?
?
?
T_C
T_C
R^2
?
R^2
?
?
?
(T_C)
$f(X)$
X
$y(T_C)$
(X)
?
?
?
?
?
?
(N)
(P)
(G)
(AW)
(MN)
(μ)
(KS)
(T_M)
(ε)
(R)
(V)
s
p
d
f

x_{min}
x_{max}
Δx
$\underline{x}$
$\overline{x}$
$\langle x \rangle$

(AW)
(AW_{min})
(AW_{max})
(ΔAW)
$(\widetilde{AW})$
$(\overline{AW})$
$\langle AW \rangle$
$v_{chem} =$
$\{x_H, x_{He}, x_{Li}, x_{Be}...\}$
$_2O_3 might be represented by the vector \{$
$\}with 3/5 assigned to the element in 8th position (Oxygen) and 2/5 to 25th (Manganese) other positions are equal to zero. The final di$
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

l_2
$y = w^T \phi(x)$
(3)

$$J(w) = \sum_{i=1}^{n} (y_n - w^T x_n)^2$$
(4)

$$w = (\phi^T \phi + \lambda I)^{-1} \phi^T y$$
(5)
$\phi\phi^T$
$K(x_m, x_n)$

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

$$K(x_m, x_n) = \phi\phi^T$$
(7)
λ
$_m, x_n) =$
$x_m^T x_n$
$K(x_m, x_n) =$
$(x_m^T x_n +$
$r)^d$
$K(x_m, x_n) =$
$\exp\left(-\frac{||x_m - x_n||^2}{2\sigma}\right)$
$K(x_m, x_n) =$
$\exp\left(-\alpha ||x_m - x_n||^2\right)$
λ
R^2
$RMSE$
??
??
$_fig/krr_results.png[Comparisonofexperimental_C^{exp})$
(T_C^{ML})
(T_C^{exp})
(T_C^{ML})
??
$_fig/rf_scetch.png[SingleTreemodelwithdepth4fortheregressionproblemunderconsideration.]SingleTreemodelwithdepth4f$
??
??
??
$_fig/rf_convergence.png[RFmodelhyperparameterstuning.]RFmodelhyperparameterstuninga)Convergencewithrespecttoth$
$_fig/rf_results.png[OptimizedRFmodelperformance,leftcomparisonofpredictedandexperimentaldata.]OptimizedRFmode$
$300K$
R^2
R^2
??
??
$(T_C^{exp} -$
$T_C^{pred})$
$(T_C^{exp} -$
$T_C^{pred})/T_C^{exp}$
$T_C >$
$300K$
$T_C^{exp} =$
$1K$
$T_C^{pred} =$
$15K$
(y)
(y)
??
??
γ
α
$\gamma =$
1
$\alpha =$
0.5
$_fig/xgb_convergence.png[XGBoostmodelhyperparameterstuning.]XGBoostmodelhyperparameterstuning: a)Convergence$
$_fig/xgb_results.png[OptimizedXGBoostperformance]OptimizedXGBoostperformance,leftcomparisonofpredictedandexp$
$300K$
R^2
R^2
??
??