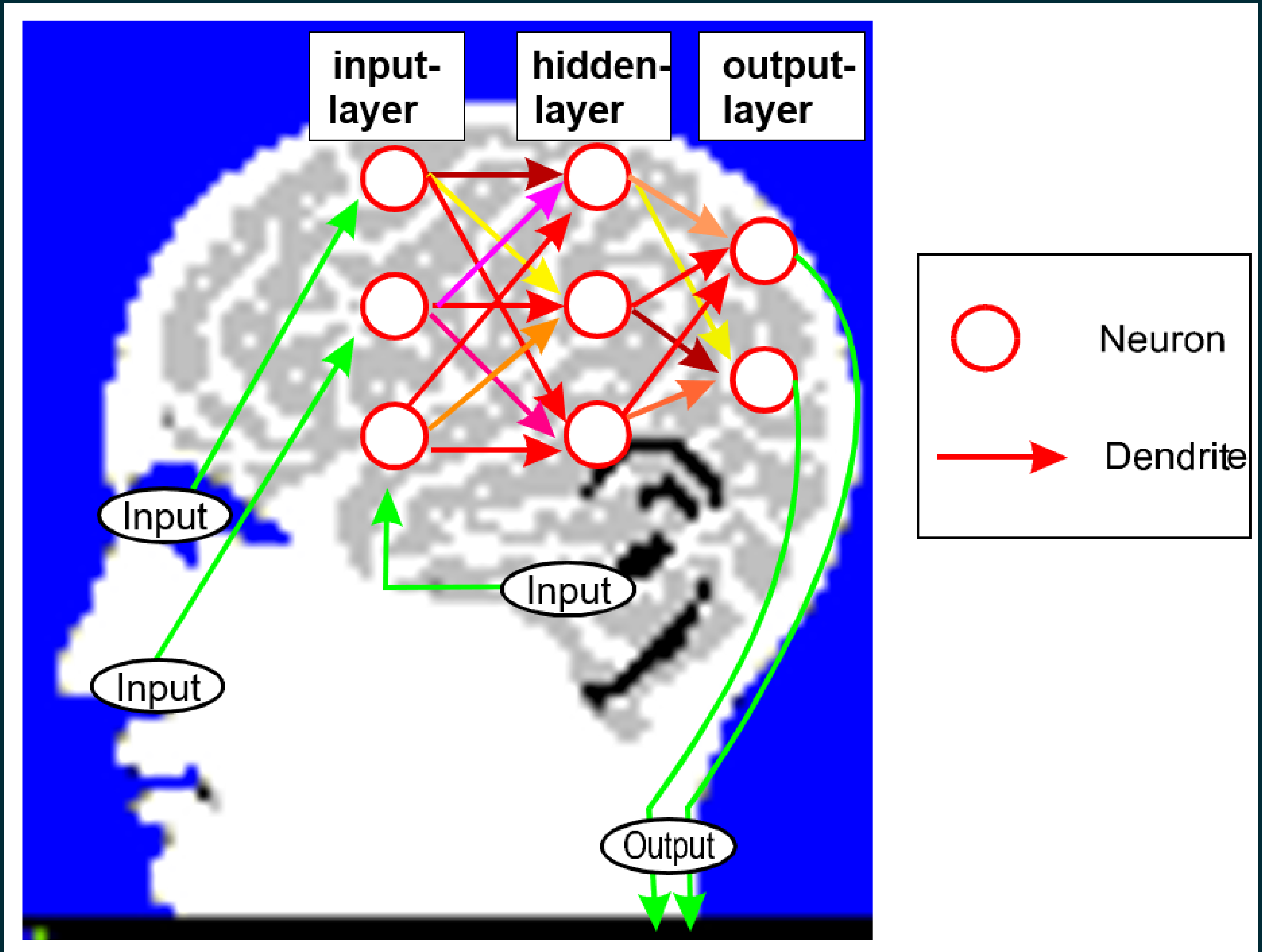
# NEURAL NETWORKS

# THE EARLY DAYS

In the early days of artificial neural networks, data scientists tried to mimic the human brain through computer models.



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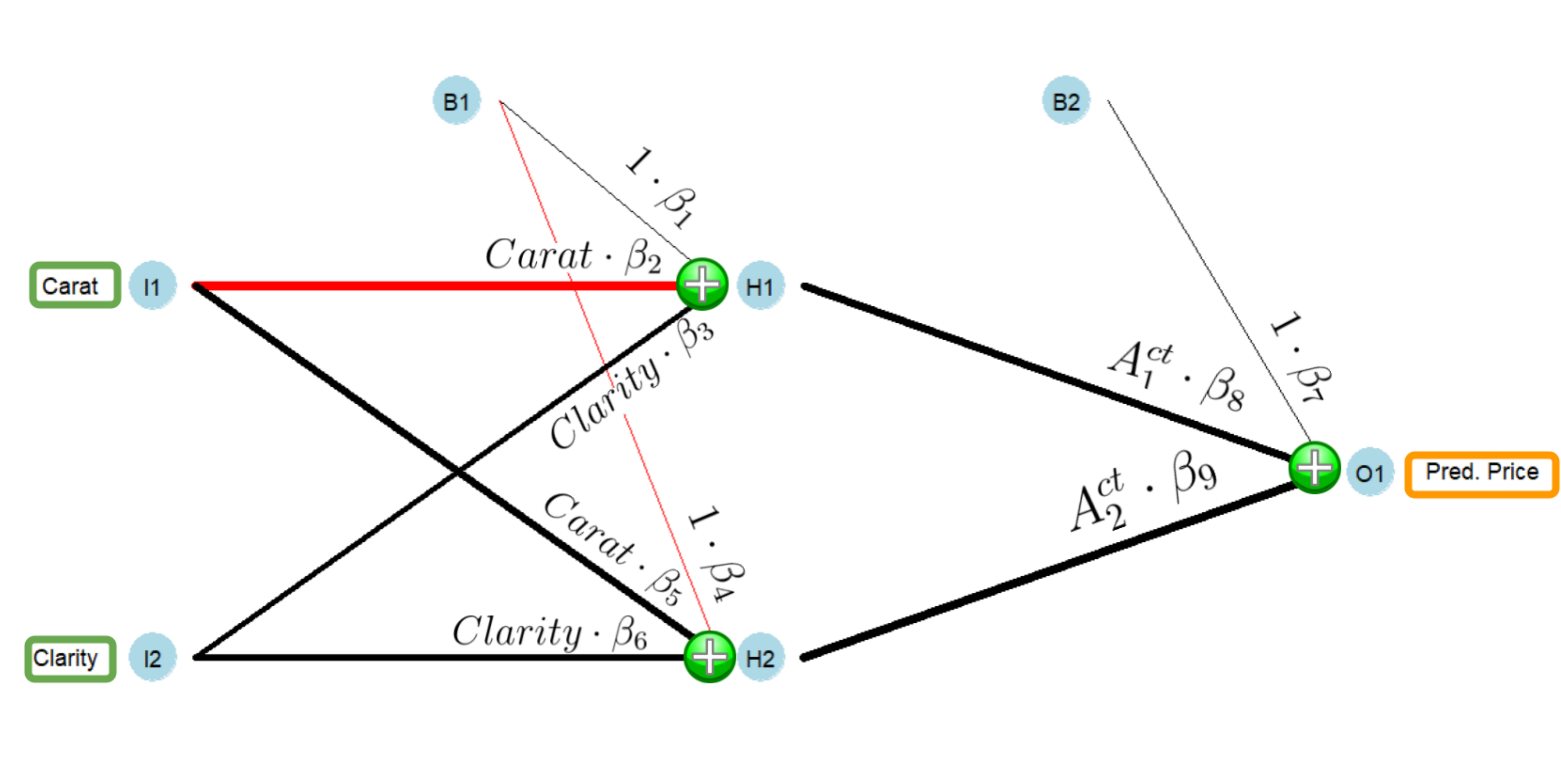
# TYPES OF NEURAL NETWORKS

- **Multi-Layer Perceptrons (MLP)** neural networks (covered here)
- Convolutional Neural Networks (CNN)
- Recurrent Neural Networks (e.g. Long Short Term Memory recurrent networks)
- Generative Adversarial Networks
- AutoEncoders
- Transformers»

# MULTI-LAYER PERCEPTRONS (MLP) NEURAL NETWORK

- **Input Layer:** with one or more input neurons.
- **Hidden Layer(s)** one or more hiden layers with one or more hidden neurons.
- **Output Layer:** with one or more output neurons.
- **Fully connected:** each neuron in each of the layers is connected to all neurons of the following layer.

# EXAMPLE FOR AN MLP NEURAL NETWORK WITH ONE HIDDEN LAYER



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# THE DATA

We will estimate diamond prices based on their physical properties and use the well-known `diamonds` dataset automatically loaded together with `tidymodels`:

▶ Code

```
tibble [53,940 × 10] (S3: tbl_df/tbl/data.frame)
 $ carat  : num [1:53940] 0.23 0.21 0.23 0.29 0.31 0.24 0.24 0.26 0.22 0.23 ...
 $ cut    : Ord.factor w/ 5 levels "Fair"<"Good"<..: 5 4 2 4 2 3 3 3 1 3 ...
 $ color  : Ord.factor w/ 7 levels "D"<"E"<"F"<"G"<..: 2 2 2 6 7 7 6 5 2 5 ...
 $ clarity: Ord.factor w/ 8 levels "I1"<"SI2"<"SI1"<..: 2 3 5 4 2 6 7 3 4 5 ...
 $ depth  : num [1:53940] 61.5 59.8 56.9 62.4 63.3 62.8 62.3 61.9 65.1 59.4 ...
 $ table  : num [1:53940] 55 61 65 58 58 57 57 55 61 61 ...
 $ price  : int [1:53940] 326 326 327 334 335 336 336 337 337 338 ...
 $ x      : num [1:53940] 3.95 3.89 4.05 4.2 4.34 3.94 3.95 4.07 3.87 4 ...
 $ y      : num [1:53940] 3.98 3.84 4.07 4.23 4.35 3.96 3.98 4.11 3.78 4.05 ...
 $ z      : num [1:53940] 2.43 2.31 2.31 2.63 2.75 2.48 2.47 2.53 2.49 2.39 ...
```

# DOMAIN KNOWLEDGE: THE FOUR C S TO APPRAISE A DIAMOND

1. **Cut:** Refers to the facets, symmetry, and reflective qualities of a diamond. The cut of a diamond is directly related to its overall sparkle and beauty.
2. **Color:** Refers to the natural color or lack of color visible within a diamond. The closer a diamond is to “colorless,” the higher its value.
3. **Clarity:** Is the visibility of natural microscopic inclusions and imperfections within a diamond. Diamonds with little to no inclusions are considered particularly rare and highly valued.
4. **Carat:** Is the unit of measurement used to describe the weight of a diamond. It is often the most visually apparent factor when comparing diamonds.

# DATA ENGENEERING

We start with a very basic model with 2 predictors for \(Price\):

- \(Carat\) (the weight of the diamond in metric grams),
- \(Clarity\) (eight categories with \(8\) being the best).

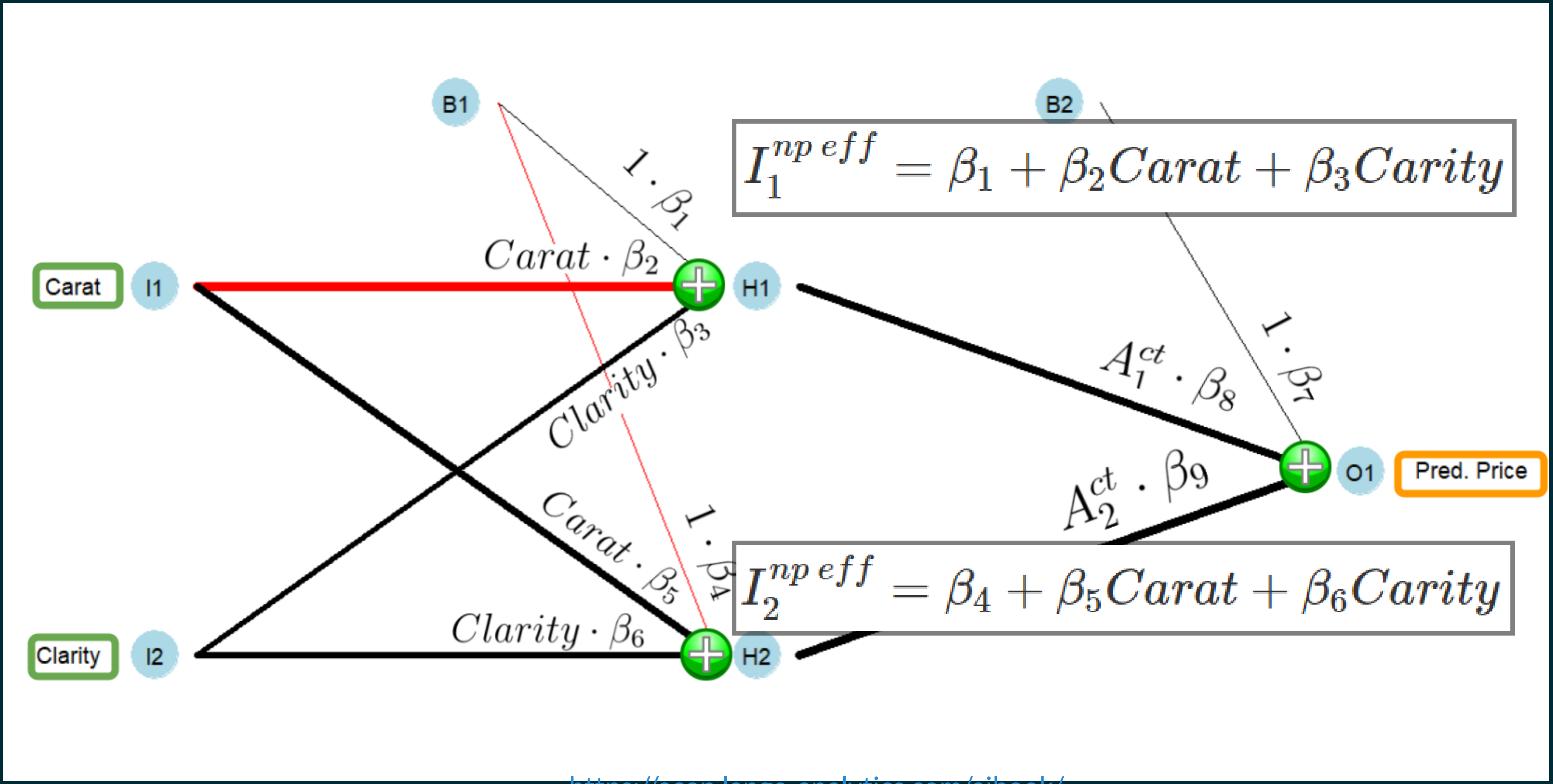
To later increase training speed, we use only 10,000 observations.

▶ Code

```
# A tibble: 6,999 × 3
   Price Carat Clarity
   <int> <dbl>   <int>
 1   506  0.3        3
 2   628  0.28       6
 3   753  0.3        7
 4   766  0.3        6
 5   552  0.35       5
 6   743  0.33       5
 7   698  0.31       4
 8   526  0.3        4
 9   675  0.3        5
10   544  0.31       4
# … with 6,989 more rows
```

# USE A TRAINED NEURAL NEWORK (\(\BETA S\) ARE KNOWN) TO PREDICT

## Effectiv Inputs to Hidden Neurons:



$$I_1^{np\,eff} = \beta_1 + \beta_2 Carat + \beta_3 Carity$$

$$I_2^{np\,eff} = \beta_4 + \beta_5 Carat + \beta_6 Carity$$

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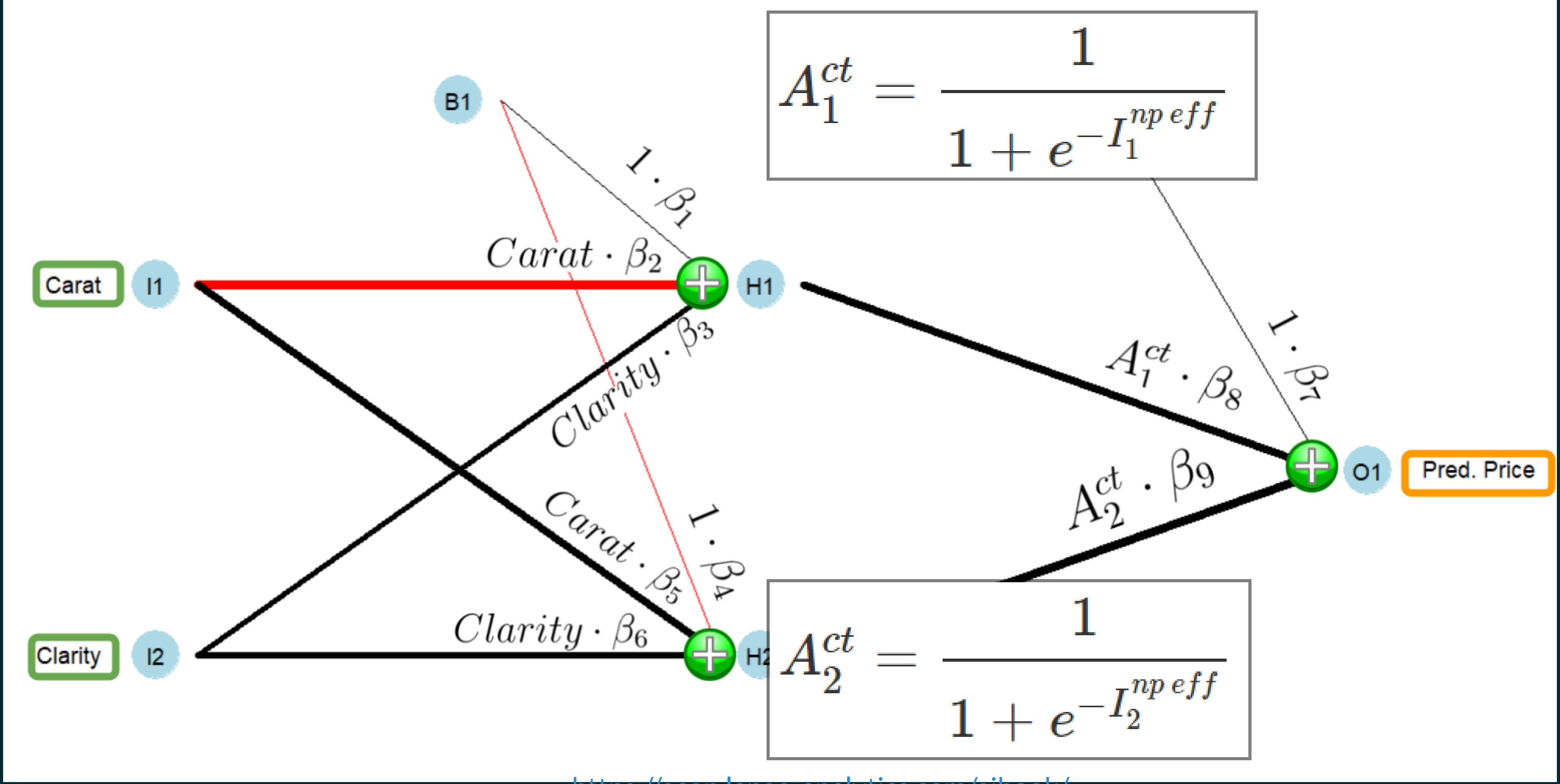
# USE A TRAINED NEURAL NEWORK (\(\BETA S\) ARE KNOWN) TO PREDICT

## Calculate Activity in Hidden Neurons with Logistic Function



$$A_1^{ct} = \frac{1}{1 + e^{-I_1^{np\,eff}}}$$

$$A_2^{ct} = \frac{1}{1 + e^{-I_2^{np\,eff}}}$$

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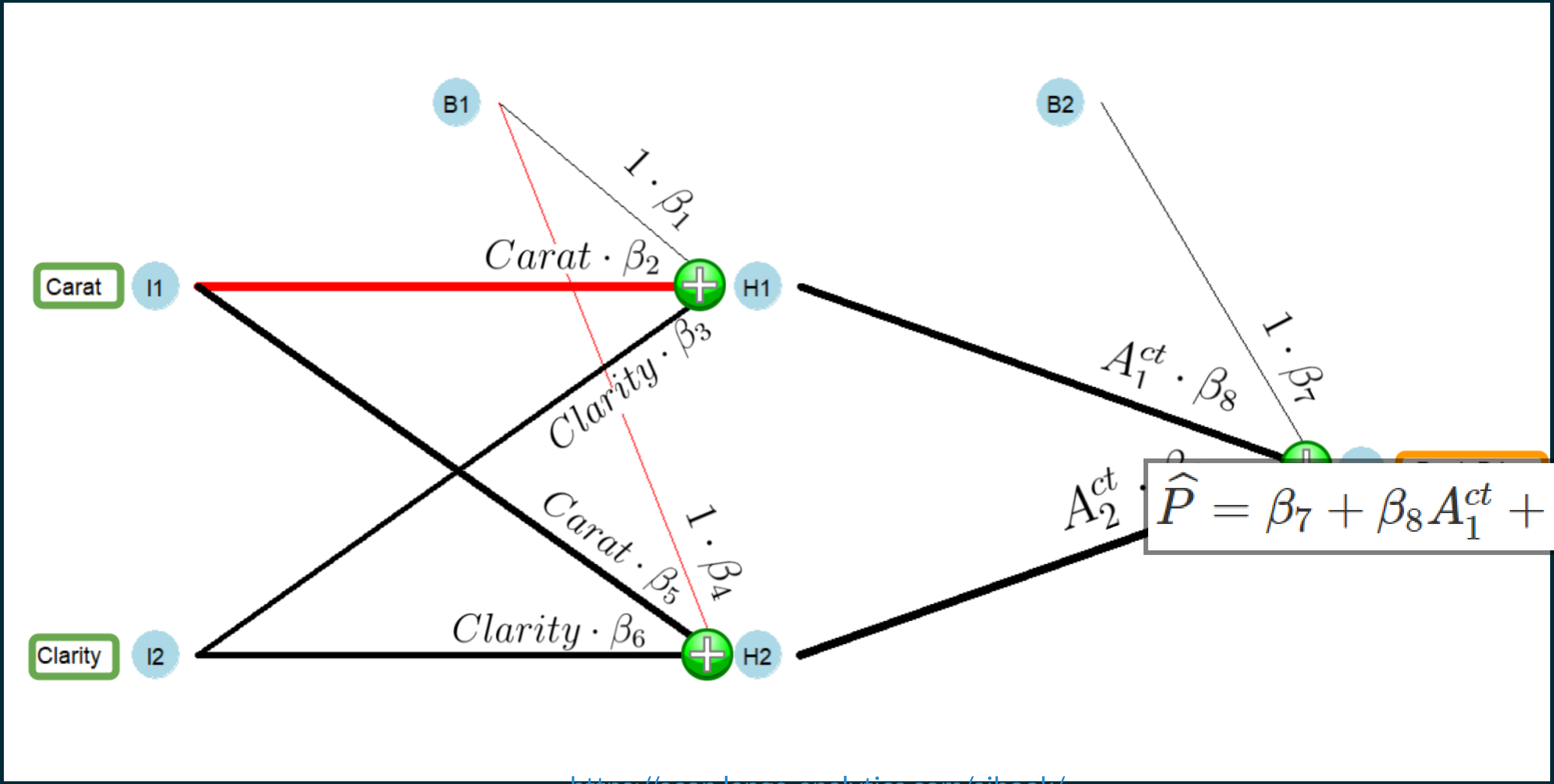
# USE A TRAINED NEURAL NEWORK (\(\BETA S\) ARE KNOWN) TO PREDICT

## Calculate Prediction from Activities in Hidden Neurons:



$$\widehat{P} = \beta_7 + \beta_8 A_1^{ct} + \beta_9 A_2^{ct}$$

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# PREDICTION OF THE NEURAL NETWORK

\[\widehat P =\beta_7 + \beta_8 A^{ct}_1 + \beta_9 A^{ct}_2\] A neural network can be transformed into a prediction equation that depends only on the \(\beta s\) and the values of the predictor variables!

We will show this in more detail on the following slides.»

# TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

$$\widehat P =\beta_7 + \beta_8 A^{ct}_1 + \beta_9 A^{ct}_2$$

- $A^{ct}_1$ and $A^{ct}_2$ depend on $I^{np\ eff}_1$ and $I^{np\ eff}_2$ (and the $\beta s$)
- $I^{np\ eff}_1$ and $I^{np\ eff}_2$ depend on the values of predictor variables $Carat$ and $Clarity$ (and the $\beta s$)
- Consequently, prediction depends only on the values of predictor variables and the $\beta s$!»

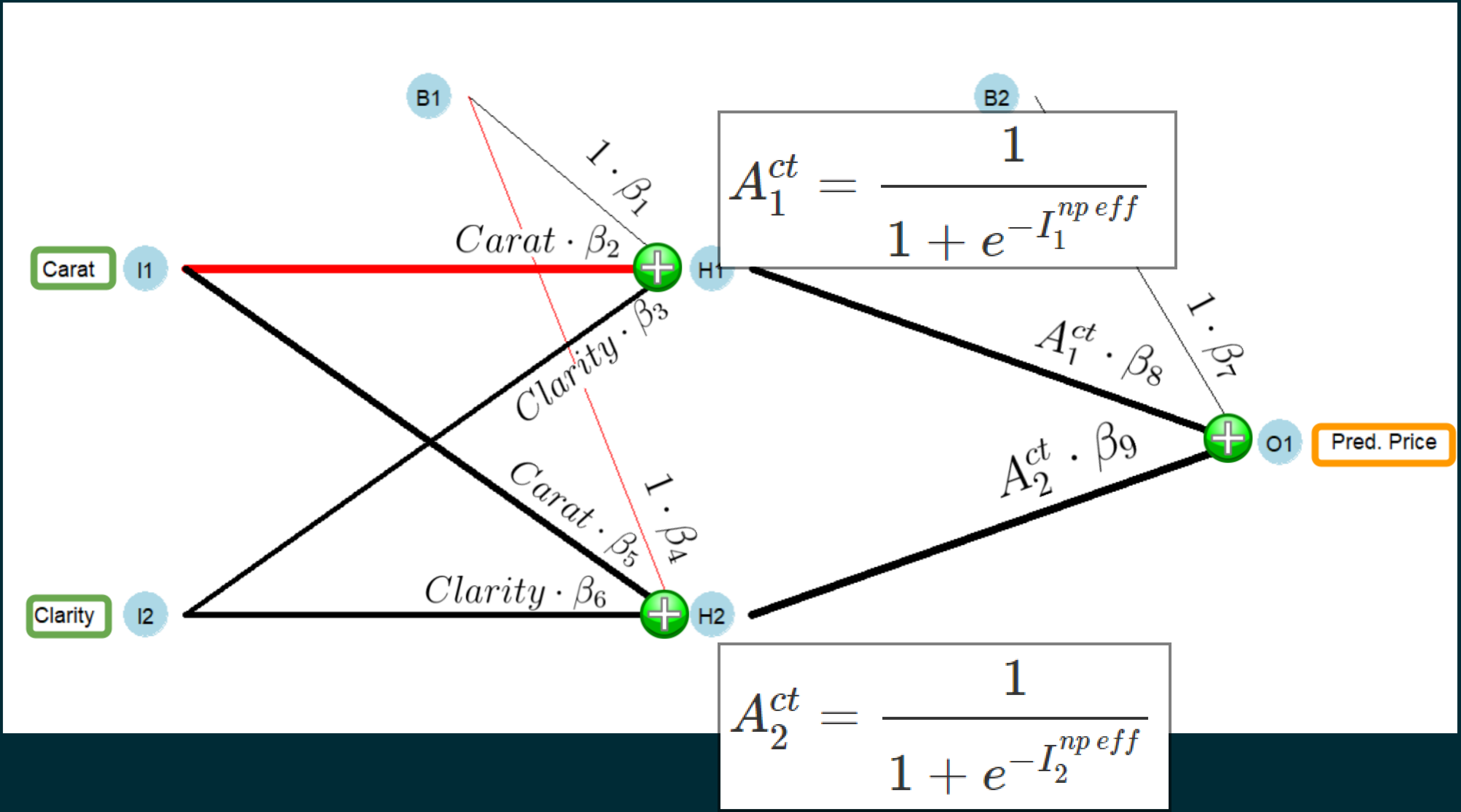
# TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

To show the transformation, we move backwards from right to left through the neural network.

$$\widehat P =\beta_7 + \beta_8 A^{ct}_1 + \beta_9 A^{ct}_2$$

# TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

## Inside the Hidden Neurons:



$$A_1^{ct} = \frac{1}{1 + e^{-I_1^{np\,eff}}}$$

$$A_2^{ct} = \frac{1}{1 + e^{-I_2^{np\,eff}}}$$

# TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

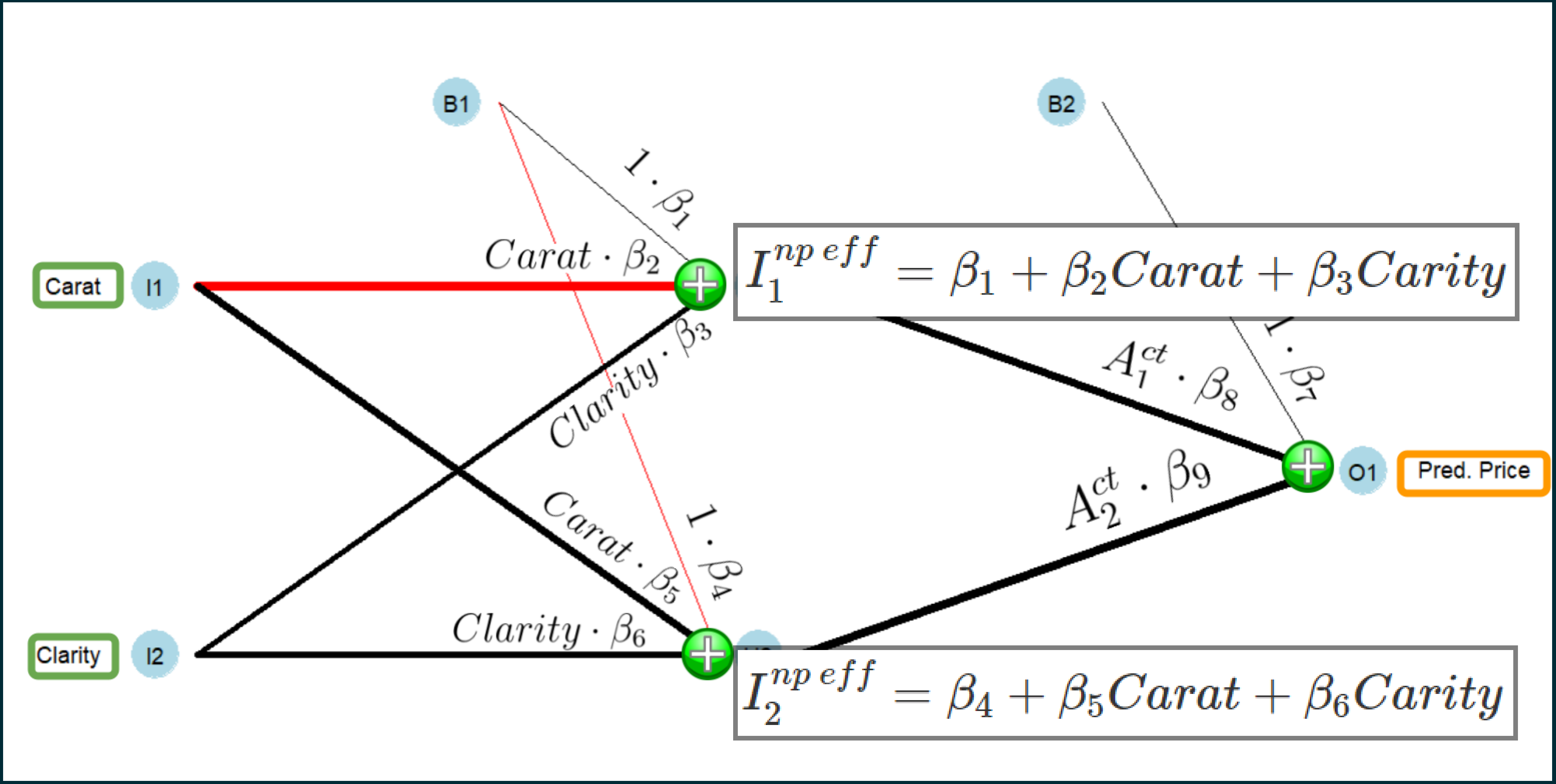
## Inside the Hidden Neurons

$$\widehat P =\beta_7 + \beta_8 A^{ct}_1 + \beta_9 A^{ct}_2$$

$$\widehat{P_i}=\beta_7+ \overbrace{ \frac{1}{1+e^{-I^{np\ eff}_1}} }^{A^{ct}_1}\cdot \beta_8+ \overbrace{ \frac{1}{1+e^{-I^{np\ eff}_2}} }^{A^{ct}_1}\cdot\beta_9$$

# TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

## Between the Input and the Hidden Layer:



$$I_1^{np\,eff} = \beta_1 + \beta_2 Carat + \beta_3 Carity$$

$$I_2^{np\,eff} = \beta_4 + \beta_5 Carat + \beta_6 Carity$$

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# TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

**Between the Input and the Hidden Layer:**

\[\widehat P =\beta_7 + \beta_8 A^{ct}_1 + \beta_9 A^{ct}_2\]

\[ \widehat{P_i}=\beta_7+ \overbrace{ \frac{1}{1+e^{-I^{np\ eff}_1}} }^{A^{ct}_1}\cdot \beta_8+ \overbrace{ \frac{1}{1+e^{-I^{np\ eff}_2}} }^{A^{ct}_1}\cdot\beta_9 \]

\[\begin{eqnarray*} \widehat{P_i}&=&\beta_7+ \overbrace{ \frac{1} {1+e^{-(\beta_1 +\beta_2 Carat_i+\beta_3 Clarity_i)}} }^{A^{ct}_1}\cdot \beta_8\\ &&+ \overbrace{ \frac{1}{1+e^{-(\beta_4 +\beta_5 Carat_i+\beta_6 Clarity_i)}} }^{A^{ct}_2}\cdot\beta_9 \end{eqnarray*}\]

# IF WE KNOW THE \(\BETA S\) WE CAN GENERATE PREDICTIONS!

\[\begin{eqnarray*} \widehat{P_i}&=&\beta_7\\ &+&\overbrace{ \frac{1}{1+e^{-(\beta_1 +\beta_2 Carat_i+\beta_3 Clarity_i)}} }^{\mbox{$A^{ct}_1$}}\cdot \beta_8 \\ &+&\overbrace{ \frac{1}{1+e^{-(\beta_4 +\beta_5 Carat_i+\beta_6 Clarity_i)}} }^{\mbox{$A^{ct}_2$}}\cdot\beta_9 \end{eqnarray*}\]

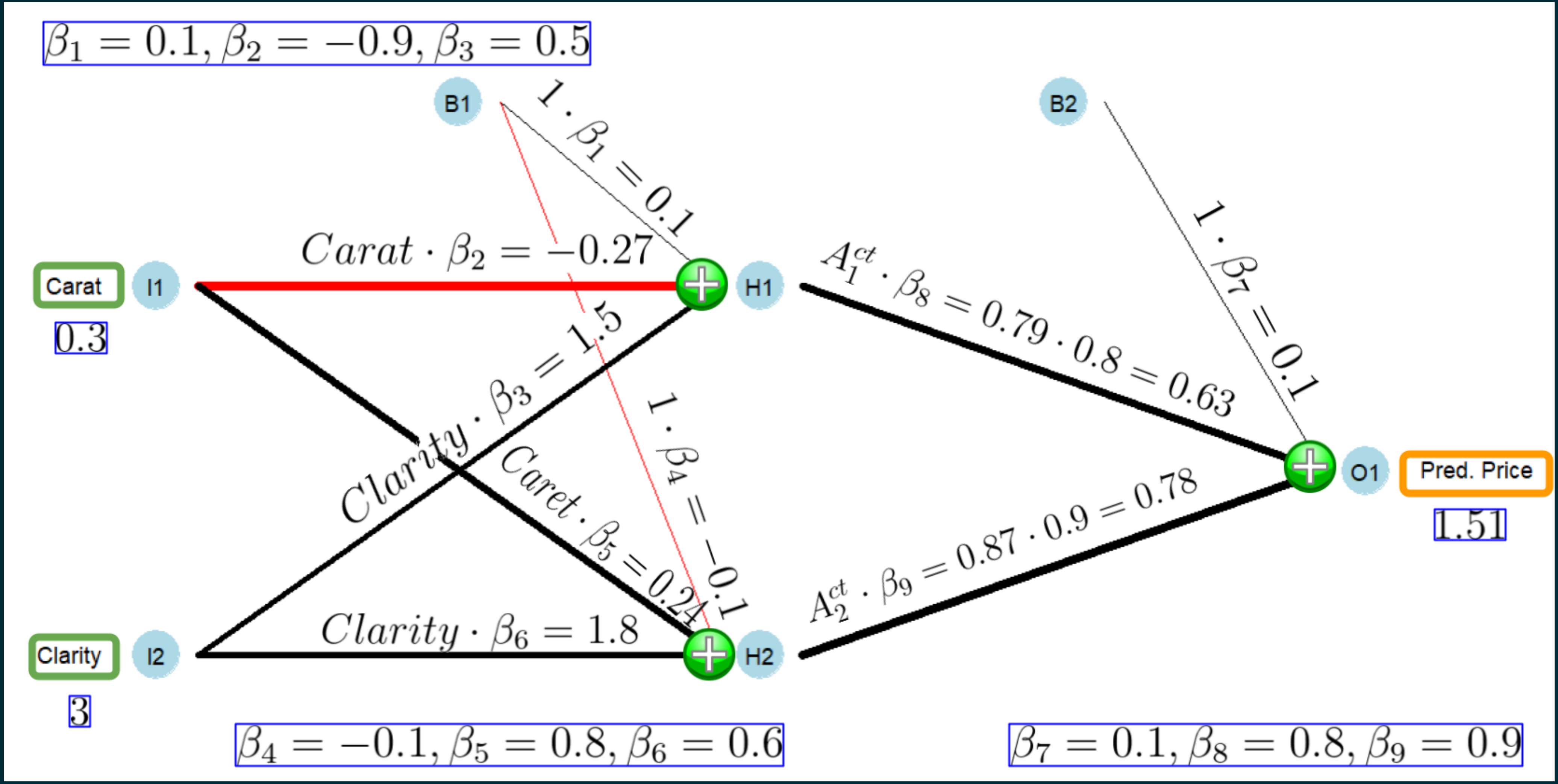
- initial \(\beta s\) are chosen at random.
- optimal \(\beta s\) are found with the *optimizer*.»

# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Predictor Variables' Values:** \(Carat=0.3\) and \(Clarity=3\)

# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Effective Inputs:** \(Carat=0.3\) and \(Clarity=3\)


$\beta_1 = 0.1, \beta_2 = -0.9, \beta_3 = 0.5$
B1
$1 \cdot \beta_1 = 0.1$
B2
$1 \cdot \beta_7 = 0.1$
$Carat \cdot \beta_2 = -0.27$
Carat
I1
$0.3$
H1
$A_1^{ct} \cdot \beta_8 = 0.79 \cdot 0.8 = 0.63$
$Clarity \cdot \beta_3 = 1.5$
$1 \cdot \beta_4 = -0.1$
$Caret \cdot \beta_5 = 0.24$
O1
Pred. Price
$1.51$
$A_2^{ct} \cdot \beta_9 = 0.87 \cdot 0.9 = 0.78$
$Clarity \cdot \beta_6 = 1.8$
Clarity
I2
H2
$3$
$\beta_4 = -0.1, \beta_5 = 0.8, \beta_6 = 0.6$
$\beta_7 = 0.1, \beta_8 = 0.8, \beta_9 = 0.9$

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# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Effective Input 1:** $Carat=0.3$ and $Clarity=3$

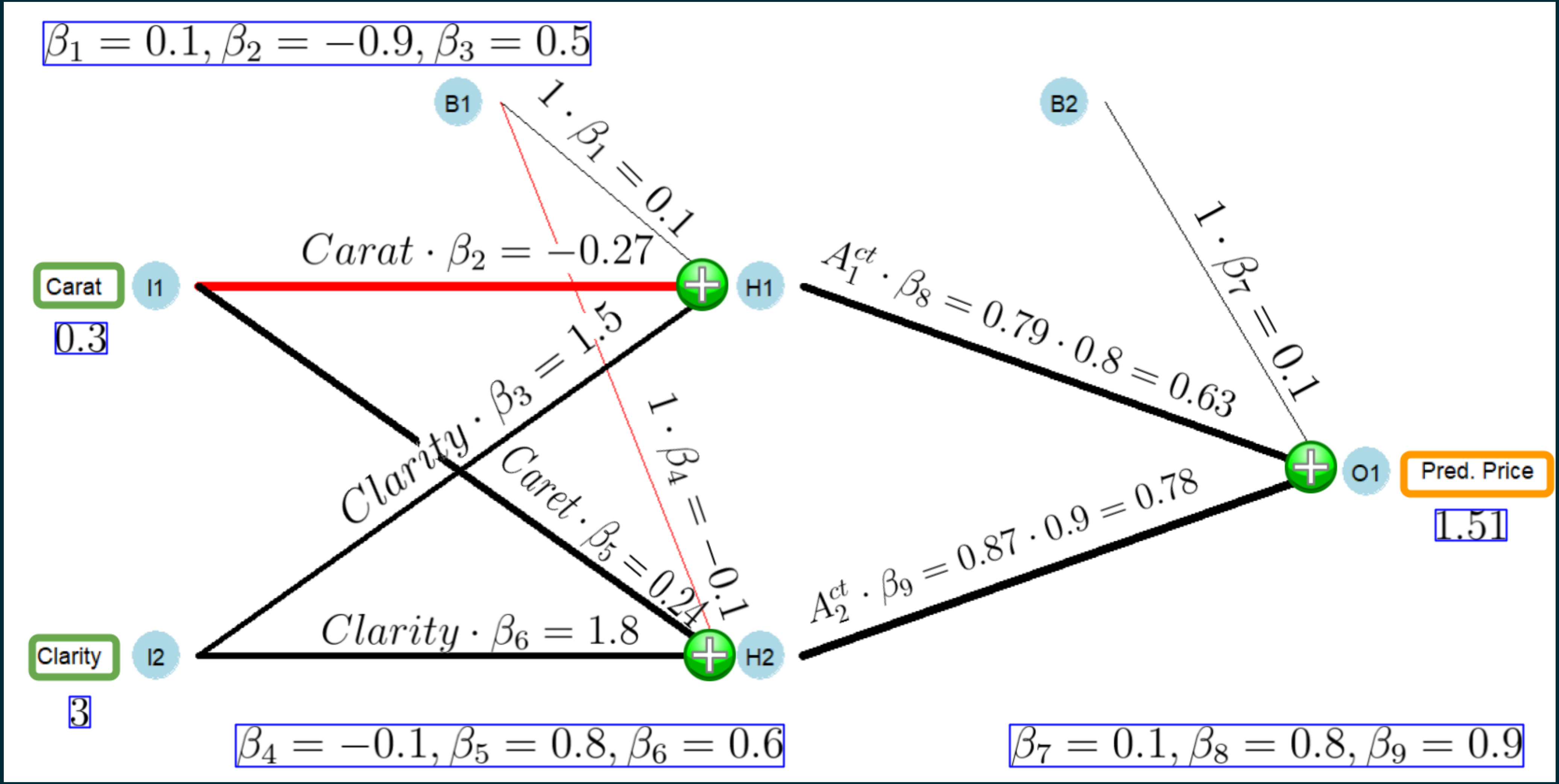
$$\beta_1 = 0.1, \beta_2=-0.9 ,\beta_3 =0.5$$

$$I_1^{np\ eff}=\beta_1+ \beta_2 Carat + \beta_3 Clarity$$

$$I_1^{np\ eff}=\underbrace{1 \cdot 0.1}_{1 \cdot \beta_1=0.1}+\underbrace{0.3\cdot(-0.9)}_{Carat\cdot \beta_2=-0.27}+\underbrace{3\cdot 0.5}_{Clarity \cdot\beta_2=First5}=1.33$$

# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Effective Input 2:** \(Carat=0.3\) and \(Clarity=3\)



$\beta_1 = 0.1, \beta_2 = -0.9, \beta_3 = 0.5$
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Clarity
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H2
3
$\beta_4 = -0.1, \beta_5 = 0.8, \beta_6 = 0.6$
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# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Effective Input 2:** \(Carat=0.3\) and \(Clarity=3\)

\[\beta_4 = -0.1,\beta_5 = 0.8,\beta_6 =0.6\]

\[I_2^{np\ eff}=\beta_4+ \beta_5 Carat + \beta_6 Clarity\]

\[I_2^{np\ eff}=\underbrace{1 \cdot (-0.1)}_{1 \cdot \beta_4=-0.1}+\underbrace{0.3\cdot0.8}_{Carat\cdot \beta_5=0.24}+\underbrace{3\cdot 0.6}_{Clarity \cdot\beta_6=1.8}=1.94\]

# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Hidden Neurons' Activity:** \(I_1^{np\ eff}=1.33\) \(I_2^{np\ eff}=1.94\)

# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Hidden Neurons' Activity:** $I_1^{np\ eff}=1.33$ and $I_2^{np\ eff}=1.94$

$$A^{ct}_1=\frac{1}{1+e^{-I_1^{np\ eff}}}$$

$$A^{ct}_1= \frac{1}{1+e^{-1.33}}=0.79$$

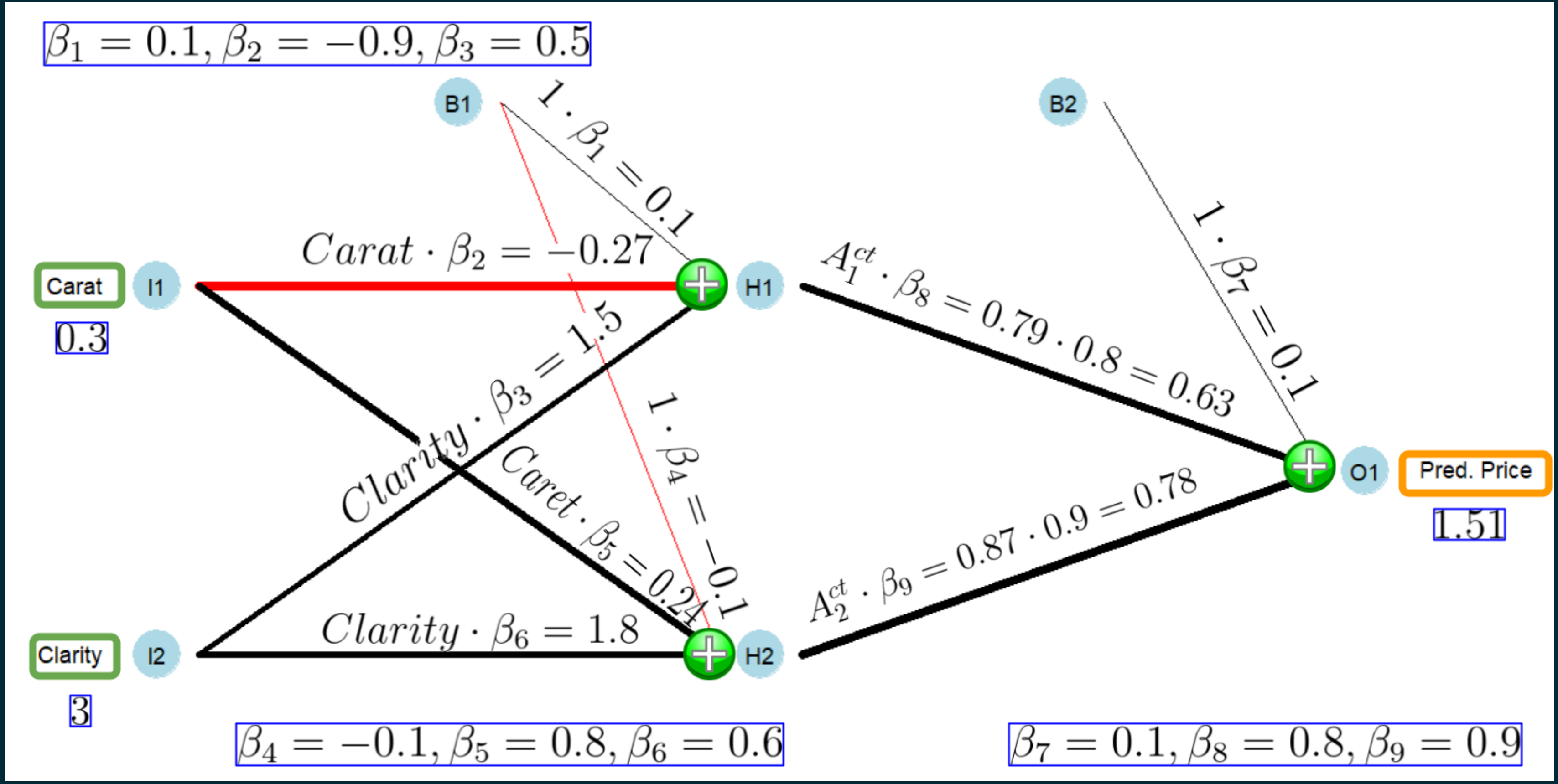
$$A^{ct}_2=\frac{1}{1+e^{-I_2^{np\ eff}}}$$

$$A^{ct}_2=\frac{1}{1+e^{-1.94}}=0.87$$

# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Prediction:**

\(\beta_7=0.1\), \(\beta_8=0.8\), \(\beta_9=0.9\), \(A^{ct}_1=0.79\) and \(A^{ct}_2=0.87\)



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O1
Pred. Price
1.51
$A^{ct}_2 \cdot \beta_9 = 0.87 \cdot 0.9 = 0.78$
Clarity
I2
3
$Clarity \cdot \beta_6 = 1.8$
H2
$\beta_4 = -0.1, \beta_5 = 0.8, \beta_6 = 0.6$
$\beta_7 = 0.1, \beta_8 = 0.8, \beta_9 = 0.9$

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# PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

**Prediction:**

$\beta_7=0.1$, $\beta_8=0.8$, $\beta_9=0.9$, $A^{ct}_1=0.79$ and $A^{ct}_2=0.87$

$$ \widehat P =\beta_7 + \beta_8 A^{ct}_1 + \beta_9 A^{ct}_2 $$

$$ \widehat P = 0.1+0.8\cdot 0.79 +0.9 \cdot 0.87 = 1.51 $$

The predicted price for a 0.3 g diamond with a clarity level of three is $1.51.

**$1.51 for a diamond???**

# SUMMARY

- We can make prediction with the neural network if we know the values for the \(\beta s\). We do know the \(\beta s\) because
  - they are randomly chosen at the beginning, or
  - they are adjusted by the Optimizer.
- when \(\beta's\) are randomly chosen the predictions are useually bad, but they can be improved by the *Optimizer*.

This raises the question:

**How does the *Optimizer* gradually change the** \(\beta s\) to improve the prediction quality of the neural network?

# STEEPEST GRADIENT DESCENT

\[MSE= \frac{\sum^N_{i=1}(\widehat P_i - P_i)^2}{N}\]

\[\begin{eqnarray*} \widehat{P_i}&=&\beta_7\\ &+&\overbrace{ \frac{1}{1+e^{-(\beta_1 +\beta_2 Carat_i+\beta_3 Clarity_i)}} }^{A^{ct}_1}\cdot \beta_8 \\ &+&\overbrace{ \frac{1}{1+e^{-(\beta_4 +\beta_5 Carat_i+\beta_6 Clarity_i)}} }^{A^{ct}_2}\cdot\beta_9 \end{eqnarray*}\]

# STEEPEST GRADIENT DESCENT

\[MSE= \frac{\sum^N_{i=1}(\widehat P_i - P_i)^2}{N}\]

\[\begin{eqnarray*} MSE= \frac{\sum^N_{i=1}\left(\widehat P_i - \left (\underbrace{\beta_7 +\overbrace{ \frac{1}{1+e^{-(\beta_1 +\beta_2 Carat_i+\beta_3 Clarity_i)}} }^{A^{ct}_1}\cdot \beta_8 +\overbrace{ \frac{1}{1+e^{-(\beta_4 +\beta_5 Carat_i+\beta_6 Clarity_i)}} }^{A^{ct}_2}\cdot\beta_9}_{P_i} \right ) \right )^2}{N} \end{eqnarray*}\]

# STEEPEST GRADIENT DESCENT

- Initially \(\beta s\) are chosen randomly.
- Optimizer adjusts \(\beta s\) incrementally (iteration by iteration; the iterations are called **epochs**)
- Each epoch:
    - Find if individual \(\beta\) needs to be increased or decreased.
        - Increase \(\beta_i\) and see if \(MSE\) increases or not.
        - Decrease \(\beta_i\) and see if \(MSE\) increases or not.
        - Reset \(\beta_i\) and note if \(\beta_i\) needs to be increased or decreased.
        - Repeat for all \(\beta s\)
    - In/Decrease \(\beta`s\) proportional to change of \(MSE\) caused — multiply by learning rate (e.g., 0.01) to keep change small.
- run process for several hundreds or thousands epochs.»

# EXAMPLE: APPROXIMATION PROPERTIES OF NEURAL NETWORKS

Let us run an example to see how well a Neural Network can approximate.

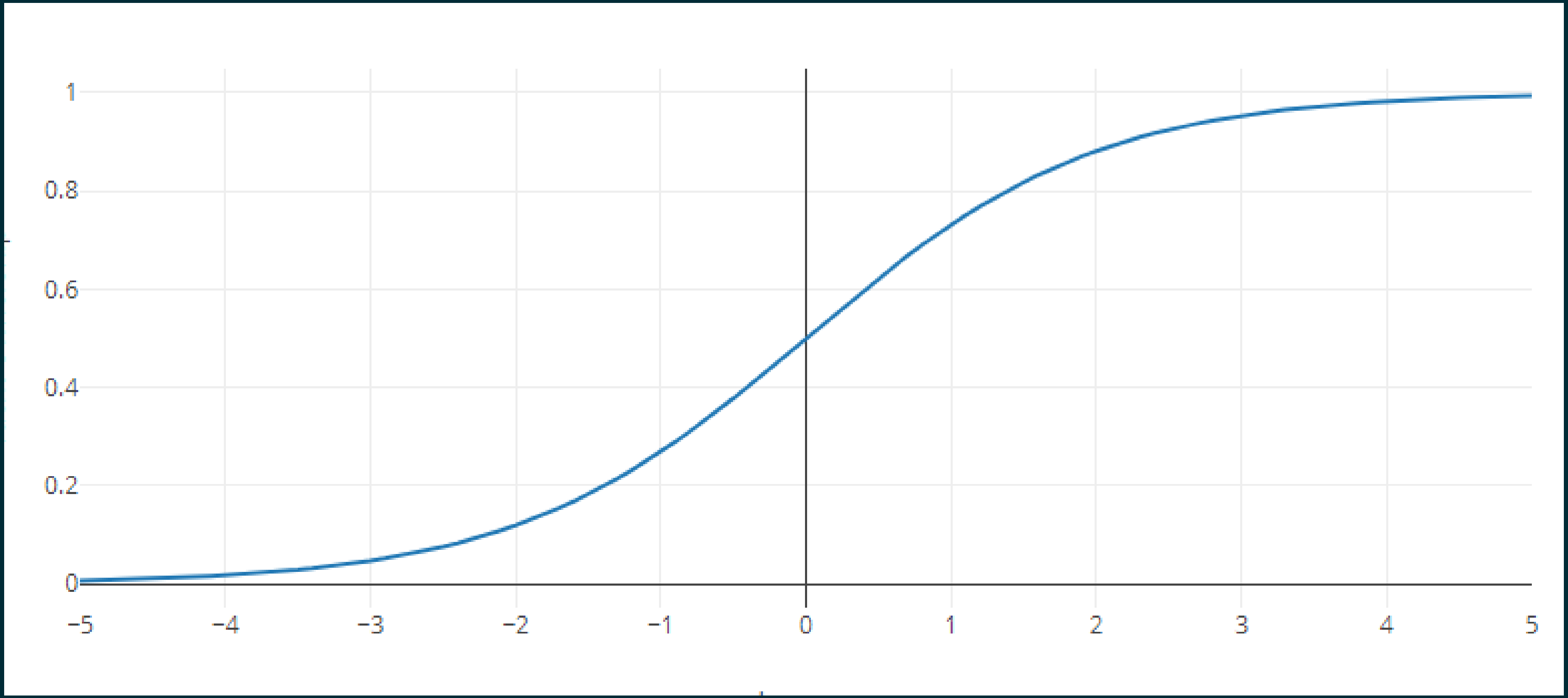
In the example we will z-normalize the predictors.

Are interested why?

Then use the **down-arrow** to proceed with the slides.

Otherwise, use the **left-arrow**.

# WHY IS SCALING OF PREDICTORS NEEDED?



Logistic Activation Function

If inputs are not scaled and if they lead to very big effective inputs, the slope of the activation function will be very close to 0 and different effective inputs are indistinguishable.

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# EXAMPLE: APPROXIMATION PROPERTIES OF NEURAL NETWORKS

To run the R-script with an example to see how well a Neural Network can approximate:

Click the link in the footer of this slide.

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# THEOREM: APPROXIMATION PROPERTIES OF NEURAL NETWORKS

“Feedforward networks are capable of arbitrarily accurate approximation to any real-valued continuous function over a compact set.”

I.e.: Single hidden layer feedforward networks can approximate any measurable function arbitrarily well.

Kurt Hornik, Maxwell Stinchcombe and Halber White (1989), p. 361

# INTUITION: APPROXIMATION PROPERTIES OF NEURAL NETWORKS

\[\begin{eqnarray*} \widehat{y_i}&=&\beta_{10}+ \overbrace{ \frac{1}{1+e^{-(\beta_1 x_i + \beta_2)}} }^{\mbox{$A^{ct}_1$}}\cdot \beta_7\\ &&+ \overbrace{ \frac{1}{1+e^{-(\beta_3 x_i + \beta_4)}} }^{\mbox{$A^{ct}_2$}}\cdot \beta_8\\ &&+ \overbrace{ \frac{1}{1+e^{-(\beta_5 x_i + \beta_6)}} }^{\mbox{$A^{ct}_3$}}\cdot \beta_9 \end{eqnarray*}\]

The app linked in the footer of this slide provides intuition for the Hornik, Stinchcombe, White proof.

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# REAL WORLD EXAMPLE TO ESTIMATE DIAMOND PRICES

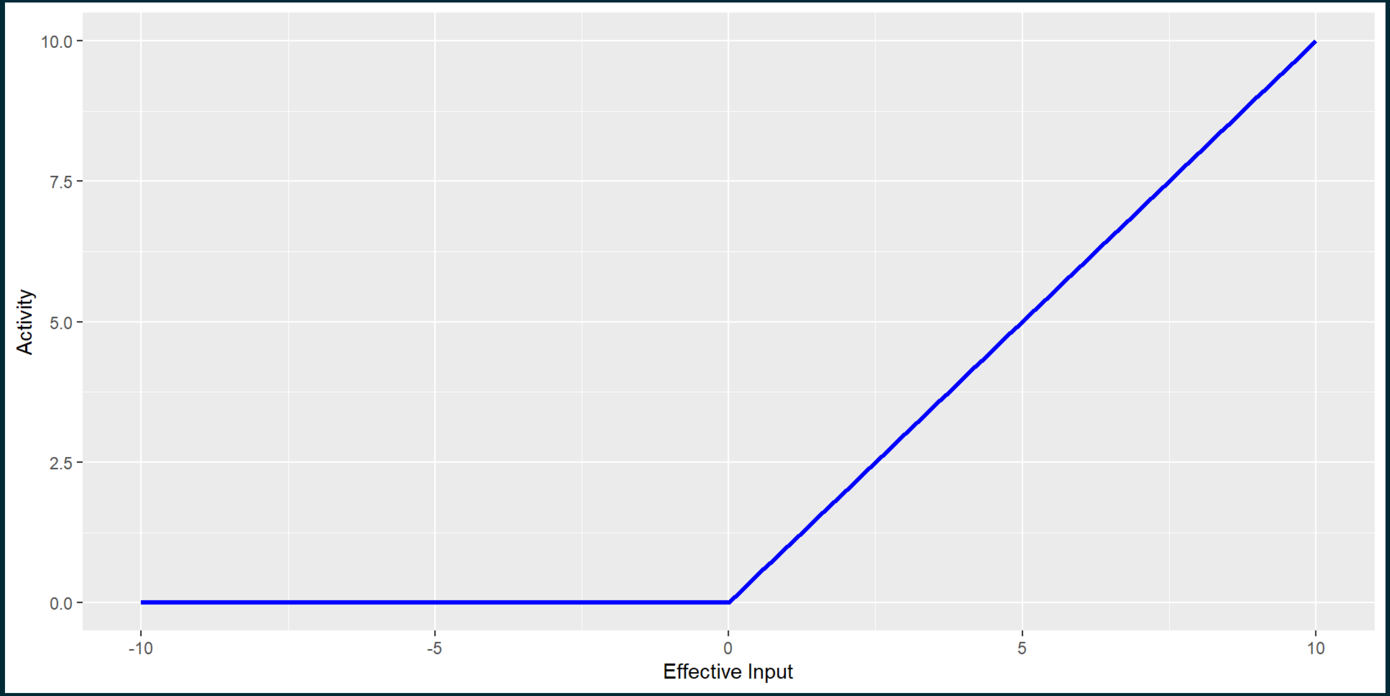
1. You will use all big C variables \(Carat\), \(Clarity\), \(Cut\), and \(Color\).
   \(Cut\) describes the quality of the cut of the diamond rated from 1 (lowest) to 6 (highest) and \(Color\) rates the color of a diamond from 1 (highest) to 7 (lowest)
2. Instead of using the `nnet` package, you will use the more advanced `brulee` package which is based on *PyTorch*, which is a Python library originally developed by *Facebook*.
3. We will tune the hyper-parameters of the neural network (e.g., the number of hidden units) using *cross validation*.

# MAJOR DIFFERENCES: `nnet` AND `brulee`/`PyTorch`

- `brulee` uses internally stop learning.
  - `epoch` setting refers to maximum *epochs*
  - from the *training* data set a *validation* set is held back.
  - when *validation error* stops decreasing for 5 epochs training is stopped.
- `brulee` allows to use **ReLu Activation Functions**

# RELU ACTIVATION FUNCTION

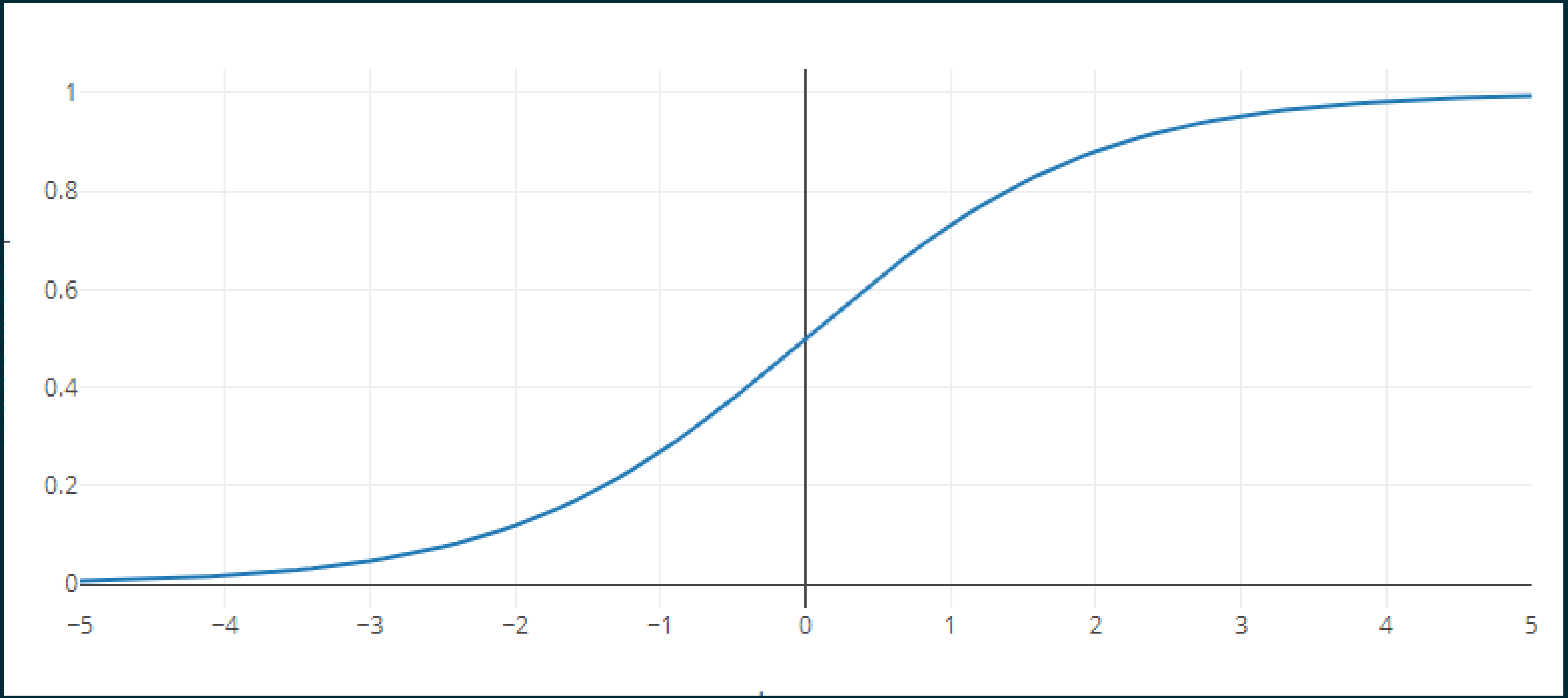
\[Act_i=max\left (0, I_i^{eff}\right )\]



Two *ReLU* functions can be combined into one step function similar to *sigmoid* functions.

See the link in the footer for a demo.

# LOGISTIC ACTIVATION FUNCTION: PROBLEM OF VANISHING GRADIENT



Logistic Activation Function

Even when activation is determined somewhere in the middle of the activation function the slope is smaller than one. With multiple layers this can propagate to a gradient that is zero because slopes from multiple layers are multiplied (chain rule).

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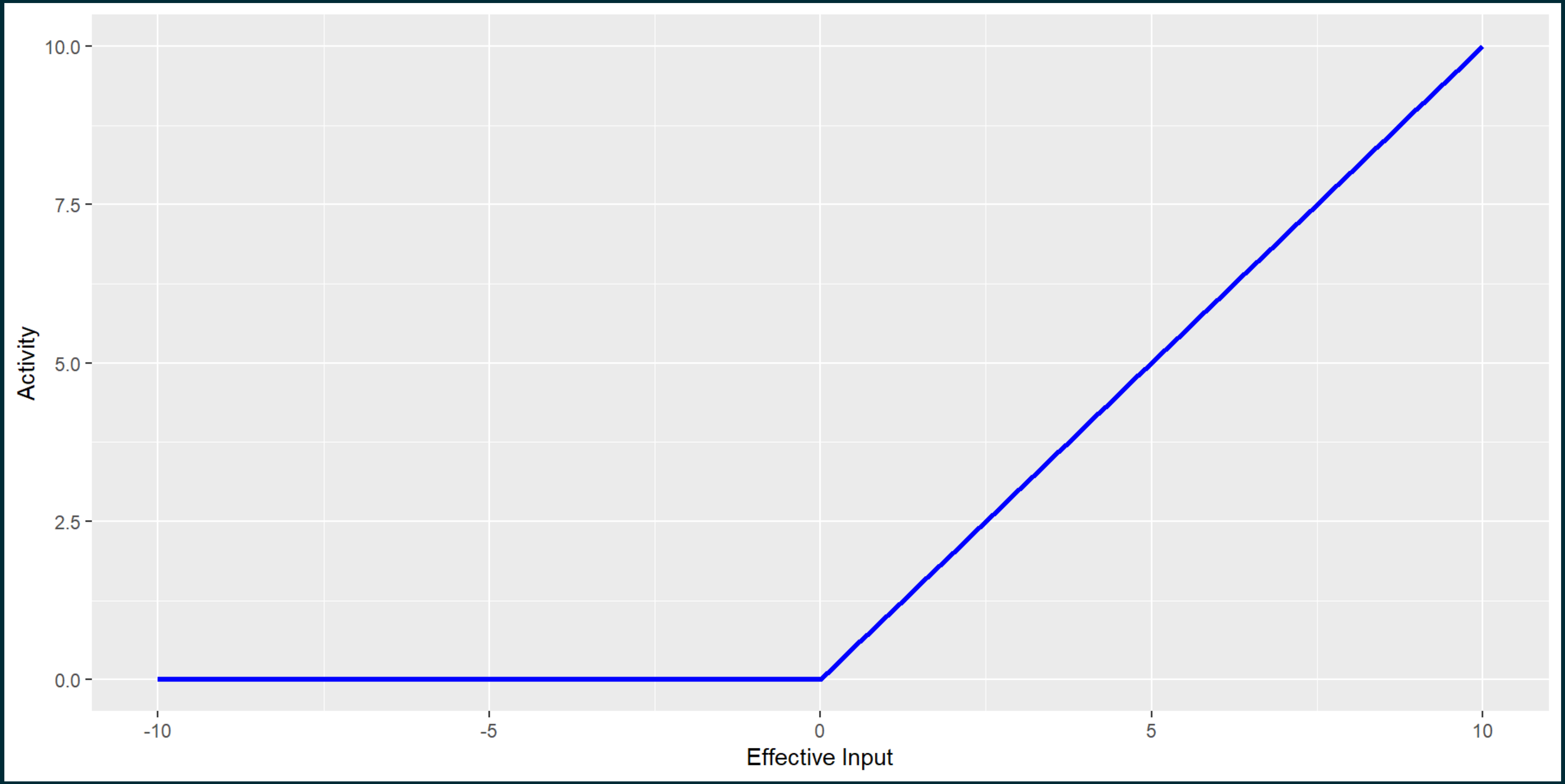
# RELU ACTIVATION FUNCTION: NO PROBLEM OF VANISHING GRADIENT

\[Act_i=max\left (0, I_i^{eff}\right )\]



*ReLu* has a slope of one.

# NOW IT'S TIME TO RUN THE REAL-WORLD ANALYSIS

Go to the AI Book and find the analysis at the end of the Neural Network chapter:

Neural Network Real World Application

Alternatively you can run uncommented R-script with the same code here.