From where do Neural Networks derive their power ?

Neural Networks seem to be more powerful than the models obtained from Classical Machine Learning.

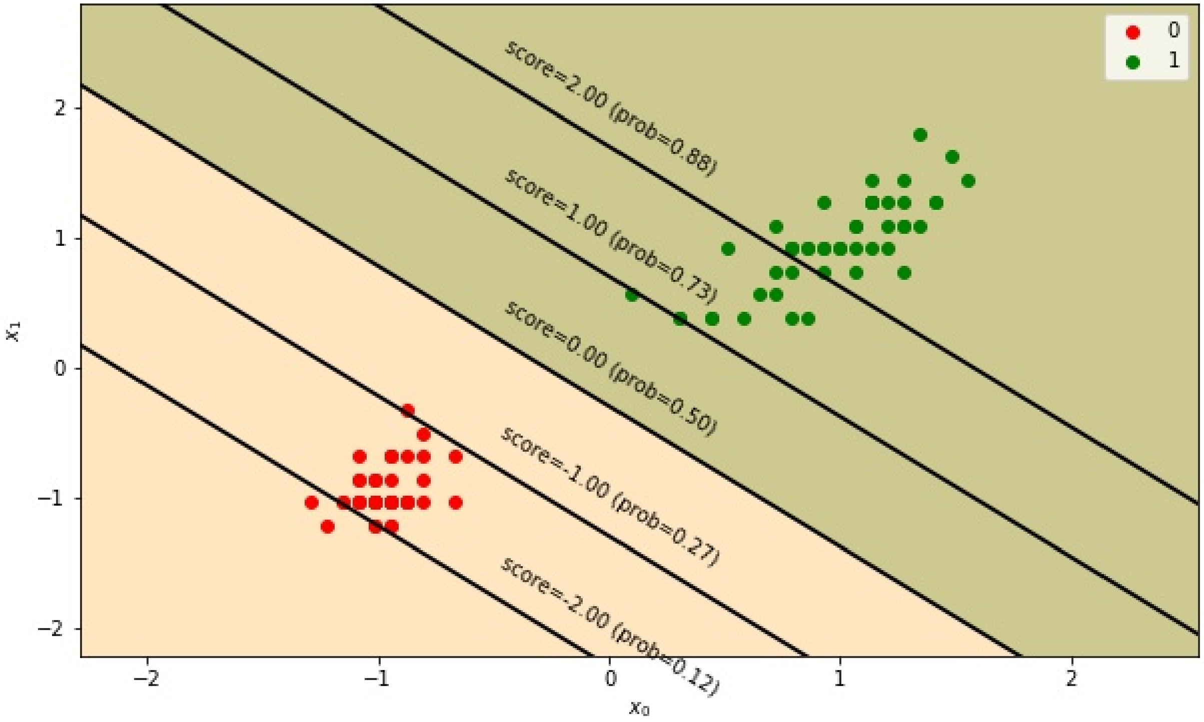
Why might that be ?

To be concrete: let us consider the Classification task.

A Classifier can be viewed as creating a decision boundary

- regions within feature space (e.g., $\mathbb{R}^n$) in which all examples have the same Class.

For example, a linear classifier like Logistic Regression creates linear boundaries



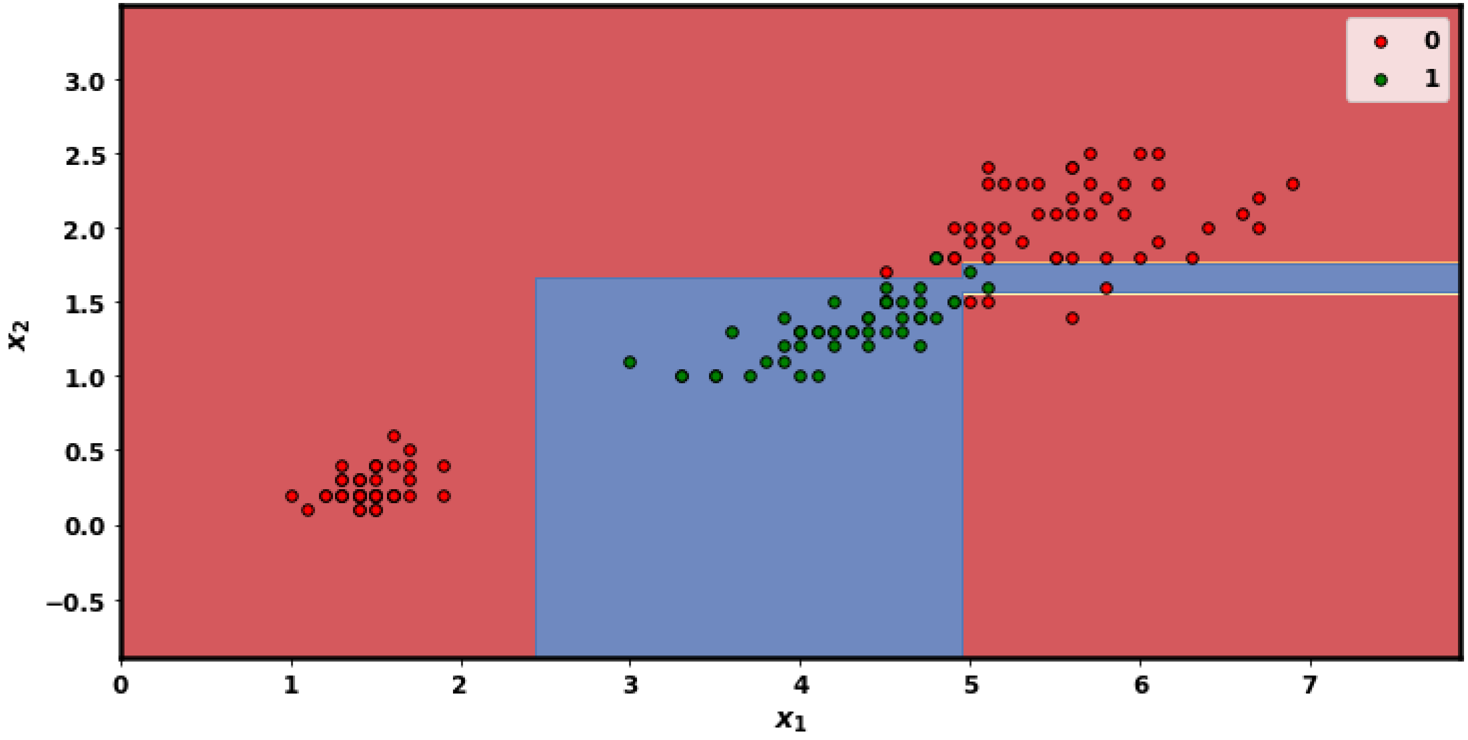
The boundaries of Decision Trees are more complex, but are perpendicular to one feature axis

- due to the nature of the question that labels a node n of the tree

$$\mathbf{x}_j^{(\mathbf{i})} < t_{\mathrm{n},j}$$

In [5]:
```
X_2c, y_2c = bh.make_iris_2class()

fig, ax = plt.subplots(figsize=(12,6))
_= bh.make_boundary(X_2c, y_2c, depth=4, ax=ax)
```



As we will see:

- the shape of decision boundaries (and functions, for Regression tasks) created by Neural Networks can be much more complex
- the complexity is obtained due to the non-linear activation functions

The power of non-linear activation functions

In our introduction to Neural Networks, we identified non-linear activation functions as a key ingredient.

Let's examine, in depth, why this is so.

Many activation functions behave like a binary "switch"

- Converting the scalar value computed by the dot product
- Into a True/False answer
- To the question: "Is a particular feature present" ?

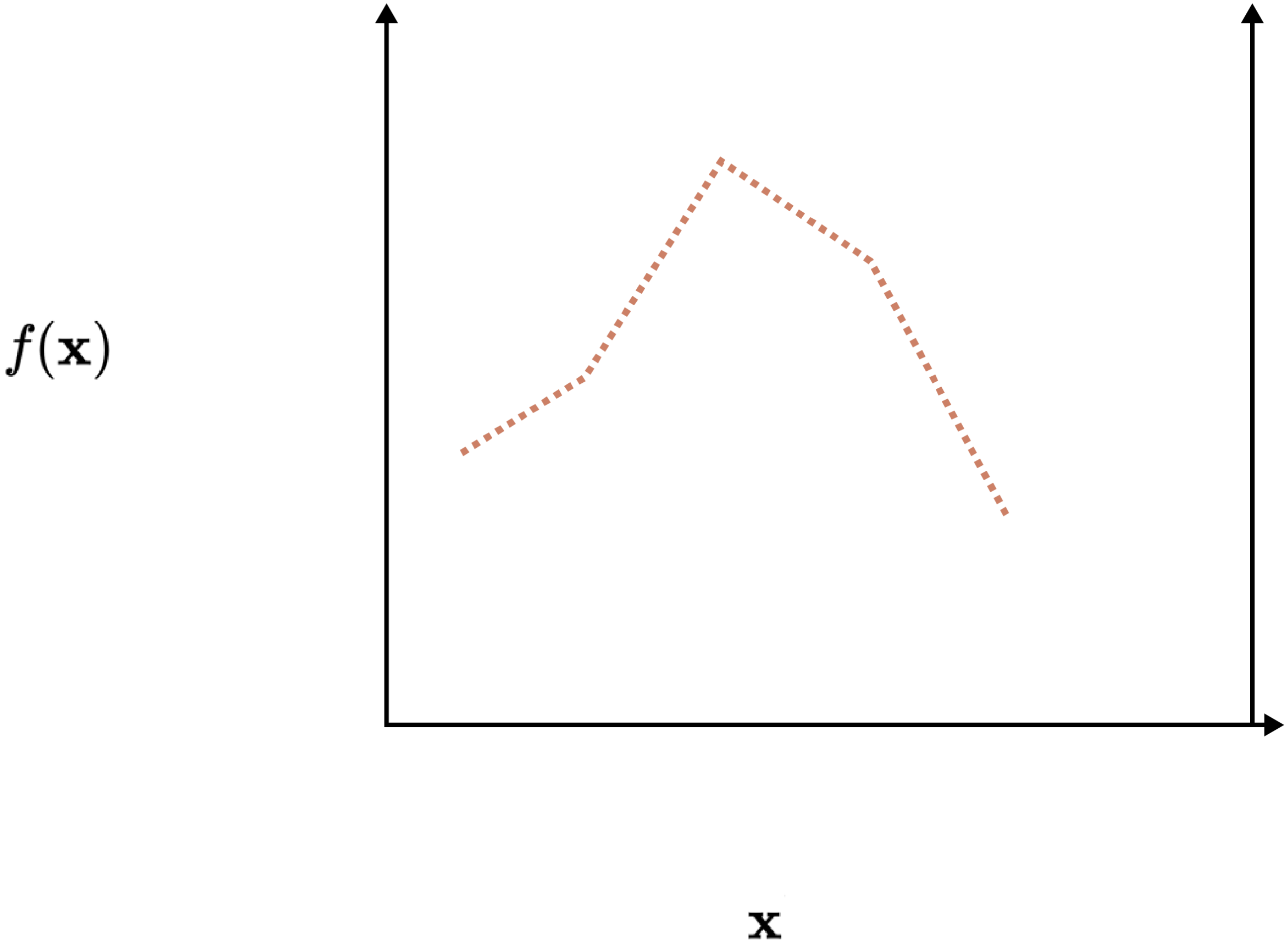
By changing the "bias" from 0, we can move the threshold of the switch to an arbitrary value.

This allows us to construct a *piece-wise* approximation of a function

- The switch, in the region in which it is active, defines one piece
- Changing the bias/threshold allows us to relocate the piece

Consider the following function f:

Function to approximate

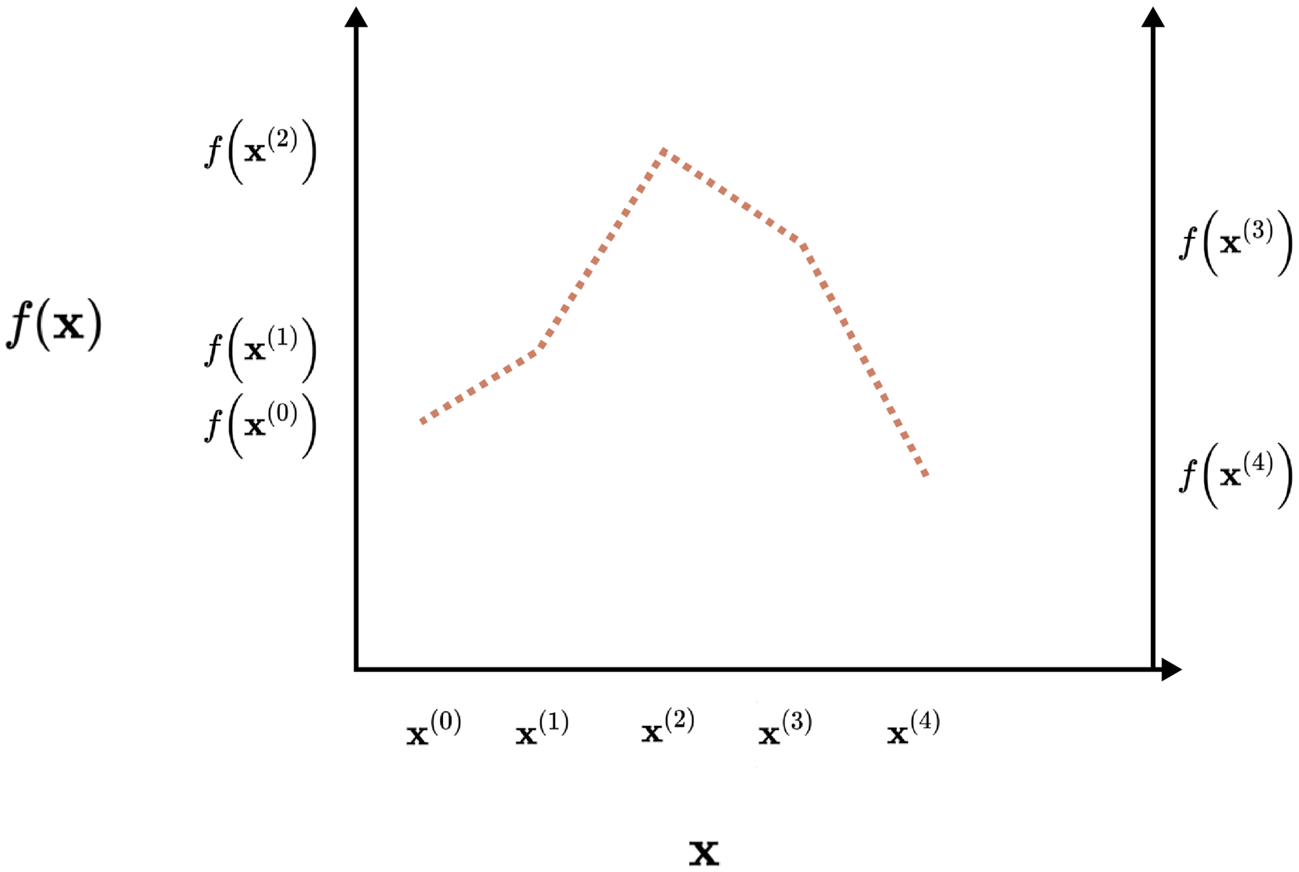


This function is

- Not continuous
- Define over set of discrete examples
$$\langle \mathbf{X}, \mathbf{y} \rangle = [\mathbf{x^{(i)}}, \mathbf{y^{(i)}} | 1 \le i \le m]$$

For ease of presentation, we will assume the examples are sorted in increasing value of $\mathbf{x^{(i)}}$:
$$\mathbf{x}^{(0)} < \mathbf{x}^{(1)} < \ldots \mathbf{x}^{(m)}$$

Function to approximate, defined by examples x



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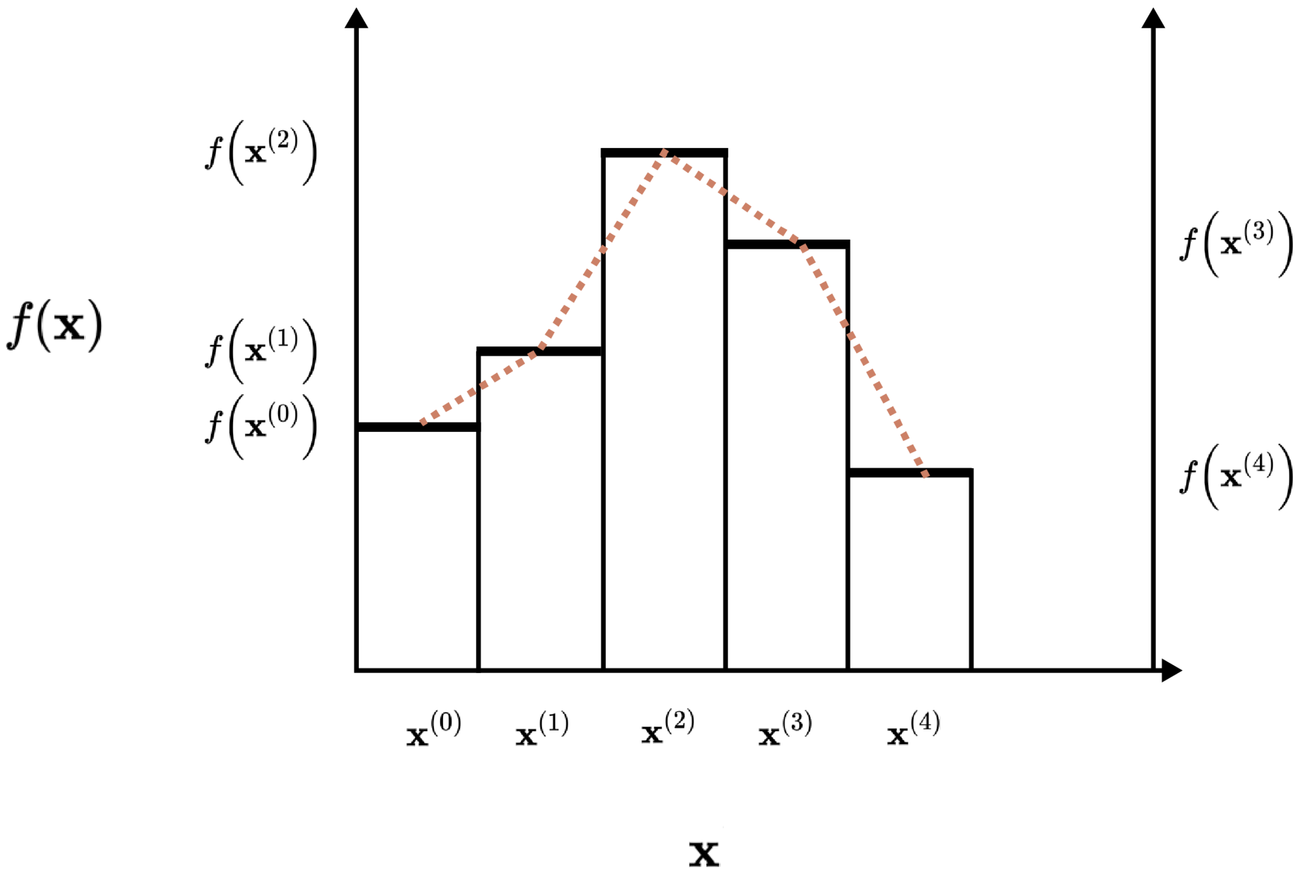
We can replicate the discrete function

- By a sequence of *step functions*
- Which create a piece-wise approximation of the function f

Piece-wise function approximation by step functions



We will show how to construct a step function using

- Dot product
- ReLU activation with 0 threshold

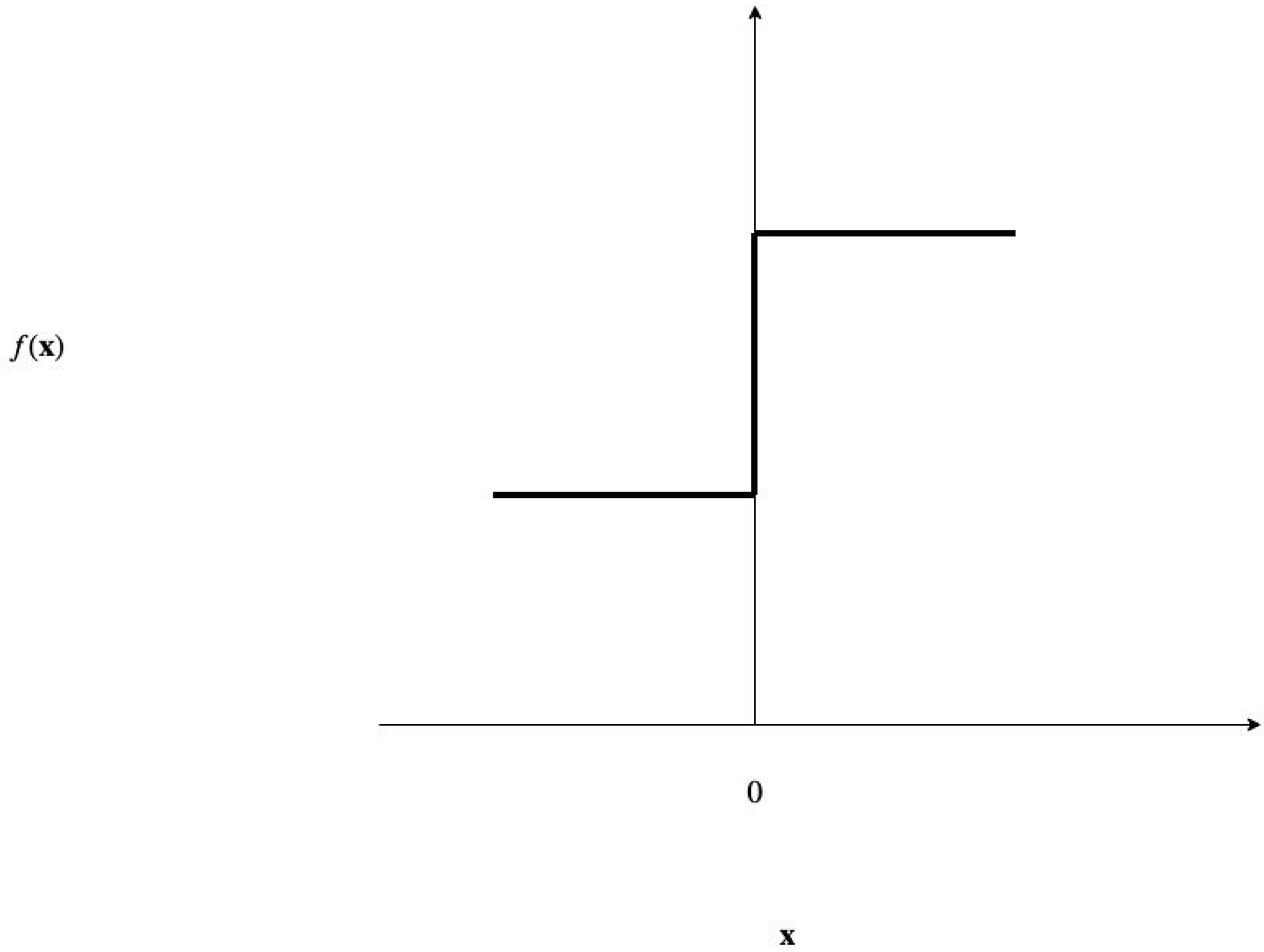
Once we have a step, we can place the center of the step anywhere along the $\mathbf{x}$ axis

- By adjusting the threshold of the ReLU

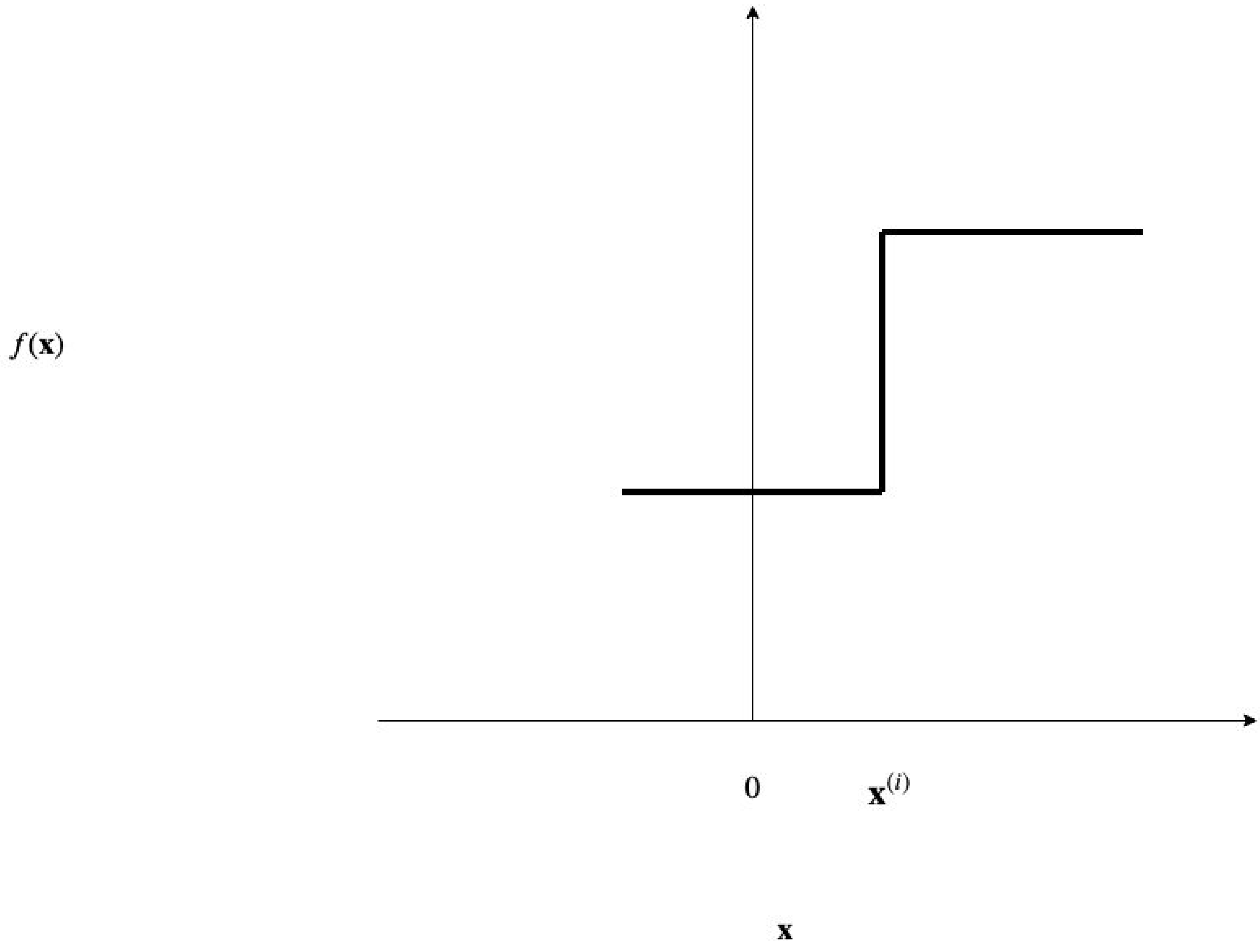
The plan is:

- Construct a step function for the i^{th} example
- Step i becomes "active" when its input is at least $\mathbf{x^{(i)}}$, using the bias of the ReLU
- Height of i^{th} step is $f(\mathbf{x^{(i)}})$
- The amount by which $f(\mathbf{x})$ increases between steps is $(f(\mathbf{x}^{(i+1)}) - f(\mathbf{x^{(i)}}))$

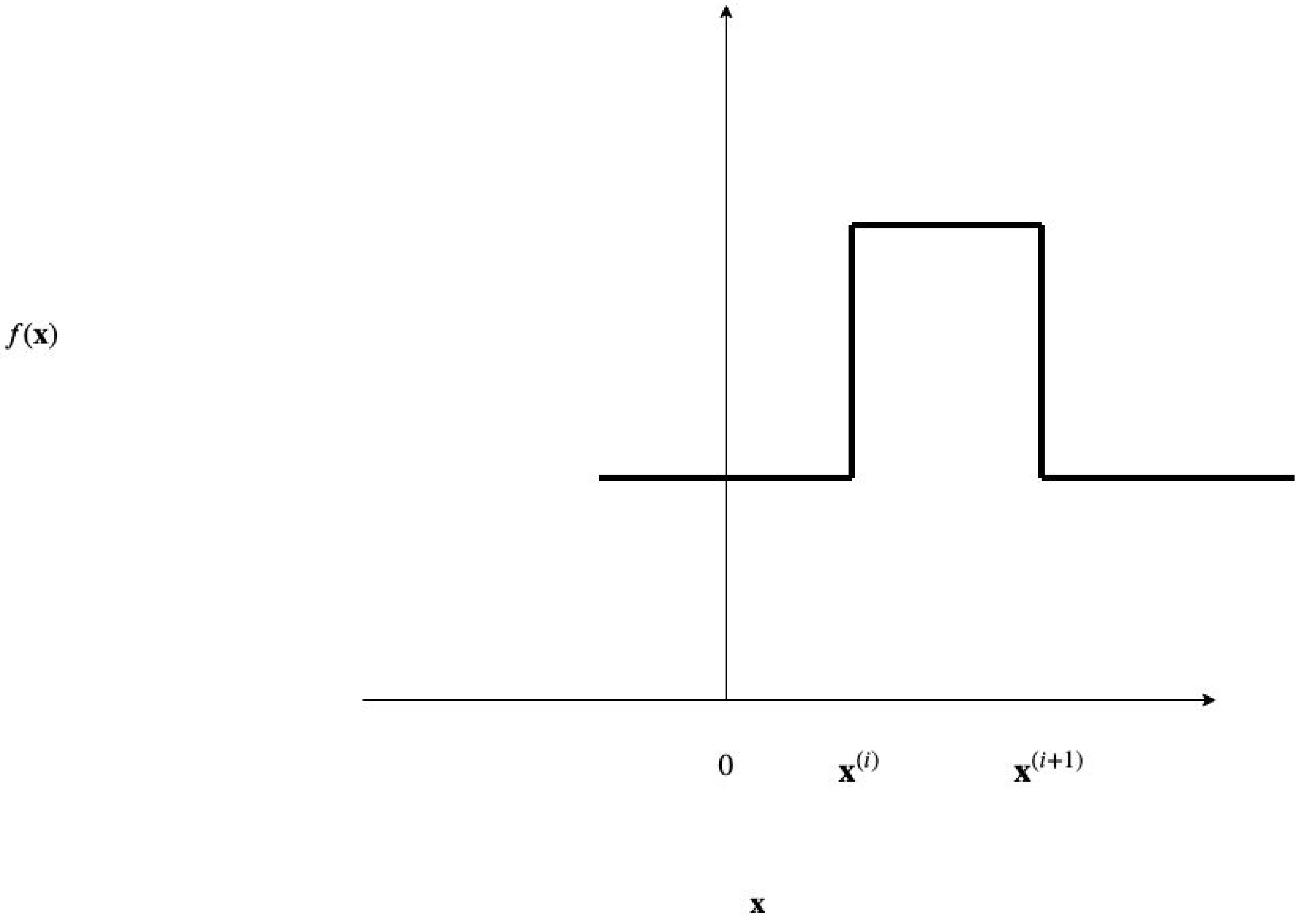
Step function: binary switch with threshold 0



Step function: binary switch with threshold - x^(i)



Impulse function: Center xˆ(i); width (xˆ(i+1) - xˆ(i))



That's the idea at a very intuitive level.

The rest of the notebook demonstrates exactly how to achieve this.

Universal function approximator

A Neural Network is a Universal Function Approximator.

This means that an NN that is sufficiently

- wide (large number of neurons per layer)
- and deep (many layers; deeper means the network can be narrower)

can approximate (to arbitrary degree) the function represented by the training set.

Recall that the training data $\langle \mathbf{X}, \mathbf{y} \rangle = [(\mathbf{x^{(i)}}, \mathbf{y^{(i)}}) | 1 \le i \le m]$ is a sequence of input/target pairs.

This may look like a strange way to define a function

- but it is indeed a mapping from the domain of $\mathbf{x}$ (i.e., $\mathcal{R}^n$) to the domain of $\mathbf{y}$ (i.e., $\mathcal{R}$)
- subject to $\mathbf{y}^i = \mathbf{y}^{i'} \text{ if } \mathbf{x}^i = \mathbf{x}^{i'}$ (i.e., mapping is unique).

We give an intuitive proof for a one-dimensional function

- all vectors $\mathbf{x}, \mathbf{y}, \mathbf{W}, \mathbf{b}$ are length 1.

For simplicity, let's assume that the training set is presented in order of increasing value of $\mathbf{x}$, i.e.

$$\mathbf{x}^{(0)} < \mathbf{x}^{(1)} < \ldots \mathbf{x}^{(m)}$$

Consider a single neuron with a ReLU activation, computing

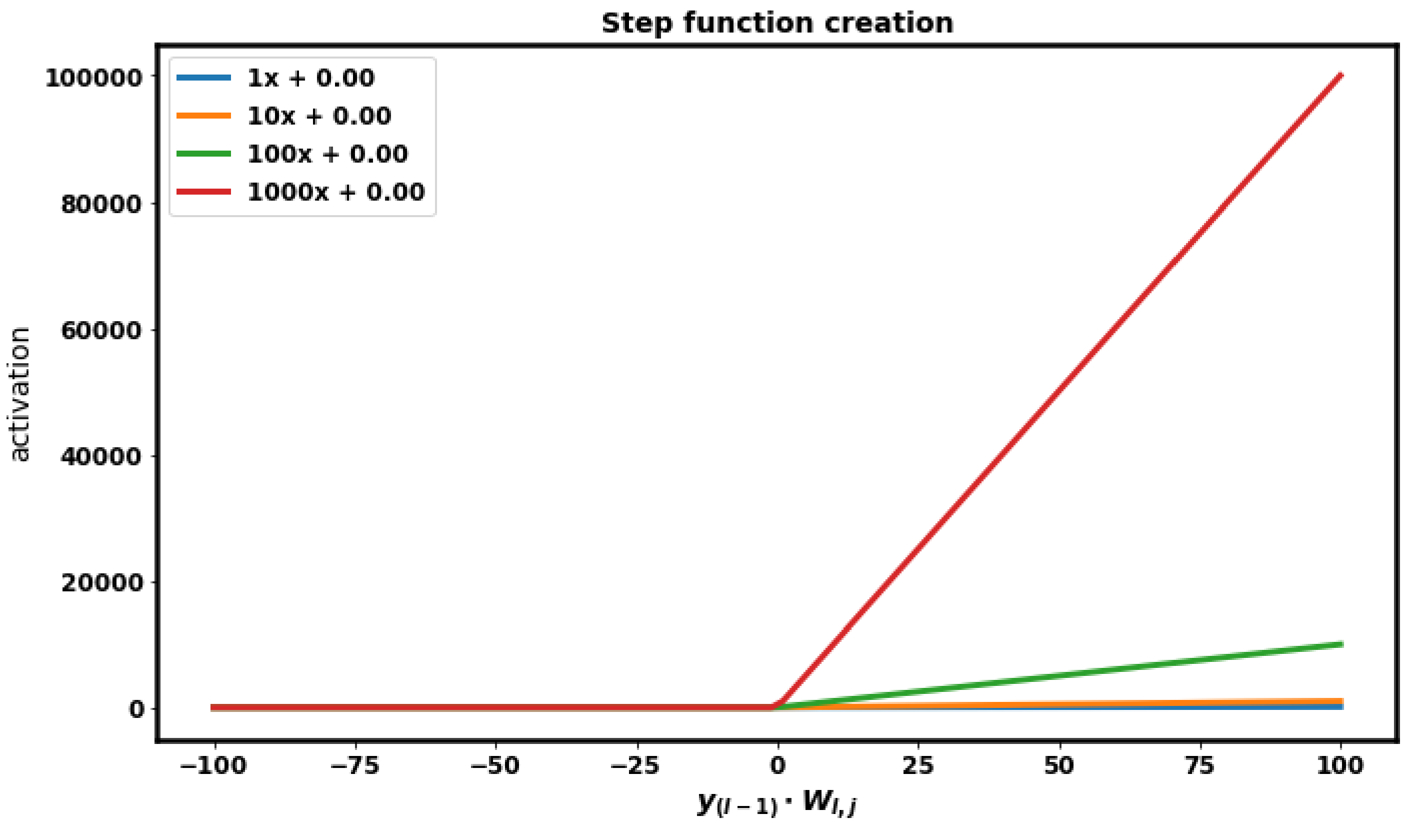
$$\max(0, \mathbf{W}\mathbf{x} + \mathbf{b})$$

Let's plot the output of this neuron, for varying $\mathbf{W}, \mathbf{b}$.

The slope of the neuron's activation is $\mathbf{W}$ and the intercept is $\mathbf{b}$.

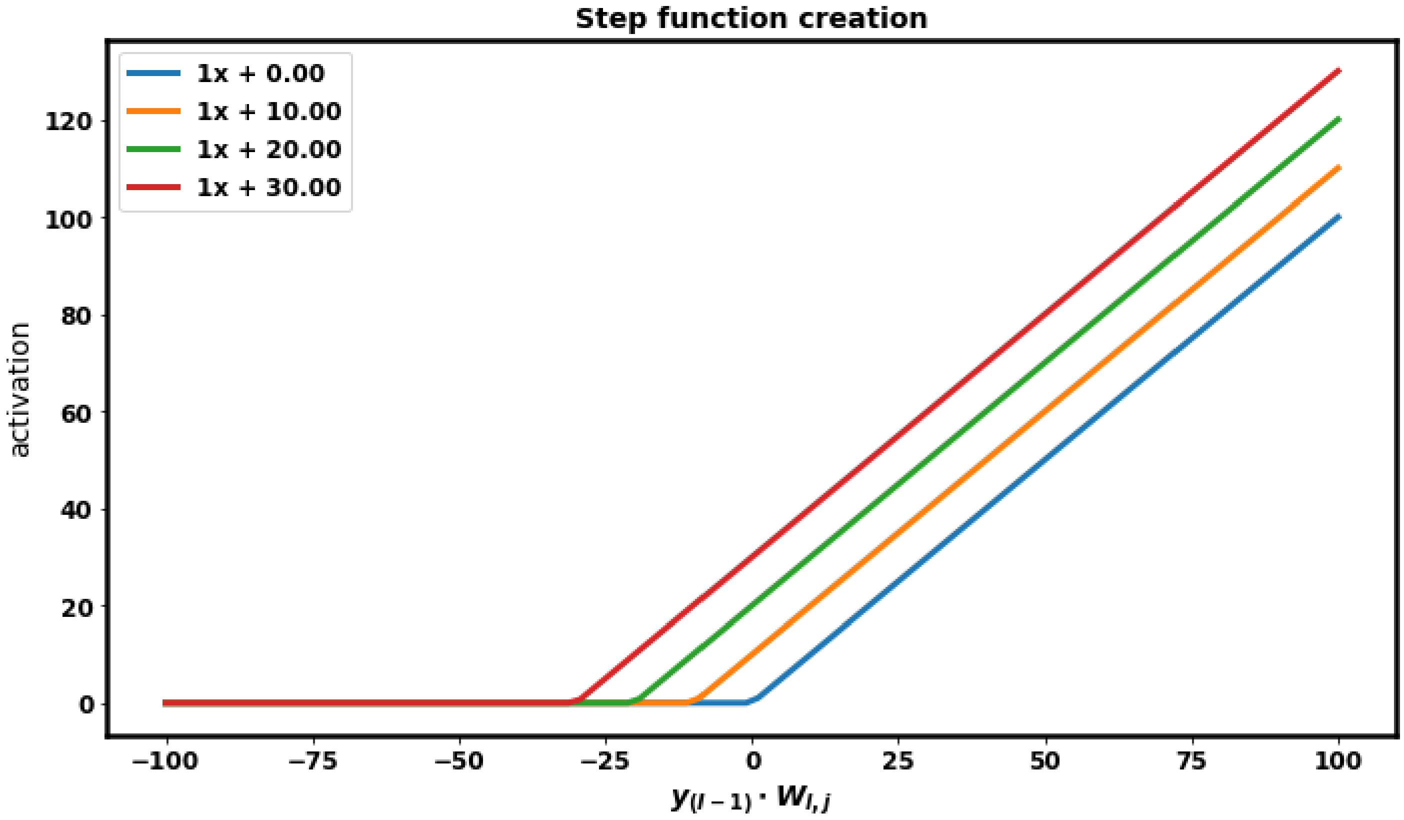
By making slope $\mathbf{w}$ extremely large, we can approach a vertical line.

In [6]:
```
_ = nnh.plot_steps( [ nnh.NN(1,0), nnh.NN(10,0), nnh.NN(100,0), nnh.NN(1000,0),
])
```



And by varying the intercept (bias) we can shift this vertical line to any point on the feature axis.

In [7]:
```
_ = nnh.plot_steps( [ nnh.NN(1,0), nnh.NN(1,10), nnh.NN(1,20), nnh.NN(1,30), ])
```



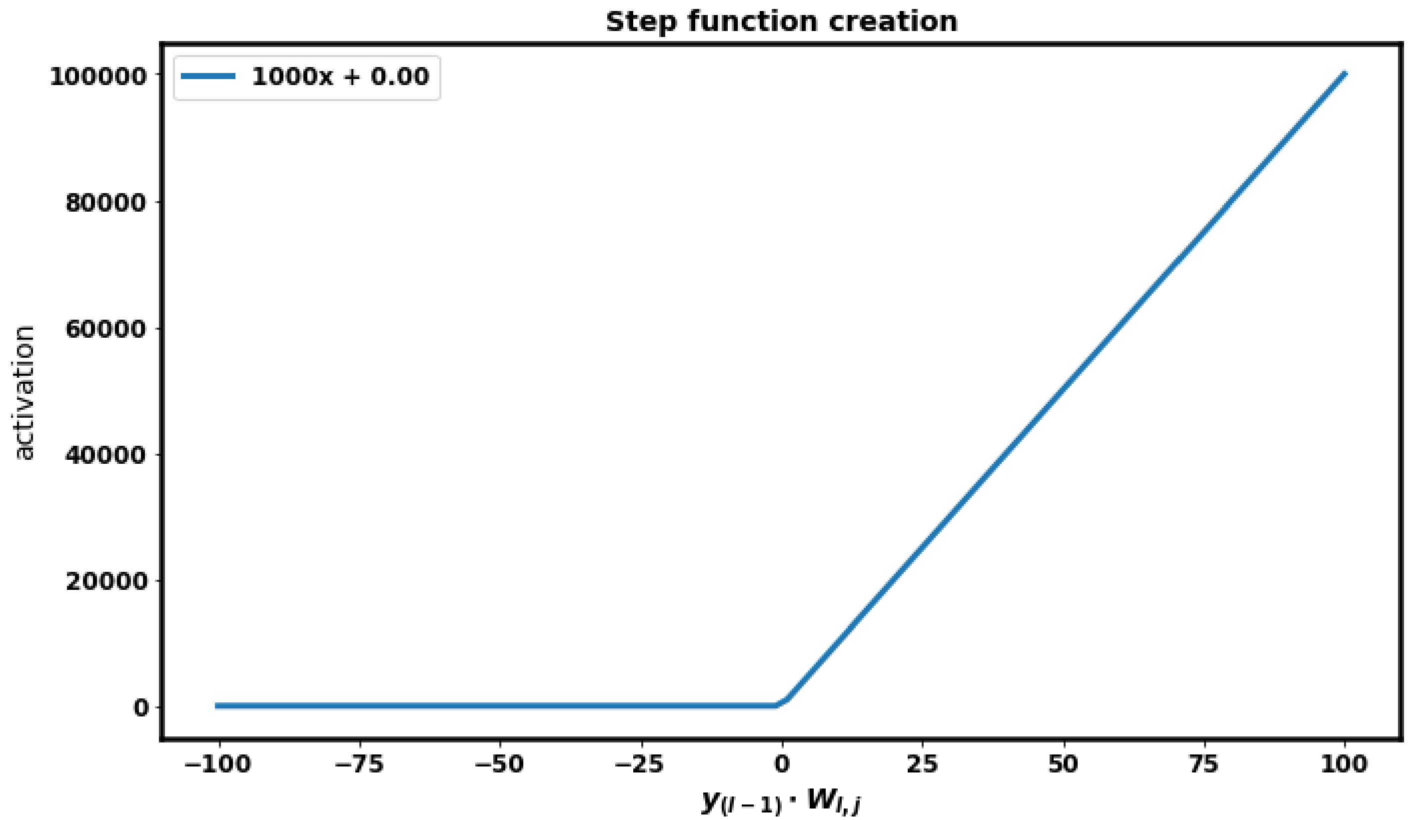
With a little effort, we can construct a neuron

- With near infinite slope
- Rising from the x-axis at any offset.

In [8]:
```
slope = 1000
start_offset = 0

start_step = nnh.NN(slope, -start_offset)

_= nnh.plot_steps( [  start_step ] )
```



If we create a neuron with intercept "epsilon" from the first neuron

In [9]:

```
end_offset = start_offset + .0001

end_step = nnh.NN(slope,- end_offset)
```

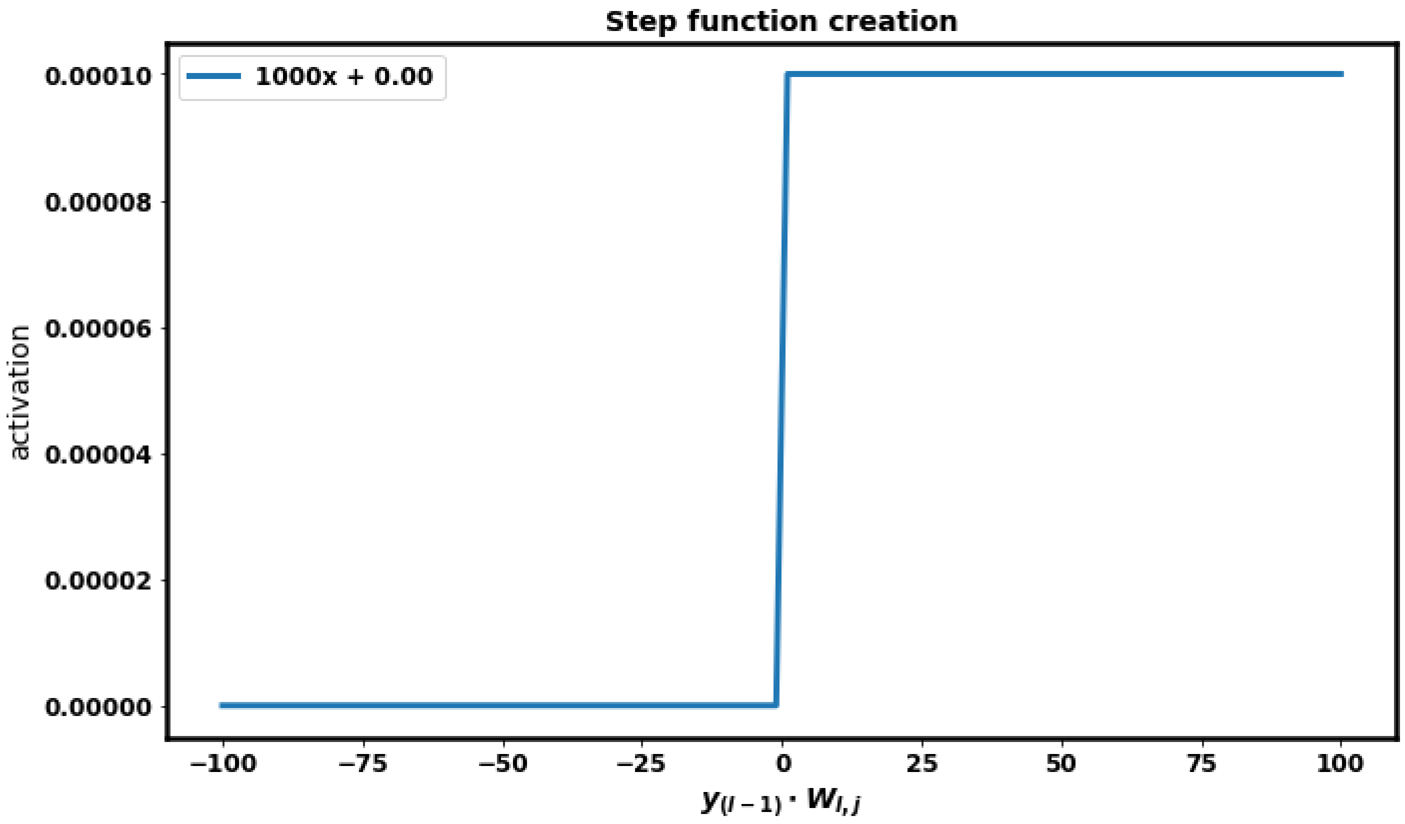
and add the two neurons together, we can approximate a step function

- unit height
- 0 output at inputs less than the x-intercept
- unit output for all inputs greater than the intercept).

(The sigmoid function is even more easily transformed into a step function).

In [10]:

```
step= {"x": start_step["x"],
       "y": start_step["y"] - end_step["y"],
       "W": slope,
       "b": 0
      }
_= nnh.plot_steps( [  step ] )
```



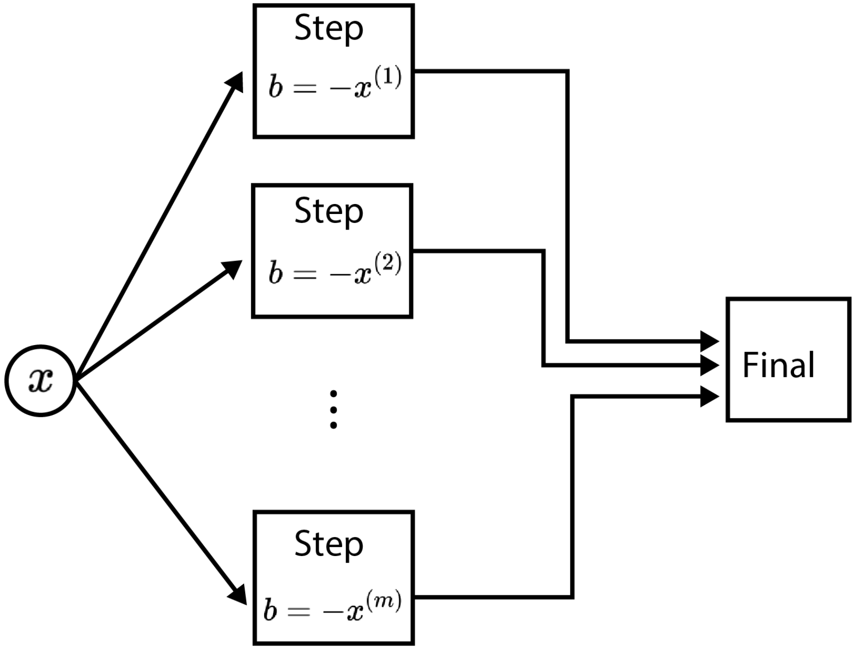
Let us construct m step neurons

- step neuron i with intercept $\mathbf{x^{(i)}}$, for $1 \le i \le m$

If we connect the m step neurons to a "final" neuron with 0 bias, linear activation, and weights

$$\begin{array}{lll} \mathbf{W}_1 & = & \mathbf{y}^{(1)} \\ \mathbf{W}_i & = & \mathbf{y}^{(i)} - \sum_{i'=1}^{i-1} \mathbf{W}_{i'} \end{array}$$

Function Approximation by Step functions



$$W_1 = y^{(1)}$$
$$W_2 = y^{(2)} - y^{(1)}$$
$$W_i = y^{(i)} - \sum_{i'=1}^{i-1} y^{(i')}$$

We claim that the output of this neuron approximates the training set.

To see this:

- Consider what happens when we input $\mathbf{x}^{(\mathbf{i})}$ to this network.
- The only step neurons that are active (non-zero) are those corresponding to inputs $1 \leq i' \leq i$.
- The output of the final neuron is the sum of the outputs of the first i step neurons.
- By construction, this sum is equal to $\mathbf{y}^{(\mathbf{i})}$.

Thus, our two layer network outputs $\mathbf{y}^{(\mathbf{i})}$ given input $\mathbf{x}^{(\mathbf{i})}$.

Financial analogy: if we have call options with completely flexible strikes and same expiry, we can mimic an arbitrary payoff in a similar manner.

In [11]:
```
print("Done")
```

```
Done
```