

PREDICTION OF LC50 VALUE USING QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP MODELS (QSAR MODELS)

Machine learning model



OBJECTIVE



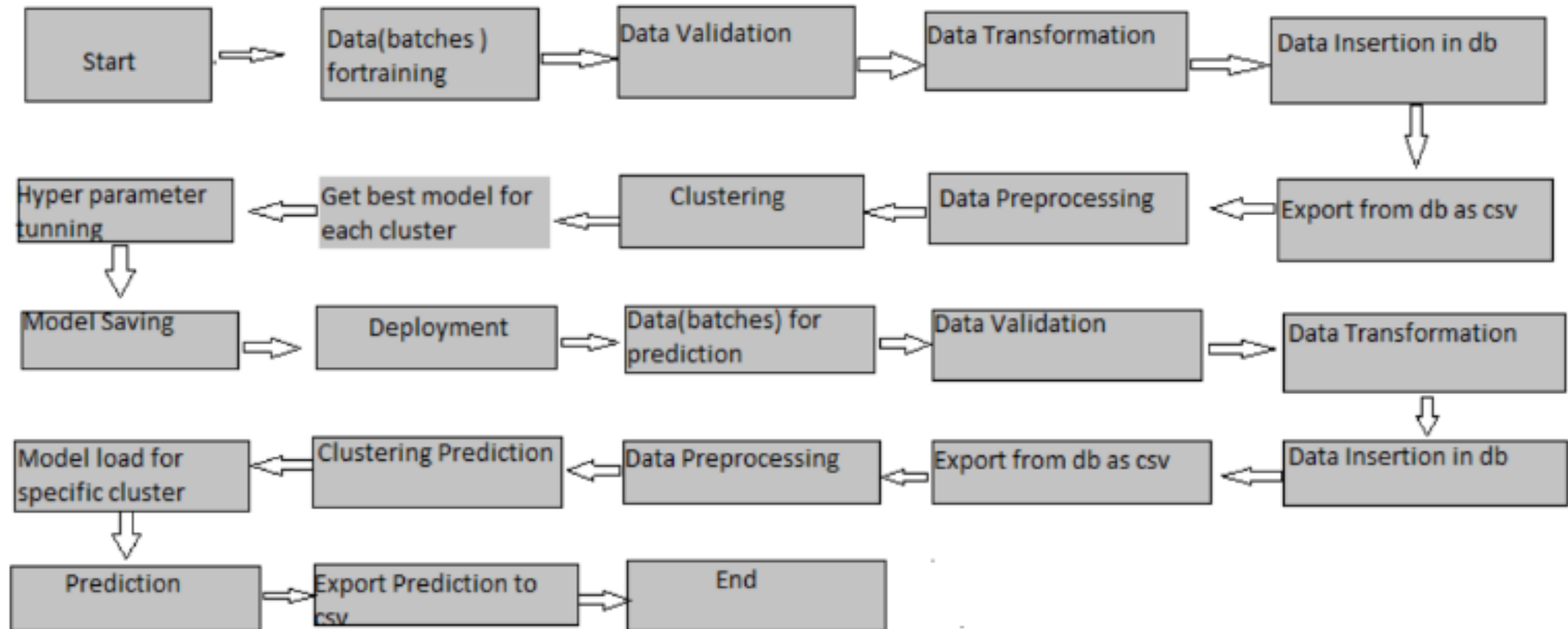
The objective of the project is to develop Quantitative Structure-Activity Relationship (QSAR) models to predict the LC50 value for acute aquatic toxicity towards the fish fathead minnow (*Pimephales promelas*) based on a dataset of 908 chemicals and 6 molecular descriptors. The project involves the development of various regression models, including linear regression, ridge, lasso, elastic net, XGBoost regressor, support vector machine regressor, and random forest regressor. After model development, the project aims to calculate predictions, R-squared value, mean absolute error (MAE), and root mean square error (RMSE) for each model, save the results to a CSV file, and serialize the most optimal model using pickle dump. Additionally, the project will involve dynamically loading data into a MySQL database, saving logging times of the code to the database, and setting up a Flask web application.

BENEFITS OF DEVELOPING QSAR MODELS FOR

Benefits of developing QSAR models for predicting LC50 values:

1. Cost Savings
2. Faster Decisions
3. Ethical Testing
4. Insights into Toxicity

ARCHITECTURE





THANK YOU

