Supplementary materials

Enhanced phase prediction of high-entropy alloys through machine learning and data augmentation

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Table S1 Input parameters and the corresponding formula for ML models.

Parameters	Formula
Mean atomic radius	$a = \sum\limits_{i=1}^{n} c_i r_i$
Atomic size difference	$R_d = \sqrt{\sum\limits_{i=1}^{n} c_i (1 - \dfrac{r_i}{a})^2}$
Average of the melting points of constituent elements	$T_m = \sum\limits_{i=1}^{n} c_i T_{mi}$
Standard deviation of melting temperature	$D\_T_m = \sqrt{\sum\limits_{i=1}^{n} c_i (1 - \dfrac{T_i}{T_m})^2}$
Average mixing enthalpy	$H_{mix} = 4 \sum\limits_{i \neq j} c_i c_j H_{ij}$
Standard deviation of mixing enthalpy	$D\_H_{mix} = \sqrt{\sum\limits_{i \neq j} c_i c_j (H_{ij} - H_{mix})^2}$
Ideal mixing entropy	$S_{id} = -k_B \sum\limits_{i=1}^{n} c_i \ln c_i$
Electronegativity	$Elec\_nega = \sum\limits_{i=1}^{n} c_i (Elec\_nega)_i$
Standard deviation of electronegativity	$D\_elec\_nega = \sqrt{\sum\limits_{i=1}^{n} c_i (elec\_nega_i - \overline{elec\_nega})^2}$
Average VEC	$VEC = \sum\limits_{i=1}^{n} c_i VEC_i$

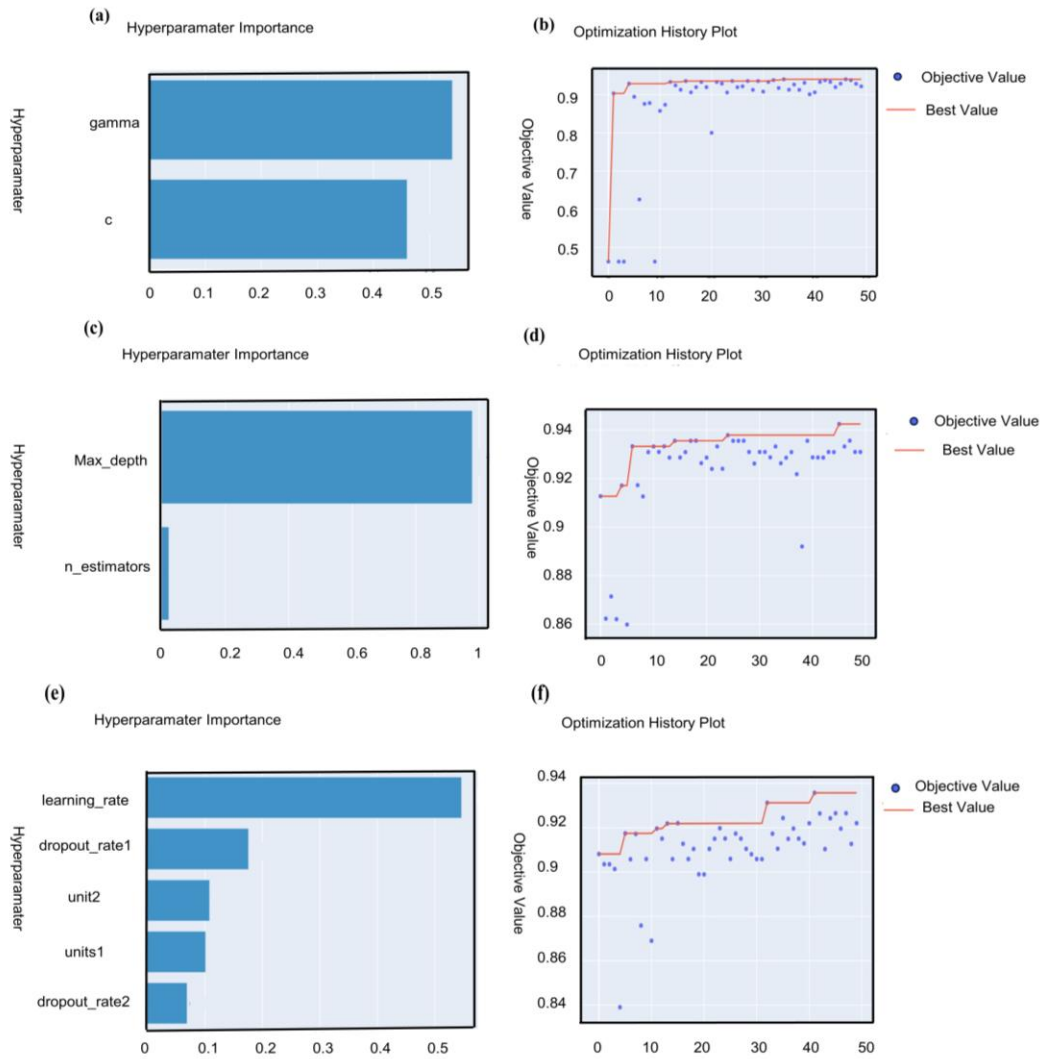| Standard deviation of VEC	$$D\_VEC = \sqrt{\sum_{i=1}^{n} c_i (VEC_i - \overline{VEC})^2}$$
Mean bulk modulus	$$Bulk\,modulus = \sum_{i=1}^{n} c_i Bulk\,modulus_i$$
Standard deviation of bulk modulus	$$D\_Bulk = \sqrt{\sum_{i=1}^{n} c_i (Bulk\,modulus_i - \overline{Bulk\,modulus})^2}$$

Fig. S1. The process of hyperparameter tuning. (a) (c) (e) represent the importance of SVM, RF, and ANN hyperparameters respectively. (b) (d) (f) represent the renderings of 50 iterations of SVM, RF, and ANN hyperparameters respectively.
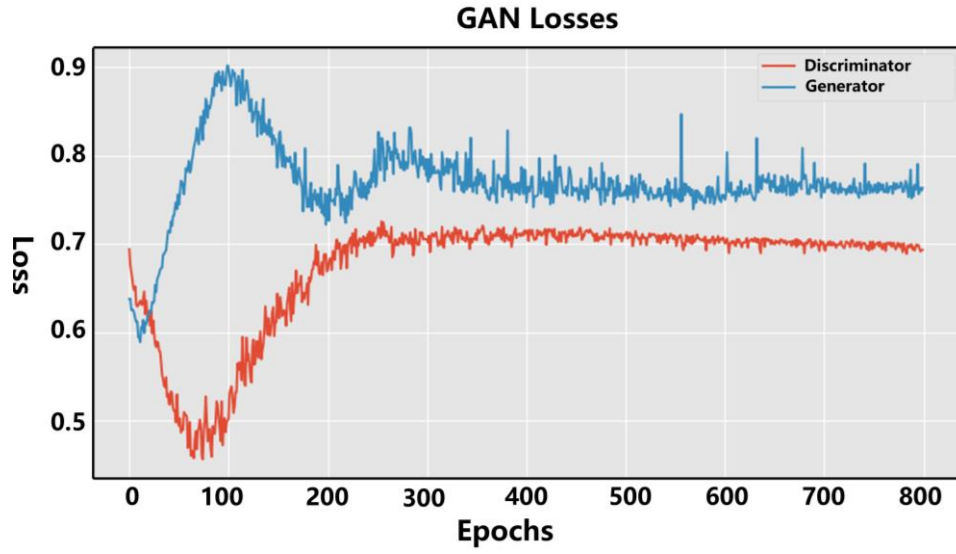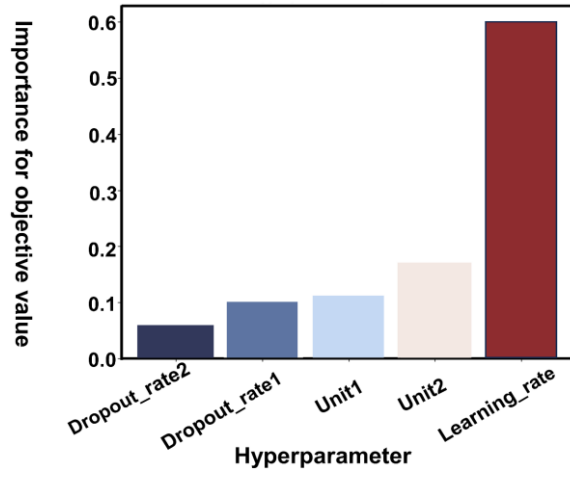
Fig. S2. the generator and discriminator loss curves

Fig. S3. Significance of each hyperparameter in the ANN.