Predicting fatigue crack growth rate of austenitic stainless steels in water reactors using machine learning algorithms

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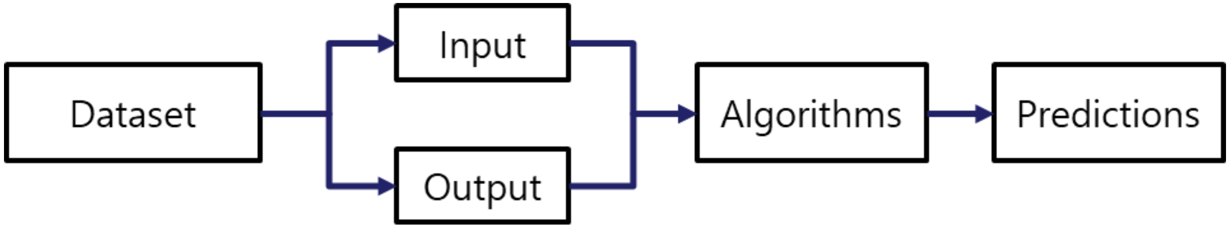
Background

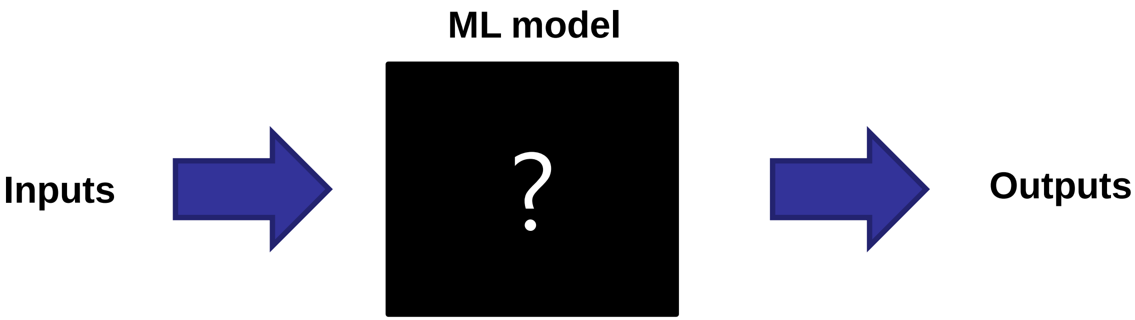
- **Cyclic loading + corrosive environment → corrosion fatigue (CF)**
- **CF has caused some cracking incidents in austenitic stainless steel (SS) components**
- **Modeling CF crack growth rate is necessary**
  - ✓ Empirical models incorporating the concept of fracture mechanics have been developed
  - ✓ There are inconsistencies among these models regarding the considered influencing factors and model forms
  - ✓ Performing model simulations involving numerous variables through traditional empirical methods is hard

Background

- **Machine learning**
  - ✓ Ability to effectively handle tons of input variables
  - ✓ Data-driven → no pre assumption and often no physical knowledge are required



- **Machine learning model = black box**



  - ✓ High complexity
  - ✓ Low interpretability/explainability

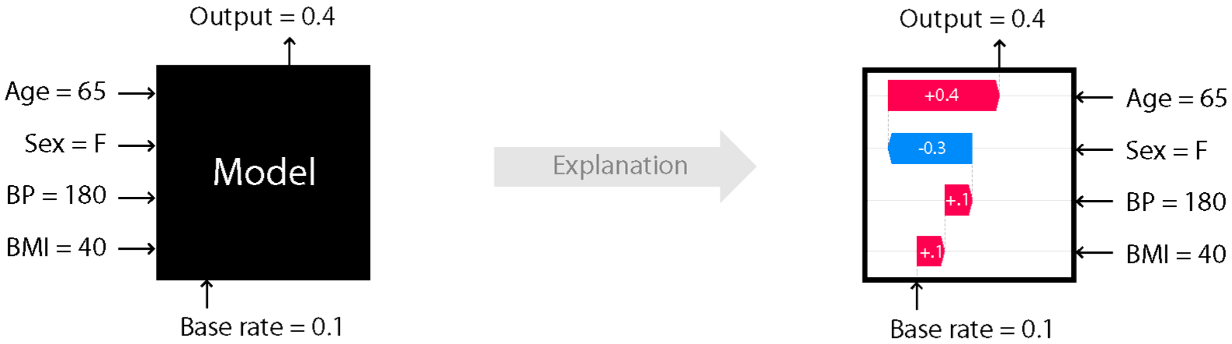
Background

- **Black box explainer/interpreter: SHAP (Shapley additive explanation) [1]**
  - ✓ Linear regression at *local level* (e.g., per individual data point). The output $\hat{y}$ is:

$$\hat{y} = y_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

  - ✓ y_0 is the baseline output, $\theta_i x_i$ is the contribution of feature x_i

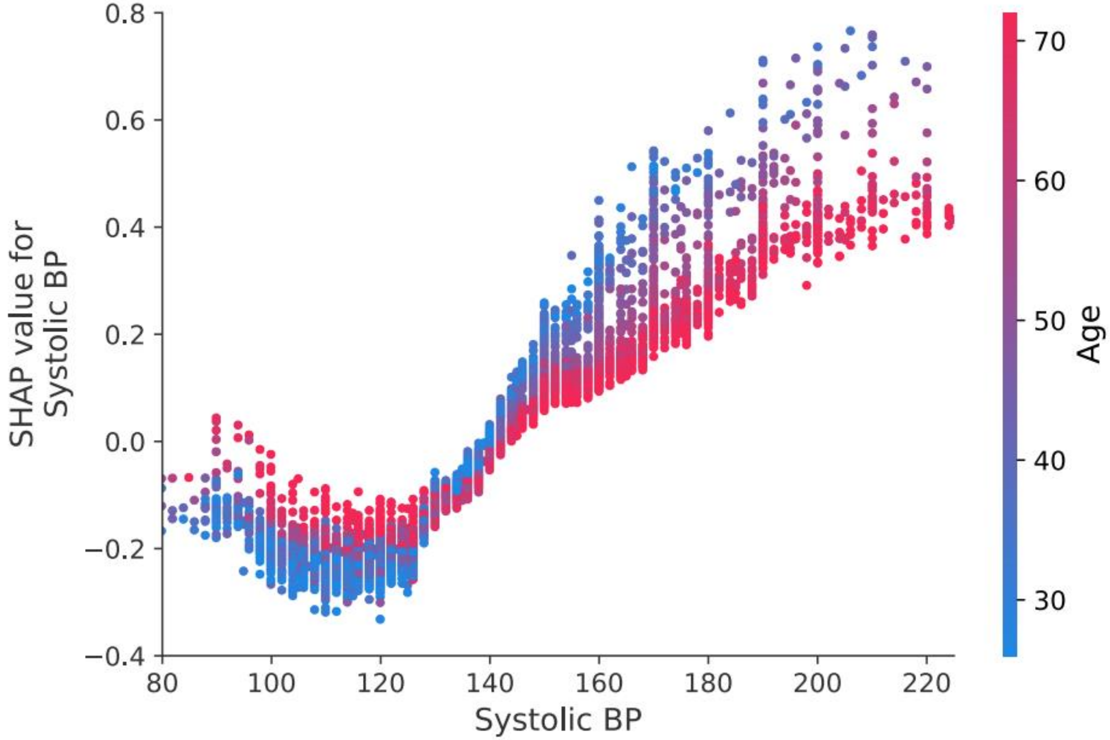
Ex) Prediction of mortality risk [1]



[1] Lundberg, S. M. & Lee, S.-I. A unified approach to interpreting model predictions. Adv. Neural Inf. Process. Syst. 20, 4765–4774 (2017).

Background

- **Black box explainer/interpreter: SHAP (Shapley additive explanation)**



SHAP values for systolic BP as a function of systolic BP [2]

- ✓ SHAP values show the effect of BP on the mortality risk
- ✓ Vertical spread is due to interaction effect

[2] Lundberg SM, Erion GG, Lee SI. Consistent individualized feature attribution for tree ensembles. arXiv preprint arXiv:1802.03888. 2018 Feb 12.

Objectives

- **Applicability of ML model for prediction of CF crack growth rate**
- **Explain ML model**

Database

- **806 experimental data of CF crack growth rate in AuSSs [3-5]**
  - ✓ 632 data of 304 SS and 174 data of 316 SS
  - ✓ Data were from tests in pressurized water reactor (PWR) and hydrogen water chemistry-boiling water reactor (HWC-BWR)

[3] Nomura Y, Tsutsumi K, Kanasaki H, Chigusa N, Jokati K, Shimizu H, Hirose T, Ohata H. Fatigue crack growth curve for austenitic stainless steels in PWR environment. Pres. Ves. Pip. 2004;480:63–70.
[4] Cipolla RC, Bamford WH, Hojo K, Nomura Y. Technical Basis for Revision of Code Case N-809 on Reference Fatigue Crack Growth Curves for Austenitic Stainless Steels in Pressurized Water Reactor Environments. In Pressure Vessels and Piping Conference (Vol. 85314 p. V001T01A001); 2021.
[5] Barron KC and Paraventi DJ. A Fatigue Crack Growth Model for Type 304 Austenitic Stainless Steels In a Pressurized Water Reactor Environment. In Pressure Vessels and Piping Conference (Vol. 85314 p. V001T01A015); 2021.

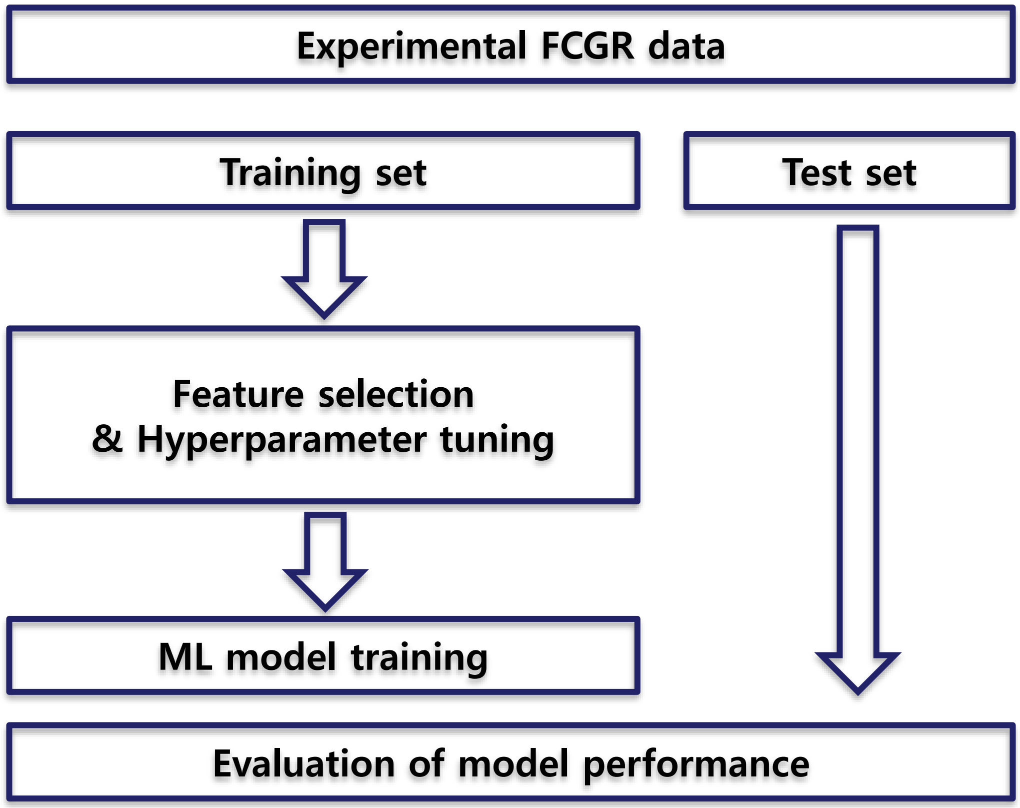
Database

- **Summary of database → 15 input features**

Variables	Means	SD	Min	Max	% Missing values
Stress intensity range, ΔK (MPa√m)	18.4	9.77	2.35	46	0
Load ratio, R	0.387	0.3	0.1	0.95	0
Rising time, t_r (s)	316.79	1597.14	1	34020	0
Water temperature, T (℃)	280.72	41.81	100	338	0
Dissolved hydrogen, DH (ppm)	2.77	0.78	0.125	4.5	0
Molybdenum content, Mo (wt%)	0.7	0.95	0.00	2.3	29
Carbon content, C (wt%)	0.035	0.012	0.005	0.07	0
Chromium content, Cr (wt%)	18.41	1.15	16.39	20.36	10
Nickel content, Ni (wt%)	9.96	1.16	8.06	12.55	10
Manganese content, Mn (wt%)	1.56	0.17	1.11	1.93	10
Silicon content, Si (wt%)	0.36	0.11	0.03	0.71	10
Phosphorous content, P (wt%)	0.023	0.006	0.005	0.034	10
Sulphur content, S (wt%)	0.002	0.001	0.001	0.007	0
Yield strength at 25 ℃, σ_{YS} (MPa)	269.54	37.1	240	434	30
Tensile strength at 25 ℃, σ_u (MPa)	560.99	24.95	531	601	12
Crack growth rate, da/dN (m/cycle)	4.3×10^{-7}	4.5×10^{-7}	1.0×10^{-10}	2.9×10^{-6}	0

Method

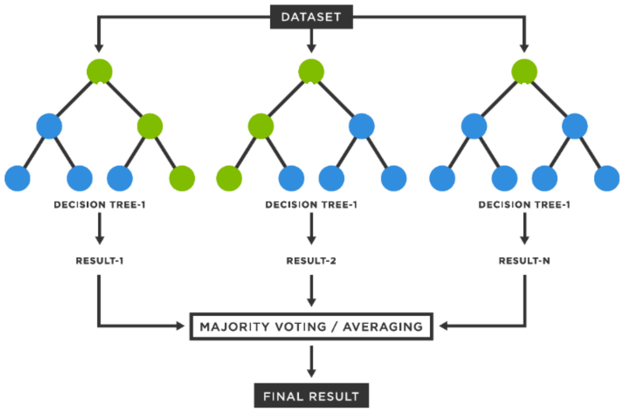
- **Modeling procedure**



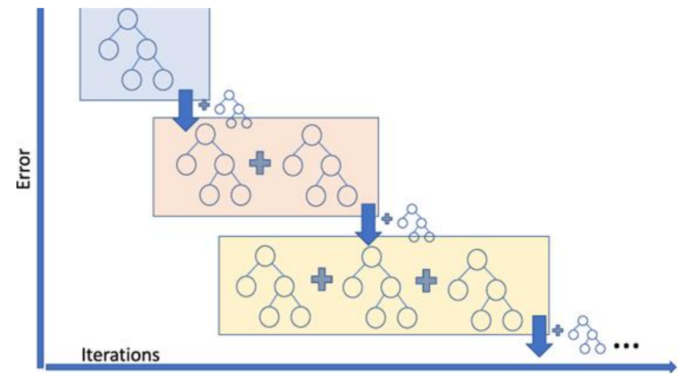
Method

- **Considered machine learning algorithms [6]**

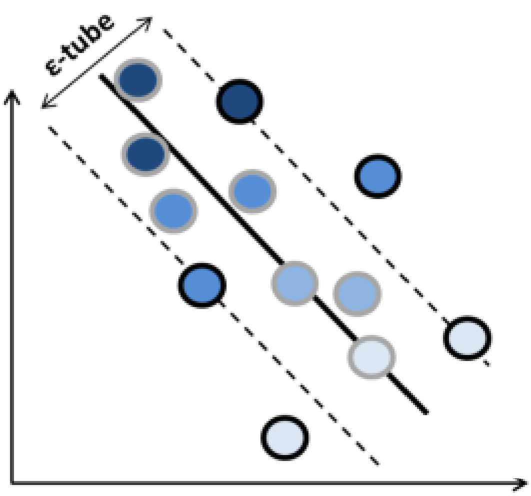
Random forest



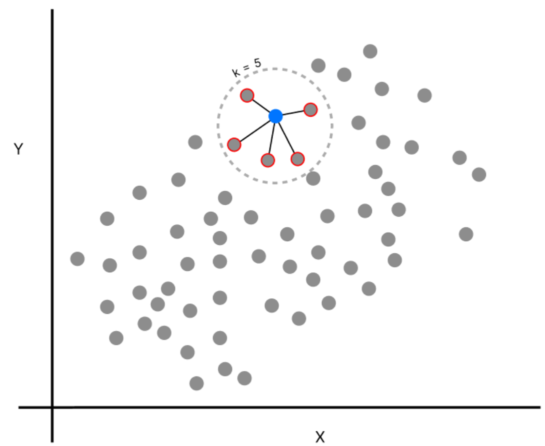
Boosted decision trees = Gboost, XGBoost, and CatBoost



Support Vector Regression



K-Nearest Neighbors

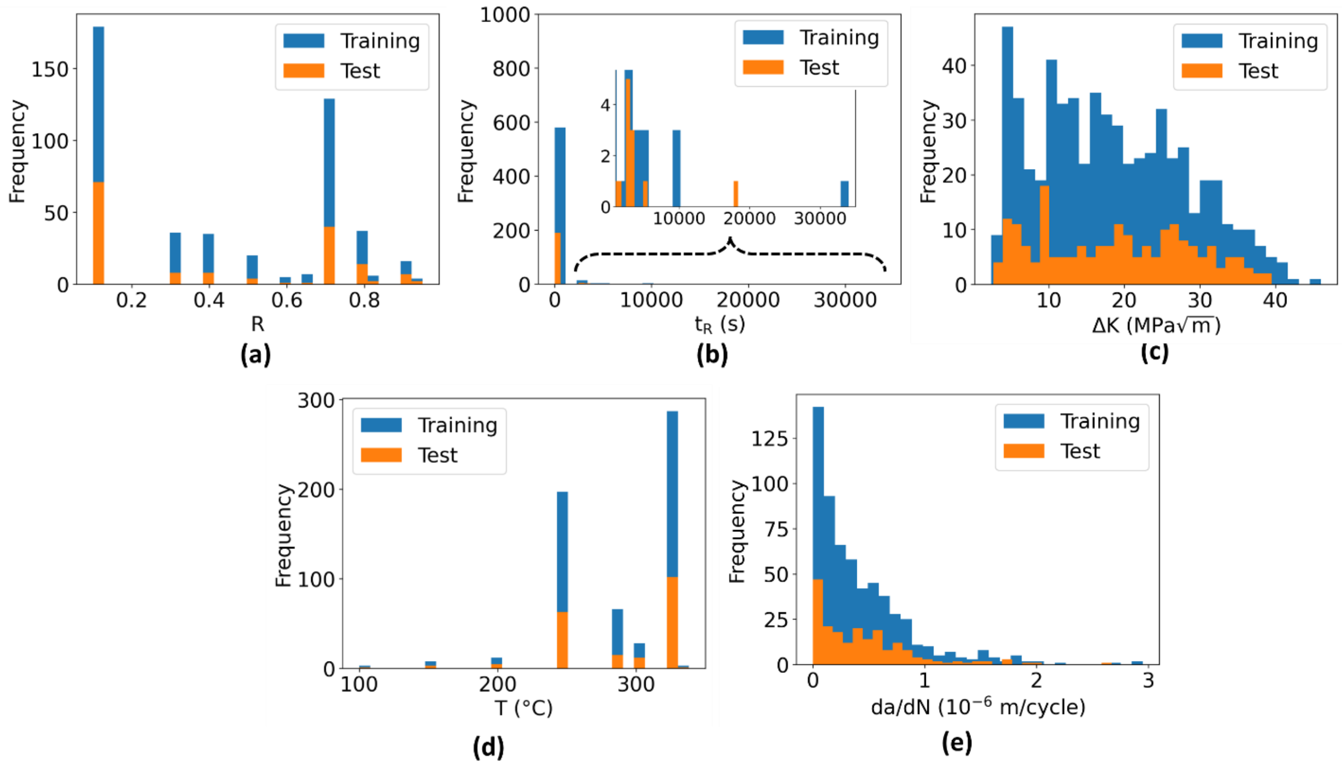


[6] Géron A. Hands-on machine learning with Scikit-Learn, Keras, and TensorFlow. " O'Reilly Media, Inc."; 2022 Oct 4.

Results

Data splitting

- ✓ Train : test = 80% : 20%
- ✓ Variables in both subsets should possess approximately similar distributions → Kolmogorov - Smirnov test



- ✓ Missing value imputation was performed using k-NN imputer

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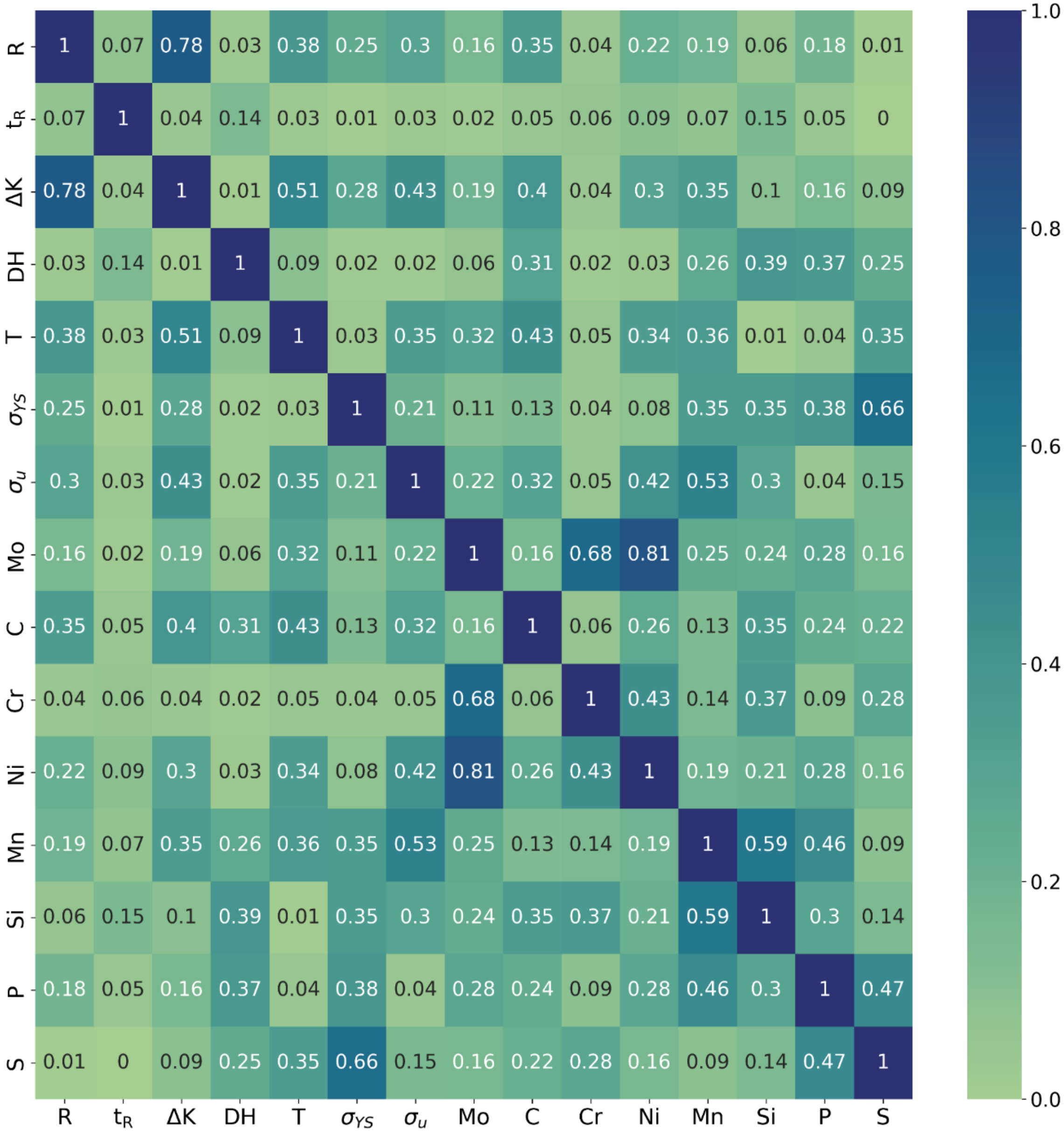
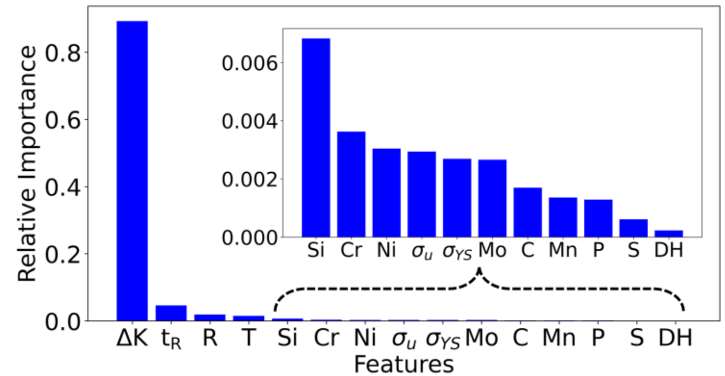


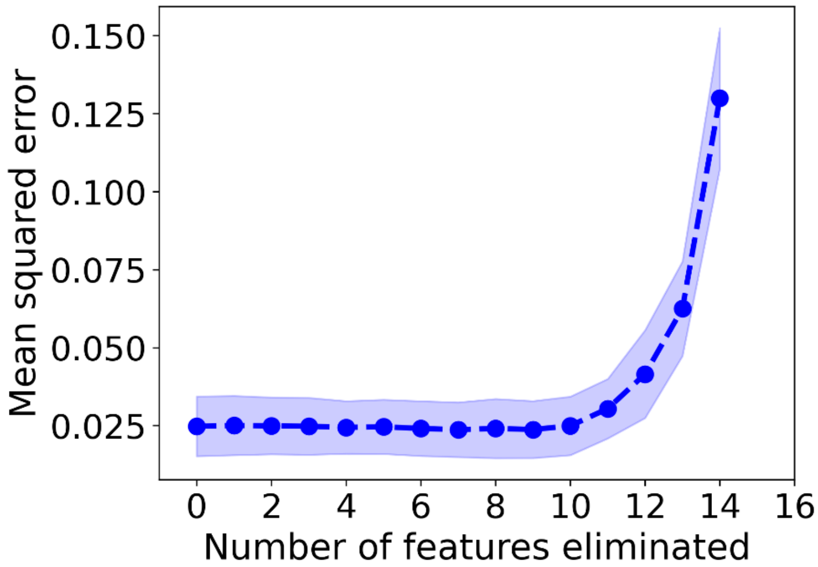
- **Feature correlations**
  - ✓ No significant multicollinearity
  - ✓ It is ok to take all features
- **Feature importance**



  - ✓ Feature importance from random forest was used
  - ✓ Loading parameters are the most important

Results

- **Feature selection**

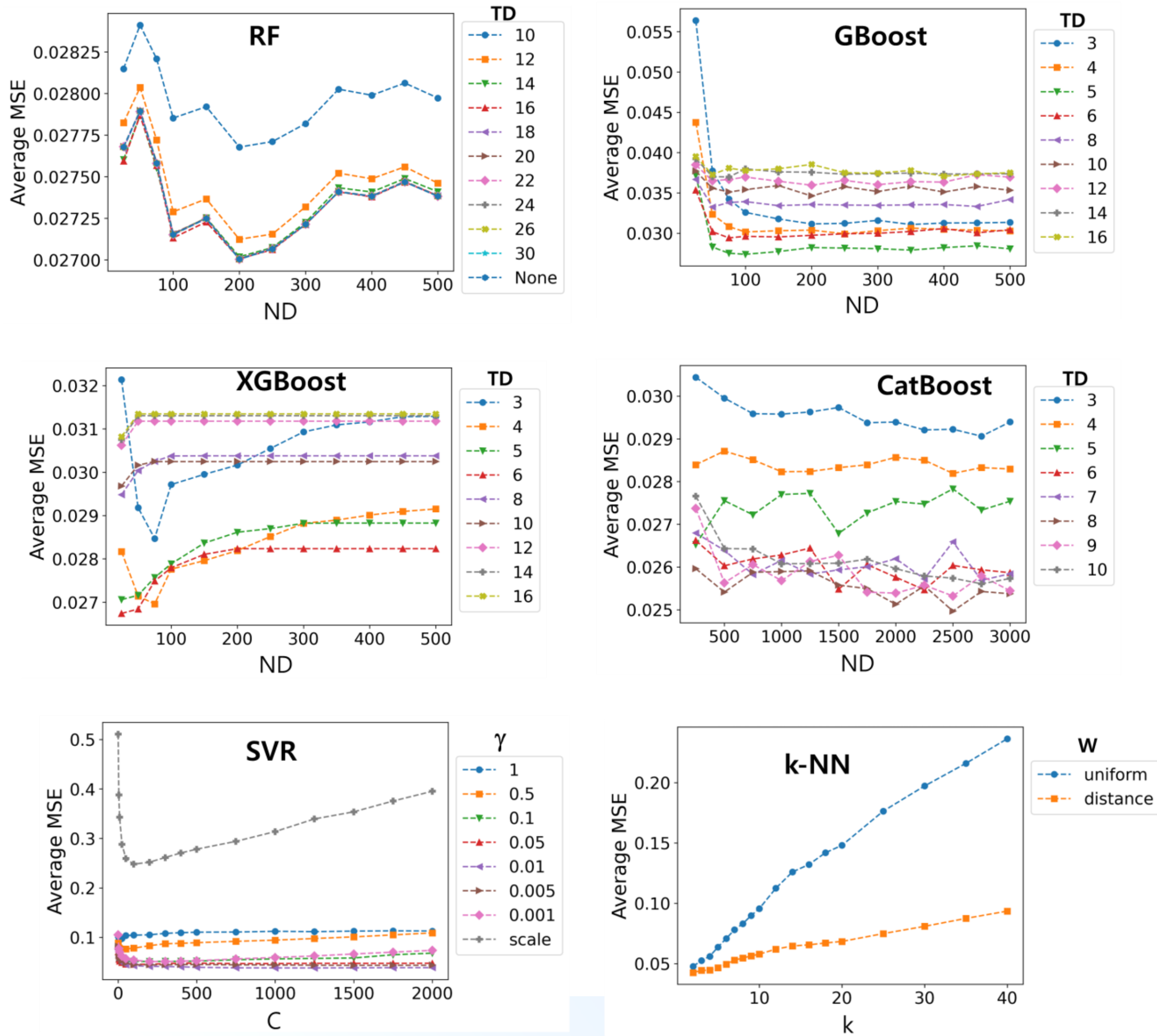


✓ Removing features does not decrease MSE

✓ It seems ok to take all features

Results

- **Hyperparameter tuning**



Results

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- **Tunned hyperparameters**

Model	Candidate space	Default value	Selected value
RF	ND = [25, 50, 75, 100, 150, 200, 250, 300, 350, 400, 450, 500] TD = [10, 12, 14, 16, 18, 20, 22, 24, 26, 30, None]	ND = 100 TD = None*	ND = 200 TD = 22
GB	ND = [25, 50, 75, 100, 150, 200, 250, 300, 350, 400, 450, 500] TD = [3, 4, 5, 6, 8, 10, 12, 14, 16]	ND = 100 TD =3	ND = 100 TD = 5
XGB	ND = [25, 50, 75, 100, 150, 200, 250, 300, 350, 400, 450, 500] TD = [3, 4, 5, 6, 8, 10, 12, 14, 16]	ND = 100 TD = 6	ND = 25 TD = 6
CB	ND = [250, 500, 750, 1000, 1250, 1500, 1750, 2000, 2250, 2500, 2750, 3000] TD = [3, 4, 5, 6, 7, 8, 9, 10]	ND = 1000 TD = 6	ND = 2500 TD = 8
SVR	C = [1, 5, 10, 25, 50, 100, 200, 300, 400, 500] γ = [3, 2.5, 2, 1.5, 1, 0.5, 0.1, 0.05, 0.01, 0.005, 0.001, scale]	C = 1 γ = scale**	C = 1250 γ = 0.01
k-NN	k = [2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 16, 18, 20, 25, 30, 35, 40] W = [uniform, distance]	ND = 5 TD = uniform	ND = 2 TD = distance

Note: * The default TD of RF, i.e., 'None', implies that each DT is grown until all leaves are *pure*.

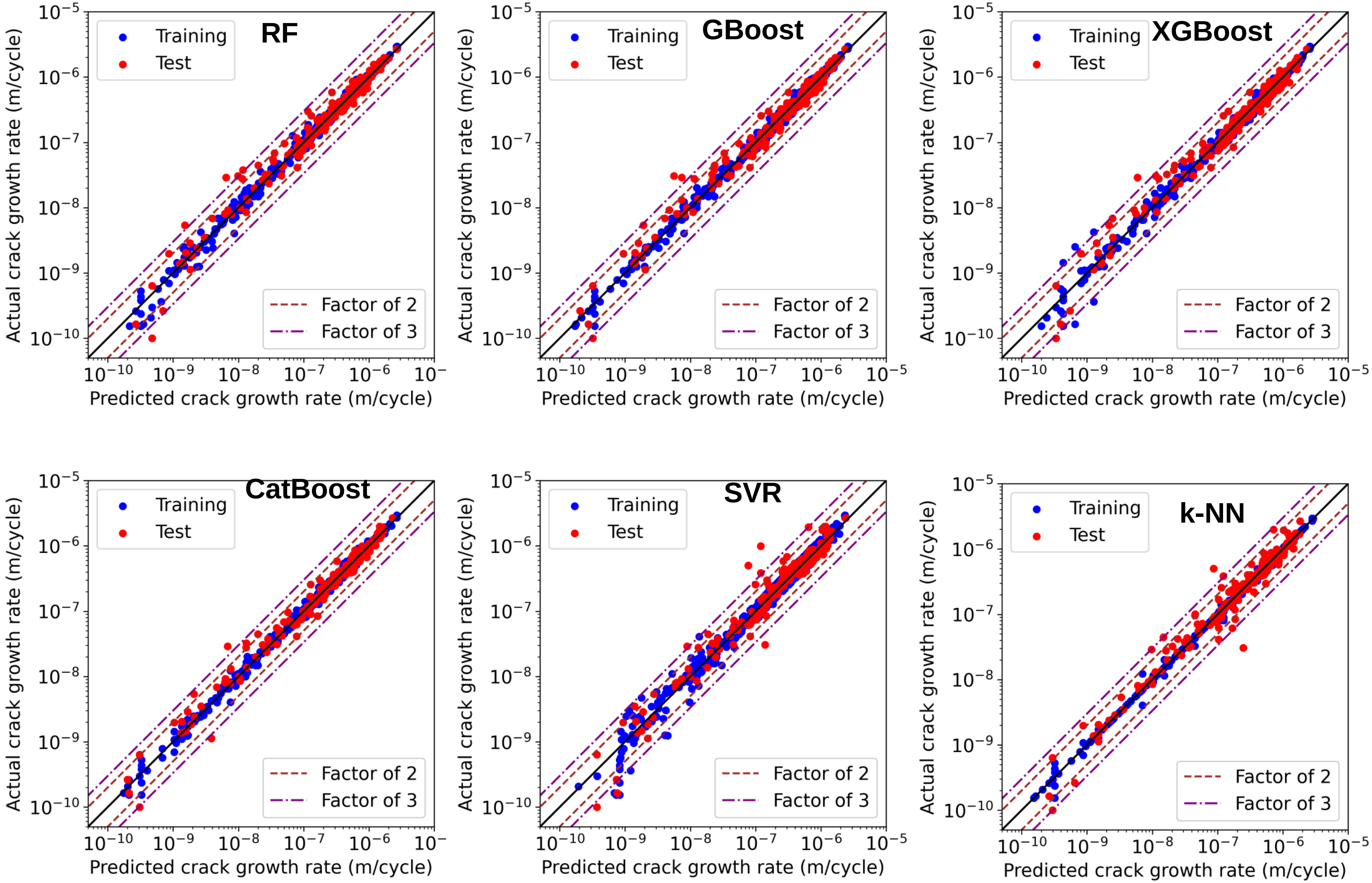
** The default γ of SVR, i.e., 'scale, implies that γ = 1/(number of features × feature variance).

- **Model training**

✓ ML models were trained with selected hyperparameters and input features

Results

- **Model evaluation on test set**



Results

- **Model evaluation on test set**

Model	MAPE		MAE		MSE		RMSE		R^2	
	Training	Test	Training	Test	Training	Test	Training	Test	Training	Test
RF	0.005	0.012	0.039	0.086	0.004	0.02	0.063	0.141	0.994	0.97
GB	0.006	0.012	0.041	0.086	0.003	0.018	0.056	0.136	0.995	0.972
XGB	0.007	0.013	0.046	0.091	0.006	0.019	0.078	0.139	0.991	0.971
CB	0.005	0.011	0.035	0.074	0.002	0.015	0.05	0.121	0.996	0.978
SVR	0.012	0.016	0.083	0.111	0.013	0.032	0.116	0.178	0.98	0.952
k-NN	0.001	0.014	0.008	0.097	0.001	0.026	0.031	0.161	0.999	0.961

Comparison to empirical models

✓ JSME Code [3]

$$da/dN = 1.61 \times 10^{-13} T^{0.63} {t_R}^{0.33} \Delta K^{3.0} (1-R)^{-1.56}$$

✓ ASME Code [4]

$$da/dN = C_0 \, \Delta K^{2.3}$$

$$C_0 = C S_T S_R S_{ENV}$$

$C = 9.10 \times 10^{-6}$ (Type 304/316)

$C = 1.39 \times 10^{-5}$ (Type 304L/316L)

$S_T = \exp\left(-\frac{2516}{T+273}\right)$ (150 °C≤T ≤343 °C)

$S_T = 3.39 \times 10^5 \exp\left(-\frac{2516}{T+273} - 0.0301T\right)$ (T≤150°C)

$S_R = 1 + 1.53R^3$ (nominal carbon grade)

$S_R = 1 + 1.11R^3$ (low carbon grade)

$S_{ENV} = {t_R}^{0.3}$ (t_R < 1s, use t_R = 1s)

$$\Delta K_{th} = 5.6(1 - 0.7R)$$

✓ Baron's model [5]

$$da/dN = C_0 \, \Delta K^n$$

$$C_0 = C S_T S_R {t_R}^{0.227}$$

$$\Delta K_C = 6.737 \text{ MPa}\sqrt{\text{m}}$$

$$n = \begin{cases} 5.08 \ (\Delta K < \Delta K_C) \\ 2.46 \ (\Delta K \geq \Delta K_C) \end{cases}$$

$C = \begin{cases} 5.005 \times 10^{-8} \ (\Delta K < \Delta K_C) \\ 7.499 \times 10^{-6} \ (\Delta K \geq \Delta K_C) \end{cases}$ (wrought metals)

$C = \begin{cases} 2.791 \times 10^{-8} \ (\Delta K < \Delta K_C) \\ 4.181 \times 10^{-6} \ (\Delta K \geq \Delta K_C) \end{cases}$ (weld metals)

$$S_T = \exp\left(-\frac{2403}{T+273}\right)$$

$$S_R = (1-R)^{-0.559}$$

[3] Nomura Y, Tsutsumi K, Kanasaki H, Chigusa N, Jokati K, Shimizu H, Hirose T, Ohata H. Fatigue crack growth curve for austenitic stainless steels in PWR envir onment. Pres. Ves. Pip. 2004;480:63–70.
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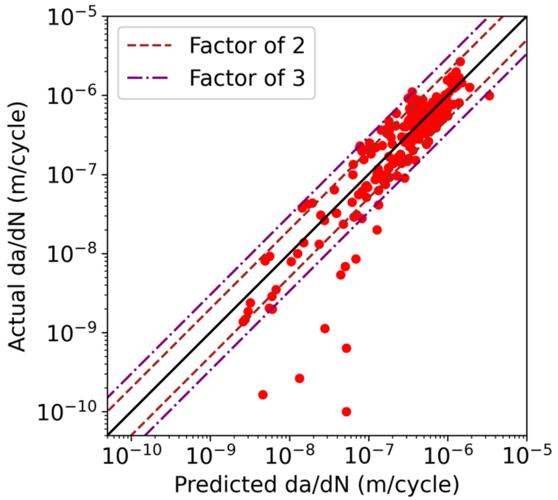
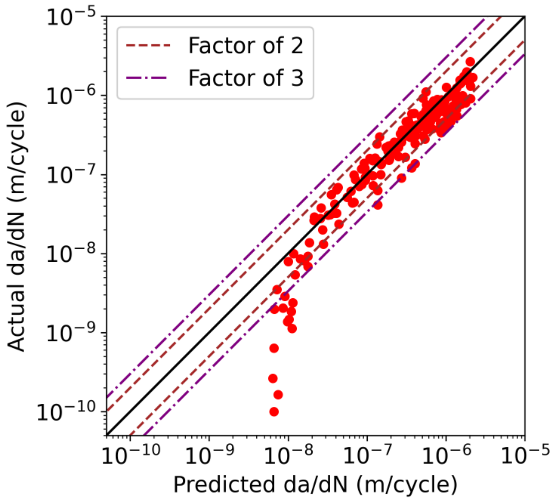
Results

- **Comparison to empirical models**

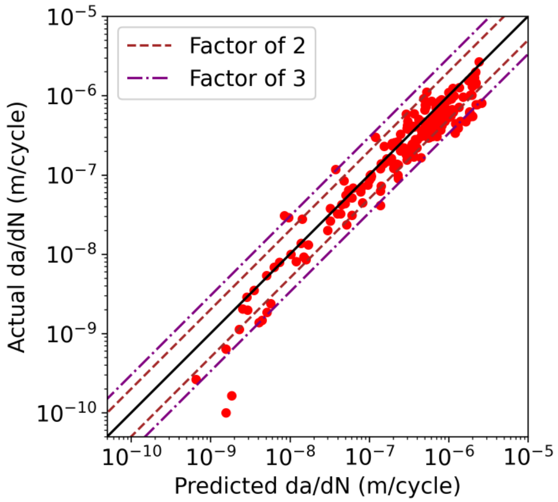
JSME



ASME



Baron



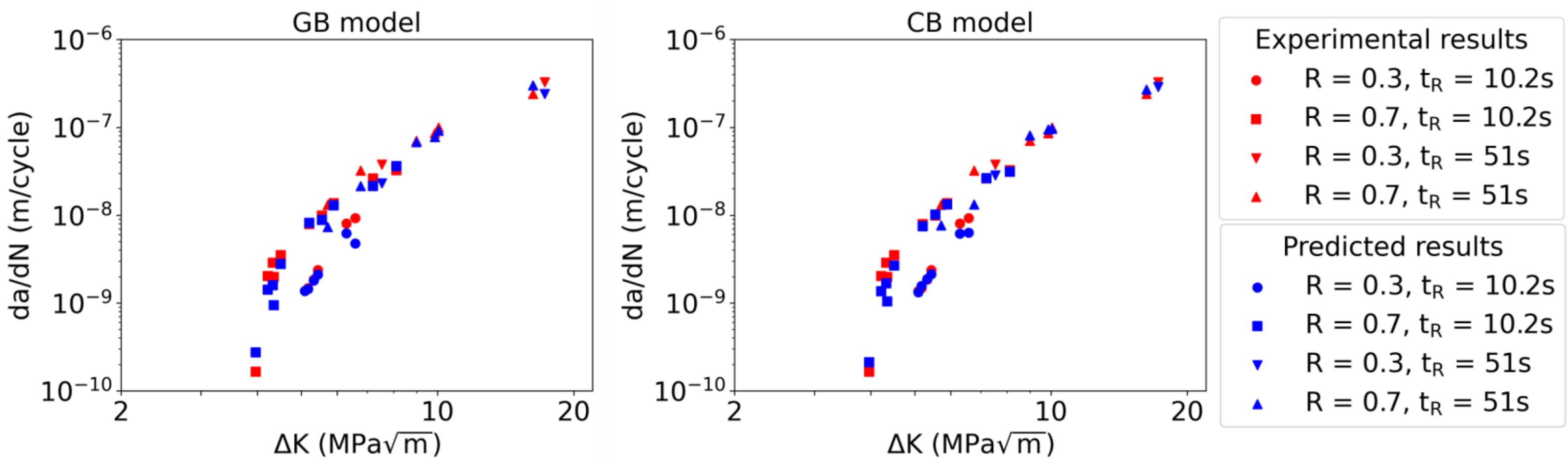
- ✓ Baron's model is the best
- ✓ ML model can be even better

Model	MAPE	MAE	MSE	RMSE	R^2
JSME	0.035	0.249	0.156	0.394	0.765
ASME	0.026	0.19	0.1	0.316	0.85
Baron	0.028	0.19	0.066	0.258	0.9

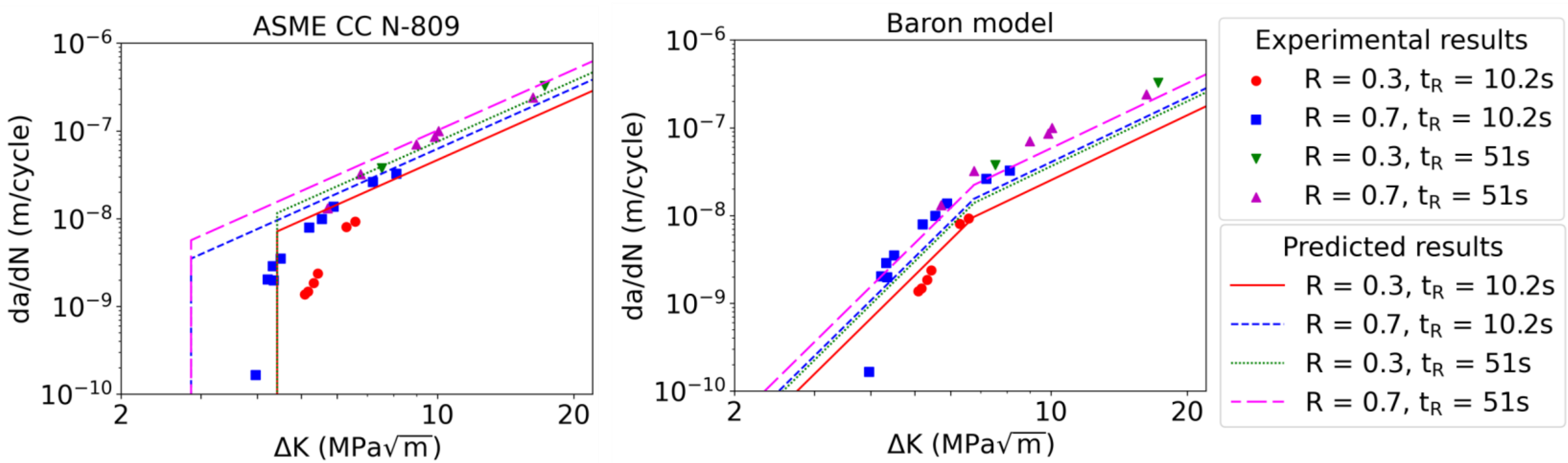
Results

- **Comparison to empirical models**

ML models



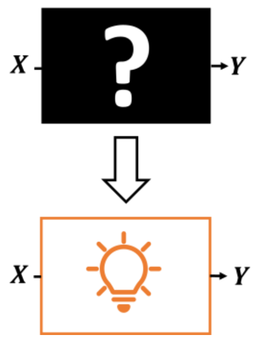
Empirical models



Results

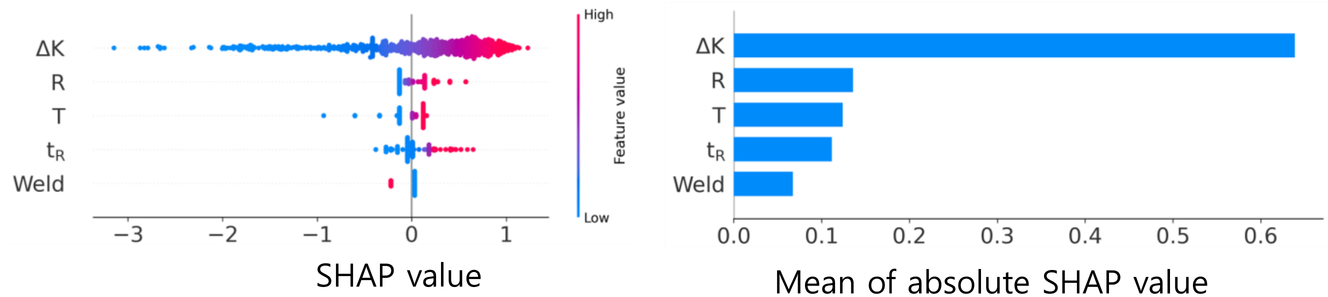
- **Why ML model is better than empirical model?**

✓ Model explanation

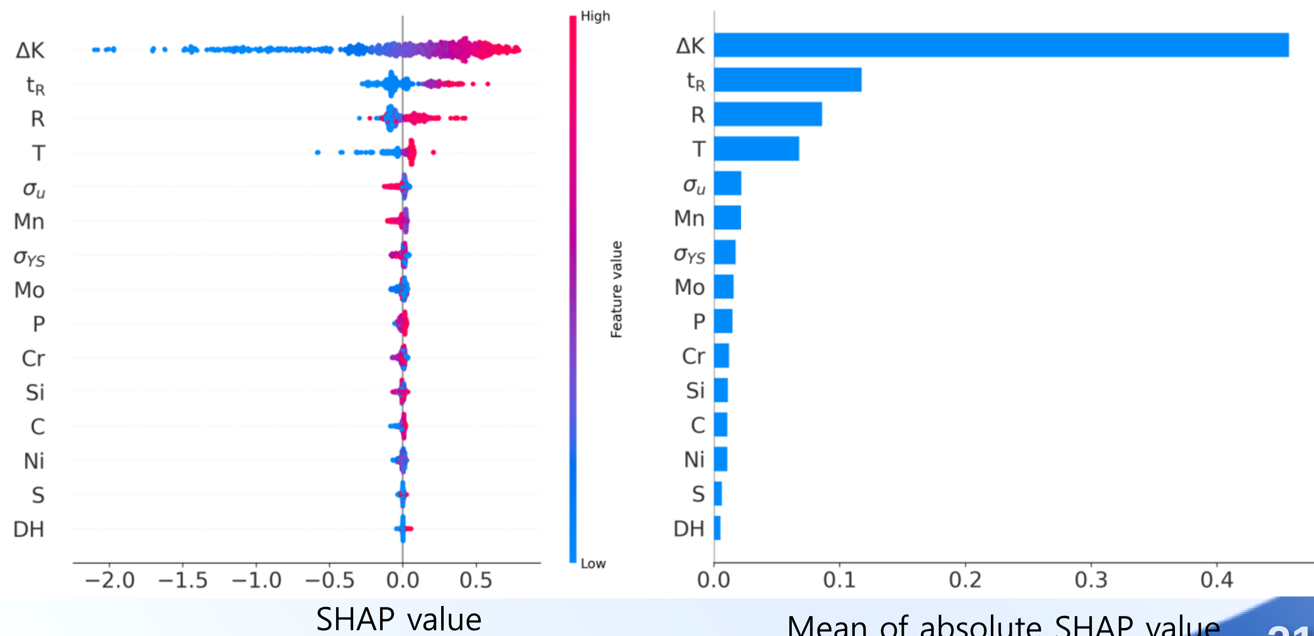


✓ SHAP values for each feature are computed

Baron

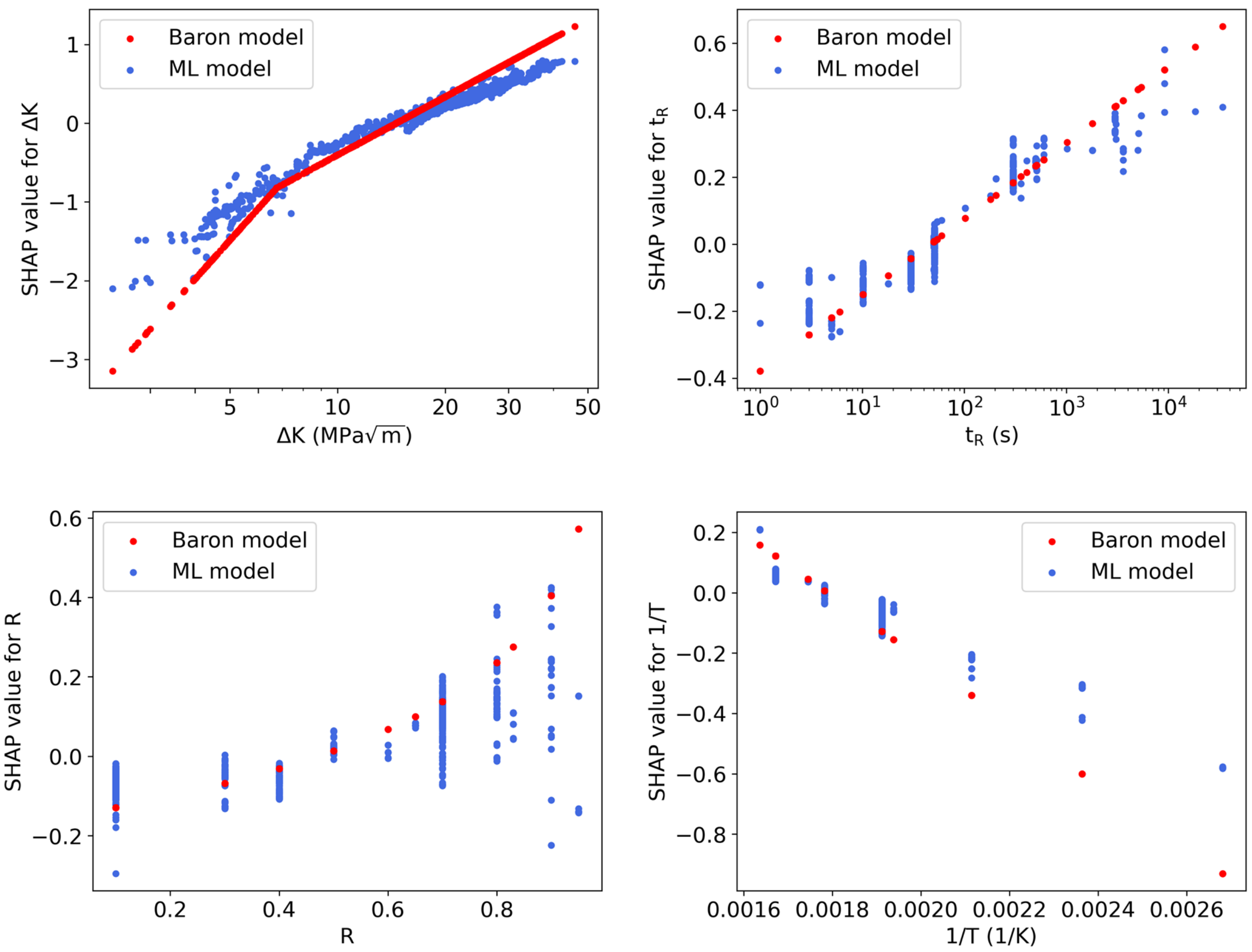


CatBoost



Results

- **Why ML model is better than empirical models?**



✓ Slope of ΔK dependence:

$da/dN = C_0\,\Delta K^{2.2}$ is better than $da/dN = C_0\,\Delta K^{2.46}$

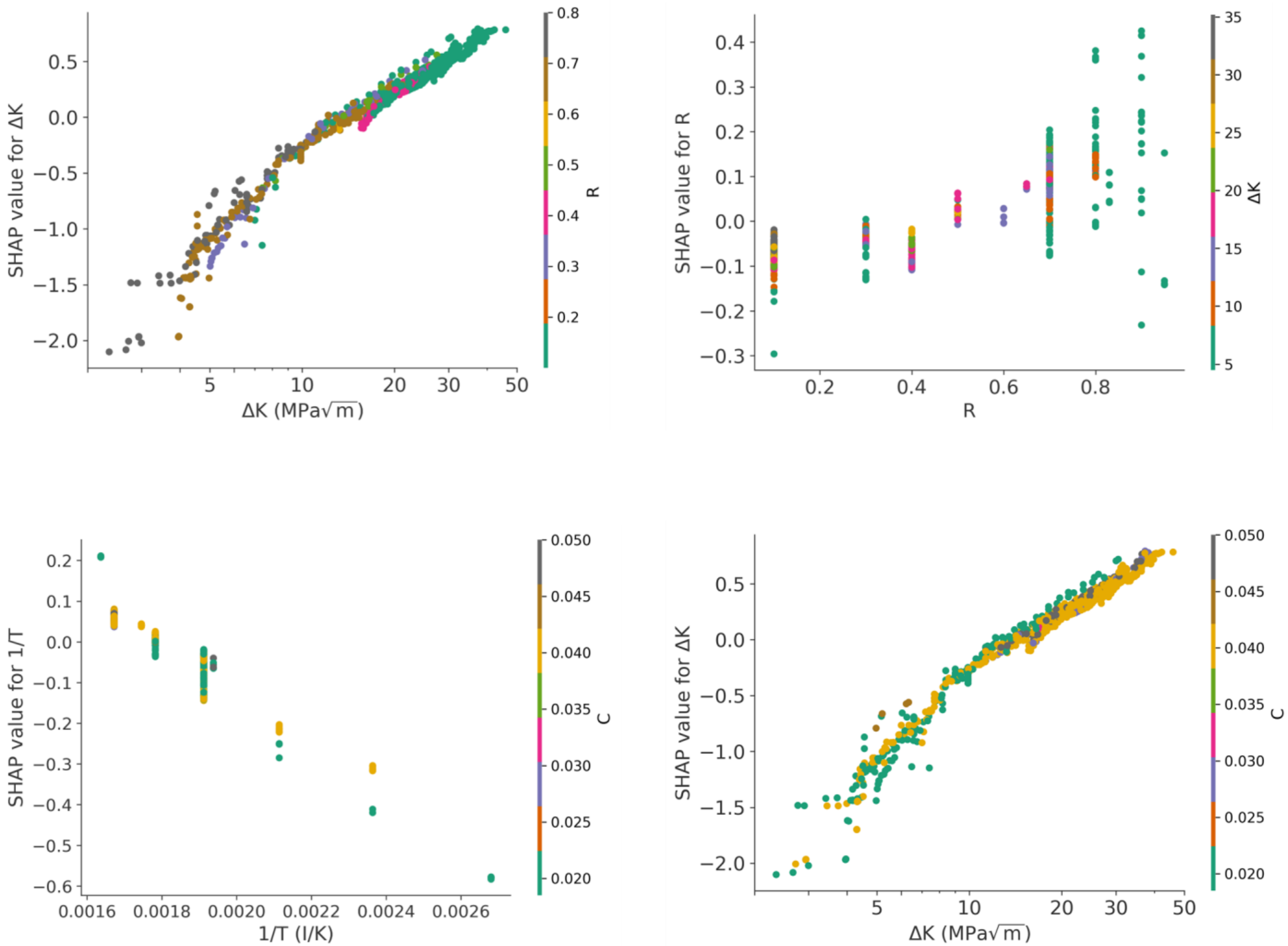
✓ Slope of T dependence:

$S_T = \exp\left(-\frac{1899}{T+273}\right)$ is better than $S_T = \exp\left(-\frac{2403}{T+273}\right)$

✓ Vertical spread of SHAP values→interaction effects

Results

▪ Interaction effects



- ✓ At near threshold, the decrease of CGR with ΔK is steeper at lower R
- ✓ Wide spread of SHAP values for R is due to low ΔK
- ✓ Different Arrhenius dependences due to C contents
- ✓ Higher slope of CGR vs ΔK for lower C steels

Summary and future works

- **Conclusion:**
  - ✓ Some commonly used supervised ML algorithms (GBoost, XGBoost, CatBoost) were considered to find the best suited one for the purpose of the current study.
  - ✓ Each of them has been shown to perform reasonably well. Among the trained ML models, CatBoost model, has been shown to outperform the other models.
  - ✓ More accurate prediction for the CF crack growth rate of austenitic SSs can be attained through the implementation of ML techniques.
  - ✓ SHAP successfully explain why ML model is better than empirical models

- **Future work:**
  - ✓ Implementation of ML algorithms for other degradation mechanism, i.e., stress corrosion cracking

Thank You for

Your Attention