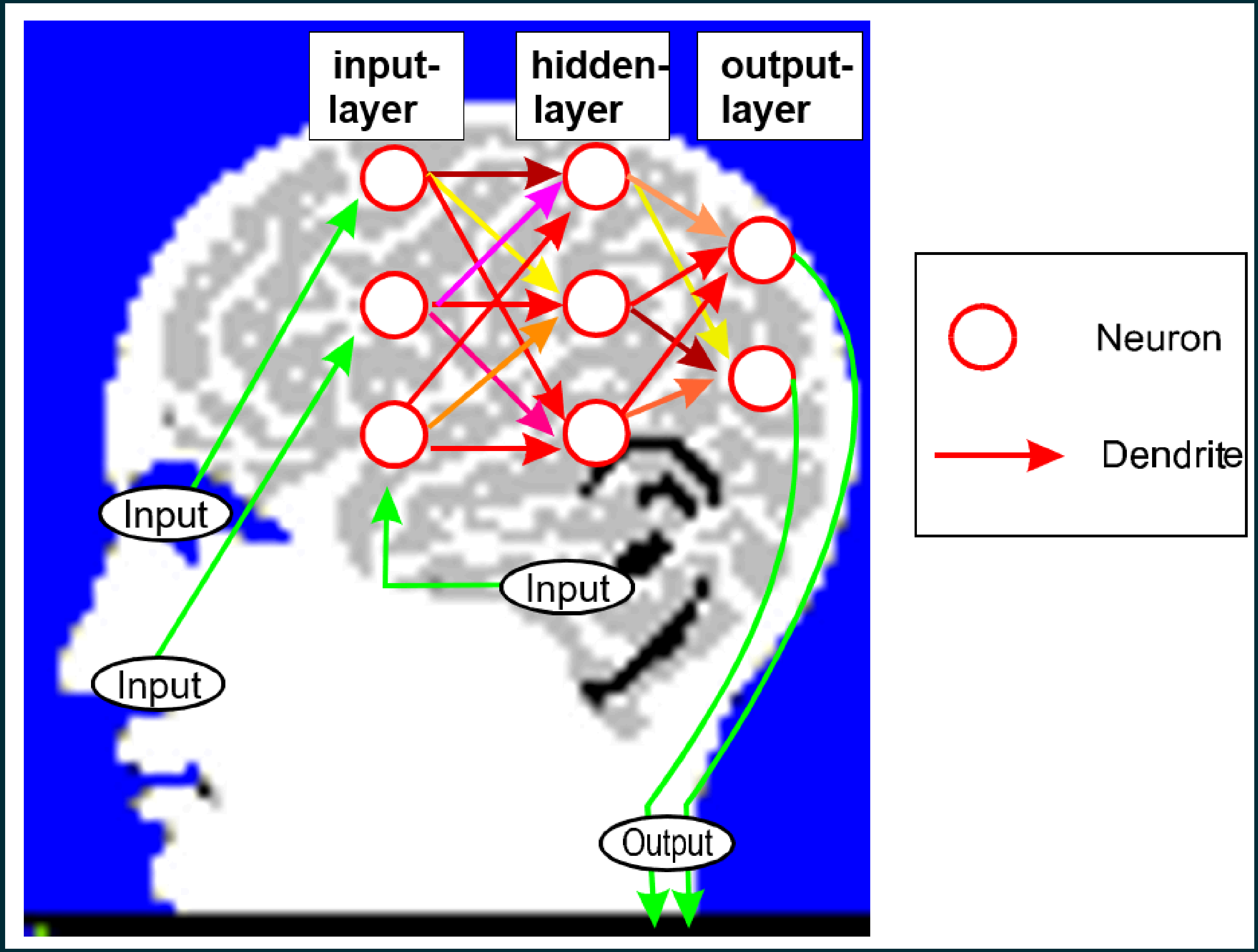
NEURAL NETWORKS

LEARNING OUTCOMES

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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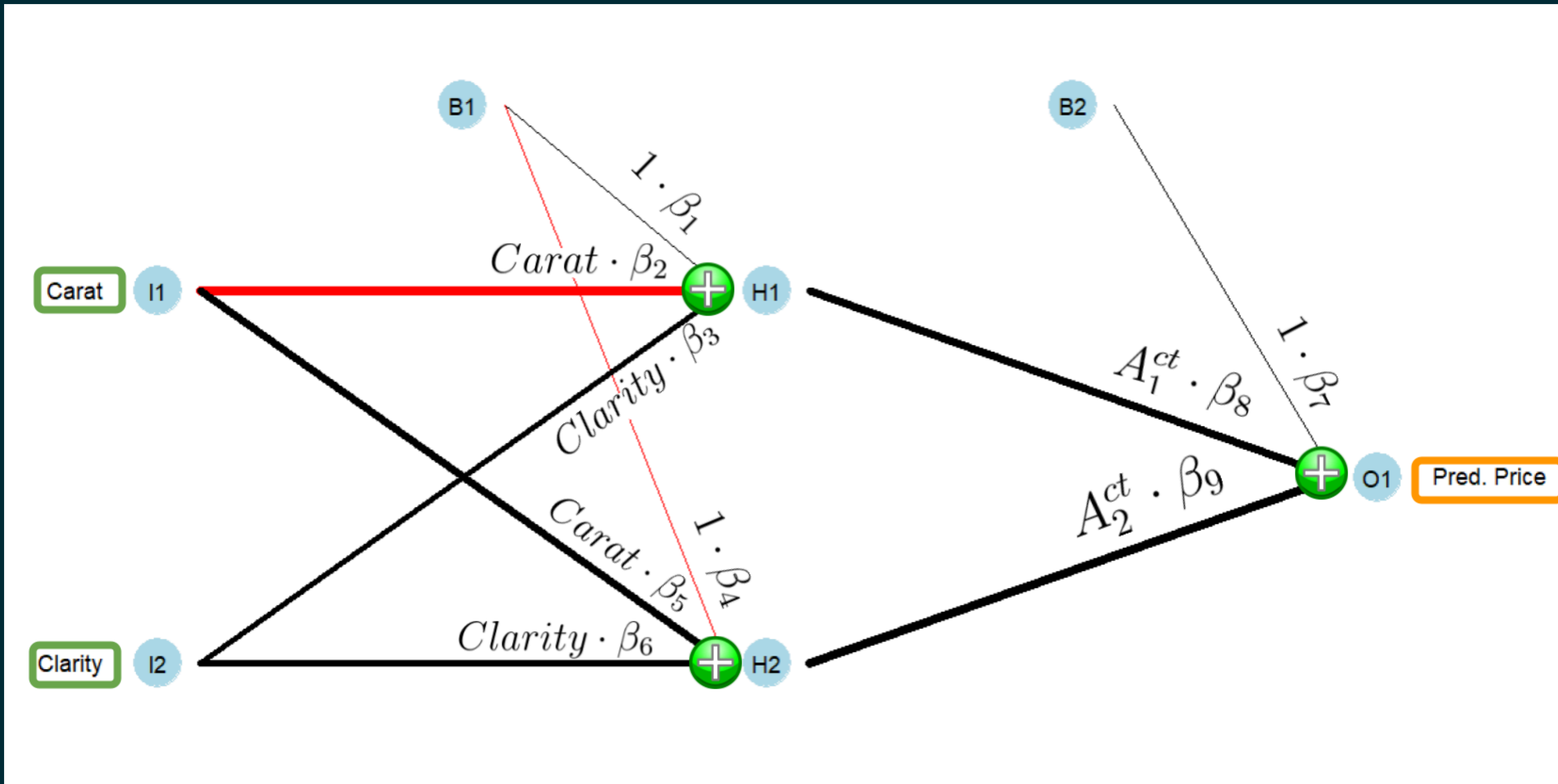
TYPES OF NEURAL NETWORKS

- **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



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).

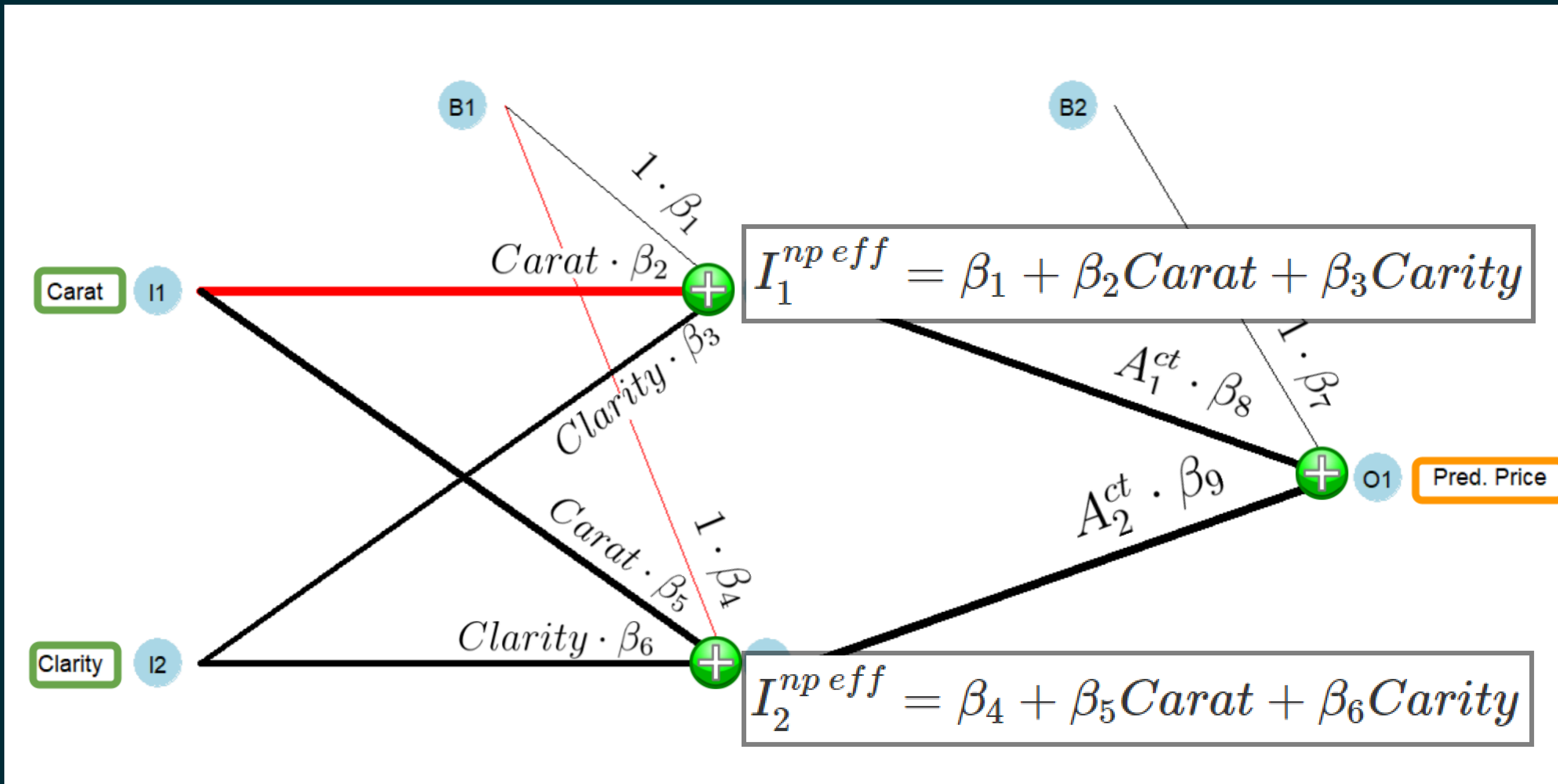
To later increase training speed, we use only 10,000 observations.

▶ 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
# ℹ 6,989 more rows
```

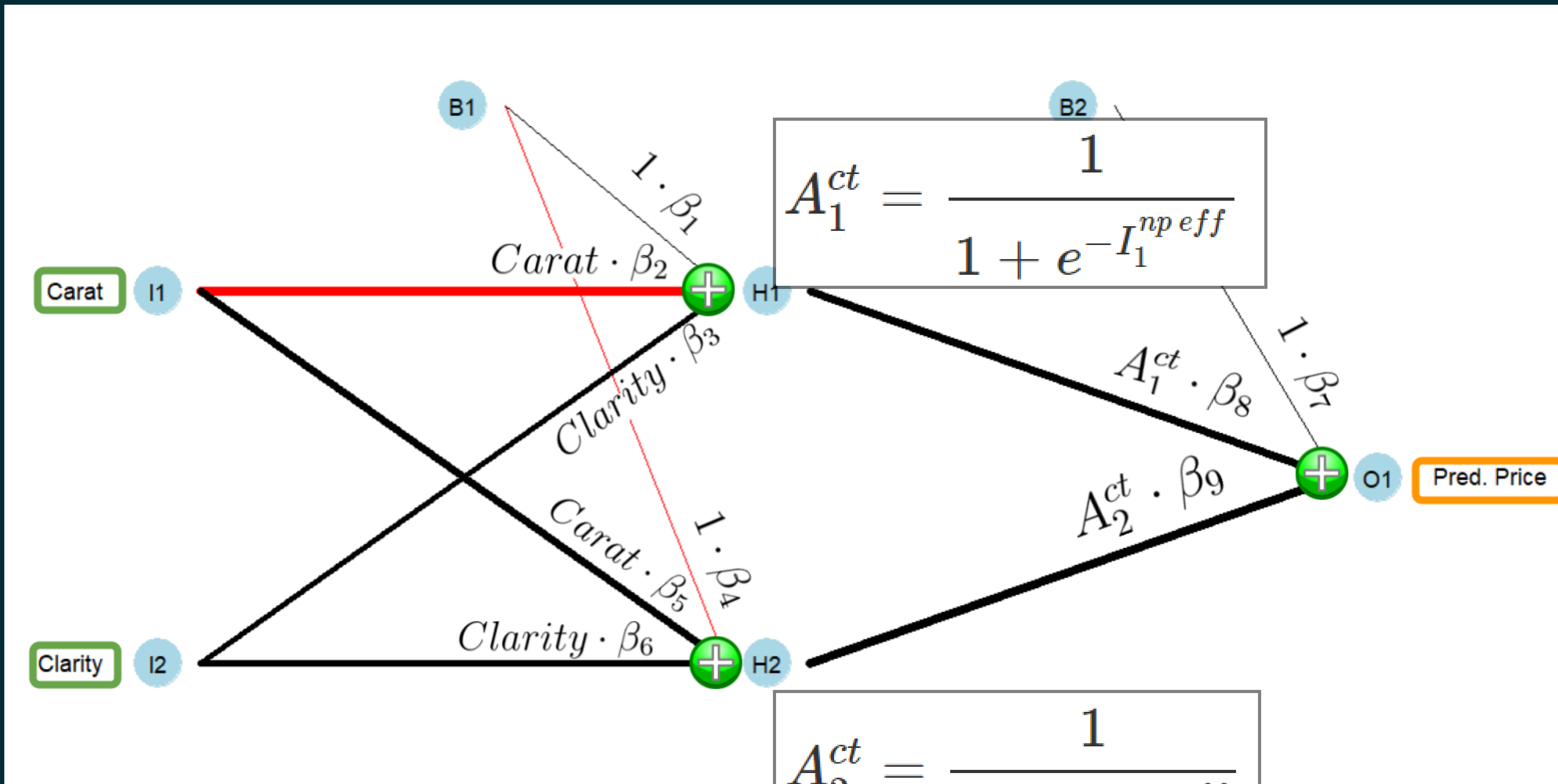
USE A TRAINED NEURAL NEWORK (βs ARE KNOWN) TO PREDICT

Effectiv Inputs to Hidden Neurons:



USE A TRAINED NEURAL NEWORK (βs 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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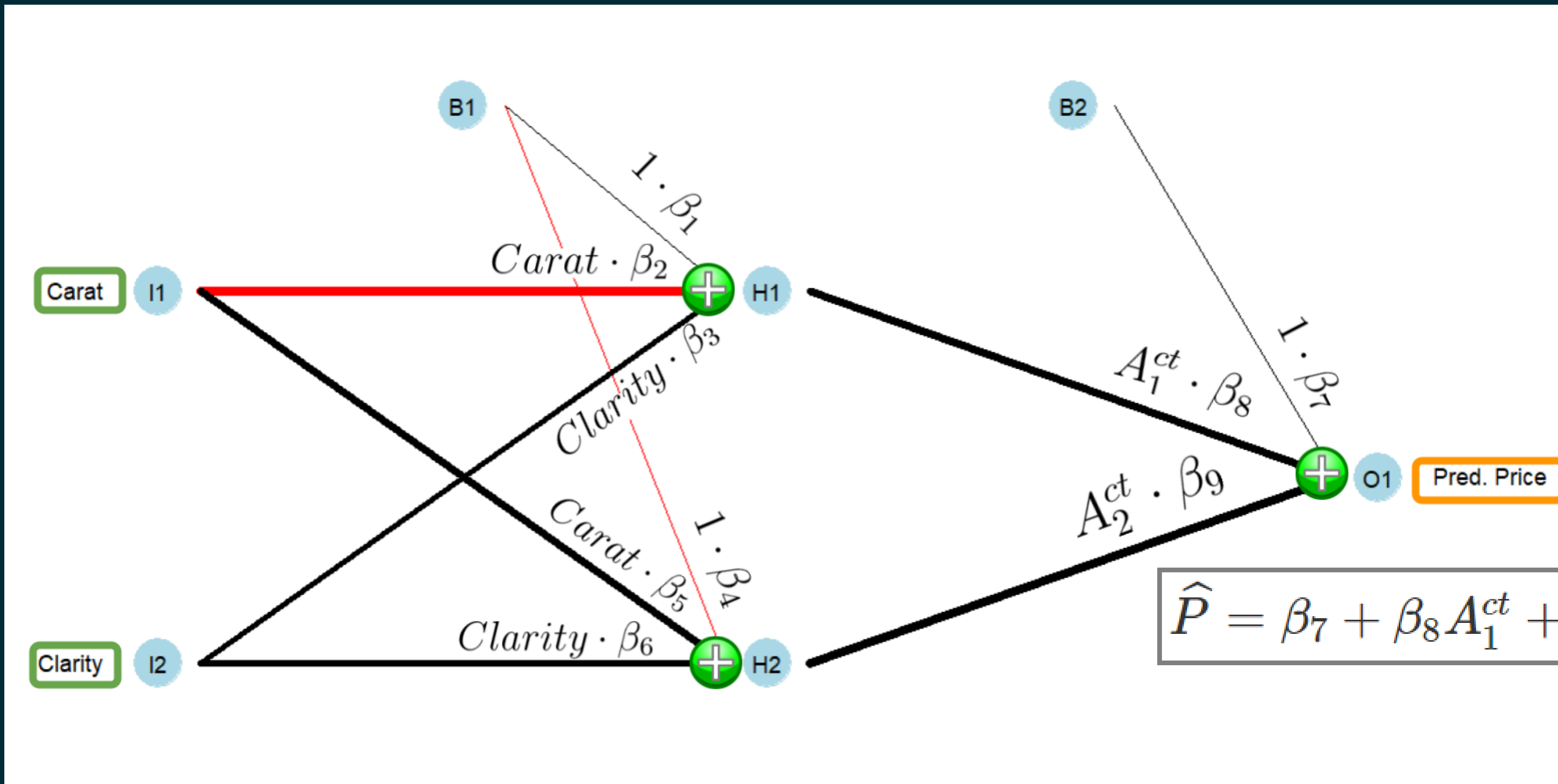
USE A TRAINED NEURAL NEWORK (βs ARE KNOWN) TO PREDICT

Calculate Prediction from Activities in Hidden Neurons:



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

PREDICTION OF THE NEURAL NETWORK

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

A neural network can be transformed into a prediction equation that depends only on the βs 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

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

- A_1^{ct} and A_2^{ct} depend on $I_1^{np\,eff}$ and $I_2^{np\,eff}$ (and the βs)
- $I_1^{np\,eff}$ and $I_2^{np\,eff}$ depend on the values of predictor variables $Carat$ and $Clarity$ (and the βs)
- Consequently, prediction depends only on the values of predictor variables and the βs!»

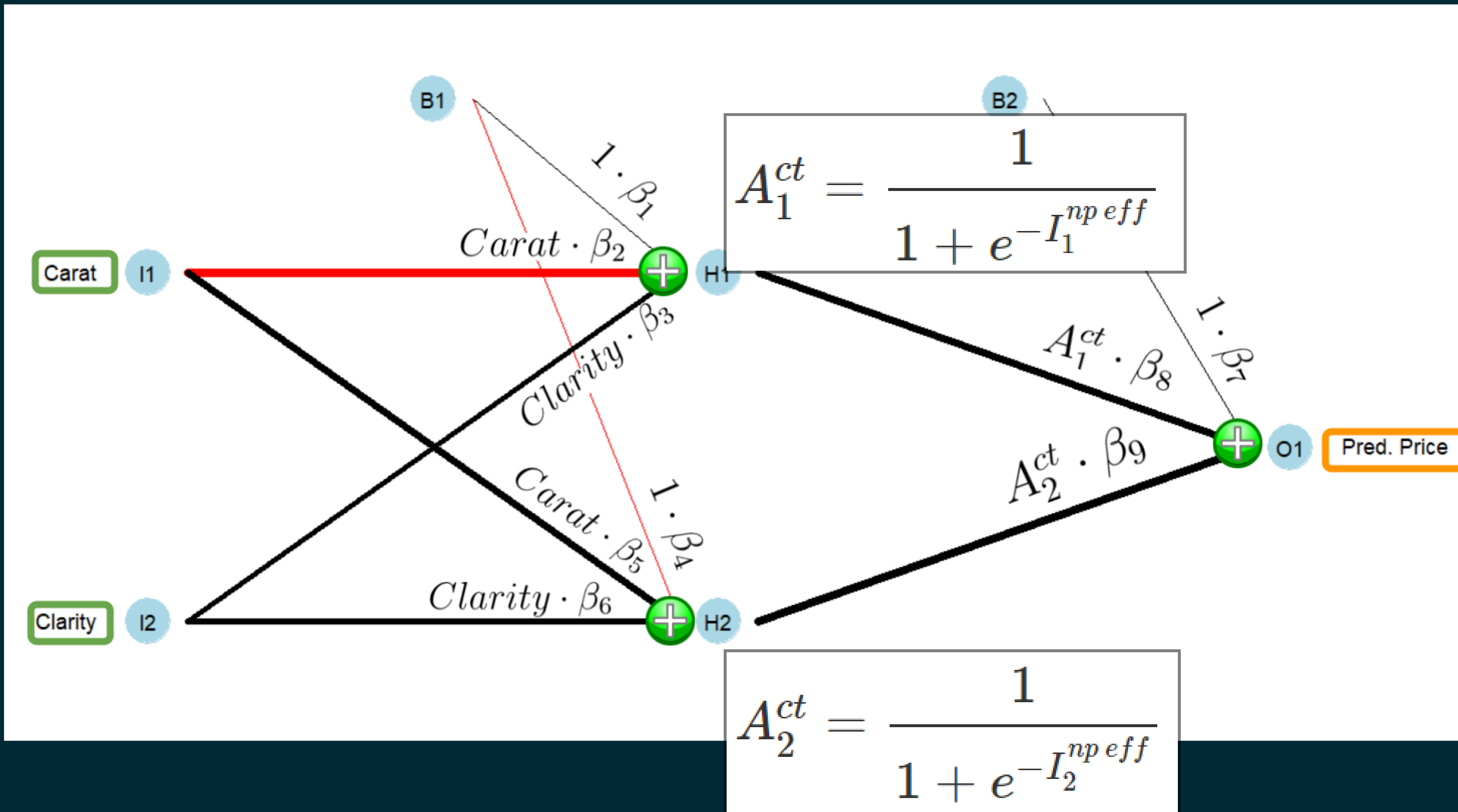
TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

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

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

TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

Inside the Hidden Neurons:



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TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

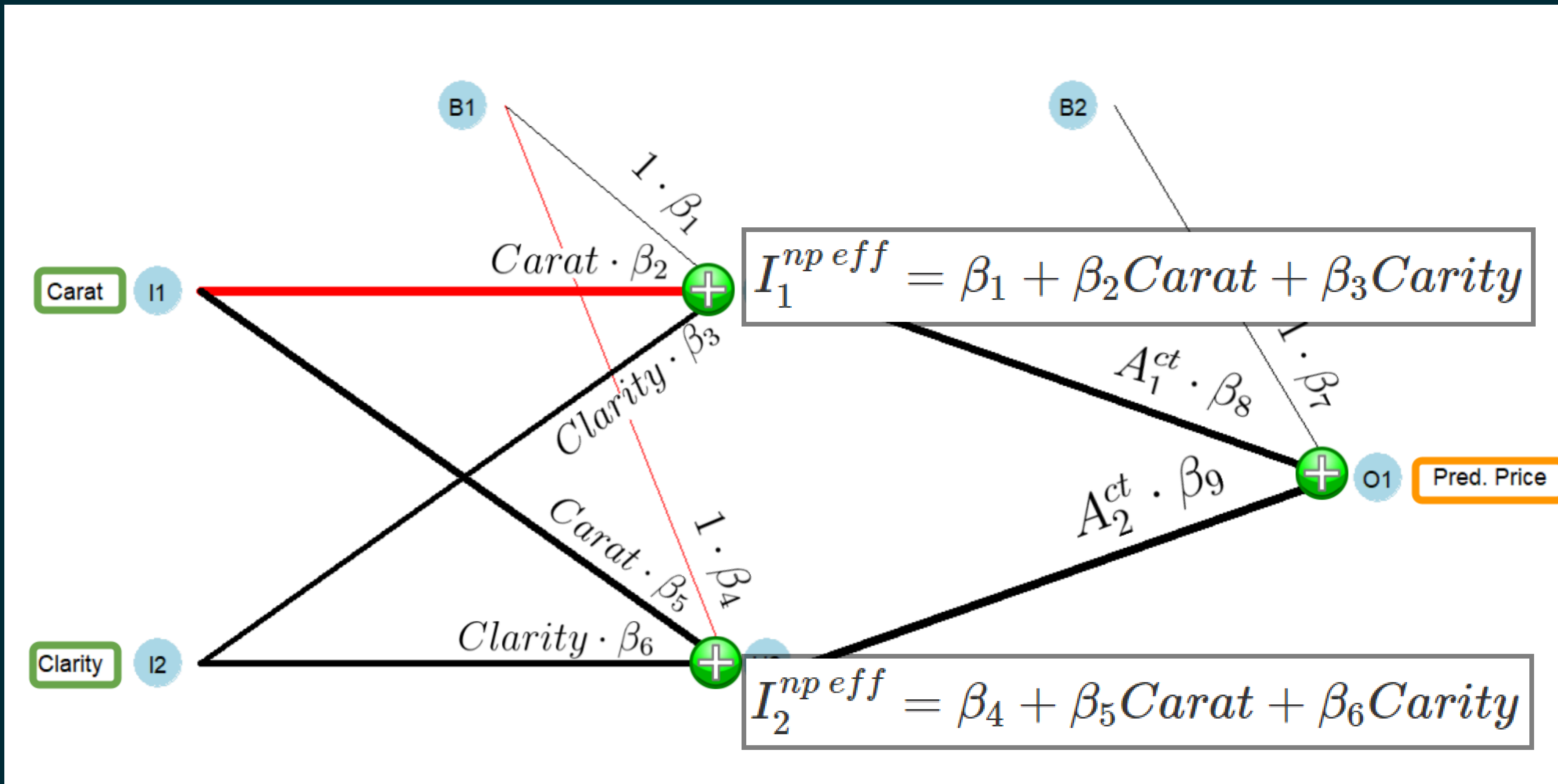
Inside the Hidden Neurons

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

$$\widehat{P_i} = \beta_7 + \overbrace{\frac{1}{1 + e^{-I_1^{np\,eff}}}}^{A_1^{ct}} \cdot \beta_8 + \overbrace{\frac{1}{1 + e^{-I_2^{np\,eff}}}}^{A_1^{ct}} \cdot \beta_9$$

TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

Between the Input and the Hidden Layer:



TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

Between the Input and the Hidden Layer:

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

$$\widehat{P_i} = \beta_7 + \overbrace{\frac{1}{1+e^{-I_1^{np\,eff}}}}^{A_1^{ct}} \cdot \beta_8 + \overbrace{\frac{1}{1+e^{-I_2^{np\,eff}}}}^{A_1^{ct}} \cdot \beta_9$$

$$\widehat{P_i} = \beta_7 + \overbrace{\frac{1}{1+e^{-(\beta_1+\beta_2 Carat_i+\beta_3 Clarity_i)}}}^{A_1^{ct}} \cdot \beta_8$$

$$+ \overbrace{\frac{1}{1+e^{-(\beta_4+\beta_5 Carat_i+\beta_6 Clarity_i)}}}^{A_2^{ct}} \cdot \beta_9$$

IF WE KNOW THE βs WE CAN GENERATE PREDICTIONS!

$$\widehat{P_i} = \beta_7 + \overbrace{\frac{1}{1+e^{-(\beta_1+\beta_2 Carat_i+\beta_3 Clarity_i)}}}^{A_1^{ct}} \cdot \beta_8 + \overbrace{\frac{1}{1+e^{-(\beta_4+\beta_5 Carat_i+\beta_6 Clarity_i)}}}^{A_2^{ct}} \cdot \beta_9$$

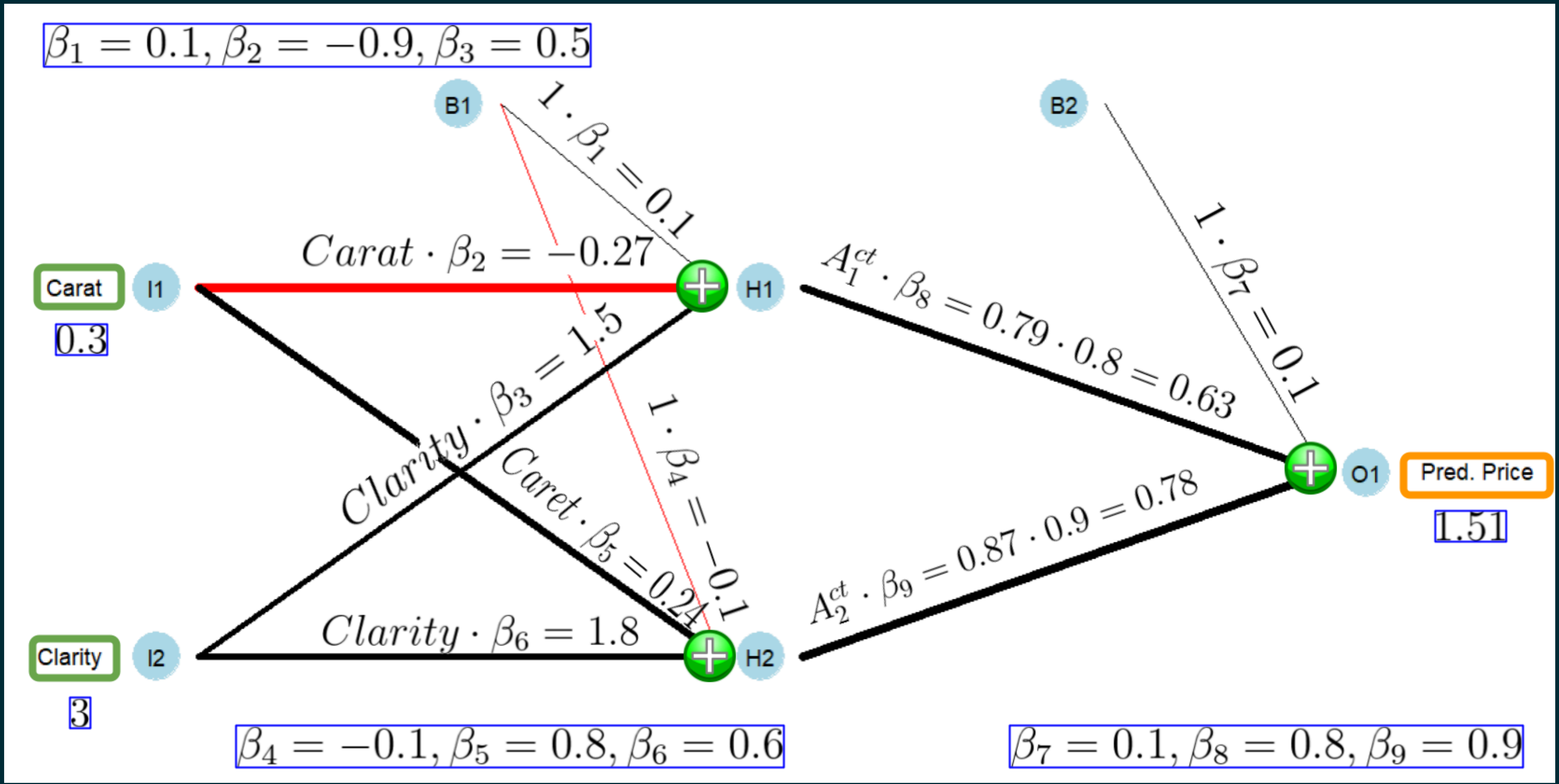
- initial βs are chosen at random.
- optimal βs are found with the *optimizer*.»

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 $Clarity = 3$



PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

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

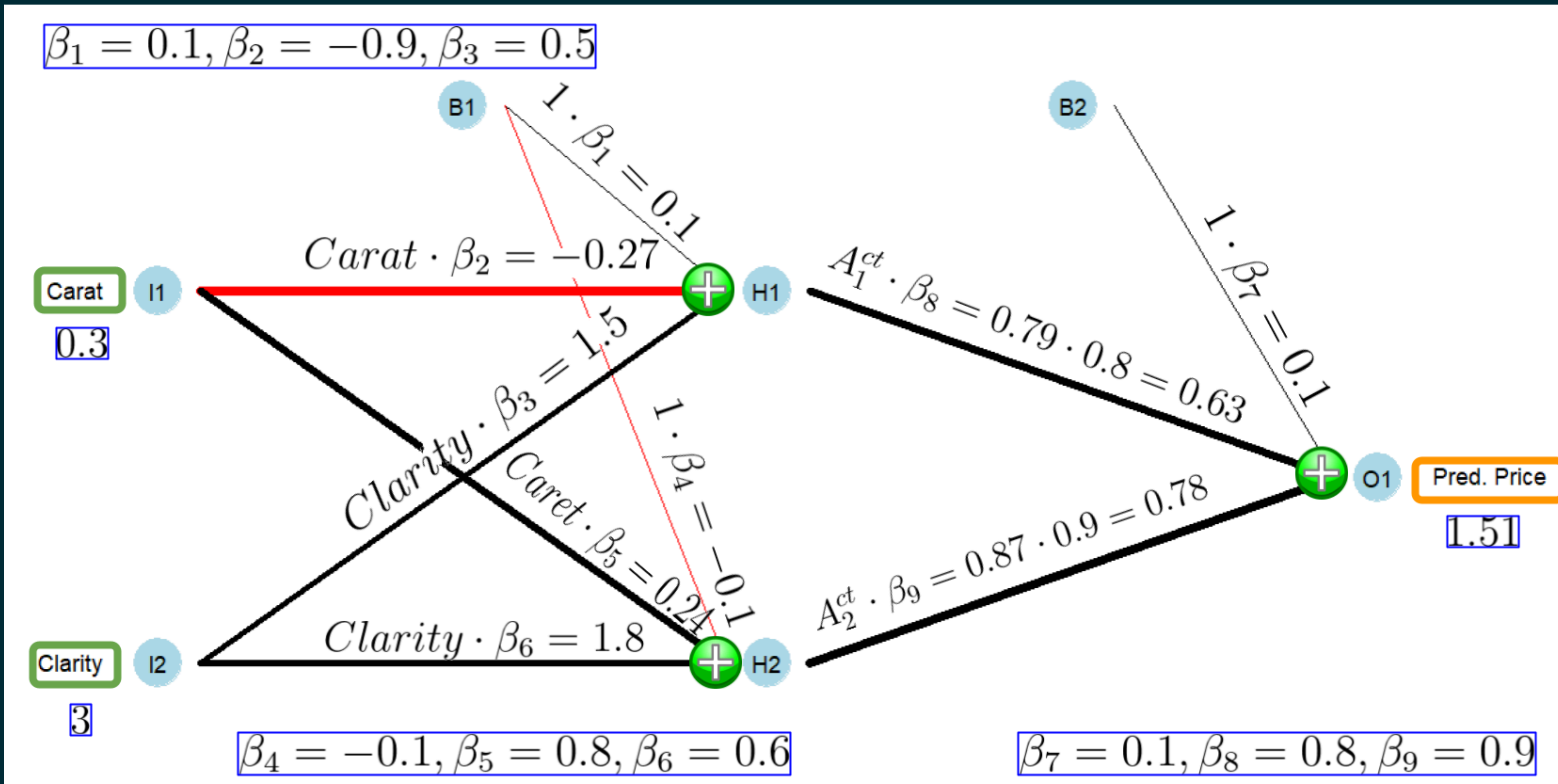
$$\beta_1 = 0.1, \beta_2 = -0.9, \beta_3 = 0.5$$

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

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

PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

Effective Input 2: $Carat = 0.3$ and $Clarity = 3$



PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

Effective Input 2: $Carat = 0.3$ and $Clarity = 3$

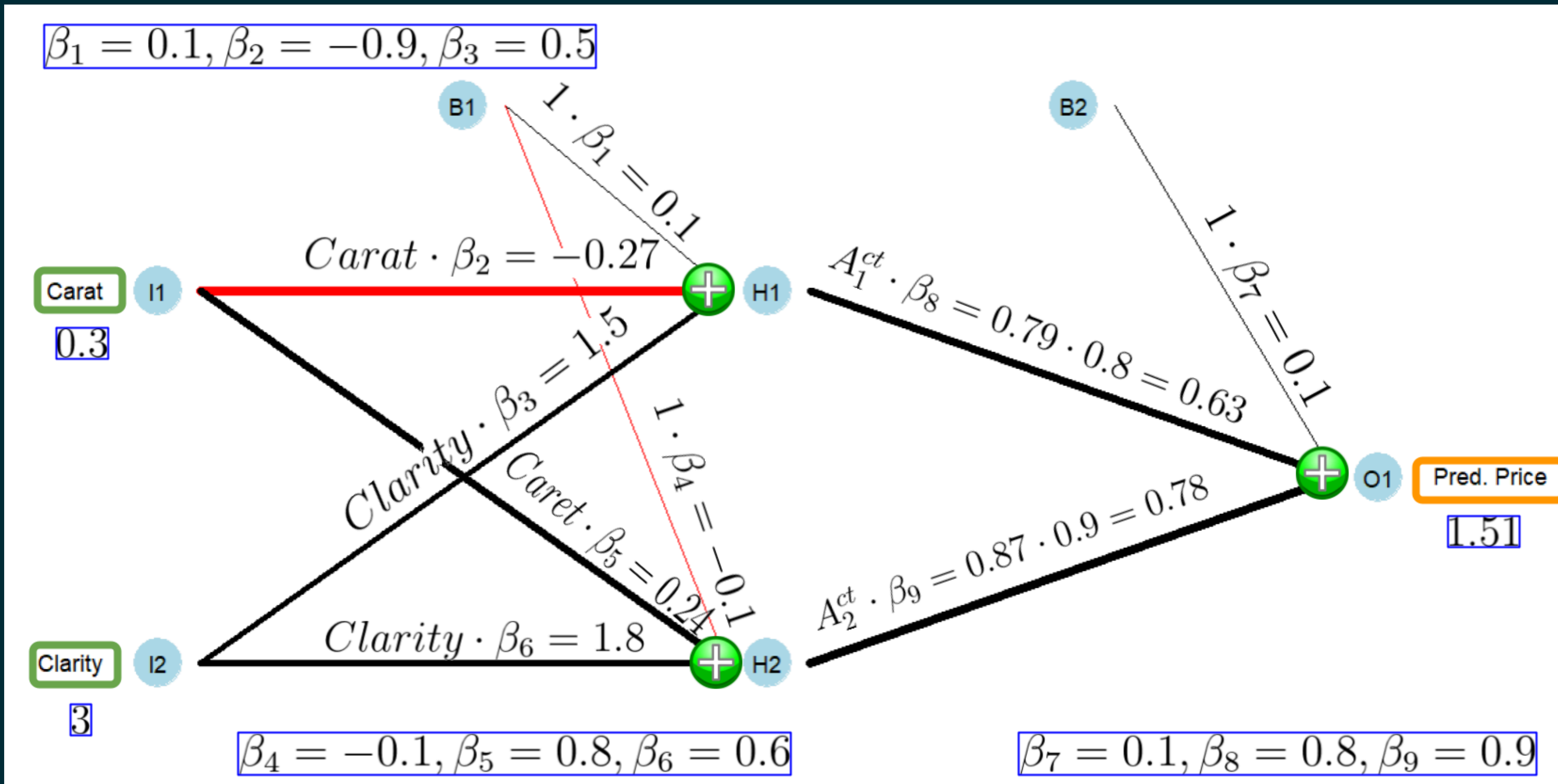
$$\beta_4 = -0.1, \beta_5 = 0.8, \beta_6 = 0.6$$

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

$$I_2^{np\,eff} = \underbrace{1 \cdot (-0.1)}_{1 \cdot \beta_4 = -0.1} + \underbrace{0.3 \cdot 0.8}_{Carat \cdot \beta_5 = 0.24} + \underbrace{3 \cdot 0.6}_{Clarity \cdot \beta_6 = 1.8} = 1.94$$

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 $I_2^{np\,eff} = 1.94$

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

$$A_1^{ct} = \frac{1}{1 + e^{-1.33}} = 0.79$$

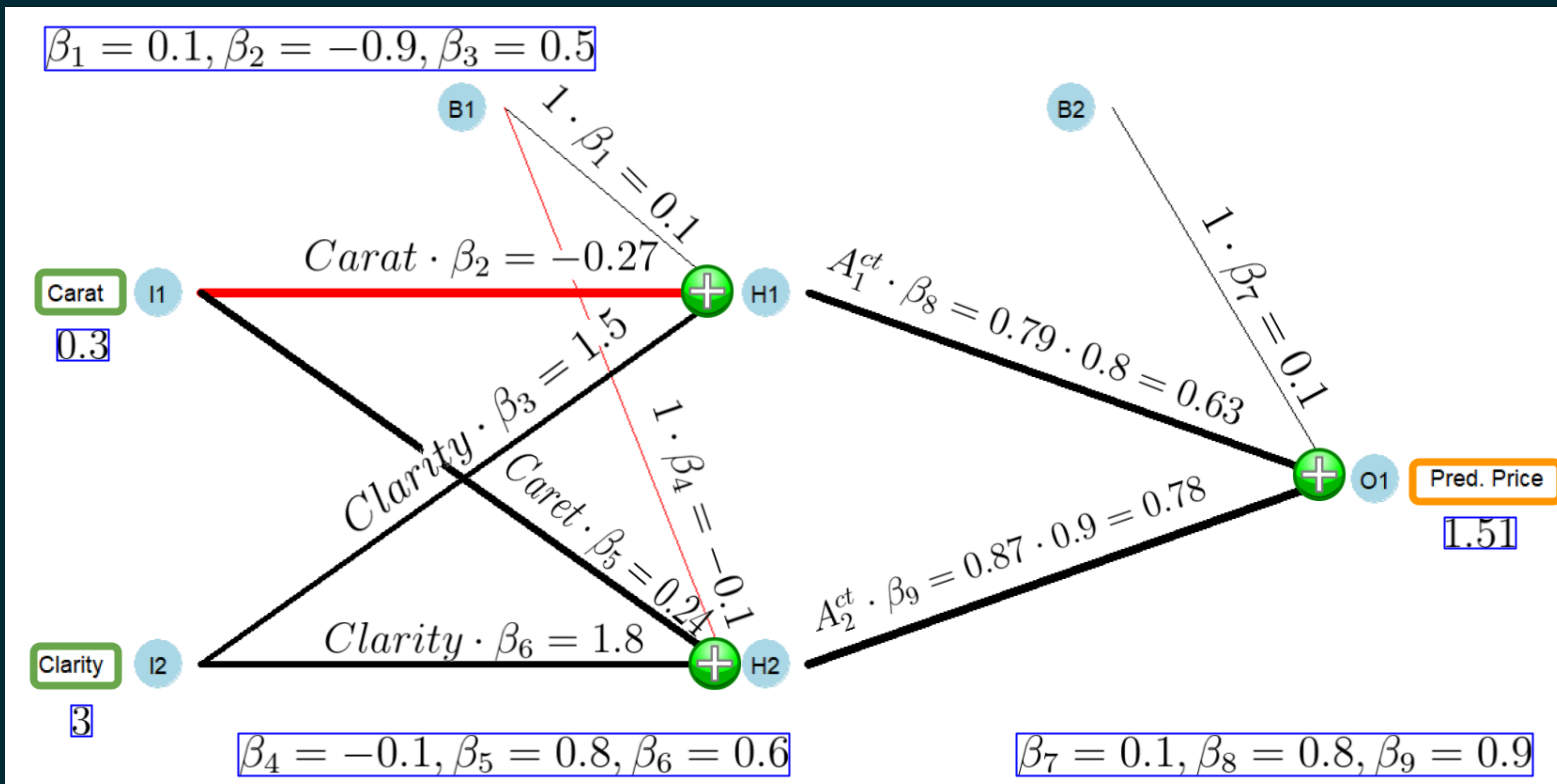
$$A_2^{ct} = \frac{1}{1 + e^{-I_2^{np\,eff}}}$$

$$A_2^{ct} = \frac{1}{1 + e^{-1.94}} = 0.87$$

PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

Prediction:

$\beta_7 = 0.1, \beta_8 = 0.8, \beta_9 = 0.9, A_1^{ct} = 0.79$ and $A_2^{ct} = 0.87$



PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

Prediction:

$\beta_7 = 0.1, \beta_8 = 0.8, \beta_9 = 0.9, A_1^{ct} = 0.79$ and $A_2^{ct} = 0.87$

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

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

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 βs. We do know the βs 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 βs to improve the prediction quality of the neural network?

STEEPEST GRADIENT DESCENT

$$MSE = \frac{\sum_{i=1}^{N} (\widehat{P}_i - P_i)^2}{N}$$

$$\widehat{P_i} = \beta_7 + \overbrace{\frac{1}{1 + e^{-(\beta_1 + \beta_2 Carat_i + \beta_3 Clarity_i)}}}^{A_1^{ct}} \cdot \beta_8 + \overbrace{\frac{1}{1 + e^{-(\beta_4 + \beta_5 Carat_i + \beta_6 Clarity_i)}}}^{A_2^{ct}} \cdot \beta_9$$

STEEPEST GRADIENT DESCENT

$$MSE = \frac{\sum_{i=1}^{N} (\widehat{P}_i - P_i)^2}{N}$$

$$MSE = \frac{\sum_{i=1}^{N} \left(\left(\underbrace{\beta_7 + \overbrace{\frac{1}{1+e^{-(\beta_1+\beta_2 Carat_i+\beta_3 Clarity_i)}}}^{A_1^{ct}} \cdot \beta_8 + \overbrace{\frac{1}{1+e^{-(\beta_4+\beta_5 Carat_i+\beta_6 Clarity_i)}}}^{A_2^{ct}} \cdot \beta_9}_{\widehat{P}_i} \right) - P_i \right)^2}{N}$$

STEEPEST GRADIENT DESCENT

- Initially βs are chosen randomly.
- Optimizer adjusts βs incrementally (iteration by iteration; the iterations are called **epochs**)
- Each epoch:
  - Find if individual β needs to be increased or decreased.
    - Increase β_i and see if MSE increases or not.
    - Decrease β_i and see if MSE increases or not.
    - Reset β_i and note if β_i needs to be increased or decreased.
    - Repeat for all βs
  - 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.

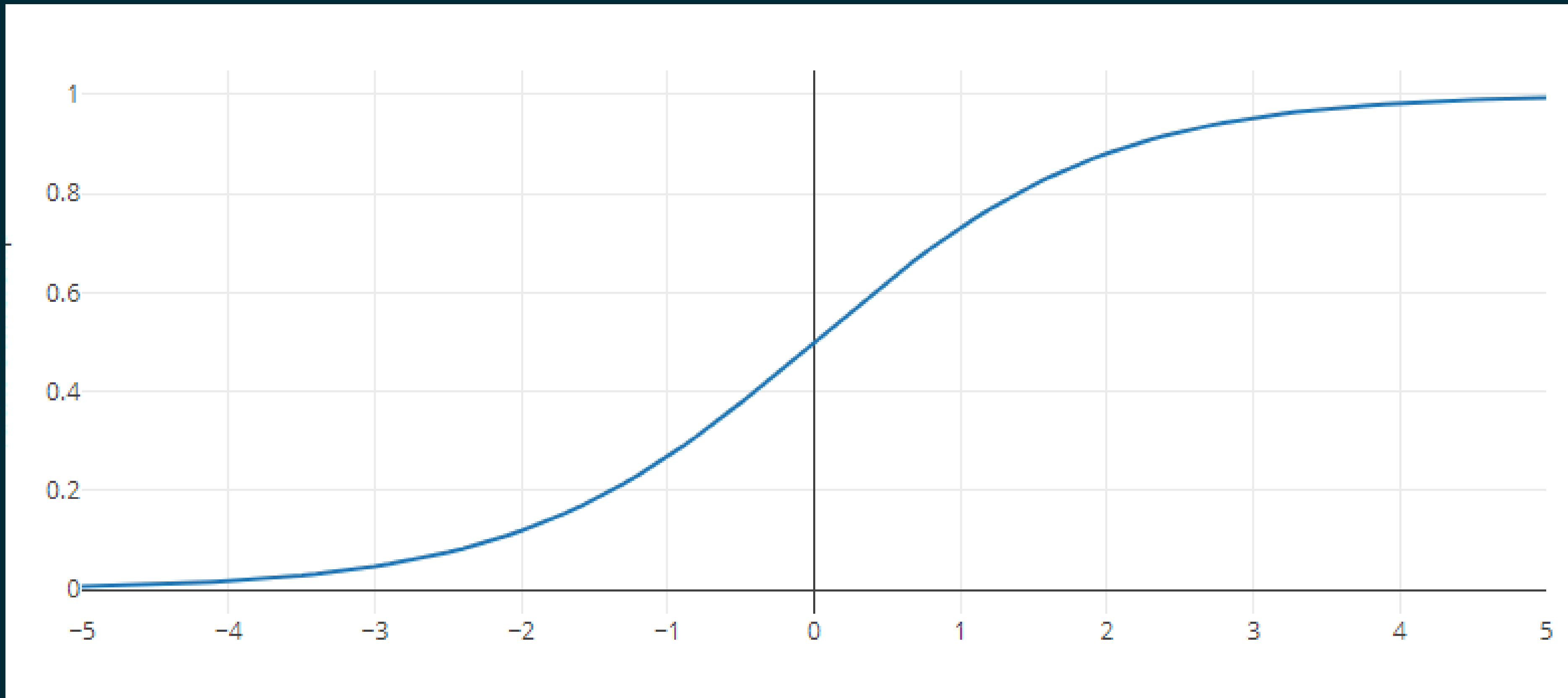
In the example we will z-normalize the predictors.

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.

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.

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

REAL WORLD EXAMPLE TO ESTIMATE DIAMOND PRICES

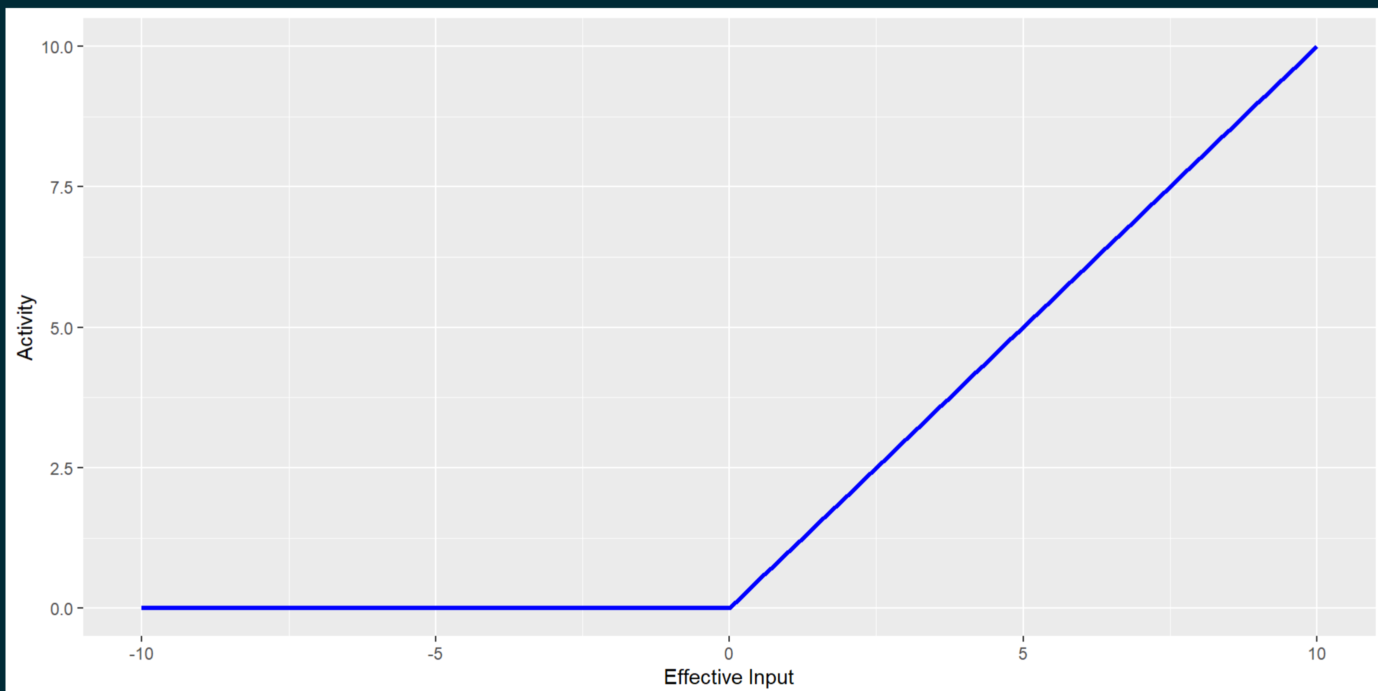
1. You will use all big C variables $Carat$, $Clarity$, Cut, and $Color$. Cut describes the quality of the cut of the diamond rated from 1 (lowest) to 6 (highest) and $Color$ rates the color of a diamond from 1 (highest) to 7 (lowest)
2. Instead of using the `nnet` package, you will use the more advanced `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**

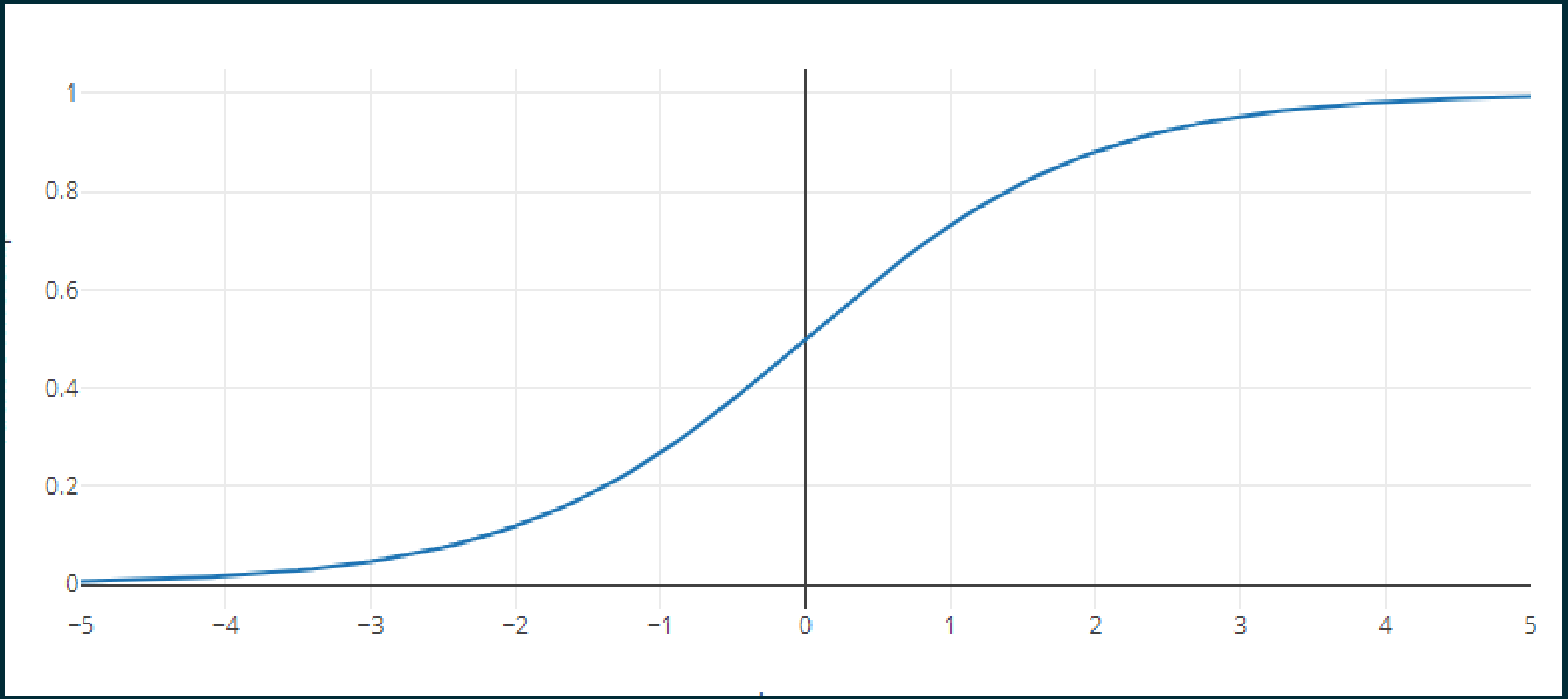
RELU ACTIVATION FUNCTION

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



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

LOGISTIC ACTIVATION FUNCTION: PROBLEM OF VANISHING GRADIENT

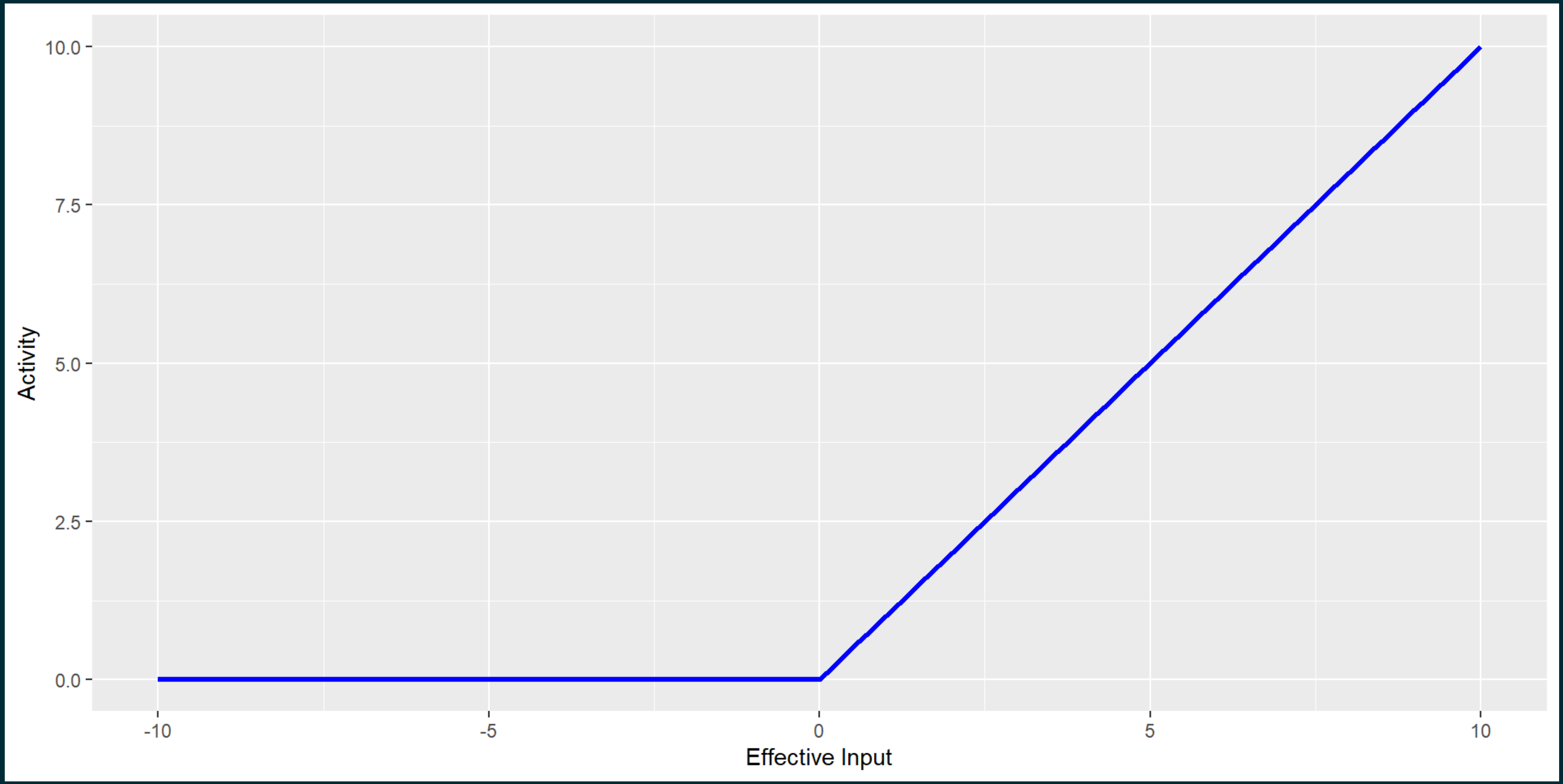


Logistic Activation Function

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).

RELU ACTIVATION FUNCTION: NO PROBLEM OF VANISHING GRADIENT

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



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

Neural Network Real World Application

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

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