$assignment_2_sofia_gonzalez$

April 10, 2025

1 Task 1: EDA

First 5 rows of the dataset:

	instant	dteday	season	yr	mnth	hr	holiday	weekday	workingday	\
0	1	2011-01-01	1	0	1	0	0	6	0	
1	2	2011-01-01	1	0	1	1	0	6	0	
2	3	2011-01-01	1	0	1	2	0	6	0	
3	4	2011-01-01	1	0	1	3	0	6	0	
4	5	2011-01-01	1	0	1	4	0	6	0	

	weathersit	temp	${\tt atemp}$	hum	windspeed	casual	registered	cnt
0	1	0.24	0.2879	0.81	0.0	3	13	16
1	1	0.22	0.2727	0.80	0.0	8	32	40
2	1	0.22	0.2727	0.80	0.0	5	27	32
3	1	0.24	0.2879	0.75	0.0	3	10	13
4	1	0.24	0.2879	0.75	0.0	0	1	1

Dataset Info:

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 17379 entries, 0 to 17378
Data columns (total 17 columns):

#	Column	Non-Null Count	Dtype
0	instant	17379 non-null	int64
1	dteday	17379 non-null	object
2	season	17379 non-null	int64
3	yr	17379 non-null	int64
4	mnth	17379 non-null	int64
5	hr	17379 non-null	int64
6	holiday	17379 non-null	int64
7	weekday	17379 non-null	int64
8	workingday	17379 non-null	int64
9	weathersit	17379 non-null	int64
10	temp	17379 non-null	float64
11	atemp	17379 non-null	float64
12	hum	17379 non-null	float64
13	windspeed	17379 non-null	float64
14	casual	17379 non-null	int64

15 registered 17379 non-null int64 16 cnt 17379 non-null int64

dtypes: float64(4), int64(12), object(1)

memory usage: 2.3+ MB

None

Missing values per column:

instant dteday season 0 0 yr mnth 0 hr 0 holiday weekday workingday weathersit 0 temp 0 atemphum 0 windspeed casual registered cntdtype: int64

Summary Statistics:

, bodorboros	•				
instant	season	yr	mnth	hr '	\
17379.0000	17379.000000	17379.000000	17379.000000	17379.000000	
8690.0000	2.501640	0.502561	6.537775	11.546752	
5017.0295	1.106918	0.500008	3.438776	6.914405	
1.0000	1.000000	0.000000	1.000000	0.000000	
4345.5000	2.000000	0.000000	4.000000	6.000000	
8690.0000	3.000000	1.000000	7.000000	12.000000	
13034.5000	3.000000	1.000000	10.000000	18.000000	
17379.0000	4.000000	1.000000	12.000000	23.000000	
holiday	y weekday	workingda	y weathersit	temp	\
17379.000000	17379.000000	17379.00000	0 17379.000000	17379.000000	
0.028770	3.003683	0.68272	1 1.425283	0.496987	
0.16716	5 2.005771	0.46543	1 0.639357	0.192556	
0.000000	0.000000	0.00000	0 1.000000	0.020000	
0.000000	1.000000	0.00000	0 1.000000	0.340000	
0.000000	3.000000	1.00000	0 1.000000	0.500000	
0.000000	5.000000	1.00000	0 2.000000	0.660000	
1.000000	6.000000	1.00000	0 4.000000	1.000000	
atemp	hum	n windspeed	d casual	registered	\
	instant 17379.0000 8690.0000 5017.0295 1.0000 4345.5000 8690.0000 13034.5000 17379.00000 0.028770 0.167169 0.000000 0.0000000 0.0000000 1.00000000	instant season 17379.0000 17379.000000 8690.0000 2.501640 5017.0295 1.106918 1.0000 1.000000 4345.5000 2.000000 8690.0000 3.000000 13034.5000 3.000000 17379.0000 4.000000 holiday weekday 17379.00000 17379.000000 0.028770 3.003683 0.167165 2.005771 0.000000 0.000000 0.000000 1.0000000 0.000000 5.0000000 1.0000000 6.0000000000000000000000000000	instant season yr 17379.0000 17379.000000 17379.000000 8690.0000 2.501640 0.502561 5017.0295 1.106918 0.500008 1.0000 1.000000 0.000000 4345.5000 2.000000 0.000000 8690.0000 3.000000 1.000000 13034.5000 3.000000 1.000000 17379.0000 4.000000 1.000000 17379.00000 17379.000000 17379.00000 0.028770 3.003683 0.68272 0.167165 2.005771 0.46543 0.000000 0.000000 0.000000 0.000000 1.0000000 0.000000 0.000000 3.000000 1.0000000 0.000000 5.000000 1.0000000 0.0000000 5.000000 1.0000000000000000000	instant season yr mnth 17379.0000 17379.000000 17379.000000 17379.000000 8690.0000 2.501640 0.502561 6.537775 5017.0295 1.106918 0.500008 3.438776 1.0000 1.000000 0.000000 1.000000 4345.5000 2.000000 0.000000 4.000000 8690.0000 3.000000 1.000000 7.000000 13034.5000 3.000000 1.000000 10.000000 17379.0000 4.000000 1.000000 12.000000 17379.00000 17379.000000 17379.000000 17379.000000 0.028770 3.003683 0.682721 1.425283 0.167165 2.005771 0.465431 0.639357 0.000000 0.000000 0.000000 1.000000 0.000000 1.000000 0.000000 1.000000 0.000000 1.000000 0.000000 1.000000 0.000000 3.000000 1.000000 1.000000 0.000000 5.000000 1.000000 2.000000 0.000000 5.000000 1.000000 4.000000	instant season yr mnth hr 17379.0000 17379.000000 17379.000000 17379.000000 17379.000000 8690.0000 2.501640 0.502561 6.537775 11.546752 5017.0295 1.106918 0.500008 3.438776 6.914405 1.0000 1.000000 0.000000 1.000000 0.000000 4345.5000 2.000000 0.000000 7.000000 12.000000 8690.0000 3.000000 1.000000 7.000000 12.000000 13034.5000 3.000000 1.000000 10.000000 18.000000 17379.0000 4.000000 1.000000 12.000000 23.000000 17379.000000 17379.000000 17379.000000 17379.000000 17379.000000 0.028770 3.003683 0.682721 1.425283 0.496987 0.167165 2.005771 0.465431 0.639357 0.192556 0.000000 1.000000 1.000000 0.340000 0.000000 3.000000 1.000000 1.

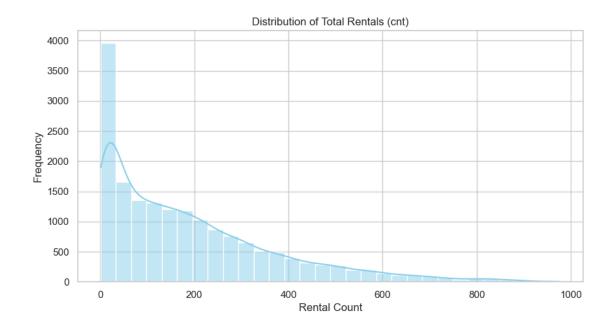
count	17379.000000	17379.000000	17379.000000	17379.000000	17379.000000
mean	0.475775	0.627229	0.190098	35.676218	153.786869
std	0.171850	0.192930	0.122340	49.305030	151.357286
min	0.000000	0.000000	0.000000	0.000000	0.000000
25%	0.333300	0.480000	0.104500	4.000000	34.000000
50%	0.484800	0.630000	0.194000	17.000000	115.000000
75%	0.621200	0.780000	0.253700	48.000000	220.000000
max	1.000000	1.000000	0.850700	367.000000	886.000000
	cnt				
count	17379.000000				
mean	189.463088				
std	181.387599				
min	1.000000				
25%	40.000000				
50%	142.000000				
75%	281.000000				
max	977.000000				

We removed the following columns from the dataset:

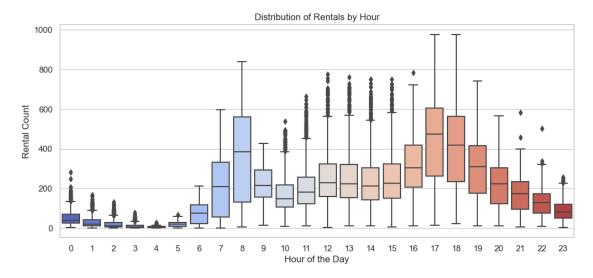
- Instant: it is just a unique id for each row, doesnt add any predictive value
- dteday: A string version of the date. Since we already have features like year (yr), month (mnth), and day of the week (weekday), this becomes redundant.
- casual and registered: These two columns together directly sum up to the target variable (cnt), which represents the total bike rentals. Keeping them would be a form of data leakage because the model would learn the target from its components instead of actual predictors.

1.0.1 EDA Visualizations

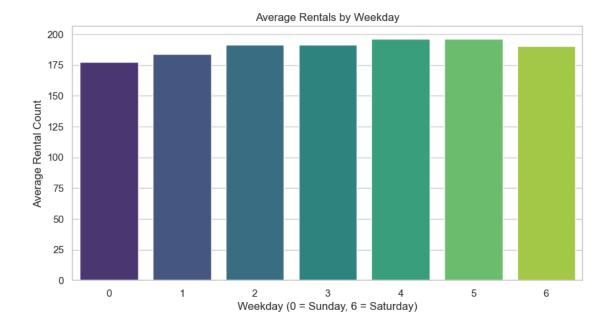
<Figure size 1200x600 with 0 Axes>



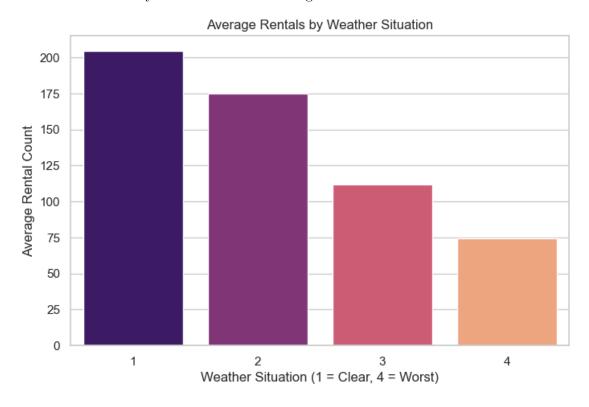
Helps us understand how bike rentals are distributed. The histogram shows that most bike rental sessions fall on the lower end of the scale, with a noticeable right skew. This makes sense because high rental spikes are rarer, while lower or moderate rental volumes are more common. The peak is strong in the 0-100 rental range and then it gradually decreases. High rental counts are much more rare, which is somethign that we were expecting.



Shows usage trends by hour. We can see that there are 2 noticeable peaks which are morning hours around 8AM and afternoon around 5-6PM. This makes sense as they are likely the typical commuting hours. We can also see that early in the morning there are far few less people who rent bikes (2-5AM)

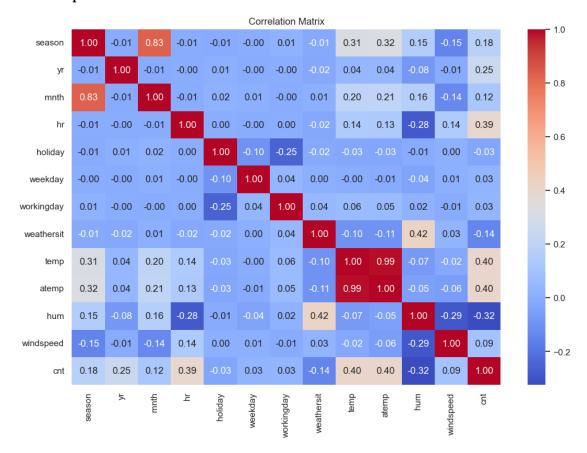


Helps spot trends across weekdays. We can see that the rentals stay pretty consistent during weekends as well as weekdays. There are more rentals on Thursdays-Fridays, but in general it stays pretty consistent. Although Sunday is the day with the least rentals, its not highly significant. We can assume then that they use bikes for commuting as well as for leisure.



Explores how external weather conditions affect bike usage. As we would expect in our data there is a negative correlation between poor weather and bike rental. The highest rental count occurs when the weather is clear and it drops as the weather also drops.

Correlation plot



We probably should drop atemp as it is highly correlated with temp

2 Task 2: Data Splitting

Training set shape: (10427, 12) Validation set shape: (3476, 12)

Test set shape: (3476, 12)

I split the data into 3 sets: 60% for training, 20% for validation, and 20% for testing. I did this by using train_test_split, ensuring that the model has enough data to learn from patters, enough separate data to tune parameters, and untouched data in order to evaluate performance.

We are doing this before of feature engineering in order to avoid data leakage. We don't want any over optimistic performance and poor generalization.

3 Task 3: Feature Engineering

We have to encode cyclical features because there is a circular nature. hour 0 and hour 23 are right next to each other, not that far away. The same thing happens with weekdays, monday and sunday are right next to each other. We used sine and cosine in order to capture patterns that repeat cyclically so now it will be between -1 and 1.

Previewing original 'hr' and 'weekday' before encoding:

	hr	weekday
14779	0	4
16914	13	3
15863	4	0
4204	2	3
1554	5	4

After cyclical encoding:

```
hr sin
                   hr cos
                            weekday sin
                                         weekday cos
      0.000000
                 1.000000
                              -0.433884
                                            -0.900969
14779
16914 -0.258819 -0.965926
                               0.433884
                                            -0.900969
15863
      0.866025
                 0.500000
                               0.000000
                                             1.000000
4204
       0.500000
                 0.866025
                               0.433884
                                            -0.900969
1554
       0.965926 0.258819
                              -0.433884
                                            -0.900969
```

I also applied one-hot econding to season, weathersit, and month. This will convert them into binary variables, this is done because these variables are cateogrical. We dont want the labels to be seen as magnitudes.

```
Before One-Hot Encoding:
```

Season unique values: [3 4 1 2] Weathersit unique values: [1 2 3 4]

Month unique values: [9 12 10 6 3 2 5 11 1 7 8 4]

After One-Hot Encoding (sample of columns):										
	season_	2 seaso	n_3 sea	son_4	weathersi	t_2 we	eathersit_	3 weath	ersit_4	\
14779	Fals	e T	rue	False	Fa	lse	Fals	е	False	
16914	Fals	e Fa	lse.	True	T	rue	Fals	е	False	
15863	Fals	e Fa	lse	True	T	rue	Fals	е	False	
4204	Fals	e T	rue	False	Fa	lse	Fals	е	False	
1554	Fals	e Fa	lse	False	Fa	lse	Tru	е	False	
	mnth_2	mnth_3	$mnth_4$	mnth_5	mnth_6	mnth_7	mnth_8	mnth_9	\	
14779	False	False	False	False	False	False	e False	True		
16914	False	False	False	False	False	False	e False	False		
15863	False	False	False	False	False	False	e False	False		
4204	False	False	False	False	True	False	e False	False		
1554	False	True	False	False	False	False	e False	False		

mnth_11 mnth_10 mnth_12 False False False 14779

16914	False	False	True
15863	True	False	False
4204	False	False	False
1554	False	False	False

I did scaling because it ensures that features with different ranges are brought to a similar scale. So it makes everything fair as it is working on the same scale instead of giving more importance to variables which ranges are with bigger numbers.

Before Scaling:

	temp	atemp	hum	windspeed
count	10427.000000	10427.000000	10427.000000	10427.000000
mean	0.496436	0.475479	0.626612	0.190609
std	0.193049	0.172721	0.192536	0.121860
min	0.020000	0.000000	0.000000	0.000000
25%	0.340000	0.333300	0.480000	0.104500
50%	0.500000	0.484800	0.620000	0.194000
75%	0.660000	0.621200	0.780000	0.253700
max	1.000000	1.000000	1.000000	0.850700

After Scaling:

	temp	atemp	hum	windspeed
count	1.042700e+04	1.042700e+04	1.042700e+04	1.042700e+04
mean	-1.454885e-16	-2.524754e-16	-4.054598e-16	1.011946e-16
std	1.000048e+00	1.000048e+00	1.000048e+00	1.000048e+00
min	-2.468067e+00	-2.753011e+00	-3.254674e+00	-1.564243e+00
25%	-8.103813e-01	-8.232137e-01	-7.615134e-01	-7.066588e-01
50%	1.846157e-02	5.396689e-02	-3.434163e-02	2.782758e-02
75%	8.473044e-01	8.437189e-01	7.967118e-01	5.177587e-01
max	2.608596e+00	3.036960e+00	1.939410e+00	5.417070e+00

I added an interaction term between temp and humidity. This was because of the idea that hot + humid conditions might impact bike usage differently than hot + dry weather. We noticed in EDA that both features independently affected usage, so combining them may help uncover non-linear relationships.

We did hr and working day because rush hour peaks only happen on working days and weekend patterns are different even at the same hour

We also added season and weathersit because they don't operate independently and their combined context can strongly influence bike rental behavior. A rainy or foggy day (weathersit) in summer might still result in high rentals because it's warm and people are more likely to go out. But the same weathersit in winter could drastically reduce rentals due to already low temperatures and less daylight. This can be a great interaction to look out for

Sample interaction terms:

season_weathersit	hr_workingday	${\tt temp_hum}$	
False	1.000000	0.176825	14779
False	-0.965926	0.869668	16914
False	0.000000	0.000325	15863

4204	0.895106	0.866025	False
1554	2.300325	0.258819	False

After reviewing the correlation matrix in Task 1, I found that atemp (feels-like temperature) is highly correlated with temp. Including both might introduce multicollinearity. So I dropped atemp to reduce redundancy and make the model more interpretable.

4 Task 4: Baseline Model - Linear Regression

Lets first reload the original dataset and split it, then we can start training a simple linear regression without the encoding and evaluate how it works.

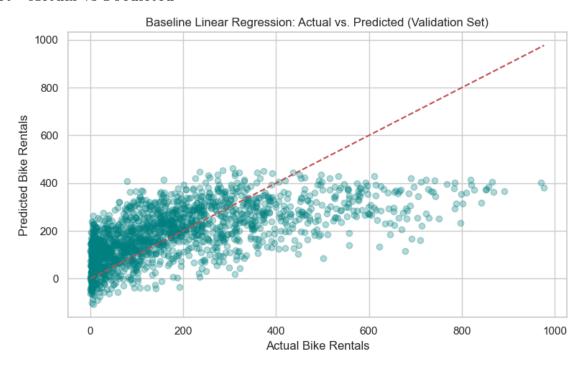
Baseline Model Evaluation on Validation Set:

Mean Squared Error (MSE): 20150.19 Mean Absolute Error (MAE): 106.13 Root Mean Squared Error (RMSE): 141.95

R² Score: 0.3991

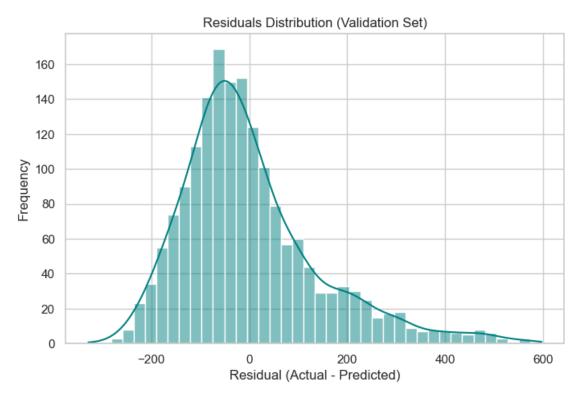
We can see that the model's prediction on the baseline are off by 142 rentals which is a lot. We can also see by the MAE that on average predictions are off by 106, regardless of the direction of the error. The MSE is 20,150 which means that the model is making significant prediction mistakes. The model also explains roughly 40% of the variance in bike rentals meaning that there is a lot of the data's behavior that it doesn't capture in the model.

Plot - Actual vs Predicted



The model is underestimating high rental counts as we can see by the points falling under the dotted line.

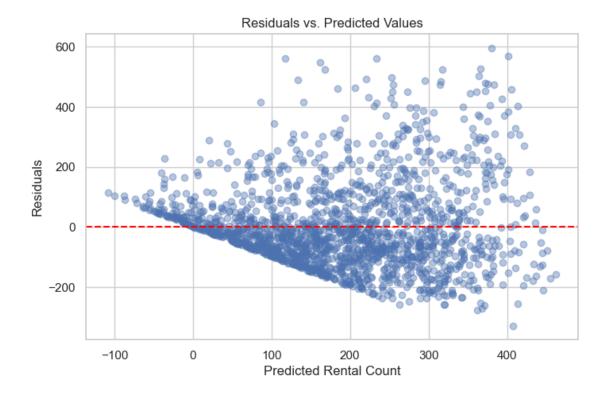
Plot - Residual Distribution



We can see that the residuals are centered around 0, which is a good sign because it menans that its not significantly overpredicting or underpredicting. It is clearly skewed to the right though, which means that it underestimates the bike rentals on the higher end.

We would ideally like it to be more tilightly concentrated around 0. This just means that the model is struggling with complex scenarios, so might be a bit biased right now.

Plot - Residuals vs Predicted



We can see that the model performs worse whenever there's a higher number of rentals. We can see heteroscedasticity, which means that its errors are not consistent at all levels of prediction.

We can see that predictions for smaller rentals counts tend to be more accurate but as there are more rental counts there are more residuals meaning that there are underpredicting them.

5 Task 5: Random Forest Regressor

Here we will be using the already processed data.

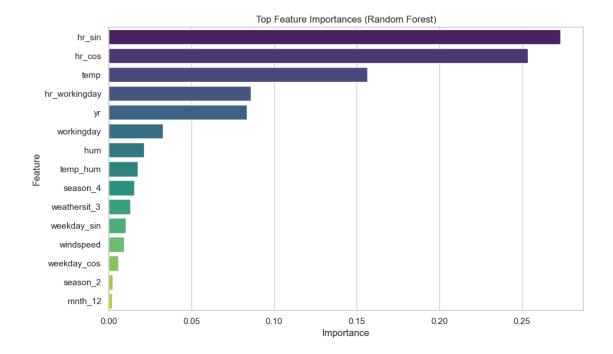
Random Forest Evaluation on Validation Set:

Mean Squared Error (MSE): 2139.29 Mean Absolute Error (MAE): 28.19 Root Mean Squared Error (RMSE): 46.25

R² Score: 0.9364

We can see that the random forest regressor performs better than the baseline model across all metrics. It reduces the MAE from 106 to 28, which is a great improvement. Also the RMSE went from 142 to 46, which is also huge improvement. Most importantly the R^2 went from 40% to 94% which means that it explains 94% of the variance in bike rentals. Really good.

We can see that the bike rental patterns are non-linear thats why the linear regression didnt do a great job, because it wasnt flexible enough.

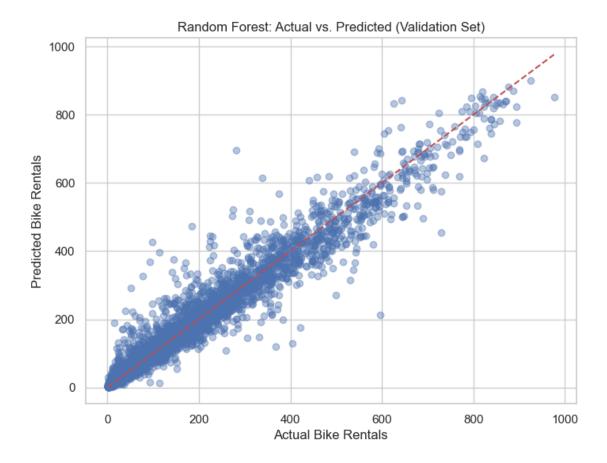


We can see that the most important features by far are the cyclically encoded hour values (hr_sin and hr_cos), which makes perfect sense because bike rental patterns follow daily cycles, with peaks likely during commute/rush hours.

Temperature is also a strong predictor, which aligns with the idea that people are more likely to rent bikes in warmer conditions. The interaction between hour and working day (hr_workingday) also ranks highly, which reflects how work schedules affect bike usage.

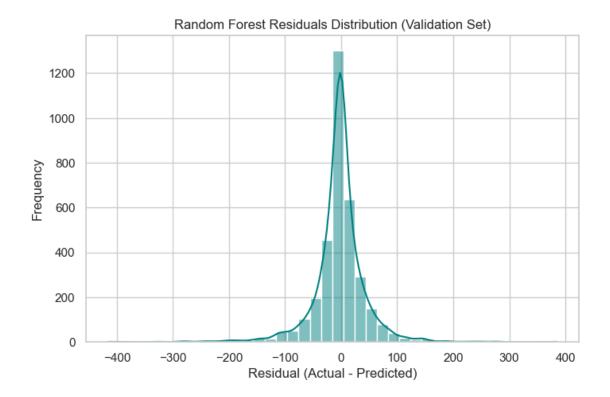
The year (yr) is also significant, suggesting an increasing trend in bike rentals over time. Other relevant features include working day status, humidity, and the interaction between temperature and humidity (temp_hum), all of which likely influence the comfort and practicality of biking.

Plot - Actual vs Predicted



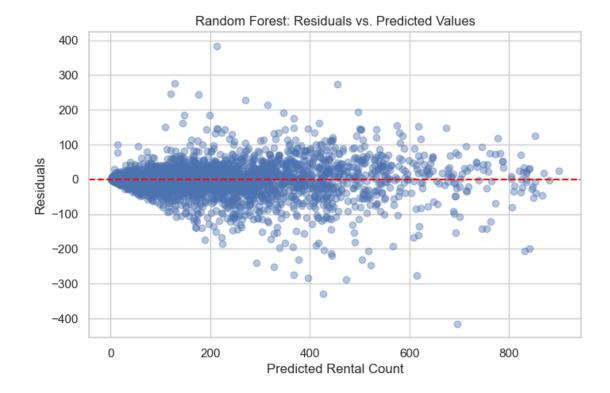
The predictions align much more closely with the actual bike rentals compared to the baseline model. Most of the points fall tightly around the diagonal line, which is a great sign. This indicates that the model is accurately capturing the patterns in the data and making reliable predictions.

Plot - Residuals Distribution



The residuals are now tightly clustered around 0, showing that the prediction errors are generally small. The distribution is sharply peaked and more symmetric than in the linear regression model, although there is still a slight right skew. Overall, the Random Forest model is making consistently accurate predictions.

Plot - Residuals vs Predicted



The residuals appear randomly scattered with no clear pattern, which is exactly what we want. This randomness suggests the model is not missing any obvious nonlinear relationships. Additionally, the residuals are more homoscedastic, which means that they're evenly spread across the range of predicted values, which indicates a good model fit across different rental counts

Overall, the Random Forest model shows both low bias and low variance on the validation set. It captures the underlying structure of the data very well and generalizes effectively. While these results are promising, we'll validate further performance on the test set to ensure robustness.

6 Task 6: Gradient Boosting Regressor

Requirement already satisfied: xgboost in
/Users/sofiagonzalez/anaconda3/lib/python3.11/site-packages (3.0.0)
Requirement already satisfied: numpy in
/Users/sofiagonzalez/anaconda3/lib/python3.11/site-packages (from xgboost)
(1.24.3)
Requirement already satisfied: scipy in
/Users/sofiagonzalez/anaconda3/lib/python3.11/site-packages (from xgboost)
(1.10.1)
Note: you may need to restart the kernel to use updated packages.
XGBoost Evaluation on Validation Set:

XGBoost Evaluation on Validation Set: Mean Squared Error (MSE): 1907.75 Mean Absolute Error (MAE): 27.97 Root Mean Squared Error (RMSE): 43.68

R² Score: 0.9433

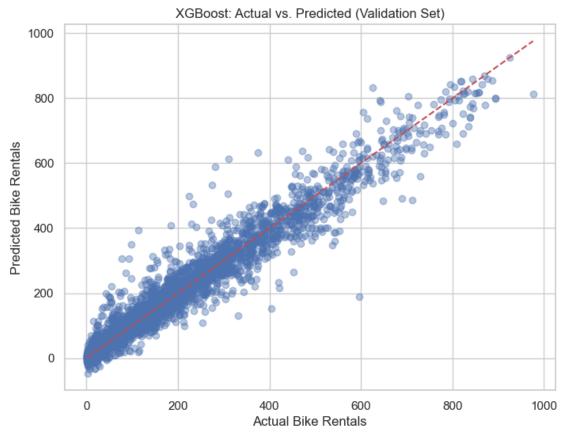
We can see that Linear Regression performed the worst across all evaluation metrics. It had a high Mean Absolute Error (MAE) of 106, and a Root Mean Squared Error (RMSE) of 142, indicating that its predictions were quite far off from the actual values. The model could only explain 40% of the variance in bike rental counts, which is relatively low and reflects its inability to capture the complex, non-linear patterns present in the data.

In contrast, the Random Forest Regressor made a significant improvement. It reduced the MAE from 106 to 28, and the RMSE dropped from 142 to 46, making the predictions much more accurate overall. The R² score increased dramatically from 0.40 to 0.94, meaning it could now explain 94% of the variance in bike rentals — a huge leap in performance. This clearly demonstrates the advantage of using non-linear ensemble models that can capture interactions between features.

Finally, XGBoost slightly outperformed Random Forest. It achieved the lowest RMSE at 43.68, a slightly lower MAE of 27.97, and the highest R² score of 0.9433. These results suggest that XGBoost was able to capture even more subtle patterns in the data, likely due to its boosting mechanism that corrects errors made by earlier trees in the ensemble.

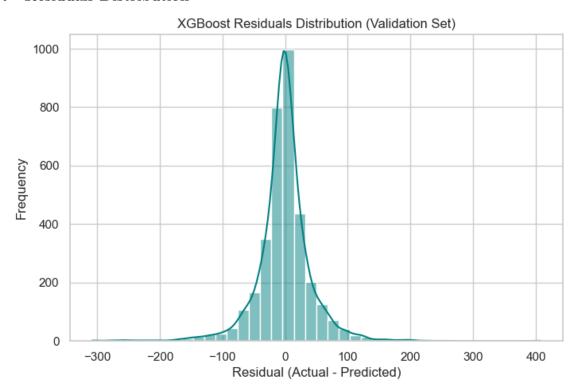
Overall, both RF and XGB models show a major improvement over the baseline, and XGBoost stands out as the best performer in this task.

Plot - Actual vs Predicted



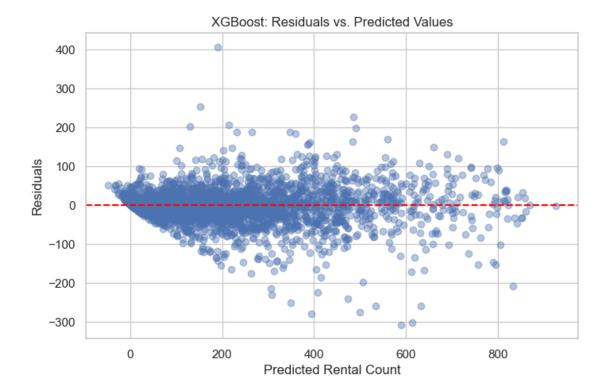
The predictions from the XGBoost model align extremely well with the actual rental values, clustering closely around the diagonal line. This suggests that the model has captured the underlying patterns in the data with high accuracy. There are still a few outliers, especially at higher rental counts, but overall, the points are much more concentrated compared to the linear regression plot; showing tighter and more reliable predictions.

Plot - Residuals Distribution



The residuals are tightly concentrated around zero, with a clear peak and relatively symmetric shape, indicating that most predictions are very close to the actual values. Compared to the baseline and even the Random Forest model, this distribution appears narrower and more focused, which a strong sign of low prediction error. There's still a bit of right skew, but it's minimal. This supports the earlier metrics showing that XGBoost produces highly accurate predictions.

Plot - Residuals vs Predicted



This plot shows that the residuals are fairly centered around zero across the range of predicted values, which is exactly what we want to see. There's no strong visible pattern, indicating that the model doesn't consistently overpredict or underpredict for certain rental volumes. While there's some increased spread at higher predicted values (a bit of heteroscedasticity), it's much more controlled than with Linear Regression. This reinforces that the model generalizes well and doesn't suffer from major bias or variance issues.

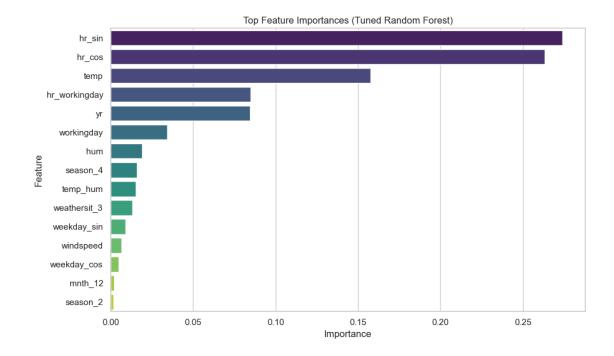
7 Task 7: Hyperparameter Tuning

7.1 Random Forest

```
Fitting 5 folds for each of 30 candidates, totalling 150 fits Tuned Random Forest Results: Best Hyperparameters: {'max_depth': 19, 'min_samples_leaf': 1, 'min_samples_split': 8, 'n_estimators': 58} RMSE: 46.71 MAE: 28.63 R^2: 0.9351
```

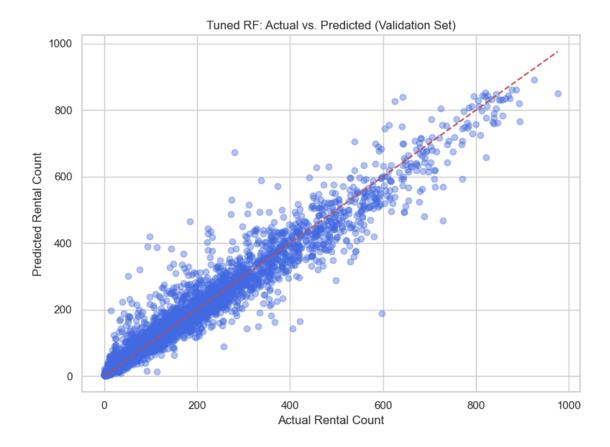
Compared to the untuned Random Forest (RMSE: 46.25, R²: 0.9364), performance slightly dropped, indicating that tuning didn't significantly improve results.

The best hyperparameter combination suggests the model performs best with moderately deep trees and a relatively low number of estimators.



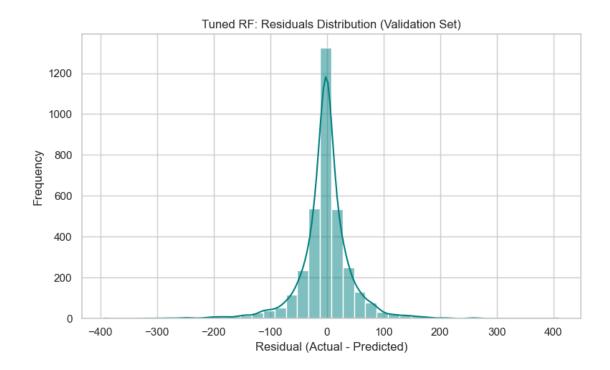
The top features remained consistent: hr_sin, hr_cos, and temp were still the most influential. This shows that even after tuning, the model relies on similar patterns in the data, confirming the robustness of the original feature engineering

Plot - Actual vs Predicted



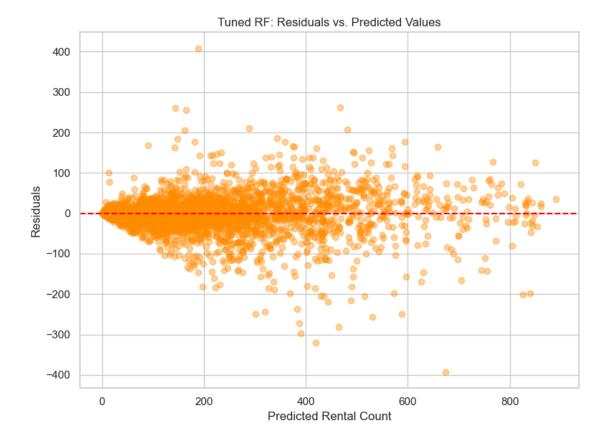
The predictions remain closely aligned with the actual values, following the diagonal line quite well. This indicates that the tuned Random Forest continues to make accurate predictions with little deviation from the real thing.

Plot - Residual Distribution



The residuals are still tightly centered around zero, suggesting low bias. The peak is slightly sharper than before, indicating that the tuning may have helped reduce moderate errors and focus the predictions even more.

Plot - Residuals vs Predicted



The residuals remain fairly homoscedastic, though we still observe a slightly funnel-shaped pattern with increasing variance at higher predicted counts. However, there is no major pattern, so the model appears to generalize well.

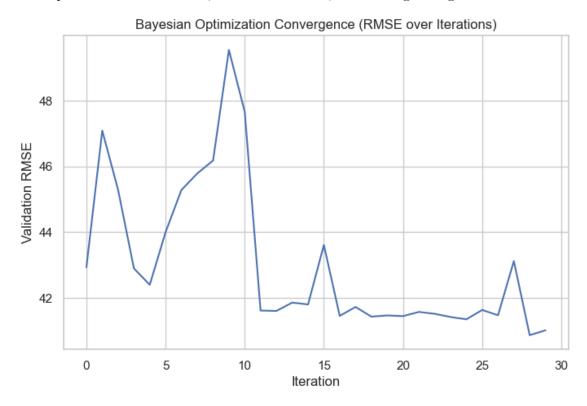
7.2 XGB

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optimize) (1.3.0)
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pyaml>=16.9->scikit-optimize) (6.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in
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learn>=1.0.0->scikit-optimize) (3.5.0)
Note: you may need to restart the kernel to use updated packages.
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Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Fitting 5 folds for each of 1 candidates, totalling 5 fits
Tuned XGBoost Results:
Best Hyperparameters: OrderedDict([('learning_rate', 0.05624593012982076),
('max_depth', 8), ('n_estimators', 300), ('subsample', 0.5)])
RMSE: 40.95
MAE: 24.91
R^2: 0.9501
```

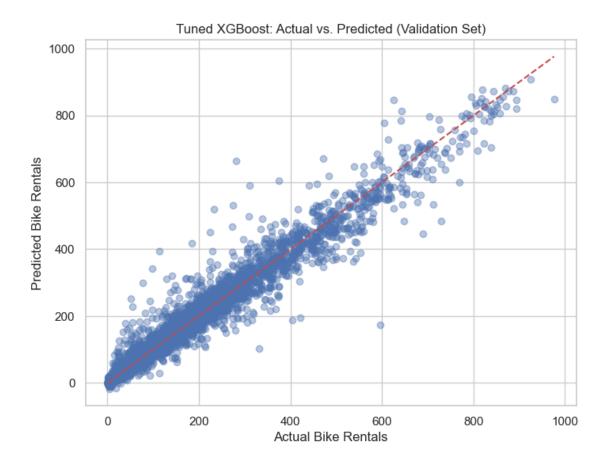
These are the best scores yet! Compared to the untuned XGBoost (RMSE: 43.68, R²: 0.9433), this shows a noticeable boost in performance. The lower learning rate likely helped prevent overfitting while maintaining accuracy by using more estimators. The subsample of 0.5 encourages diversity in the trees, which can also reduce variance and improve generalization.

This shows that hyperparameter tuning via Bayesian Optimization was worth it. The tuned model is better at capturing the underlying patterns in the data and generalizes better on the validation set. The improvement isn't massive, but it's consistent, which is a good sign of a well-tuned model.



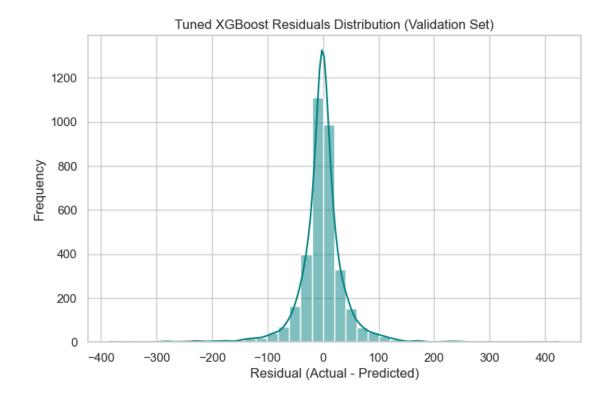
This plot shows that early iterations had a wide range of RMSE values (some even above 48), but after around iteration 10, the RMSE drops significantly and stabilizes near 41, which is a clear sign that Bayesian Optimization found a good region in the hyperparameter space. The relatively flat curve afterward suggests that the optimizer converged — further tuning would likely give diminishing returns.

Plot - Actual vs Predicted



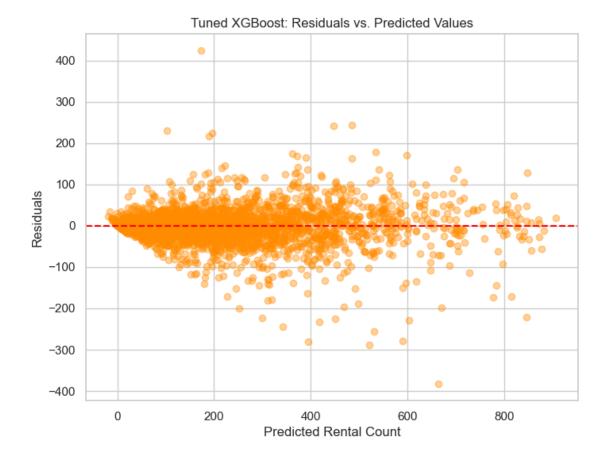
The points align very closely with the diagonal, showing that the tuned XGBoost model makes highly accurate predictions. There is minimal spread, especially in the mid-range values, which reflects improved generalization.

Plot - Residuals Distribution



The residuals are tightly centered around 0 with a sharp peak, indicating that most predictions are very close to the actual values. This suggests low bias and fewer large errors.

Plot - Residuals vs Predictions



The residuals are evenly spread across the predicted range with no clear pattern, confirming the model's errors are randomly distributed. The slight fan shape is still present but less pronounced compared to the untuned version.

For Random Forest, tuning slightly reduced performance on the validation set (RMSE increased from 46.25 to 46.71, and R² dropped from 0.9364 to 0.9351). This suggests that the untuned model was already near-optimal and the randomized search may have landed on a configuration that slightly underperformed. The feature importance plot remained nearly identical, reinforcing that the model's interpretation and decision structure didn't change significantly. Overall, there were no signs of overfitting, but tuning didn't provide a clear advantage.

In contrast, XGBoost showed more meaningful gains from tuning. The RMSE improved from 43.68 to 40.95, and R² increased from 0.9433 to 0.9501. This improvement suggests that Bayesian Optimization effectively identified better hyperparameter combinations, enabling the model to capture more subtle patterns without overfitting. The convergence plot confirmed steady progress in reducing validation error over iterations.

8 Task 8: Iterative Evaluation and Refinement

After comparing the performance of all three models, Linear Regression, Random Forest, and XGBoost, it became clear that the tuned XGBoost Regressor outperformed the others across all

evaluation metrics. It achieved the lowest error values (RMSE: 40.95, MAE: 24.91) and the highest R² score of 0.9501, indicating that it explains over 95% of the variance in bike rental demand.

This strong performance, coupled with its ability to model complex non-linear relationships, makes XGBoost the most promising candidate for final refinement. Task 8 is about iterating and polishing, and it makes the most sense to apply those refinements to the model that is already working best.

By focusing our efforts here, we can ensure that we get the most out of our data and push this already high-performing model to its full potential before locking it in for final testing in Task 9.

So first we should see the current model performance, which is: - RMSE: 40.95 - MAE: 24.91 - R^2 : 0.9501

This is already really good but let's see if we can tweak it a bit with better features

In Task 3, we initially added a few interaction terms based on intuition and EDA: - temp \times hum: because high temperature and high humidity together likely affect user comfort and thus rentals. - hr_cos \times workingday: to model how rental patterns change across work hours vs. weekends. - season_2 \times weathersit_2: a basic example to test the interaction between weather and time of year.

We also dropped atemp as it was highly correlated to temp. Let's see if we can drop more things, and we do! According to the correlation matrix done in Task 1 we can also see that holiday has zero correlation and might just be noise and weekday, which is also has very little correlation

We can also see if we can drop month or season, since they are both strongly correlated

lets retrain the XGB

Tuned XGBoost on Cleaned Features:

RMSE: 43.62 MAE: 26.68 R²: 0.9434

We can see that dropping holiday and mnth actually made the model slightly worse. So, we should keep mnth and holiday in our final feature set.

Even though holiday and mnth showed low correlation with cnt, XGBoost was likely using subtle patterns in those features.

Lets now try to drop one of our correlations to see if it was actually helping: temp_hum

Tuned XGBoost without temp_hum:

RMSE: 40.86 MAE: 24.84 R²: 0.9504

So we will keep this one dropped. Although temperature and humidity seemed correlated during EDA, removing the temp_hum interaction actually improved model performance slightly across all metrics. This suggests the model already captures the relationship between temp and hum independently, so the interaction term wasn't helpful.

We are now going to try to drop hr_workingday to see how much it was actually helping

Tuned XGBoost without hr_workingday:

RMSE: 41.28

MAE: 25.14 R²: 0.9493

Removing hr_workingday slightly worsened the model's performance across all metrics. Even though the difference is small, it suggests that hr_workingday provides marginal value, likely helping the model capture behavioral patterns tied to work hours.

Now we will see season_weathersit

Tuned XGBoost without season_weathersit:

RMSE: 40.95 MAE: 24.88 R²: 0.9501

We can see that removing season_weathersit had almost no impact on the model's performance. This is a good sign, it means that the model is robust and not overly reliant on a specific interaction term. We will remove it as it is better to keep the model simpler

We iteratively pruned redundant interactions (like temp_hum) and retained useful ones (like hr_workingday), guided not just by correlation but also model performance impacts. This aligns with his suggested workflow: start with low-variance filtering, prune highly correlated inputs, and consider dimensionality tradeoffs through validation

So for the final model I ended up choosing XGB Regressor as it was the one that performed better and it generalized very well. It was also balanced and it had low variance and bias

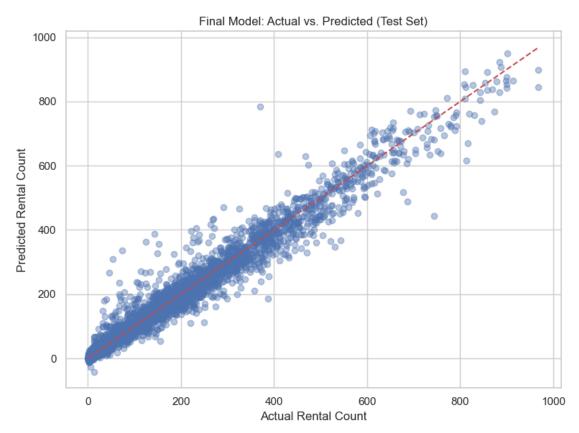
9 Task 9: Final Model Selection and Training

Final Model Performance on Test Set:
Mean Squared Error (MSE): 1366.23
Mean Absolute Error (MAE): 22.84
Root Mean Squared Error (RMSE): 36.96
R² Score: 0.9579

After retraining the model on the combined training and validation sets and evaluating on the untouched test set, we obtained the following results: - Mean Squared Error (MSE): 1366.23 - Mean Absolute Error (MAE): 22.84 - Root Mean Squared Error (RMSE): 36.96 - R^2 Score: 0.9579

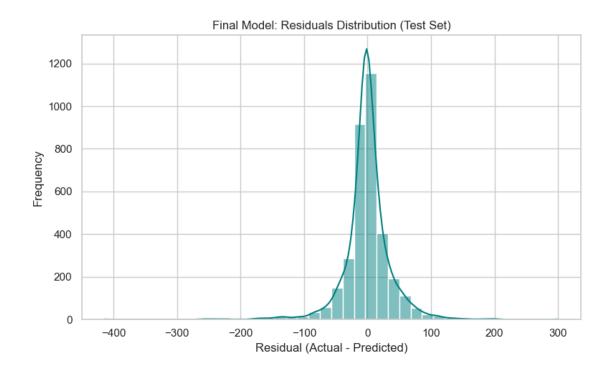
These metrics confirm that the final model generalizes extremely well to unseen data. It explains 95.8% of the variance in bike rentals and has a very low average prediction error, which demonstrates both low bias and low variance.

Plot - Actual vs Predicted



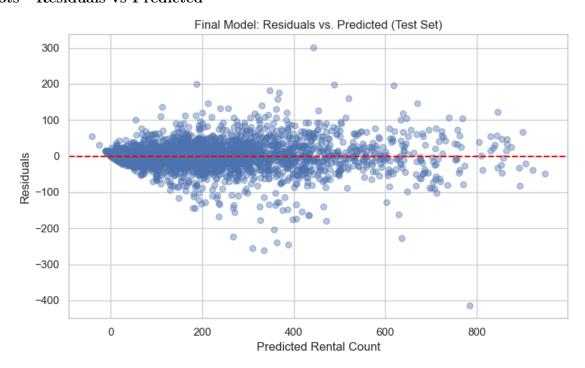
Predictions align very closely with the actual values, forming a tight cluster around the diagonal. This indicates that the model generalizes extremely well and has low bias on unseen data

Plots - Residual Distribution



The residuals are sharply centered around zero and symmetrically distributed, showing low variance and no major outliers or skew. This confirms that prediction errors are small and normally distributed, which is ideal for a well-performing model.

Plots - Residuals vs Predicted



Residuals are evenly spread without a clear pattern, which is a good sign of homoscedasticity. This means the model's errors are consistent across different prediction values and not systematically biased.

10 Conclusions

```
Metric Validation (Before Tuning) Validation (After Tuning)
0
        RMSE
                                  43.6800
                                                              40.9500
1
         MAE
                                  27.9700
                                                              24.9100
 R^2 Score
                                   0.9433
                                                               0.9501
   Test Set (Final)
            36.9600
0
1
            22.8400
             0.9579
```

The progressive improvements in RMSE, MAE, and R² demonstrate how impactful model tuning and iterative refinement can be. Starting with a strong baseline XGBoost model, we significantly enhanced its predictive power through Bayesian optimization and targeted feature engineering.

Tuning reduced the RMSE from 43.68 to 40.95 on the validation set, and further refining the features dropped the final test RMSE to 36.96, showing great generalization. Likewise, MAE decreased by over 5 points, and the R^2 score rose from 0.9433 to 0.9579, confirming the model's improved ability to explain variance in bike rentals.

These gains reflect not just better hyperparameters, but also smarter features and a model that now balances bias and variance more effectively. Overall, the final XGBoost model captures the complexity of rental patterns while remaining robust across unseen data.

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pdf) (6.5.4)
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  Obtaining dependency information for websockets<11.0,>=10.0 from https://files
.pythonhosted.org/packages/cc/19/2f003f9f81c0fab2eabb81d8fc2fce5fb5b5714f1b4abfe
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Installing collected packages: websockets
  Attempting uninstall: websockets
   Found existing installation: websockets 14.2
   Uninstalling websockets-14.2:
      Successfully uninstalled websockets-14.2
ERROR: pip's dependency resolver does not currently take into account all
the packages that are installed. This behaviour is the source of the following
dependency conflicts.
realtime 2.4.1 requires websockets<15,>=11, but you have websockets 10.4 which
is incompatible.
Successfully installed websockets-10.4
Note: you may need to restart the kernel to use updated packages.
[NbConvertApp] Converting notebook assignment_2_sofia_gonzalez.ipynb to pdf
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unsupported version of pandoc (3.6.3).
Your version must be at least (1.12.1) but less than (3.0.0).
Refer to https://pandoc.org/installing.html.
Continuing with doubts...
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[NbConvertApp] Writing 1791080 bytes to assignment_2_sofia_gonzalez.pdf
[NbConvertApp] WARNING | pattern 'assignment_2_sofia_gonzalez-no-input.ipynb'
matched no files
This application is used to convert notebook files (*.ipynb)
        to various other formats.
        WARNING: THE COMMANDLINE INTERFACE MAY CHANGE IN FUTURE RELEASES.
Options
The options below are convenience aliases to configurable class-options,
as listed in the "Equivalent to" description-line of the aliases.
To see all configurable class-options for some <cmd>, use:
    <cmd> --help-all
--debug
    set log level to logging.DEBUG (maximize logging output)
    Equivalent to: [--Application.log_level=10]
```

```
--show-config
    Show the application's configuration (human-readable format)
    Equivalent to: [--Application.show_config=True]
--show-config-json
    Show the application's configuration (json format)
    Equivalent to: [--Application.show_config_json=True]
--generate-config
    generate default config file
   Equivalent to: [--JupyterApp.generate_config=True]
    Answer yes to any questions instead of prompting.
   Equivalent to: [--JupyterApp.answer_yes=True]
--execute
    Execute the notebook prior to export.
   Equivalent to: [--ExecutePreprocessor.enabled=True]
--allow-errors
    Continue notebook execution even if one of the cells throws an error and
include the error message in the cell output (the default behaviour is to abort
conversion). This flag is only relevant if '--execute' was specified, too.
    Equivalent to: [--ExecutePreprocessor.allow_errors=True]
--stdin
    read a single notebook file from stdin. Write the resulting notebook with
default basename 'notebook.*'
   Equivalent to: [--NbConvertApp.from_stdin=True]
--stdout
   Write notebook output to stdout instead of files.
   Equivalent to: [--NbConvertApp.writer_class=StdoutWriter]
--inplace
    Run nbconvert in place, overwriting the existing notebook (only
            relevant when converting to notebook format)
    Equivalent to: [--NbConvertApp.use_output_suffix=False
--NbConvertApp.export_format=notebook --FilesWriter.build_directory=]
--clear-output
    Clear output of current file and save in place,
            overwriting the existing notebook.
    Equivalent to: [--NbConvertApp.use_output_suffix=False
--NbConvertApp.export_format=notebook --FilesWriter.build_directory=
--ClearOutputPreprocessor.enabled=True]
--no-prompt
   Exclude input and output prompts from converted document.
    Equivalent to: [--TemplateExporter.exclude_input_prompt=True
--TemplateExporter.exclude_output_prompt=True]
--no-input
    Exclude input cells and output prompts from converted document.
            This mode is ideal for generating code-free reports.
    Equivalent to: [--TemplateExporter.exclude_output_prompt=True
--TemplateExporter.exclude_input=True
--TemplateExporter.exclude_input_prompt=True]
```

```
--allow-chromium-download
    Whether to allow downloading chromium if no suitable version is found on the
system.
   Equivalent to: [--WebPDFExporter.allow_chromium_download=True]
--disable-chromium-sandbox
    Disable chromium security sandbox when converting to PDF..
    Equivalent to: [--WebPDFExporter.disable sandbox=True]
--show-input
   Shows code input. This flag is only useful for dejavu users.
   Equivalent to: [--TemplateExporter.exclude_input=False]
--embed-images
    Embed the images as base64 dataurls in the output. This flag is only useful
for the HTML/WebPDF/Slides exports.
    Equivalent to: [--HTMLExporter.embed_images=True]
--sanitize-html
    Whether the HTML in Markdown cells and cell outputs should be sanitized..
    Equivalent to: [--HTMLExporter.sanitize_html=True]
--log-level=<Enum>
    Set the log level by value or name.
    Choices: any of [0, 10, 20, 30, 40, 50, 'DEBUG', 'INFO', 'WARN', 'ERROR',
'CRITICAL']
   Default: 30
   Equivalent to: [--Application.log_level]
--config=<Unicode>
   Full path of a config file.
   Default: ''
   Equivalent to: [--JupyterApp.config_file]
--to=<Unicode>
    The export format to be used, either one of the built-in formats
            ['PDFviaHTML', 'asciidoc', 'custom', 'html', 'latex', 'markdown',
'notebook', 'pdf', 'pdfviahtml', 'python', 'rst', 'script', 'slides', 'webpdf']
            or a dotted object name that represents the import path for an
            ``Exporter`` class
   Default: ''
   Equivalent to: [--NbConvertApp.export_format]
--template=<Unicode>
   Name of the template to use
   Default: ''
    Equivalent to: [--TemplateExporter.template_name]
--template-file=<Unicode>
   Name of the template file to use
    Default: None
    Equivalent to: [--TemplateExporter.template_file]
--theme=<Unicode>
    Template specific theme(e.g. the name of a JupyterLab CSS theme distributed
    as prebuilt extension for the lab template)
   Default: 'light'
    Equivalent to: [--HTMLExporter.theme]
```

```
--sanitize_html=<Bool>
    Whether the HTML in Markdown cells and cell outputs should be sanitized. This
    should be set to True by nbviewer or similar tools.
    Default: False
    Equivalent to: [--HTMLExporter.sanitize html]
--writer=<DottedObjectName>
    Writer class used to write the
                                        results of the conversion
    Default: 'FilesWriter'
    Equivalent to: [--NbConvertApp.writer_class]
--post=<DottedOrNone>
    PostProcessor class used to write the
                                        results of the conversion
    Default: ''
    Equivalent to: [--NbConvertApp.postprocessor_class]
--output=<Unicode>
    overwrite base name use for output files.
                can only be used when converting one notebook at a time.
    Default: ''
    Equivalent to: [--NbConvertApp.output_base]
--output-dir=<Unicode>
    Directory to write output(s) to. Defaults
                                  to output to the directory of each notebook.
To recover
                                  previous default behaviour (outputting to the
current
                                  working directory) use . as the flag value.
    Default: ''
    Equivalent to: [--FilesWriter.build_directory]
--reveal-prefix=<Unicode>
    The URL prefix for reveal.js (version 3.x).
            This defaults to the reveal CDN, but can be any url pointing to a
сору
            of reveal.js.
            For speaker notes to work, this must be a relative path to a local
            copy of reveal.js: e.g., "reveal.js".
            If a relative path is given, it must be a subdirectory of the
            current directory (from which the server is run).
            See the usage documentation
            (https://nbconvert.readthedocs.io/en/latest/usage.html#reveal-js-
html-slideshow)
            for more details.
    Default: ''
    Equivalent to: [--SlidesExporter.reveal_url_prefix]
--nbformat=<Enum>
    The nbformat version to write.
            Use this to downgrade notebooks.
    Choices: any of [1, 2, 3, 4]
```

```
Default: 4
```

Equivalent to: [--NotebookExporter.nbformat_version]

Examples

The simplest way to use nbconvert is

> jupyter nbconvert mynotebook.ipynb --to html

Options include ['PDFviaHTML', 'asciidoc', 'custom', 'html', 'latex', 'markdown', 'notebook', 'pdf', 'pdfviahtml', 'python', 'rst', 'script', 'slides', 'webpdf'].

> jupyter nbconvert --to latex mynotebook.ipynb

 $\ensuremath{\mathtt{Both}}$ HTML and LaTeX support multiple output templates. LaTeX includes

'base', 'article' and 'report'. HTML includes 'basic', 'lab' and 'classic'. You can specify the flavor of the format used.

> jupyter nbconvert --to html --template lab mynotebook.ipynb

You can also pipe the output to stdout, rather than a file

> jupyter nbconvert mynotebook.ipynb --stdout

PDF is generated via latex

> jupyter nbconvert mynotebook.ipynb --to pdf

You can get (and serve) a Reveal.js-powered slideshow

> jupyter nbconvert myslides.ipynb --to slides --post serve

Multiple notebooks can be given at the command line in a couple of different ways:

- > jupyter nbconvert notebook*.ipynb
- > jupyter nbconvert notebook1.ipynb notebook2.ipynb

or you can specify the notebooks list in a config file, containing::

- c.NbConvertApp.notebooks = ["my_notebook.ipynb"]
- > jupyter nbconvert --config mycfg.py

To see all available configurables, use `--help-all`.