

The EMBRACE Checklist

Version 1.0. Last Updated Date: September, 2024.

The main purpose of EMBRACE Checklist is to facilitate the reporting of basic data and methods used for supervised machine learning (ML) research in environmental science and engineering (ESE). It also aims to provide a comprehensive evaluation of important preparation and analysis steps. We warmly encourage researchers to include the checklist as a reference, and if interested list it as supplementary materials in their publications.

Detailed instructions and additional resources are available open access for download from the author's GitHub: <https://github.com/starfriend10/EMBRACE>

- Future updates and new resources will be available in the above GitHub repository, which is also served as a community-owned platform to share data and codes, refine forms/checklists, discuss ML-ESE topics, promote research outcomes, and continuously identify/avoid pitfalls and follow good practices.
- We encourage you to direct share your checklists, but you can also save it as a read-only document. See instructions for detailed steps.
- Please cite the Viewpoint when using the checklist. If you have any questions or suggestions, please contact Dr. Jun-Jie Zhu at Princeton University (junjiez@princeton.edu or ranmuweijie@gmail.com).

Project Overview			
Project Title			
Contributing Authors			
Date		Completed by	
Contact Email		DOI (if published)	
Domain Category		Or Specify:	
Learning Type	Regression	Classification	Regression+ Classification
Prediction Type	Deterministic	Probabilistic	Deterministic+ Probabilistic
Other Information			

I. Problem Formulation							
Project Objective(s)							
Feasibility Assessment	Data Availability	Model Accessibility	Computation Resources	Knowledge Preparation	Time Availability	Financial Availability	Risk Tolerance
Levels							

II. Data Collection							
Data Sources		Time-series Monitoring			Field Campaigns		
		Laboratory Experiments			Simulation Outputs		Others. Specify:
Source Types		Ordinary		Time-series		Literature-based	Others. Specify:
Data Types		Continuous Numerical			Categorical		
		Graphical			Auditory		Others. Specify:
Data Ethics		No special ethical considerations are required, or followed the necessary requirements when needed					
		No special permissions are required, or obtained the necessary permissions when needed.					
		Provided appropriate credit(s) to the data source(s)					
Data Availability		Data are publicly available through a PURL or DOI				Data are available as requested	
Raw Data Quantity		Raw Sample Size		Raw Variable Size		Raw Total Data volume	
Raw Data Quality		The raw data had an internal QA/QC before data retrieval?				Yes	No
		The raw data went through a peer-review or similar process?				Yes	No

III. Data Preprocessing											
Data Cleaning		Abnormal Data Management				Statistical Outlier Management				Technical Outlier Management	
		Data Correction due to Technical Limitations					Others. Specify:				
Data Enrichment		Missing Data Management			Data Augmentation			Data Aggregation			Data Balancing
		Upper sample ratio among groups:					Others. Specify:				
Feature Engineering		Initial Variable(s) Exclusion				Feature Importance Analysis				Feature Extraction	
		Categorical Feature Transformation					Dummy Feature Removal				
		Ordinal Encoding			Encoded variable(s):						
		Feature Selection			Feature Scaling (for X)			Feature Scaling (for Y)			Circular Feature Scaling
		New Feature Development			Ordinary Mathematical Transformation(s)				Time-Dependent Feature Transformation(s)		
				Spatial Feature Transformation(s)				Others. Specify:			
		Sparse Dataset?	Yes	No	Preprocessed to increase information density?			Yes	No		
	Normality Test (before/after transformation)					Others. Specify:					
Data Splitting	Framework			Training-Testing			(Pre-)Training-Validation-Testing				Cross-Validation-Testing
	Splitting Method			Simple Random			Grouped Random			Simple Block	Sub-Group R/B
	Ensured training dataset covered most possible scenarios (e.g., different seasons)										
Final Data Quantity	Testing Ratio		Preprocessed Sample Size		Preprocessed Feature Size		Sample-Feature Ratio		Training SFR		

IV. Methods Selection and Model Initialization										
Methods Selection		Selected supervised learning methods to be tested based on case needs (e.g., data, computation resources, etc.)?								
	Methods Studied: N ML and M Statistical					N =		M =		
	ML Family			Tree-based			Neural Network			Others
	ML Type			Shallow ML			Deep ML		Final Optimal Method(s):	
Model Uncertainty	Examined Random Seeds				Replicated Modeling Process					
	Assessed probabilistic prediction results				Others. Specify:					

V. Model Evaluation and Model Optimization											
Model Evaluation	Set a goal model performance before evaluation										
	Specify Evaluation Metrics:										
	Studied under-fitting issue					Studied over-fitting issue					
	Final evaluation was based on the testing data					Weighted metrics were used for imbalanced data					
	ML significantly outperformed statistical models					Statistical perform similar or even better than ML models					
Hyper-parameter Optimization	HPO Method		No HPO		Trial-and-Error/Experience			Grid/Random Search (similar)		Metaheuristics	
		Other HPO. Specify:									
	Number of methods tuned by HPO:					Number of hyperparameters searched:					
	Number of values in each hyperparameter:					Continuous Search			Discrete Search. Specify the number:		
	CV Method		No CV		k-fold CV			Leave-one-out CV			Stratified CV
Pre-defined or other CV. Specify:											

VI. Model Explanation									
Model Interpretability		Reported model interpretability as intrinsic property					Described tradeoff between interpretability and complexity		
		Explained limitations of low model interpretability					Compared the methods with different interpretabilities		
Model Explainability		Reported the explanation method(s) used for FIA			Explanation method(s):				
		Reminded high accuracy might not be trustable explanation					Described application of explanation on the optimal model		
	Reflected on understanding that explanations:				couldn't cover all mechanisms			might be incorrect	
Causality		Reflected on higher accuracy not implying logical causal relationships							
		Reported understanding that explanation results do not indicate causality							
		Described alignment of explanations with environmental domain knowledge for causality							
		Identified illogical or counterintuitive parts based on environmental domain knowledge							
		Described study of illogical or counterintuitive parts based on environmental domain knowledge							

VII. Data Leakage Management											
General/ Data Source	Verified no:			response variable Y leakage			future-to-current data leakage			current-to-current data leakage	
	Confirmed that no overlapped data between training and testing						Yes			No	
	Data splitting method for literature-source data:										
Data Enrichment	Verified that missing data replacement utilized only seen dataset						N/A		Yes		No
	Verified that missing data interpolation utilized neighbor data in same subset						N/A		Yes		No
	Verified that model-based imputation utilized only seen data						N/A		Yes		No
Feature Engineering	Confirmed that feature engineering utilized only seen dataset						N/A		Yes		No
	Confirmed that feature scaling utilized only seen dataset						N/A		Yes		No
	Confirmed that data splitting method for time-dependent data:										
CV Loop	Verified that missing data replacement utilized only seen data in each split						N/A		Yes		No
	Verified that missing data interpolation with neighbor data in each split						N/A		Yes		No
	Verified that feature engineering utilized only seen data in each split						N/A		Yes		No
	Verified that feature scaling utilized only seen data in each split						N/A		Yes		No
	Data splitting method for literature-source data in CV loop:										
	Data splitting method for time-dependent data in CV loop:										
Others		Self-specify:									

VIII. Additional Items			
	PURL or DOI are publicly available. Data:	Code:	
	Email or URL are available to request. Data:	Code:	
	Self-specified Item:		