Machine Learning Model Tracking Document

1. Dataset Information

Dataset Name:	Well 782
Number of Samples:	782
Number of Features:	4 (Tf, Rs, Gg, Api)
Target Variable:	Pb
Outlier Handling:	None
Feature Engineering Applied:	None
Scaling/Normalization Applied:	Only for Neural Networks
Encoding Applied:	None

2. Preprocessing Steps

Step	Description
Train-Test Split	70% - 30%
Shuffling	Yes, using random_state=42
Handling Missing Data	None
Feature Scaling	Only for Neural Networks
Feature Selection	None

3. Models Used & Hyperparameters

Model	Hyperparameters	Training Time
XGBoost	n_estimators=200, learning_rate=0.1, max_depth=4	0.0434
CatBoost	iterations=1000, learning_rate=0.05, depth=4, l2_leaf_reg=7	0.1938
Neural Network	[128, 64], epochs=100, batch_size=16	3.1911
Stacking Ensemble	Default base models + CatBoost final estimator	0.7844
Extra Trees	n_estimators=200	0.1635
Deep Neural Network	[256, 128, 64], epochs=100, batch_size=32	2.3129

4. Evaluation Metrics

Model	MSE	RMSE	MAE	R^2 Score	Adjusted R^2
XGBoost	108293.491	329.080	178.893	0.9261	0.9253
CatBoost	94122.562	306.794	177.038	0.9358	0.9351
Neural Network	170444.040	412.849	263.698	0.8837	0.8825
Stacking Ensemble	101285.715	318.254	178.067	0.9309	0.9302
Extra Trees	108699.095	329.696	177.497	0.9259	0.9250
Deep Neural Network	162918.102	403.631	264.895	0.8889	0.8877

5. Cross-Validation Summary (5-Fold)

| Model	RMSE Mean	RMSE Std	MAE Mean	MAE Std	R^2 Mean	R^2 Std
Extra Trees Regressor	290.750	33.520	170.724	9.566	0.9407	0.0140
XGBoost	292.065	53.057	178.745	18.818	0.9389	0.0217
Stacking Ensemble	294.349	49.304	181.307	15.466	0.9381	0.0209
CatBoost	296.746	42.848	181.322	17.429	0.9380	0.0162
Deep Neural Network	496.948	26.444	358.732	13.780	0.8294	0.0132
Neural Network	499.334	25.269	362.252	12.390	0.8277	0.0132

6. Visualizations
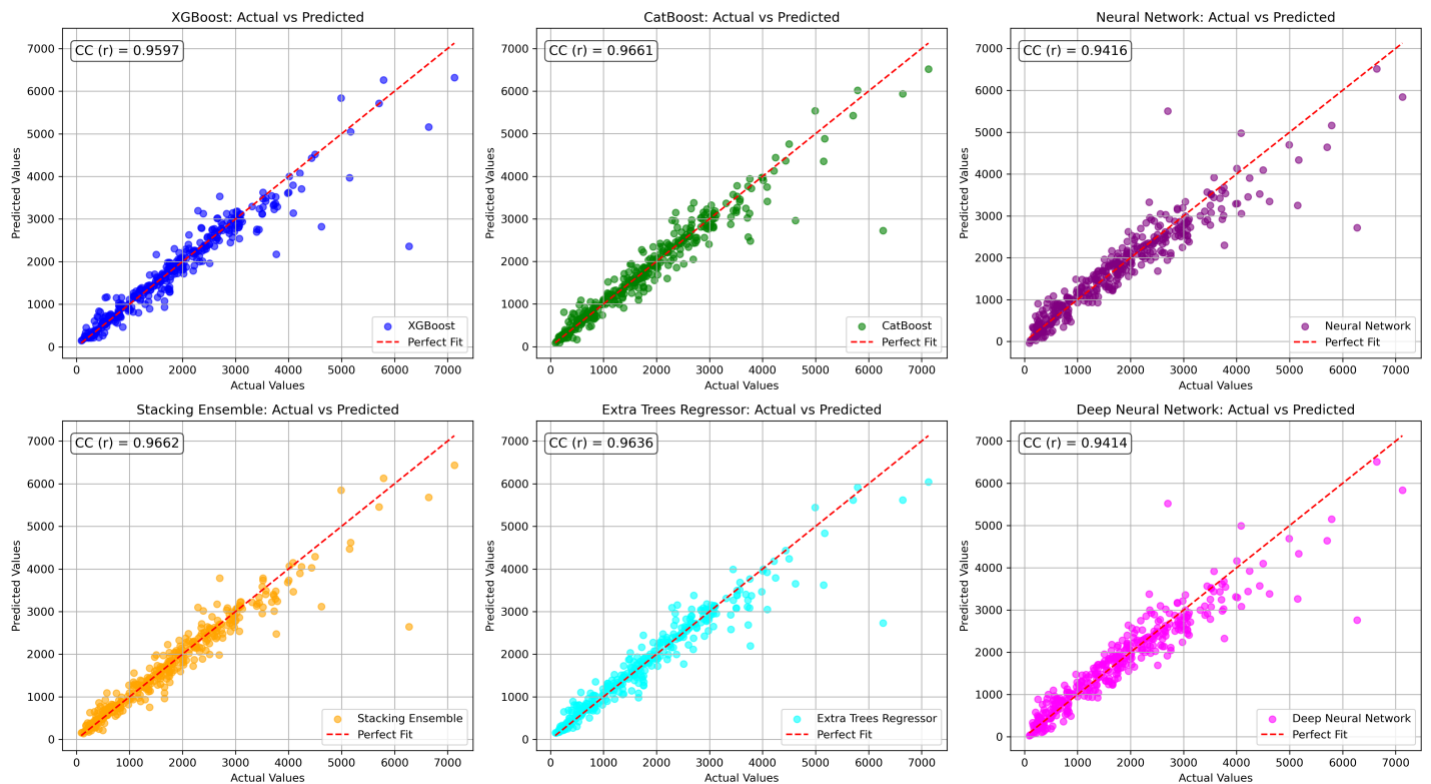
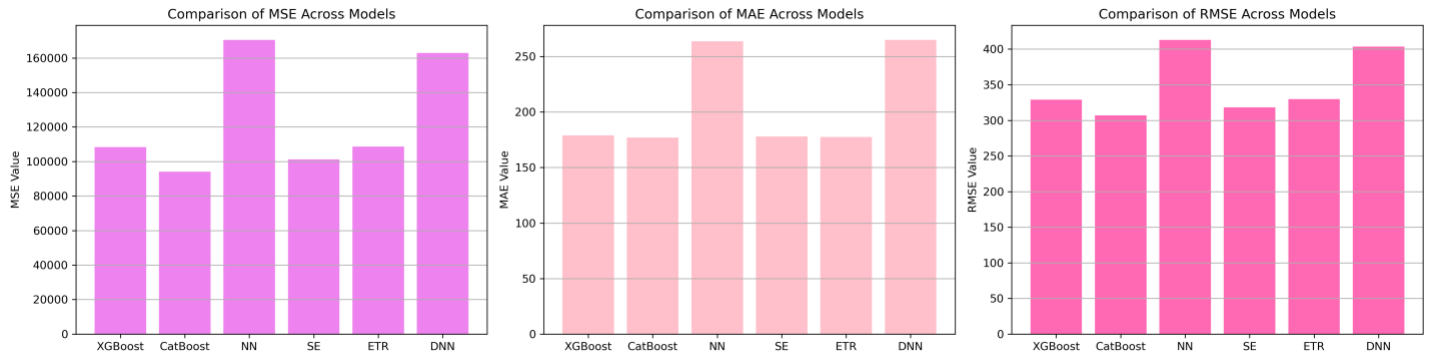*Figure 1: Actual vs. Predicted Values for Pb (Well 782)*
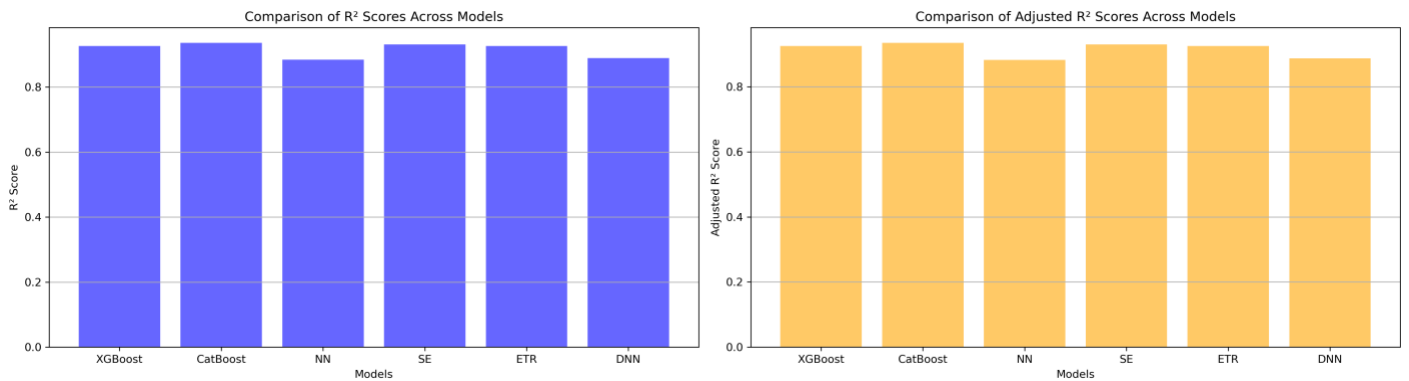
Figure 2: Bar Charts of MSE, RMSE, MAE for Pb (Well 782)

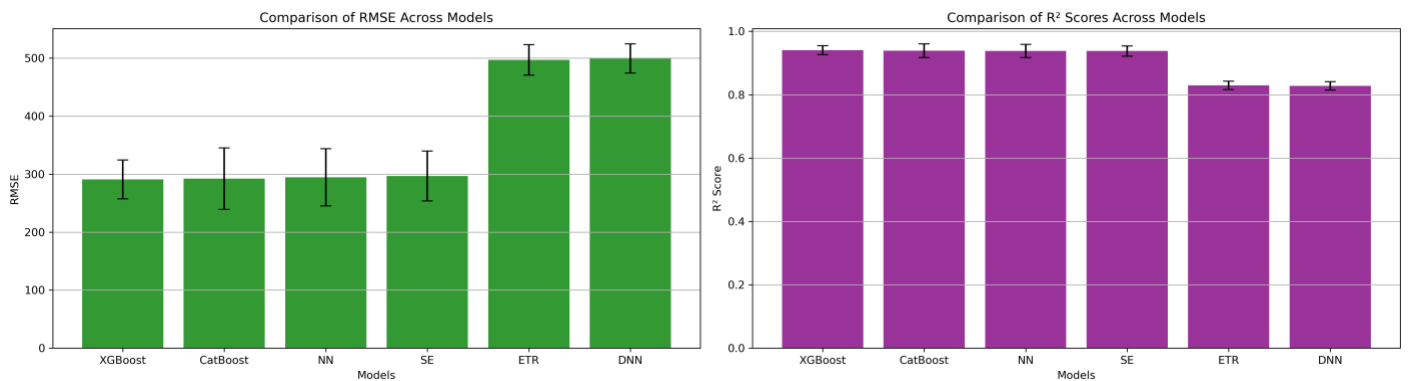*Figure 3: Bar Charts of R^2 and Adjusted R^2 for Pb (Well 782)*

Figure 4: Error Bars for RMSE and R^2 from CV for Pb (Well 782)

7. Observations & Next Steps

Best Performing Models: Extra Trees Regressor and **XGBoost** with RMSE around ~291–293 and R^2 above 0.94.

- Stacking and CatBoost closely followed in performance.
- Neural Networks (both NN and DNN) were significantly worse:
  - RMSE values exceeded 400.
  - R^2 values dropped below 0.89.
- Overall, ensemble-based tree models proved more reliable for larger structured datasets like 1225 samples

8. Code Access

The complete source code for data preprocessing, model training, evaluation, and visualization is available here. The repository includes organized Jupyter notebooks for each phase, dataset, and target, as well as requirements for reproducibility.