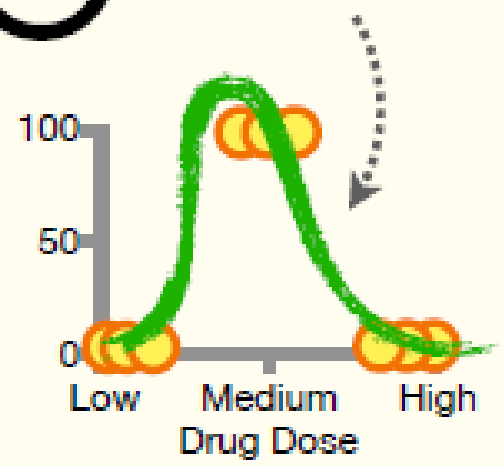


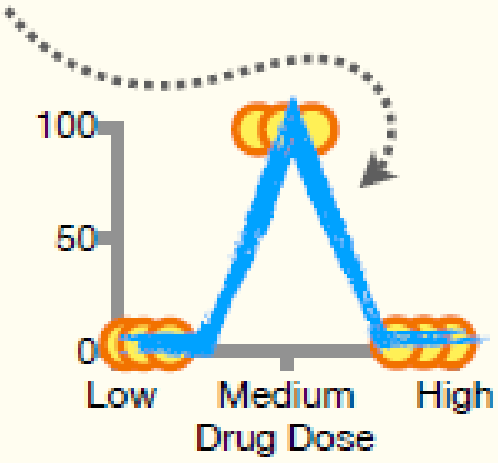
SoftPlus, which sounds like a brand of toilet paper, is a modified form of the **ReLU Activation Function**. The big difference is that instead of the line being bent at **0**, we get a nice **Curve**.

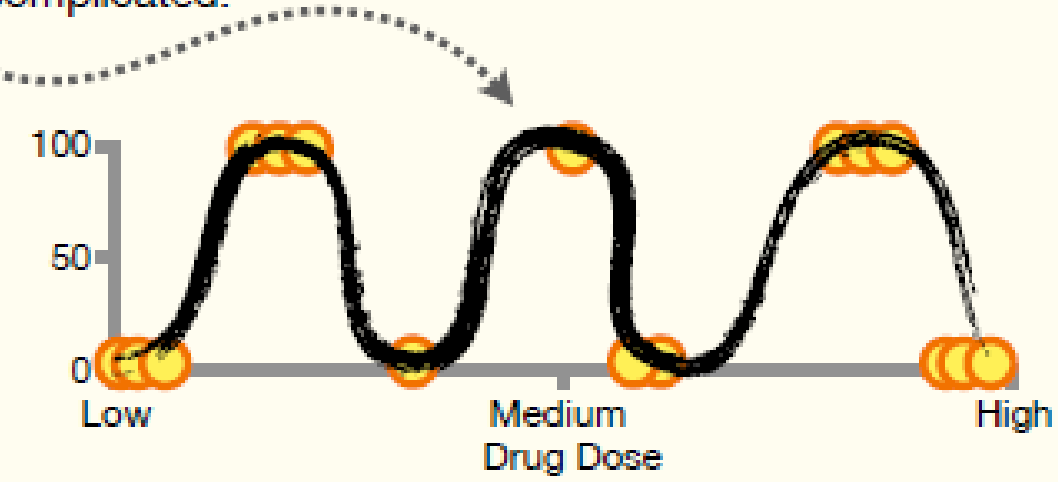


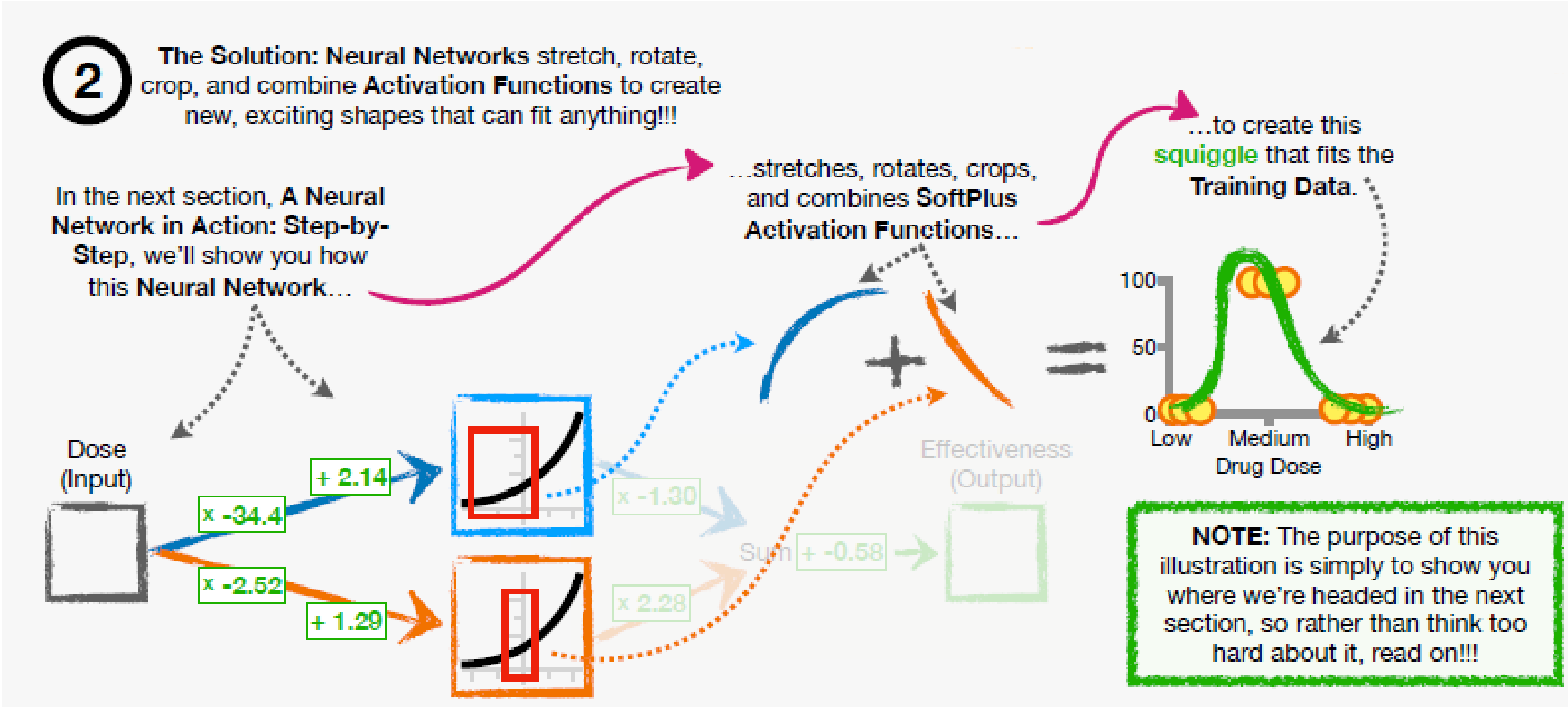
Lastly, the **Sigmoid Activation Function** is an **s-shaped squiggle** that's frequently used when people teach **Neural Networks** but is rarely used in practice.

1 **The Problem:** We need to create new, exciting shapes that can fit any dataset with a squiggle or bent lines, even when the dataset is super complicated.

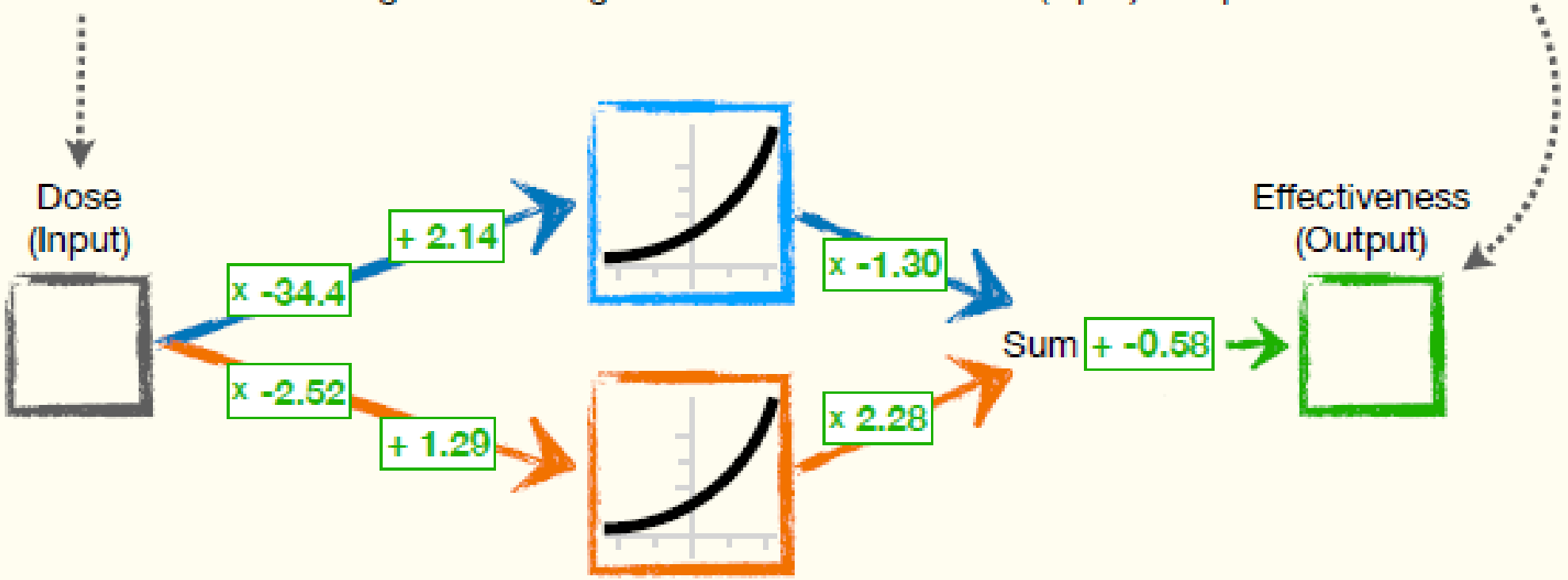






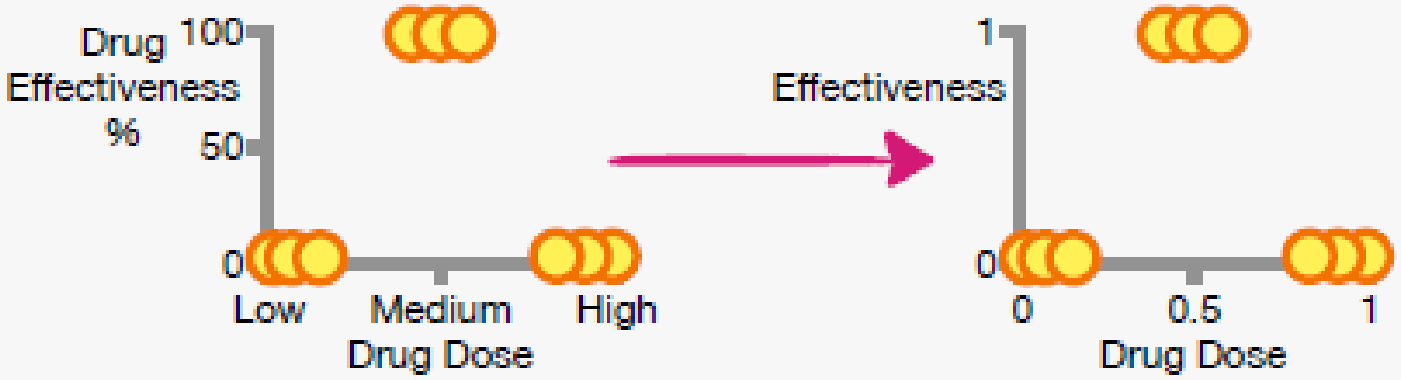

2
The Solution: Neural Networks stretch, rotate, crop, and combine Activation Functions to create new, exciting shapes that can fit anything!!!
In the next section, A Neural Network in Action: Step-by-Step, we'll show you how this Neural Network…
…stretches, rotates, crops, and combines SoftPlus Activation Functions…
…to create this squiggle that fits the Training Data.
Dose (Input)
+ 2.14
x -34.4
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)
100
50
0
Low
Medium
High
Drug Dose
NOTE: The purpose of this illustration is simply to show you where we're headed in the next section, so rather than think too hard about it, read on!!!

1 A lot of people say that **Neural Networks** are black boxes and that it's difficult to understand what they're doing. Unfortunately, this is true for big, fancy **Neural Networks**. However, the good news is that it's *not* true for simple ones. So, let's walk through how this simple **Neural Network** works, one step at a time, by plugging in Dose values from low to high and seeing how it converts the Dose (input) into predicted Effectiveness (output).



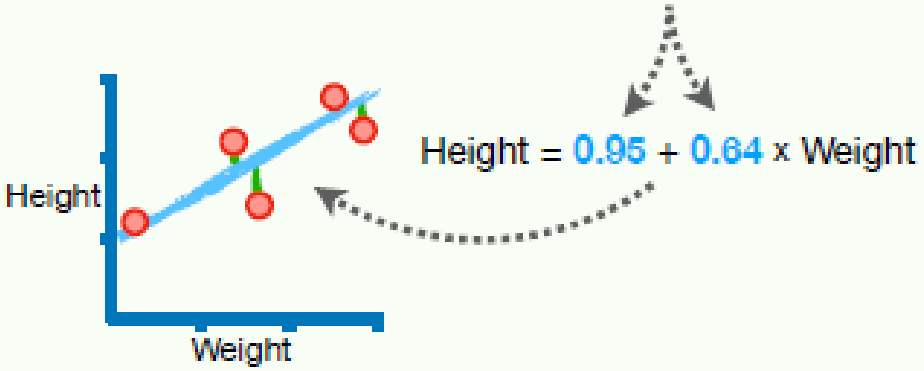
2

NOTE: To keep the math in this section simple, let's scale both the x- and y-axes so that they go from **0**, for *low* values, to **1**, for *high* values.



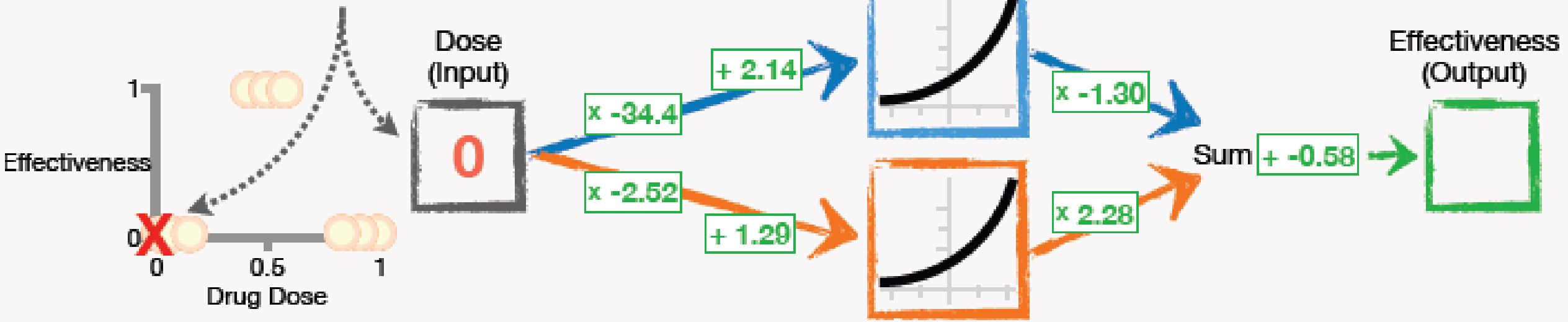
3

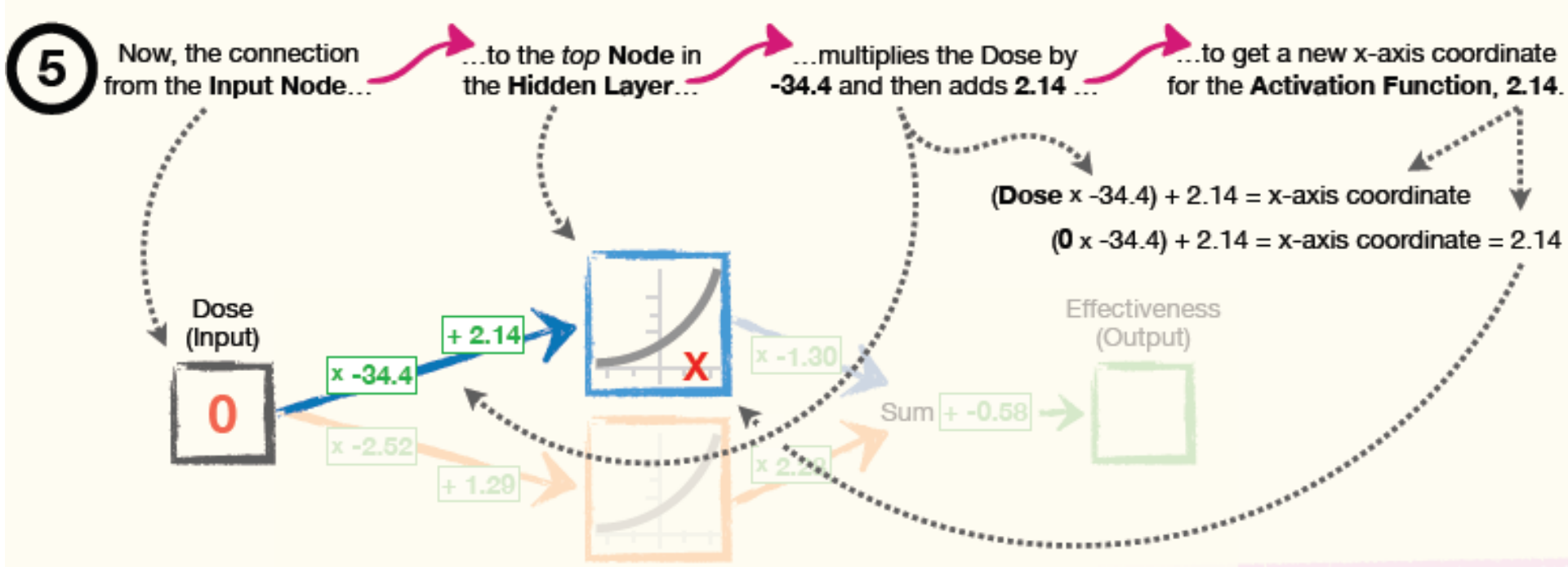
ALSO NOTE: These numbers are *parameters* that are estimated using a method called **Backpropagation**, and we'll talk about how that works, step-by-step, later. For now, just assume that these values have already been optimized, much like the slope and intercept are optimized when we fit a line to data.

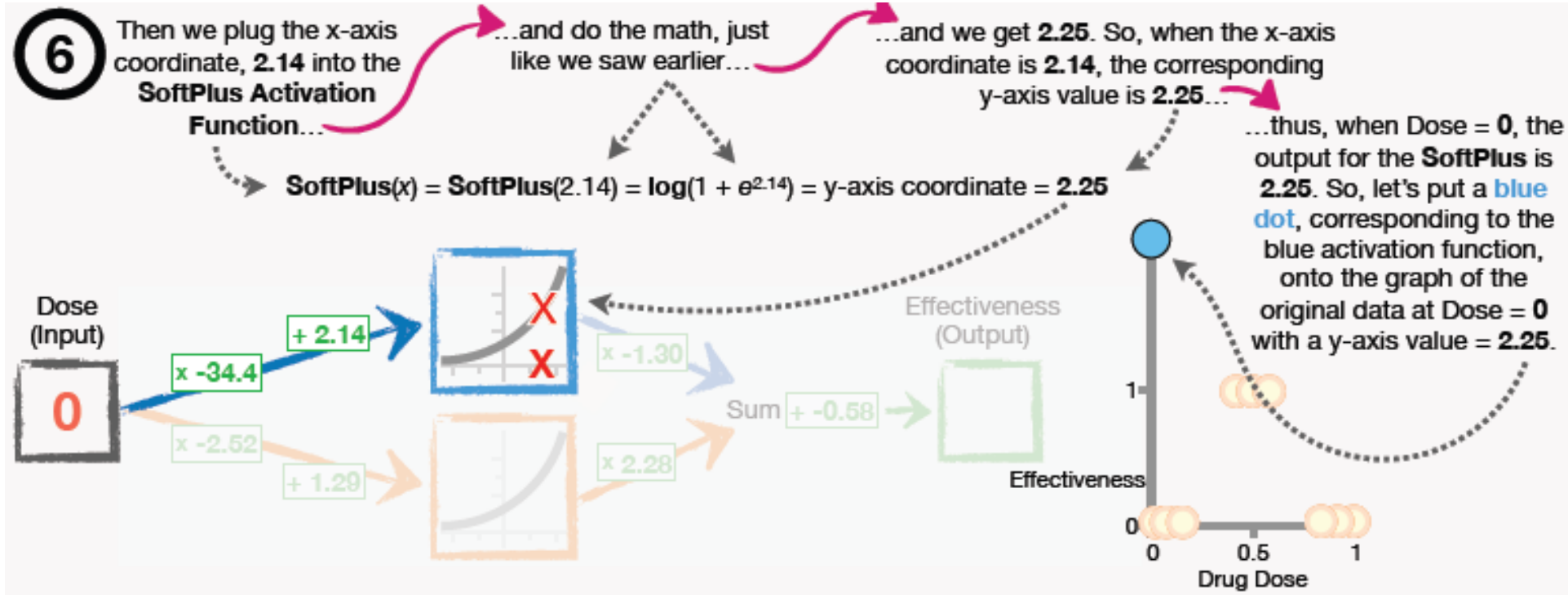


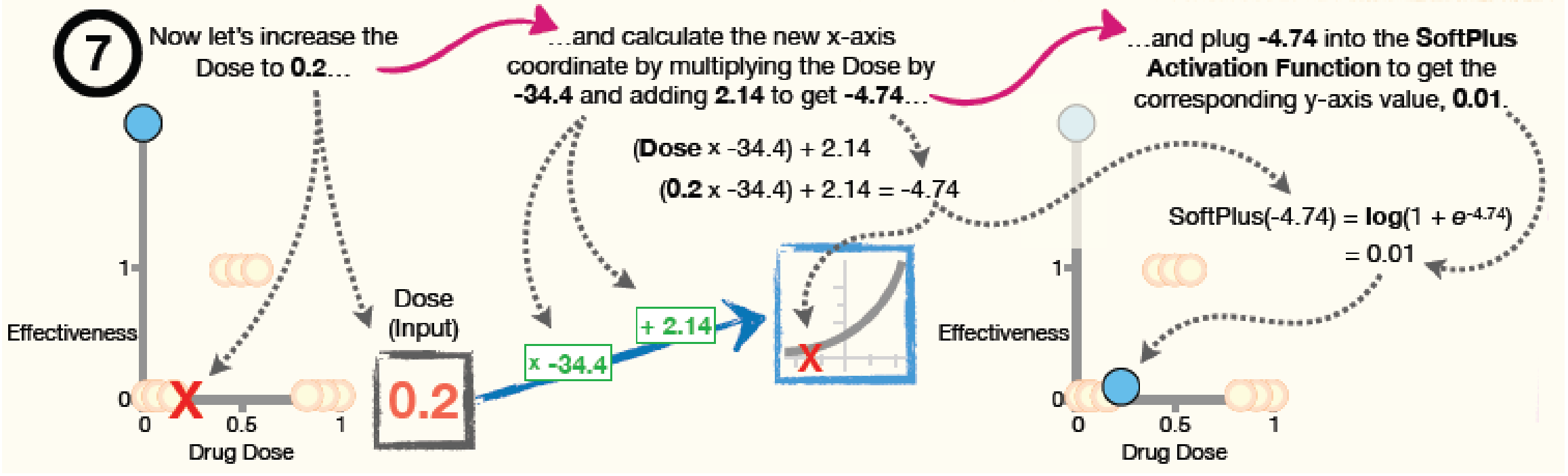
4

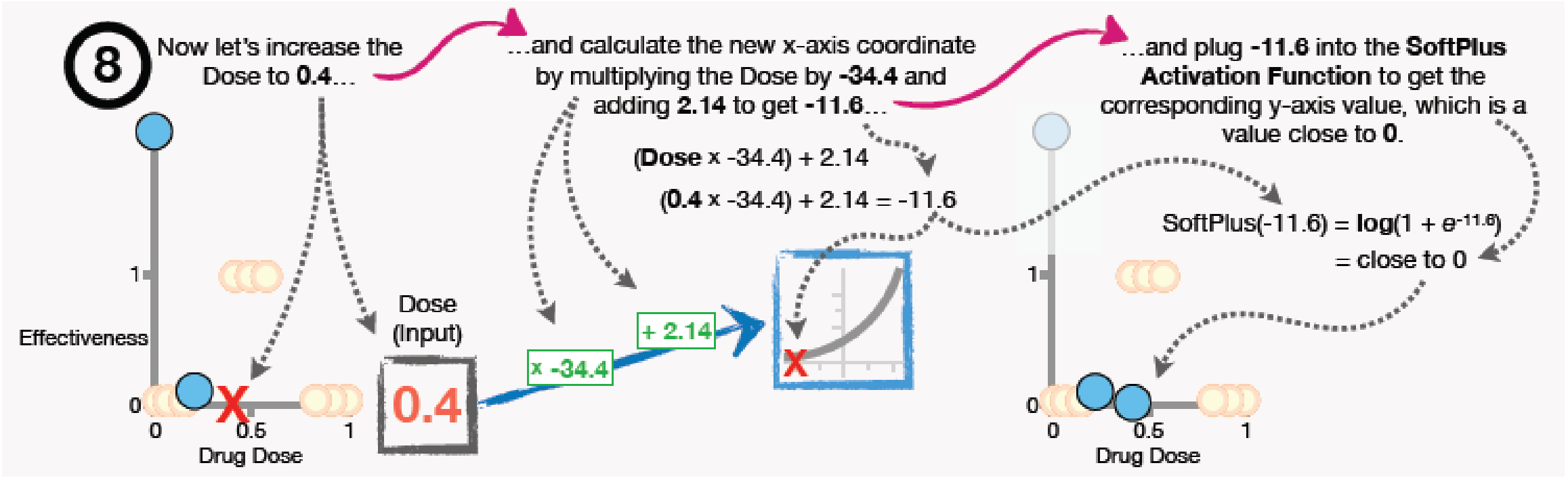
The first thing we do is plug the lowest Dose, **0**, into the **Neural Network**.

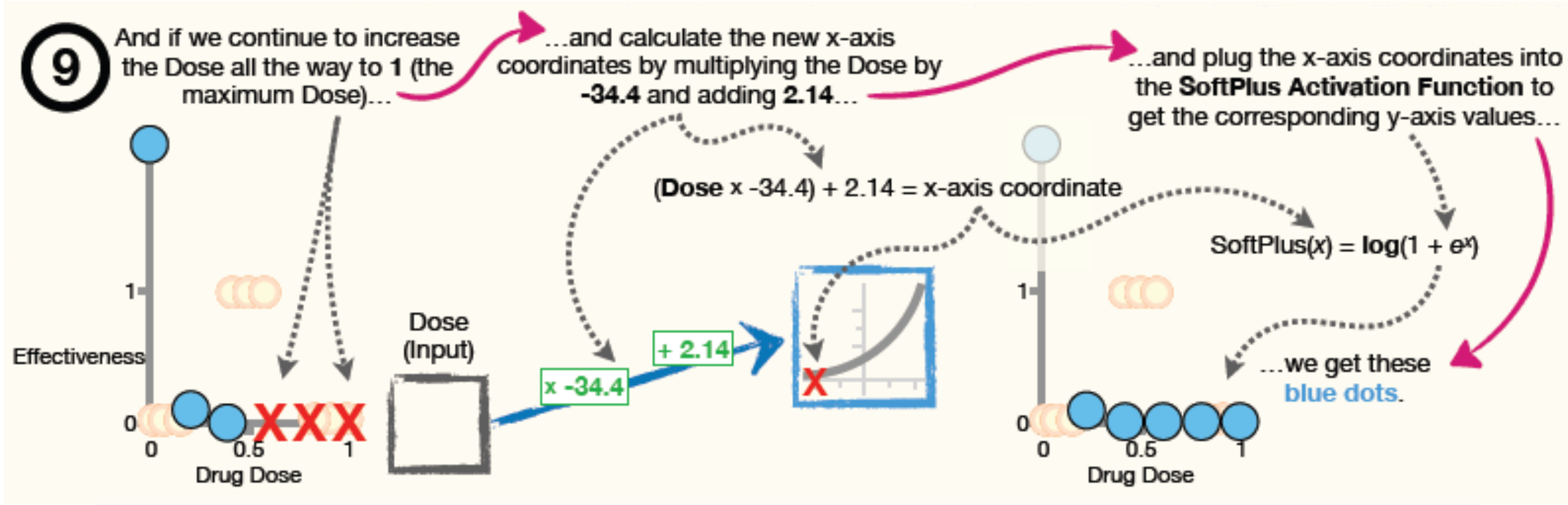


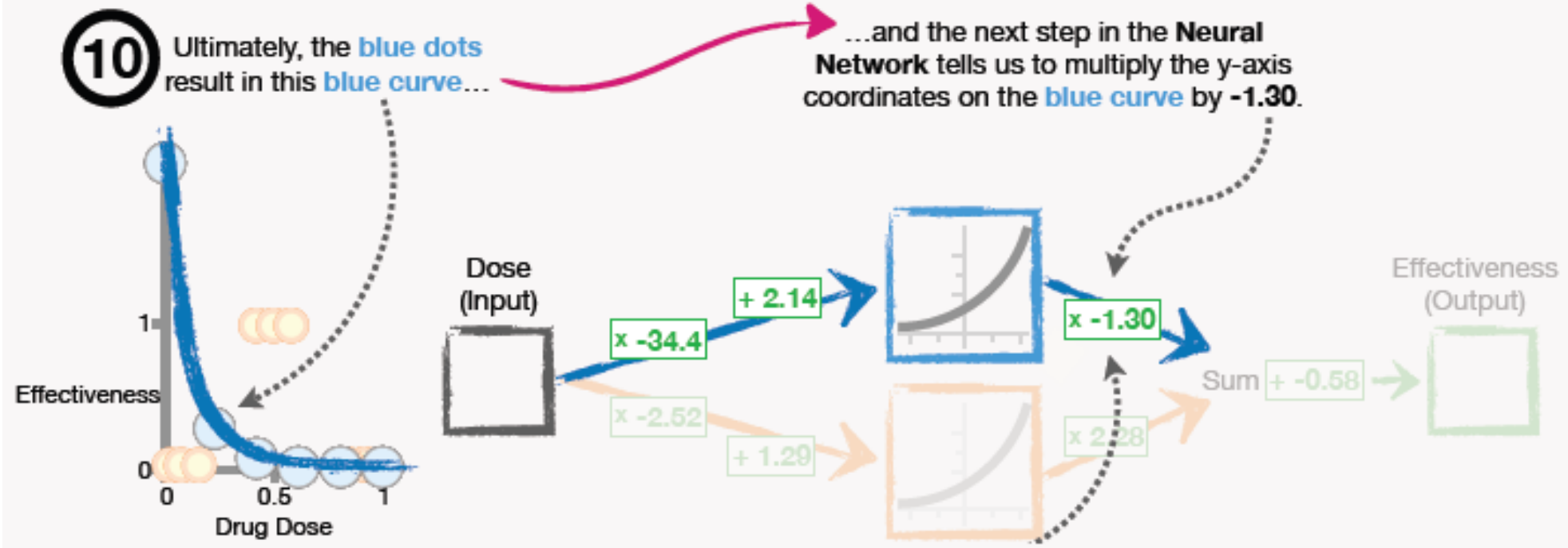

5
Now, the connection from the Input Node...
...to the top Node in the Hidden Layer...
...multiplies the Dose by -34.4 and then adds 2.14 ...
...to get a new x-axis coordinate for the Activation Function, 2.14.
(Dose x -34.4) + 2.14 = x-axis coordinate
(0 x -34.4) + 2.14 = x-axis coordinate = 2.14
Dose (Input)
0
x -34.4
+ 2.14
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)

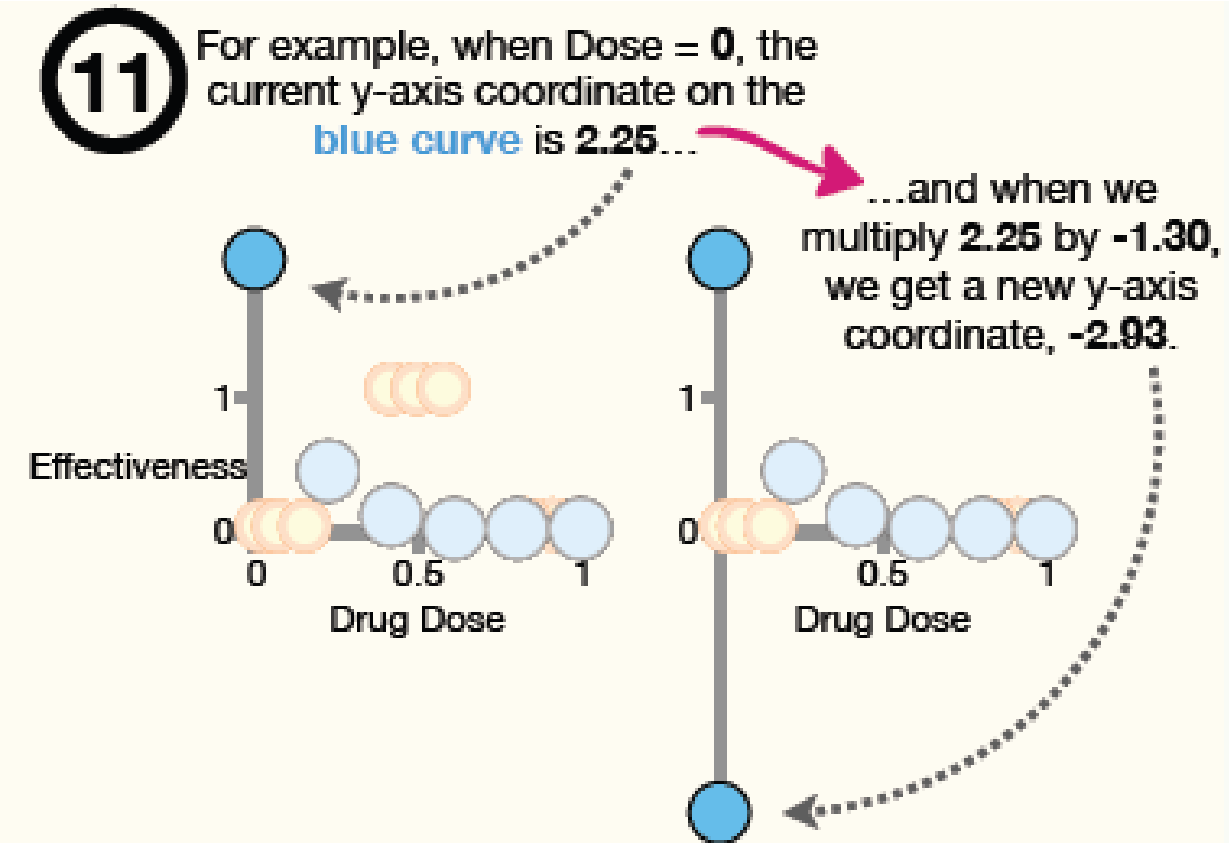

6
Then we plug the x-axis coordinate, 2.14 into the SoftPlus Activation Function...
...and do the math, just like we saw earlier...
...and we get 2.25. So, when the x-axis coordinate is 2.14, the corresponding y-axis value is 2.25...
...thus, when Dose = 0, the output for the SoftPlus is 2.25. So, let's put a blue dot, corresponding to the blue activation function, onto the graph of the original data at Dose = 0 with a y-axis value = 2.25.
SoftPlus(x) = SoftPlus(2.14) = log(1 + e^2.14) = y-axis coordinate = 2.25
Dose (Input)
0
x -34.4
+ 2.14
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)
Effectiveness
1
0
0
0.5
1
Drug Dose

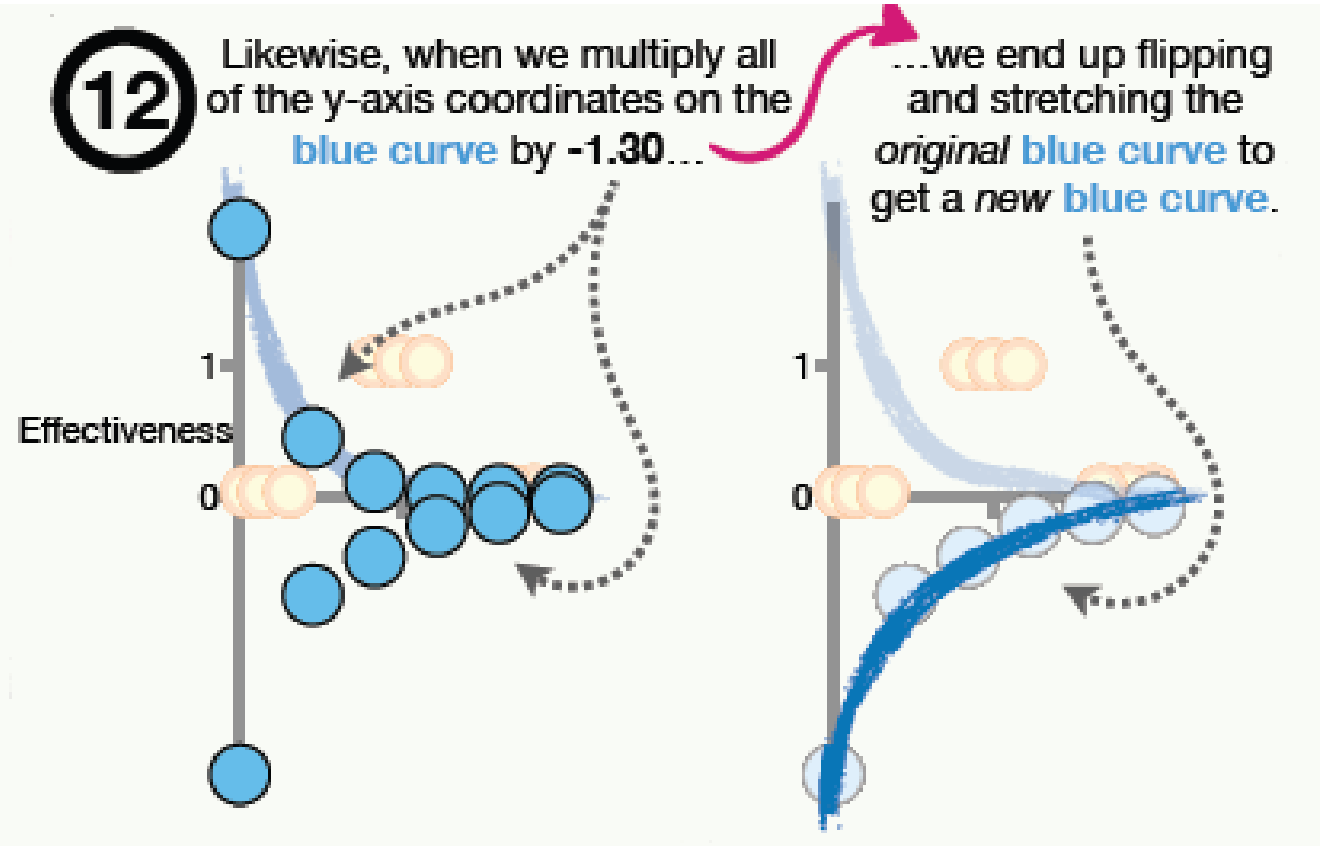

7
Now let's increase the Dose to 0.2...
...and calculate the new x-axis coordinate by multiplying the Dose by -34.4 and adding 2.14 to get -4.74...
(Dose x -34.4) + 2.14
(0.2 x -34.4) + 2.14 = -4.74
...and plug -4.74 into the SoftPlus Activation Function to get the corresponding y-axis value, 0.01.
SoftPlus(-4.74) = log(1 + e^-4.74)
= 0.01
Effectiveness
Drug Dose
Dose (Input)
0.2
x -34.4
+ 2.14
0
0.5
1

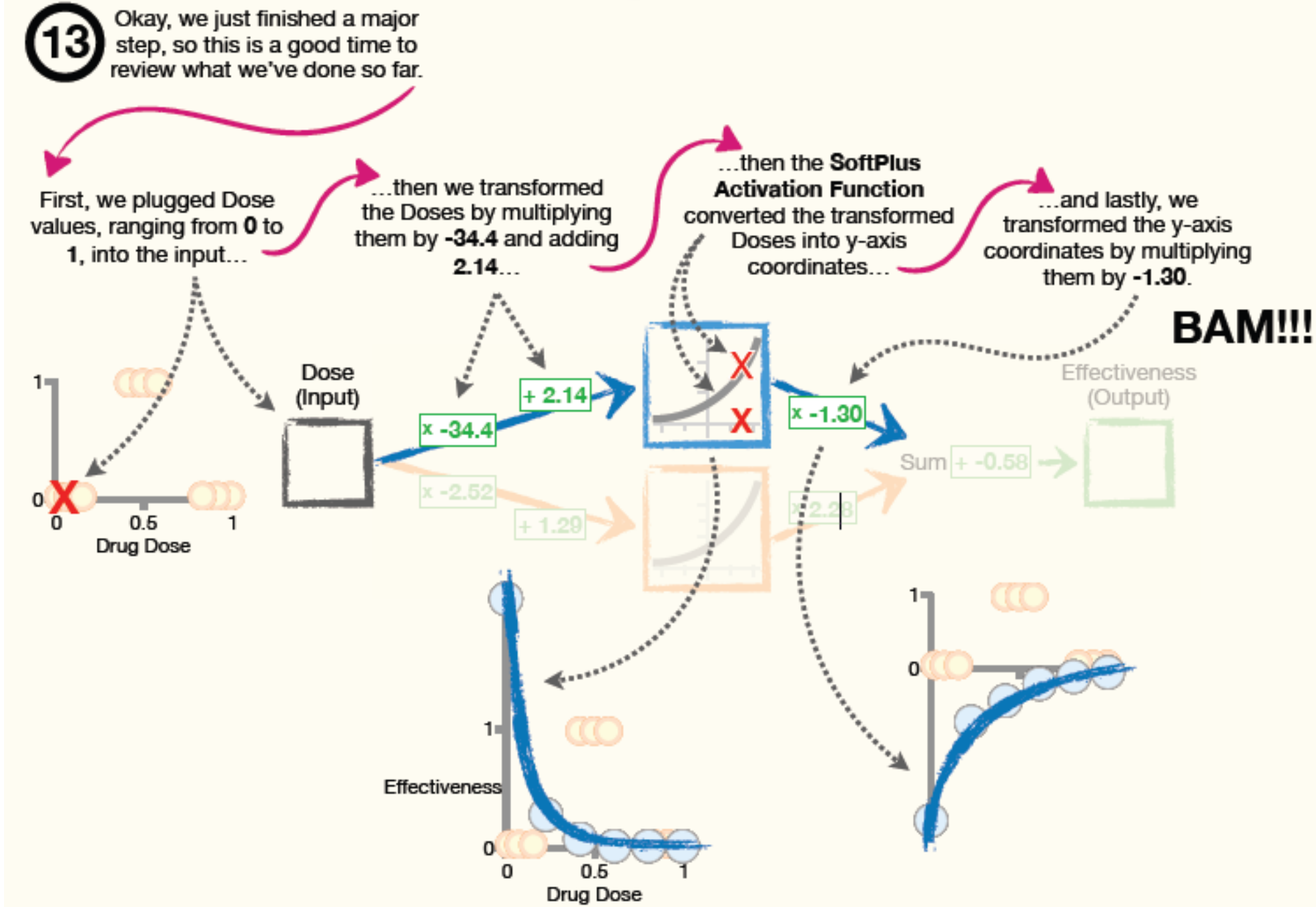

8
Now let's increase the Dose to 0.4...
...and calculate the new x-axis coordinate by multiplying the Dose by -34.4 and adding 2.14 to get -11.6...
(Dose x -34.4) + 2.14
(0.4 x -34.4) + 2.14 = -11.6
...and plug -11.6 into the SoftPlus Activation Function to get the corresponding y-axis value, which is a value close to 0.
SoftPlus(-11.6) = log(1 + e^-11.6)
= close to 0
Effectiveness
Drug Dose
Dose (Input)
0.4
x -34.4
+ 2.14
0
0.5
1

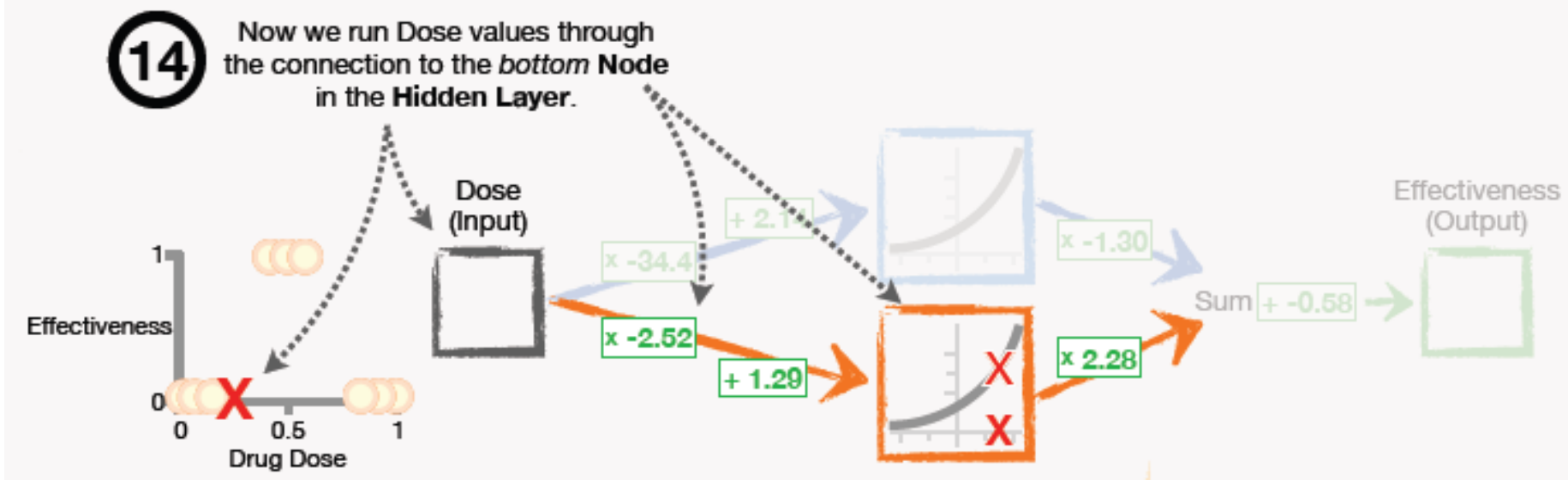

9
And if we continue to increase the Dose all the way to 1 (the maximum Dose)...
...and calculate the new x-axis coordinates by multiplying the Dose by -34.4 and adding 2.14...
...and plug the x-axis coordinates into the SoftPlus Activation Function to get the corresponding y-axis values...
(Dose x -34.4) + 2.14 = x-axis coordinate
SoftPlus(x) = log(1 + e^x)
Effectiveness
1
0
0
0.5
1
Drug Dose
Dose (Input)
x -34.4
+ 2.14
...we get these blue dots.

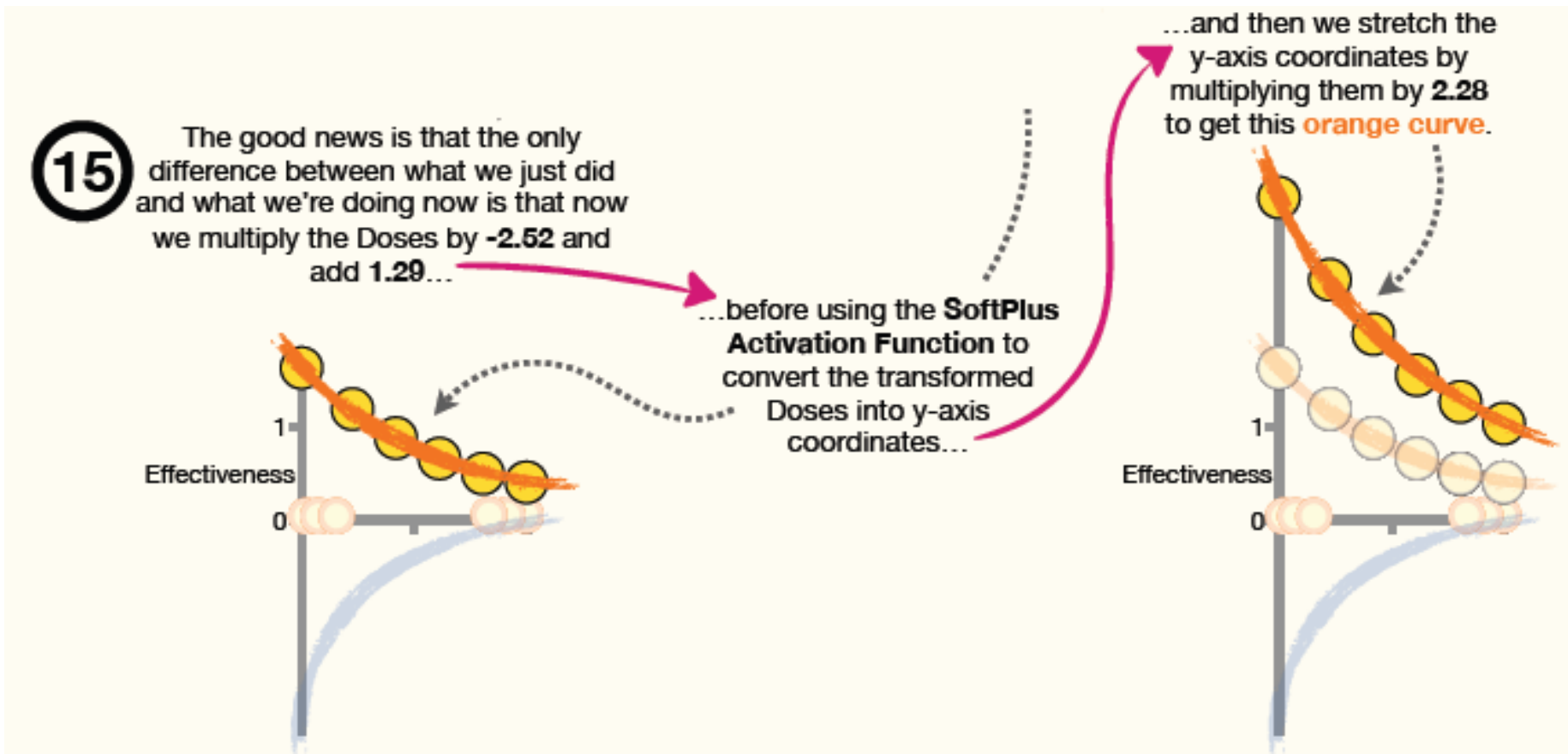

10
Ultimately, the blue dots result in this blue curve...
...and the next step in the Neural Network tells us to multiply the y-axis coordinates on the blue curve by -1.30.
Effectiveness
1
0
0
0.5
1
Drug Dose
Dose (Input)
x -34.4
+ 2.14
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)

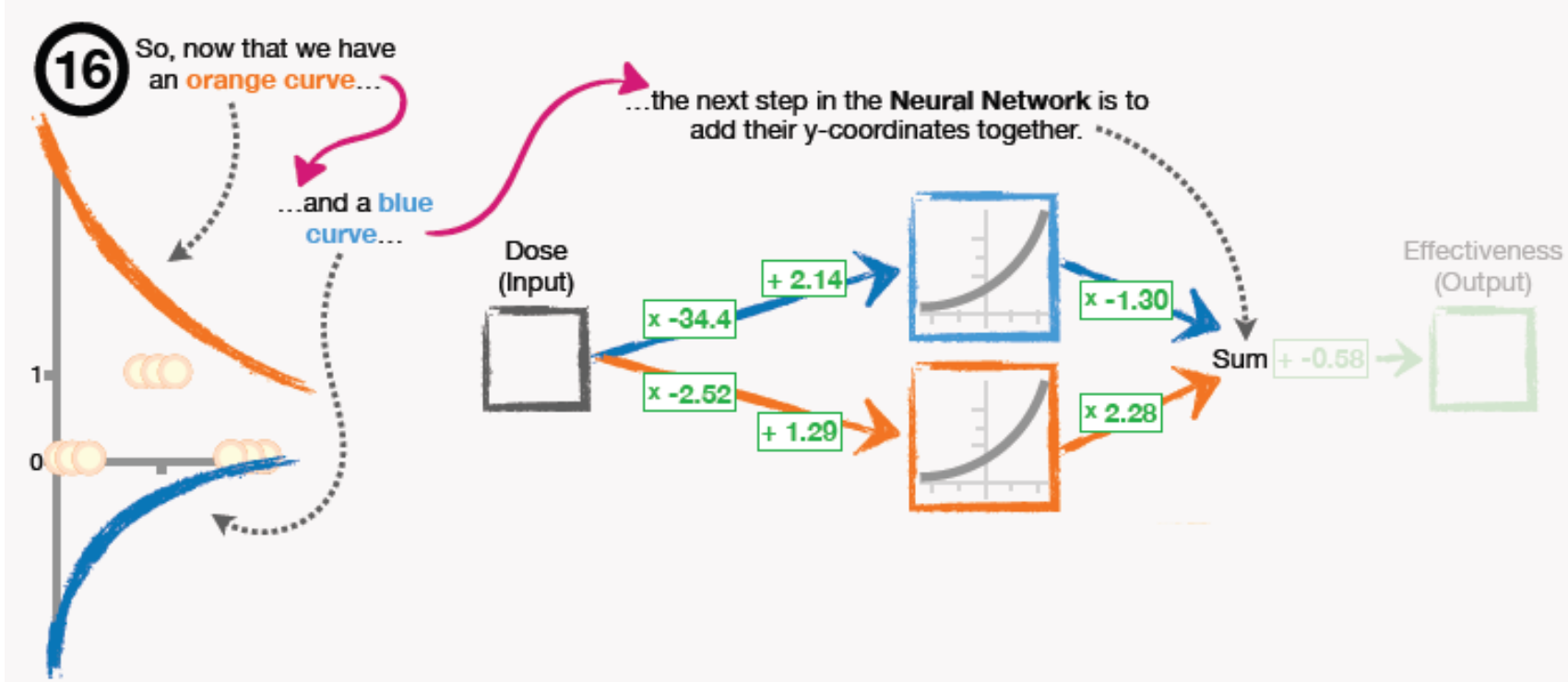

11
For example, when Dose = 0, the current y-axis coordinate on the blue curve is 2.25...
...and when we multiply 2.25 by -1.30, we get a new y-axis coordinate, -2.93.
1
Effectiveness
0
0
0.5
1
Drug Dose
1
0
0.5
1
Drug Dose

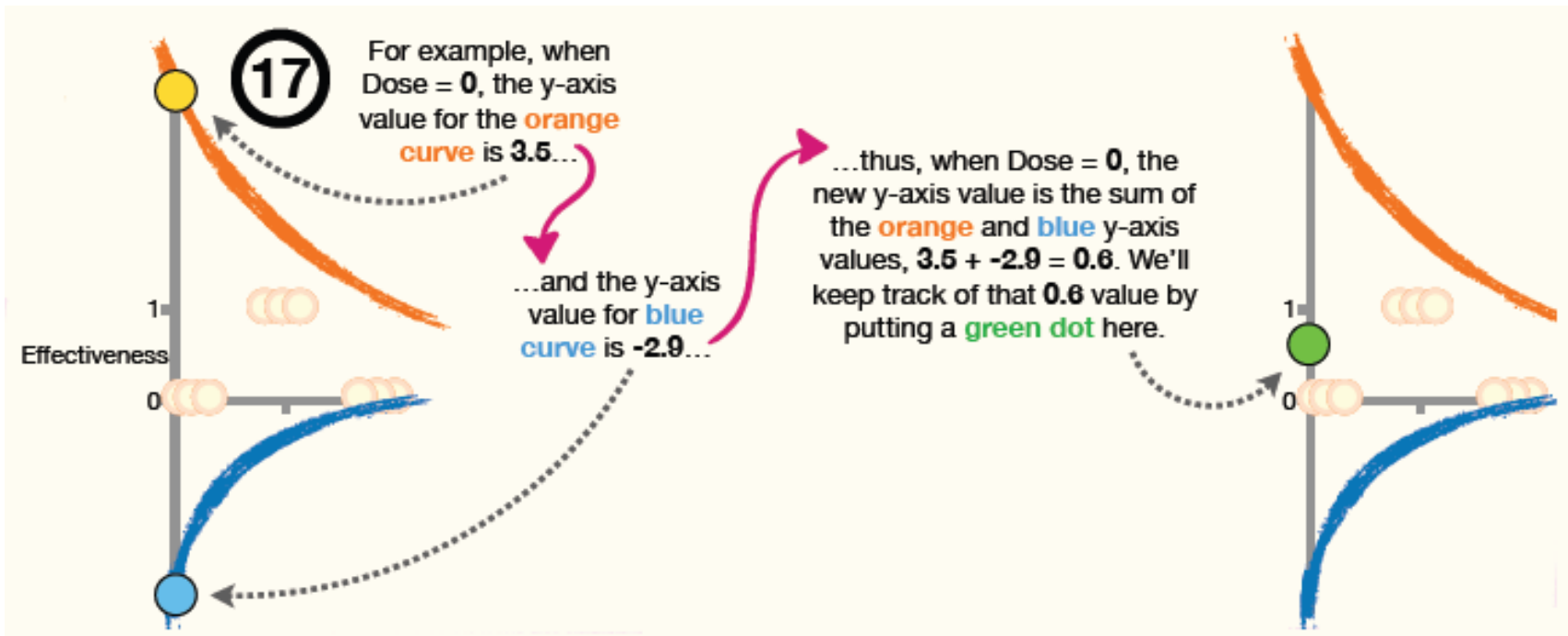

12
Likewise, when we multiply all of the y-axis coordinates on the blue curve by -1.30...
...we end up flipping and stretching the original blue curve to get a new blue curve.
1
Effectiveness
0
1
0

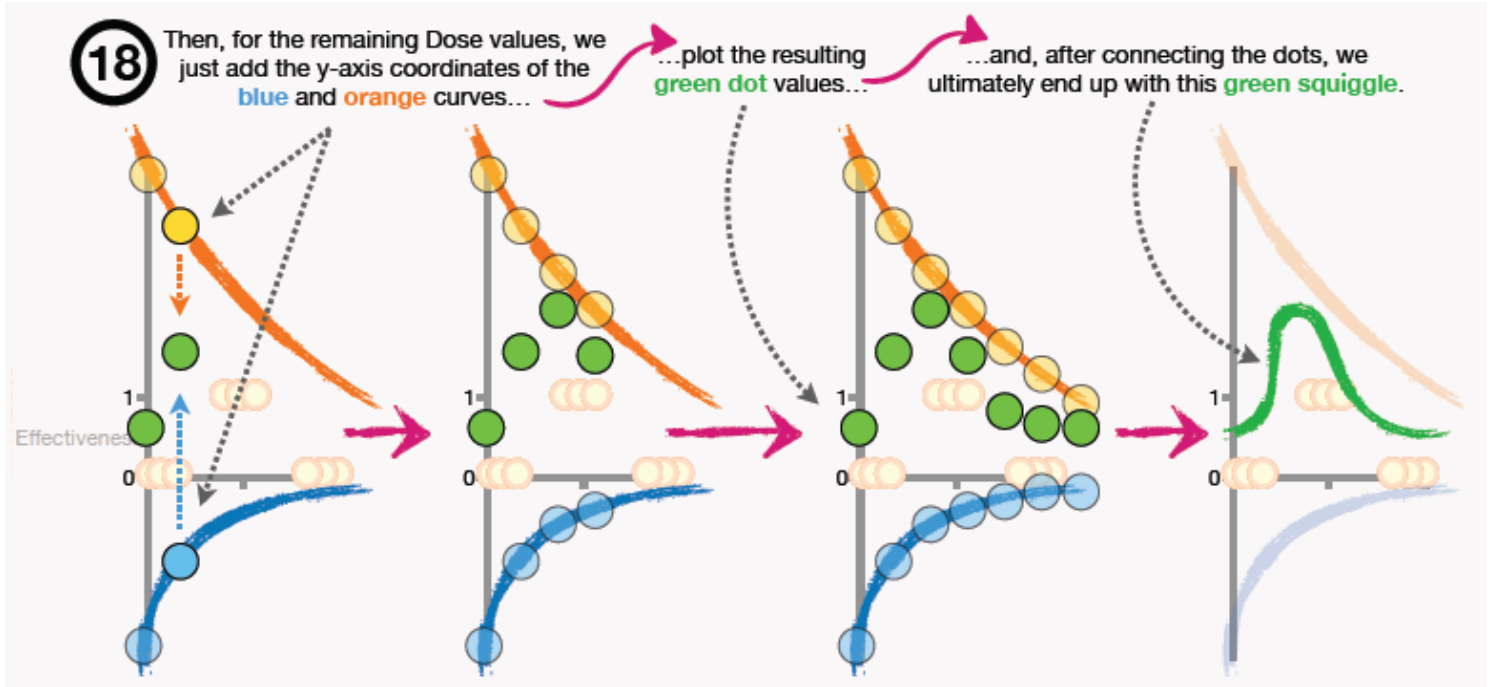

13
Okay, we just finished a major step, so this is a good time to review what we've done so far.
First, we plugged Dose values, ranging from 0 to 1, into the input...
...then we transformed the Doses by multiplying them by -34.4 and adding 2.14...
...then the SoftPlus Activation Function converted the transformed Doses into y-axis coordinates...
...and lastly, we transformed the y-axis coordinates by multiplying them by -1.30.
BAM!!!
1
0
0
0.5
1
Drug Dose
Dose (Input)
x -34.4
+ 2.14
x -2.52
+ 1.29
x -1.30
x 2.28
Sum + -0.58
Effectiveness (Output)
1
Effectiveness
0
0
0.5
1
Drug Dose
1
0

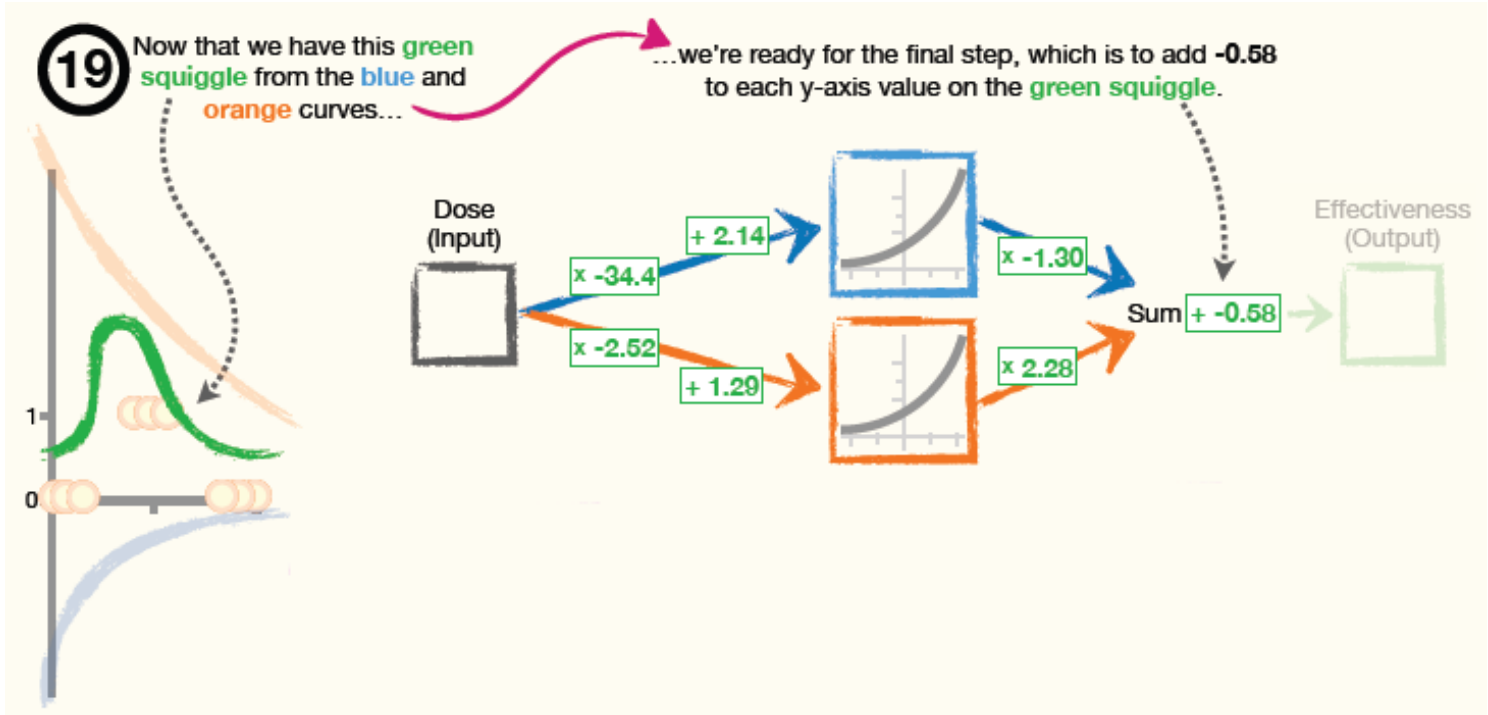

14
Now we run Dose values through the connection to the *bottom* **Node** in the **Hidden Layer**.
Dose (Input)
Effectiveness
1
0
0
0.5
1
Drug Dose
x -34.4
+ 2.14
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)


15
The good news is that the only difference between what we just did and what we're doing now is that now we multiply the Doses by **-2.52** and add **1.29**...
...before using the **SoftPlus Activation Function** to convert the transformed Doses into y-axis coordinates...
...and then we stretch the y-axis coordinates by multiplying them by **2.28** to get this orange curve.
1
Effectiveness
0
1
Effectiveness
0

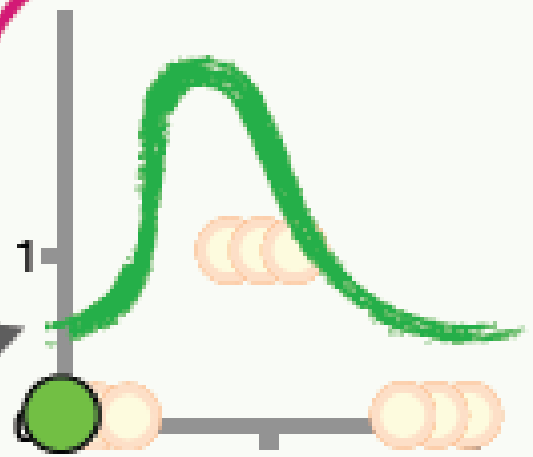

16
So, now that we have an orange curve...
...and a blue curve...
...the next step in the Neural Network is to add their y-coordinates together.
Dose (Input)
x -34.4
+ 2.14
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)
1
0


17
For example, when Dose = 0, the y-axis value for the orange curve is 3.5...
...and the y-axis value for blue curve is -2.9...
...thus, when Dose = 0, the new y-axis value is the sum of the orange and blue y-axis values, 3.5 + -2.9 = 0.6. We'll keep track of that 0.6 value by putting a green dot here.
Effectiveness
1
0
1
0


18
Then, for the remaining Dose values, we just add the y-axis coordinates of the blue and orange curves…
…plot the resulting green dot values…
…and, after connecting the dots, we ultimately end up with this green squiggle.
Effectiveness
1
0


19
Now that we have this green squiggle from the blue and orange curves…
…we're ready for the final step, which is to add -0.58 to each y-axis value on the green squiggle.
Dose (Input)
x -34.4
+ 2.14
x -2.52
+ 1.29
x -1.30
x 2.28
Sum
+ -0.58
Effectiveness (Output)
1
0

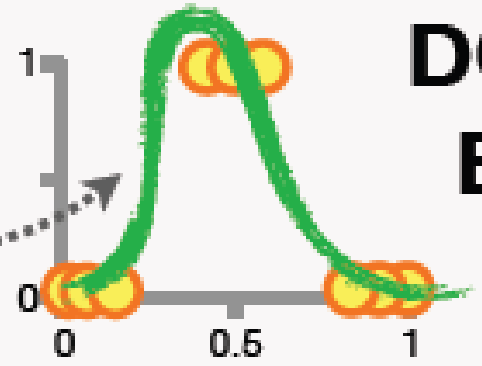
20 For example, when Dose = **0**, the y-axis coordinate on the green squiggle starts out at **0.6**...



...but after subtracting **0.58**, the new y-axis coordinate for when Dose = **0** is **0.0** (rounded to the nearest tenth).

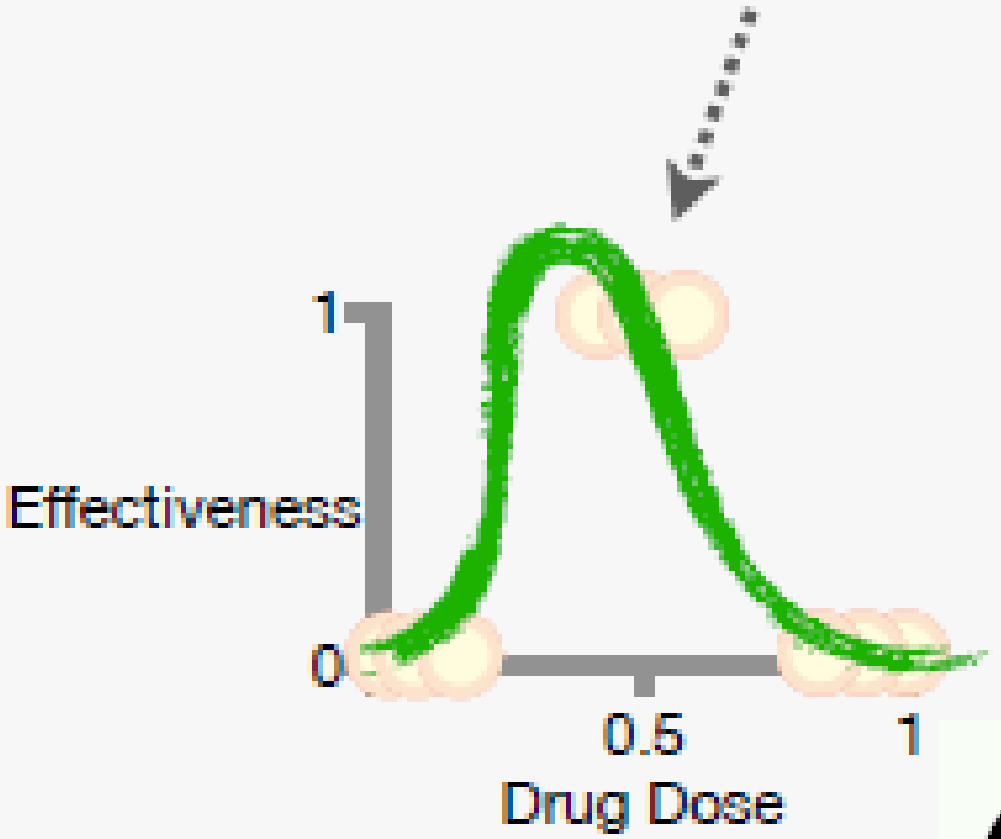
21 Likewise, subtracting **0.58** from all of the other y-axis coordinates on the green squiggle shifts it down...

...and, ultimately, we end up with a green squiggle that fits the **Training Data**.



DOUBLE BAM!!!

23 Now, if we're wondering if a medium Dose of **0.5** will be effective, we can look at the **green squiggle** and see that the output from the **Neural Network** will be **1**, and thus, Dose = **0.5** will be effective.



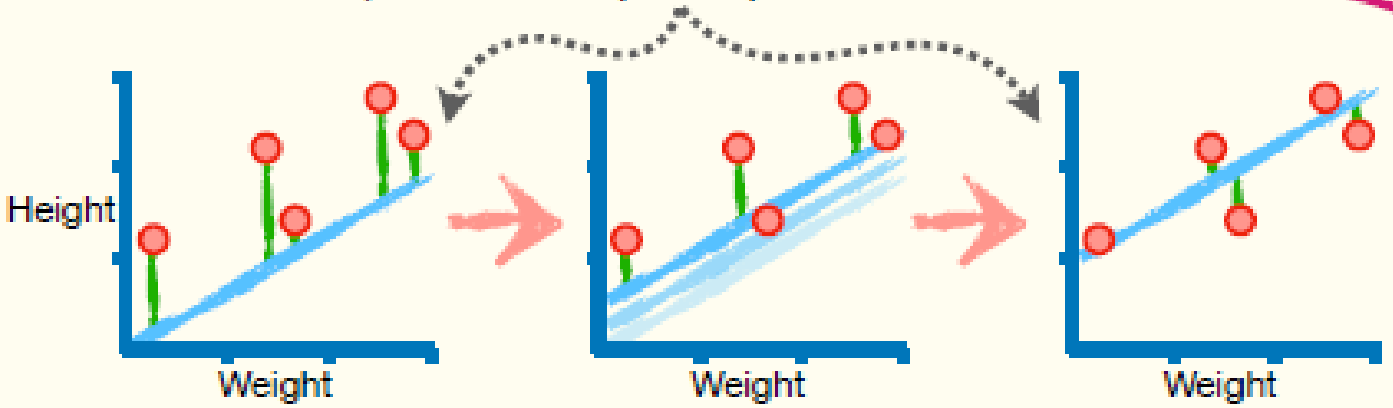
24 Alternatively, if we plug **Dose** = **0.5** into the **Neural Network** and do the math, we get **1**, and thus, Dose = **0.5** will be effective.

1

The Problem: Just like for **Linear Regression**, **Neural Networks** have parameters that we need to optimize to fit a squiggle or bent shape to data. How do we find the optimal values for these parameters?

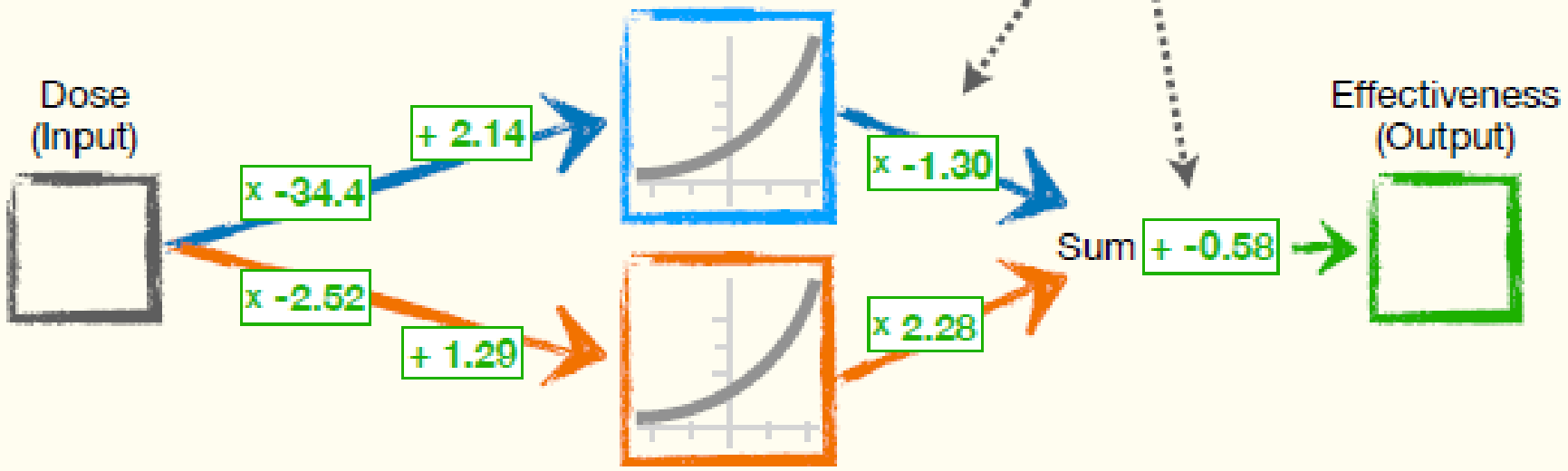
2

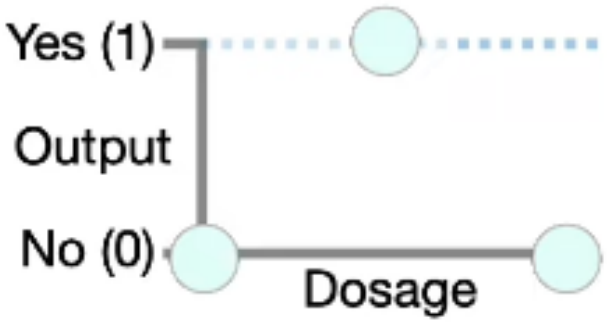
A Solution: Just like for **Linear Regression**, we can use **Gradient Descent** (or **Stochastic Gradient Descent**) to find the optimal parameter values…

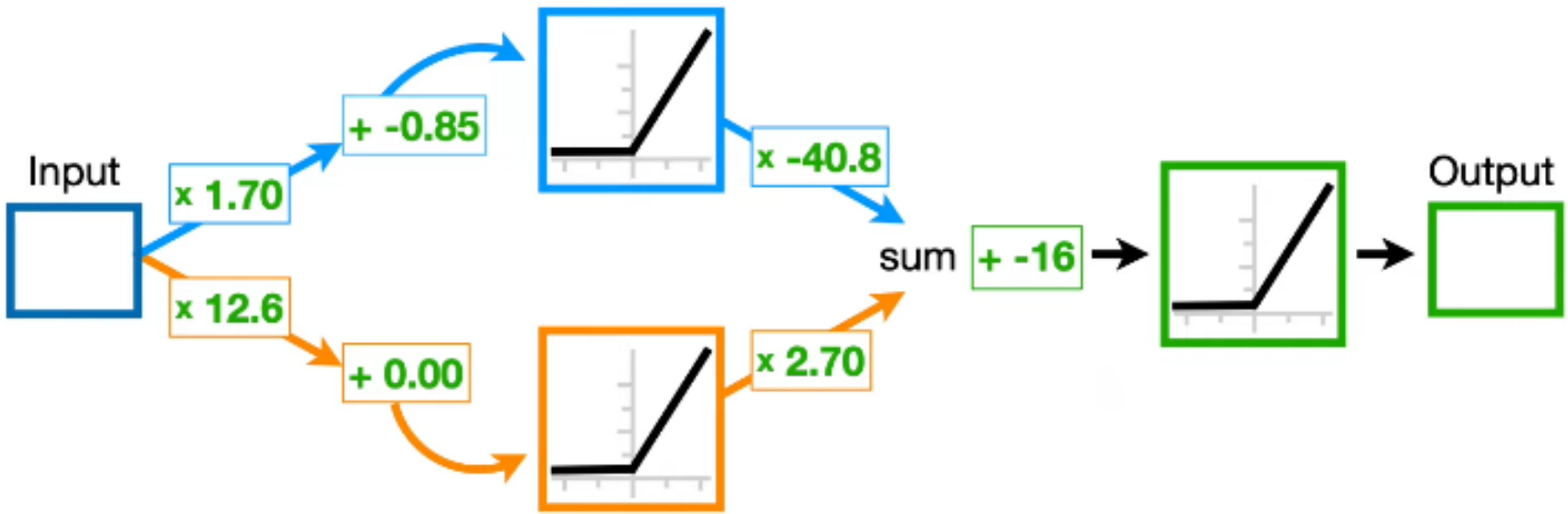


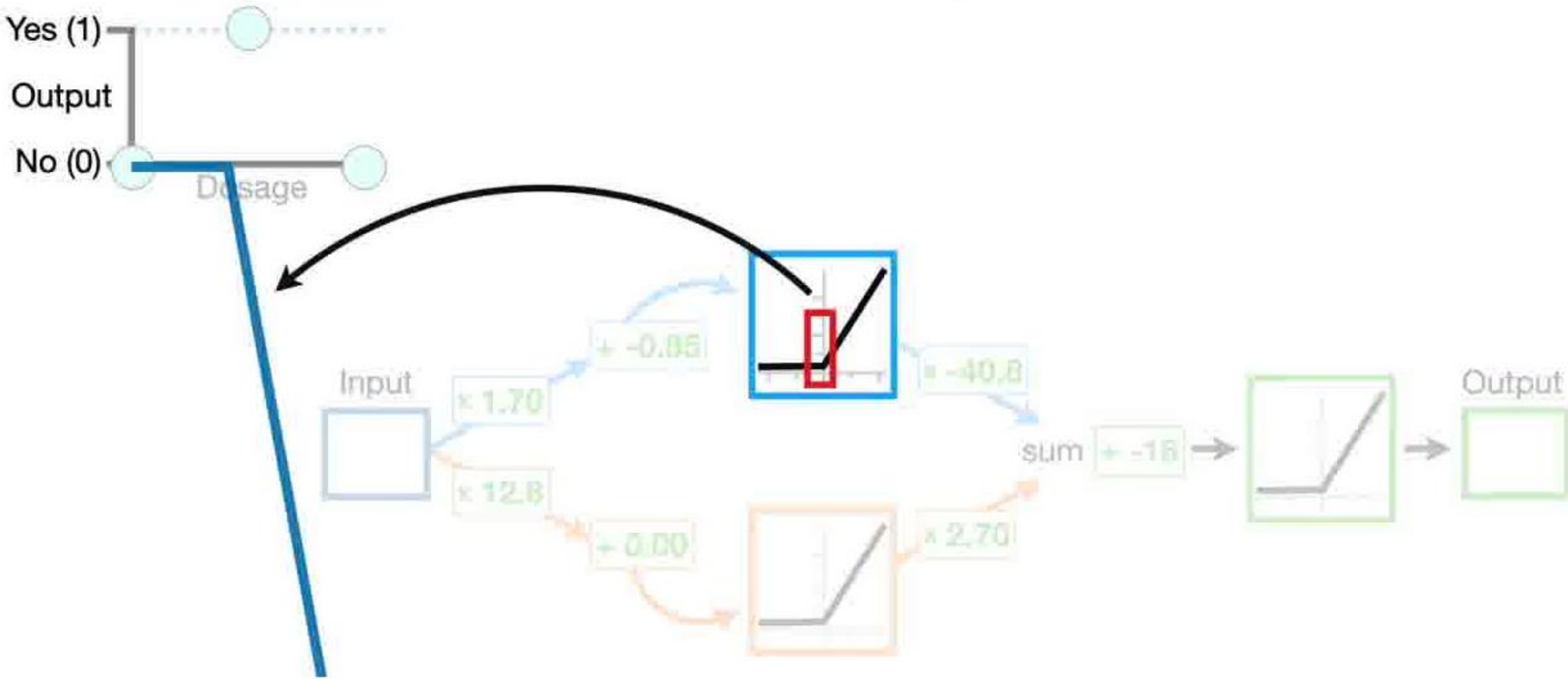
…however, we don't call it **Gradient Descent**. That would be too easy. Instead, because of how the derivatives are found for each parameter in a **Neural Network** (from the back to the front), we call it **Backpropagation**.

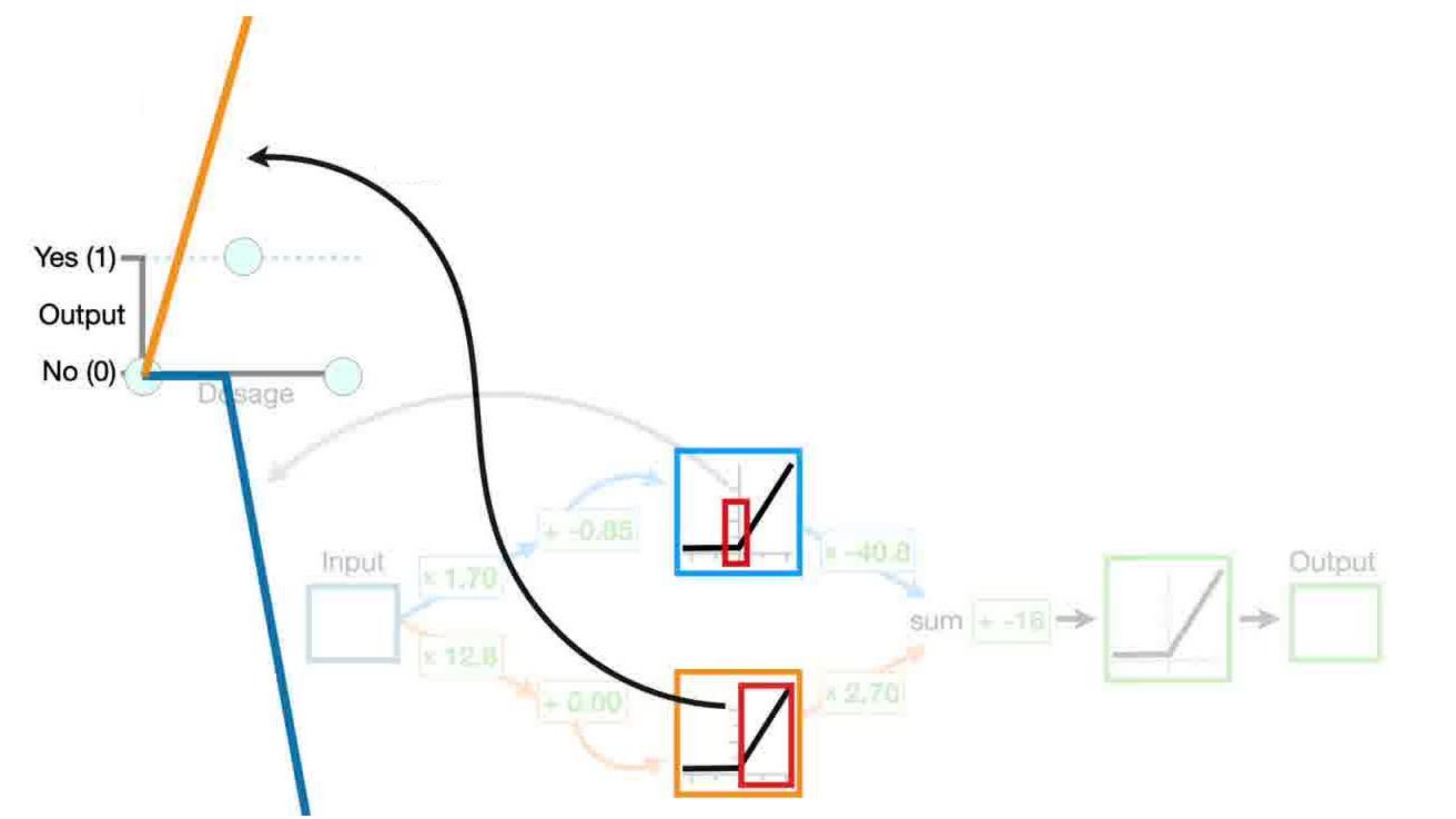
BAM!!!

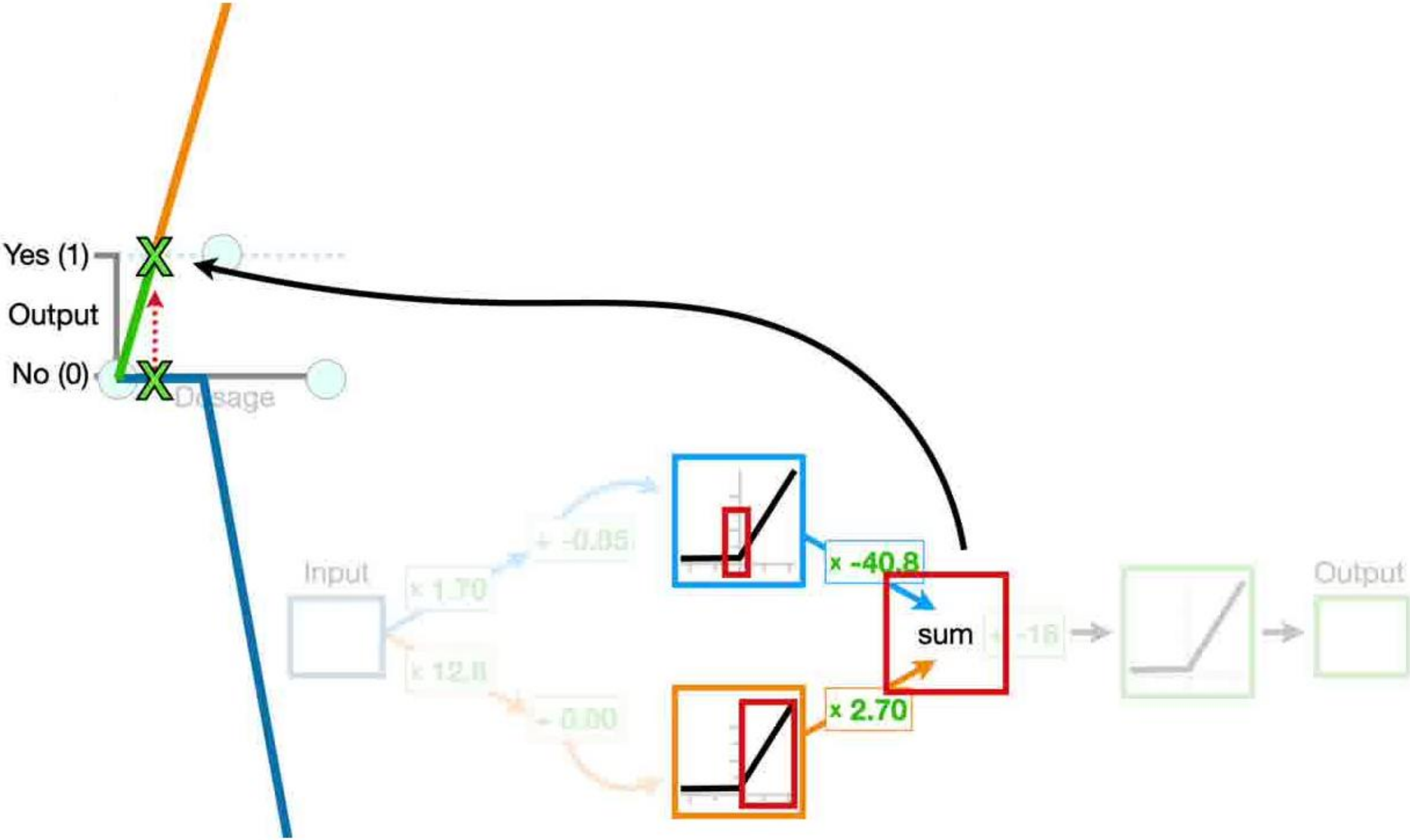


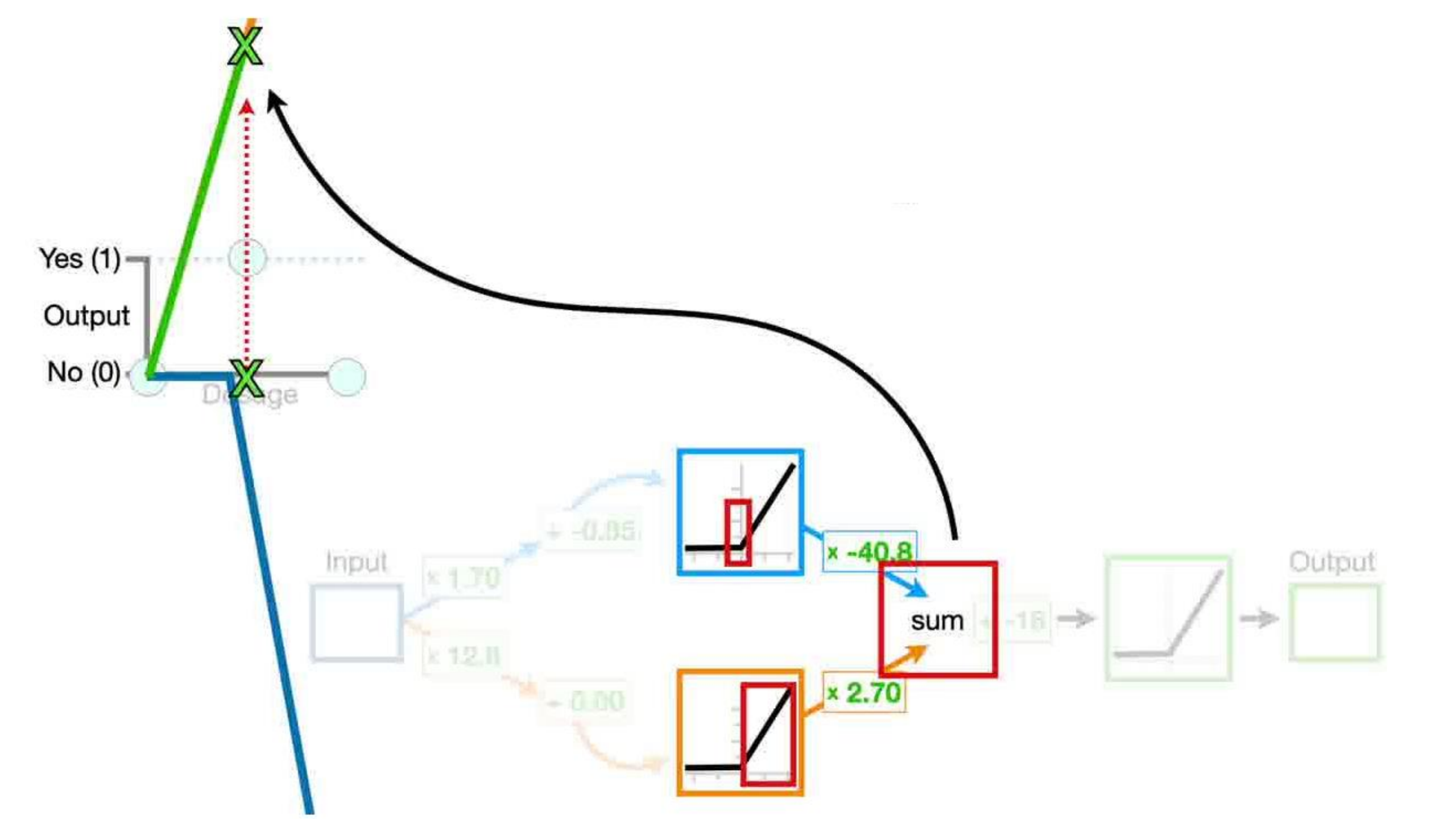

Yes (1)
Output
No (0)
Dosage

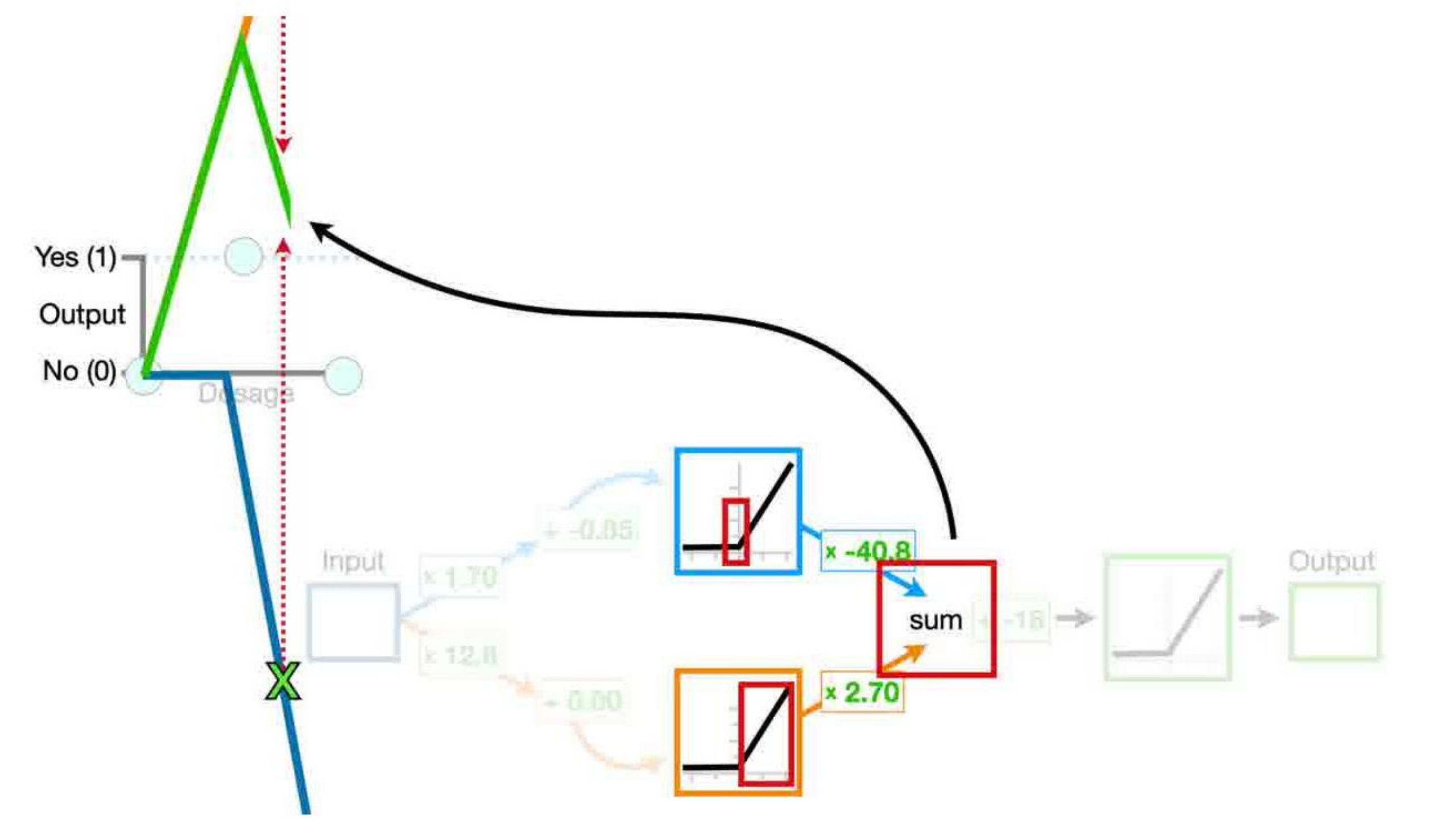

Input
x 1.70
+ -0.85
x -40.8
x 12.6
+ 0.00
x 2.70
sum
+ -16
Output

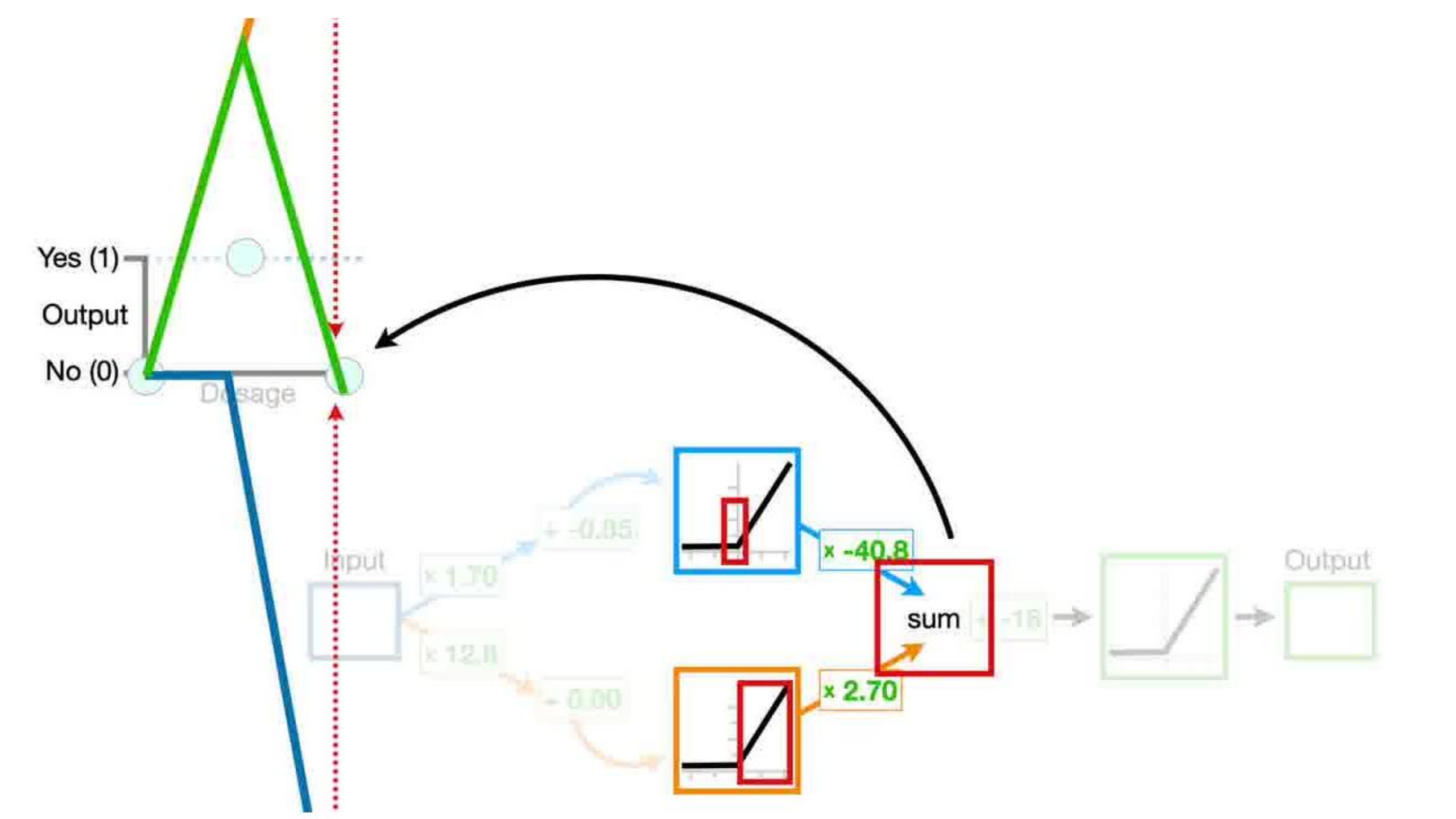

Yes (1)
Output
No (0)
Dosage
Input
× 1.70
+ -0.86
× 12.8
+ 0.00
× -40.8
× 2.70
sum
+ -16
Output

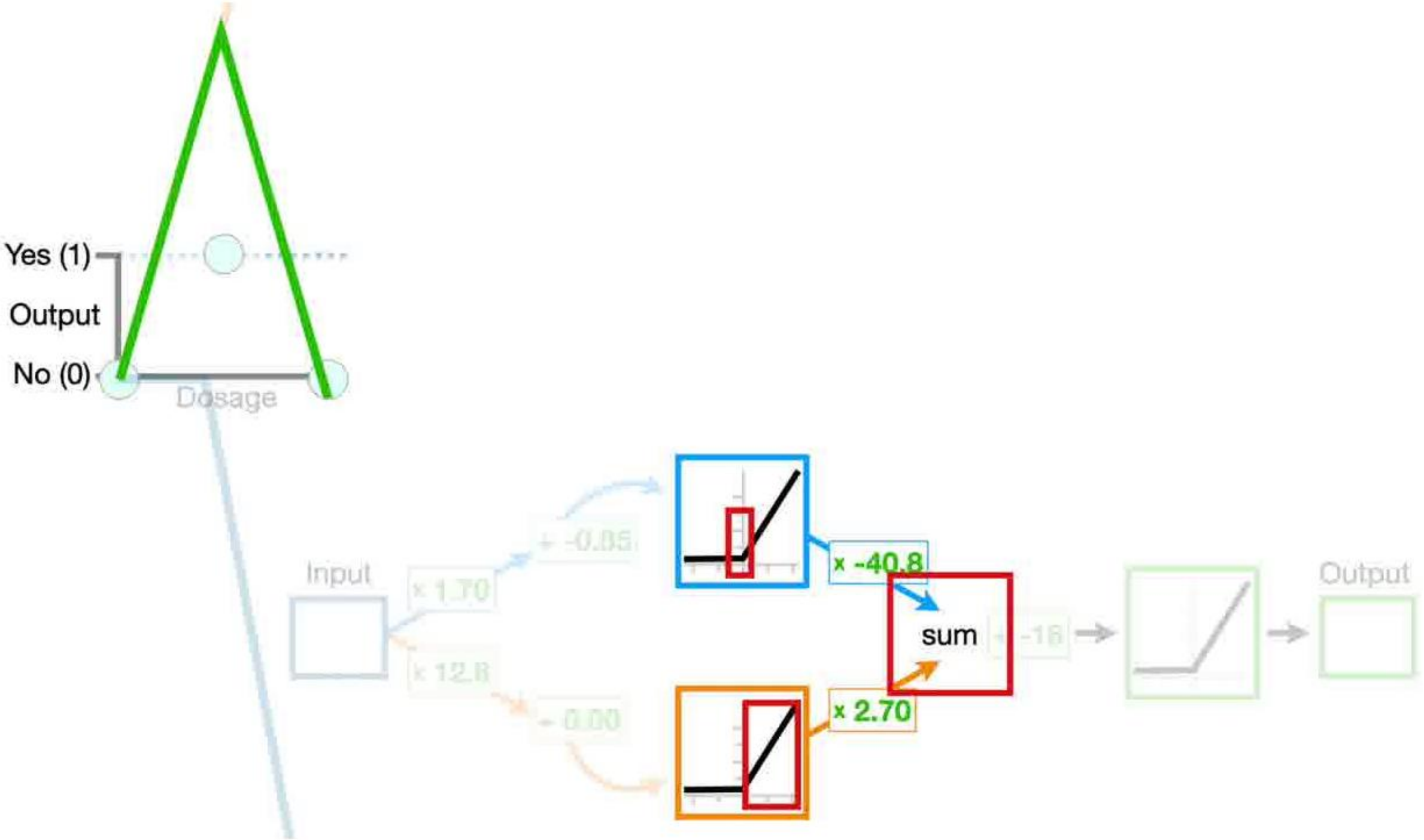

Yes (1)
Output
No (0)
Dosage
Input
x 1.70
+ -0.85
x 12.8
+ 0.00
+ -40.8
x 2.70
sum
+ -16
Output

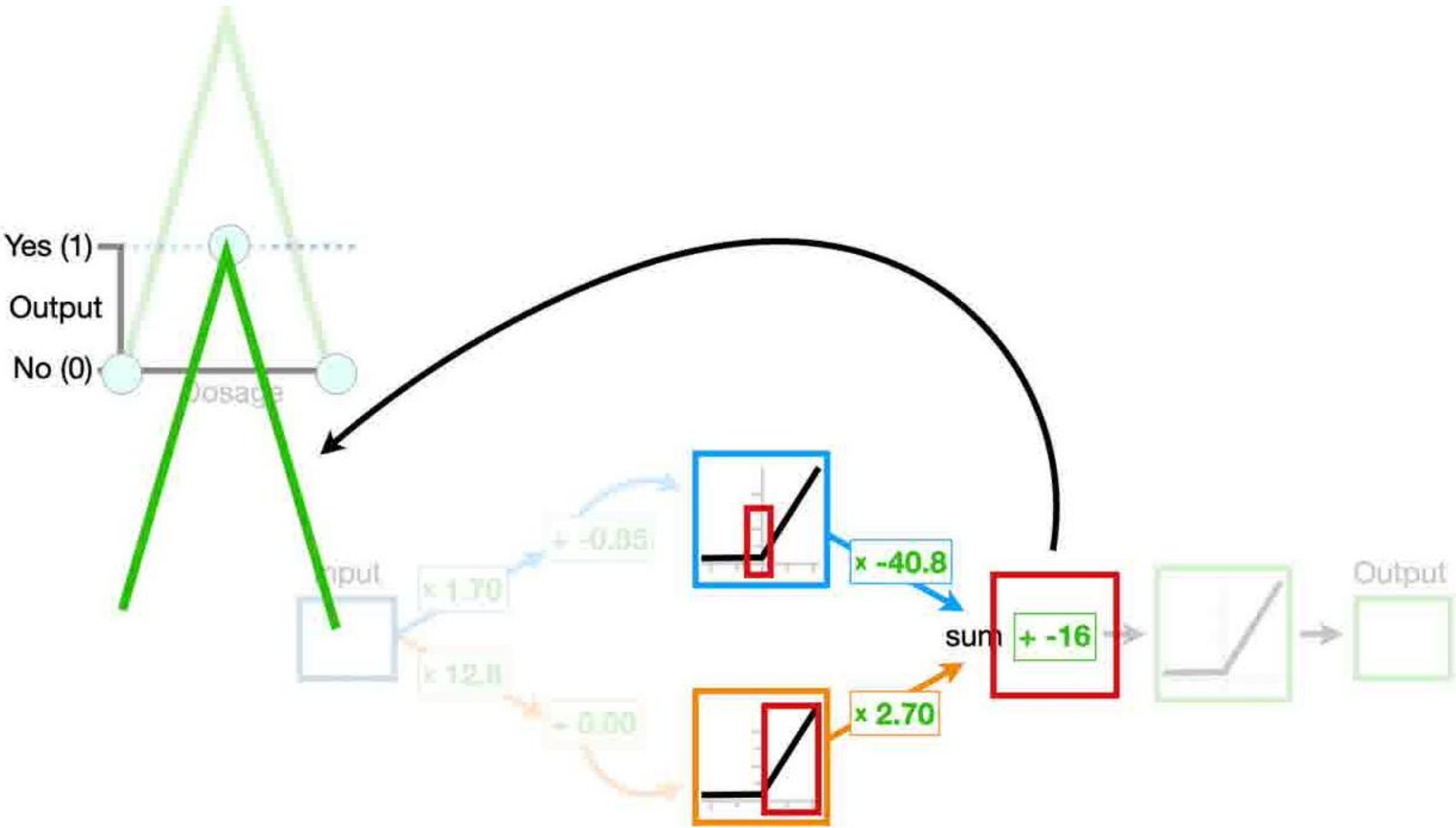

Yes (1)
Output
No (0)
Dosage
Input
+ -0.05
x 1.70
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output

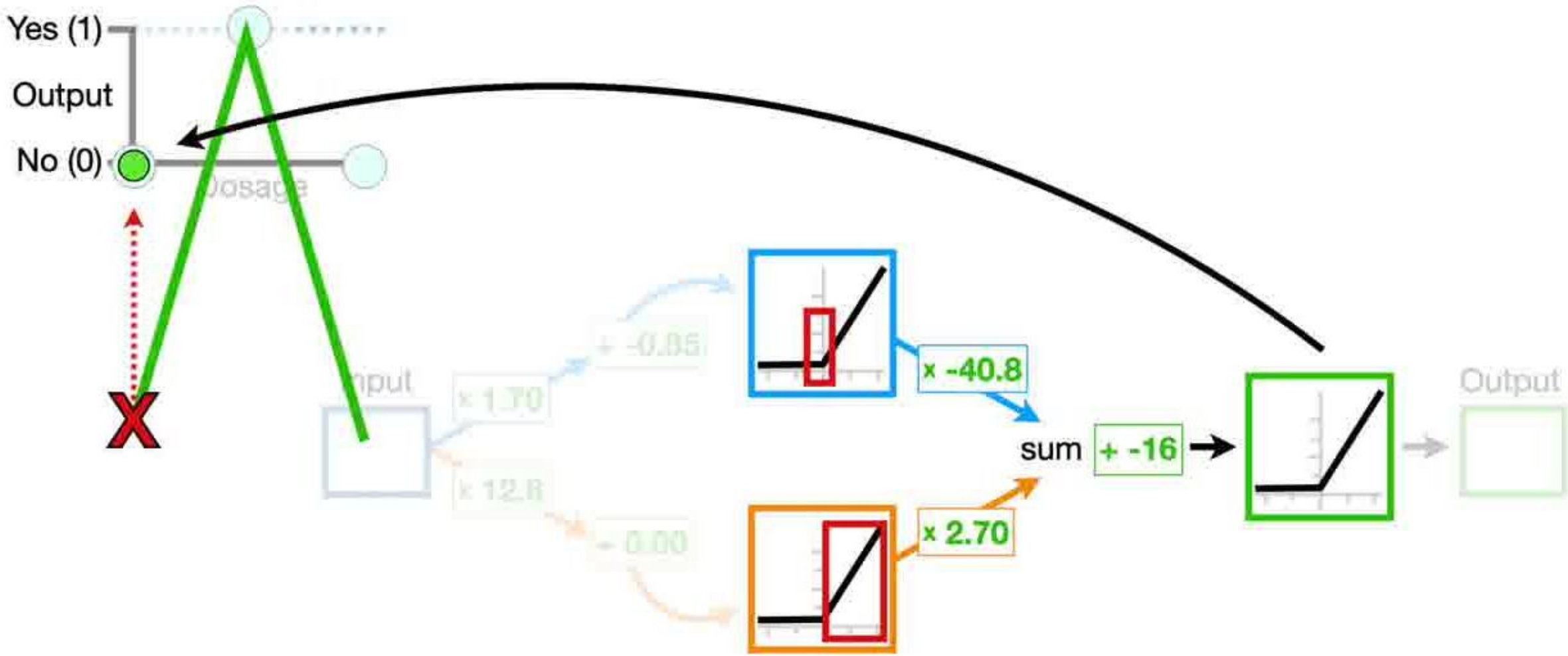

Yes (1)
Output
No (0)
Input
x -40.8
sum
x 2.70
Output

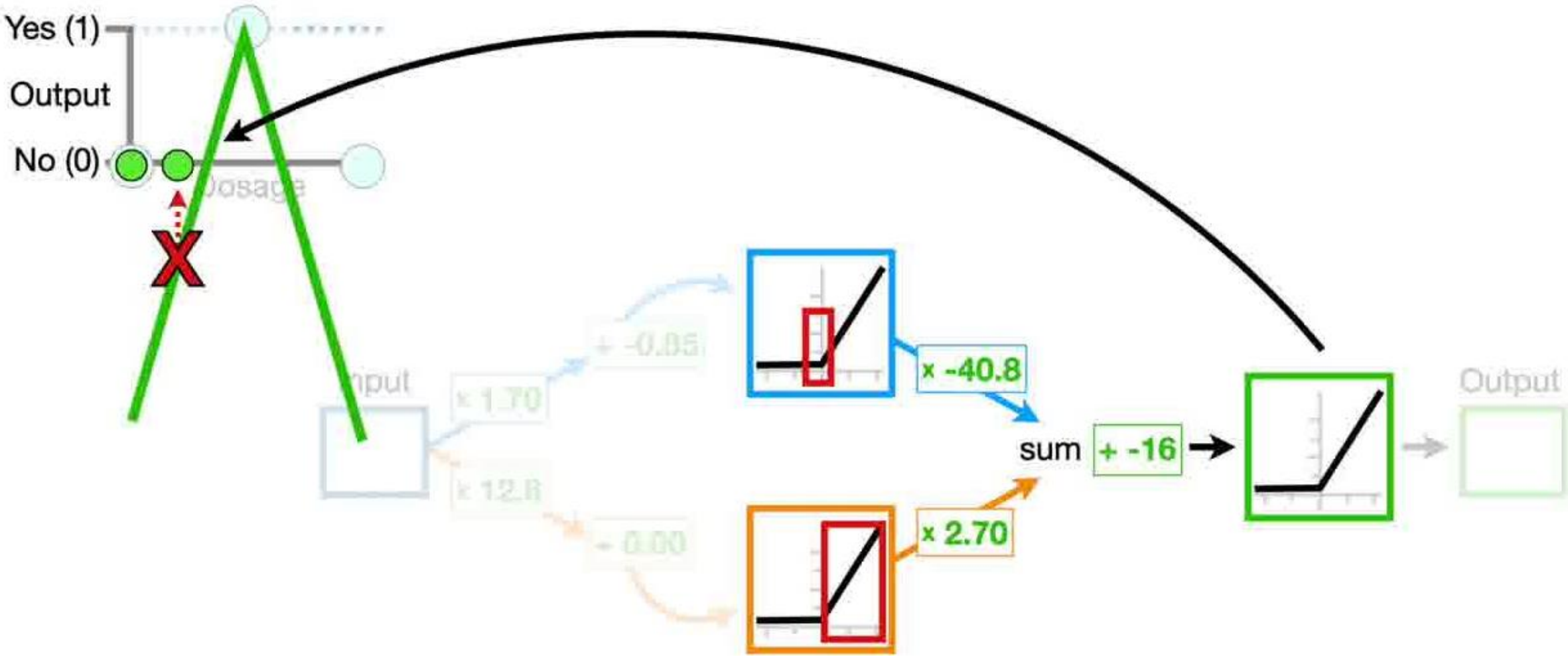

Yes (1)
Output
No (0)
Dosage
X
Input
x 1.70
+ -0.05
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output

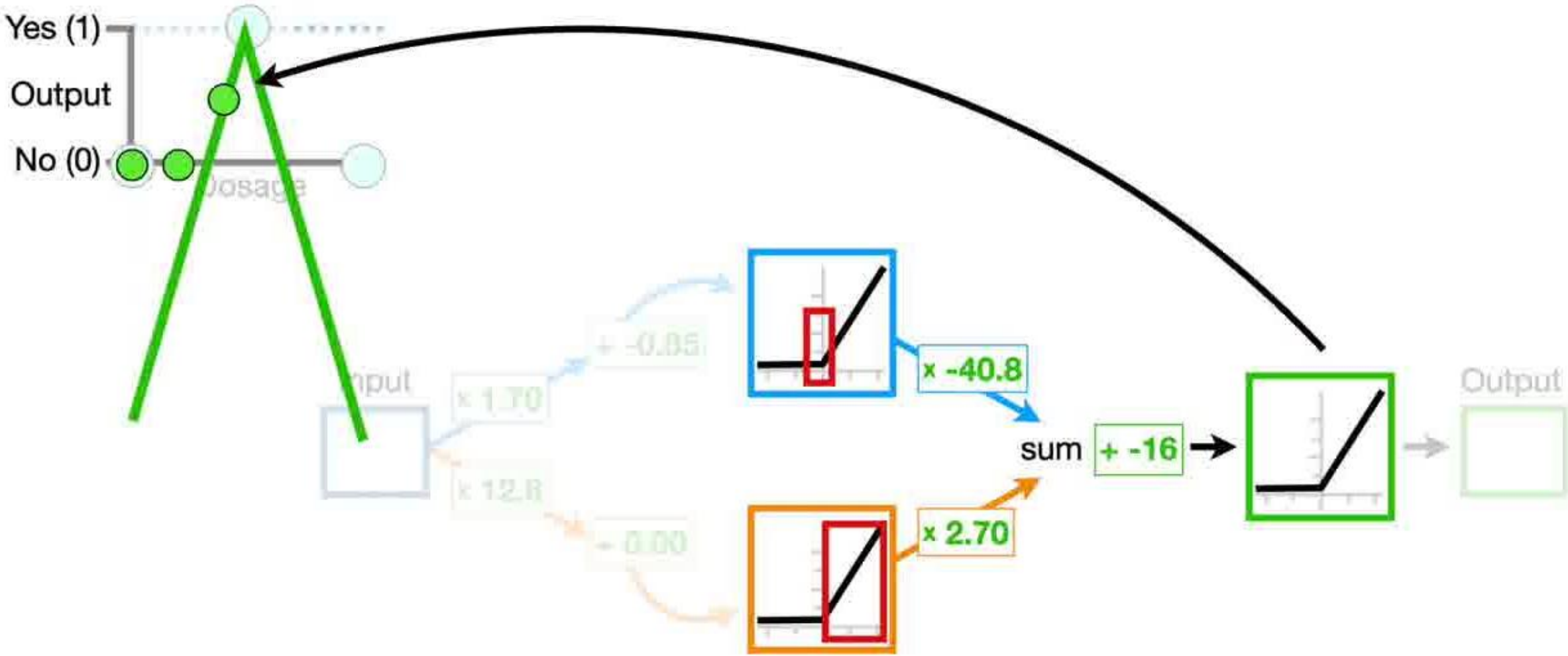

Yes (1)
Output
No (0)
Dosage
Input
× 1.70
+ -0.05
× 12.8
+ 0.00
× -40.8
× 2.70
sum
+ -16
Output

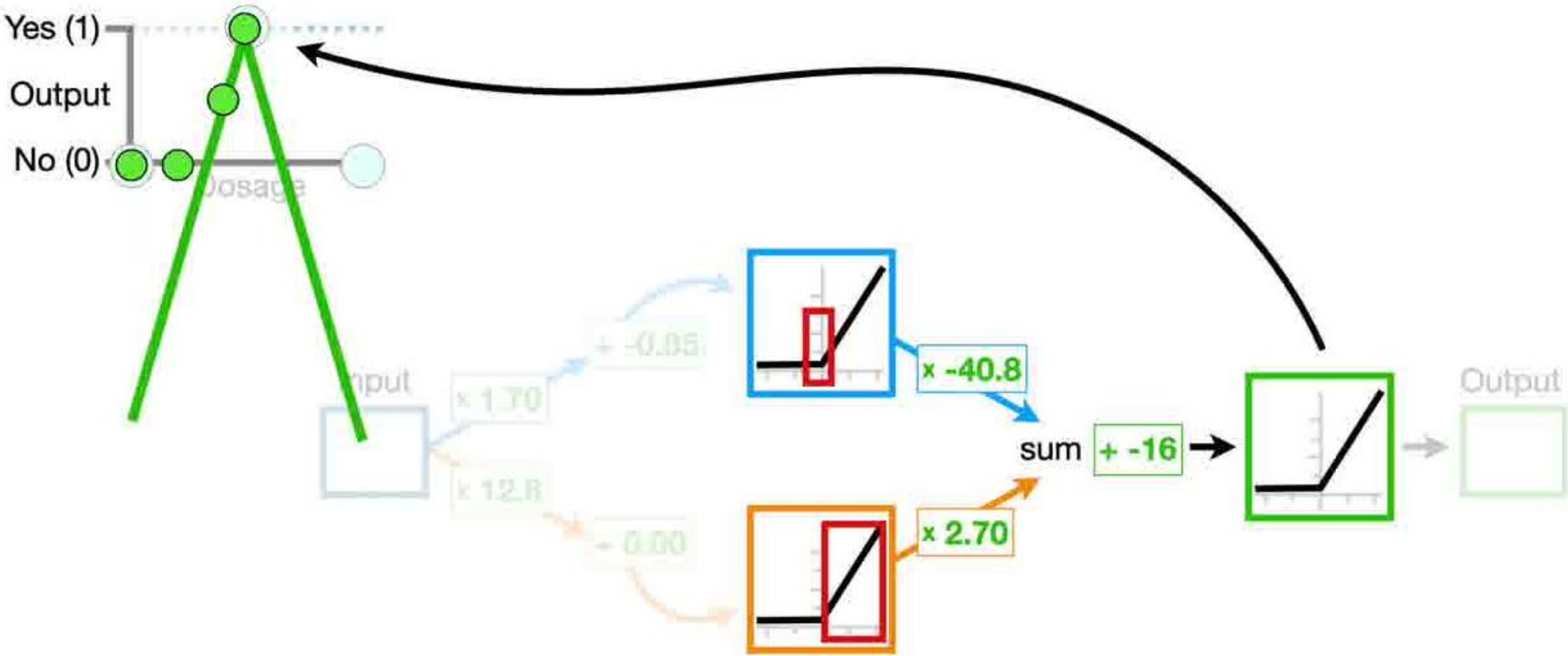

Yes (1)
Output
No (0)
Dosage
Input
x 1.70
+ -0.85
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output

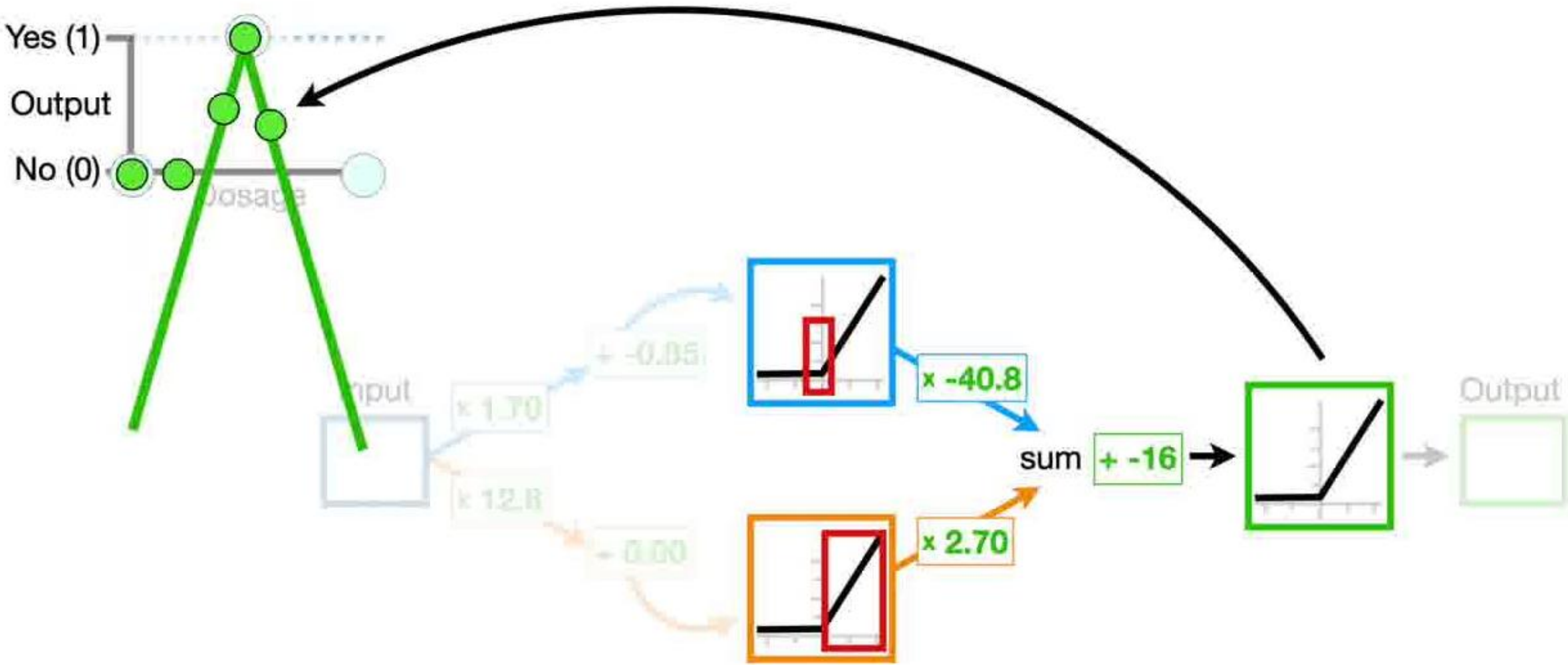

Yes (1)
Output
No (0)
Dosage
+ -0.05
x 1.70
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output

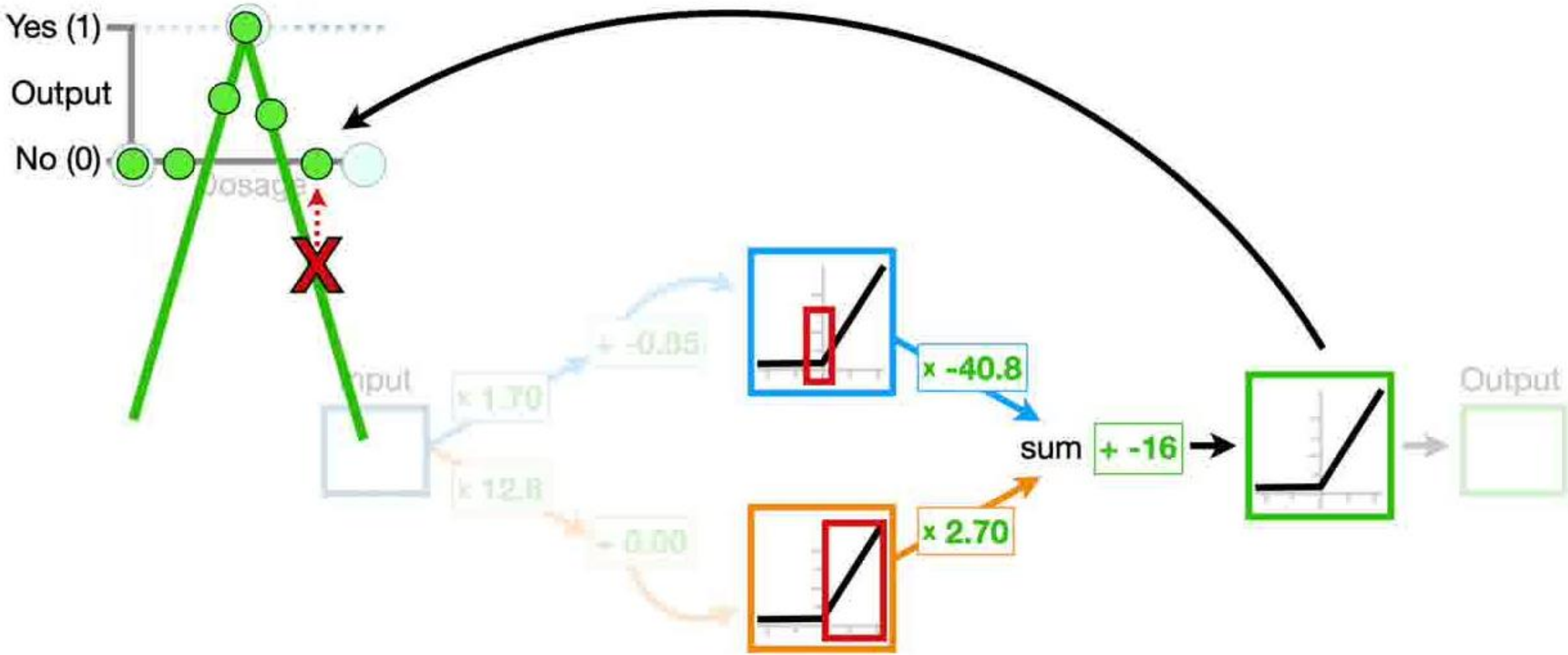

Yes (1)
Output
No (0)
Dosage
X
nput
x 1.70
+ -0.85
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output

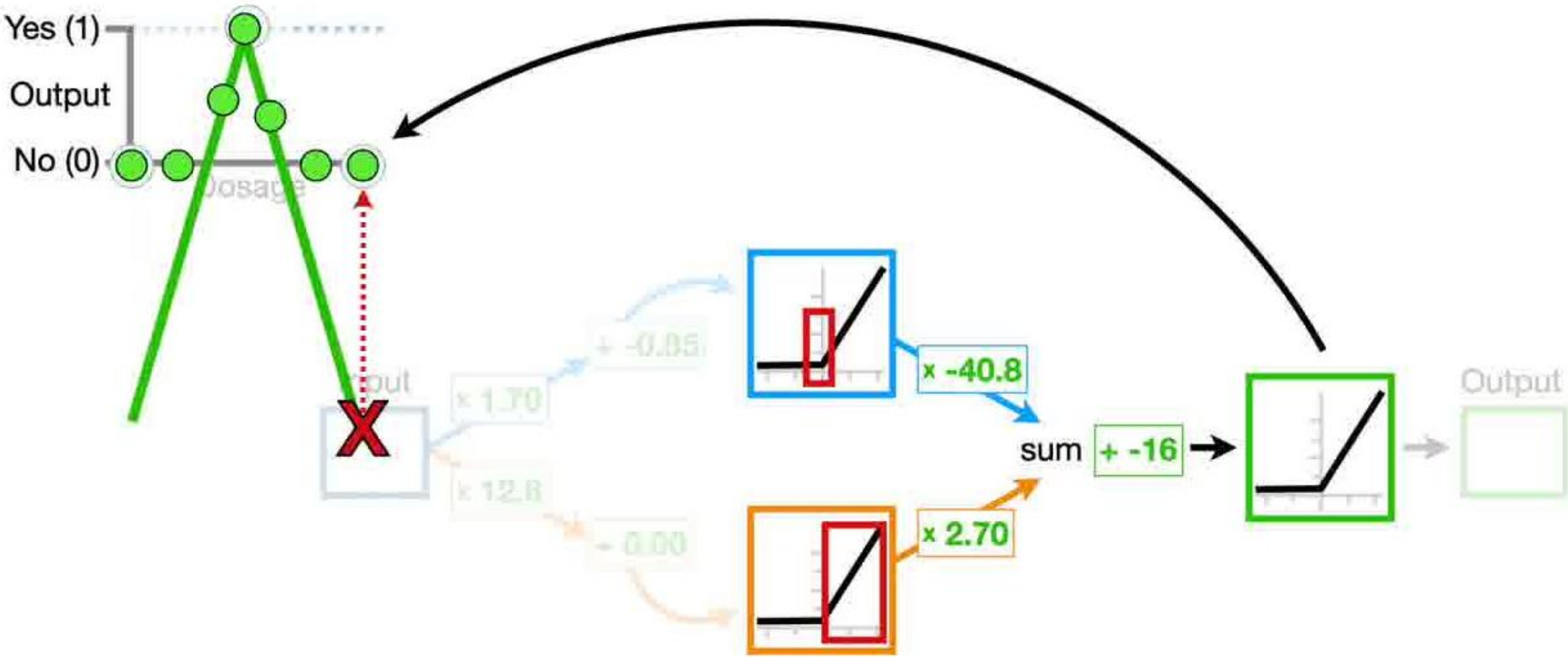

Yes (1)
Output
No (0)
Dosage
× -40.8
sum
+ -16
Output
× 2.70

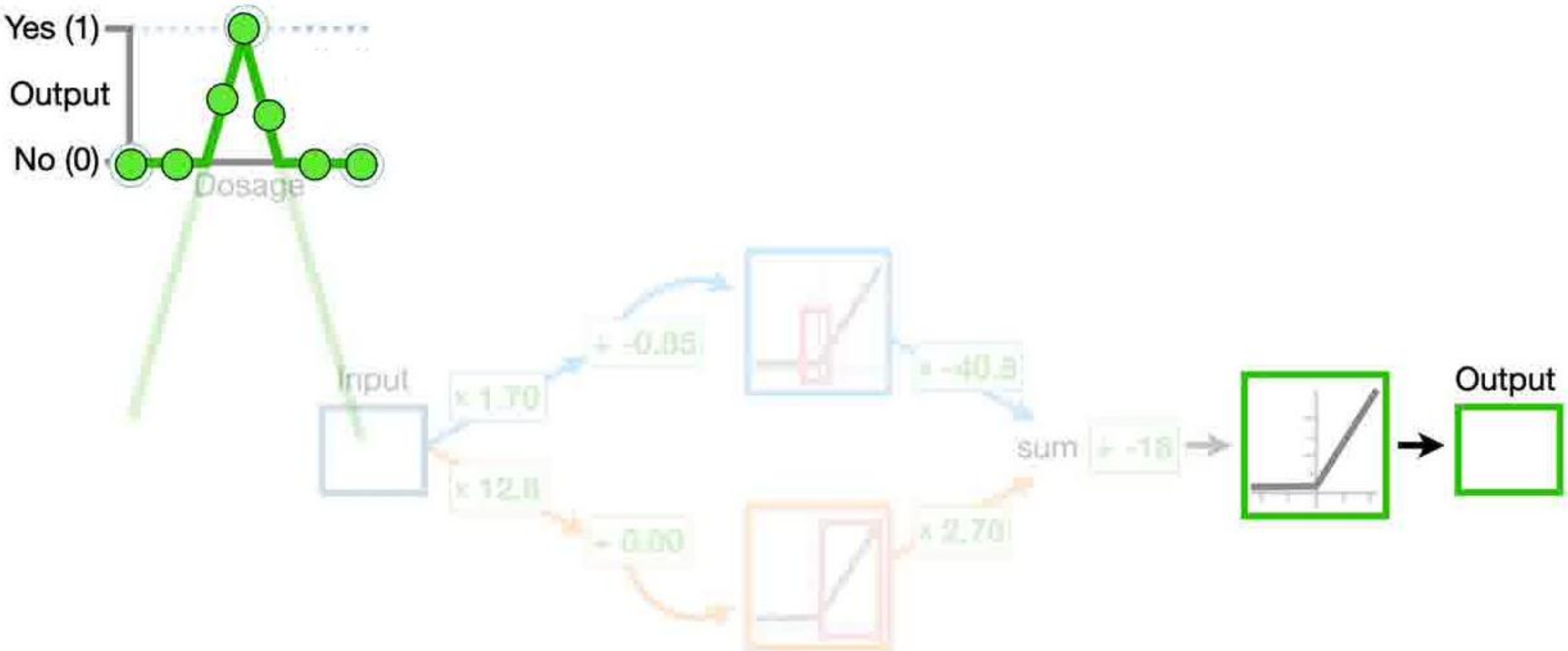

Yes (1)
Output
No (0)
× -40.8
sum
+ -16
Output
× 2.70

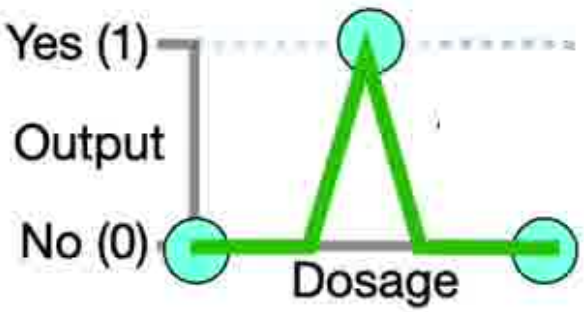

Yes (1)
Output
No (0)
x -40.8
sum
+ -16
Output
x 2.70

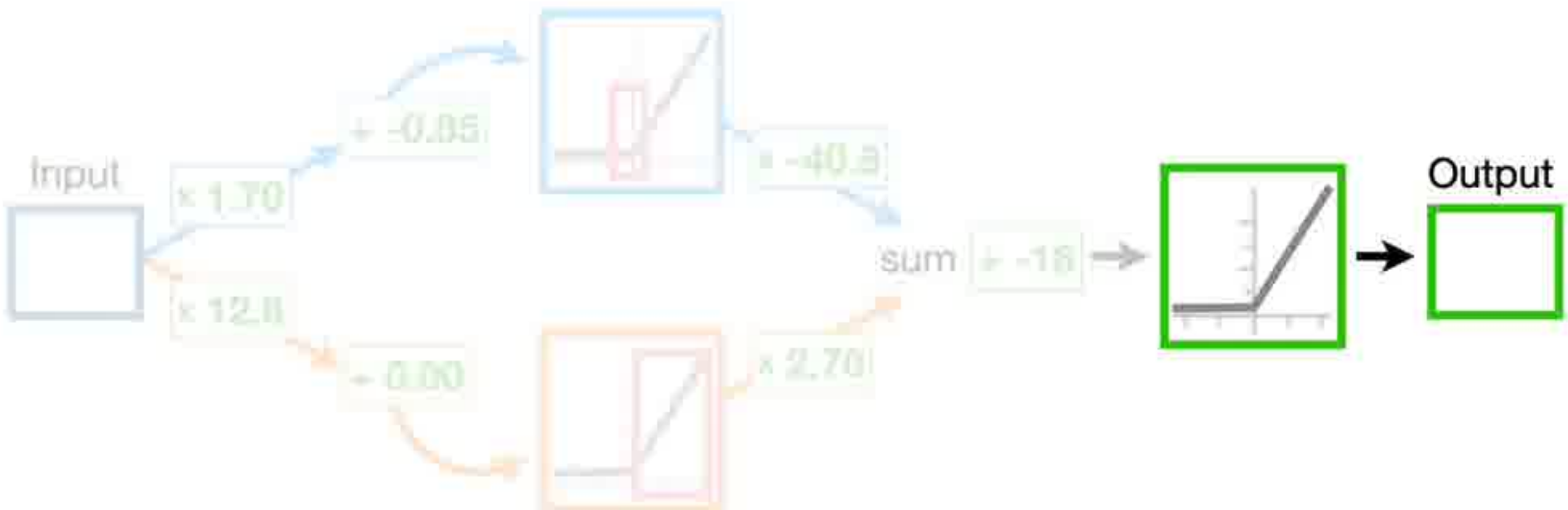

Yes (1)
Output
No (0)
Dosage
nput
+ -0.05
x 1.70
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output


Yes (1)
Output
No (0)
Dosage
X
+ -0.05
x 1.70
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output


Yes (1)
Output
No (0)
Dosage
Input
+ -0.85
x 1.70
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output


Yes (1)
Output
No (0)
Dosage
Input
x 1.70
+ -0.05
x 12.8
+ 0.00
x -40.8
x 2.70
sum
+ -16
Output


Yes (1)
Output
No (0)
Dosage

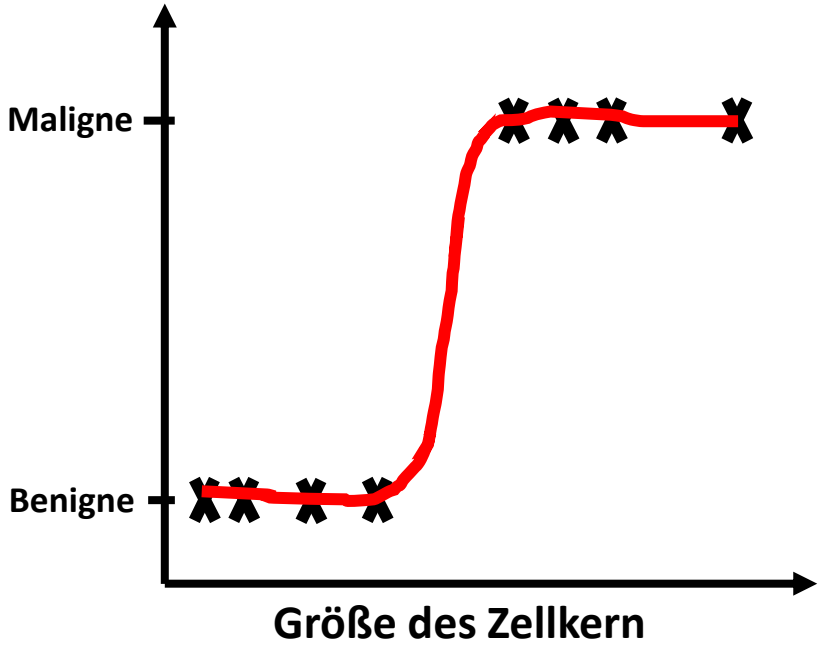

Input
× 1.70
+ -0.85
× 12.8
+ 0.00
× -40.8
× 2.70
sum
+ -16
Output

Schritt 1: Man füttere eine KI mit einem gewaltigen Trainingsdatensatz.

Schritt 2: KI versucht die Daten notfalls sogar in einem mehrdimensionalen Koordinatensystem darzustellen.

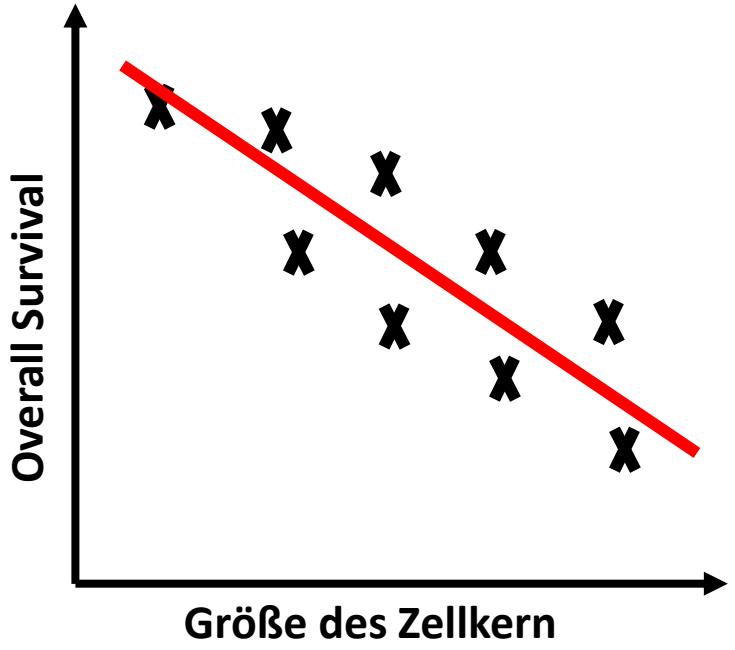
Schritt 3: KI versucht eine Funktion in die Datenpunkte zu erzwingen

bei Logistic Regression…



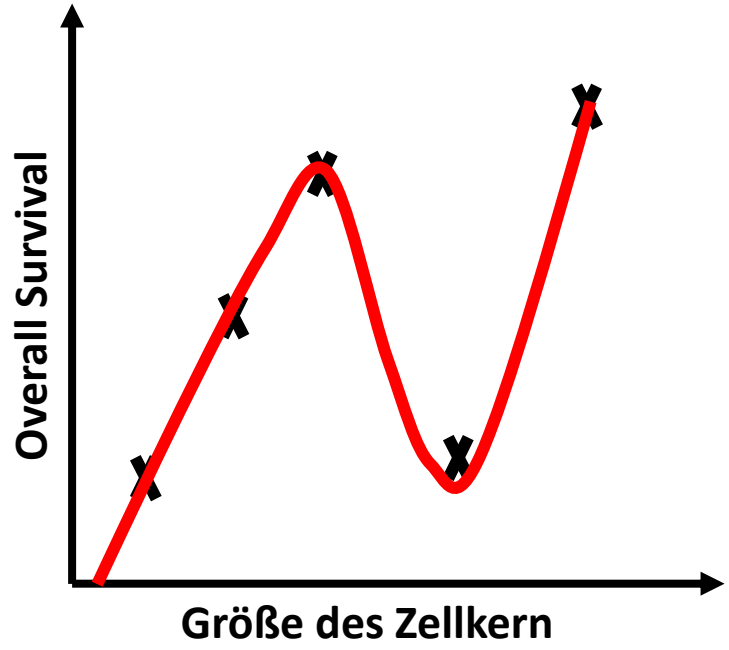
… eine sigmoide Funktion

bei Linear Regression…



… eine lineare Funktion

bei neuronalen Netzen …

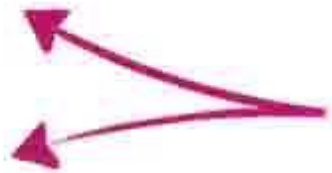


… eine komplexere Funktion

Schritt 4: Abgleich der modellierten Funktion mit einem Trainingsdatensatz -> Berechnung der Accuracy…

Und wie kann man ein Neuronales Netz programmieren?

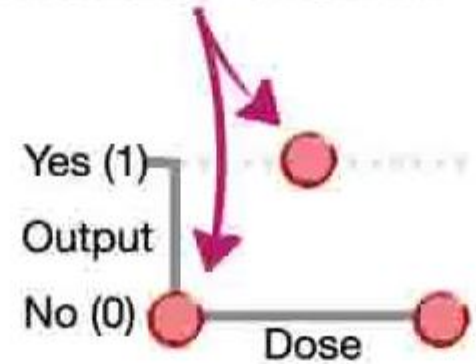
```
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.optim import SGD

import matplotlib.pyplot as plt
import seaborn as sns
```



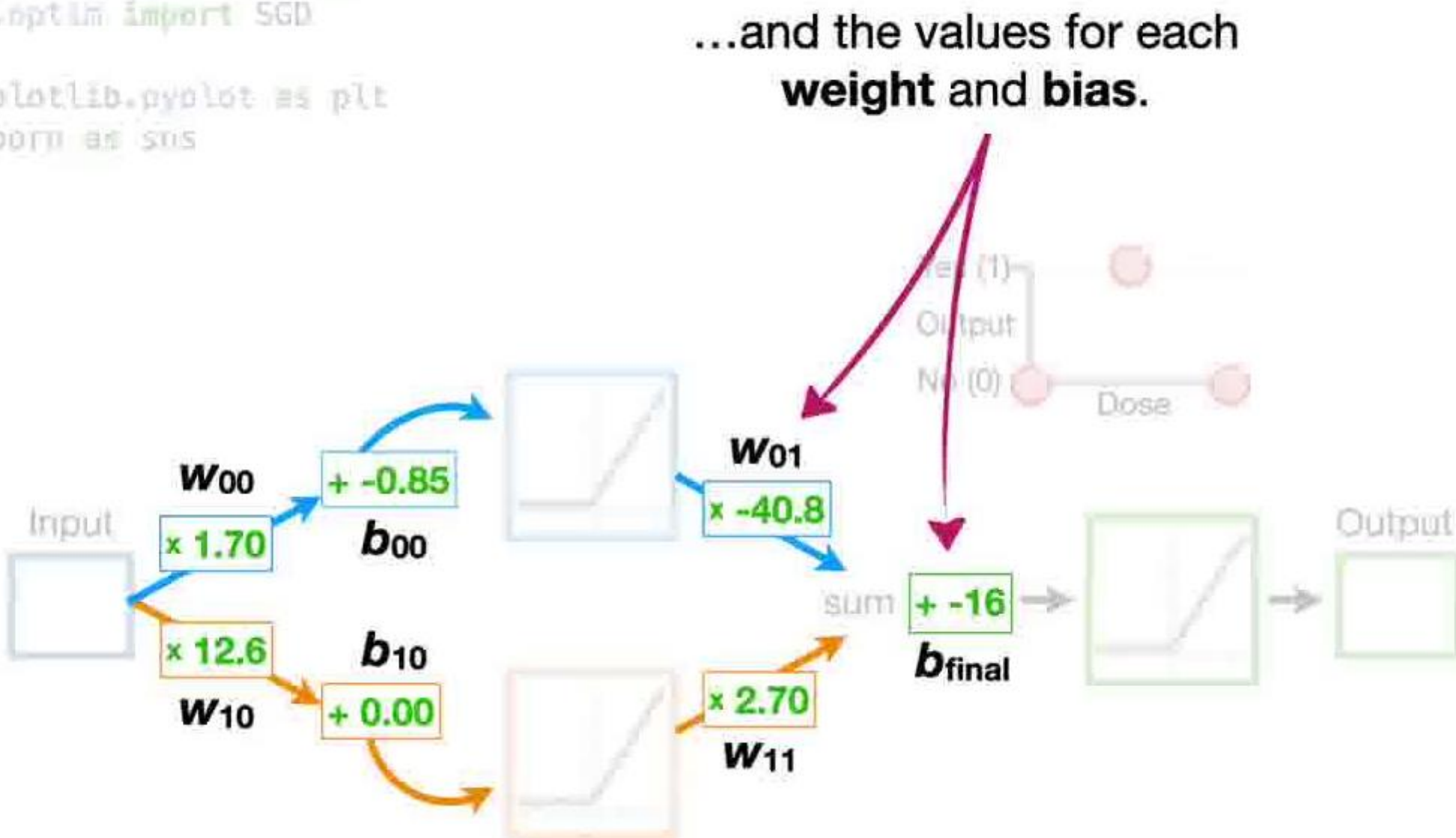
The first thing we do is import the **Python** modules that we will use.

```
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.optim import SGD

import matplotlib.pyplot as plt
import seaborn as sns
```

We will use **torch** to create **tensors** to store all of the numerical values, including the raw data…

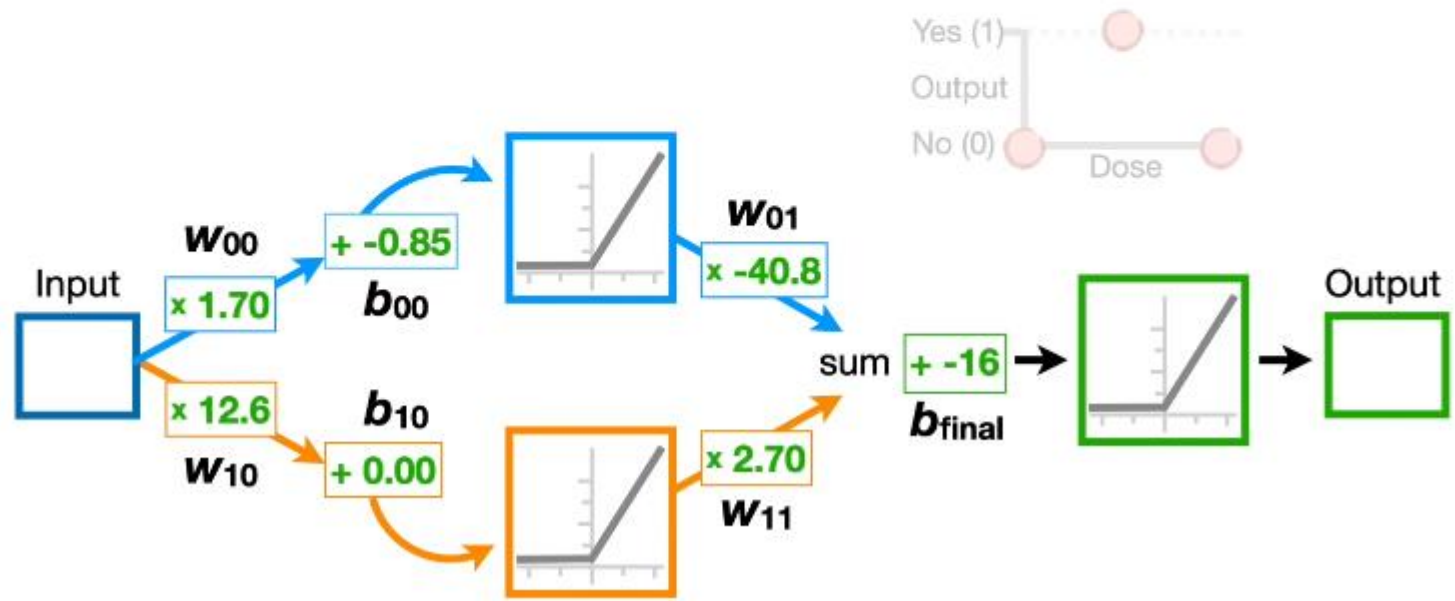


```
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.optim import SGD

import matplotlib.pyplot as plt
import seaborn as sns
```



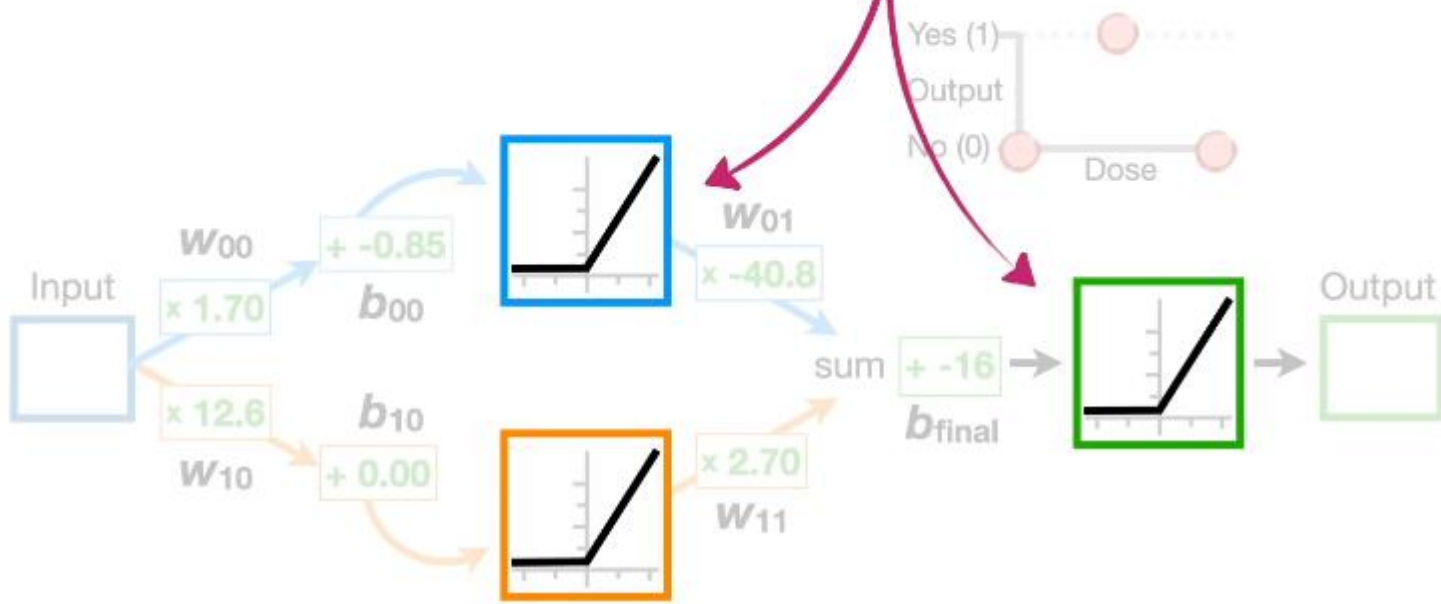
```
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.optim import SGD

import matplotlib.pyplot as plt
import seaborn as sns
```

Then we import **torch.nn**, which we will use to make the **weight** and **bias tensors** part of the neural network.



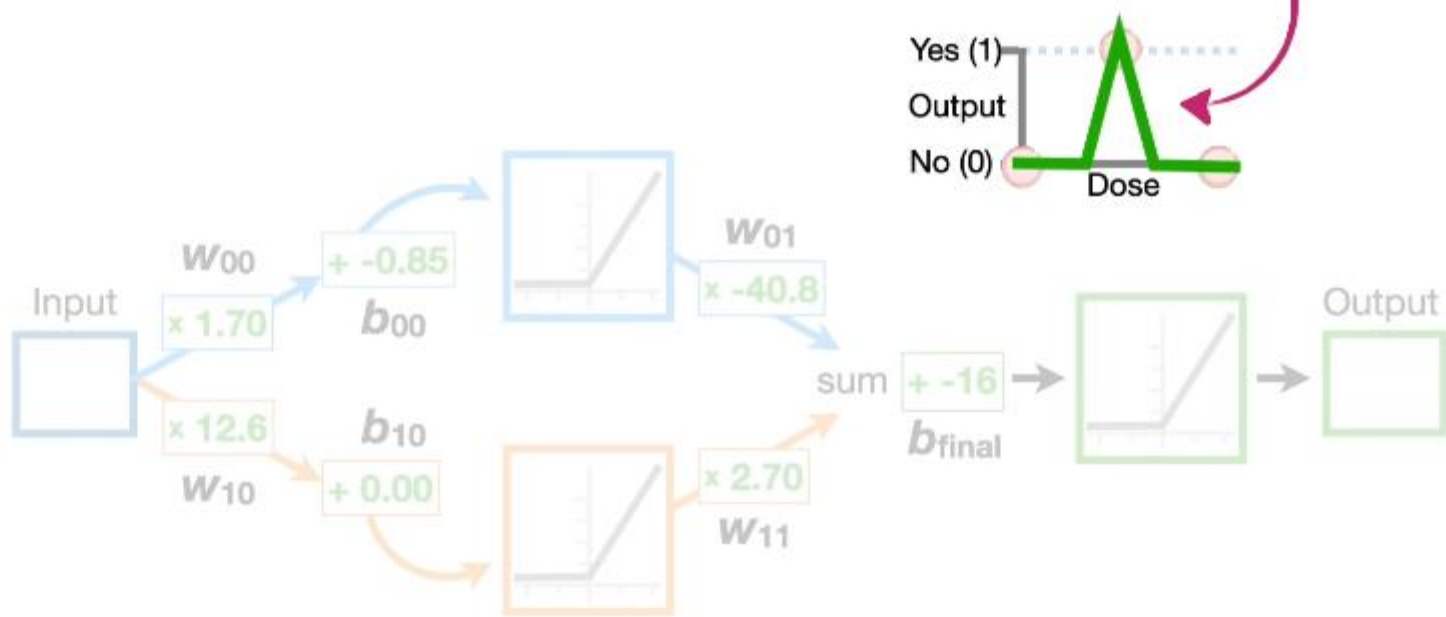
```python
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.optim import SGD

import matplotlib.pyplot as plt
import seaborn as sns
```

Then we import **torch.nn.functional**, which gives us the **activation functions.**



```
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.optim import SGD

import matplotlib.pyplot as plt
import seaborn as sns
```

Then we import **SGD**, which is short for **Stochastic Gradient Descent**, to fit the neural network to the data.



```
class BasicNN(nn.Module):
```

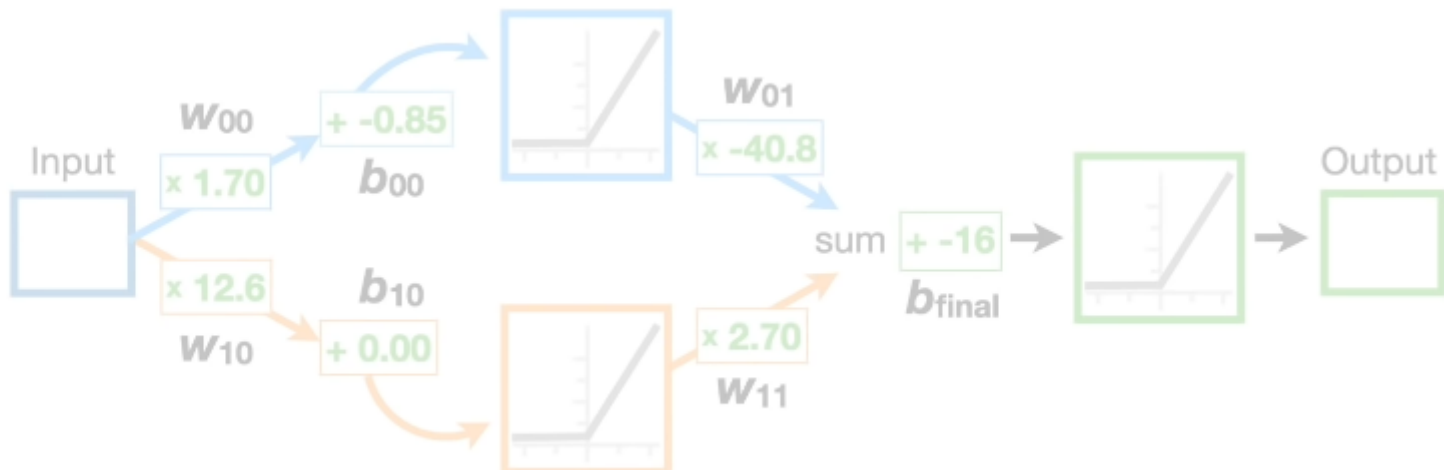
With **PyTorch**, creating a new neural network means creating a new **class**.

```
class BasicNN(nn.Module):
```

So we start by creating a new **class**…

…that, in this example, we call **BasicNN**…

…and **BasicNN** will inherit from a **PyTorch** class called **Module**.



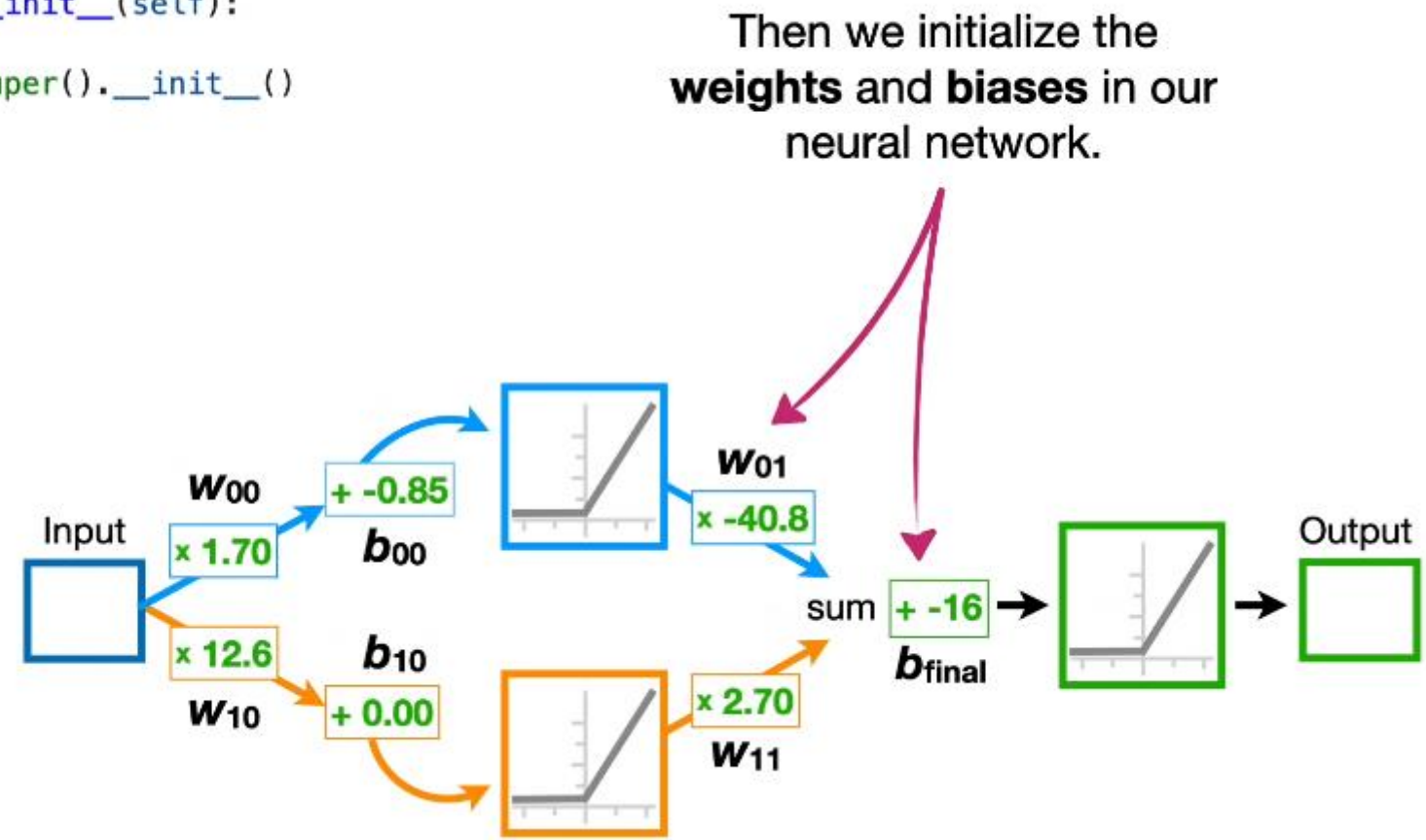
```
class BasicNN(nn.Module):

    def __init__(self):
```

Now we create an initialization method for the new class…

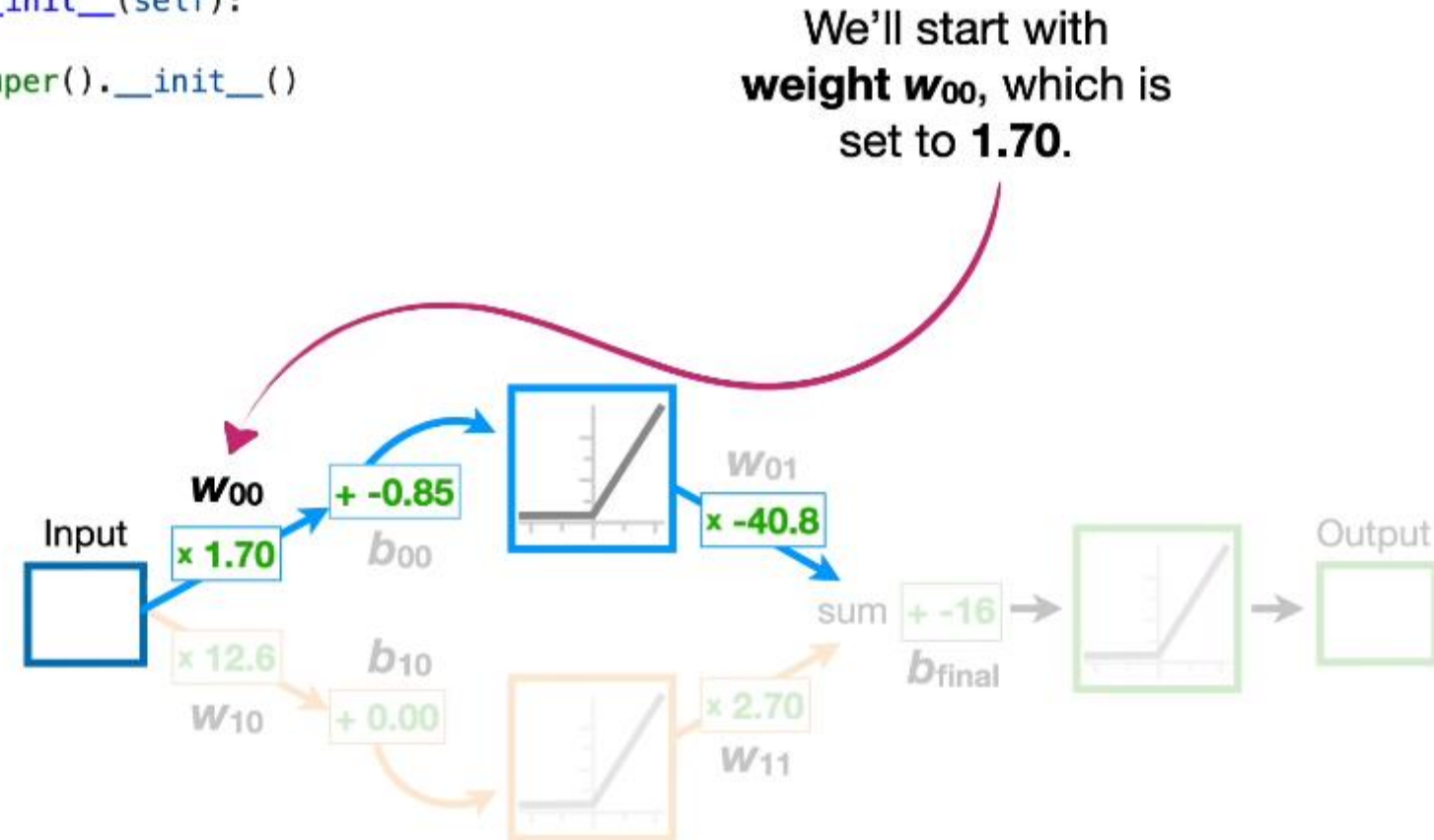
```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()
```

…and the first thing we do is call the initialization method for the parent class, **nn.Module**.

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()
```

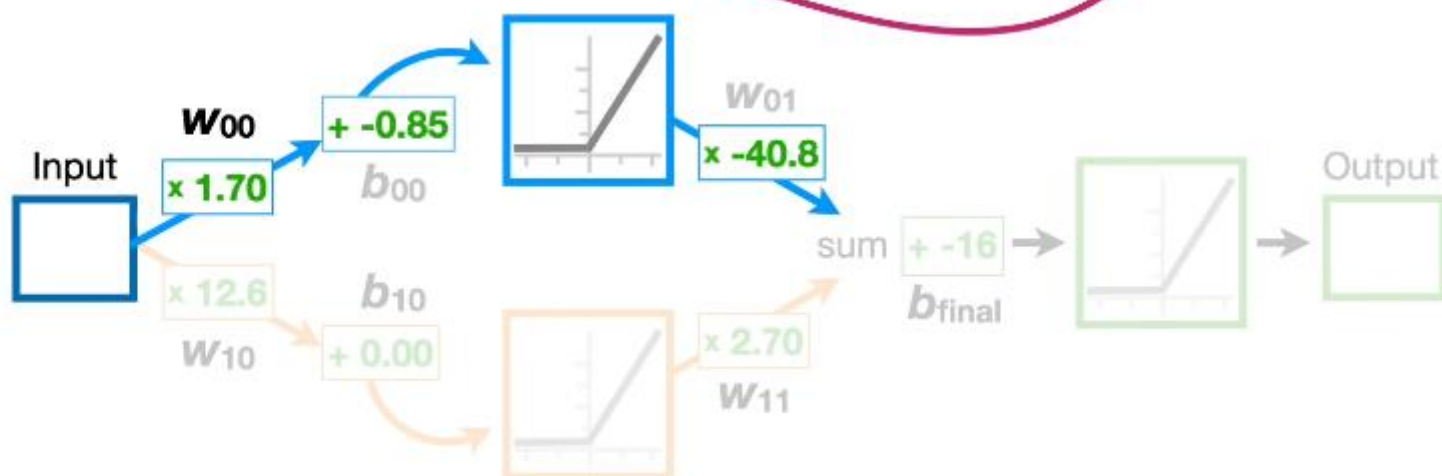


```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()
```



```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
```

So we create a new variable called **w00**...



```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
```

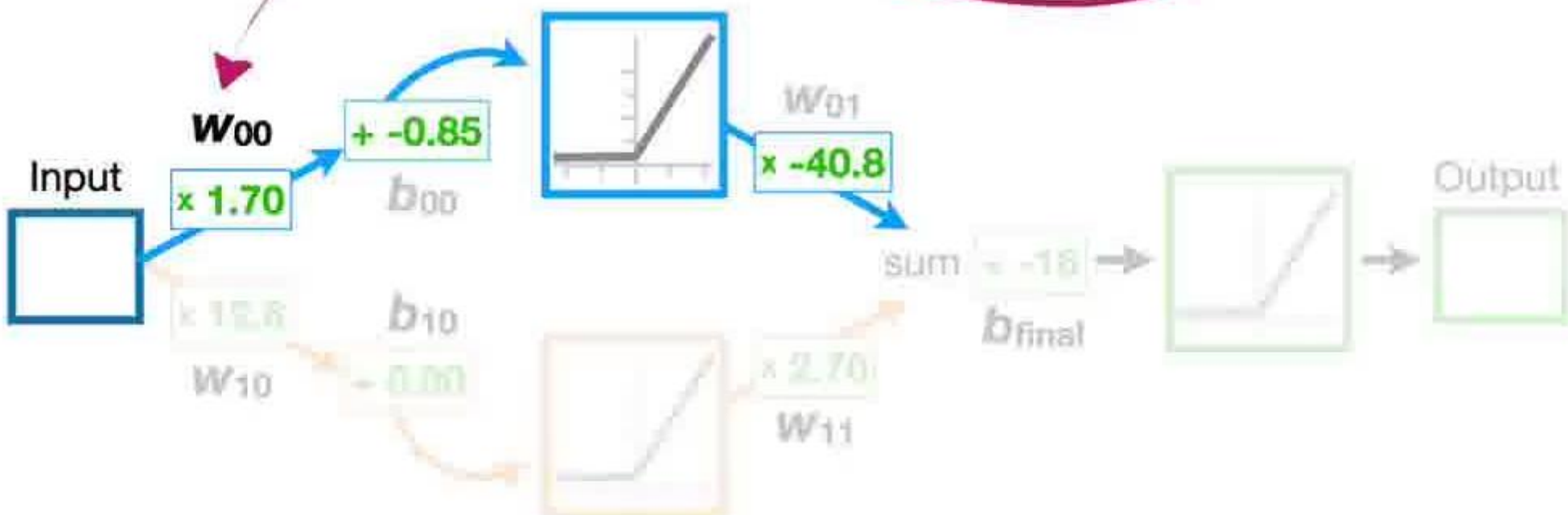
...and make it a neural network **Parameter**.

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
```

Making this **weight** a parameter for the neural network gives us the option to optimize it.

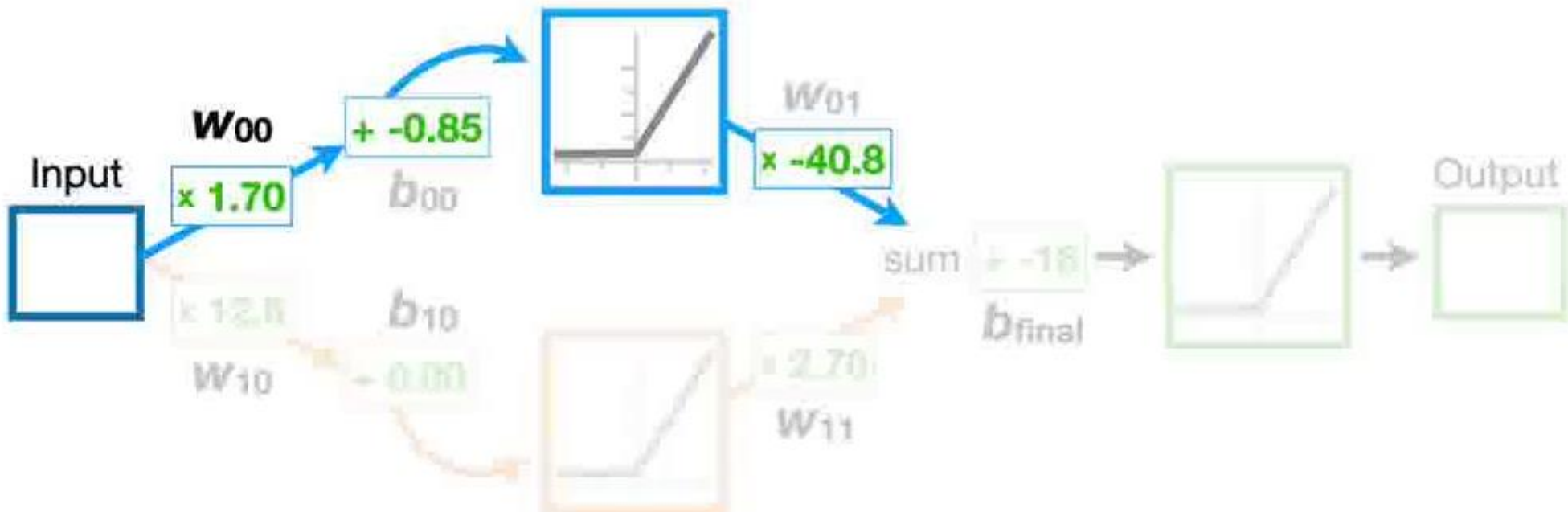
```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
```

Now, since **weight** w_{00} is **1.70**...



```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
```

...we initialize the new parameter with a **tensor** set to **1.7**.

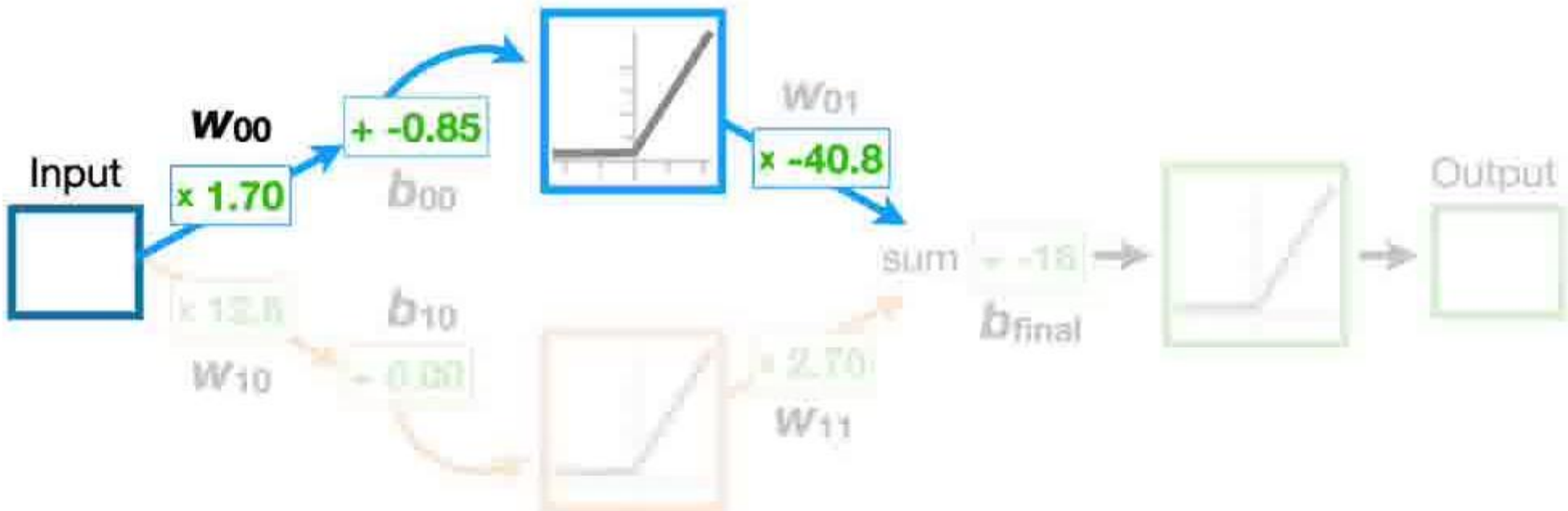


```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
```

NOTE: Since this is a **tensor**, the neural network can take advantage of the accelerated arithmetic and automatic differentiation that it provides.

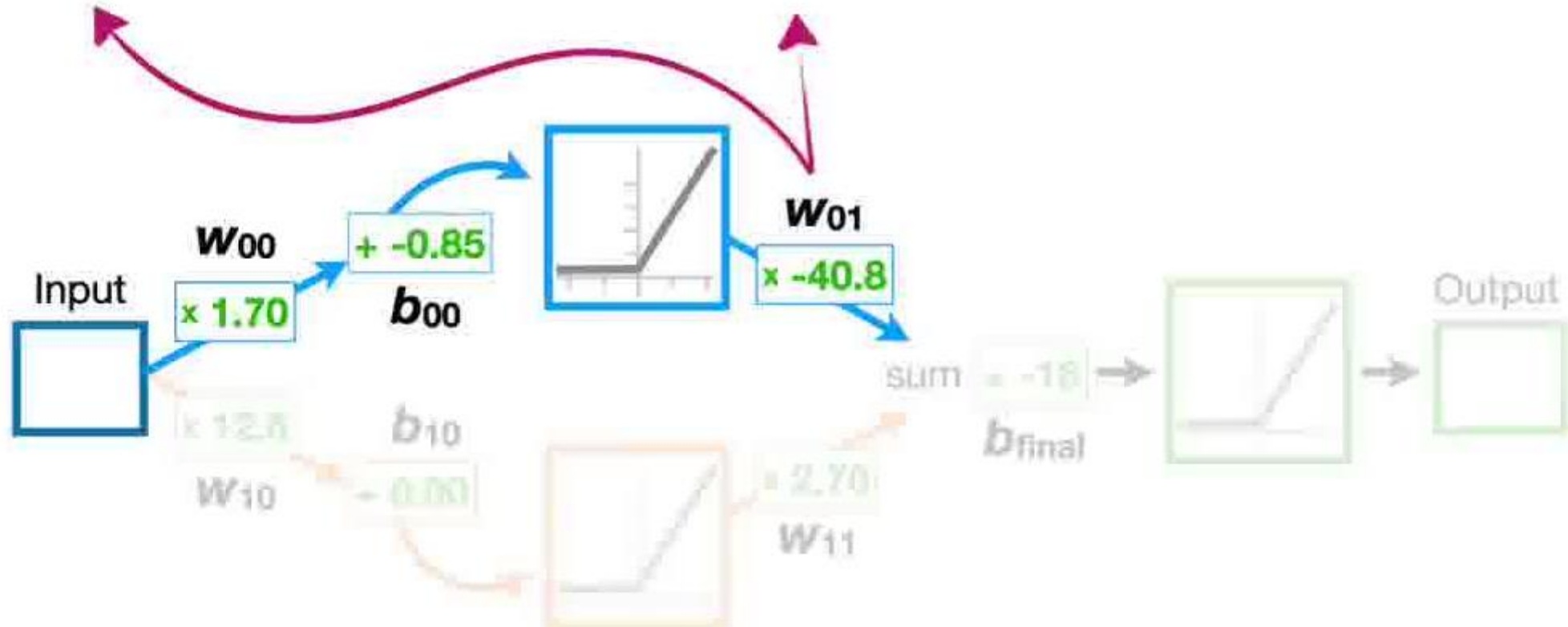
```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
```

Lastly, because we don't need to optimize this **weight**, we'll set **requires_grad**, which is short for **requires gradient**, to **False**.



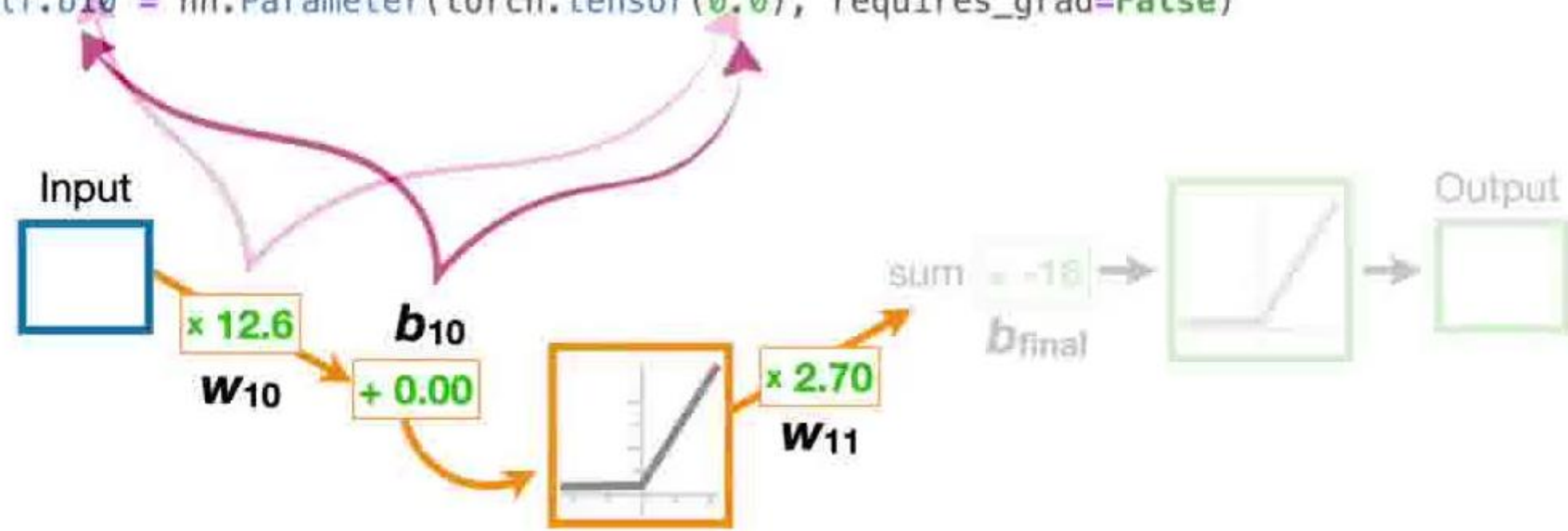
```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)
```

Likewise, we create new variables for the **bias b_{00}** and the **weight w_{01}**.



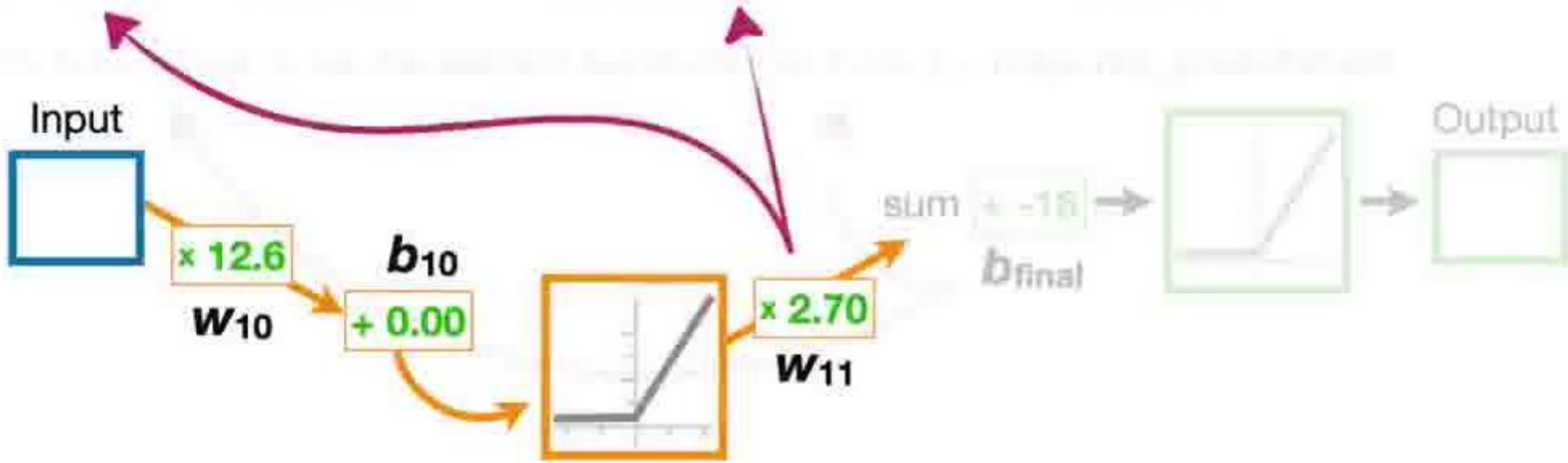
```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
```

And then we create variables for the remaining **weights** and **biases**.



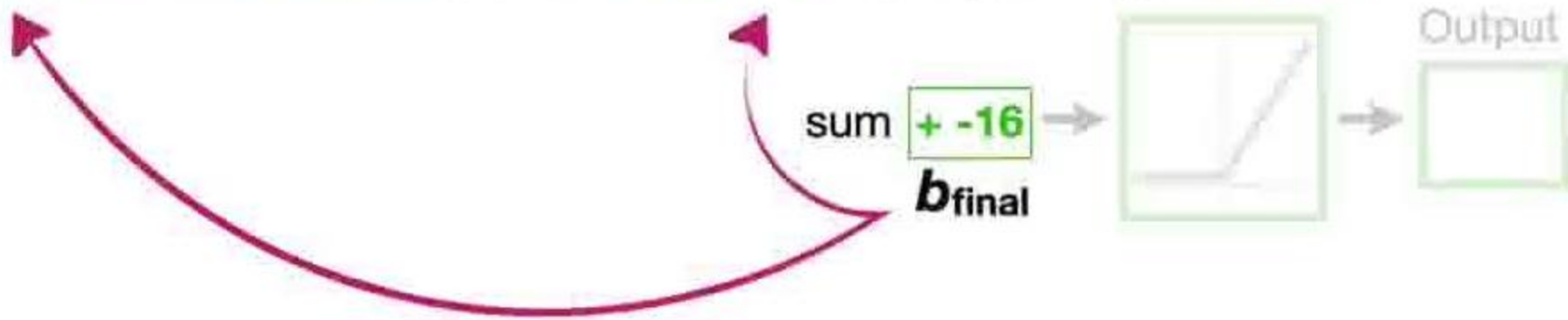
```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)
```

And then we create variables for the remaining **weights** and **biases**.



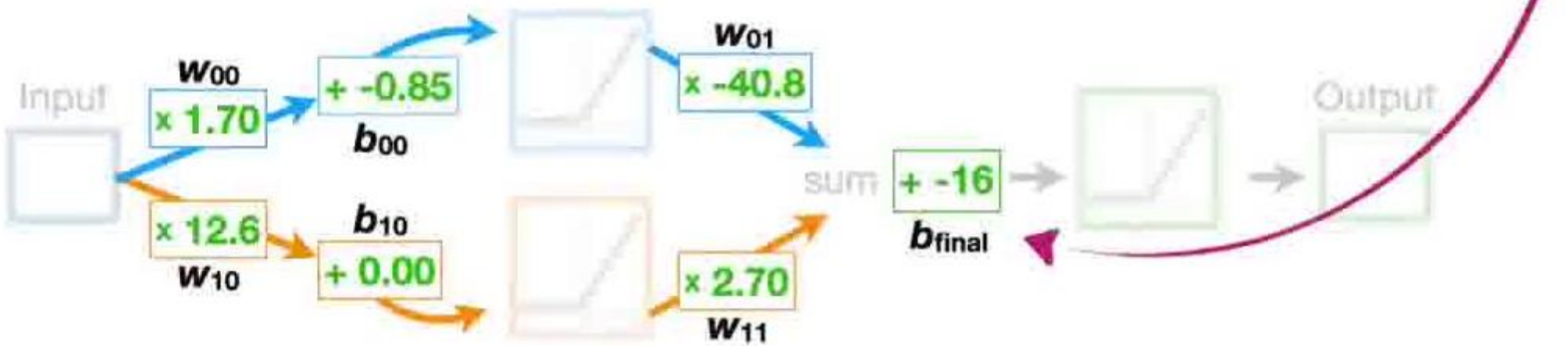
```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)
```

And then we create variables for the remaining **weights** and **biases**.



```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)
```

Bam! We have created neural network parameters for each **weight** and **bias**.



```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)
```

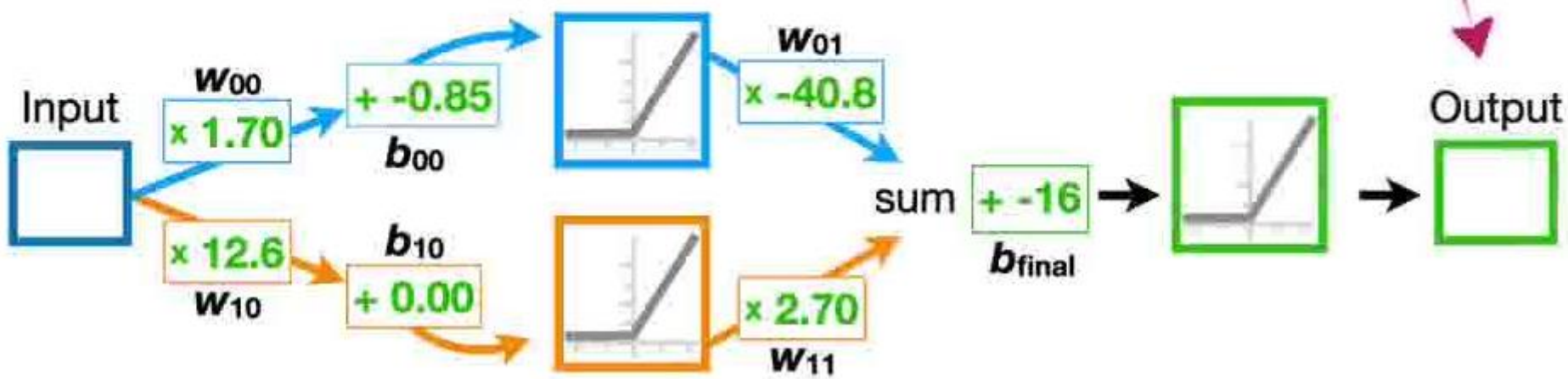
Now we need to connect them to the input…

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)
```

…the **activation functions**…

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)
```

…and, ultimately, to the output.



```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)
```

In other words, we need a way to make a **forward pass** through the neural network that uses the **weights** and **biases** that we just initialized.

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)

    def forward(self, input):
```

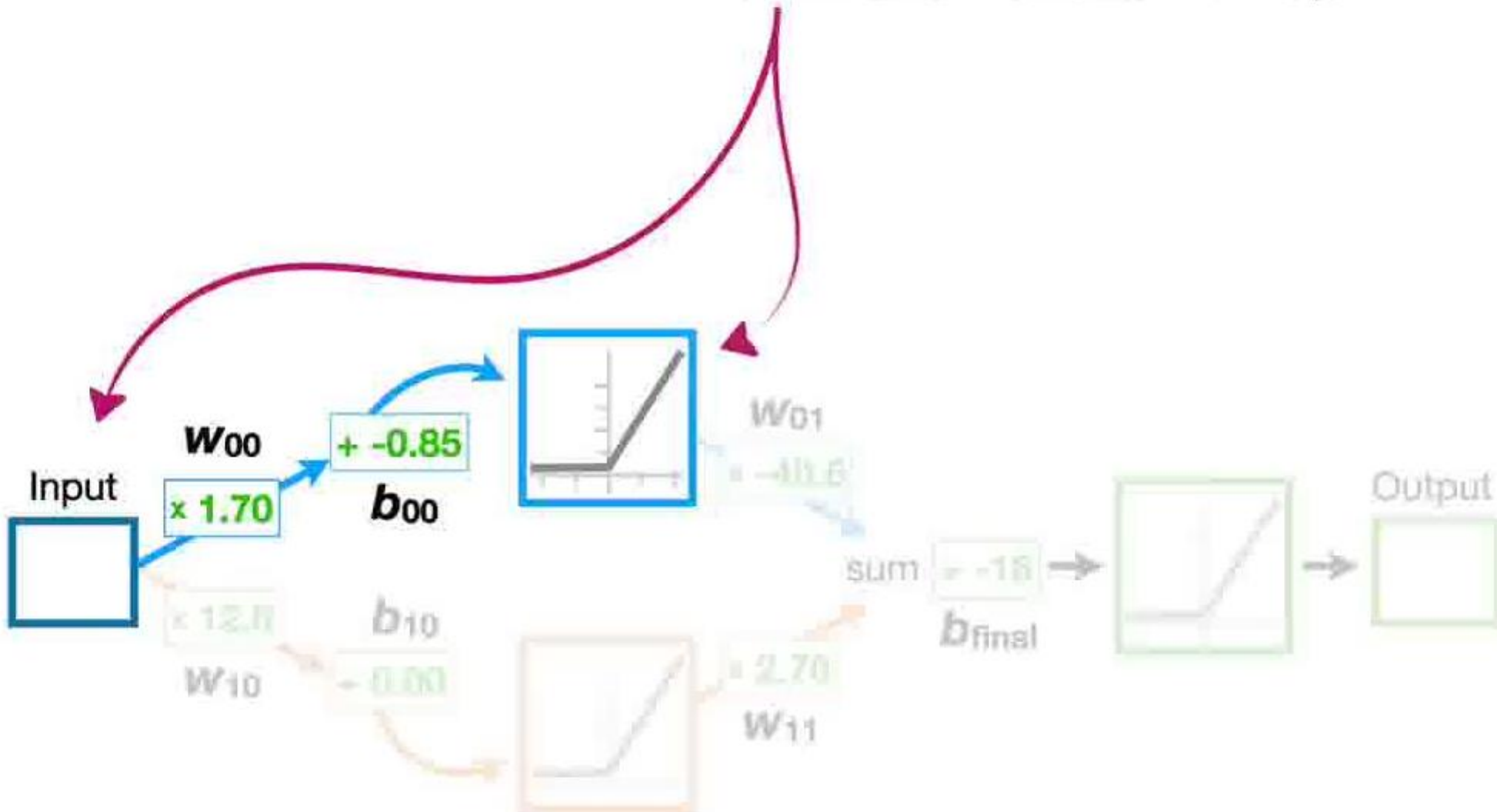
So we do that by creating a second method inside **BasicNN** called **forward()**.

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)

    def forward(self, input):
```

So we can see what's going on, let's move the code for **forward()** to the top of the screen.

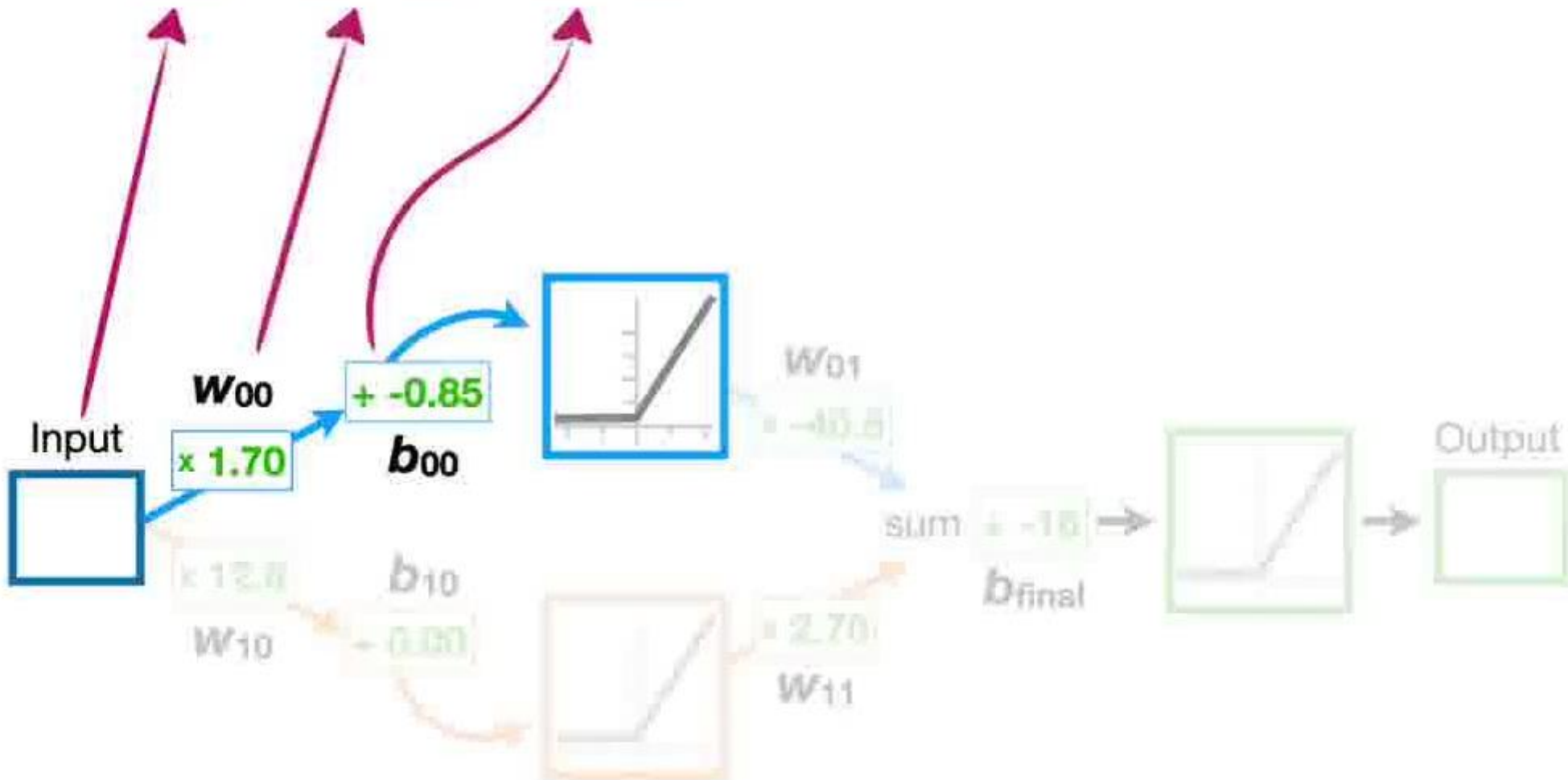
```
def forward(self, input):
```

Now, the first thing we want to do is connect the input to the **activation function** on top.



So we create a new variable, **input_to_top_relu**, that is equal to...

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
```



Then we pass **input_to_top_relu** to the **ReLU** activation function with **F.relu()**.

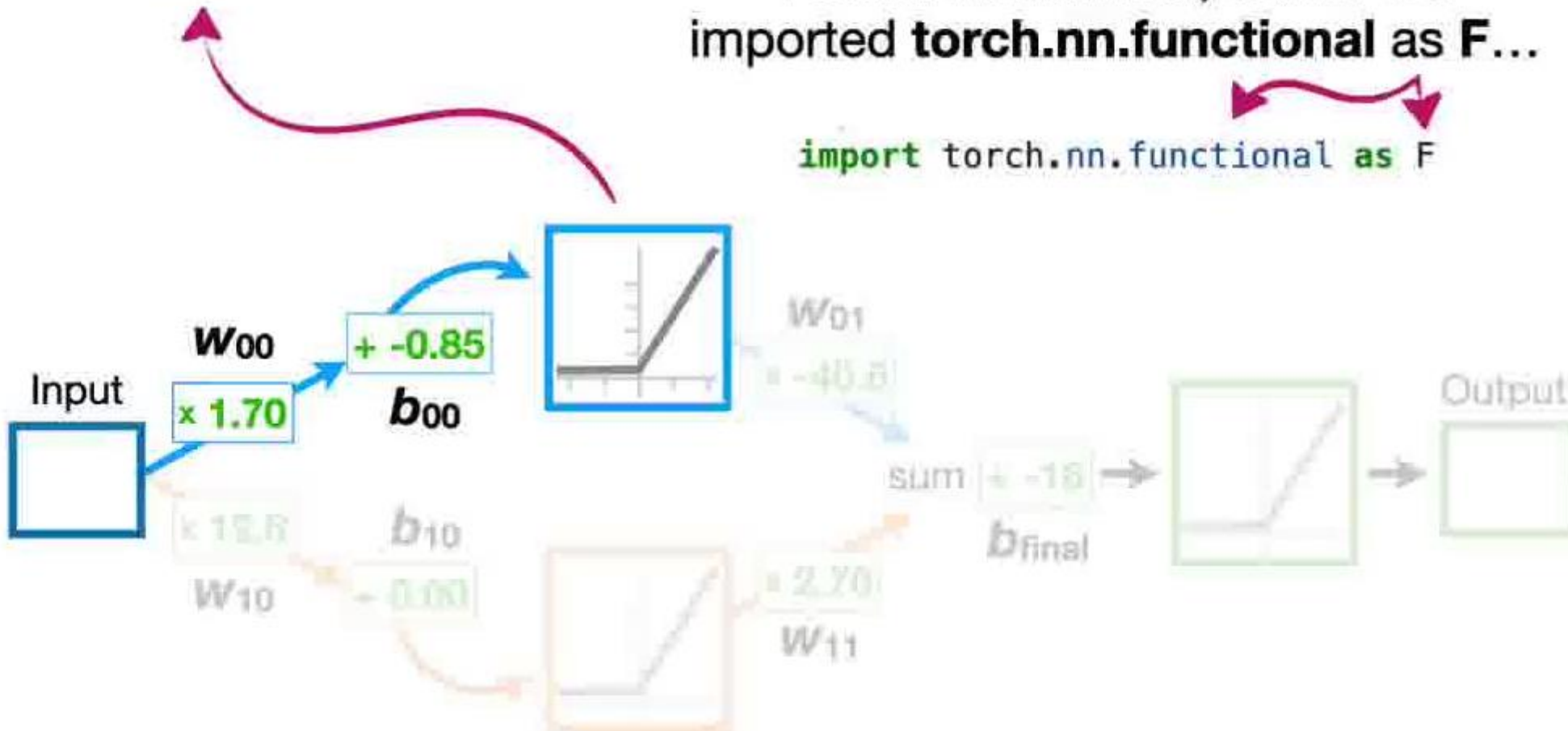
```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
```

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
```

Then we pass **input_to_top_relu** to the **ReLU** activation function with **F.relu()**.

Psst… Remember, earlier we imported **torch.nn.functional** as **F**…

```
import torch.nn.functional as F
```

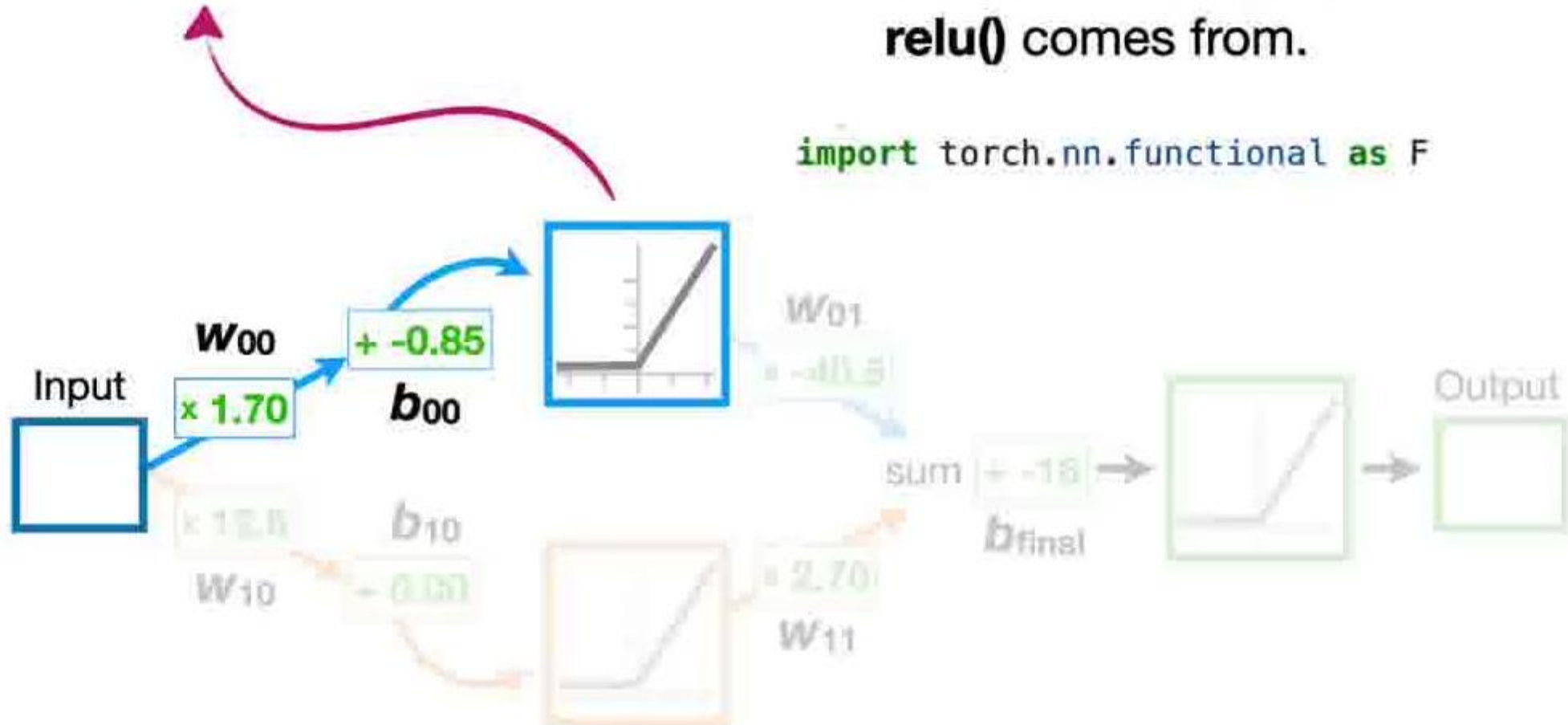


```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
```

Then we pass **input_to_top_relu** to the **ReLU** activation function with **F.relu()**.

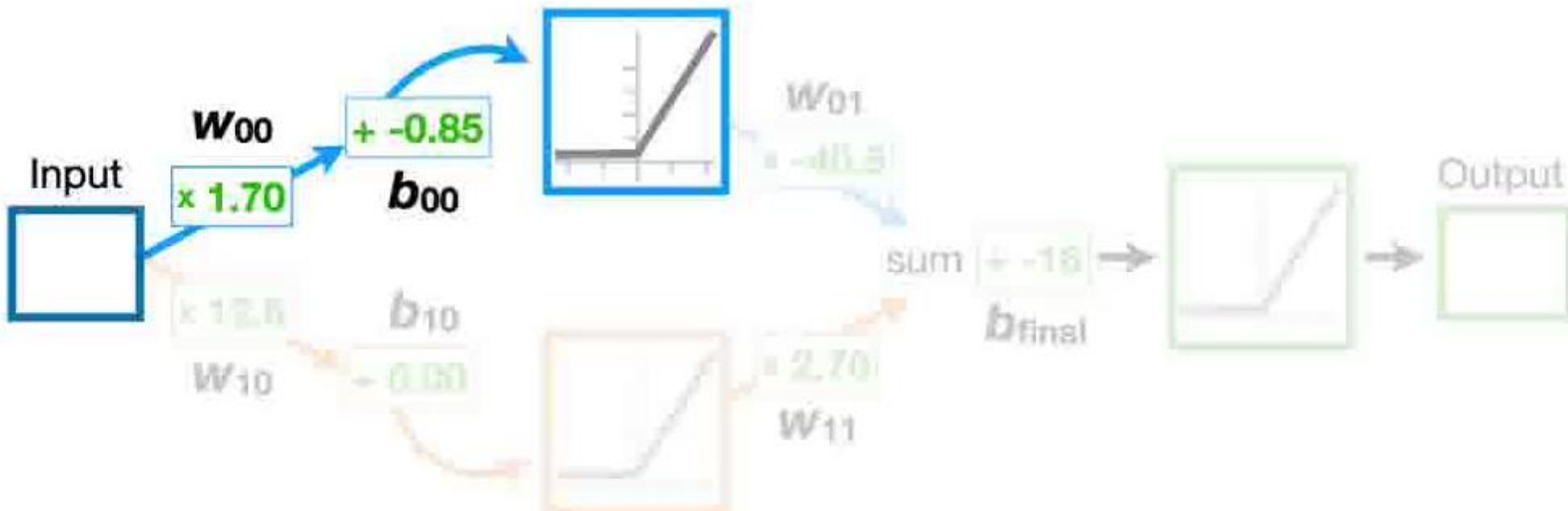
...so that is where the **relu()** comes from.

```
import torch.nn.functional as F
```



Then we save the output of the **ReLU** in **top_relu_output**.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
```

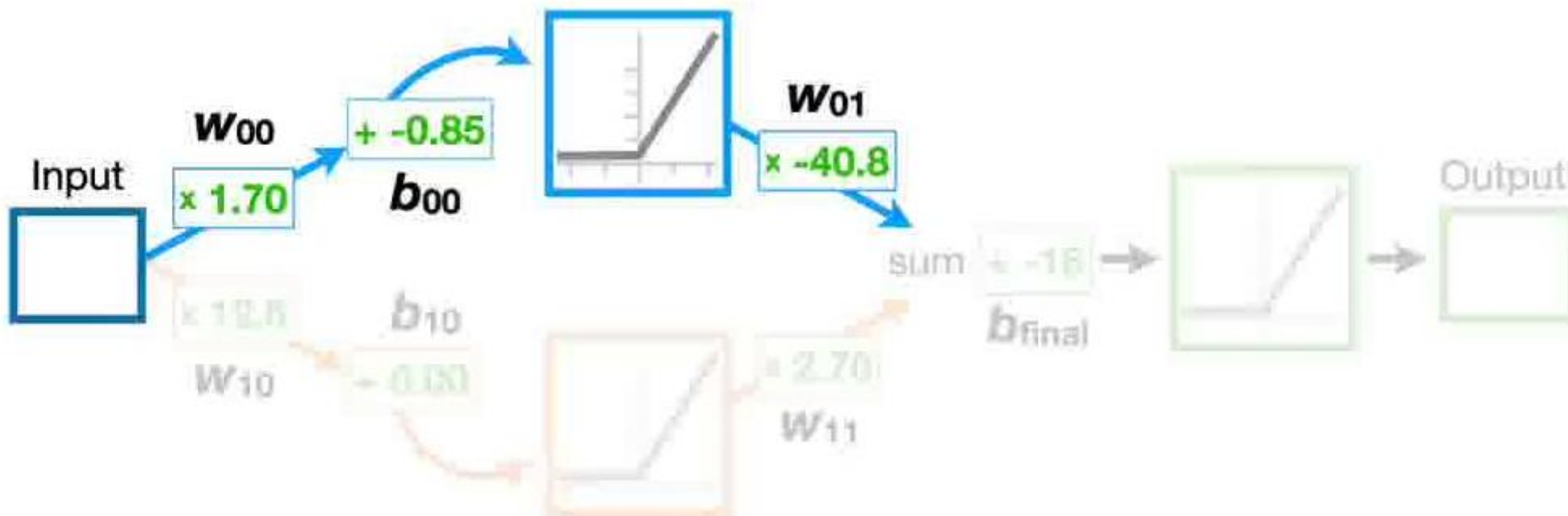


```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01
```

Now we scale **top_relu_output** by the **weight w_{01}**...

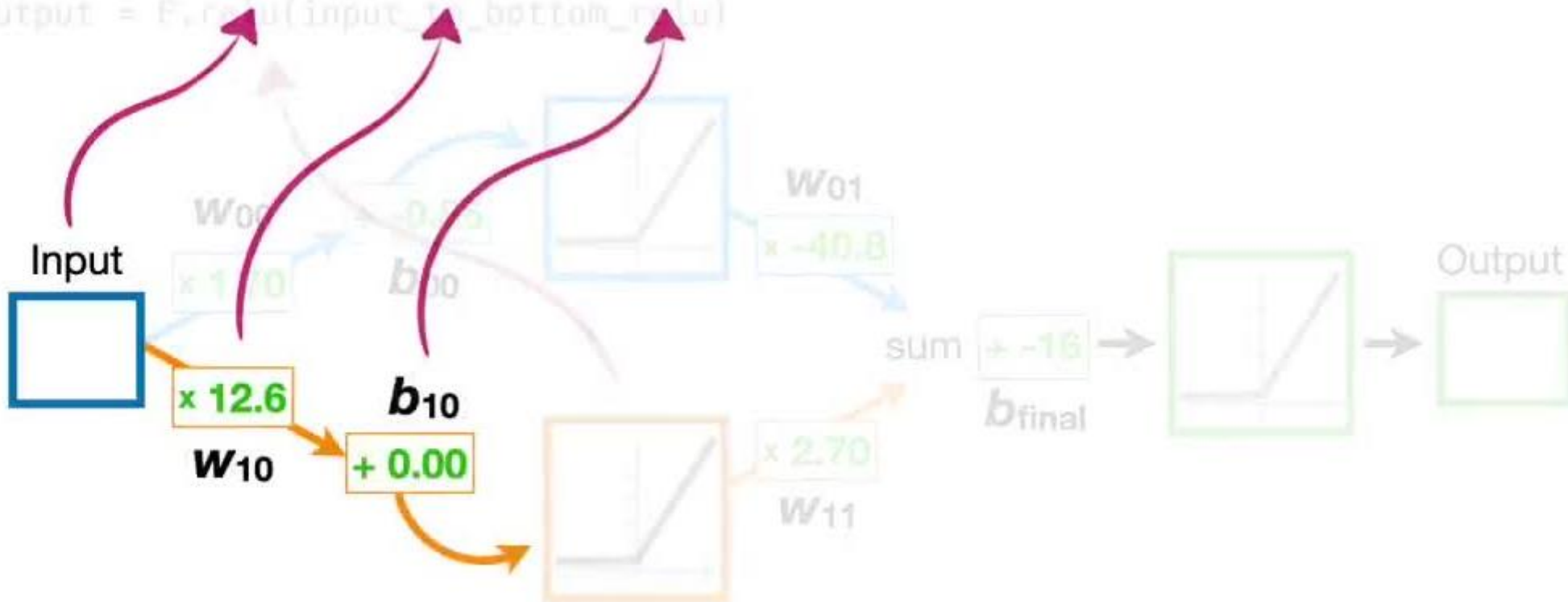
…and save the result in **scaled_top_relu_output.**

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01
```



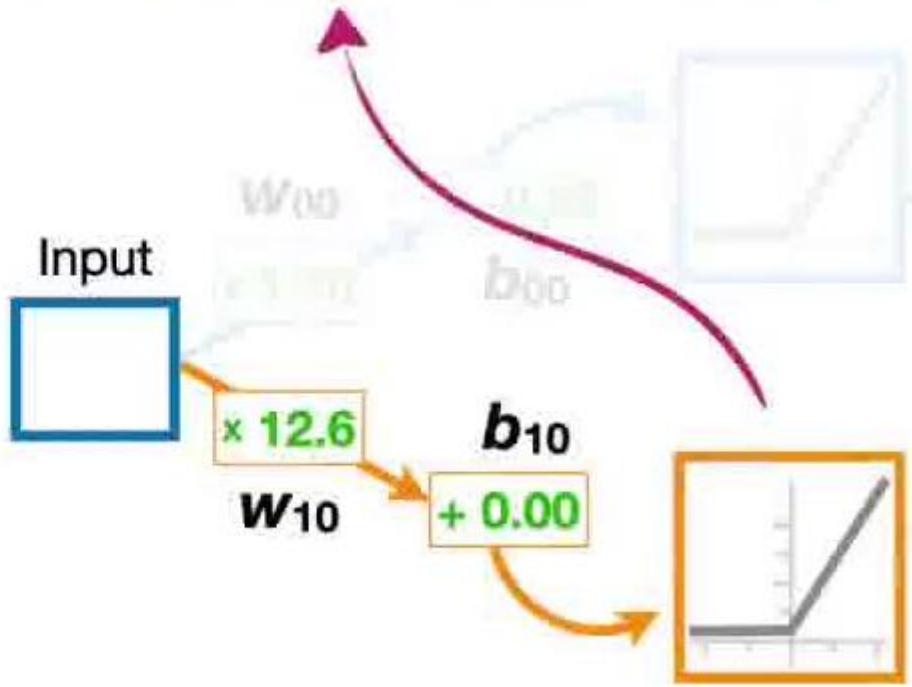
Likewise, we connect the input to the bottom **ReLU** and scale the activation function's output.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
```



Likewise, we connect the input to the bottom **ReLU** and scale the activation function's output.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
```

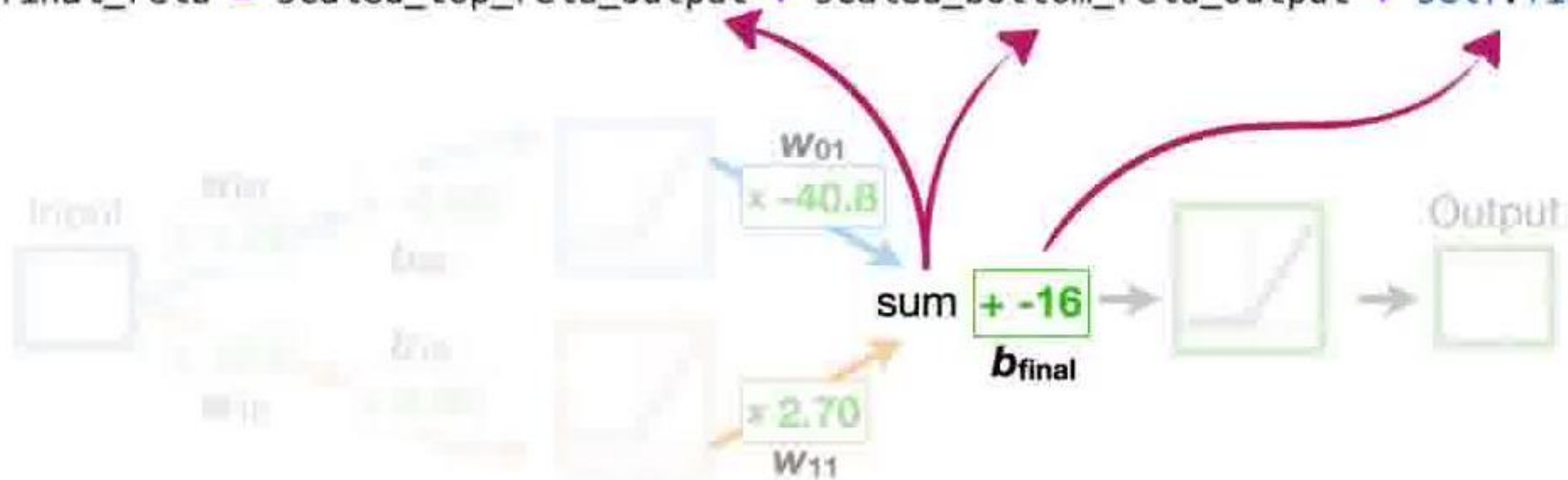


Likewise, we connect the input to the bottom **ReLU** and scale the activation function's output.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
    scaled_bottom_relu_output = bottom_relu_output * self.w11
```

Then we add the top and bottom scaled values to the final **bias**…

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
    scaled_bottom_relu_output = bottom_relu_output * self.w11

    input_to_final_relu = scaled_top_relu_output + scaled_bottom_relu_output + self.final_bias
```



…and use the sum as the input to the final **ReLU** to get the output value.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
    scaled_bottom_relu_output = bottom_relu_output * self.w11

    input_to_final_relu = scaled_top_relu_output + scaled_bottom_relu_output + self.final_bias

    output = F.relu(input_to_final_relu)
```

...and use the sum as the input to the final **ReLU** to get the output value.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
    scaled_bottom_relu_output = bottom_relu_output * self.w11

    input_to_final_relu = scaled_top_relu_output + scaled_bottom_relu_output + self.final_bias

    output = F.relu(input_to_final_relu)
```

Lastly, the **forward()** function returns the **output**.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
    scaled_bottom_relu_output = bottom_relu_output * self.w11

    input_to_final_relu = scaled_top_relu_output + scaled_bottom_relu_output + self.final_bias

    output = F.relu(input_to_final_relu)

    return output
```

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)

    def forward(self, input):

        input_to_top_relu = input * self.w00 + self.b00
        top_relu_output = F.relu(input_to_top_relu)
        scaled_top_relu_output = top_relu_output * self.w01

        input_to_bottom_relu = input * self.w10 + self.b10
        bottom_relu_output = F.relu(input_to_bottom_relu)
        scaled_bottom_relu_output = bottom_relu_output * self.w11

        input_to_final_relu = scaled_top_relu_output + scaled_bottom_relu_output + self.final_bias

        output = F.relu(input_to_final_relu)

        return output
```

Now, if we look at the entire class that we created, **BasicNN**…

```
class BasicNN(nn.Module):

    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)

    def forward(self, input):

        input_to_top_relu = input * self.w00 + self.b00
        top_relu_output = F.relu(input_to_top_relu)
        scaled_top_relu_output = top_relu_output * self.w01

        input_to_bottom_relu = input * self.w10 + self.b10
        bottom_relu_output = F.relu(input_to_bottom_relu)
        scaled_bottom_relu_output = bottom_relu_output * self.w11

        input_to_final_relu = scaled_top_relu_output + scaled_bottom_relu_output + self.final_bias

        output = F.relu(input_to_final_relu)

        return output
```

...we see two methods, **__init__()** and **forward()**.

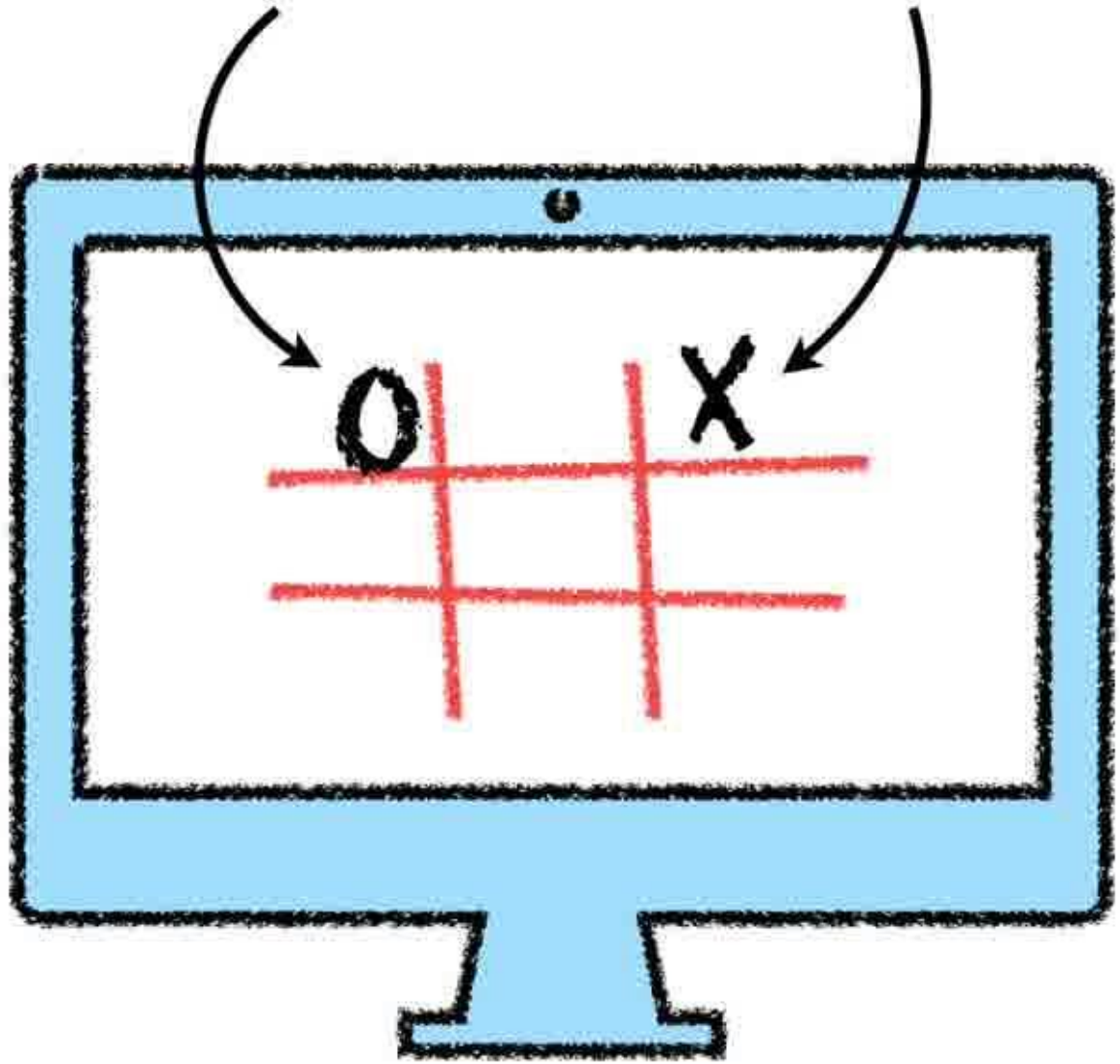
```
    def __init__(self):

        super().__init__()

        self.w00 = nn.Parameter(torch.tensor(1.7), requires_grad=False)
        self.b00 = nn.Parameter(torch.tensor(-0.85), requires_grad=False)
        self.w01 = nn.Parameter(torch.tensor(-40.8), requires_grad=False)

        self.w10 = nn.Parameter(torch.tensor(12.6), requires_grad=False)
        self.b10 = nn.Parameter(torch.tensor(0.0), requires_grad=False)
        self.w11 = nn.Parameter(torch.tensor(2.7), requires_grad=False)

        self.final_bias = nn.Parameter(torch.tensor(-16.), requires_grad=False)
```

__init__() creates and initializes the **weights** and **biases**...

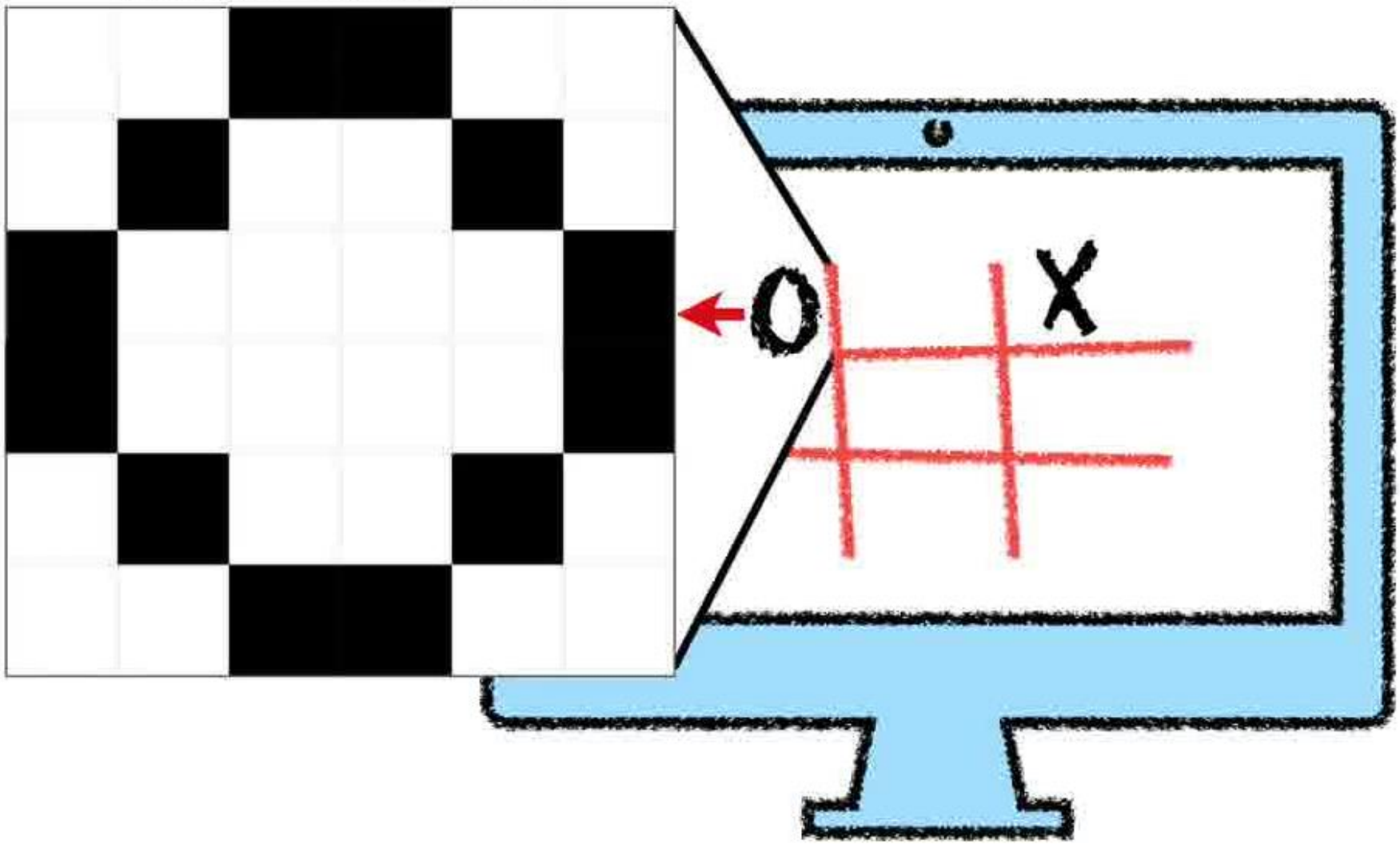
…and **forward()** does a **forward pass** through the neural network by taking an input value and calculating the output value with the **weights**, **biases** and **activation functions**.

```
def forward(self, input):

    input_to_top_relu = input * self.w00 + self.b00
    top_relu_output = F.relu(input_to_top_relu)
    scaled_top_relu_output = top_relu_output * self.w01

    input_to_bottom_relu = input * self.w10 + self.b10
    bottom_relu_output = F.relu(input_to_bottom_relu)
    scaled_bottom_relu_output = bottom_relu_output * self.w11

    input_to_final_relu = scaled_top_relu_output + scaled_bottom_relu_output + self.final_bias

    output = F.relu(input_to_final_relu)

    return output
```

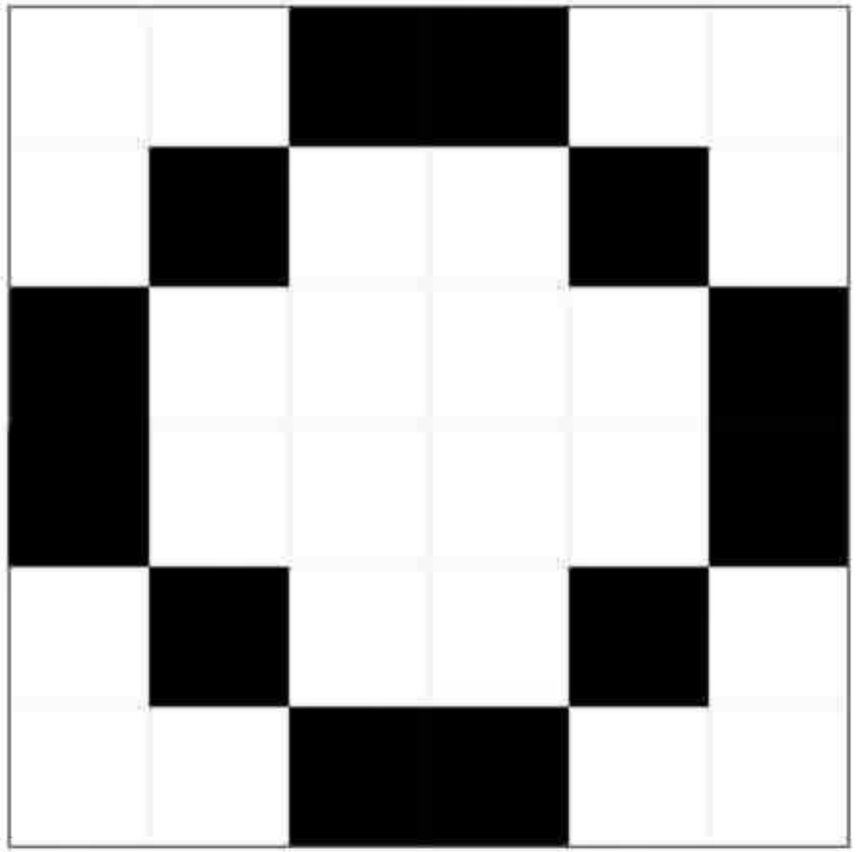
Wie geht ein Neuronales Netz bei Bilddaten vor?


O
X

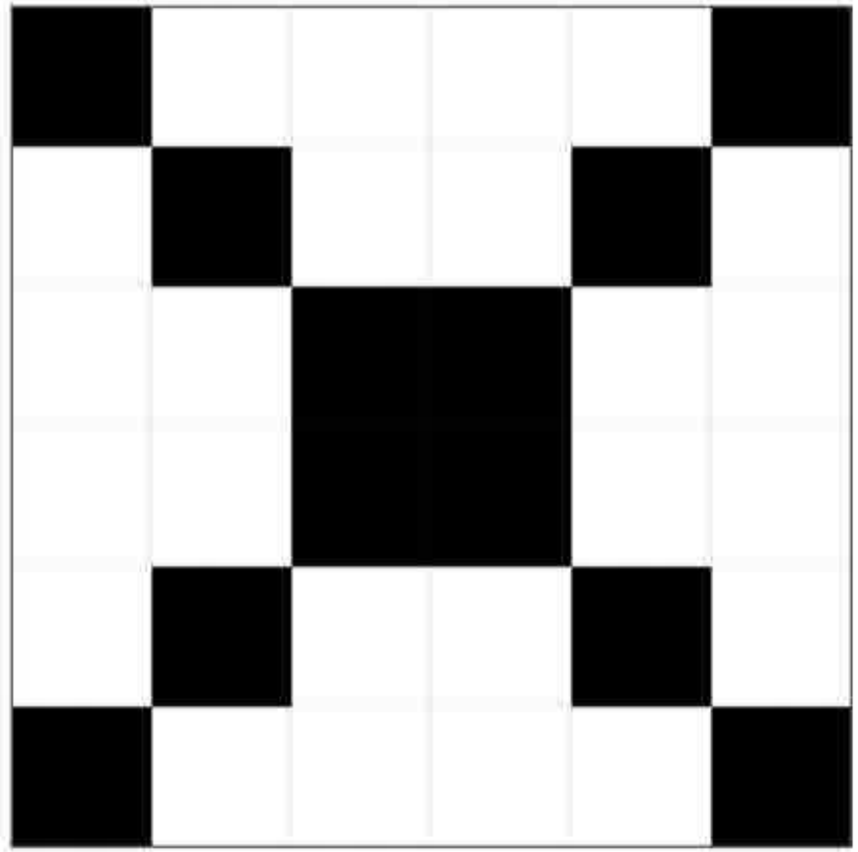
The letter “O”, zoomed in.

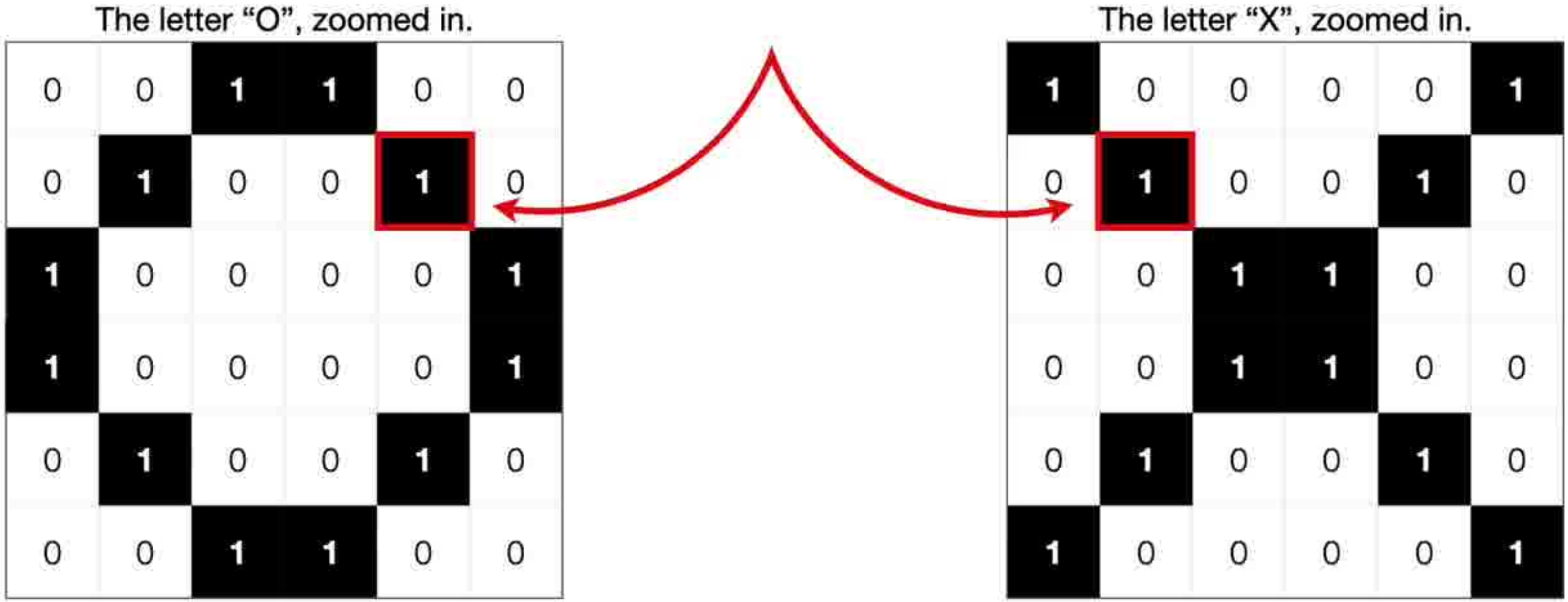


The letter “O”, zoomed in.



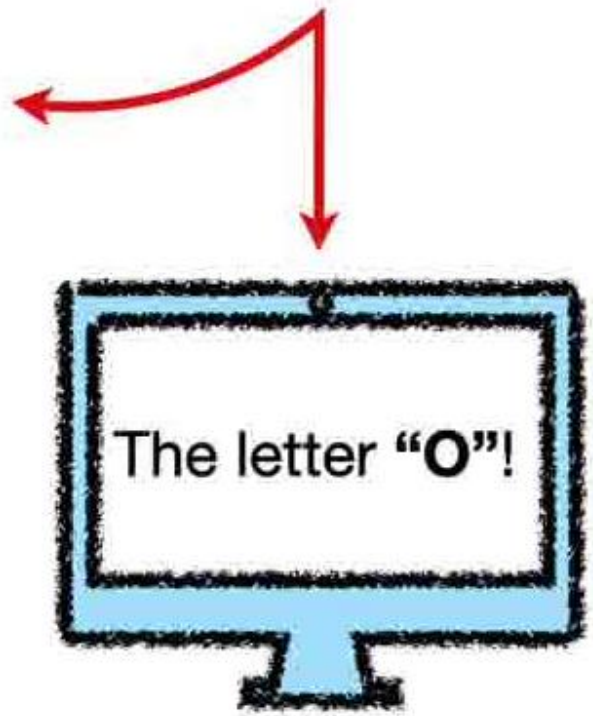
The letter “X”, zoomed in.




The letter “O”, zoomed in.
0 0 1 1 0 0
0 1 0 0 1 0
1 0 0 0 0 1
1 0 0 0 0 1
0 1 0 0 1 0
0 0 1 1 0 0
The letter “X”, zoomed in.
1 0 0 0 0 1
0 1 0 0 1 0
0 0 1 1 0 0
0 0 1 1 0 0
0 1 0 0 1 0
1 0 0 0 0 1

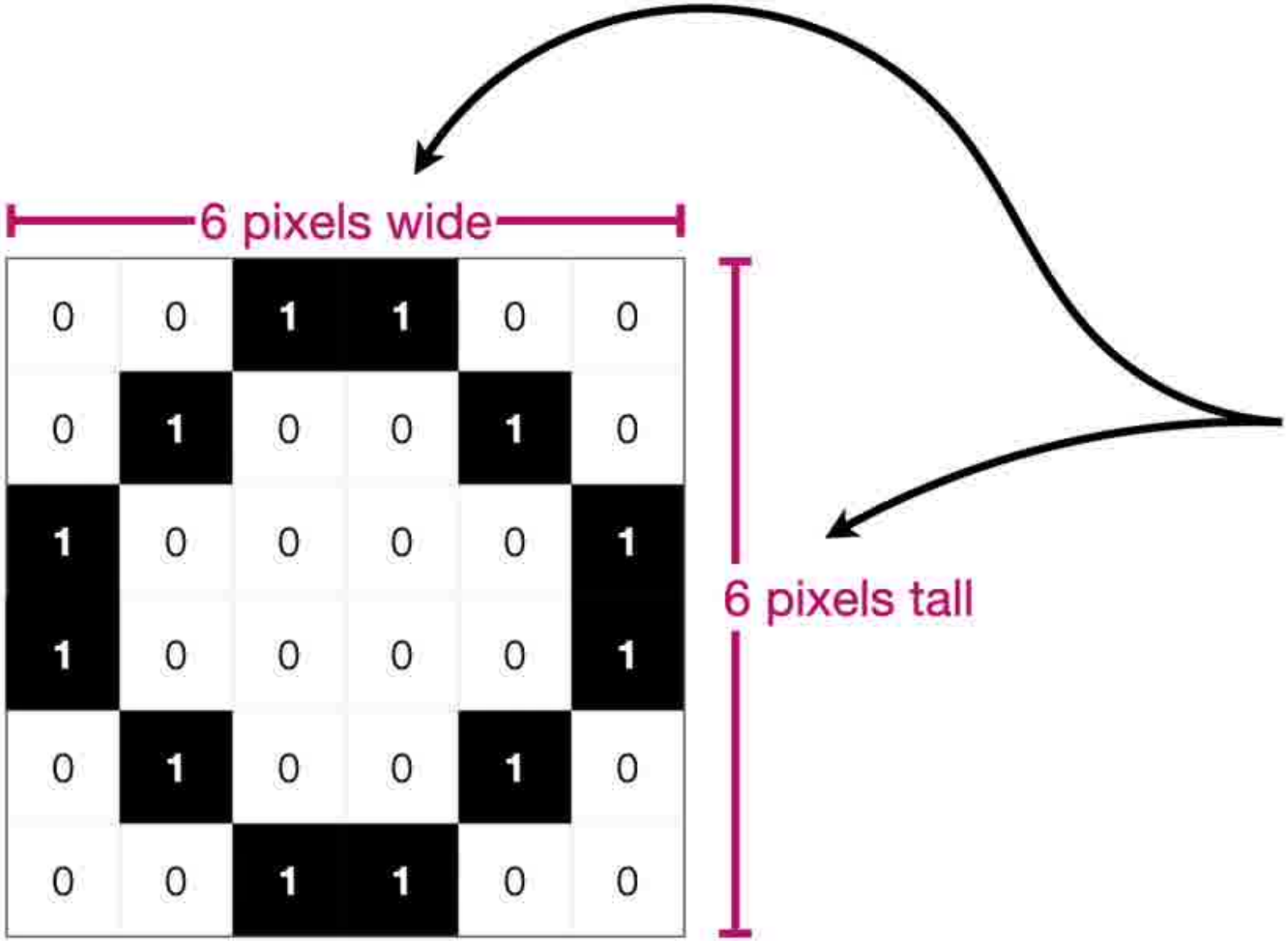
The letter “O”, zoomed in.

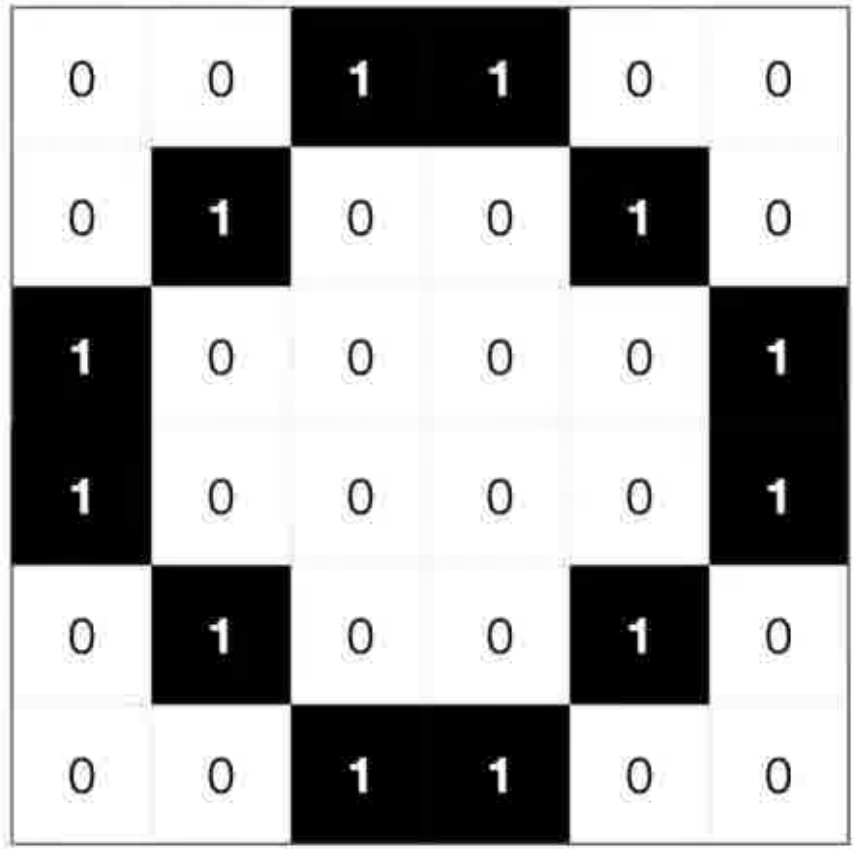
0	0	1	1	0	0
0	1	0	0	1	0
1	0	0	0	0	1
1	0	0	0	0	1
0	1	0	0	1	0
0	0	1	1	0	0

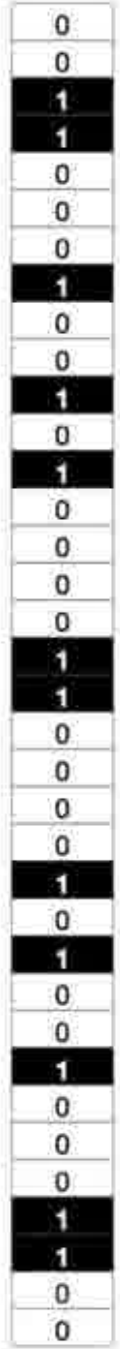


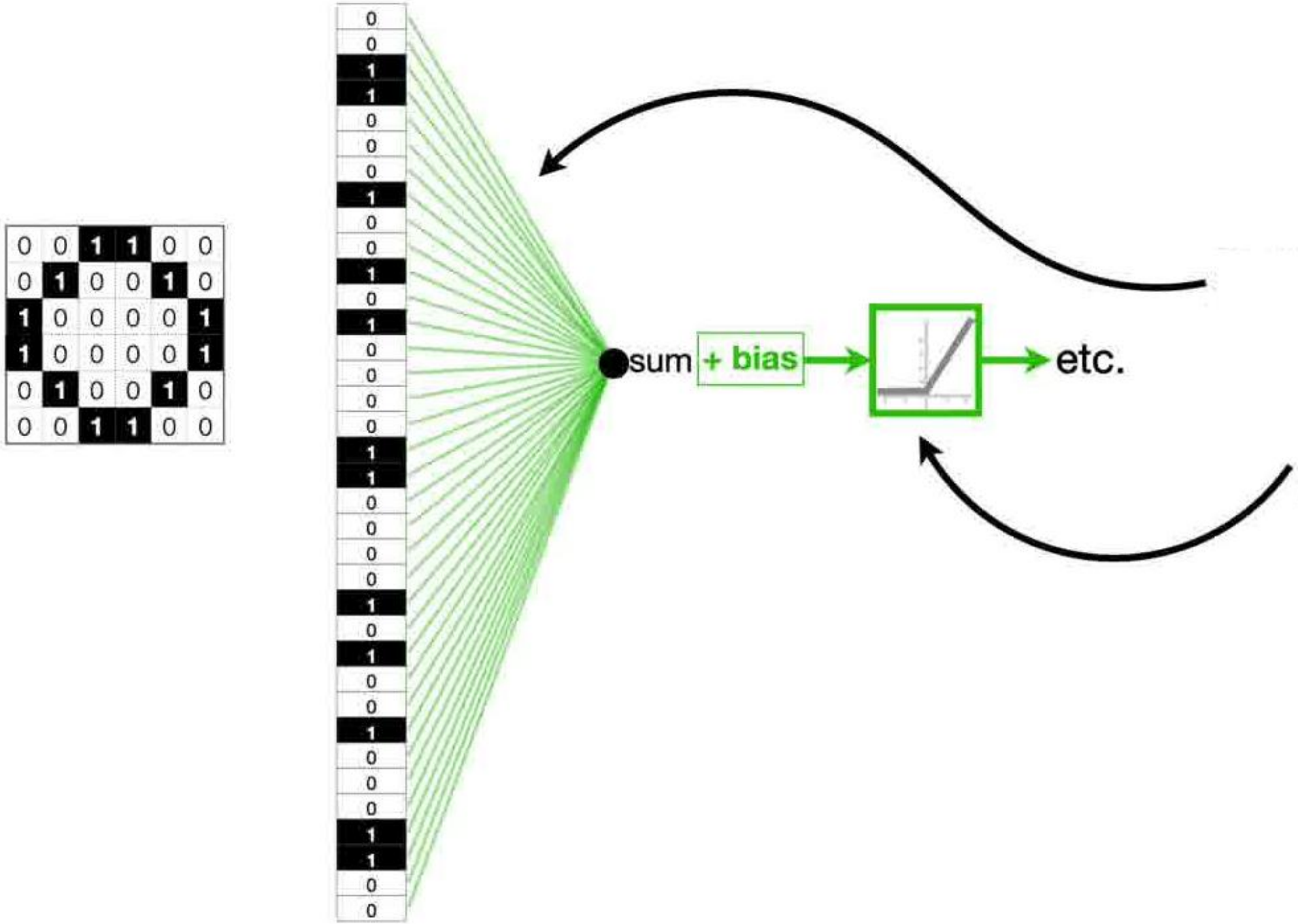
The letter “X”, zoomed in.

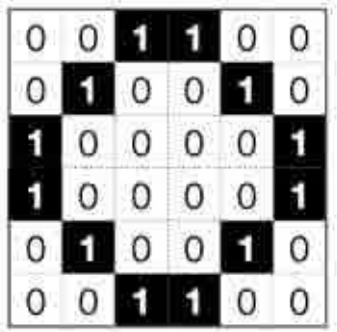
1	0	0	0	0	1
0	1	0	0	1	0
0	0	1	1	0	0
0	0	1	1	0	0
0	1	0	0	1	0
1	0	0	0	0	1

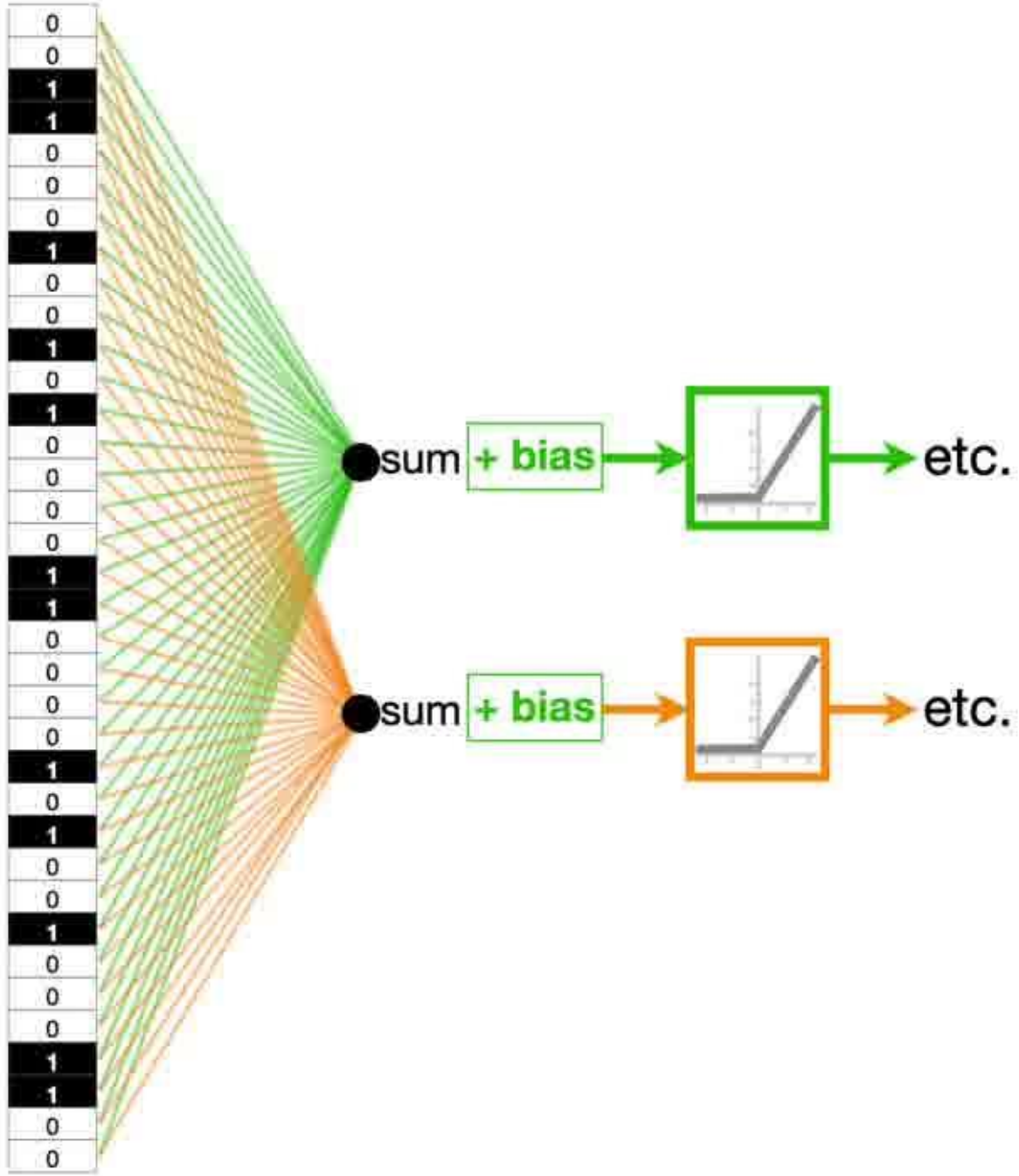

6 pixels wide
6 pixels tall
0 0 1 1 0 0
0 1 0 0 1 0
1 0 0 0 0 1
1 0 0 0 0 1
0 1 0 0 1 0
0 0 1 1 0 0


0 0 1 1 0 0
0 1 0 0 1 0
1 0 0 0 0 1
1 0 0 0 0 1
0 1 0 0 1 0
0 0 1 1 0 0


0
0
1
1
0
0
0
1
0
0
1
0
1
0
0
0
0
1
1
0
0
0
0
1
0
1
0
0
1
0
0
0
1
1
0
0


0 0 1 1 0 0
0 1 0 0 1 0
1 0 0 0 0 1
1 0 0 0 0 1
0 1 0 0 1 0
0 0 1 1 0 0
0 0 1 1 0 0 1 1 0 0 1 0 0 1 0 0 1 0 0 1 0 0 1 0 0 0 1 1 0 0 0 0 1 0 1 0 0 0 1 0 0 0 1 1 0 0
sum
+ bias
etc.

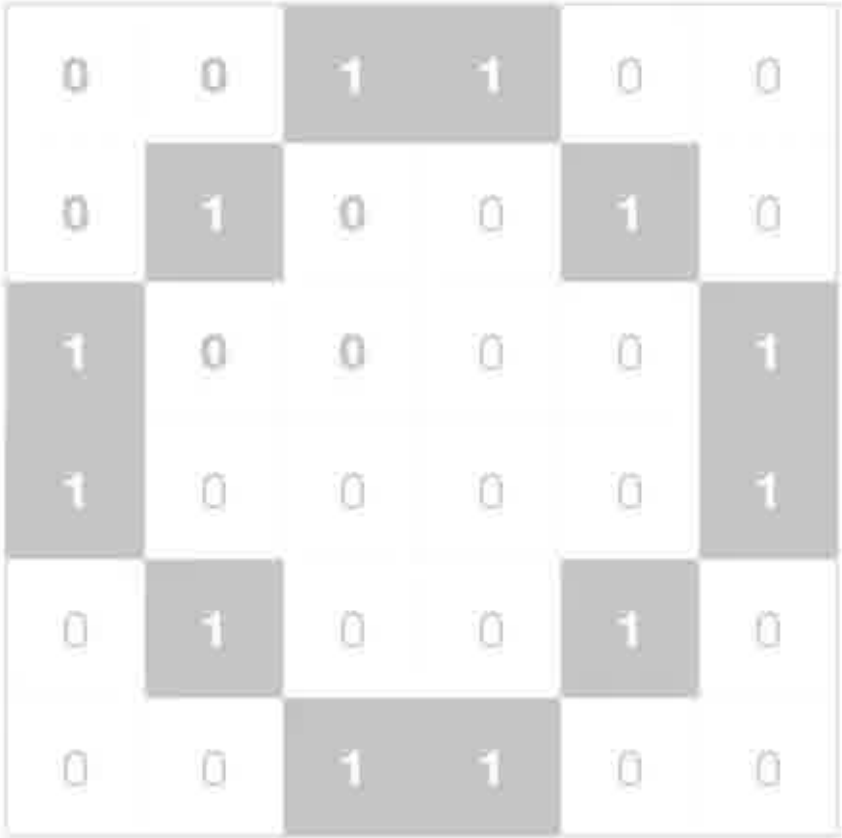




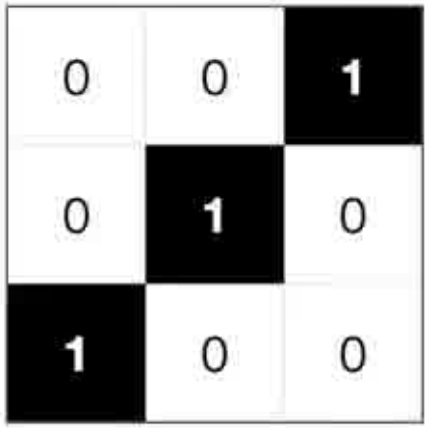
Bei großen Bilddaten und komplexeren Neuronalen Netzen wäre ein solches Verfahren viel zu aufwändig!

Lösung:
CONVOLUTIONAL NEURAL NETWORK

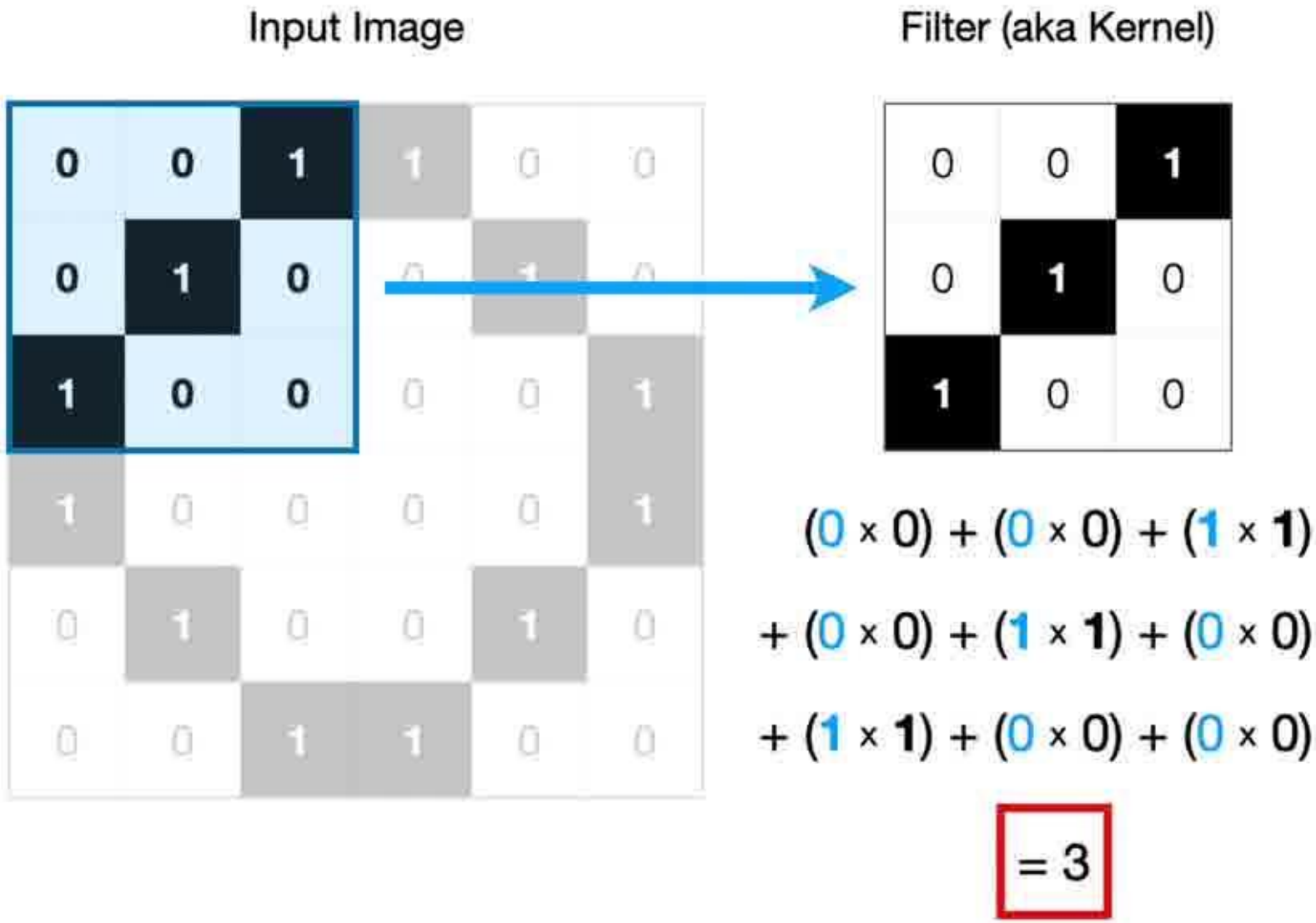
Input Image



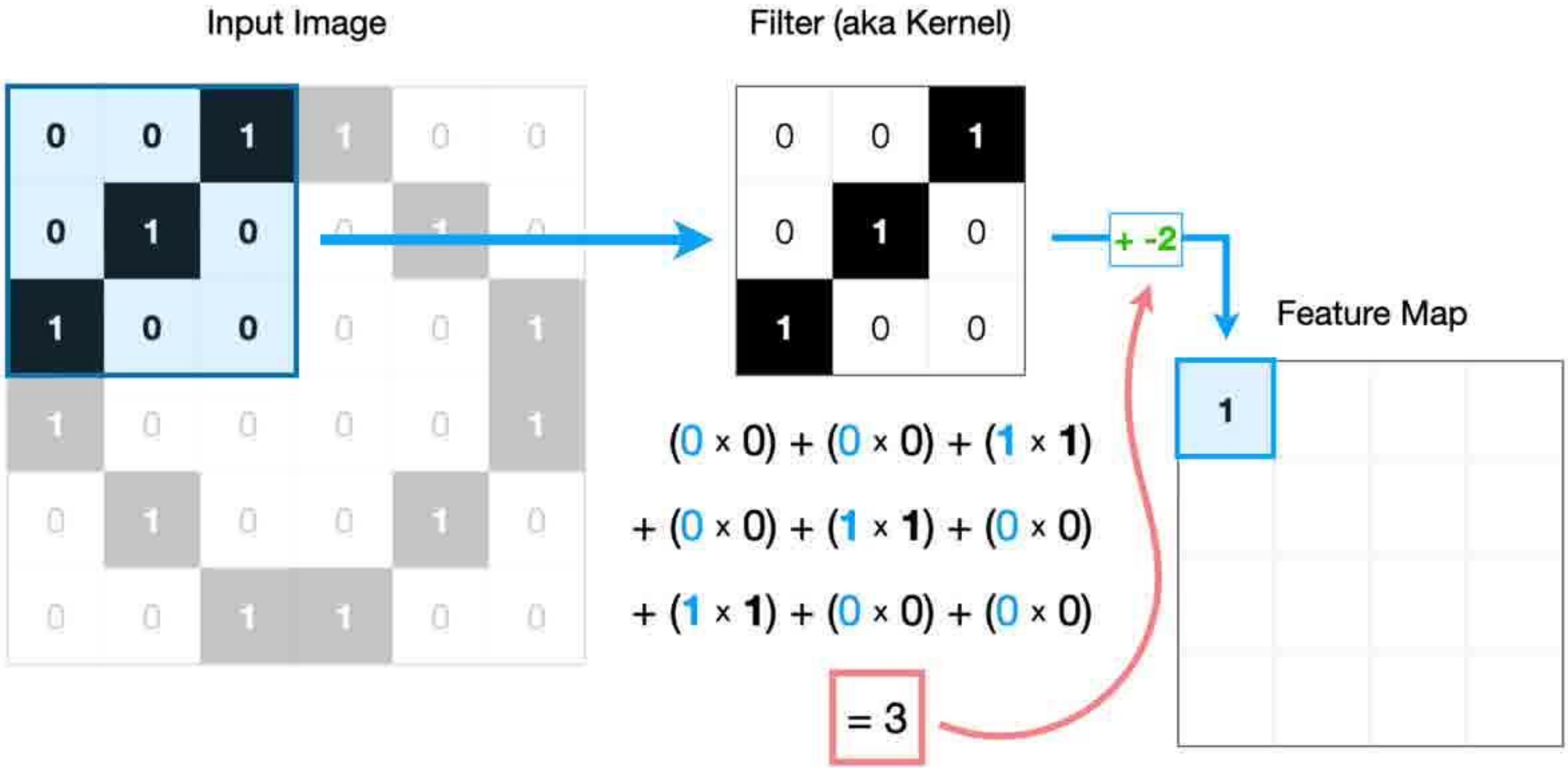
Filter (aka Kernel)

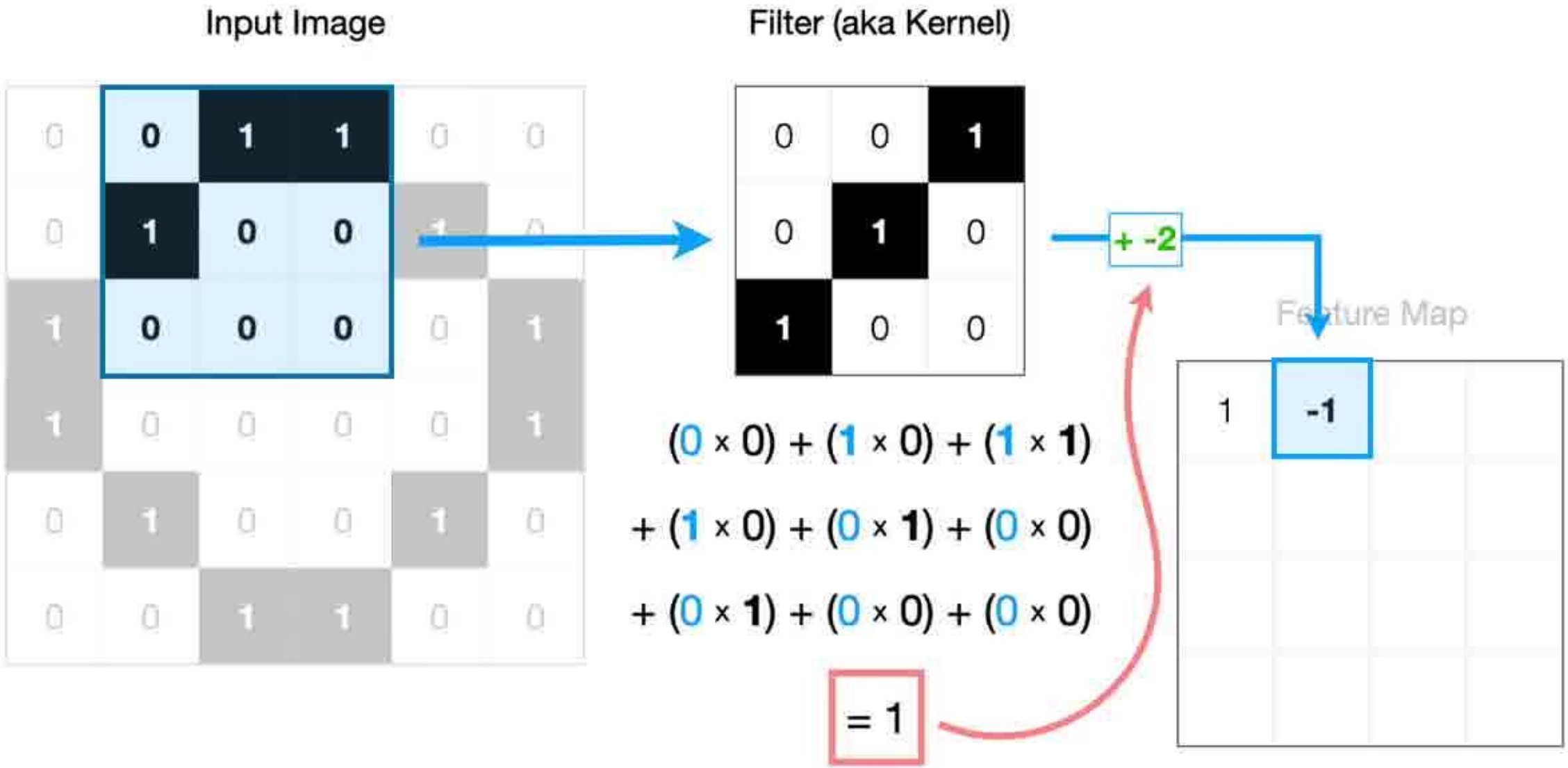


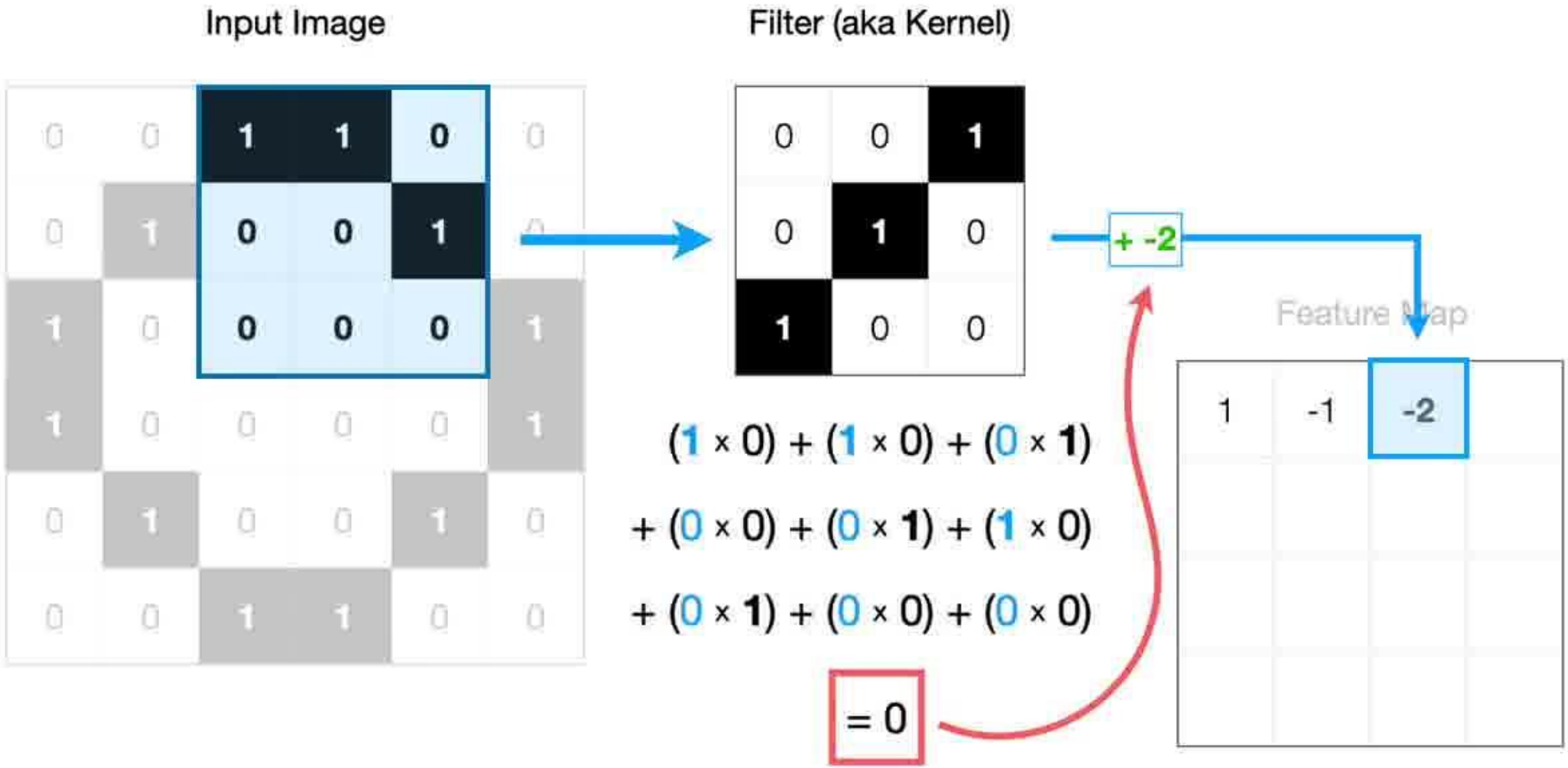
Ein CNN wendet zunächst einen **Filter** auf das Input Image an.



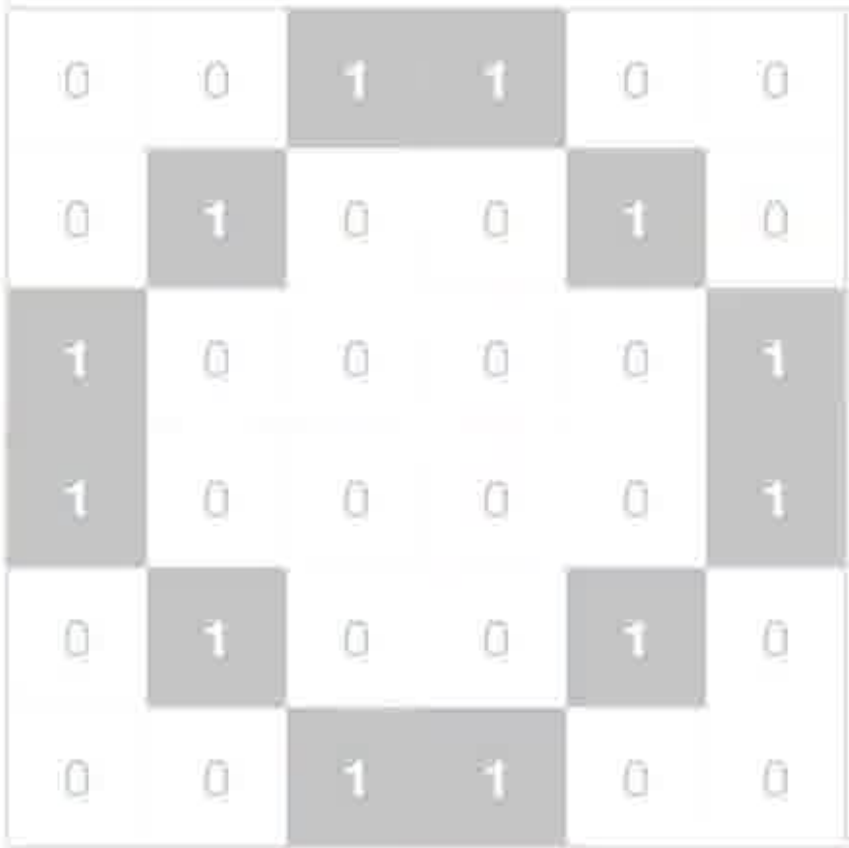
Durch das **Skalarprodukt** zwischen Input und Filter, wird der Filter mit dem Input „**convolved**“ (zusammengefaltet).


Input Image
Filter (aka Kernel)
0 0 1
0 1 0
1 0 0
+ -2
Feature Map
1
(0 × 0) + (0 × 0) + (1 × 1)
+ (0 × 0) + (1 × 1) + (0 × 0)
+ (1 × 1) + (0 × 0) + (0 × 0)
= 3

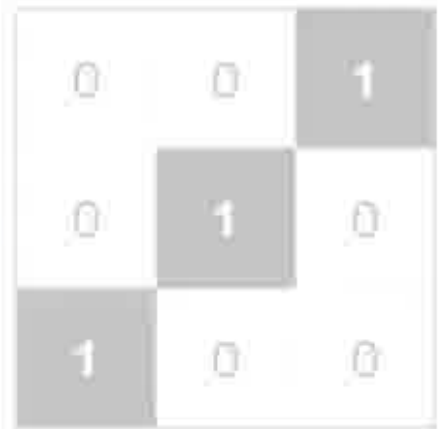

Input Image
Filter (aka Kernel)
0 0 1
0 1 0
1 0 0
(0 × 0) + (1 × 0) + (1 × 1)
+ (1 × 0) + (0 × 1) + (0 × 0)
+ (0 × 1) + (0 × 0) + (0 × 0)
= 1
+ -2
Feature Map
1
-1


Input Image
Filter (aka Kernel)
0 0 1
0 1 0
1 0 0
(1 × 0) + (1 × 0) + (0 × 1)
+ (0 × 0) + (0 × 1) + (1 × 0)
+ (0 × 1) + (0 × 0) + (0 × 0)
= 0
+ -2
Feature Map
1 -1 -2

Input Image

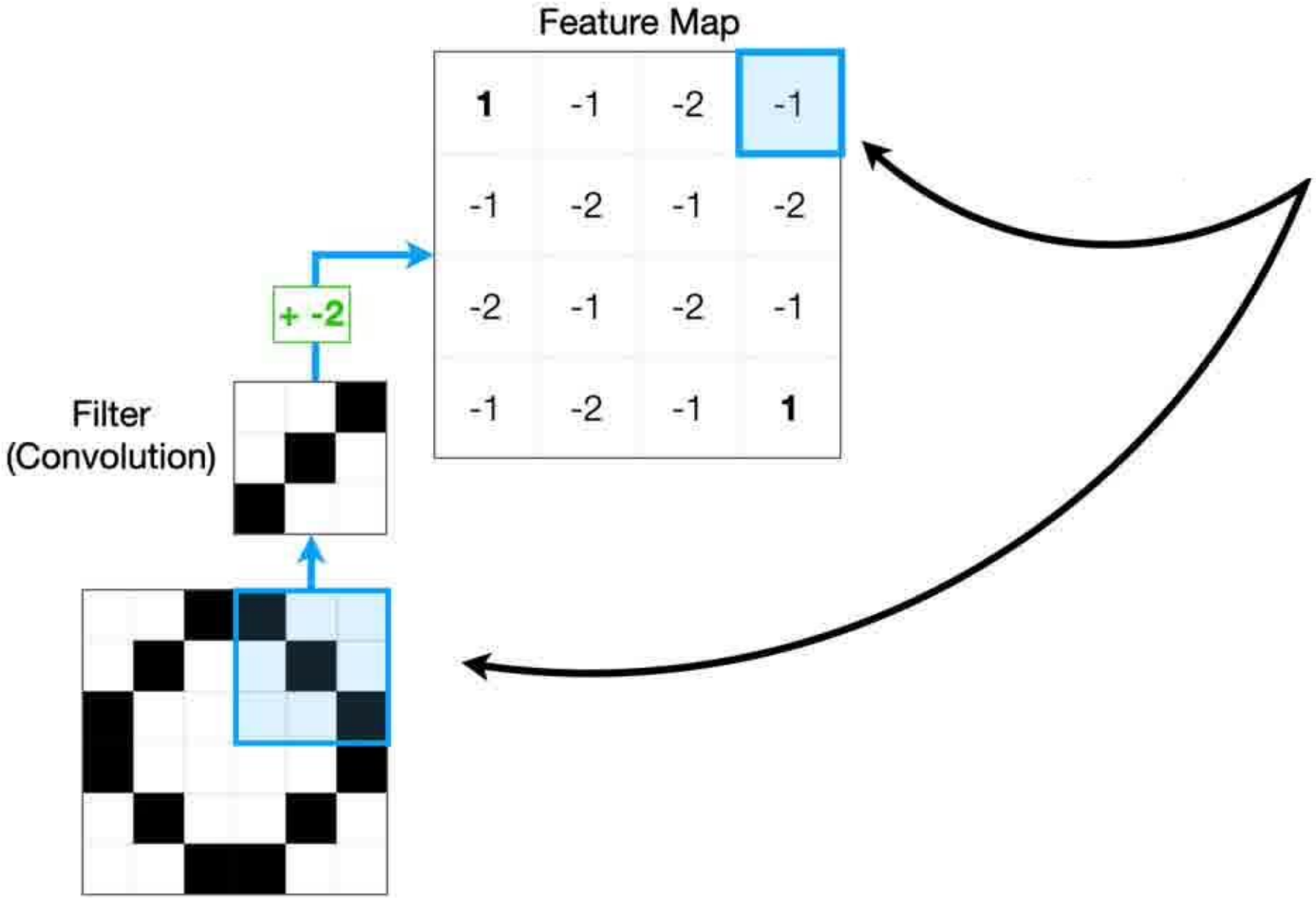


Filter (aka Kernel)



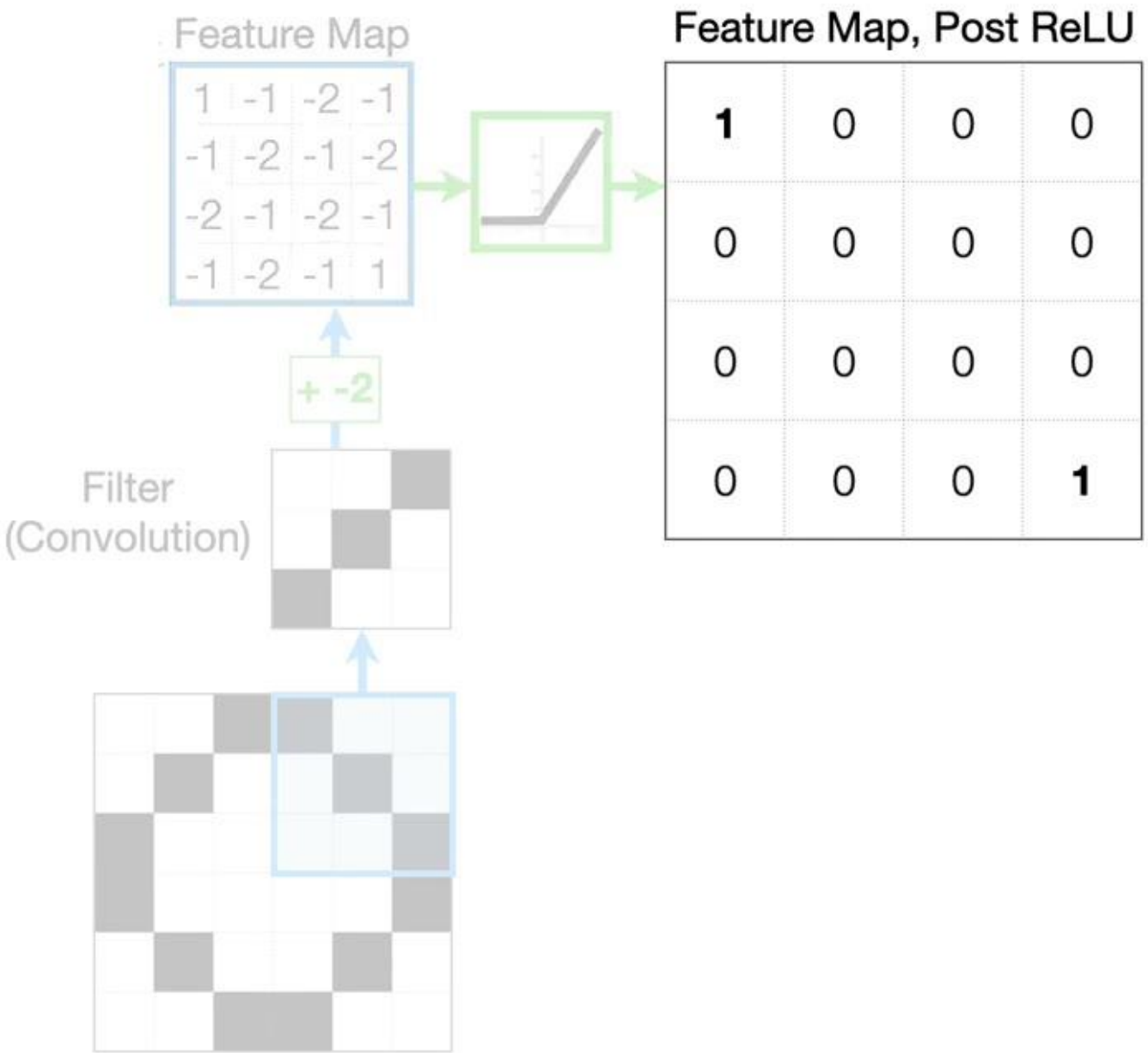
Feature Map

1	-1	-2	-1
-1	-2	-1	-2
-2	-1	-2	-1
-1	-2	-1	1


Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
+ -2
Filter
(Convolution)

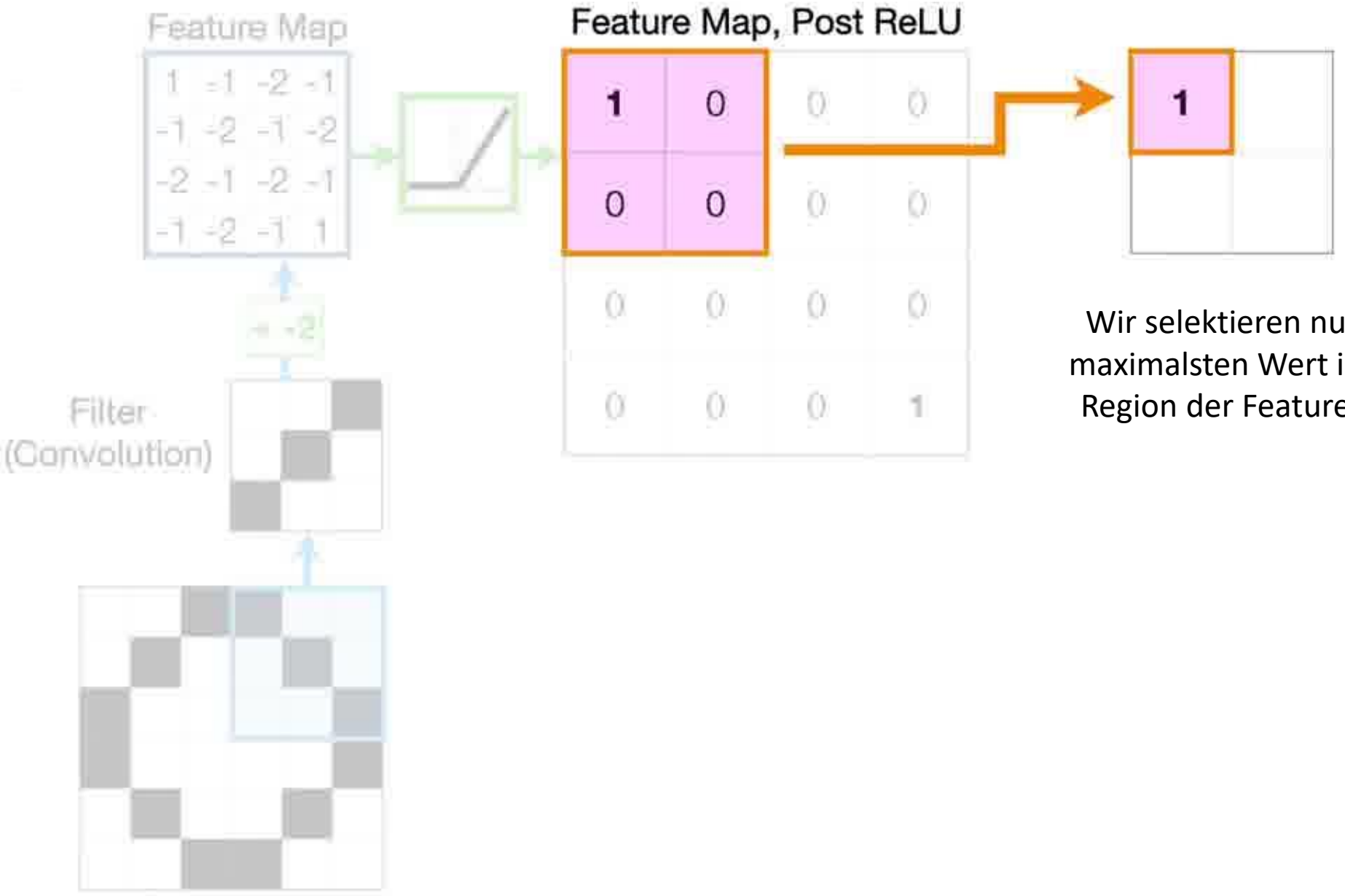

Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
Filter
(Convolution)


Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
Feature Map, Post ReLU
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 1
Filter
(Convolution)

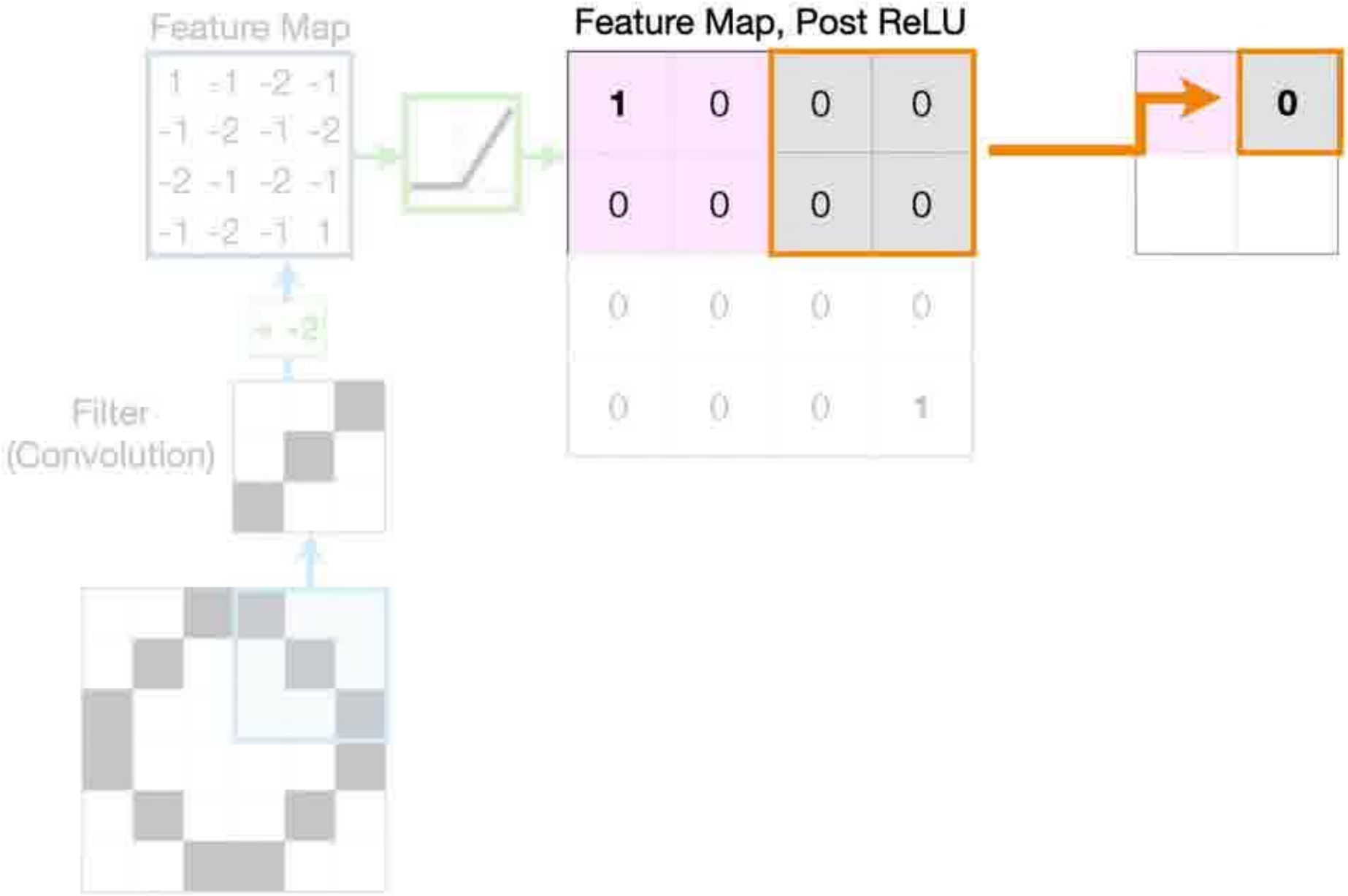


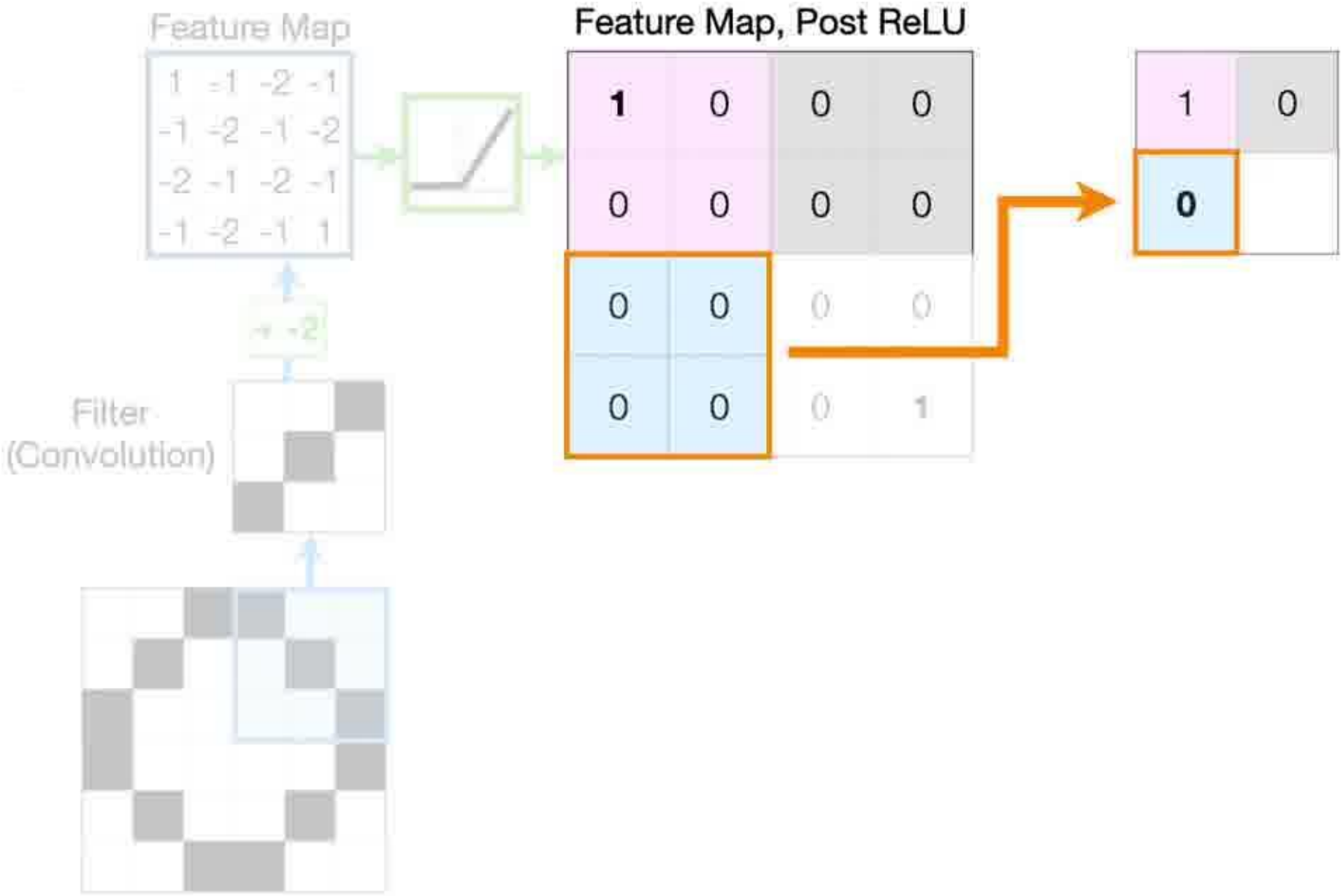
Feature Map, Post ReLU

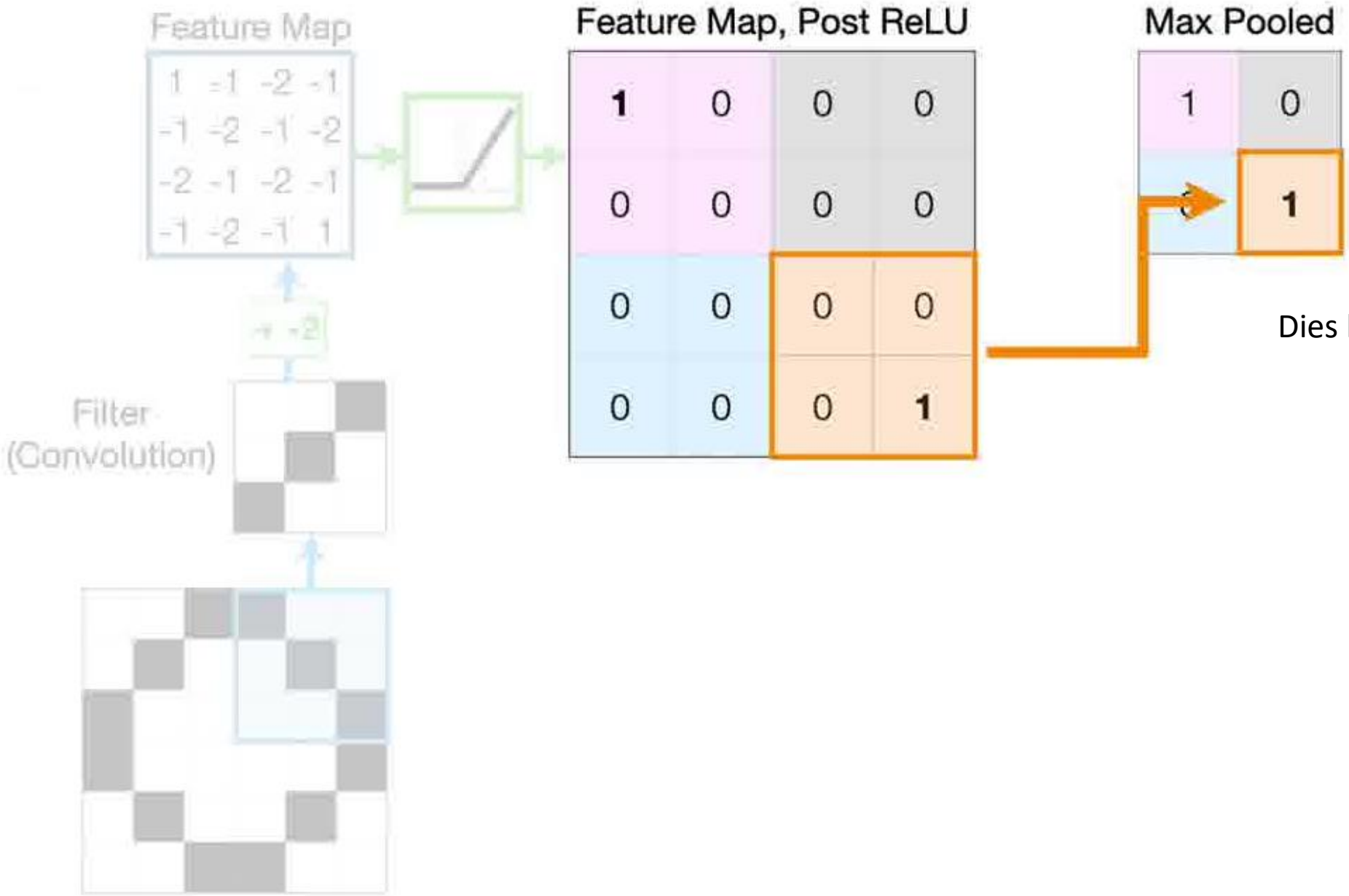
1	0	0	0
0	0	0	0
0	0	0	0
0	0	0	**1**



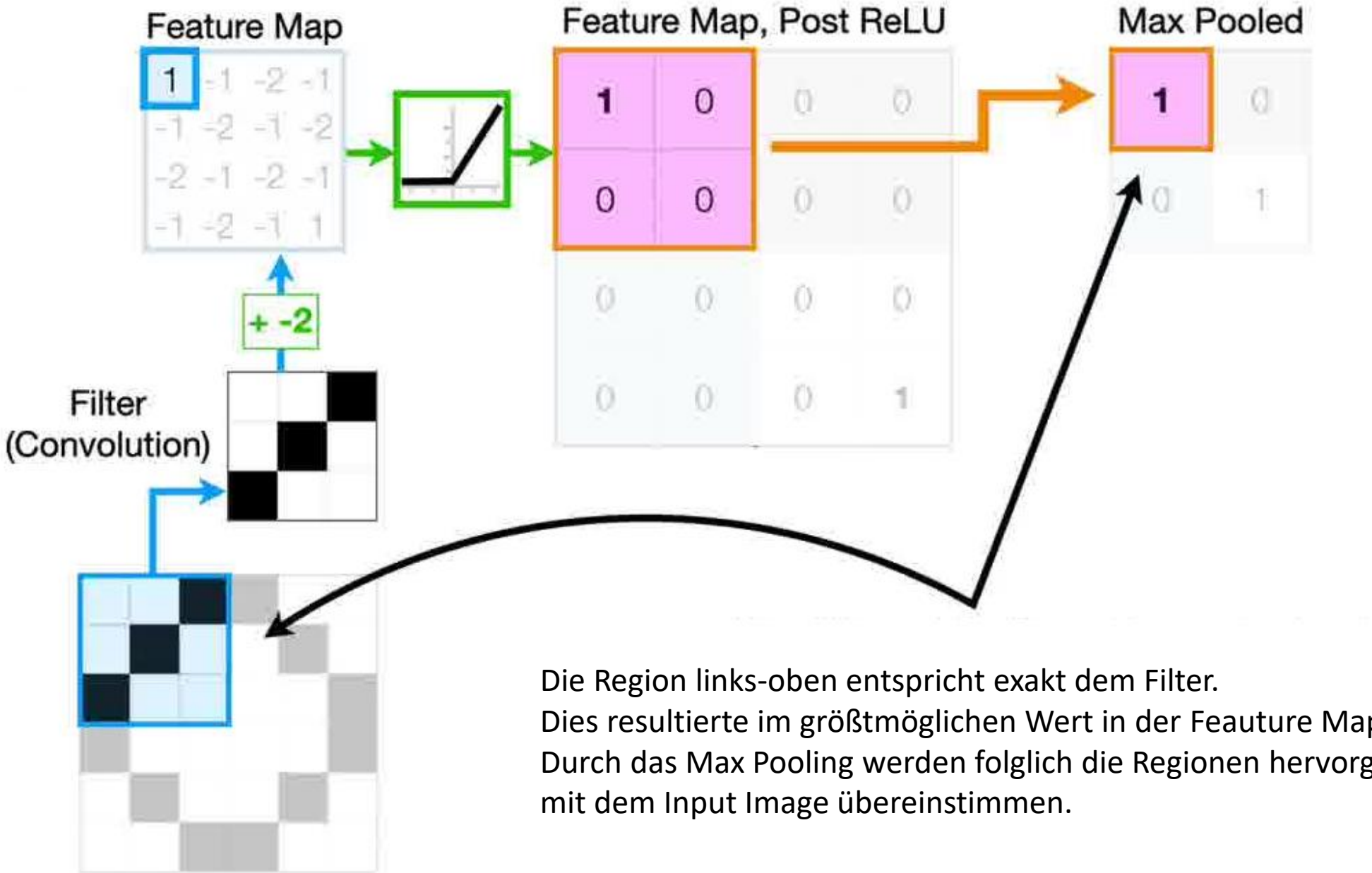
Wir selektieren nun den maximalsten Wert in einer Region der Feature Map.


Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
Filter
(Convolution)
Feature Map, Post ReLU
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 1
0

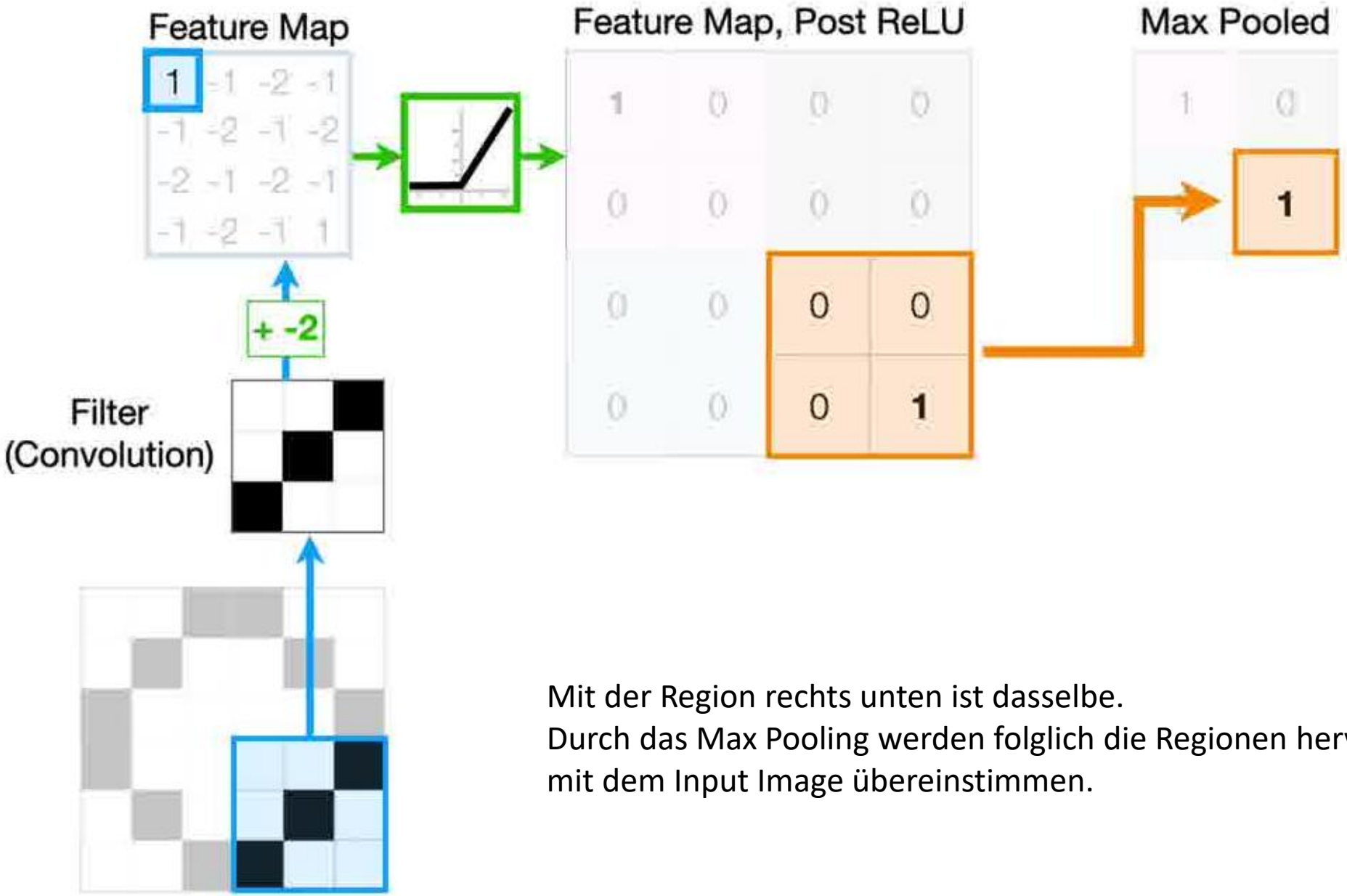

Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
Filter
(Convolution)
Feature Map, Post ReLU
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 1
1 0
0



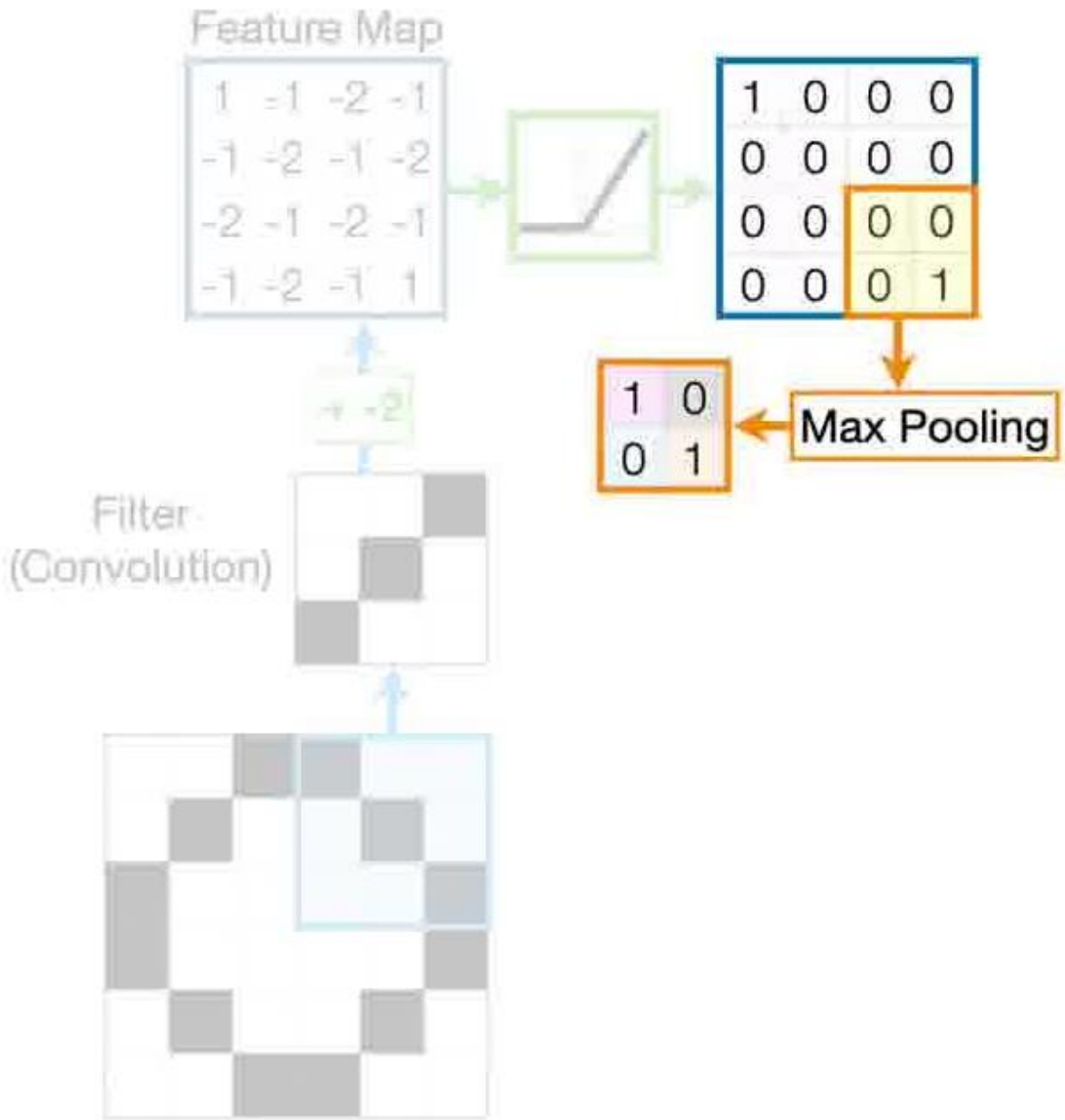
Dies bezeichnet man als **Max Pooling**.

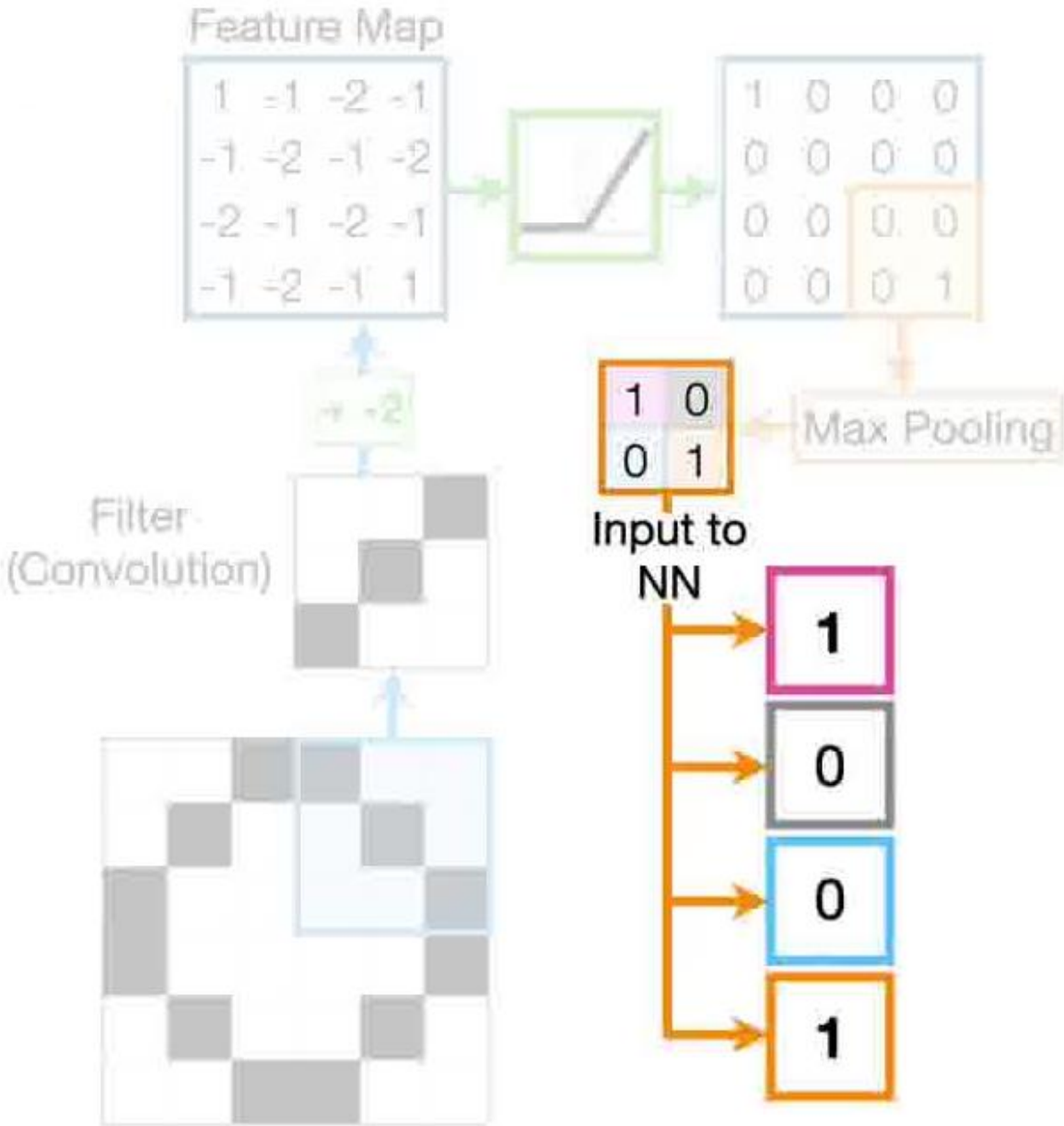


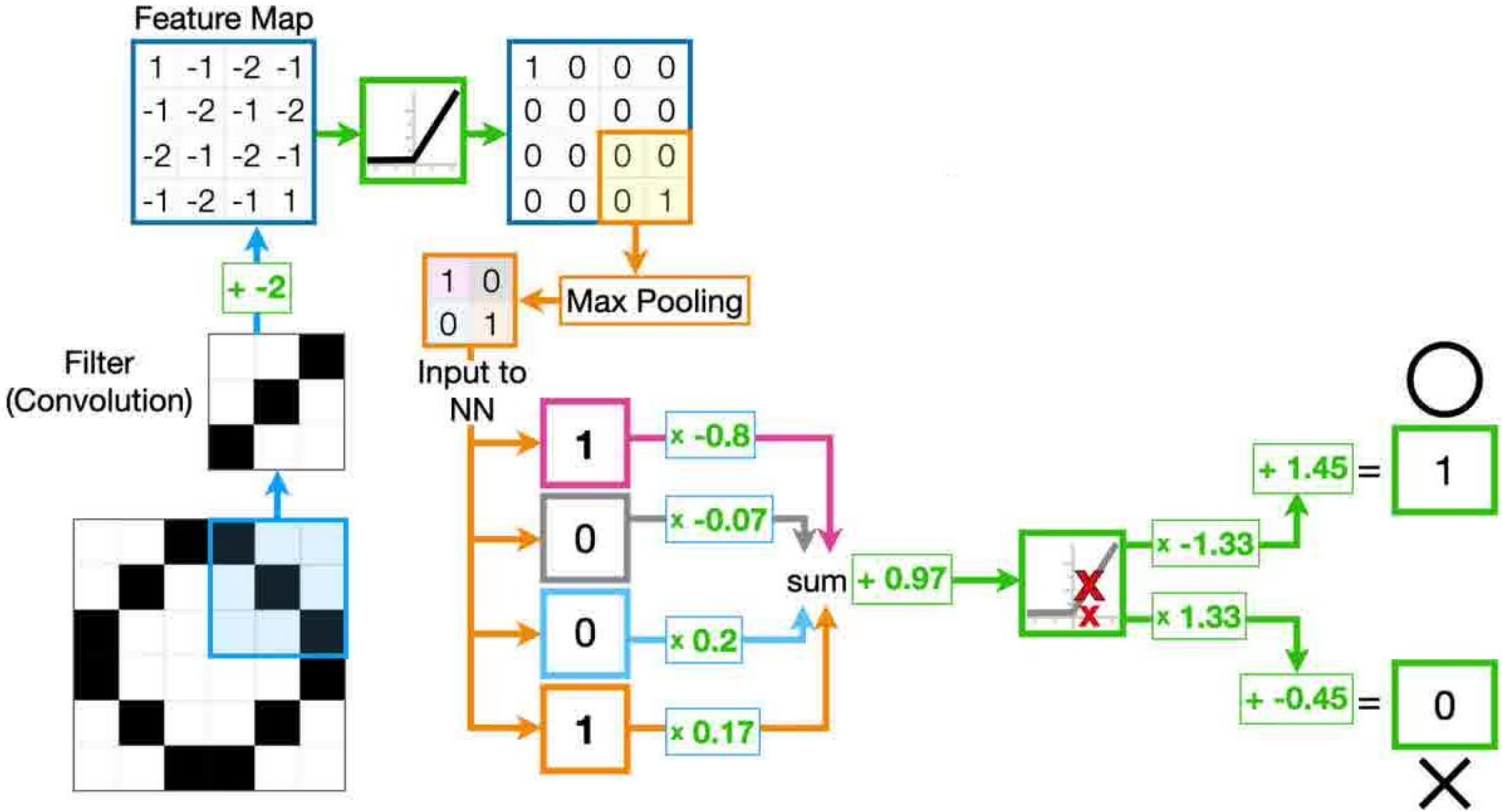
Die Region links-oben entspricht exakt dem Filter.
Dies resultierte im größtmöglichen Wert in der Feauture Map.
Durch das Max Pooling werden folglich die Regionen hervorgehoben, die am besten mit dem Input Image übereinstimmen.

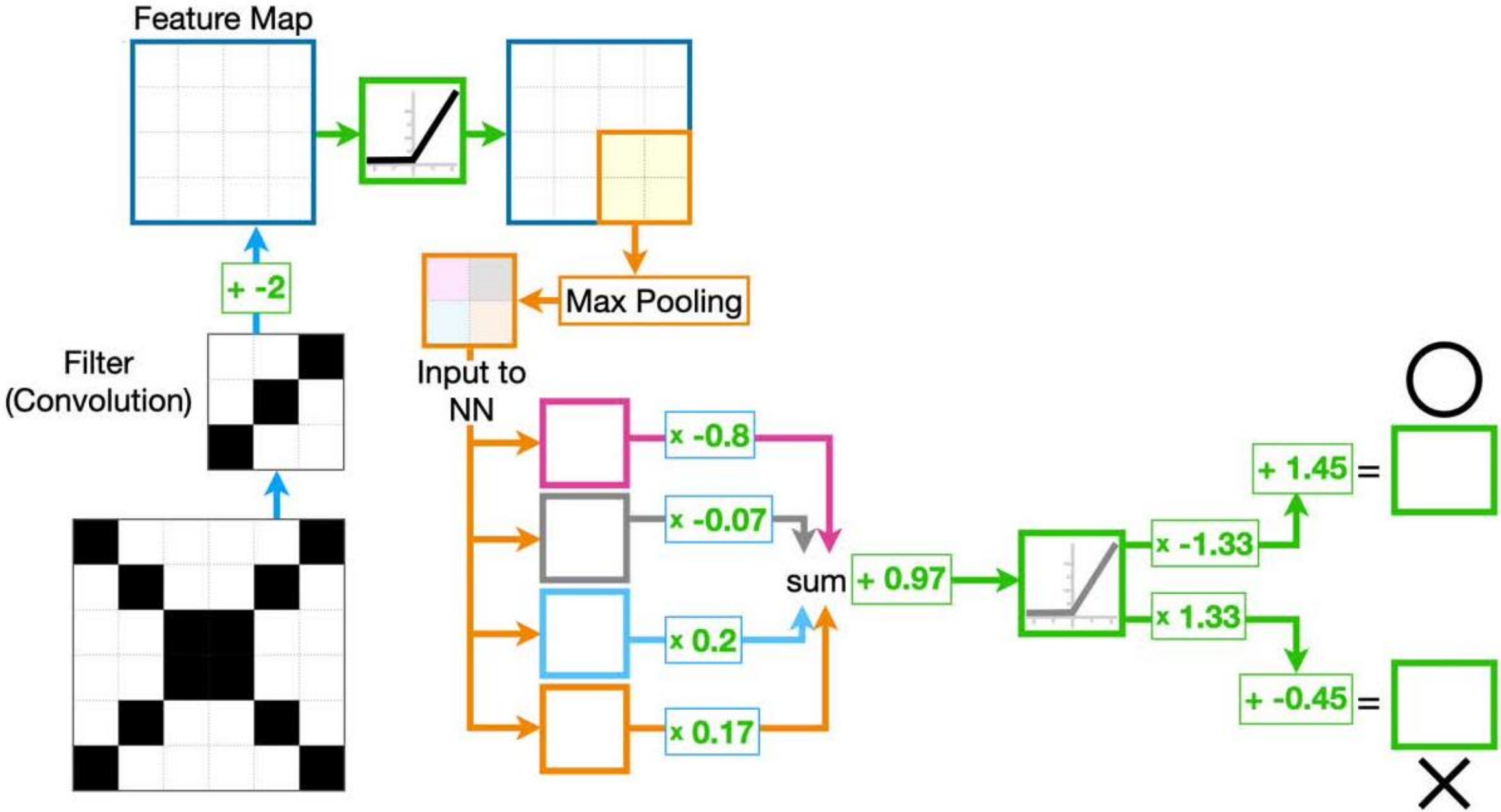


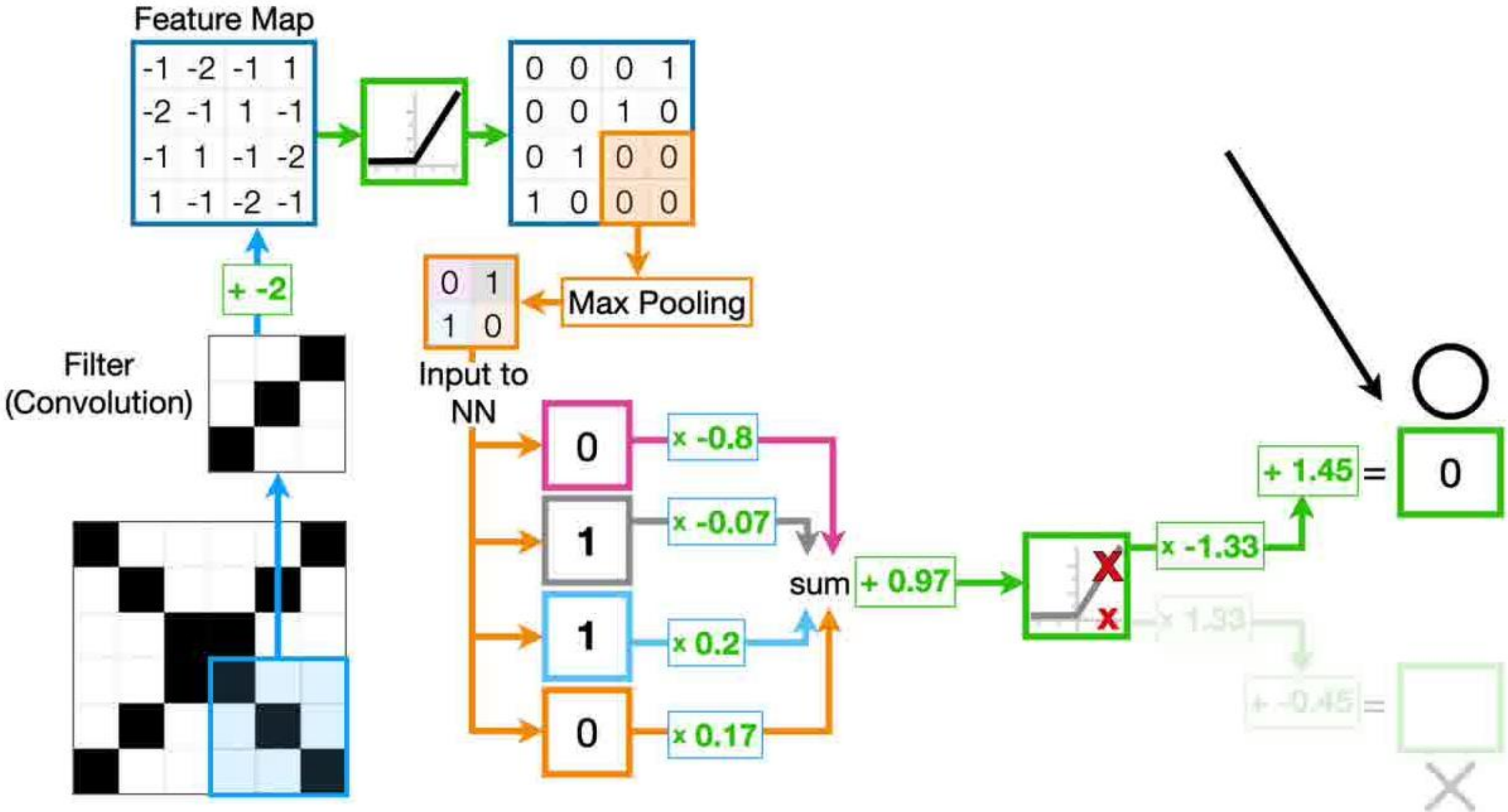
Mit der Region rechts unten ist dasselbe.
Durch das Max Pooling werden folglich die Regionen hervorgehoben, die am besten mit dem Input Image übereinstimmen.

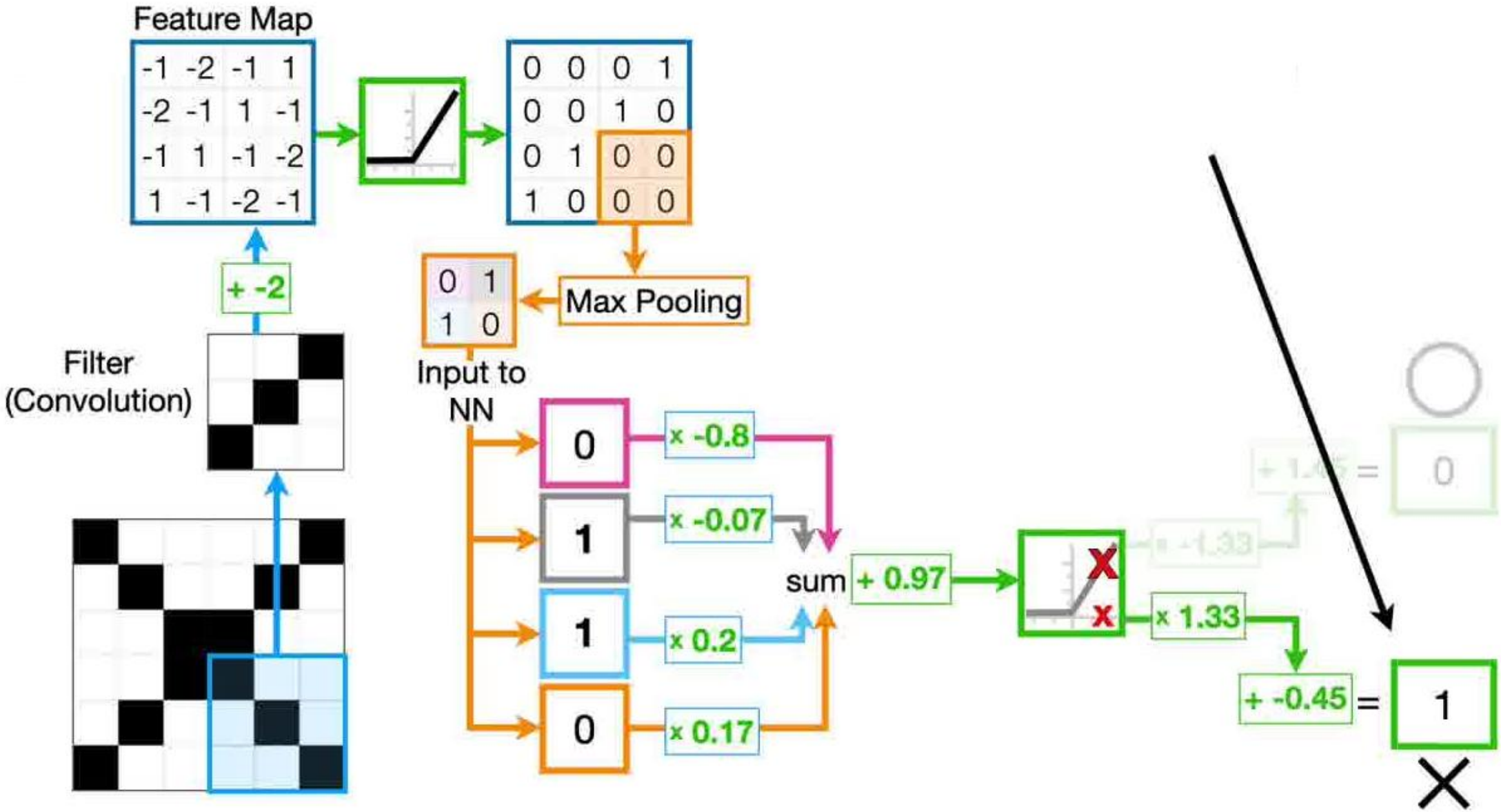

Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 1
1 0
0 1
Max Pooling
Filter
(Convolution)

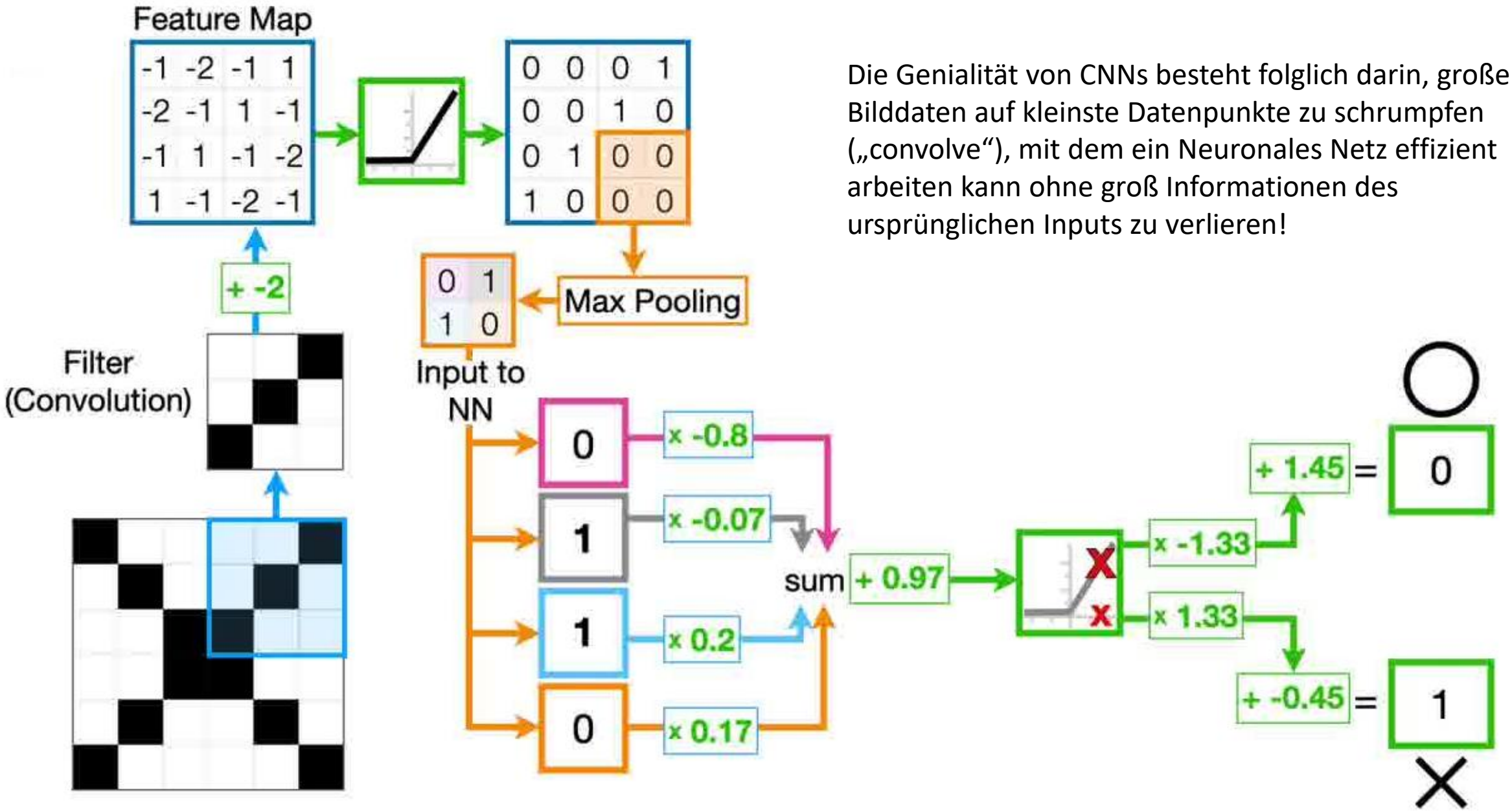

Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 1
Max Pooling
1 0
0 1
Input to NN
Filter (Convolution)
1
0
0
1


Feature Map
1 -1 -2 -1
-1 -2 -1 -2
-2 -1 -2 -1
-1 -2 -1 1
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 1
Max Pooling
1 0
0 1
Input to NN
+ -2
Filter (Convolution)
1
0
0
1
x -0.8
x -0.07
x 0.2
x 0.17
sum
+ 0.97
x -1.33
x 1.33
+ 1.45 = 1
+ -0.45 = 0

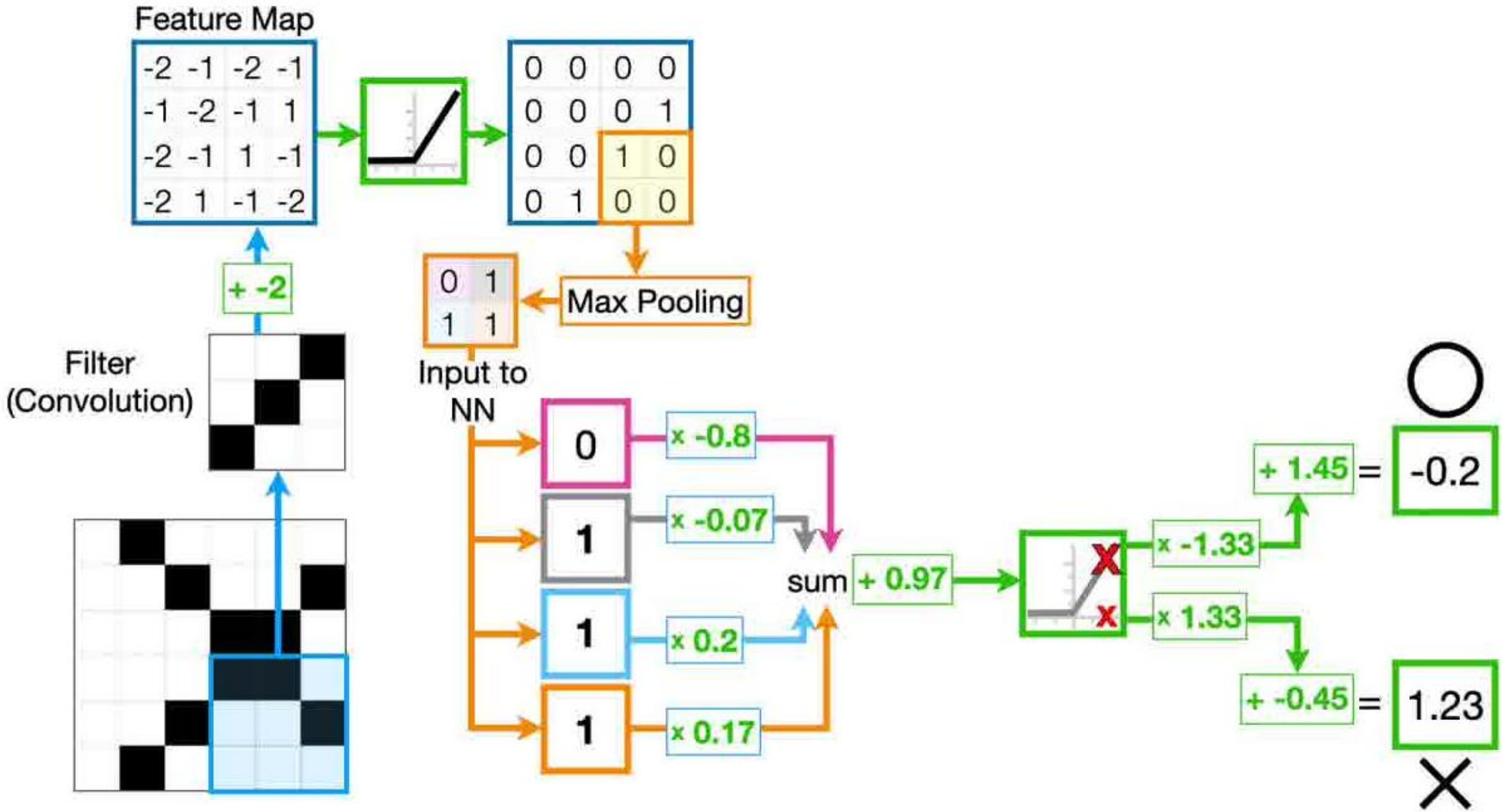

Feature Map
+ -2
Filter
(Convolution)
Max Pooling
Input to
NN
x -0.8
x -0.07
x 0.2
x 0.17
sum
+ 0.97
x -1.33
x 1.33
+ 1.45 =
+ -0.45 =


Feature Map
-1 -2 -1 1
-2 -1 1 -1
-1 1 -1 -2
1 -1 -2 -1
0 0 0 1
0 0 1 0
0 1 0 0
1 0 0 0
0 1
1 0
Max Pooling
+ -2
Filter
(Convolution)
Input to
NN
0
1
1
0
x -0.8
x -0.07
x 0.2
x 0.17
sum
+ 0.97
x -1.33
+ 1.45 =
0


Feature Map
-1 -2 -1 1
-2 -1 1 -1
-1 1 -1 -2
1 -1 -2 -1
0 0 0 1
0 0 1 0
0 1 0 0
1 0 0 0
0 1
1 0
Max Pooling
Input to NN
+ -2
Filter (Convolution)
0
1
1
0
x -0.8
x -0.07
x 0.2
x 0.17
sum
+ 0.97
x
x
x 1.33
+ -0.45
=
1
=
0

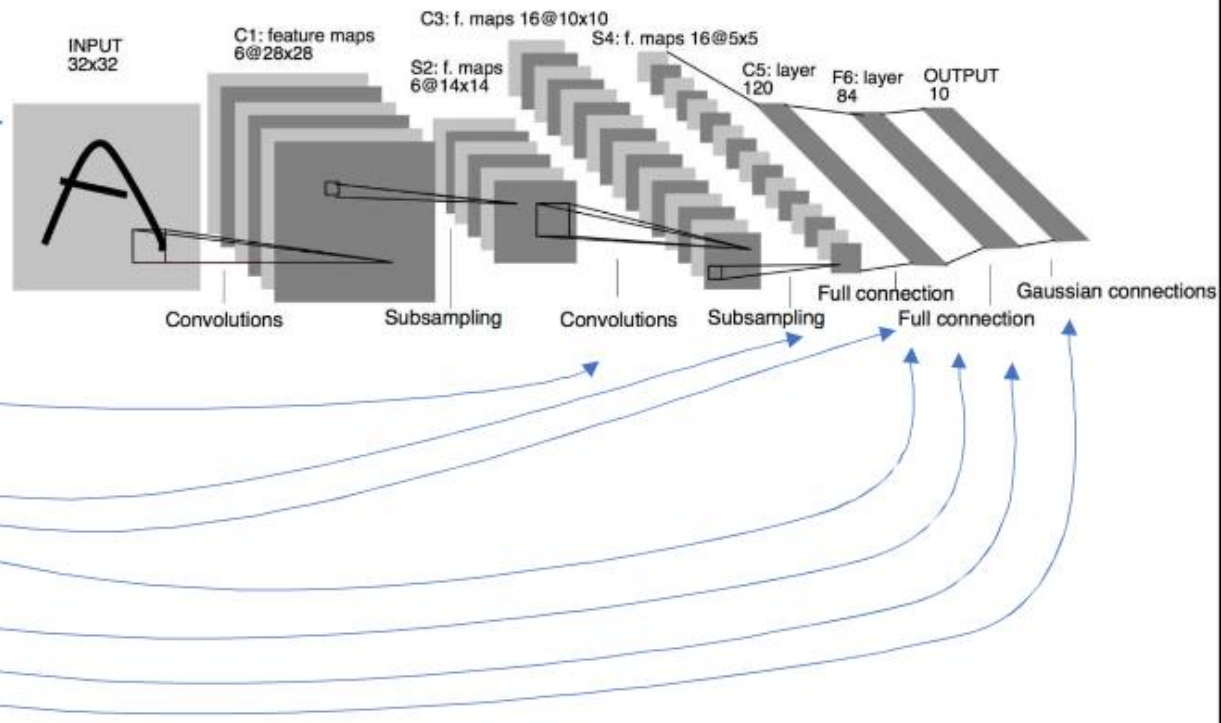


Die Genialität von CNNs besteht folglich darin, große Bilddaten auf kleinste Datenpunkte zu schrumpfen („convolve“), mit dem ein Neuronales Netz effizient arbeiten kann ohne groß Informationen des ursprünglichen Inputs zu verlieren!


Feature Map
-2 -1 -2 -1
-1 -2 -1 1
-2 -1 1 -1
-2 1 -1 -2
0 0 0 0
0 0 0 1
0 0 1 0
0 1 0 0
Max Pooling
0 1
1 1
Input to NN
+ -2
Filter (Convolution)
0
1
1
1
x -0.8
x -0.07
x 0.2
x 0.17
sum
+ 0.97
x -1.33
x 1.33
+ 1.45 = -0.2
+ -0.45 = 1.23

https://poloclub.github.io/cnn-explainer/

```python
import torch
import torch.nn as nn
import torch.nn.functional as F


class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        # 1 input image channel, 6 output channels, 3x3 square convolution
        # kernel
        self.conv1 = nn.Conv2d(1, 6, 3)
        self.conv2 = nn.Conv2d(6, 16, 3)
        # an affine operation: y = Wx + b
        self.fc1 = nn.Linear(16 * 6 * 6, 120)  # 6*6 from image dimension
        self.fc2 = nn.Linear(120, 84)
        self.fc3 = nn.Linear(84, 10)

    def forward(self, x):
        # Max pooling over a (2, 2) window
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))
        # If the size is a square you can only specify a single number
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(-1, self.num_flat_features(x))
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x

    def num_flat_features(self, x):
        size = x.size()[1:]  # all dimensions except the batch dimension
        num_features = 1
        for s in size:
            num_features *= s
        return num_features


net = Net()
print(net)
```



https://pytorch.org/tutorials/beginner/blitz/neural_networks_tutorial.html

– Bernhard Kainz

Layer

nn.Linear(m, n): Fully Connected Layer (oder Dense Layer) von m auf n Neuronen

nn.Flatten(): Reduziert die Dimensionen eines Tensors auf 1

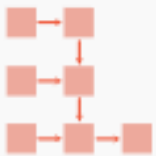
nn.Dropout(p=0.5): Setzt während des Trainings zufällig Eingaben auf 0; hilft Overfitting zu vermeiden

nn.Embedding(m, n): Bildet Indizes aus Verzeichnis mit Größe m auf Vektoren der Dimension n ab

nn.ConvXd(m, n, s): X-dimensionaler Convolution Layer von m auf n Kanäle mit Kernelgröße s; X ∈ {1, 2, 3}

nn.MaxPoolXd(s): X-dimensionaler Pooling Layer mit Kernelgröße s; X ∈ {1, 2, 3}

nn.BatchNormXd(n): Normalisiert einen X-dimensionalen Eingabebatch mit n Features; X ∈ {1, 2, 3}



nn.RNN/LSTM/GRU: Recurrent Networks verbinden Neuronen einer Schicht mit Neuronen derselben oder vorheriger Schichten

torch.nn bietet zudem viele weitere Bausteine.
"State of the art"-Architekturen gibt es unter https://paperswithcode.com/sota

Daten laden

Ein Datensatz wird durch eine Klasse repräsentiert, die von **Dataset** erbt (Liste von (Features, Label)-Tupeln).

Mit **DataLoader** erfolgt das Laden strukturunabhängig in Batches.

Üblicherweise wird der Datensatz in Trainings- (z.B. 80%) und Testdaten (z.B. 20%) aufgeteilt.

```
from torch.utils.data
 import Dataset, TensorDataset,
        DataLoader, random_split

train_data, test_data =
 random_split(
    TensorDataset(inps, tgts),
    [train_size,test_size]
 )

train_loader =
      DataLoader(
         dataset=train_data,
         batch_size=16,
         shuffle=True)
```

Aktivierungsfunktionen

Zu den häufigsten Aktivierungsfunktionen zählen **ReLU**, **Sigmoid** und **Tanh**. Daneben existieren noch eine Reihe weiterer Aktivierungsfunktionen.

nn.ReLU() *erzeugt ein* **nn.Module** *etwa für Sequential Modelle.* **F.relu()** *ist nur Aufruf der ReLU Funktion etwa für eine Verwendung in der* **forward** *Methode.*

nn.ReLU() oder **F.relu()**

Ausgabe zwischen 0 und ∞,
häufigste Aktivierungsfunktion

nn.Sigmoid() oder **F.sigmoid()**

Ausgabe zwischen 0 und 1,
oft für Wahrscheinlichkeiten verwendet

nn.Tanh() oder **F.tanh()**

Ausgabe zwischen -1 und 1,
oft für zwei Klassen verwendet

Modelldefinition

Es gibt verschiedene Wege ein neuronales Netz in PyTorch zu definieren, z.B. mit **nn.Sequential** (a), als Klasse (b) oder auch als Kombination aus beidem.

```
model = nn.Sequential(
    nn.Conv2D(■,■,■)
    nn.ReLU()
    nn.MaxPool2D(■)
    nn.Flatten()
    nn.Linear(■,■)
)
```

a

```
class Net(nn.Module):
  def __init__():
    super(Net, self).__init__()

      self.conv
        = nn.Conv2D(■,■,■)

      self.pool
        = nn.MaxPool2D(■)

      self.fc = nn.Linear(■,■)

  def forward(self, x):
      x = self.pool(
            F.relu(self.conv(x))
          )

      x = x.view(-1,■)

      x = self.fc(x)

    return x
model = Net()
```

b

Training

VERLUSTFUNKTION

PyTorch bietet bereits verschiedene Möglichkeiten den Fehler zu berechnen, u.a.:

nn.L1Loss	Mittlerer absoluter Fehler
nn.MSELoss	Mittlere quadratische Abweichung (L2Loss)
nn.CrossEntropyLoss	Kreuzentropie, u.a. für Single-Label, unausgewogene Trainingsdaten
nn.BCELoss	Binäre Kreuzentropie, u.a. für Multi-Label oder Autoencoder

OPTIMIERUNGSALGORITHMEN (torch.optim)

Optimierungsalgorithmen werden genutzt, um im Gradientenabstiegsverfahren Gewichte zu aktualisieren und die Lernrate dynamisch anzupassen, u.a.:

optim.SGD	Stochastic Gradient Descent
optim.Adam	Adaptive Moment Estimation
optim.Adagrad	Adaptive Gradient
optim.RMSProp	Root Mean Square Prop

Auf zu Colab!

Supervised Learning with scikit-learn

Rückblick: Was haben wir alles in diesem Wahlfach gelernt?

Grundlagen von Python:

- Grundlegendes Verständnis der Python Syntax
- lists, dictionaries, functions, if/else, for-loops
- matplotlib zur Darstellung Graphen
- Pandas DataFrames

Supervised Learning mit scikit-learn:

- Classification: k-nearest-neighbors
- Regression: linear regression, lasso
- Statistik: overfitting/underfitting, cross-validation, AUROC, Confusion-Matrix

Classification und Regression Trees:

- Decision Trees
- Random Forest

Grundlagen zu Neuronalen Netzen

FAQ: Woher habe ich die ganzen Datensätze?

Tutorials

Python

- https://geeksforgeeks.org/python-basics/
- https://coursera.org/specializations/python
- https://codecademy.com/learn/learn-python

Machine Learning and Deep Learning

- https://coursera.org/learn/machine-learning
- https://coursera.org/specializations/deep-learning
- https://pytorch.org/tutorials/
- https://youtube.com/playlist?list=PLTuOKAhhBkunnUQlOYD0PtxC7EZk2TQMv
- https://course.fast.ai
- https://nvidia.com/en-us/deep-learning-ai/education/
- https://d2l.ai/
- https://explained.ai/
- https://deeplearningbook.org/
- https://lelon.io/blog/2018/02/08/pytorch-with-baby-steps

codecademy

datacamp

CS4MS - S23

This repository contains the exercises - provided in form of Jupyter notebooks - for the course CS4MS taught in the summer semester of 2023.

How to Run

Refer to the colab_setup for running the notebooks on Google Colaboratory.

Python and machine learning tutorials

More information and additional material can be found here Summary of Tutorials.


szmuenchen
Markus Söder
Ministerpräsident
„Die TU ist eine der geilsten Unis, die es überhaupt gibt, echt. Die LMU ist größer, ist auch super, aber die TUM ist schon ein sehr schnittiges Schiffchen."
Foto: Robert Haas
Süddeutsche Zeitung

Bitte evaluieren!