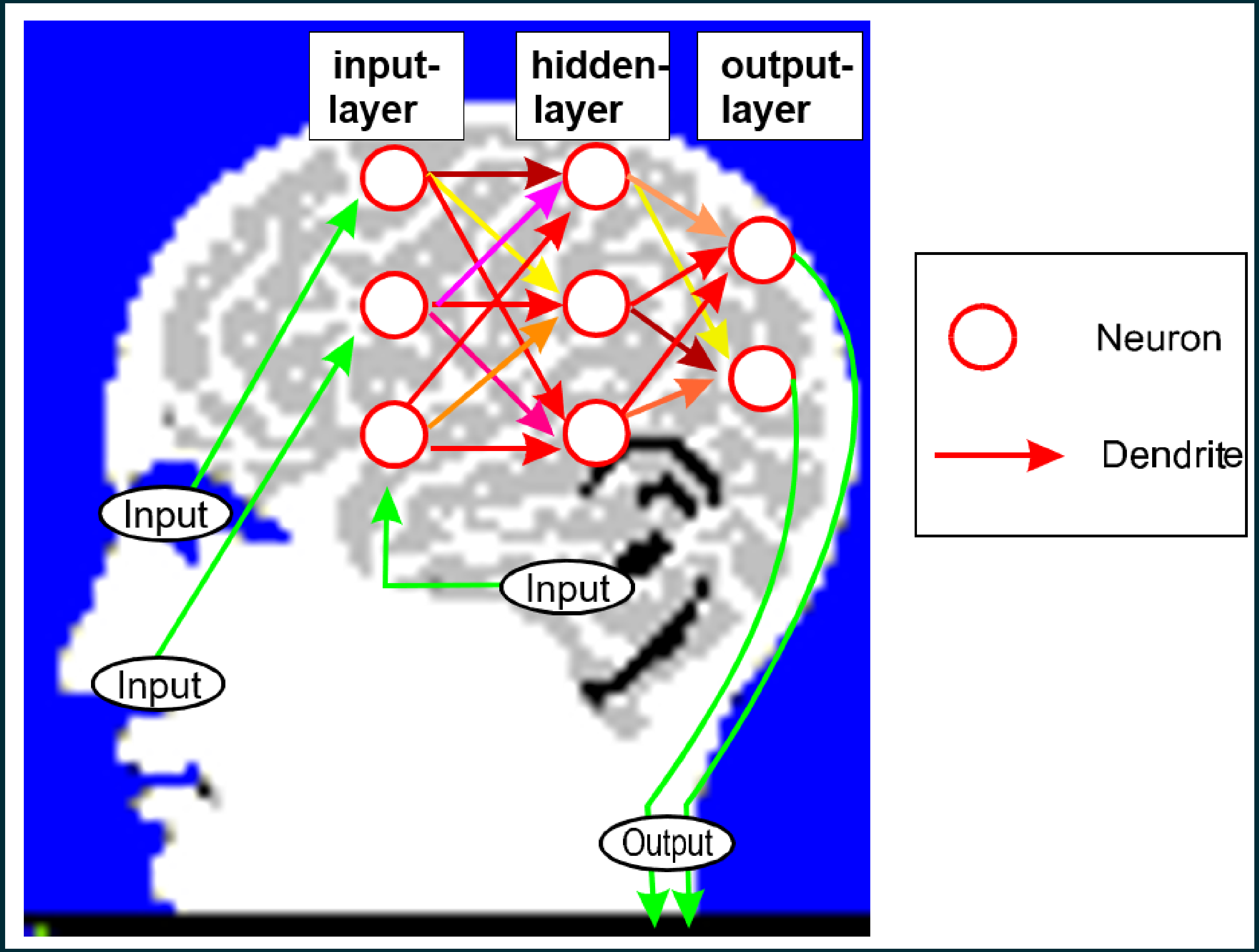
NEURAL NETWORKS

THE EARLY DAYS

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



https://econ.lange-analytics.com/aibook/

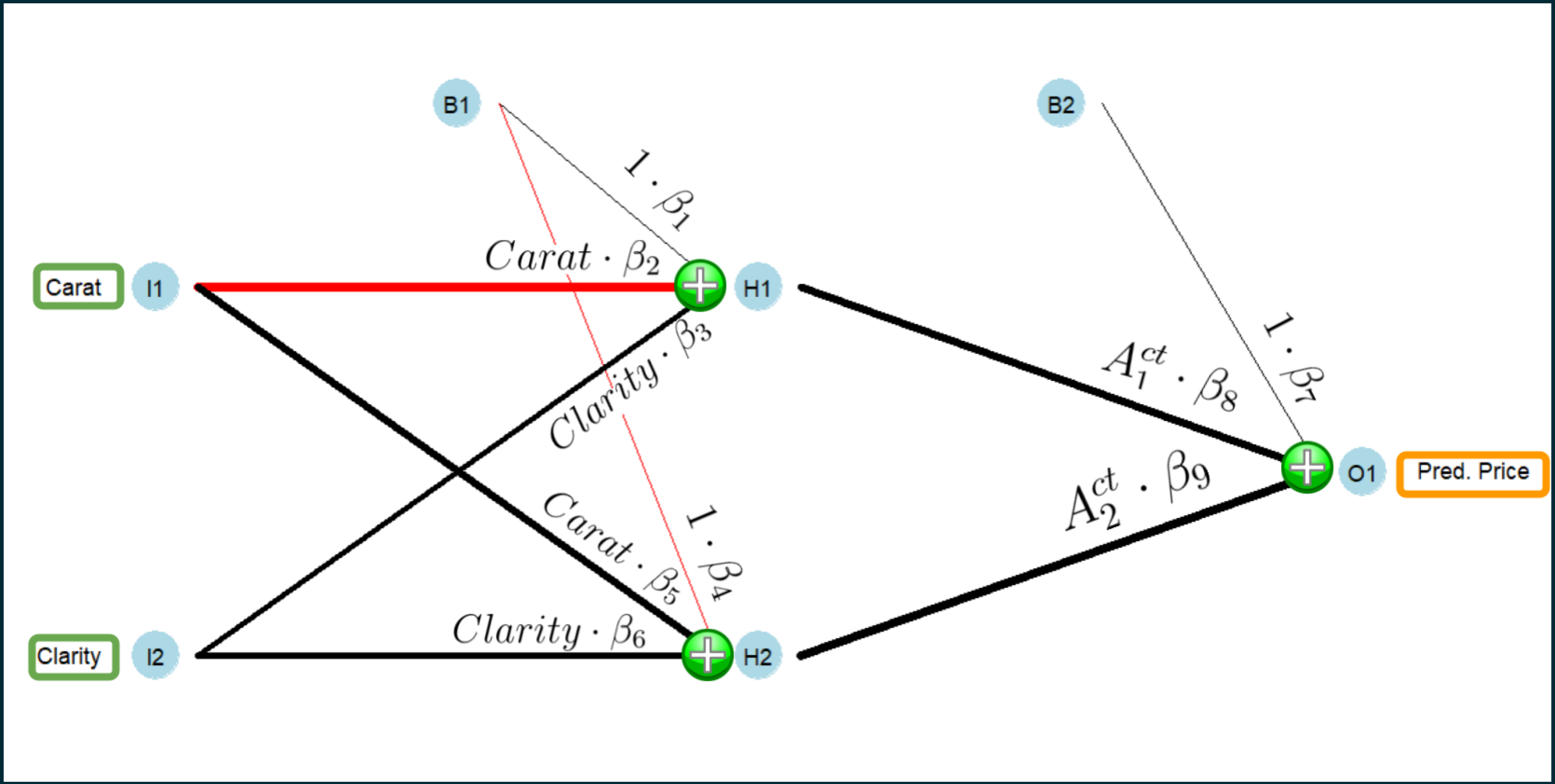
TYPES OF NEURAL NETWORKS

- **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



https://econ.lange-analytics.com/aibook/

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).

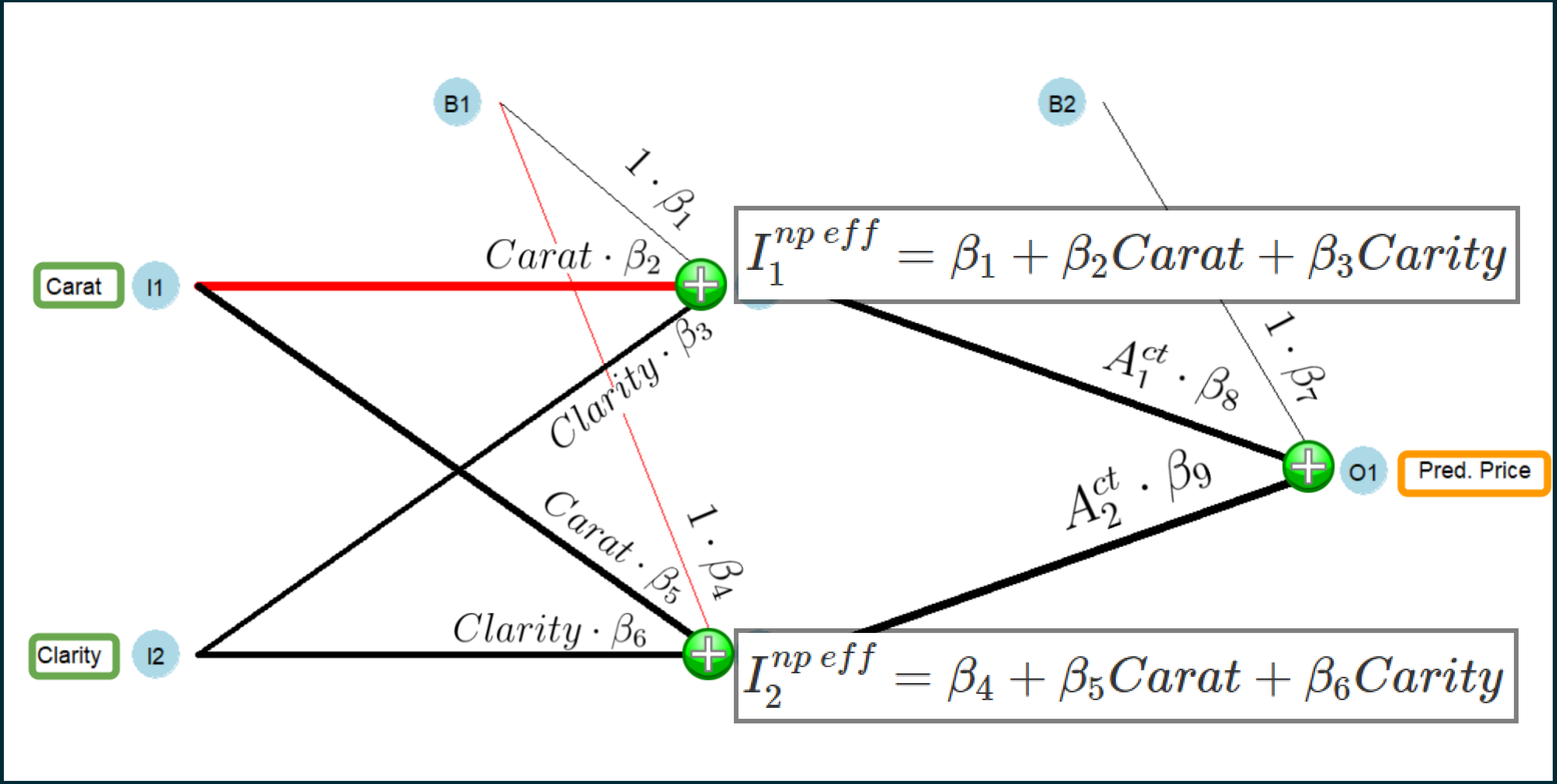
To later increase training speed, we use only 10,000 observations.

▶ 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
```

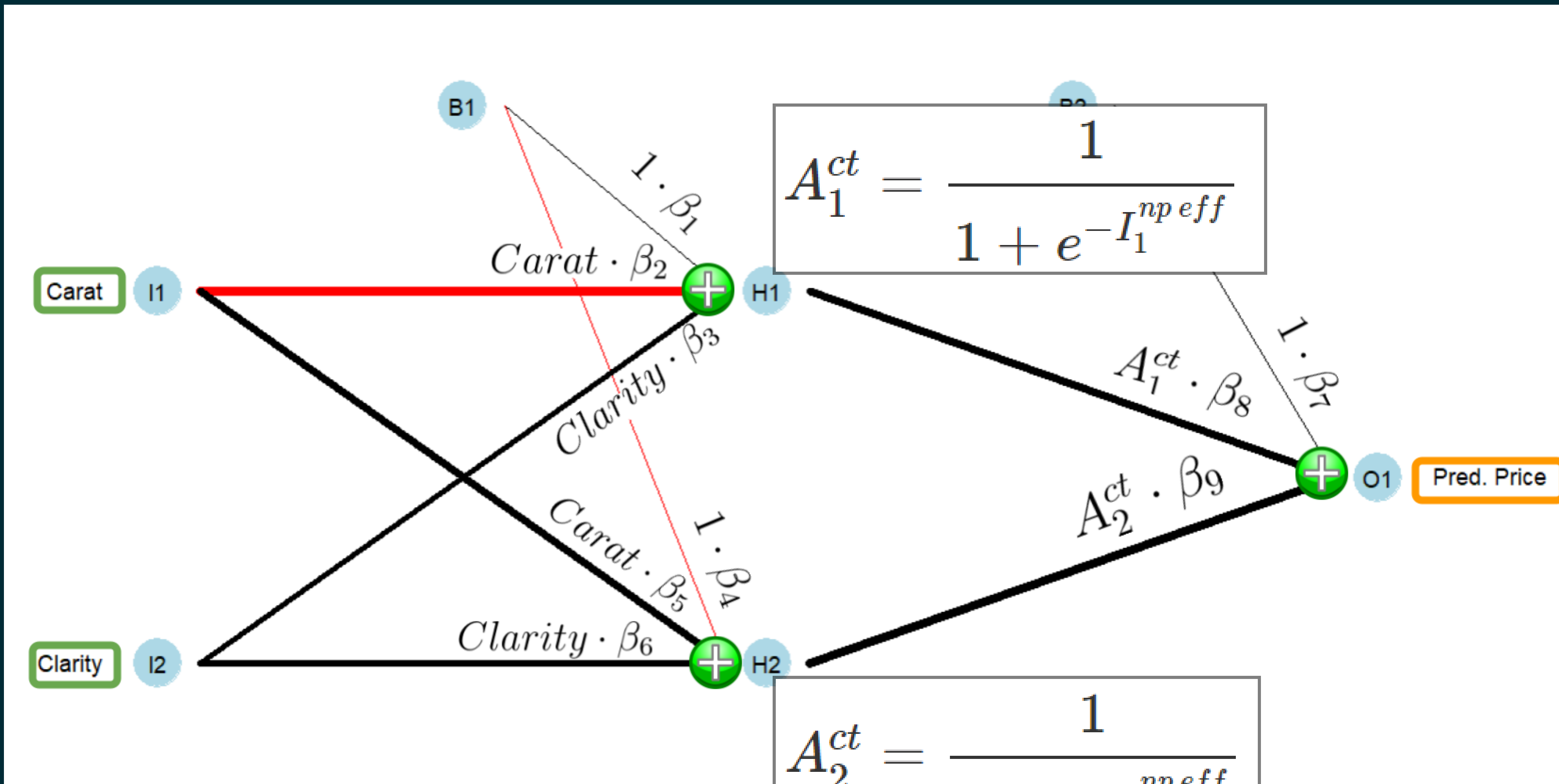
USE A TRAINED NEURAL NEWORK (βs ARE KNOWN) TO PREDICT

EFFECTIV INPUTS TO HIDDEN NEURONS



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

CALCULATE ACTIVITY IN HIDDEN NEURONS WITH LOGISTIC FUNCTION



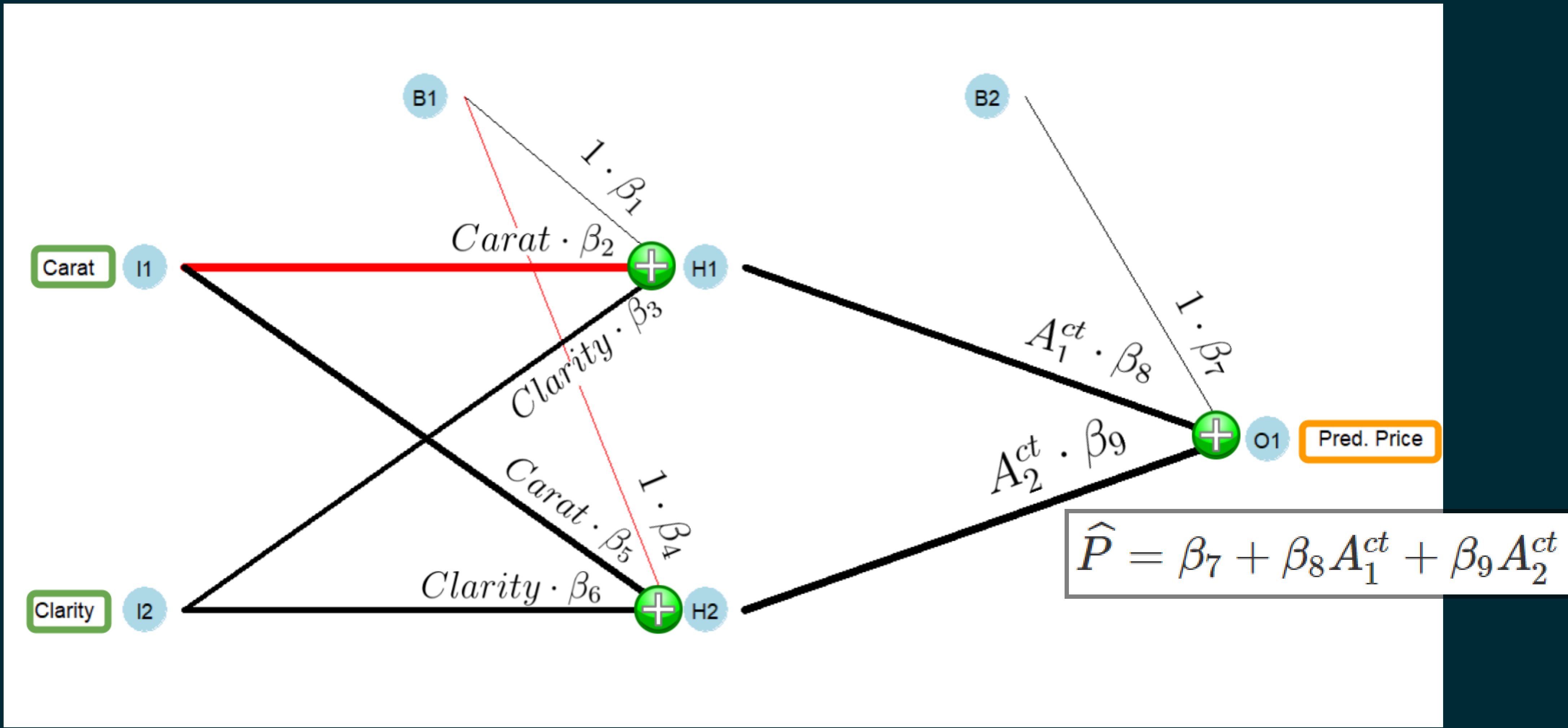
$$A_1^{ct} = \frac{1}{1 + e^{-I_1^{np\,eff}}}$$

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

https://econ.lange-analytics.com/aibook/

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

CALCULATE PREDICTION FROM ACTIVITIES IN HIDDEN NEURONS



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!

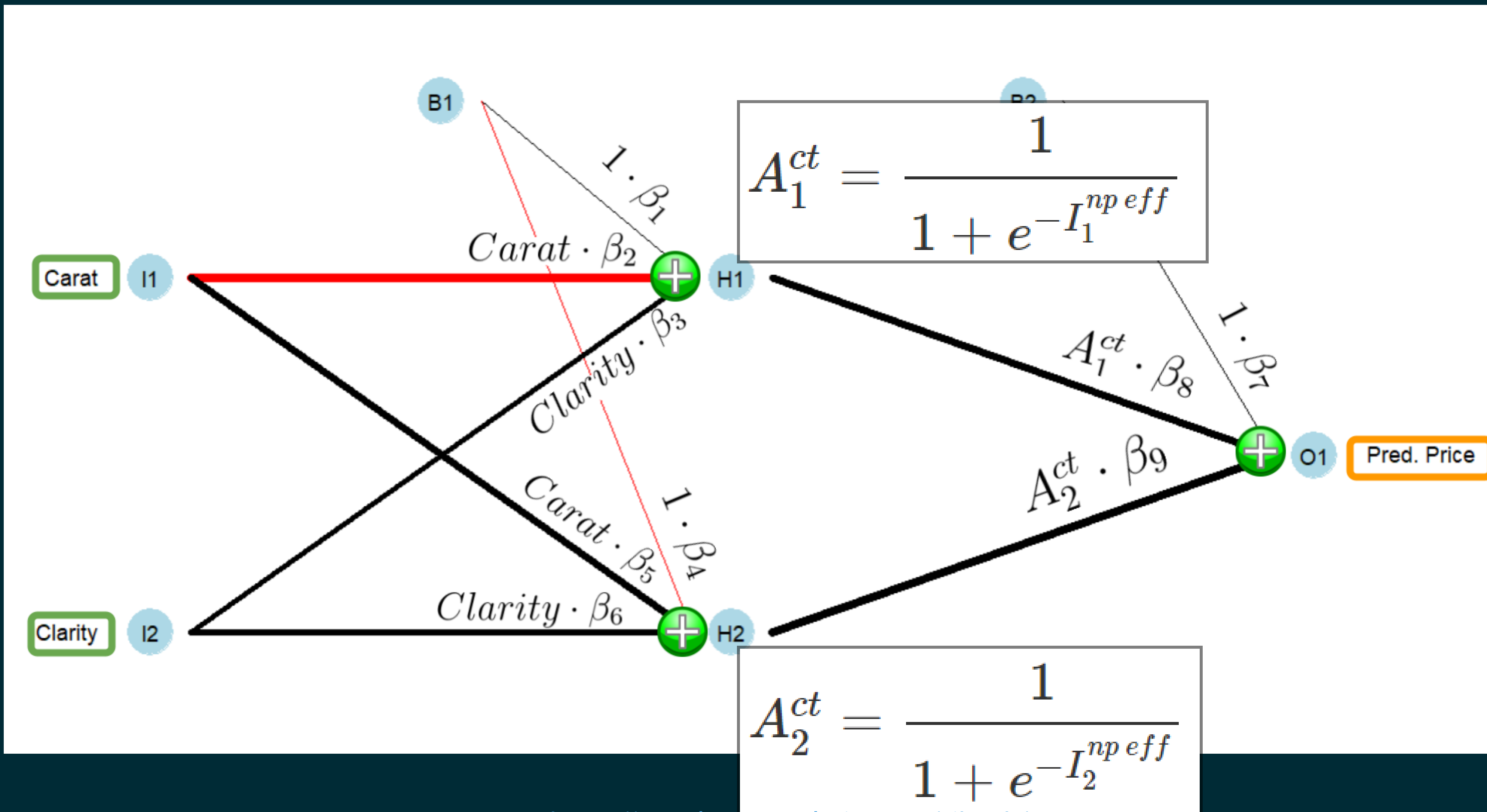
TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

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



TRANSFORMATION FROM NEURAL NETWORK TO PREDICTION EQUATION

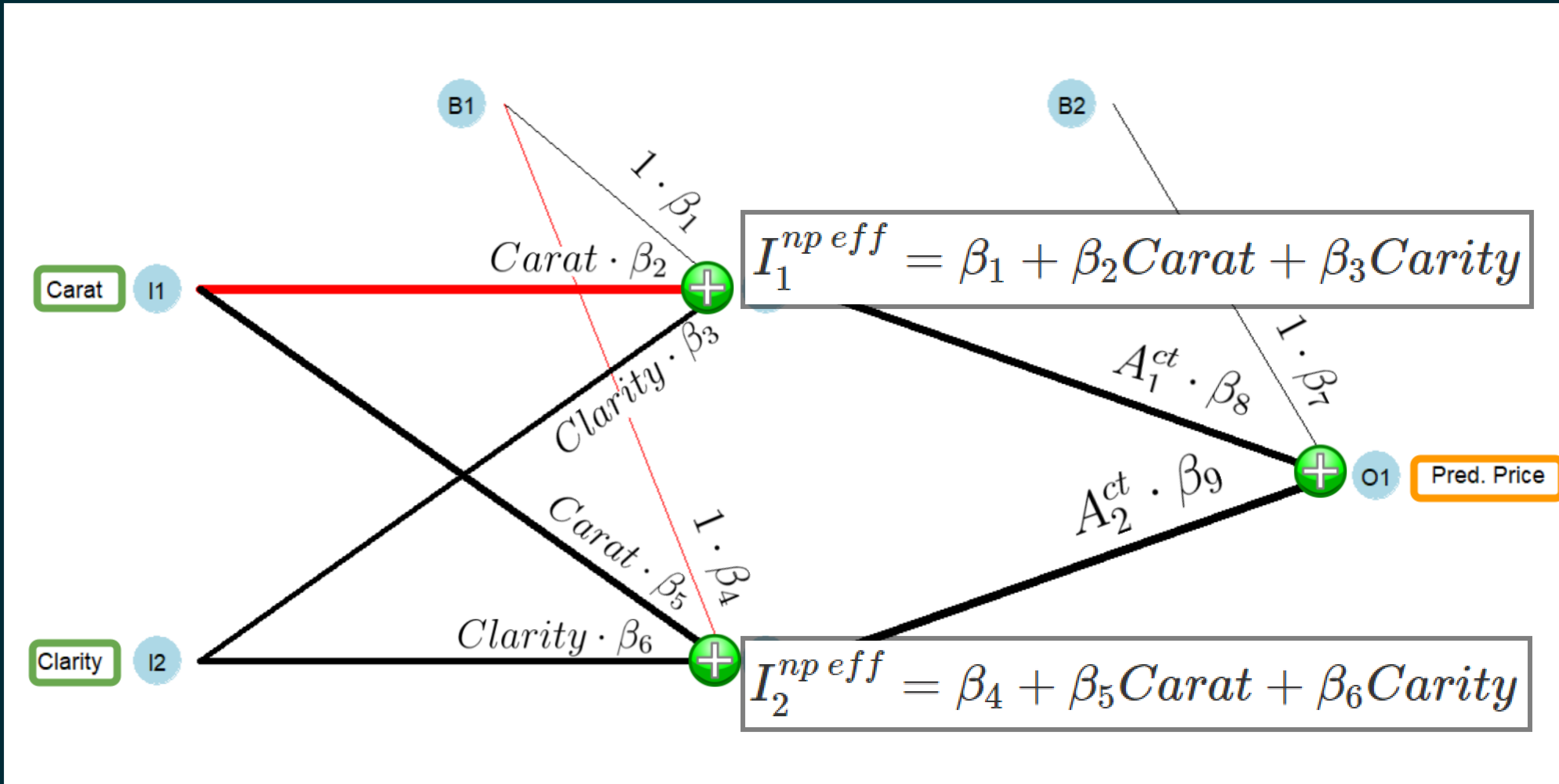
XX INSIDE THE HIDDEN NEURONS

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

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

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!

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

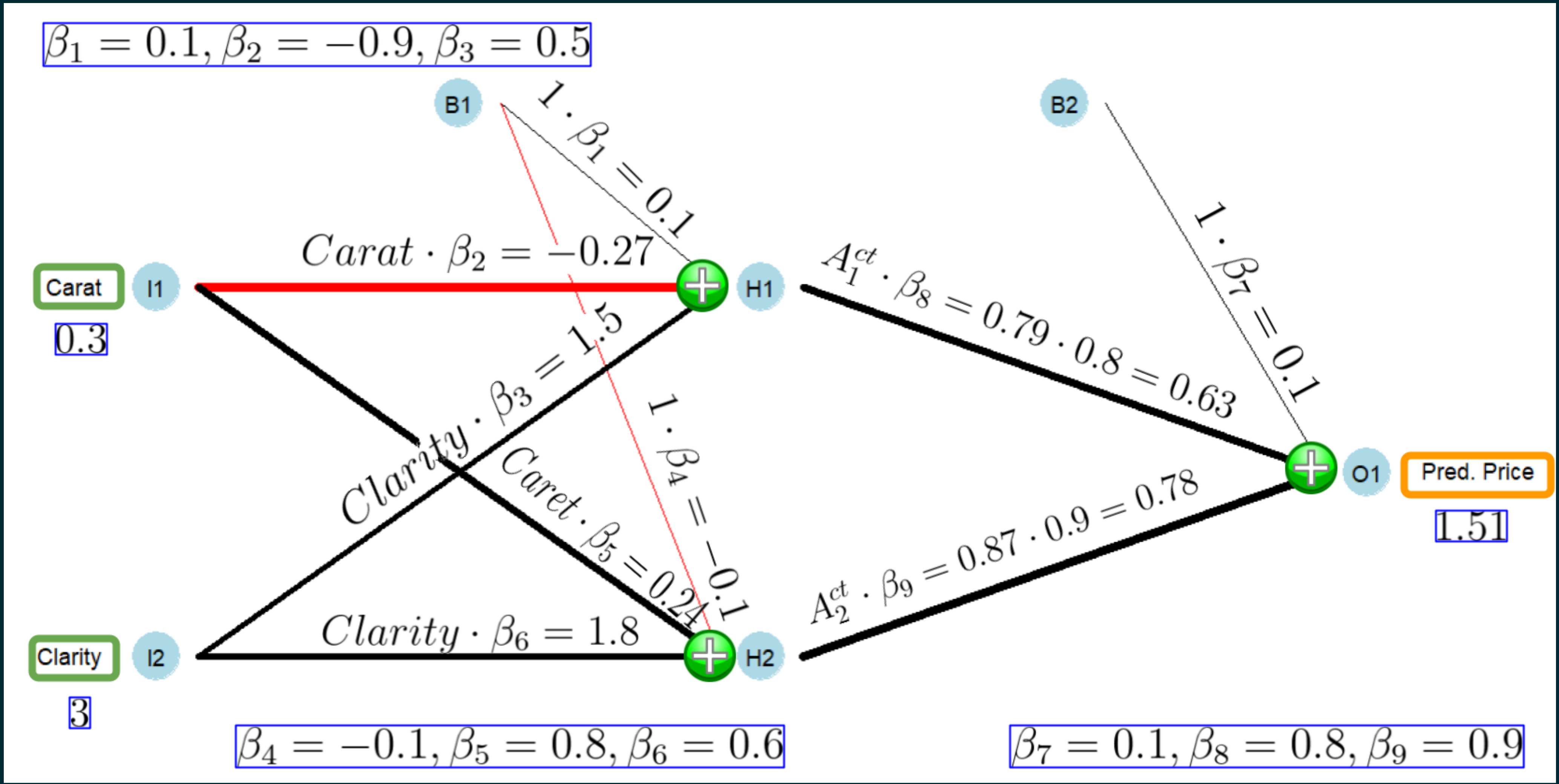
- initial βs are chosen at random.
- optimal βs are found with the *optimizer*.

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 $Clarity = 3$

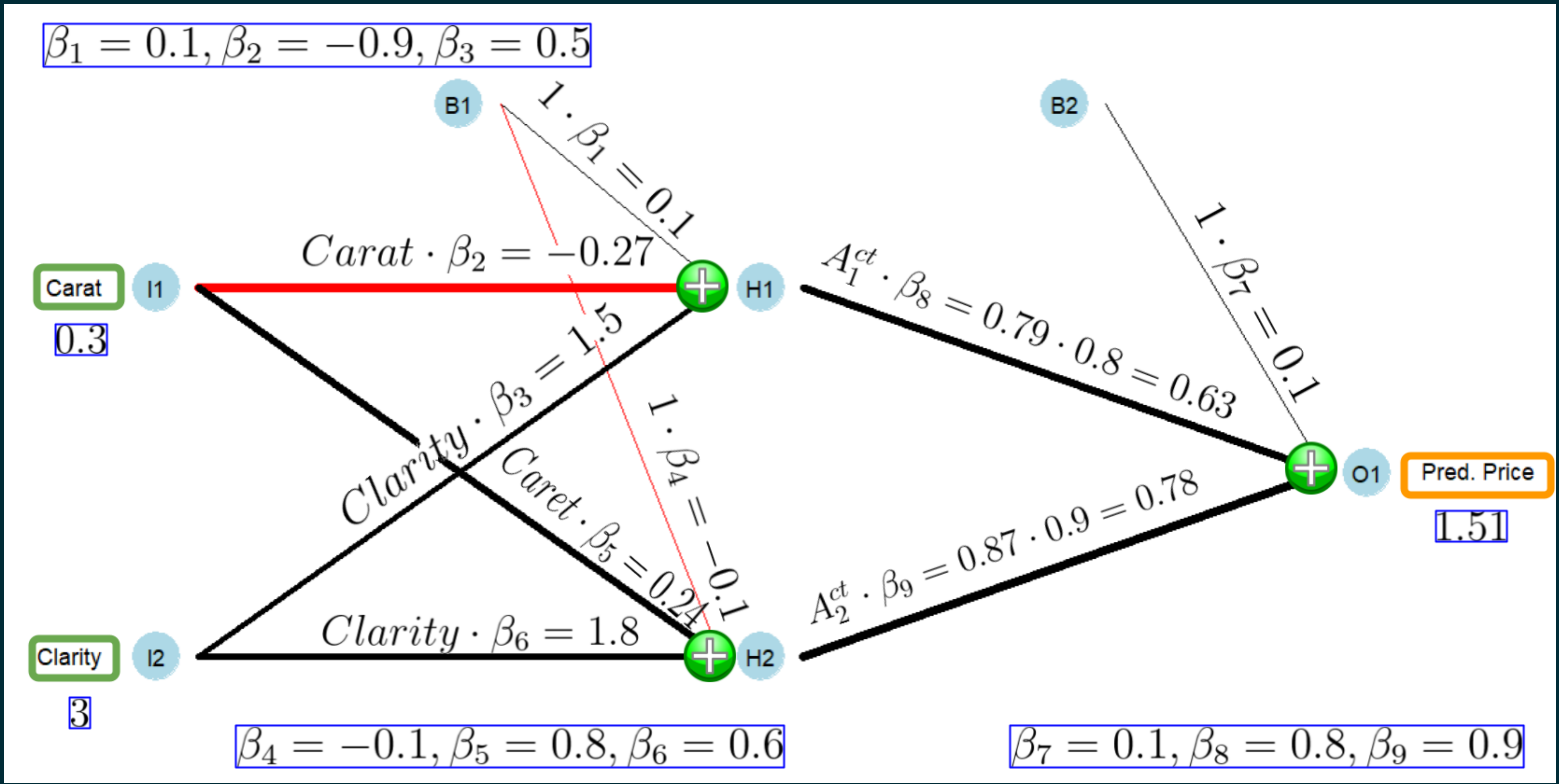
$$\beta_1 = 0.1, \beta_2 = -0.9, \beta_3 = 0.5$$

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

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

PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

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



https://econ.lange-analytics.com/aibook/

PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

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

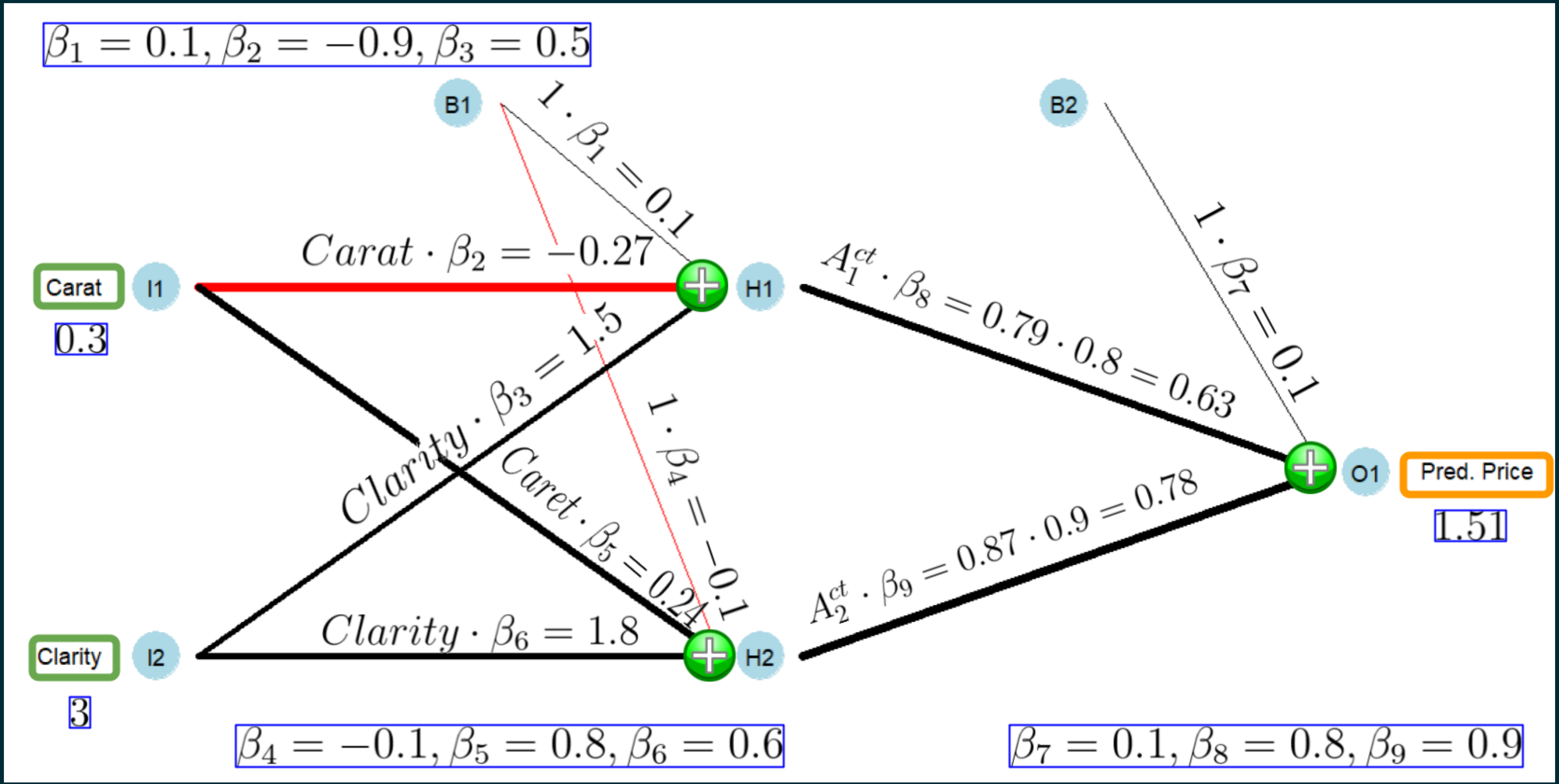
$$\beta_4 = -0.1, \beta_5 = 0.8, \beta_6 = 0.6$$

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

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

PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

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



https://econ.lange-analytics.com/aibook/

PREDICTING THE FIRST OBSERVATION OF THE TRAINING DATA

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

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

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

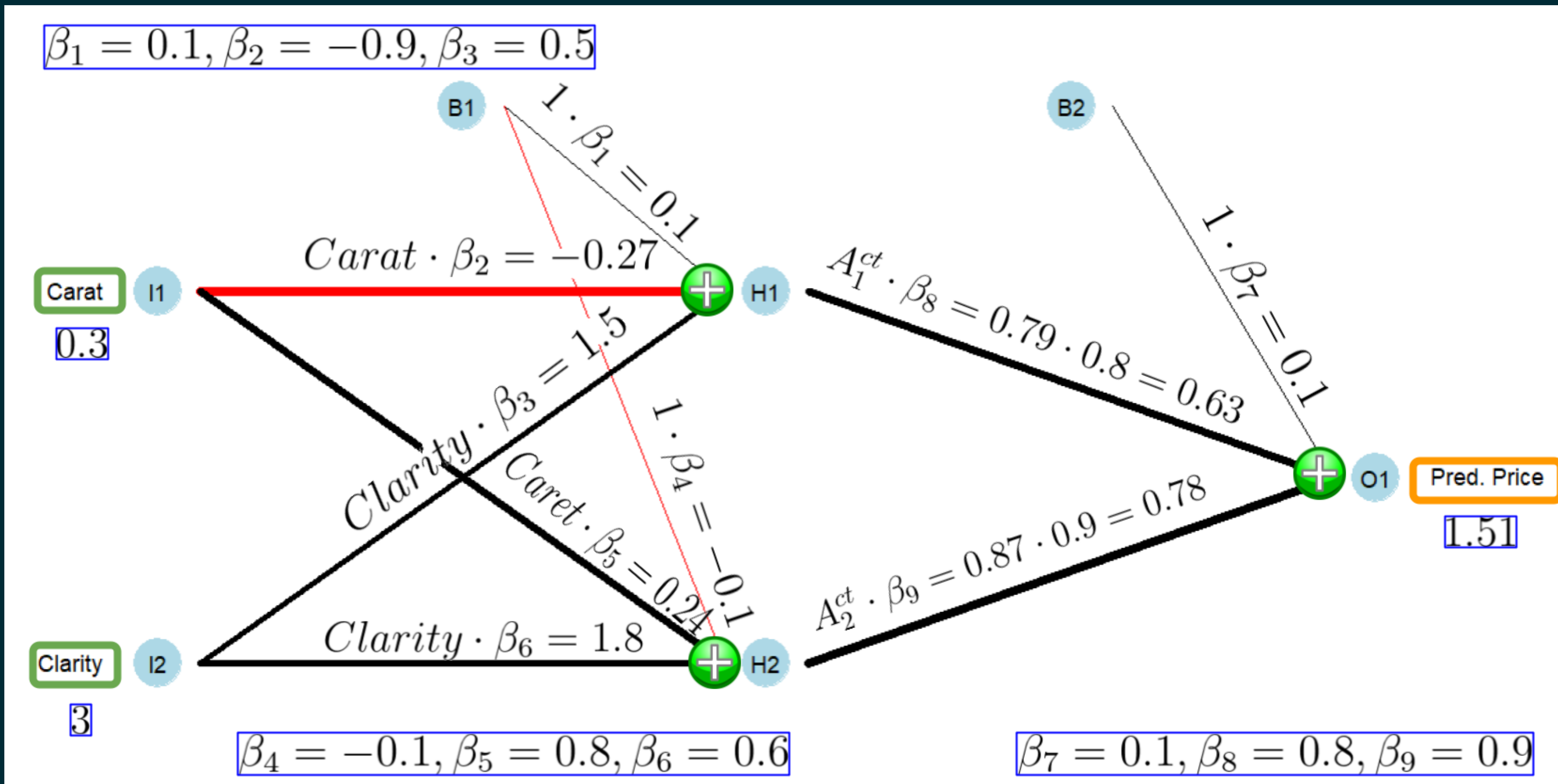
$$A_2^{ct} = \frac{1}{1 + e^{-I_2^{np\,eff}}}$$

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

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

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

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

https://econ.lange-analytics.com/aibook/

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
  - Increase/Decrease the $\beta`s$ proportional to the change of MSE they triggered when changed individually — 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.

The link to the example is in the footer of this slide.

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

$$
\begin{aligned}
\widehat{y_i} = \beta_{10} &+ \overbrace{\frac{1}{1+e^{-(\beta_1 x_i + \beta_2)}}}^{A_1^{ct}} \cdot \beta_7 \\
&+ \overbrace{\frac{1}{1+e^{-(\beta_3 x_i + \beta_4)}}}^{A_2^{ct}} \cdot \beta_8 \\
&+ \overbrace{\frac{1}{1+e^{-(\beta_5 x_i + \beta_6)}}}^{A_3^{ct}} \cdot \beta_9
\end{aligned}
$$