XAI 3: Model-agnostic methods

Exercise 5. Model-agnostic: Partial Dependency Plot (PDP)

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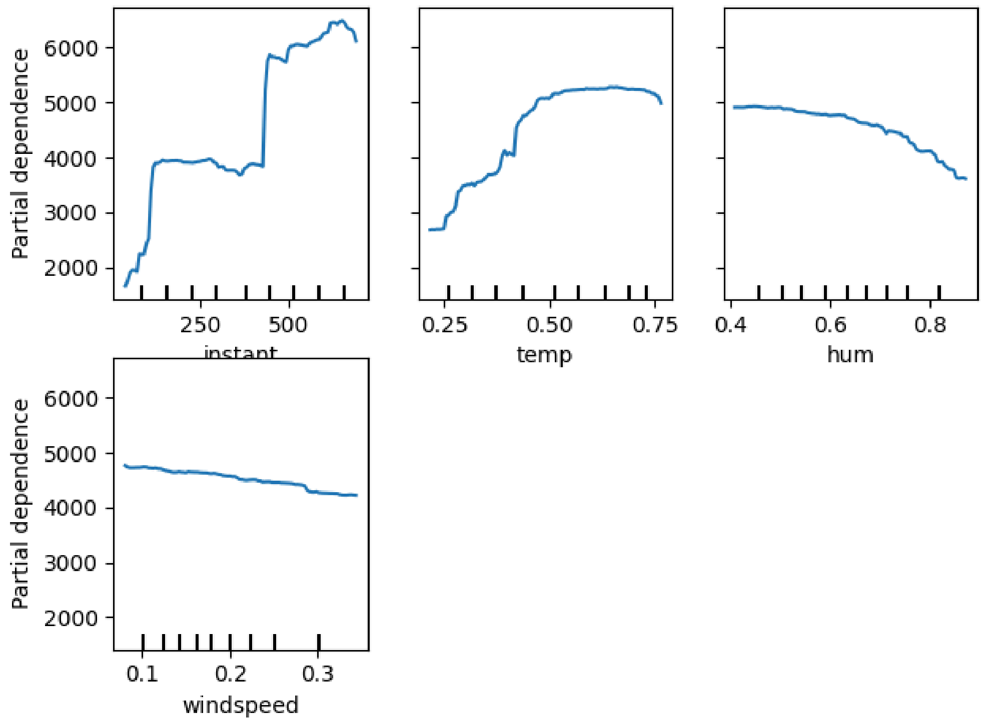
Evaluation, deployment and monitoring of models

Data Science Degree UPV

EXERCISE 1:

To analyze the influence of the variables “days since 2011,” temperature, humidity, and wind speed on the predicted number of bike rentals, we employed Partial Dependence Plots (PDPs) using a Random Forest Regressor trained on the day.csv dataset. The goal of these plots is to visualize how the model's predictions for bike rentals (cnt) change when each individual feature is varied while keeping all others fixed.



- Day:

The variable representing days since 2011 is instant, which corresponds to a sequential count of days from the start of the dataset (January 1st, 2011). The PDP for instant shows a noticeable upward trend in predicted bike counts as time progresses. This suggests that the usage of the bike-sharing system has steadily increased over time. This trend is likely attributable to factors such as increased user adoption, expansion of the service, greater public awareness, or enhancements in infrastructure. The sharp rise observed around mid-range values could indicate specific milestones, such as marketing campaigns, service expansions, or seasonal effects becoming more prominent in later years.

- Temperature:

Regarding temperature (temp), the partial dependence plot reveals a strong positive relationship with bike rentals. As temperature increases, the predicted number of bike rentals rises sharply, particularly between normalized values of approximately 0.3 and 0.6. This aligns with real-world behavior: people are more likely to use bicycles in comfortable weather conditions. After a certain threshold (around 0.6–0.7), the increase levels off, indicating a saturation point where higher temperatures no longer contribute significantly to further increases in demand. This plateau might reflect a thermal comfort limit beyond which usage does not continue to grow—or could even slightly decline if excessively hot temperatures were included in the dataset (though they may not be, given the normalized scale).

- Humidity:

Humidity (hum) displays a clear negative relationship with bike rental predictions. As humidity rises from 0.4 to 0.8, the model predicts fewer rentals. This is intuitive, as high humidity often corresponds to unpleasant or rainy conditions, which typically discourage outdoor activity and bike usage. The downward slope is gradual but consistent, indicating that the impact of humidity is steady and meaningful, though perhaps not as sharp as that of temperature.

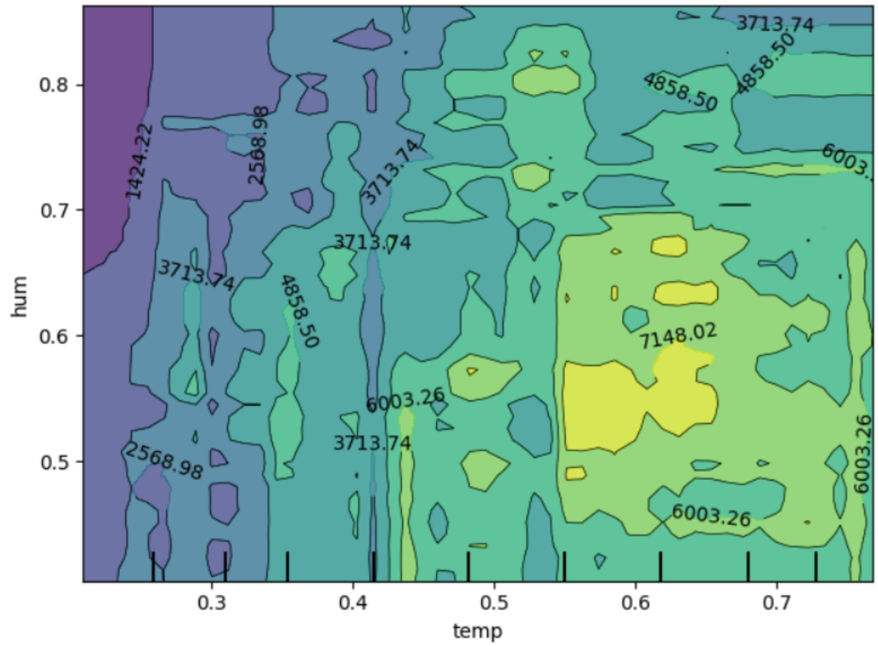
- Wind speed:

Wind speed (windspeed) also exhibits a negative effect, though less pronounced. As wind speed increases, there is a slight but persistent decrease in predicted bike counts. This subtle effect suggests that while wind is not the most influential factor, it still contributes to lower demand. This is reasonable, as strong winds can make cycling physically uncomfortable or unsafe, leading some users to opt for other modes of transport.

In summary, the PDPs demonstrate that temperature has the most substantial positive impact on bike rental predictions, while humidity and wind speed both negatively influence demand, with humidity having a stronger effect. Time (as represented by instant) also shows a significant positive trend, reflecting the growing use of the bike-sharing system over the period covered by the dataset. These insights are coherent with expectations and validate that the model is capturing meaningful real-world behavior patterns.

EXERCISE 2:

The two-dimensional Partial Dependence Plot (PDP) generated with temp (temperature) and hum (humidity) allows us to examine how these two features, considered jointly, influence the model's predictions of bike rental counts (cnt). The contour map displays the predicted values across a grid of temperature and humidity values. The color scale progresses from darker shades (lower predictions) to lighter and yellow tones (higher predicted counts).



A prominent high-prediction region can be seen in the central-right area of the plot, where temperature ranges between approximately 0.55 and 0.7, and humidity lies around 0.5 to 0.6. This region forms a clear "hot spot" in the graph, where the predicted number of rentals is above 7000 in some zones. This suggests that the model has learned that bike usage is highest when temperatures are warm but not extreme, and when the humidity is comfortable. These conditions likely correspond to pleasant spring or early summer days, when outdoor cycling is most appealing.

In contrast, the upper-left region of the plot, where humidity exceeds 0.75, is consistently associated with low rental predictions, even when temperatures are moderate. This area appears in dark blue and purple shades, with predicted values below 3000. This indicates that high humidity significantly suppresses demand, likely due to user discomfort or increased chance of rain. The model clearly interprets highly humid conditions as unfavorable for bike usage.

Another low-prediction area is visible in the lower-left corner, where temperature is below 0.35 and humidity is above 0.6. These are cold and damp conditions that naturally discourage cycling. The model reflects this by predicting minimal rental activity in this region.

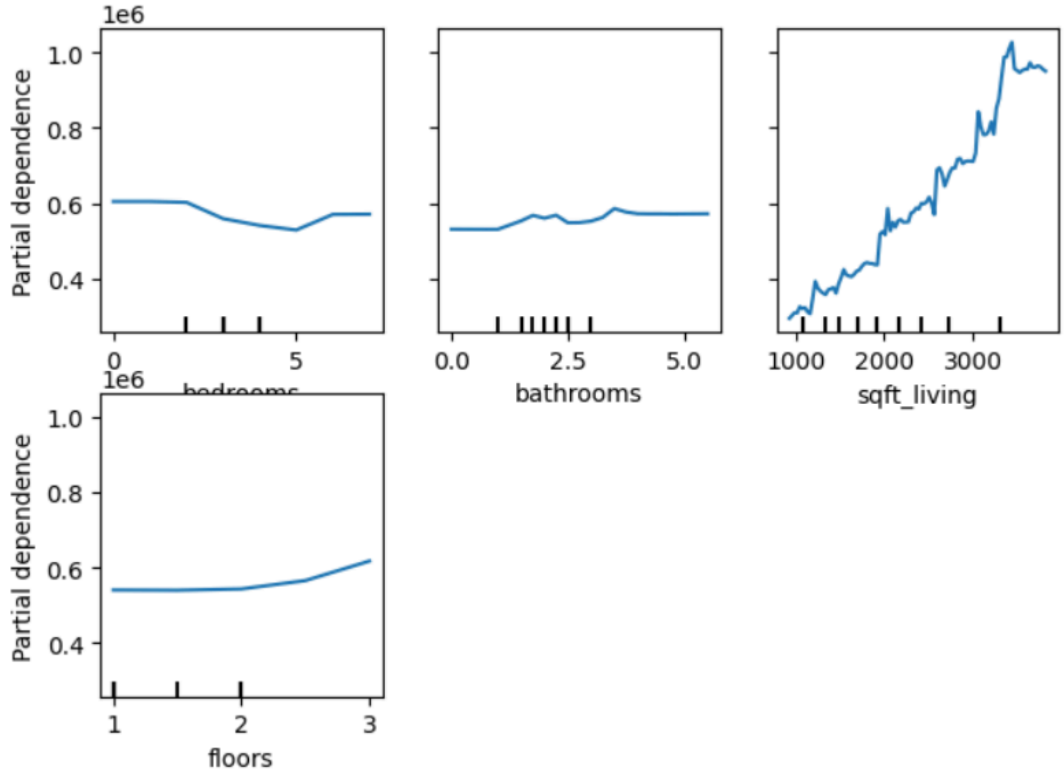
The distribution of values and the contour transitions in the plot suggest that the model has captured a non-linear and interactive relationship between these two variables. The effect of increasing temperature on rental counts is not uniform across humidity levels. For instance, while higher temperatures generally lead to increased predictions, this effect is much less pronounced (or even negligible) when humidity is too high. In other words, the influence of temperature is conditional upon humidity being within a certain comfortable range.

It is also worth noting that the contours are not perfectly smooth, and some areas show abrupt changes. This could be due to the use of a limited sample (as required by the exercise) or a relatively coarse grid resolution. However, the overall trend is clear and consistent with expectations based on human behavior and weather conditions.

In conclusion, the PDP reveals that the optimal conditions for bike rental demand are those with moderate to high temperatures combined with moderate humidity. Both low temperatures and high humidity suppress demand significantly, and the interaction between these two variables is essential to understanding user behavior. The model reflects these patterns well, demonstrating its ability to capture realistic, context-dependent relationships between features and the target variable.

EXERCISE 3:

The Partial Dependence Plots (PDPs) below display how the features bedrooms, bathrooms, sqft_living, and floors influence the model's predictions of house prices (price) in the kc_house_data.csv dataset. These visualizations help us understand the learned relationships between each individual variable and the predicted outcome, while holding all other features constant.



The most significant pattern appears in the PDP for sqft_living. The graph shows a strong and consistent positive relationship: as the square footage of the house increases, the predicted price rises sharply. This result is highly intuitive and expected — larger homes tend to be more expensive, and the model reflects this trend with a near-linear increase that steepens beyond roughly 2000–2500 square feet. The steep slope of the curve indicates that sqft_living is one of the most influential features in the model.

In contrast, the PDP for bedrooms suggests a very limited and mostly flat influence on price. While there is a slight dip in predicted value as the number of bedrooms increases from 3 to 5, the changes are small and non-linear, implying that the number of bedrooms alone does not have a strong or direct impact on the price when controlling for other factors such as size or bathrooms. This could be due to the fact that bedrooms is often correlated with sqft_living, which captures the effect more clearly.

The bathrooms feature shows a slightly positive but weak influence on price. There is a modest increase in predicted value around 2–3 bathrooms, after which the effect plateaus. This suggests that having more than two bathrooms may provide some added value, but additional bathrooms beyond that do not significantly increase the price in the model's estimation.

The PDP for floors indicates a small upward trend in predicted price as the number of floors increases. Homes with more floors tend to have slightly higher predicted values, particularly when going from one to two floors. However, the effect is relatively minor compared to sqft_living. The curve is smooth and stable, suggesting the model recognizes a real, but limited, relationship.

In conclusion, the PDPs confirm that sqft_living is by far the most influential of the four variables examined, showing a strong and consistent impact on house prices. The other features (bedrooms, bathrooms, and floors) contribute to a lesser extent and show weaker or flatter trends. This aligns well with real-world expectations, where the size of a property is typically the most important determinant of its market value.