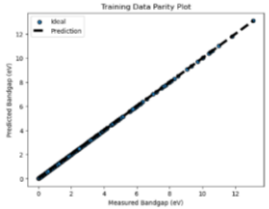
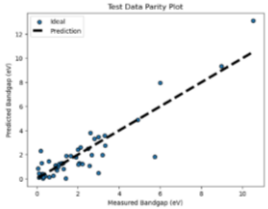
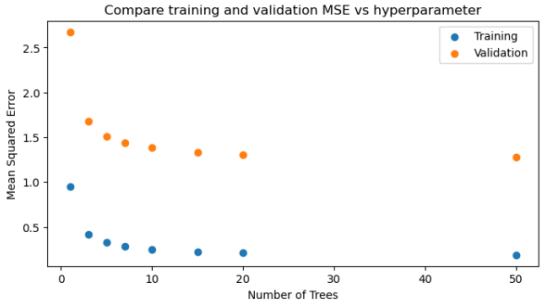
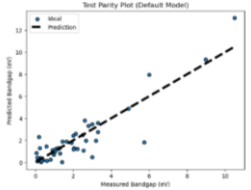
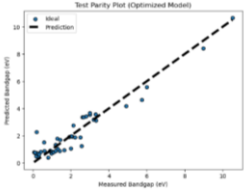
Assessment Figures











ML4ER Assignment 3

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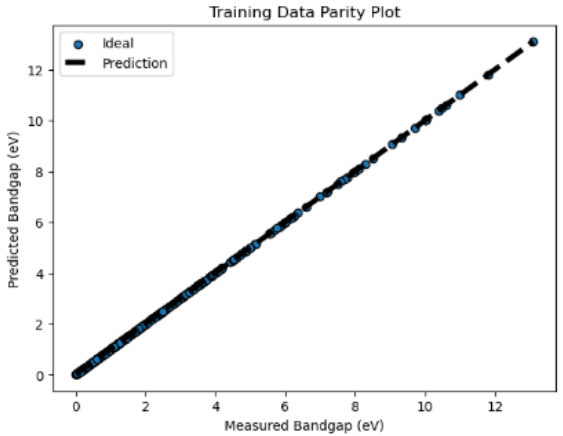
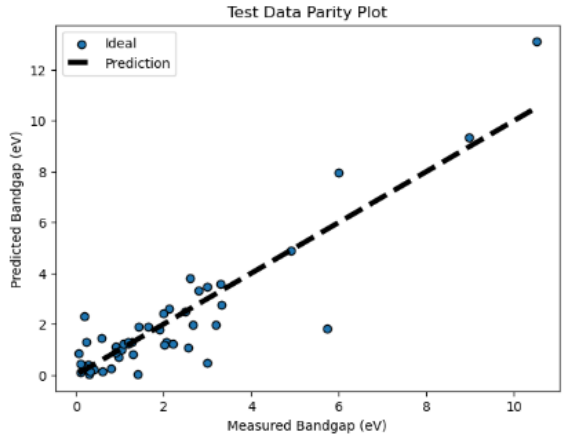
Informatics Skunkworks
MSE 401, 3 Credits
Jul 24 2024

Progress

- Default model test data parity plot from above exercise 5.1



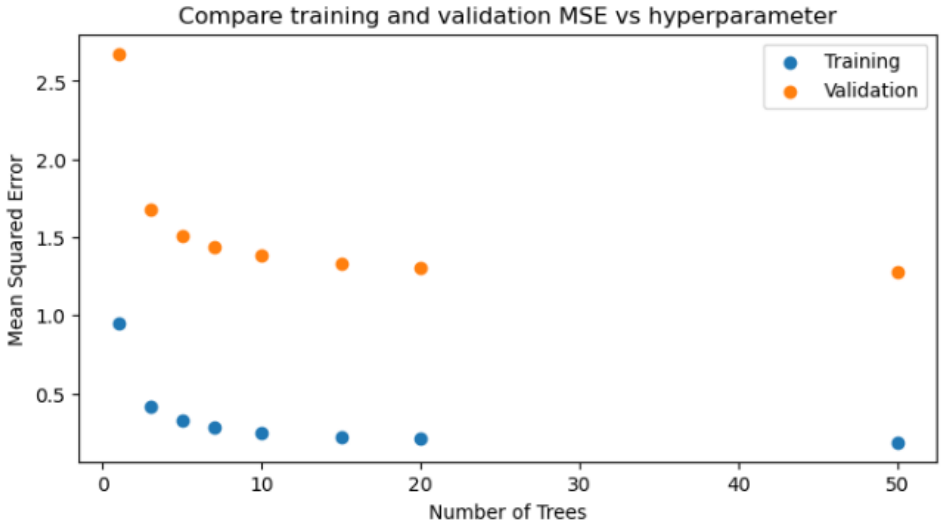


	Error Metric	Training Data	Test Data	Note
0	RMSE	0.0003 (eV)	1.0492 (eV)	(0.0 for perfect prediction)
1	RMSE/std	0.0001	0.4884	(0.0 for perfect prediction)
2	MAE	0.0 (eV)	0.6811 (eV)	(0.0 for perfect prediction)
3	R2	1.0	0.7614	(1.0 for perfect prediction)

Training Data Parity Plot: Data points align closely with the ideal dashed line. **Test Data Parity Plot:** Data points are more scattered compared to the training plot, indicating prediction errors.

Progress

- Learning curve plot from above exercise 6.1



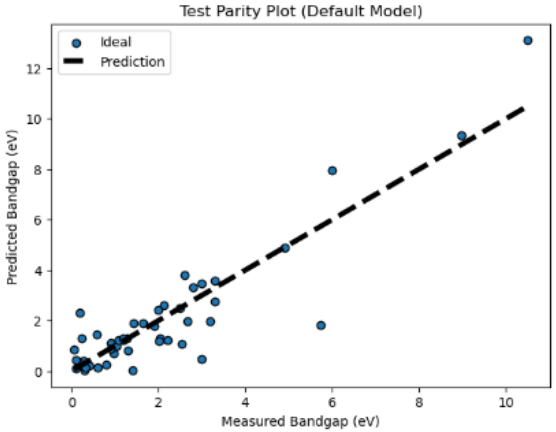

```
Minimum Mean Squared Error of test:  1.2795
Number of Trees at minimum of test:  50
Minimum Mean Squared Error of train:  0.1881
Number of Trees at minimum of train:  50
```

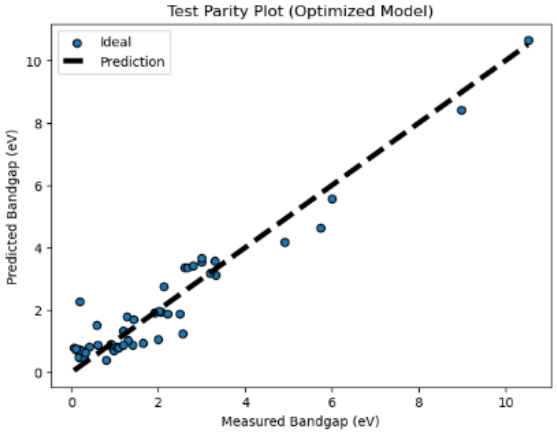
MSE decreases as the number of trees increases, with training error consistently lower than validation error.

Progress

Test Parity Plot (Default Model): Data points scatter around the ideal dashed line, with noticeable deviations. **Test Parity Plot (Optimized Model):** Data points align more closely to the ideal dashed line, indicating improved predictions.

- Optimized model test data parity plot from exercise 6.4





6]:

	Error Metric	Test Set (Default Model)	Test Set (Optimized Model)	Note
0	RMSE	1.0492 (eV)	0.6062 (eV)	(0.0 for perfect prediction)
1	RMSE/std	0.4884	0.2822	(0.0 for perfect prediction)
2	MAE	0.6811 (eV)	0.4776 (eV)	(0.0 for perfect prediction)
3	R2	0.7614	0.9204	(1.0 for perfect prediction)

Problems

- I have no problems with the sections I need to go through this week.

Questions

- Could you recommend any detailed textbooks on machine learning algorithms? I understand the working principles of most ML models but would like to delve deeper into the specifics.

Hours Summary

Date	Hours	Description of Work
07/24/2024	1.0 hours	Complete through section 7 of module 1