Exploring Tools for Interpretable Machine Learning

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PyData Global 2021

Outline

Introduction

Aim and Scope of the Talk

What? In this talk we want to test various ways of getting a better understanding on how machine learning (ML) models generate predictions and how features interact with each other. This is in general not straight forward and key components are

- Domain knowledge on the problem.
- Understanding on the input data.
- Understanding the logic behind the ML algorithms.

How? We are going to wor out a concrete example.

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- Understanding the logic behind the ML algorithms.

How? We are going to wor out a concrete example.

References

This talk is based on this blog post ([3]), which itself is based on these two amazing references:

- Interpretable Machine Learning, A Guide for Making Black Box Models Explainable by Christoph Molnar
- Interpretable Machine Learning with Python by Serg Masís

Interpretable ML $\neq$ Causality

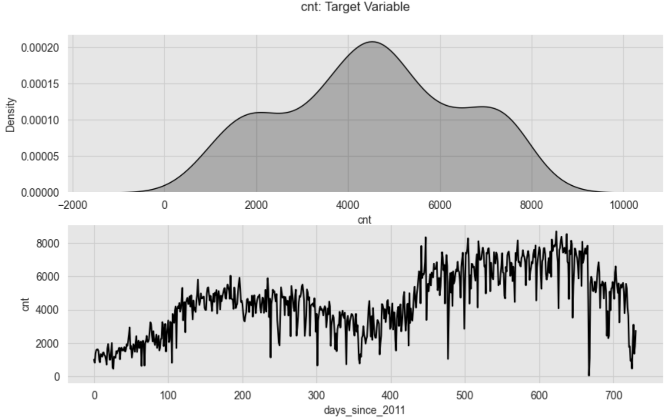
Note that the methods discussed in this notebook are not related with causality.

References

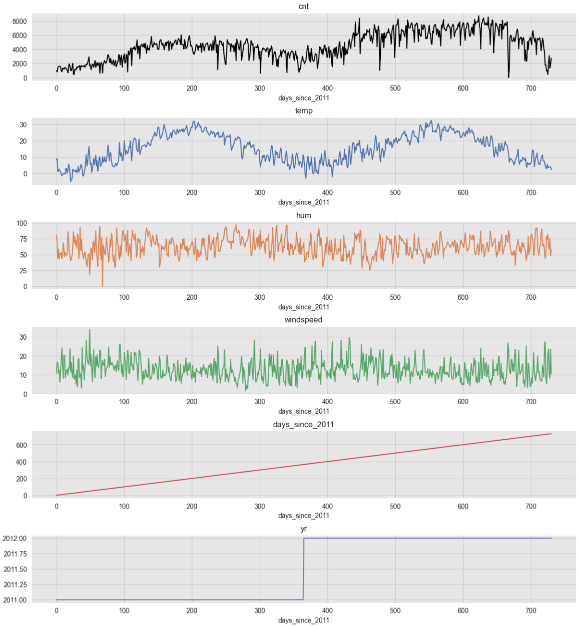
- Be Careful When Interpreting Predictive Models in Search of Causal Insights by Scott Lundberg(one of the core developers of SHAP)
- Statistical Rethinking, A Bayesian Course with Examples in R and Stan by Richard McElreath
- Causal Inference: The Mixtape by Scott Cunningham

Target Variable - cnt: Daily Bike Rents

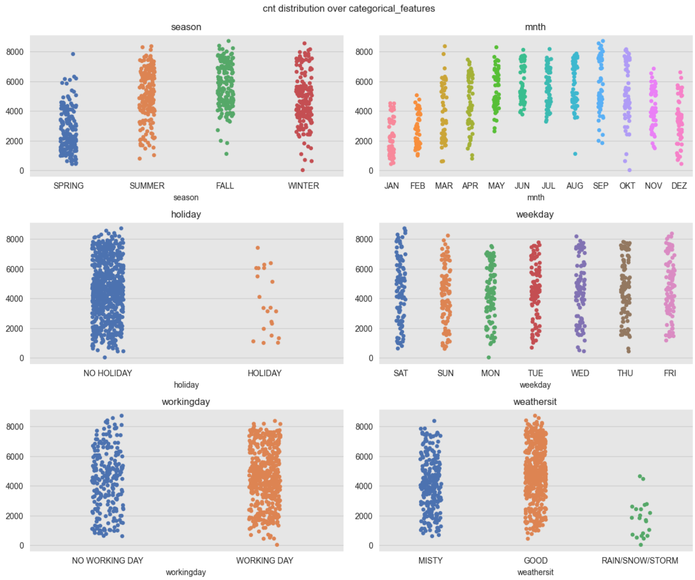
	season	yr	mnth	holiday	weekday	workingday	weathersit	temp	hum	windspeed	cnt	days_since_2011
0	SPRING	2011	JAN	NO HOLIDAY	SAT	NO WORKING DAY	MISTY	8.175849	80.5833	10.749882	985	0
1	SPRING	2011	JAN	NO HOLIDAY	SUN	NO WORKING DAY	MISTY	9.083466	69.6087	16.652113	801	1
2	SPRING	2011	JAN	NO HOLIDAY	MON	WORKING 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



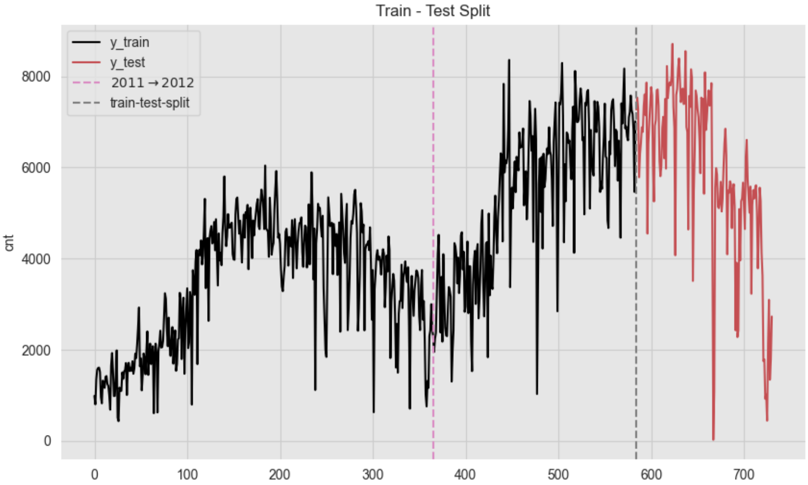
Continuous Regressors



Categorical Regressors



Train-Test Split



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Models

Two model flavours

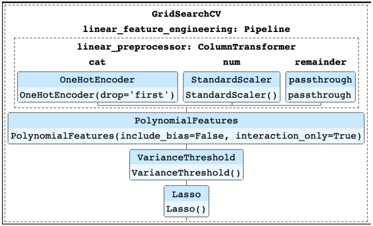


Figure: Lasso model with second order polynomial interactions.

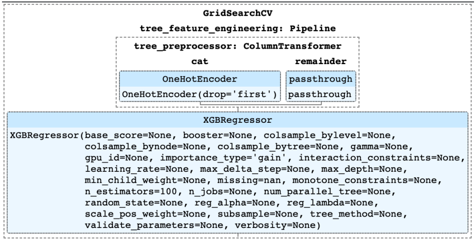
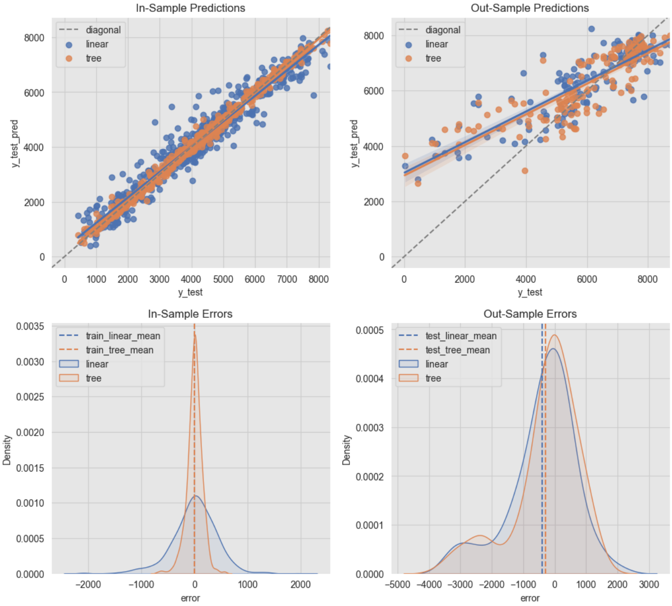
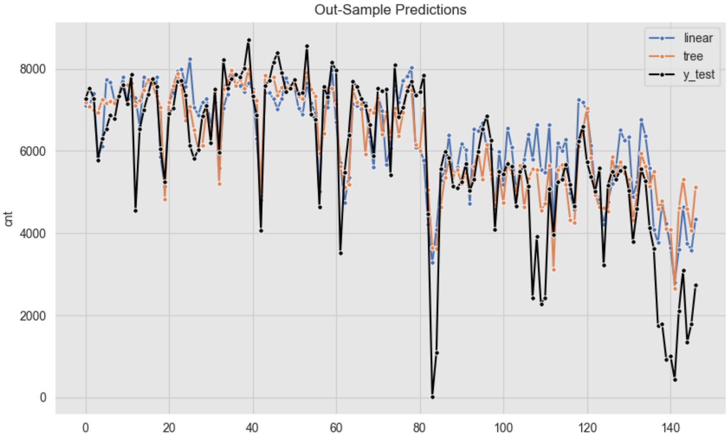


Figure: XGBoost regression model.

Out of sample performance - Erros Distribution



Out of sample performance - Predictions



β coeffiecients

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

	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 $\beta_i x_i$

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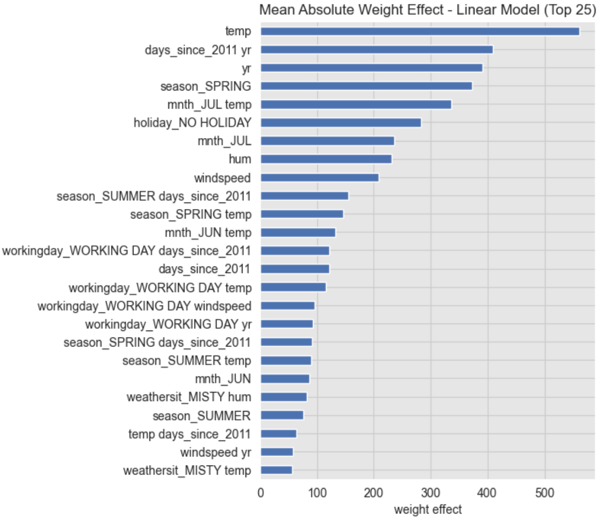
Weight Effects Importance $w_i = \frac{1}{n}\sum_{i=1}^{n} |\beta_i x_i|$



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Weight Effects: Temperature (z-transform)

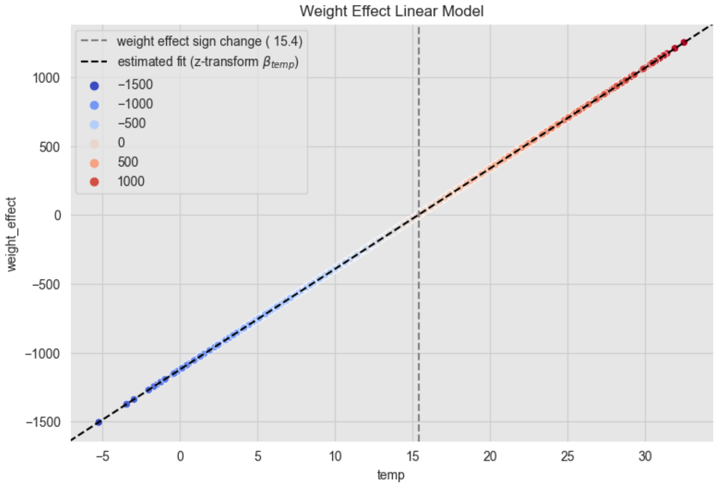


Figure: This plot just shows the effect of the linear term *temp* and not the interactions.

Weight Effects: Interatctions

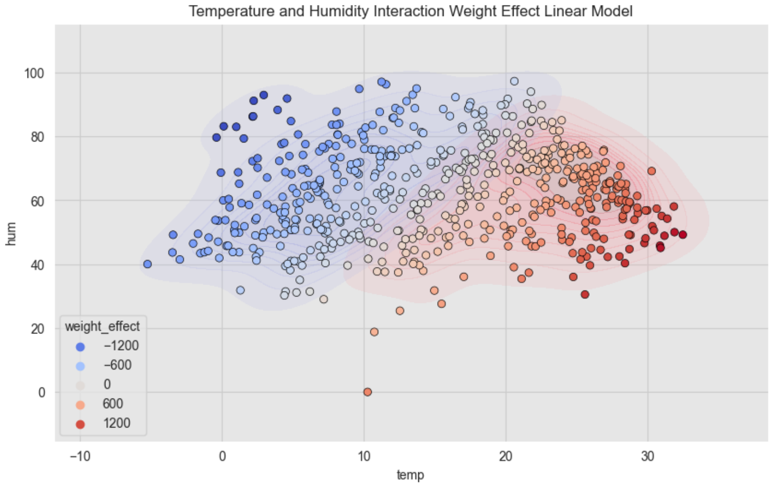
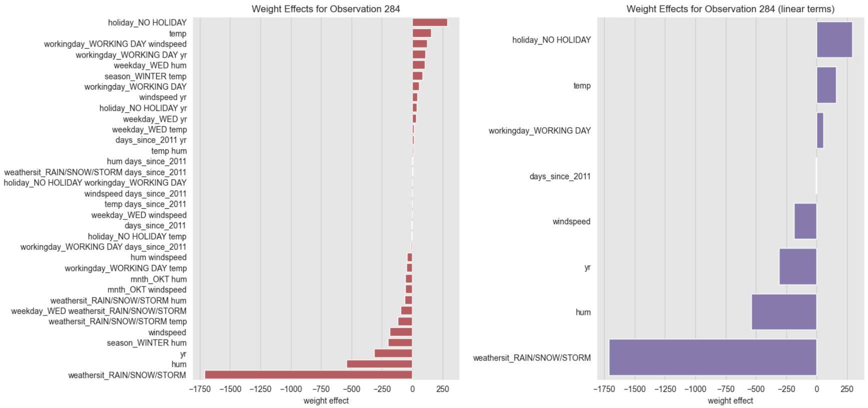
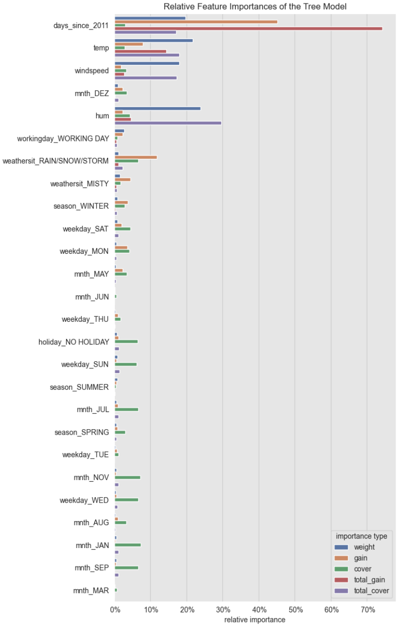


Figure: We can visualize the interaction between *temp* and *hum* by computing the total weight effect as $\beta_{temp}x_{temp} + \beta_{hum}x_{hum} + \beta_{temp\times hum}x_{temp}x_{hum}$.

Explaining Individual Predictions



Feature Importance Metrics: XGBoost



Partial Dependence Plot (PDP) & Individual Conditional Expectation (ICE) ([2, 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.

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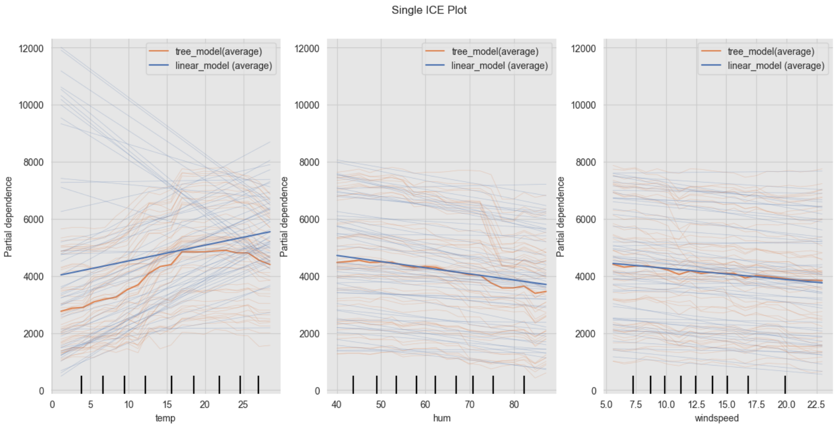
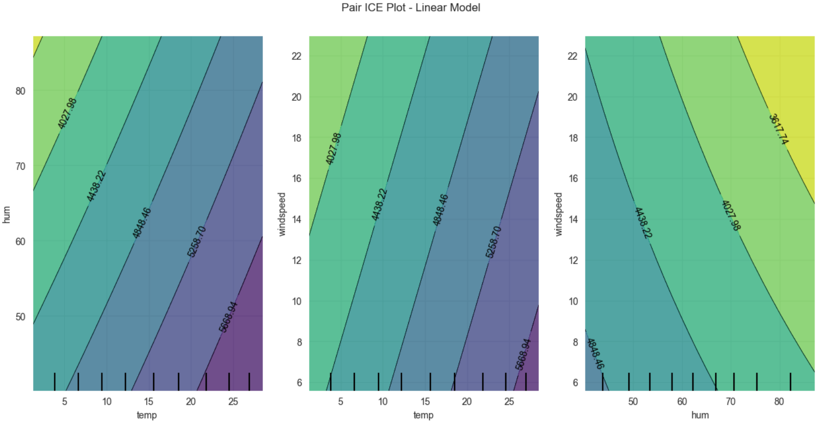
PDP & ICE Examples (1D)



PDP & ICE Examples (2D)



	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 ([2, Section 5.6]).

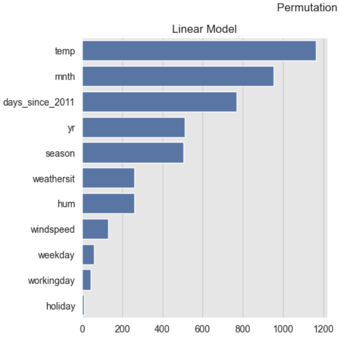


Figure: The permutation importance for these two models have *days_since_2011* and *temp* on their top 3 ranking, which partially explain the trend and seasonality components respectively (see [2, Figure 5.32]).

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SAHP Values

Definition

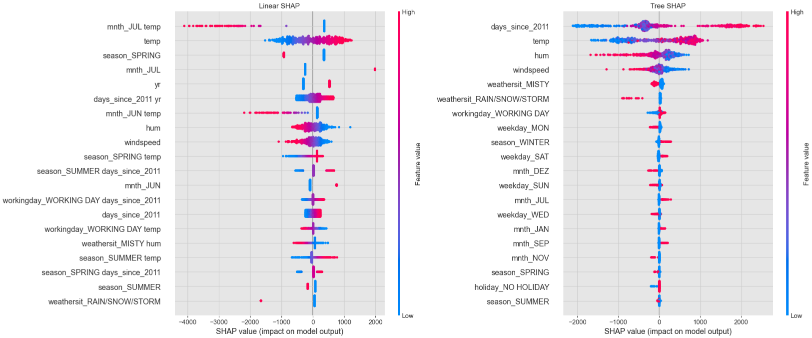
For each data instance x

- Sample coalitions $z'_k \in \{0, 1\}^M$, where M, is the maximum coalition size.
- Get prediction for each z'_k. For features not in the coalition we replace their values with random samples from the dataset (background data).
- Compute the weight for each z'_k, with the SHAP kernel,

$$\pi_x(z') = \frac{(M-1)}{\binom{M}{|z'|}|z'|(M-|z'|)}$$

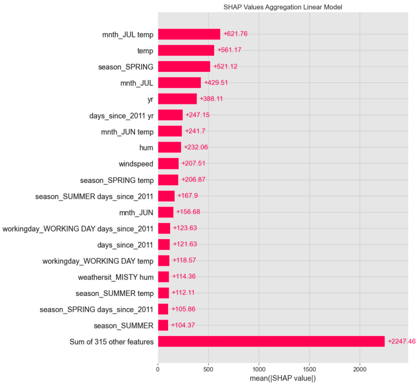
- Fit weighted linear model.
- Return Shapley values, i.e. the coefficients from the linear model.

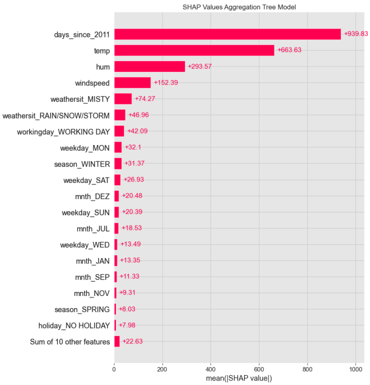
SHAP Values



Linear SHAP
mnth_JUL temp
temp
season_SPRING
mnth_JUL
yr
days_since_2011 yr
mnth_JUN temp
hum
windspeed
season_SPRING temp
season_SUMMER days_since_2011
mnth_JUN
workingday_WORKING DAY days_since_2011
days_since_2011
workingday_WORKING DAY temp
weathersit_MISTY hum
season_SUMMER temp
season_SPRING days_since_2011
season_SUMMER
weathersit_RAIN/SNOW/STORM
−4000 −3000 −2000 −1000 0 1000 2000
SHAP value (impact on model output)
High
Feature value
Low
Tree SHAP
days_since_2011
temp
hum
windspeed
weathersit_MISTY
weathersit_RAIN/SNOW/STORM
workingday_WORKING DAY
weekday_MON
season_WINTER
weekday_SAT
mnth_DEZ
weekday_SUN
mnth_JUL
weekday_WED
mnth_JAN
mnth_SEP
mnth_NOV
season_SPRING
holiday_NO HOLIDAY
season_SUMMER
−2000 −1000 0 1000 2000
SHAP value (impact on model output)
High
Feature value
Low

Mean Abs SHAP Values





SHAP Values: Temperature

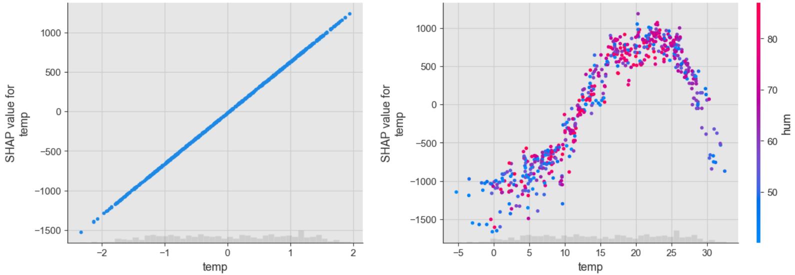


Figure: ...

SHAP Values: Observation 284

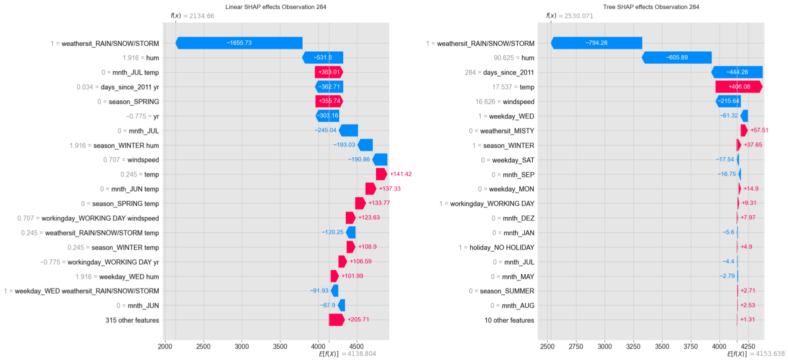


Figure: ...

References I

[1] Serg Masís.
Interpretable Machine Learning with Python.
Packrat, 2021.
https://github.com/PacktPublishing/Interpretable-Machine-Learning-with-Python.

[2] Christoph Molnar.
Interpretable Machine Learning.
2019.
https://christophm.github.io/interpretable-ml-book/.

[3] Juan Orduz.
Exploring tools for interpretable machine learning.
https://juanitorduz.github.io/interpretable_ml/, Jul 2021.

Thank You!

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