Appendix A

Illustrative Example of Model Execution

To demonstrate the mathematical transparency and reproducibility of the developed ANN-PSO model (8-15-15-1 structure), a step-by-step verification is presented using the exact learned weights and biases. A random test sample was selected to trace the signal propagation from the input layer to the final prediction.

Step 1: Input Normalization

The experimental UCS for the selected sample is 13.45 MPa. The input features were normalized using the Z-score method (Eq. 15), resulting in the following input vector (I):

$I = [0.5875, 0.5902, 1.5073, -0.4600, 0.7821, -1.1528, -0.2676, -0.6097]$

Step 2: First Hidden Layer Processing

The input vector (I) is processed by the 15 neurons of the first hidden layer. To demonstrate the calculation process, we detail the operation for the first neuron ($H1_1$). This neuron computes the weighted sum of the 8 normalized inputs using its specific weight vector ($W_1^{(1)}$) and bias ($b_1^{(1)}$).

- Incoming Weights ($W_1^{(1)}$):

$$[0.1241, -0.2105, -0.5532, 0.3341, -0.4120, 0.2215, 0.1109, -0.3056]$$

- Bias ($b_1^{(1)}$): 0.6250

The net input ($Z_1^{(1)}$) is calculated as:

$$Z_1^{(1)} = \sum_{j=1}^{8} (I_j \times W_{j,1}^{(1)}) + b_1^{(1)}$$

$$Z_1^{(1)} = (0.5875 \times 0.1241) + \cdots + (-0.6097 \times -0.3056) + 0.6250 = -0.8347$$

Applying the activation function:

$$H1_1 = \tanh(-0.8347) = \mathbf{-0.6830}$$

(Repeating this procedure for all 15 neurons yields the complete Layer 1 output vector $O^{(1)}$, listed below):

$$O^{(1)} = [-0.6830, 0.3192, -0.2559, -0.5417, -0.7184, 0.5669, 0.0296, -0.6969, -0.9201, 0.9073, -0.9774, -0.3550, -0.9296, 0.8890, 0.6276]$$

Step 3: Second Hidden Layer Calculation

To illustrate the internal mechanism, we detail the calculation for the first neuron ($H2_1$) of the second hidden layer. This neuron computes the weighted sum of the signals from Layer 1 ($O^{(1)}$) using its specific weight vector ($W_1^{(2)}$) and bias ($b_1^{(2)}$).

- Learned Weights ($W_1^{(2)}$):

$$\begin{bmatrix} -0.4998, 1.1352, 0.4037, -0.8122, -0.8129, -0.3374, -0.3237, 0.4303, -0.1667, 0.4660, \\ -0.4023, -0.3190, 0.3956, -0.2877, 0.4739 \end{bmatrix}$$

- Learned Bias ($b_1^{(2)}$)**:** 0.1056

The net input ($Z_1^{(2)}$) is calculated as:

$$Z_1^{(2)} = \sum_{j=1}^{15} (O_j^{(1)} \times W_{j,1}^{(2)}) + b_1^{(2)} = 1.9858$$

Applying the activation function:

$$H2_1 = \tanh(1.9858) = \mathbf{0.9630}$$

Following the same procedure for all 15 neurons, the complete output vector for Layer 2 ($O^{(2)}$) is obtained:

$$O^{(2)} = [0.9630, -0.6918, -0.9921, 0.4912, -0.8931, -0.9840, 0.9849, 0.9806, 0.4546, 0.8241, 0.9725, -0.7113, -0.9947, 0.9948, 0.9885]$$

Step 4: Final Prediction

The final UCS value is predicted by aggregating the signals from Layer 2 ($O^{(2)}$) using the optimized output weights ($W^{(out)}$) and the final bias ($b^{(out)}$).

- Output Weights ($W^{(out)}$):

$$\begin{bmatrix} -1.1646, 1.3629, -1.6271, 1.2413, -1.0808, -1.4293, 1.0768, 1.1486, 1.5120, 0.9631, 1.2559, \\ -1.0762, -1.2523, 1.3704, 1.3775 \end{bmatrix}$$

- Final Bias **($b^{(out)}$):** 1.2880

The calculation is performed as follows:

$$UCS_{pred} = (O^{(2)} \cdot W^{(out)}) + b^{(out)}$$

$$UCS_{pred} = (0.9630 \times -1.1646) + (-0.6918 \times 1.3629) + \cdots + (0.9885 \times 1.3775) + 1.2880$$

$$UCS_{pred} = \mathbf{13.4450} \text{ MPa}$$

Verification:

Comparing the predicted value with the experimental value (13.4500 MPa):

$$RelativeError = \frac{|\, 13.4450 - 13.4500 \,|}{13.4500} \times 100 = \mathbf{0.04}\%$$

This negligible error (0.04%) confirms the precision of the optimized weights and biases in mapping the complex nonlinear relationship between the mix design parameters and the compressive strength.