

$$\begin{array}{c} ? \\ ? \\ ? \\ T_C \\ T_C \\ R^2 \\ ? \\ R^2 \\ ? \\ ? \\ ? \\ ? \\ (T_C) \\ f(X) \\ X \\ y(T_C) \\ (X) \\ ? \\ ? \\ ? \\ ? \\ ? \\ ? \\ (N) \\ (P) \\ (G) \\ (AW) \\ (MN) \\ (\mu) \\ (KS) \\ (T_M) \\ (\varepsilon) \\ (R) \\ (V) \\ \tilde{p} \\ d_f \end{array}$$

$$\begin{array}{c} x_{min} \\ x_{max} \\ \Delta x \\ \frac{x}{x} \\ \langle x \rangle \end{array}$$

$$\begin{array}{c} (AW) \\ (AW_{min}) \\ (AW_{max}) \\ (\Delta AW) \\ (AW) \\ (AW) \\ \langle AW \rangle \\ v_{chem} = \\ \{x_H, x_{He}, x_{Li}, x_{Be} \dots \} \\ {}_2O_3 might be represented by the vector \{ \\ \} with 3/5 assigned to the element in 8th position (Oxygen) and 2/5 to 25th (Manganese) other positions are equal to zero. The final di \\ v_{chem} \\ AW_{min} AW_{max} \Delta AW \widetilde{AW} \overline{AW} \langle AW \rangle \\ P_{min} P_{max} \Delta P \widetilde{P} \overline{P} \langle P \rangle \\ G_{min} G_{max} \Delta G \widetilde{G} \overline{G} \langle G \rangle \\ MN_{min} MN_{max} \Delta MN \widetilde{MN} \overline{MN} \langle MN \rangle \\ AW_{min} AW_{max} \Delta AW \widetilde{AW} \overline{AW} \langle AW \rangle \\ V_{min} V_{max} \Delta V \widetilde{V} \overline{V} \langle V \rangle \\ \mu_{min} \mu_{max} \Delta \mu \widetilde{\mu} \overline{\mu} \langle \mu \rangle \\ KS_{min} KS_{max} \Delta KS \widetilde{KS} \overline{KS} \langle KS \rangle \\ T^M_{min} T^M_{max} \Delta T^M \widetilde{T^M} \overline{T^M} \langle T^M \rangle \\ \varepsilon_{min} \varepsilon_{max} \Delta \varepsilon \widetilde{\varepsilon} \overline{\varepsilon} \langle \varepsilon \rangle \\ R_{min} R_{max} \Delta R \widetilde{R} \overline{R} \langle R \rangle \\ N^s_{min} N^s_{max} \Delta N^s \widetilde{N^s} \overline{N^s} \langle N^s \rangle \\ N^p_{min} N^p_{max} \Delta N^p \widetilde{N^p} \overline{N^p} \langle N^p \rangle \\ N^d_{min} N^d_{max} \Delta N^d \widetilde{N^d} \overline{N^d} \langle N^d \rangle \\ N^f_{min} N^f_{max} \Delta N^f \widetilde{N^f} \overline{N^f} \langle N^f \rangle \\ T_C \\ T_C \\ T_C \\ (X) \\ (y) \\ T_C \\ T_C \end{array}$$

$$(3) \quad y = w^T \phi(x)$$

$$(4) \quad J(w) = \sum_{i=1}^n (y_i - w^T x_i)^2$$

$$(5) \quad w = (\phi^T \phi + \lambda I)^{-1} \phi^T y$$

$$\phi \phi^T$$

$$K(x_m, x_n)$$

$$(6) \quad w = (\phi^T (\phi \phi^T + \lambda I))^{-1} y$$

$$(7) \quad K(x_m, x_n) = \phi \phi^T$$

$$\lambda$$

$$m, x_n) =$$

$$x_m^T x_n$$

$$K(x_m, x_n) =$$

$$(x_m^T x_n +$$

$$r)$$

$$K(x_m, x_n) =$$

$$\exp\left(-\frac{\|x_m - x_n\|^2}{2\sigma}\right)$$

$$K(x_m, x_n) =$$

$$\exp(-\alpha \|x_m - x_n\|^2)$$

$$\lambda$$

$$R^2$$

$$RMSE$$

$$fig/krr_results.png$$

$$[Comparison of experimental^{exp}$$

$$(T_C^{ML})$$

$$(T_C^{exp})$$

$$(T_C^{ML})$$

$$fig/rf_s_cetch.png$$

$$[Single Tree model with depth 4 for the regression problem under consideration.]$$

$$Single Tree model with depth 4 for$$

$$fig/rf_convergence.png$$

$$[RF model hyperparameter tuning.]$$

$$RF model hyperparameter tuning a)$$

$$Convergence with respect to$$

$$fig/rf_results.png$$

$$[Optimized RF model performance, left comparison of predicted and experimental data.]$$

$$Optimized RF model$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_convergence.png$$

$$[XGBoost model hyperparameter tuning.]$$

$$XGBoost model hyperparameter tuning : a)$$

$$Convergence$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$

$$300K$$

$$R^2$$

$$R^2$$

$$fig/xgb_results.png$$

$$[Optimized XGBoost performance]$$

$$Optimized XGBoost performance, left comparison of predicted and experimental$$