

Exploring Tools for Interpretable Machine Learning

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PyData Global 2021

Outline

Introduction

Data Set

Models Fit

Model Explainability

- Model Specific

 - Beta Coefficients and Weight Effects

 - Tree ensembles

- Model Agnostic

 - PDP and ICE Plots

 - Permutation Importance

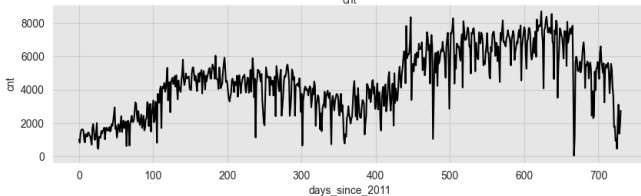
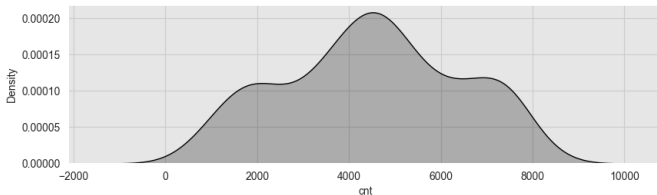
 - SHAP

References

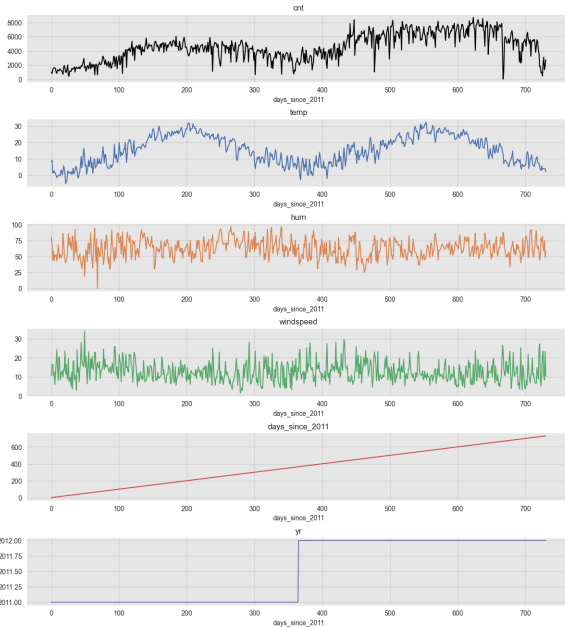
Target Variable - cnt: Daily Bike Rents

	season	yr	mnth	holiday	weekday	workingday	weathersit	temp	hum	windspeed	cnt	days_since_2011
0	SPRING	2011	JAN	NO HOLIDAY	SAT	NO WORKING DAY	MISTY	8.175849	80.5833	10.749882	985	0
1	SPRING	2011	JAN	NO HOLIDAY	SUN	NO WORKING DAY	MISTY	9.083466	69.6087	16.652113	801	1
2	SPRING	2011	JAN	NO HOLIDAY	MON	WORKING DAY	GOOD	1.229108	43.7273	16.636703	1349	2
3	SPRING	2011	JAN	NO HOLIDAY	TUE	WORKING DAY	GOOD	1.400000	59.0435	10.739832	1562	3
4	SPRING	2011	JAN	NO HOLIDAY	WED	WORKING DAY	GOOD	2.666979	43.6957	12.522300	1600	4

cnt: Target Variable

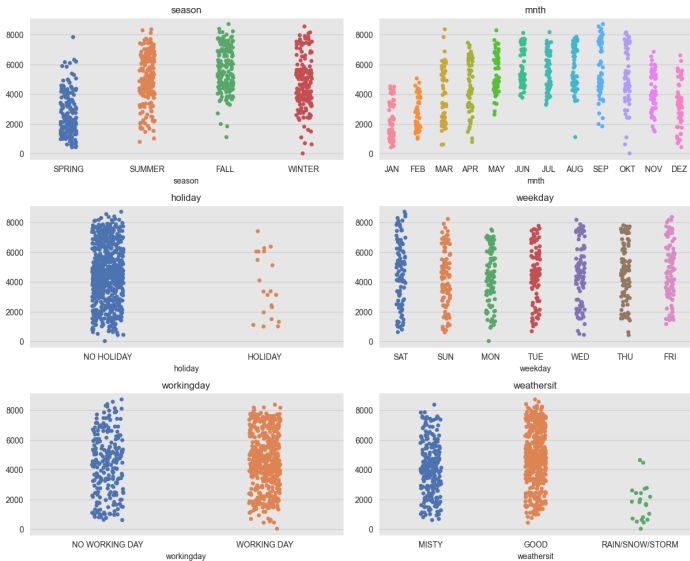


Continuous Regressors

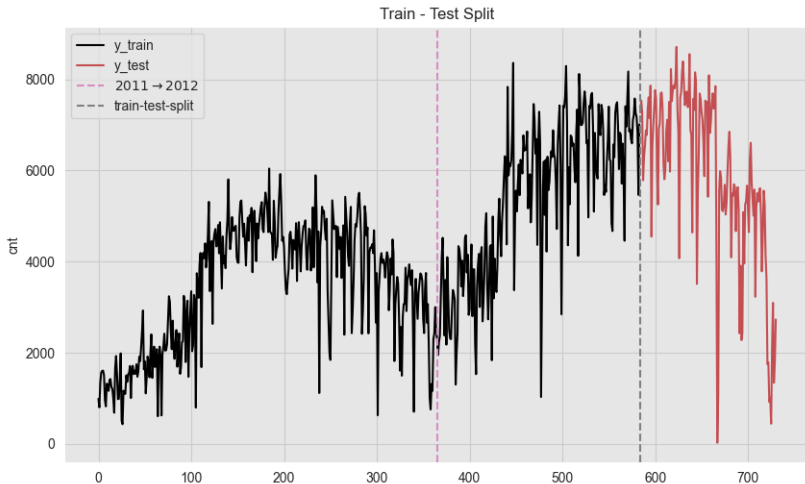


Categorical Regressors

cnt distribution over categorical_features

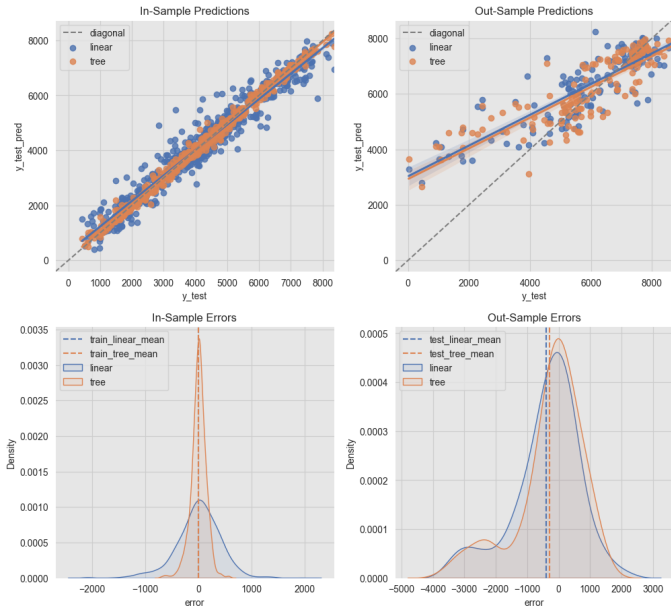


Train-Test Split

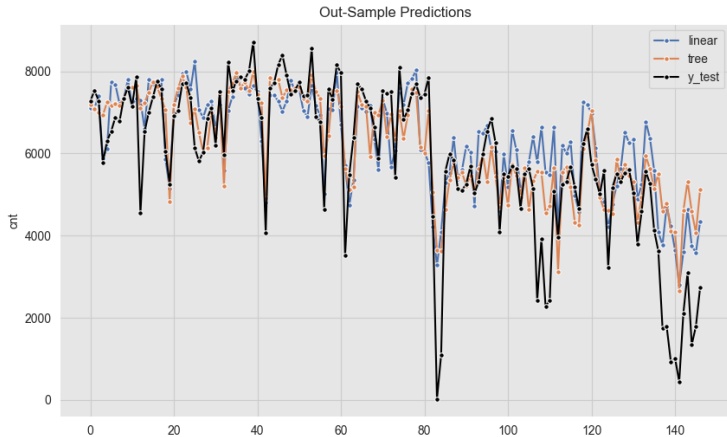


Models

Out of sample performance - Errors Distribution



Out of sample performance - Predictions



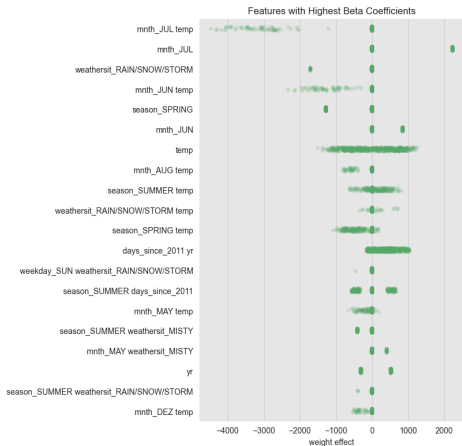
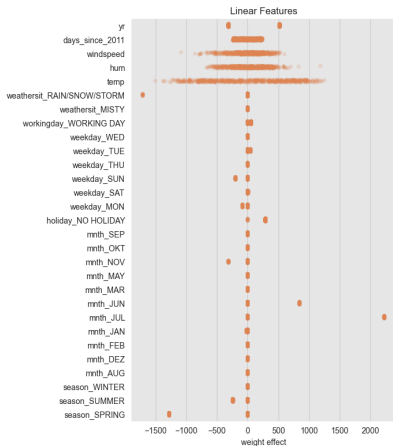
β coefficients

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \varepsilon, \quad \text{where } \varepsilon \sim N(0, \sigma^2)$$

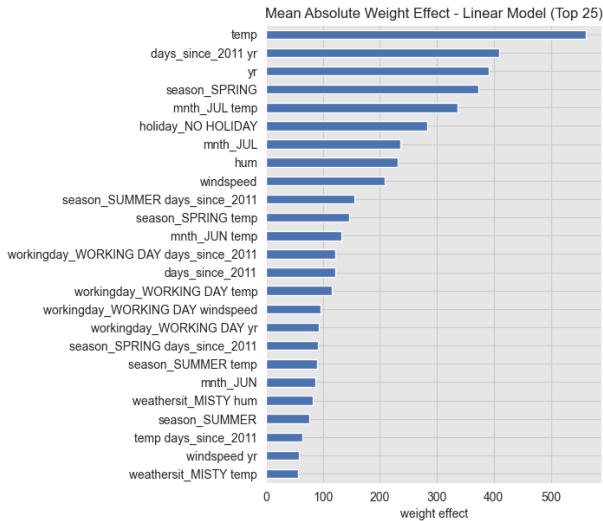
	linear_features	coef_	abs_coef_
0	mnth_JUL temp	-2305.096894	2305.096894
1	mnth_JUL	2227.672335	2227.672335
2	weathersit_RAIN/SNOW/STORM	-1710.469071	1710.469071
3	mnth_JUN temp	-1299.644413	1299.644413
4	season_SPRING	-1279.629779	1279.629779
5	mnth_JUN	845.229031	845.229031
6	temp	646.609622	646.609622
7	mnth_AUG temp	-523.011653	523.011653
8	season_SUMMER temp	489.319256	489.319256
9	weathersit_RAIN/SNOW/STORM temp	-482.660271	482.660271
10	season_SPRING temp	465.512410	465.512410
11	days_since_2011 yr	465.079169	465.079169
12	weekday_SUN weathersit_RAIN/SNOW/STORM	-462.286059	462.286059
13	season_SUMMER days_since_2011	454.137278	454.137278
14	mnth_MAY temp	-445.268148	445.268148
15	season_SUMMER weathersit_MISTY	-408.809531	408.809531
16	mnth_MAY weathersit_MISTY	404.790954	404.790954
17	yr	403.199142	403.199142
18	season_SUMMER weathersit_RAIN/SNOW/STORM	-394.157306	394.157306
19	mnth_DEZ temp	363.222114	363.222114

Weight Effects $\beta_i x_i$

Effect Weight Distribution



Weight Effects Importance $w_i = \frac{1}{n} \sum_{i=1}^n |\beta_i x_i|$



Weight Effects: Temperature (z-transform)

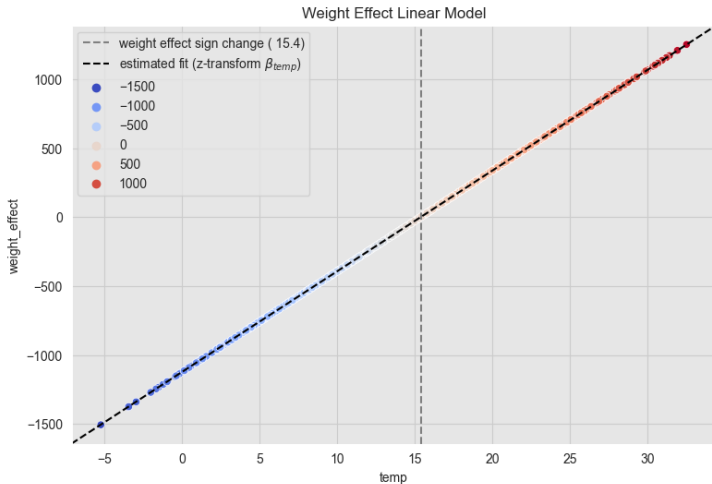


Figure: This plot just shows the effect of the linear term *temp* and not the interactions.

Weight Effects: Interactions

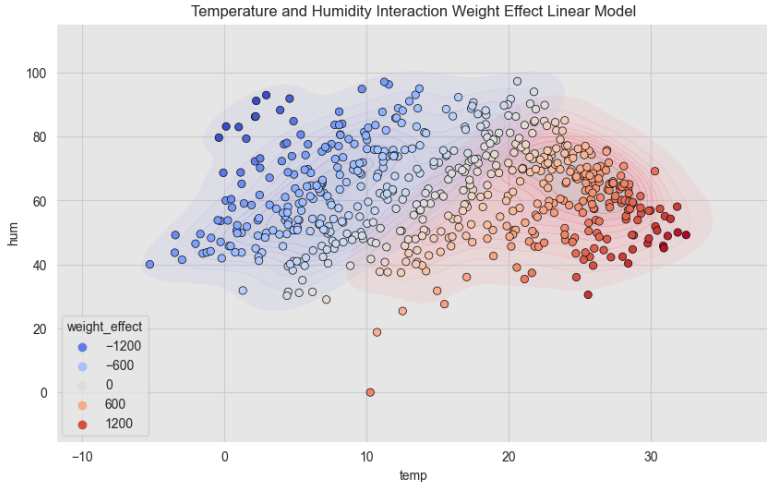
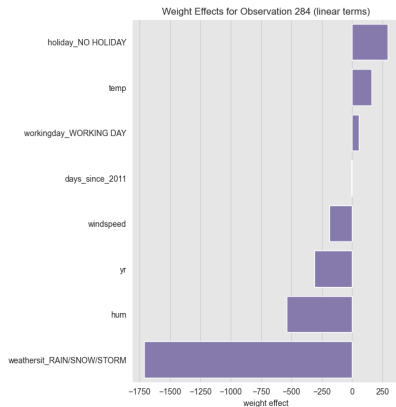
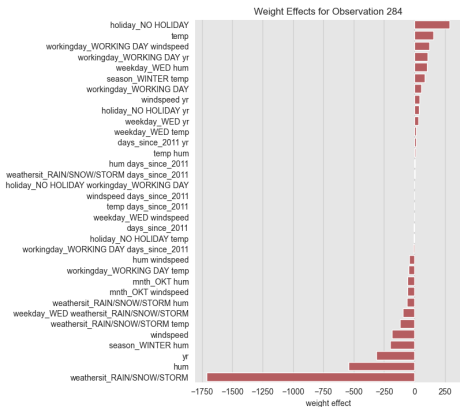
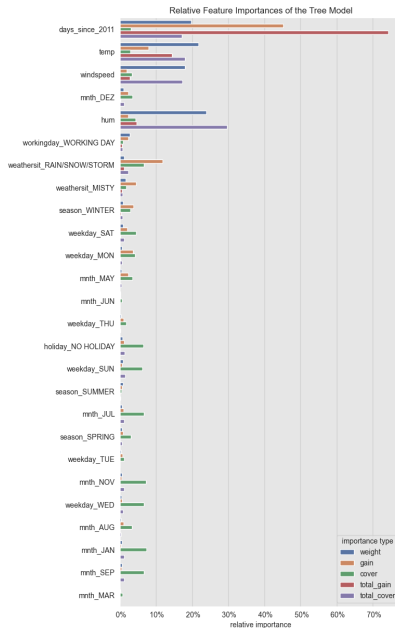


Figure: We can visualize the interaction between *temp* and *hum* by computing the total weight effect as $\beta_{temp}x_{temp} + \beta_{hum}x_{hum} + \beta_{temp \times hum}x_{temp}x_{hum}$.

Explaining Individual Predictions



Feature Importance Metrics: XGBoost



Partial Dependence Plot (PDP) & Individual Conditional Expectation (ICE) ([1, Section 5.1])

- ▶ Let x_S be the features for which the partial dependence function should be plotted and x_C be other features used in the machine learning model. One can estimate the *dependence function* as

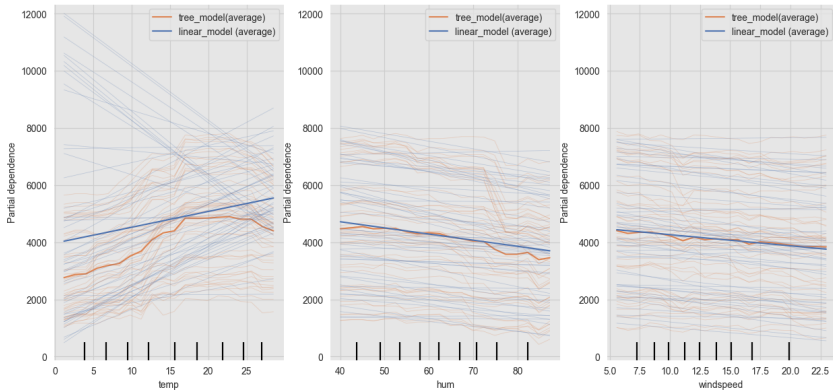
$$\hat{f}_{x_S}(x_S) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_S, x_C^i)$$

where \hat{f} is the model prediction function, x_C^i are actual feature values (not in S) and n is the number points.

- ▶ Similar to a PDP, an individual conditional expectation (ICE) plot shows one line per instance. That is, for each instance in $\{(x_S^i, x_C^i)\}_{i=1}^n$, we plot \hat{f}_S as a function of x_S^i while leaving x_C^i fixed.

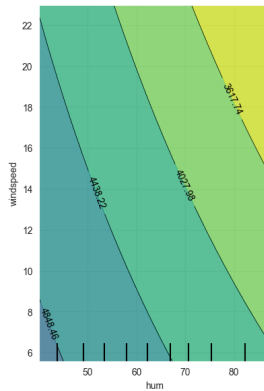
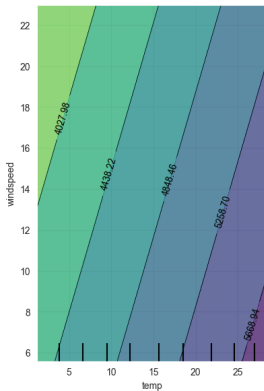
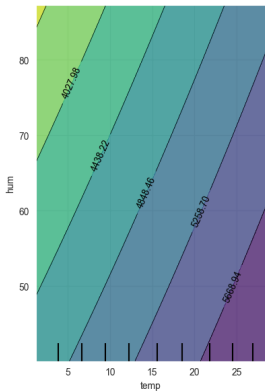
PDP & ICE Examples (1D)

Single ICE Plot



PDP & ICE Examples (2D)

Pair ICE Plot - Linear Model



	linear_features	coef_	abs_coef_
6	temp	646.609622	646.609622
29	hum	-281.701209	281.701209
32	windspeed	-264.190697	264.190697
114	hum windspeed	-31.993914	31.993914
130	temp hum	15.127133	15.127133
155	temp windspeed	-0.000000	0.000000

Permutation Importance

Measures the increase in the prediction error of the model after we permuted the feature's values, which breaks the relationship between the feature and the true outcome ([1, Section 5.5]).

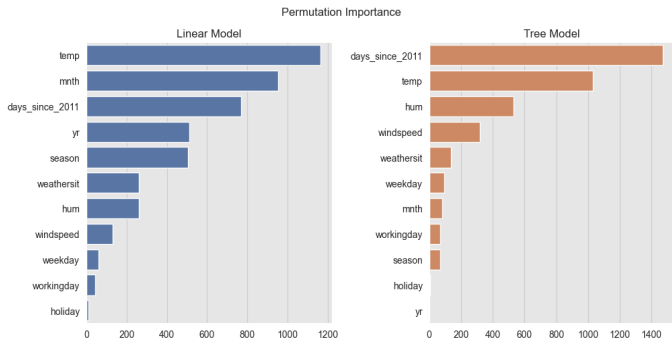


Figure: The permutation importance for these two models have *days_since_2011* and *temp* on their top 3 ranking, which partially explain the trend and seasonality components respectively (see [1, Figure 5.30]).

References I

[1] Christoph Molnar.

Interpretable Machine Learning.

2019.

<https://christophm.github.io/interpretable-ml-book/>.

Thank You!

Contact

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