
Limitations of Interpretable Machine Learning Methods



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Preface

This book explains limitations of current methods in interpretable machine learning. The methods include partial dependence plots (PDP), Accumulated Local Effects (ALE), permutation feature importance, leave-one-covariate out (LOCO) and local interpretable model-agnostic explanations (LIME). All of those methods can be used to explain the behavior and predictions of trained machine learning models. But the interpretation methods might not work well in the following cases:

- if a model models interactions (e.g. when a random forest is used)
- if features strongly correlate with each other
- if the model does not correctly model causal relationships
- if parameters of the interpretation method are not set correctly

This book is the outcome of the seminar “Limitations of Interpretable Machine Learning” which took place in summer 2019 at the Department of Statistics, LMU Munich.

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Foreword

Author: Christoph Molnar

This book is the result of an experiment in university teaching. Each semester, students of the Statistics Master can choose from a selection of seminar topics. Usually, every student in the seminar chooses a scientific paper, gives a talk about the paper and summarizes it in the form of a seminar paper. The supervisors help the students, they listen to the talks, read the seminar papers, grade the work and then ... hide the seminar papers away in (digital) drawers. This seemed wasteful to us, given the huge amount of effort the students usually invest in seminars. An idea was born: Why not create a book with a website as the outcome of the seminar? Something that will last at least a few years after the end of the semester. In the summer term 2019, some Statistics Master students signed up for our seminar entitled “Limitations of Interpretable Machine Learning”. When they came to the kick-off meeting, they had no idea that they would write a book by the end of the semester.

We were bound by the examination rules for conducting the seminar, but otherwise we could deviate from the traditional format. We deviated in several ways:

1. Each student project is part of a book, and not an isolated seminar paper.
2. We gave challenges to the students, instead of papers. The challenge was to investigate a specific limitation of interpretable machine learning methods.
3. We designed the work to live beyond the seminar.
4. We emphasized collaboration. Students wrote some chapters in teams and reviewed each others texts.

Looking back, the seminar was a lot of fun and – from our perspective – successful. Especially considering that it was an experiment. Everyone was highly motivated and we got great feedback from the students that they liked the format. For the students it was a more work than a traditional seminar. But in the end, our hope is that their effort will pay off for them as well, not only because of their increased visibility. It was also more work for us supervisors. But the extra effort was worth it, since limitations of interpretability are relevant for our research. For me the seminar was an inspiration. The students had

new ideas and new perspectives to approach the limitations of interpretable machine learning.

Technical Setup

The book chapters are written in the Markdown language. The simulations, data examples and visualizations were created with R ([R Core Team, 2018](#)). To combine R-code and Markdown, we used rmarkdown. The book was compiled with the bookdown package. We collaborated using git and github. For details, head over to the book's repository³.

³https://github.com/compstat-lmu/iml_methods_limitations

1

Introduction

Author: Emanuel Renkl

Supervisor: Christoph Molnar

1.1 Statistical Modeling: The Two Approaches

In statistics, there are two approaches to reach conclusions from data (see Breiman (2001b)). First, the data modeling approach, where one assumes that the data are generated by a given stochastic data model. More specifically, a proposed model associates the input variables, random noise and parameters with the response variables. Typical models are for instance the linear and logistic regression model. These models allow to predict what the responses are going to be to future input variables and give information on how the response variables and input variables are associated, i.e. they are interpretable. Second, the algorithmic modeling approach that uses algorithmic models and treats the underlying data mechanism as unknown. More precisely, the goal is to find an algorithm that operates on the input variables to predict the response variables. Algorithms that are used are for instance random forests and neural nets. These algorithms allow to predict what the responses are going to be to future input variables, but do not give information on how the response variables and input variables are associated. Put differently, these algorithms produce black box models, because they do not provide any direct explanation for their predictions, i.e. they are not interpretable.

Within the statistics community, the data modeling approach was prevalently dominant for a long time (Breiman (2001b)). However, especially in the last decade the increasing availability of enormous amounts of complex and unstructured data as well as the increase in processing power of computers served as a breeding ground for a strong shift to the algorithmic modeling approach, primarily for two reasons.

First, the data modeling approach is not applicable to exciting problems like text, speech and image recognition (Breiman (2001b)). Second, for complex prediction problems new algorithms such as random forests and neural nets

outperform classical models in prediction accuracy as they can model complex relationships in the data (Breiman (2001b)). For these reasons, more and more researchers switched from the data modeling approach to the algorithmic modeling approach that is much more common under the name machine learning.

But what about interpretability? As we learned in the first paragraph machine learning algorithms are black box models that do not provide any direct explanation for their predictions. Hence, the question arises whether we need to know why an algorithm makes a certain prediction? To get a better feeling for this question, it's helpful to understand how algorithms learn to make predictions and for which tasks machine learning is used.

1.2 Importance of Interpretability

Algorithms learn to make predictions from training data. Thus, algorithms also pick up biases of the training data and hence may not be robust under certain circumstances, e.g. they perform well on a test set, but not in the real world. Such behavior can lead to undesired outcomes.

For instance, consider a simple husky versus wolf classifier that misclassifies some huskies as wolves (see Ribeiro et al. (2016b)). Since the machine learning model does not give any information on how the response and input variables are associated, we do not know why it classified a husky as a wolf. However, interpretability might be useful to debug the algorithm and see if this problem is persistent or not. Using methods that make machine learning algorithms interpretable and that we will discuss later in the book, we would find that the misclassification was due to the snow on the image. The algorithm learned to use snow as a feature for classifying images as wolves. This might make sense in the training dataset, but not in the real world. Thus, in this example interpretability helps us to understand how the algorithm gets to the result and hence, we know in which cases the robustness of the algorithm is not given. In the following, we want to derive the importance of interpretability by focusing on academic and industrial settings.

Broadly speaking in academia machine learning is used to draw conclusions from data. However, off the shelf machine learning algorithms only give predictions without explanations. Thus, they answer only the “what”, but not the “why” of a certain question and hence, do not allow for actual scientific findings. Especially, in areas such as life sciences and social sciences, that aim to identify causal relationships between input and response variables interpretability is key to scientific discoveries.

For example, in a medical study researchers applying machine learning found

that patients with pneumonia who have a history of asthma have a lower risk of dying from pneumonia than the general population ([Caruana et al. \(2015\)](#)). This is of course counterintuitive. However it was a true pattern in the training data: pneumonia patients with a history of asthma were usually admitted not only to the hospital but also directly to the Intensive Care Unit. The aggressive care received by asthmatic pneumonia patients was so effective that it lowered their risk of dying from pneumonia compared to the general population. However, since the prognosis for these patients was above average, models trained on this data erroneously find that asthma reduces the risk, while asthmatics actually have a much higher risk if they are not hospitalized. Hence, in this example blind trust in the machine learning algorithm would yield misleading results. Thus, interpretability is necessary in research to help identify causal relationships and increase the reliability and robustness of machine learning algorithms. Especially in areas outside of statistics the adoption of machine learning would be facilitated by making these models interpretable by adding explanations to their predictions.

In industry, machine learning is a standard component of almost any digital product offered by the big tech companies. From Amazons Alexa, or Netflixs movie recommendation system to the search algorithm from Google and Facebooks feed. These companies use machine learning to improve their products and business models. However, their machine learning algorithms are also built on training data collected from their users. Thus, in the age af data leaks à la Cambridge Analytica people want to understand for what purposes their data is collected and how the algorithms work that keep them on the streaming platforms or urge them to buy additional products and spend more time on social media.

Thus, in the digital world, interpretability of machine learning models would yield to a broader understanding of machine learning in the society and make the technology more trustworthy and fair. Switching to the analog world we see a far slower adoption of machine learning sytsems at scale. This is due to the fact that decisions made by machine learning systems in the real world can have far more severe consequences than in the digital world.

For instance, if the wrong movie is suggested to us it really doesn't matter, but if a machine learning system that is deployed to a self driving car does not recognize a cyclist it might take the wrong decision with real lifes at stake (see [Molnar \(2019\)](#)). We need to be sure that the machine learning system is flawless, because driving over a cyclist is pretty bad. For example, an explanation might show that the most important feature is to recognize the two wheels of a bicycle, and this explanation helps you to think about certain edge cases, such as bicycles with side pockets that partially cover the wheels. Self-driving cars are just one example where machines are taking over decisions in the real world that were previously taken by humans and can involve severe and sometimes irreversible consequences. Interpretability helps to ensure the reliability and robusntess of these systems and thus makes them safer.

To conclude, adding interpretability to machine learning algorithms is necessary in both academic and industrial applications. While we distinguished between academia and industry settings, the general points, causality, robustness & reliability, trust and fairness are of course valid in both worlds.

However, for academia, interpretability is especially key to identify causal relationships and increase the reliability and robustness of scientific discoveries made by the help of machine learning algorithms.

In industrial settings establishing trust in and fairness of machine learning systems matters most in low-risk environments whereas robustness and reliability is key to high-risk environments where machines take over decisions that have far reaching consequences.

Now that we established the importance of interpretability, how do we put this into practice? A restriction to machine learning models that are considered interpretable due to their simple structure, such as short decision trees or sparse linear models has the drawback that better performing models are excluded a priori from model selection. Hence, do we trade off prediction versus information and go back to more simple models? - No!

We separate the explanations from the machine learning model and apply interpretable methods that analyze the model after the model is trained.

1.3 Interpretable Machine Learning

As discussed in the previous chapter, most machine learning algorithms produce black box models, because they do not provide any direct explanation for their predictions. However, we do not want to restrict ourselves to models that are considered interpretable due to their simple structure and thus trade prediction accuracy for interpretability. Instead, we make machine learning models interpretable by applying methods that analyze the model after the model is trained, i.e. we establish post-hoc interpretability. Moreover, we are separating the explanations from the machine learning model, i.e. we focus on so called model-agnostic interpretation methods.

Post-hoc, model-agnostic explanation systems have several advantages (Ribeiro et al. (2016a)). First, since we separate the underlying machine learning model and its interpretation, developers can work with any model as the interpretation method is independent of the model. Thus we establish model flexibility. Second, since the interpretation is independent of the underlying machine learning model, the form of the interpretation also becomes independent. For instance in some cases it might be useful to have a linear formula, in other cases a graphic with feature importances is more appropriate. Thus, we establish explanation flexibility.

So what do these explanation systems do? - As discussed before, interpretation methods for machine learning algorithms ensure causal relationships, robustness & reliability and establish trust and fairness. More specifically, they do so by shedding light on the following issues (see [Molnar \(2019\)](#)):

- Algorithm transparency - How does the algorithm create the model?
- Global, kolistic model interpretability - How does the trained model make predictions?
- Global model interpretability on a modular level - How do parts of the model affect predictions?
- Local interpretability for a single prediction - Why did the model make a certain prediction for an instance?
- Local interpretability for a group of predictions - Why did the model make specific predictions for a group of instances?

Now that we learned that post-hoc and model-agnostic methods ensure model as well as explanantion flexibility and in which ways explanation systems ensure causal relationships, robustness & reliability and establish trust and fairness, we can move on to the outline of the booklet and discuss specific interpretation methods and their limitations.

1.4 Outline of the booklet

This booklet introduces and investigates the limitations of current post-hoc and model agnostic approaches in interpretable machine learning, such as Partial Dependence Plots (PDP), Accumulated Local Effects (ALE), Permutation Feature Importance (PMI), Leave-One-Covariate Out (LOCO) and Local Interpretable Model-Agnostic Explanations (LIME). All of these methods can be used to explain the behavior and predictions of trained machine learning models. However, their reliability and compactness deteriorate when models use a high number of features, have strong feature interactions and complex feature main effects among others. In the following, the methods mentioned are introduced and the outline of the booklet is given.

To start with, PDP and ALE are methods that enable a better understanding of the relationship between the outcome and feature variables of a machine learning model. Common to both methods is that they reduce the prediction function to a function that depends on only one or two features ([Molnar \(2019\)](#)). Both methods reduce the function by averaging the effects of the other features, but they differ in how the averages are calculated.

PDP, for example, visualizes whether the relationship between the outcome and a feature variable is, for instance, linear, monotonic or nonlinear and

hence allows for a straightforward interpretation of the marginal effect of a certain feature on the predicted outcome of a model (Friedman (2001)). However, this holds only true as long as the feature in question is not correlated with any other features of the model. ALE plots are basically a faster and unbiased alternative to PDP, because they can interpret models containing correlated variables correctly (Molnar (2019)). Chapter 2 of the booklet gives a short introduction to PDP. Next, PDP and its limitations when features are correlated are investigated in Chapter 3, respectively. Chapter 4 discusses if PDP allow for causal interpretations. Chapter 5 gives then a short introduction to ALE. ALE and PDP are compared in detail in Chapter 6. The choice of intervals, problems with piece-wise constant models and categorial features in the context of ALE are investigated in Chapter 7.

Yet, PDP and ALE do not provide any insights to what extent a feature contributes to the predictive power of a model - in the following defined as feature importance. PFI and LOCO are two methods that allow us to compute and visualize the importance of a certain feature for a machine learning model. PFI by Breiman (2001a) measures the importance of a feature by calculating the increase in the model's prediction error after permuting the feature. Leave-One-Covariate-Out (LOCO) by Lei et al. (2018), requires to refit the model as the approach is based on leaving features out instead of permuting them (Casalicchio et al. (2018)). Chapter 8 gives a short introduction to PFI and LOCO and gives rise to its limitations. Chapter 9 discusses both methods in the case of correlated features. Then partial and individual PFI are discussed in Chapter 10 and the issue whether feature importance should be computed on training or test data is discussed in Chapter 11.

Finally, LIME is a method that explains individual predictions of a black box machine learning model by locally approximating the prediction using a less complex and interpretable model (Molnar (2019)). These simplifying models are referred to as surrogate models. Consider for instance a neural network that is used for a classification task. The neural network itself is of course not interpretable, but certain decision boundaries could, for example, be explained reasonably well by a logistic regression which in fact yields interpretable coefficients. To refer to the first paragraph of the introduction, we use the data modeling approach to explain the algorithmic modeling approach in this example. Chapter 12 gives a short introduction to LIME. Chapter 13 sheds light on the effect of the neighbourhood on LIME's explanation for tabular data. Chapter 14 deals with the sampling step in LIME and the resulting side effects in terms of feature weight stability of the surrogate model.

Now that we shortly introduced the different methods we can move to the respective chapters of the booklet which discuss the methods and their limitations in more detail and by the help of practical examples.

2

Introduction to Partial Dependence Plots (PDP) and Individual Conditional Expectation (ICE)

Authors: Thommy Dassen, Naiwen Hou, Veronika Kronseder

Supervisor: Gunnar König

2.1 Partial Dependence Plots (PDP)

The Partial Dependence Plot (PDP) is a rather intuitive and easy-to-understand visualization of the features' impact on the predicted outcome. If the assumptions for the PDP are met, it can show the way a feature impacts an outcome variable. More precisely, mapping the marginal effect of the selected variable(s) uncovers the linear, monotonic or nonlinear relationship between the predicted response and the individual feature variable(s) (Molnar, 2019).

The underlying function can be described as follows:

Let x_S be the set of features of interest for the PDP and x_C the complement set which contains all other features. While the general model function $f(x) = f(x_S, x_C)$ depends on all input variables, the partial dependence function marginalizes over the feature distribution in set C (Hastie et al., 2013):

$$f_{x_S}(x_S) = \mathbb{E}_{x_C}[f(x_S, x_C)]$$

The partial dependence function can be estimated by averaging predictions with actual feature values of x_C in the training data at given values of x_S or, in other words, it computes the marginal effect of x_S on the prediction. In order to obtain realistic results, a major assumption of the PDP is that the features in x_S and x_C are independent and thus uncorrelated.(Hastie et al., 2013)

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

An example of a PDP based on the ‘Titanic’ data set, which contains information on the fate of 2224 passengers and crew members during the Titanic’s maiden voyage, is given in figure 2.1.

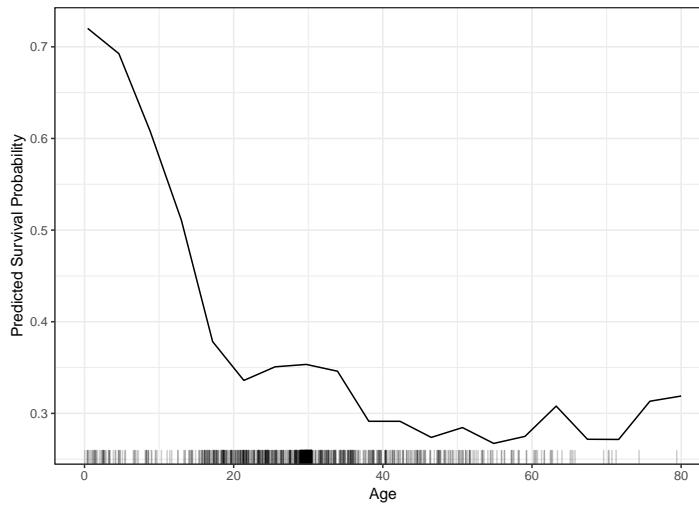


FIGURE 2.1: PDP for predicted survival probability and numeric feature variable ‘Age’. The probability to survive sharply drops at a young age and more moderately afterwards. The rug on the x-axis illustrates the distribution of observed training data.

When a feature is categorical, rather than continuous, the partial dependence function is modeled separately for all of the K different classes of said feature. It maps the predictions for each respective class at given feature values of x_S (Hastie et al., 2013).

For such categorical features, the partial dependence function and the resulting plot are produced by replacing all observed x_S -values with the respective category and averaging the predictions. This procedure is repeated for each of the features’ categories (Molnar, 2019). As an example, figure 2.2 shows the partial dependence for the survival probability prediction for passengers on the Titanic and the categorical feature ‘passenger class’.

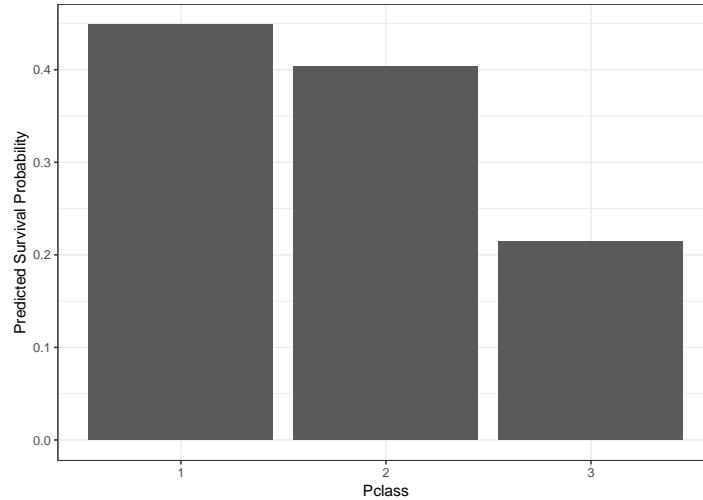


FIGURE 2.2: The PDP for survival probability and categorical feature ‘passenger class’ reveals that passengers in lower classes had a lower probability to survive than those in a higher class.

2.1.1 Advantages and Limitations of Partial Dependence Plots

Partial Dependence Plots are easy to compute and a popular way to explain insights from black box Machine Learning models. With their intuitive character, PDPs are perfect for communicating to a non-technical audience. However, due to limited visualization techniques and the restriction of human perception to a maximum of three dimensions, only one or two features can reasonably be displayed in one PDP (Molnar, 2019). 2.3 shows that the combination of one numerical (Age) and one categorical (Sex) feature still allows rather precise interpretation. The combination of two numerical features (Age & Fare) still works, but already degrades the interpretability with its colour intensity scale as shown in figure 2.4.

Drawing a PDP with one or two feature variables allows a straight-forward interpretation of the marginal effects. This holds true as long as the features are not correlated. Should this independence assumption be violated, the partial dependence function will produce unrealistic data points. For instance, a correlation between height and weight leading to a data point for someone taller than 2 meters weighing less than 50 kilos. Furthermore, opposite effects of heterogeneous subgroups might remain hidden through averaging the marginal effects, which could lead to wrong conclusions (Molnar, 2019).

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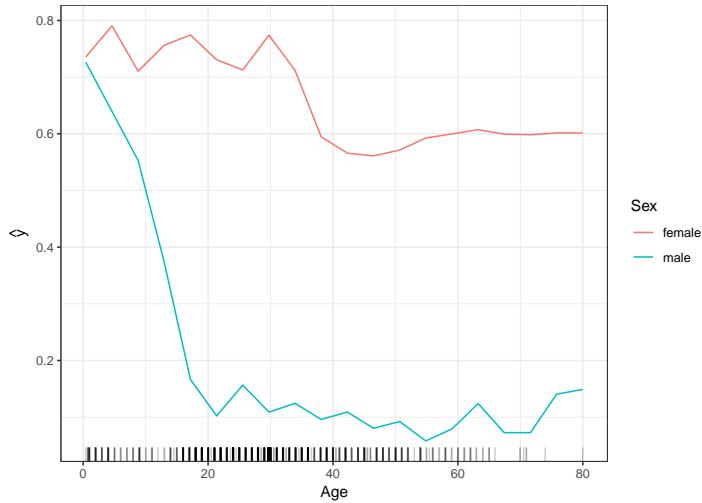


FIGURE 2.3: Two-dimensional PDP for predicted survival probability and numerical feature 'Age', together with the categorical feature 'Sex'. The PDP shows that while the survival probability for both genders declines as age increases, there is a difference between genders. It is clear that the decrease is much steeper for males.

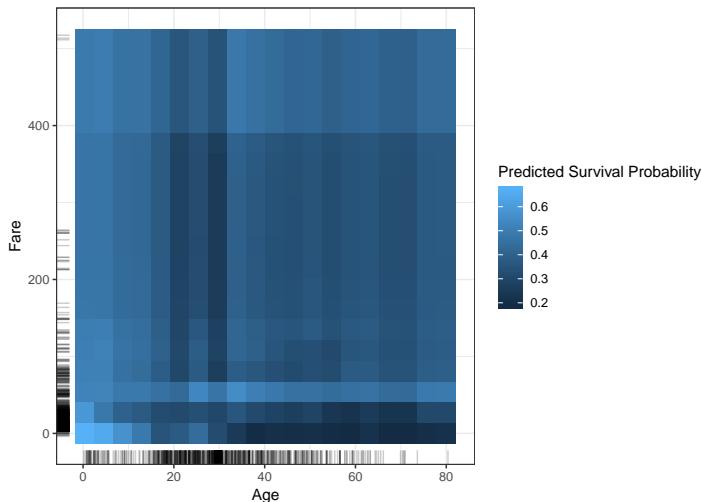


FIGURE 2.4: Two-dimensional PDP for predicted survival probability and numerical features 'Age' and 'Fare'. The PDP illustrates that the survival probability of younger passengers is fairly uniform for varying fares, while adults travelling at a lower fare also had a much lower probability to survive compared to those that paid a high fare.

2.2 Individual Conditional Expectation Curves

While partial dependence plots provide the average effect of a feature, Individual Conditional Expectation (ICE) plots are a method to disaggregate these averages. ICE plots visualize the functional relationship between the predicted response and the feature separately for each instance. In other words, a PDP averages the individual lines of an ICE plot (Molnar, 2019).

More formally, ICE plots can be derived by considering the estimated response function \hat{f} and the observations $(x_S^{(i)}, x_C^{(i)})_{i=1}^N$. The curve $\hat{f}_S^{(i)}$ is plotted against the observed values of $x_S^{(i)}$ for each of the observed instances while $x_C^{(i)}$ remains fixed at each point on the x-axis (Molnar, 2019; Goldstein et al., 2013)

As shown in figure 2.5, each line represents one instance and visualizes the effect of varying the feature value $x_S^{(i)}$ (Age) of a particular instance on the model's prediction, given all other features remain constant (c.p.). An ICE plot can highlight the variation in the fitted values across the range of a feature. This suggests where and to what extent heterogeneities might exist.

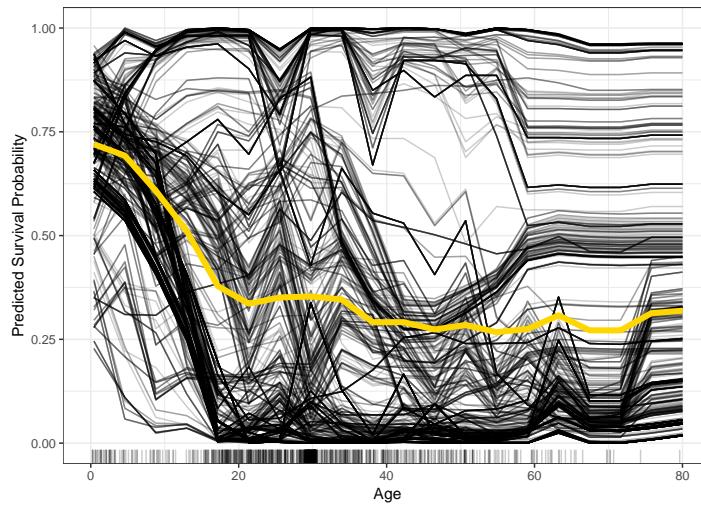


FIGURE 2.5: ICE plot of survival probability by Age. The yellow line represents the average of the individual lines and is thus equivalent to the respective PDP. The individual conditional relationships indicate that there might be underlying heterogeneity in the complement set.

2.2.1 Centered ICE Plot

If the curves of an ICE plot are stacked or have a wide range of intercepts it can be difficult to observe heterogeneity in the model. The so-called centered ICE plot (c-ICE plot) is a simple solution to this problem. The curves are centered at a certain point in the feature and display only the difference in the prediction to this point (Molnar, 2019). After anchoring a location x^a in the range of x_s and connecting all prediction lines at that point, the new curves are defined as:

$$\hat{f}_{cent}^{(i)} = \hat{f}^{(i)} - \mathbf{1}\hat{f}(x^a, x_C^{(i)})$$

Experience has shown that the most interpretable plots occur when the anchor point x^a is chosen as minimum or maximum of the observed values. Figure 2.6 shows the effect of centering the ICE curves of survival probability by Age at the minimum of observed ages in the ‘Titanic’ data set.

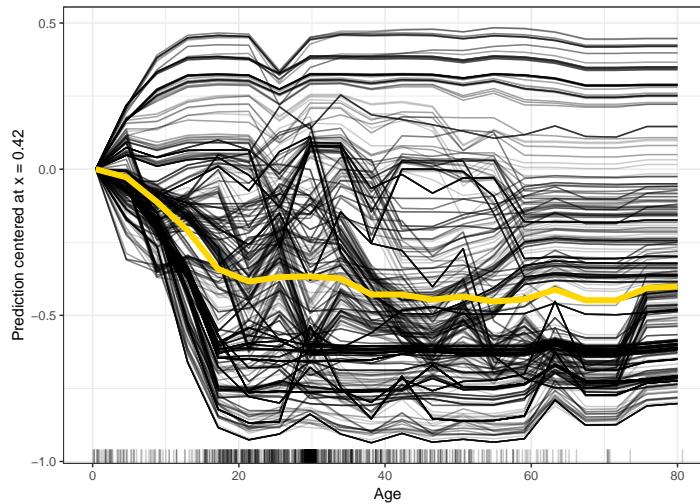


FIGURE 2.6: Centered ICE plot of survival probability by Age. All lines are fixed to 0 at the minimum observed age of 0.42. The y-axis shows the survival probability difference to age 0.42. Centred ICE plot shows that compared to age 0.42, the predictions for most passengers decrease as age increases. However, there are quite a few passengers with opposite predictions.

2.2.2 Derivative ICE Plot

Another way to explore the heterogeneity is to show plots of the partial derivative of \hat{f} with respect to x_s . Assume that x_s does not interact with the other predictors in the fitted model, the prediction function can be written as:

$$\hat{f}(x) = \hat{f}(x_s, x_C) = g(x_s) + h(x_C),$$

so that

$$\frac{\partial \hat{f}(\mathbf{x})}{\partial x_s} = g'(x_s)$$

When no interactions are present in the fitted model, all curves in the d-ICE plot are equivalent and the plot shows a single line. When interactions do exist, the derivative lines will be heterogeneous. As it can be difficult to visually assess derivatives from ICE plots, it is useful to plot an estimate of the partial derivative directly (Goldstein et al., 2013).

2.2.3 Advantages and Limitations of ICE Plots

The major advantage of ICE plots is that they are even more intuitive than PDPs which enables data scientists to drill much deeper to explore individual differences. This may help to identify subgroups and interactions between model inputs. However, there are also some disadvantages of ICE plots. Firstly, only one feature can be plotted in an ICE plot meaningfully. Otherwise, there would be a problem of overplotting and it would be hard to distinguish anything in the plot. Secondly, just like PDPs, ICE plots for correlated features may produce invalid data points. Finally, without additionally plotting the PDP it might be difficult to see the average in ICE plots (Molnar, 2019).



3

PDP and Correlated Features

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Supervisor: Giuseppe Casalicchio

3.1 Problem Description

As outlined in chapter 2, PDPs and ICE plots are meaningful graphical tools to visualize the impact of individual feature variables. This is particularly true for black box algorithms, where the mechanism of each feature and its influence on the generated predictions may be difficult to retrace (Goldstein et al., 2013).

The reliability of the produced curves, however, strongly builds on the independence assumption of the features. Furthermore, results can be misleading in areas with no or little observations, where the curve is drawn as a result of extrapolation. In this chapter, we want to illustrate and discuss the issue of dependencies between different types of variables, missing values and the associated implications on PDPs.

3.1.1 What is the issue with dependent features?

When looking at PDPs, one should bear in mind that by definition the partial dependence function does not reflect the isolated effect of x_S while the features in x_C are ignored. This approach would correspond to the conditional expectation $\tilde{f}_S(x_S) = \mathbb{E}_{x_C}[f(x_S, x_C)|x_S]$, which is only congruent to the partial dependence function $f_{x_S}(x_S) = \mathbb{E}_{x_C}[f(x_S, x_C)]$ in case of x_S and x_C being independent (Hastie et al., 2013).

Although unlikely in many practical applications, the independence of feature variables is one of the major assumptions to produce meaningful PDPs. Its violation would mean that, by calculating averages of the features in x_C , the

estimated partial dependence function $\hat{f}_{x_S}(x_S)$ takes unrealistic data points into consideration (Molnar, 2019).

Figure 3.1 illustrates the problem by contrasting simulated data with independent features x_1 and x_2 on the left with an example where the two features have a strong linear dependency, and thus are highly correlated, on the right.

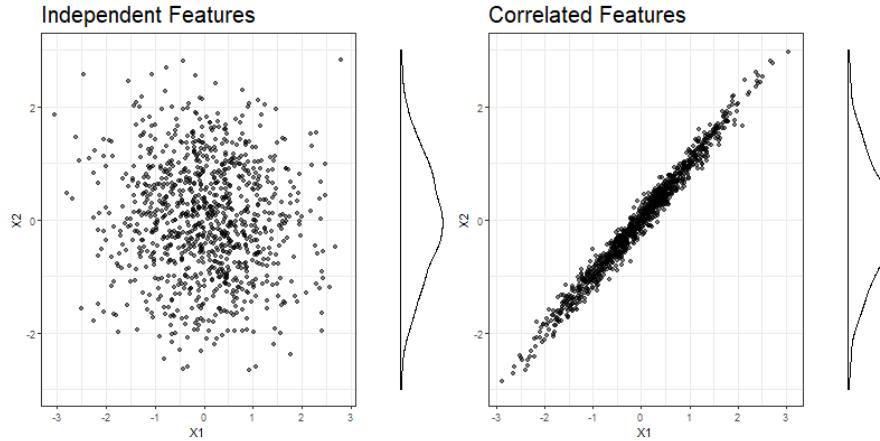


FIGURE 3.1: Simulated data for independent (left) and strongly correlated (right) features x_1 and x_2 . The marginal distribution of x_2 is displayed on the right side of each plot.

When computing the PDP for feature x_1 , we take x_2 into account by calculating the mean predictions at observed x_2 values in the training data, while the values of x_1 are given. This makes sense in the independent case, where observations are randomly scattered. However, when looking at the correlated features in the right part of figure 3.1, the average is not a realistic value in combination with certain values of x_1 , e.g. in the very left and the very right part of the feature distribution.

3.1.2 What is the issue with extrapolation?

Generally speaking, extrapolation means leaving the distribution of observed data. On the one hand, this can affect the predictions, namely in the event of the prediction function doing ‘weird stuff’ in unobserved areas. In chapter 3.4 we will see an example where this instant leads to a failure of the PDP (Molnar, 2019).

On the other hand, PDPs are also directly exposed to extrapolation problems due to the fact that the estimated partial dependence function \hat{f}_{x_S} is evaluated at each observed $x_S^{(i)}$, giving a set of N ordered pairs: $\{(x_S^{(i)}, \hat{f}_{x_S^{(i)}})\}_{i=1}^N$. The

resulting coordinates are plotted against each other and joined by lines. Not only outside the margins of observed values, but also in areas with a larger distance between neighboured x_S values, the indicated relationship with the target variable might be inappropriate and volatile in case of outliers (Goldstein et al., 2013).

In figure 3.2, a part of the previously simulated observations has been deleted from both the independent and the correlated example to visualize a data situation which might have an impact on the PDP in terms of extrapolation. An example is given in chapter 3.4.1. The shift in observed areas can also be noticed from the marginal distribution of x_2 .

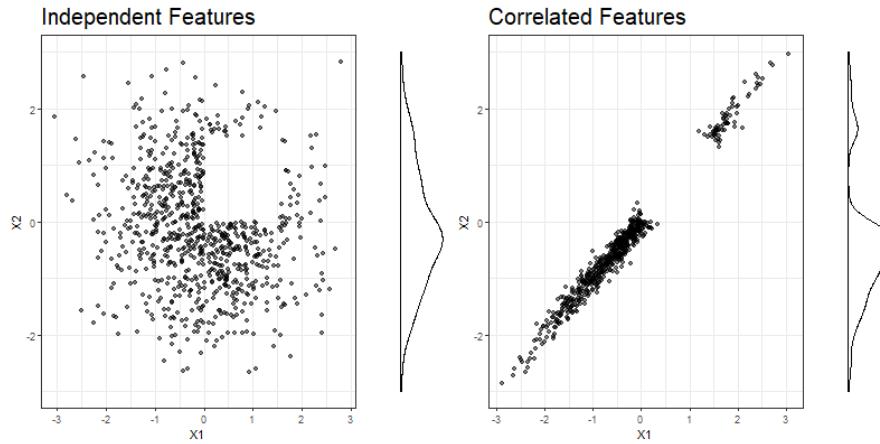


FIGURE 3.2: Manipulated simulated data for independent (left) and strongly correlated (right) features x_1 and x_2 . Observations where both the value of x_1 and x_2 lies between 0 and 1.5 have been deleted to artificially produce an extrapolation problem. The marginal distribution of x_2 , which is displayed on the right side of each plot, is obviously more affected in the correlated case.

The extrapolation problem in PDPs is strongly linked to the aforementioned independence assumption. Independent features are a prerequisite for the computation of meaningful extrapolation results, therefore one could say that both problems go hand in hand. In the following chapters, the failure of PDPs in case of a violation of the independence assumption shall be discussed by means of real data examples (chapter 3.2) and based on simulated cases (chapter 3.3).

3.2 Dependent Features: Bike Sharing Dataset

In order to investigate the impact of dependent features, we are now looking at the Bike-Sharing dataset from the rental company ‘Capital-Bikeshare’, which is available for download via the UCI Machine Learning Repository. Besides the daily count of rental bikes between the year 2011 and 2012 in Washington D.C., the dataset contains the corresponding weather and seasonal information ([Fanaee-T and Gama, 2013](#)).

For our purposes, the dataset was restricted to the following variables:

- y : cnt (count of total rental bikes including both casual and registered)
- x_1 : season: Season (1:springer, 2:summer, 3:fall, 4:winter)
- x_2 : yr: Year (0: 2011, 1:2012)
- x_3 : mnth: Month (1 to 12)
- x_4 : holiday: weather day is holiday or not
- x_5 : workingday: If day is neither weekend nor holiday is 1, otherwise is 0.
- x_6 : weathersit:
 - 1: Clear, Few clouds, Partly cloudy, Partly cloudy
 - 2: Mist + Cloudy, Mist + Broken clouds, Mist + Few clouds, Mist
 - 3: Light Snow, Light Rain + Thunderstorm + Scattered clouds, Light Rain + Scattered clouds
 - 4: Heavy Rain + Ice Pallets + Thunderstorm + Mist, Snow + Fog
- x_7 : temp: Normalized temperature in Celsius.
- x_8 : atemp: Normalized feeling temperature in Celsius.
- x_9 : hum: Normalized humidity.
- x_{10} : windspeed: Normalized wind speed.

For all machine learning models based on the Bike-Sharing dataset, ‘cnt’ is used as a target variable, while the remaining information serves as feature variables. Six out of these ten features are categorical (x_1 to x_6), the rest is measured on a numerical scale (x_7 to x_{10}). Since the appearance of a PDP depends on the class of the feature(s) of interest, we are looking at three different scenarios of dependency:

1. Dependency between numerical features
2. Dependency between categorical features
3. Dependency between numerical and categorical features

At the same time, for each of those scenarios, three different learning algorithms shall be compared:

- Linear Model (LM)
- Random Forest (RF)

- Support Vector Machines (SVM)

3.2.1 Dependency between Numerical Features

The linear dependency between two numerical features can be measured by the Pearson correlation coefficient (Fahrmeir et al., 2016). Figure 3.3 shows the correlation matrix of all numerical features used in our analysis. It is striking, but certainly not surprising, that ‘temp’ and ‘atemp’ are strongly correlated, not to say almost perfectly collinear.

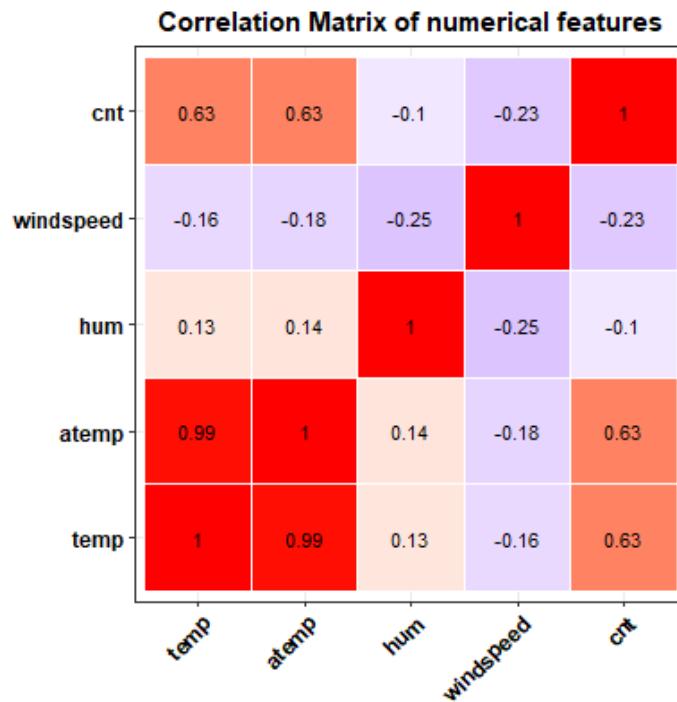


FIGURE 3.3: Matrix of Pearson correlation coefficients between all numerical variables extracted from the bike-sharing dataset.

Due to their strong correlation, ‘temp’ (x_7) and ‘atemp’ (x_8) perfectly qualify for our analysis of the impact of dependent features on PDPs. In order to compare the partial dependence curve with and without the influence of dependent features, we compute PDPs based on the following models:

$$y \sim x_1 + x_2 + x_4 + x_5 + x_6 + x_7 + x_9 + x_{10} \quad (3.1)$$

$$y \sim x_1 + x_2 + x_4 + x_5 + x_6 + \mathbf{x}_8 + x_9 + x_{10} \quad (3.2)$$

$$y \sim x_1 + x_2 + x_4 + x_5 + x_6 + \mathbf{x}_7 + \mathbf{x}_8 + x_9 + x_{10} \quad (3.3)$$

Please note that the representation of the different models with the feature variables connected via ‘+’ shall, in this context, not be read as a (linear) regression model where all coefficients are equal to 1, but rather as a combination of applicable feature variables to explain y . The (non-)linear effect of each variable is modelled individually, depending on the observed values and the learner.

While model (3.1) and (3.2) only take one of the two substituting variables into account, (3.3) considers both ‘temp’ and ‘atemp’ in one and the same model. Figures 3.4, 3.5 and 3.6 compare the associated PDPs for the different learning algorithms. Note that ‘season’ (x_1) and ‘mnth’ (x_3) are not taken into account in combination with x_7 and/or x_8 , since there are meaningful associations between those variables, too, as we will show in chapter 3.2.3. At this stage we want to illustrate the isolated effect of the dependence between the two numerical variables.

In all cases, we can see that the features’ effect on the prediction is basically the same for x_7 and x_8 , if only one of the dependent variables is used for modelling (see PDPs in top left and top right corners). If both ‘temp’ and ‘atemp’ are relevant for the prediction of y , each feature’s impact is smoothed and neither the PDP for x_7 nor the one for x_8 seems to properly reflect the true effect of the temperature on the count of bike rentals.

3.2.2 Dependency between Categorical Features

In order to measure the association between two categorical features, we calculate the corrected contingency coefficient, which is based on the χ^2 -statistic. Other than the Pearson correlation coefficient, the corrected contingency coefficient is a measure of association $\in [0, 1]$ which can only indicate the strength but not the direction of the variables’ relationship (Fahrmeir et al., 2016). For the categorical features in the Bike-Sharing dataset, we observe the values stated in figure 3.7.

The only combination of categorical features with an exceptionally high corrected contingency coefficient, is ‘season’ (x_1) and ‘mnth’ (x_3). Also from a content-related point of view, this finding is no surprise, since both variables measure the time of the year. For the computation of the respective PDPs, we use the following models:

$$y \sim \mathbf{x}_1 + x_2 + x_4 + x_5 + x_6 + x_9 + x_{10} \quad (3.4)$$

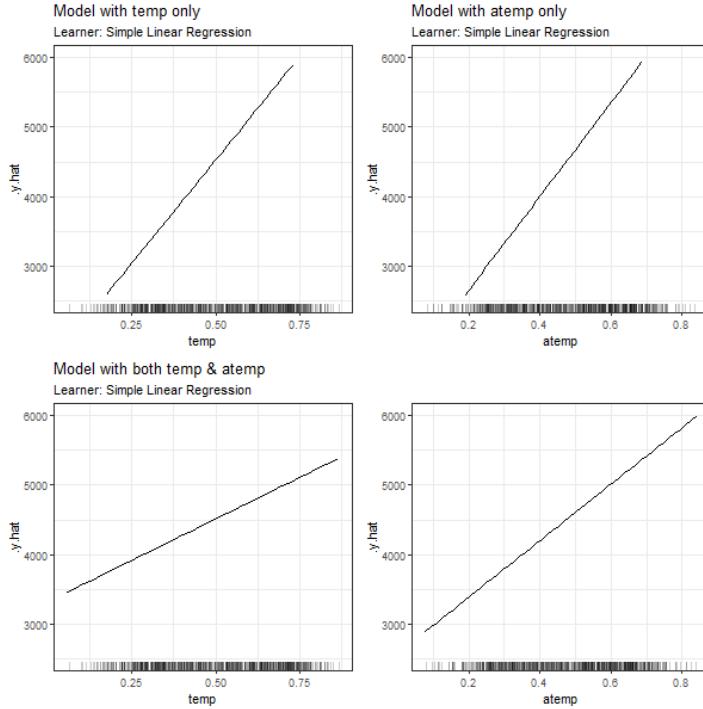


FIGURE 3.4: PDPs based on Linear Regression learner for 'temp' in model 3.1 (top left), 'atemp' in model 3.2 (top right), 'temp' in model in model 3.3 (bottom left) and 'atemp' in model 3.3 (bottom right).

$$y \sim x_2 + \mathbf{x}_3 + x_4 + x_5 + x_6 + x_9 + x_{10} \quad (3.5)$$

$$y \sim \mathbf{x}_1 + x_2 + \mathbf{x}_3 + x_4 + x_5 + x_6 + x_9 + x_{10} \quad (3.6)$$

The approach is equivalent to the numeric case, with model (3.4) containing only 'season' and (3.5) only 'mnth', while both dependent features are part of model (3.6). The impact on the PDPs for categorical features are shown in figures 3.8, 3.9 and 3.10.

Again, in all PDPs based on the different learning algorithms, the results between models with and without dependent features are diverging. The predicted number of bike rentals between the seasons/months shows a stronger variation when modelled without feature dependencies.

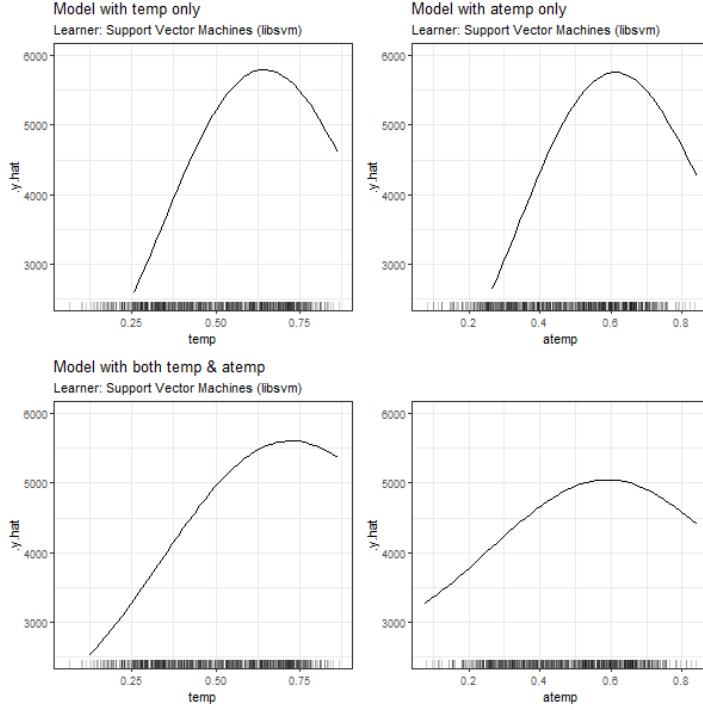


FIGURE 3.5: PDPs based on Support Vector Machines learner for 'temp' in model 3.1 (top left), 'atemp' in model 3.2 (top right), 'temp' in model in model 3.3 (bottom left) and 'atemp' in model 3.3 (bottom right).

3.2.3 Dependency between Numerical and Categorical Features

Our third dependency scenario seeks to provide an example for a strong correlation between a numerical and a categorical feature. For this constellation, neither the Pearson correlation nor the contingency coefficient are applicable as such, since both methods are limited to their respective classes of variables.

We can, however, fit a linear model to explain the numeric variable through the categorical feature. By doing so, we produce another numerical variable, the fitted values. In a next step, we can calculate the Pearson correlation coefficient between the observed and the fitted values of the numerical feature. The resulting measure of association lies within the interval $[0, 1]$ and is equivalent to the square root of the linear model's variance explained (R^2) (Fahrmeir et al., 2013). For this reason, we refer to the measure as ‘variance-explained measure’.

When applying this procedure to the categorical feature ‘season’ (x_1) and the

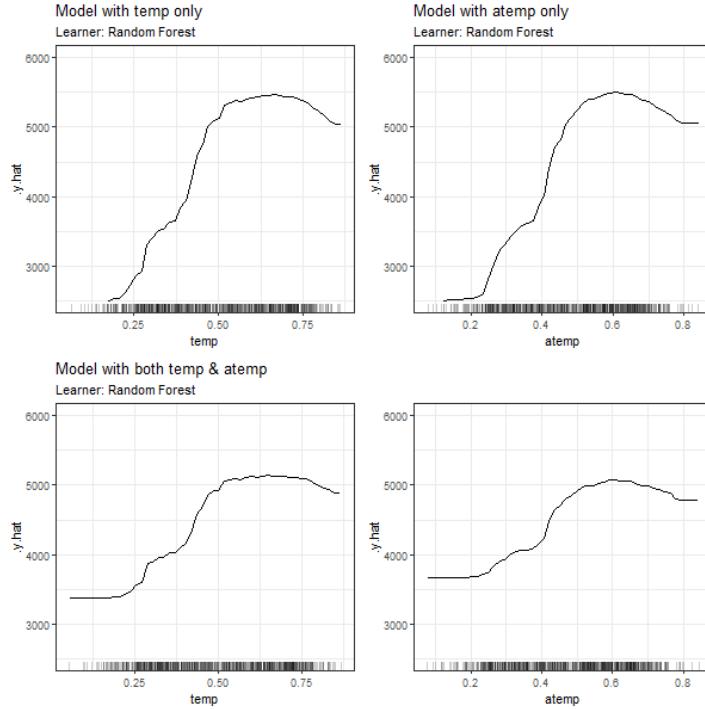


FIGURE 3.6: PDPs based on Random Forest learner for 'temp' in model 3.1 (top left), 'atemp' in model 3.2 (top right), 'temp' in model in model 3.3 (bottom left) and 'atemp' in model 3.3 (bottom right).

numerical feature 'temp' (x_7), we find that with a variance-explained value of 0.83, there seems to be a reasonable association between the two features. The PDPs are derived through the following models:

$$y \sim \mathbf{x}_1 + x_2 + x_4 + x_5 + x_6 + x_9 + x_{10} \quad (3.7)$$

$$y \sim x_1 + x_2 + x_4 + x_5 + x_6 + \mathbf{x}_7 + x_9 + x_{10} \quad (3.8)$$

$$y \sim \mathbf{x}_1 + x_2 + x_4 + x_5 + x_6 + \mathbf{x}_7 + x_9 + x_{10} \quad (3.9)$$

Figure 3.11, 3.12 and 3.13 present the partial dependence plots for the three underlying machine learning algorithms (LM, SVM and RF) defined for the purpose of our analysis.

Compared to the first two scenarios, we observe a more moderate difference between the PDPs when comparing model (3.7) and (3.8) containing just

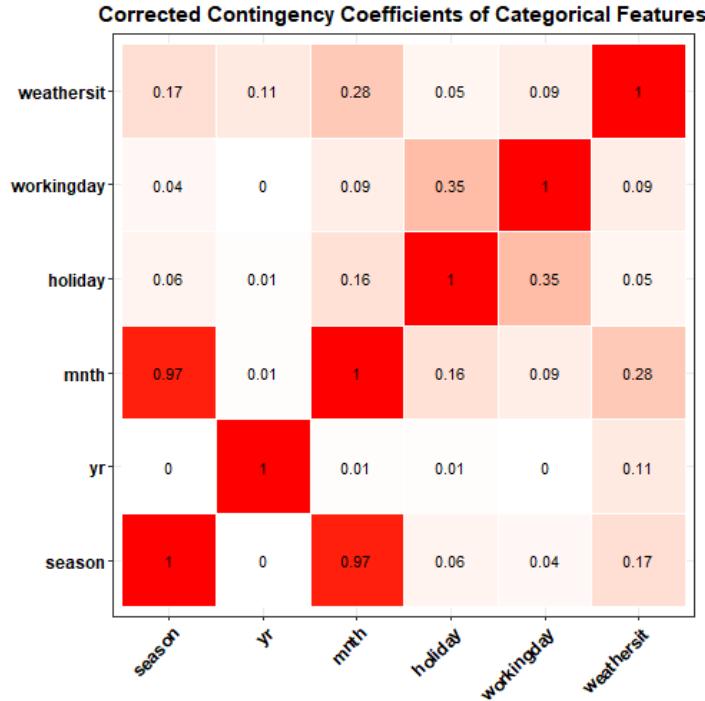


FIGURE 3.7: Matrix of corrected contingency coefficients between all categorical variables extracted from the bike-sharing dataset.

one of the dependent features to the full model (3.9). The weaker association between the two variables, in contrast to scenario 1 and 2, could be an explanation for this observation. It is, however, evident that the dependency structure between two feature variables, irrespective of their class, does impact the partial dependence plot.

3.3 Dependent Features: Simulated Data

A major disadvantage of the analysis of PDPs on the basis of real data examples is, that we cannot exclude other factors to play a role. As an example, underlying interactions could have an impact on the PDP and hide the true effect of a feature on the predicted target variable (Molnar, 2019). In order to illustrate the isolated impact of dependent variables in the feature space, we have simulated data in different settings, which we will discuss in this chapter.

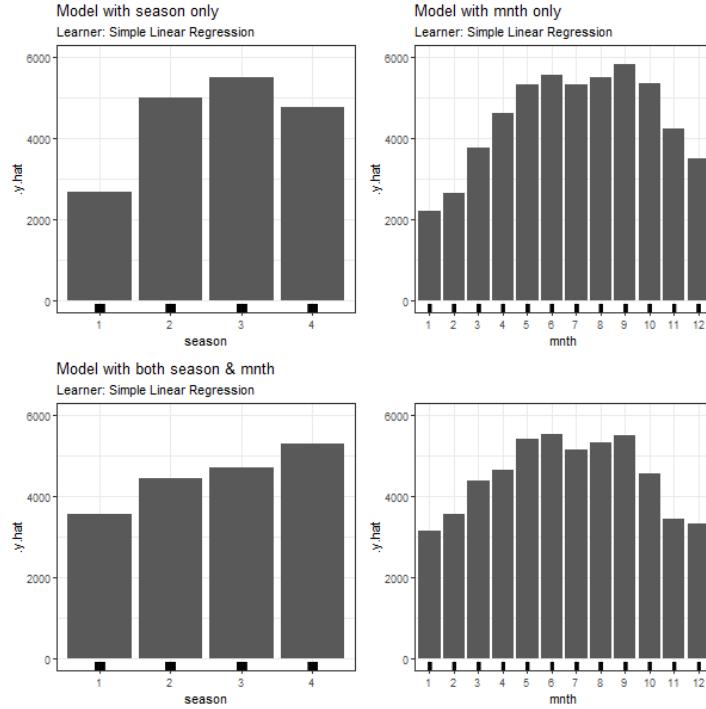


FIGURE 3.8: PDPs based on Linear Regression learner for 'season' in model 3.4 (top left), 'mnth' in model 3.5 (top right), 'season' in model in model 3.6 (bottom left) and 'mnth' in model 3.6 (bottom right).

3.3.1 Simulation Settings: Numerical Features

For a start, the different settings of simulations used for our investigation shall be introduced. Just like in chapter 2, we are separately looking at different classes of variables and different machine learning algorithms (LM, RF and SVM). PDPs for independent, correlated and dependent numerical features are computed for each of the following data generating processes (DGP), which describe the true impact of the features on y :

- Setting 1: Linear Dependence:

$$y = x_1 + x_2 + x_3 + \varepsilon \quad (3.10)$$

- Setting 2: Nonlinear Dependence in x_1 :

$$y = \sin(3 * x_1) + x_2 + x_3 + \varepsilon \quad (3.11)$$

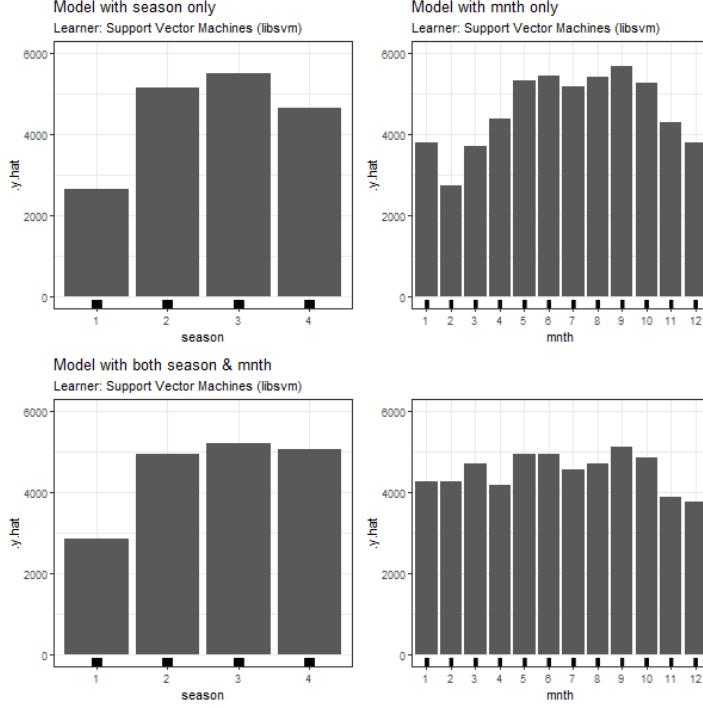


FIGURE 3.9: PDPs based on Support Vector Machines learner for 'season' in model 3.4 (top left), 'mnth' in model 3.5 (top right), 'season' in model in model 3.6 (bottom left) and 'mnth' in model 3.6 (bottom right).

- Setting 3: Missing informative feature x_3

$$y = x_1 + x_2 + x_3 + \varepsilon \quad (3.12)$$

with x_3 relevant for the DGP but unconsidered in the machine learning model.

In the independent case, the feature variables x_1 , x_2 and x_3 have been drawn from a gaussian distribution with $\mu = 0$, $\sigma^2 = 1$ and a correlation coefficient of $\rho_{ij} = 0 \forall i \neq j$, $i, j \in \{1, 2, 3\}$.

The correlated case is based on the same parameters for μ and σ^2 , but a correlation coefficient of $\rho_{12} = \rho_{21} = 0.90$, i.e. a relatively strong linear association between x_1 and x_2 , and $\rho_{ij} = 0$ otherwise.

The dependent case describes the event of perfect multicollinearity, where x_2 is a duplicate of x_1 , based on the data generated in the independent case.

The target variable y results from the respective DGP with an error term $\varepsilon \sim N(0, \sigma_\varepsilon^2)$ and σ_ε^2 depending on the feature values.

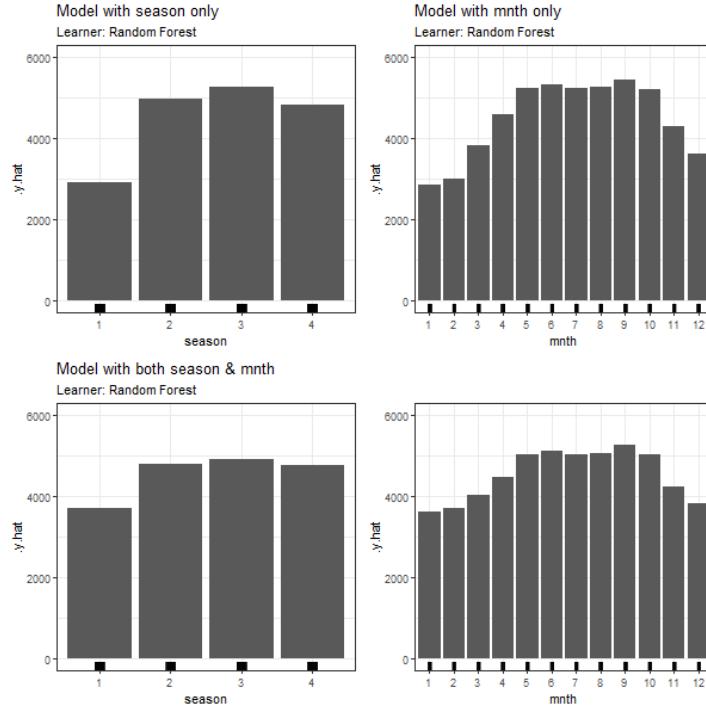


FIGURE 3.10: PDPs based on Random Forest learner for 'season' in model 3.4 (top left), 'mnth' in model 3.5 (top right), 'season' in model in model 3.6 (bottom left) and 'mnth' in model 3.6 (bottom right).

One source of variation in the PDPs is the simulation of the data itself. For this reason, the process has been repeated 20 times for each analysis and the resulting PDP curves are shown as gray lines in the plots below. The thicker, black line represents the average partial dependence curve over these 20 simulations and the error bars indicate their variation. Additionally, a red line represents the true effect of the feature for which the PDP is computed. In all cases, the simulations are based on a number of 500 observations and grid size 50.

Since in the dependent case, x_2 is simply a duplicate of x_1 , the DGP could also be written as $y = 2 * x_1 + x_3 + \varepsilon$ in setting (3.10) and (3.12) and $y = \sin(3 * x_1) + x_1 + x_3 + \varepsilon$ in setting (3.11). For the purpose of this analysis, we are looking at each of the three features' PDP separately. However, in order to illustrate the aforementioned, the common effect of x_1 and x_2 on the prediction is added to the plots as dashed blue line.

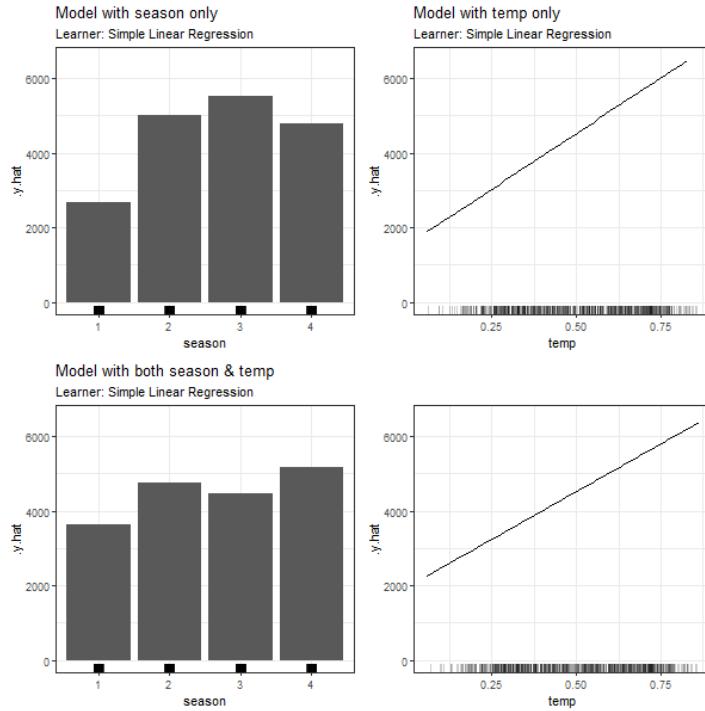


FIGURE 3.11: PDPs based on Linear Regression learner for 'season' in model 3.4 (top left), 'temp' in model 3.5 (top right), 'season' in model in model 3.6 (bottom left) and 'temp' in model 3.6 (bottom right).

3.3.2 Simulation of Setting 1: Linear Dependence

3.3.2.1 PDPs based on Linear Model

The results of our simulations in setting 1 based on the Linear Model are shown in figure 3.14:

Across all simulations, there is hardly any variation between the PDPs based on the Linear Model. In the independent case, the PDPs for each feature adequately reflect the linear dependency structure. The effect is equivalent in each PDP, since all features have the same impact and are independent from each other. From the PDPs in the second row of figure 3.14 we see that even with a relatively strong correlation of features x_1 and x_2 , the PDPs adequately reflect the linear dependency structure when predictions are computed from the Linear Model. In the event of perfect multicollinearity, the PDP for one of the dependent features (x_2) fails, while the corresponding PDP for the

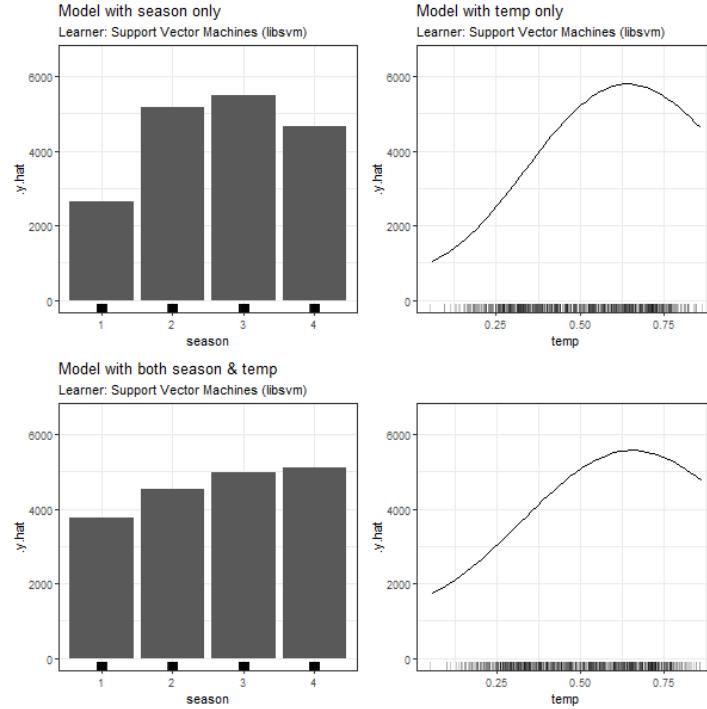


FIGURE 3.12: PDPs based on Support Vector Machines learner for 'season' in model 3.4 (top left), 'temp' in model 3.5 (top right), 'season' in model in model 3.6 (bottom left) and 'temp' in model 3.6 (bottom right).

other feature (x_1) reflects the common effect of both. The PDP for feature x_3 adequately reveals its linear effect on y .

3.3.2.2 PDPs based on Random Forest

The results of our simulations in setting 1 based on Random Forest are shown in figure 3.15:

Compared to the LM, there is a little more variance between the individual PDP curves produced from RF as learner. Furthermore, the partial dependence plots cannot adequately reflect the linear dependency structure, particularly at the margins of the feature's distribution. Again, there is no visual differentiation between the different features in the first row of figure 3.15 due to their independence. Besides, the computation of PDPs based on Random Forest does not produce significantly worse results when two features are correlated and the relationship between all variables and y is linear.

When comparing the PDPs subject to perfect multicollinearity to those in the

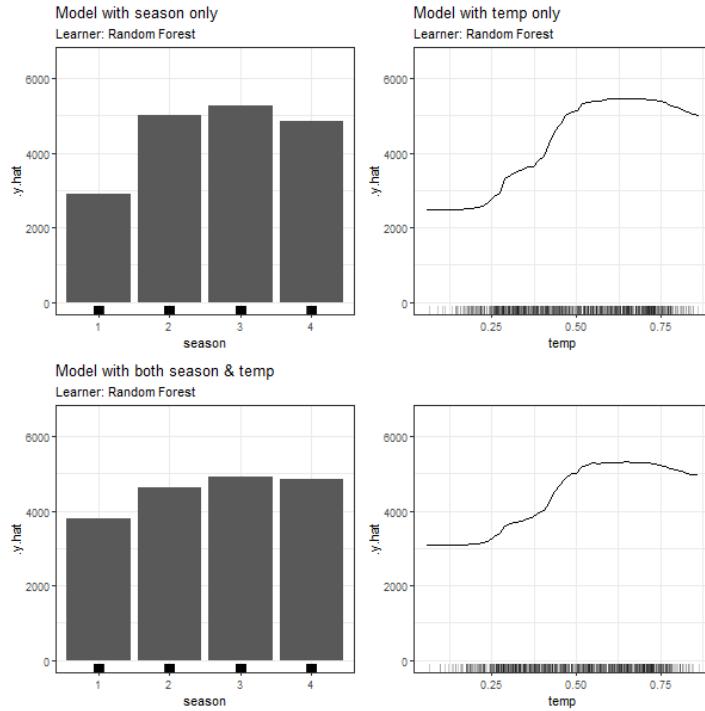


FIGURE 3.13: PDPs based on Random Forest learner for 'season' in model 3.4 (top left), 'temp' in model 3.5 (top right), 'season' in model in model 3.6 (bottom left) and 'temp' in model 3.6 (bottom right).

correlated case, a slightly increased variation in the individual PDP curves is observed. Other than in the Linear Model, the learner is not able to reveal the true common effect of x_1 and x_2 .

3.3.2.3 PDPs based on Support Vector Machines

The results of our simulations in setting 1 based on Support Vector Machines are shown in figure 3.16:

Support Vector Machines as learning algorithms are able to reproduce the respective feature's linear effect on the prediction fairly adequate in case of independence. The accuracy decreases in the margins of the feature's distribution. With two correlated features, the interval of predicted values of both correlated features becomes smaller, while the learner produces the same 'shape' of its effect, both for x_1 and x_2 . The same observation is made in the event of two identical features (dependent case), but even more evident with PDP curves increasingly deviating from the true effect. Other than in the LM, none

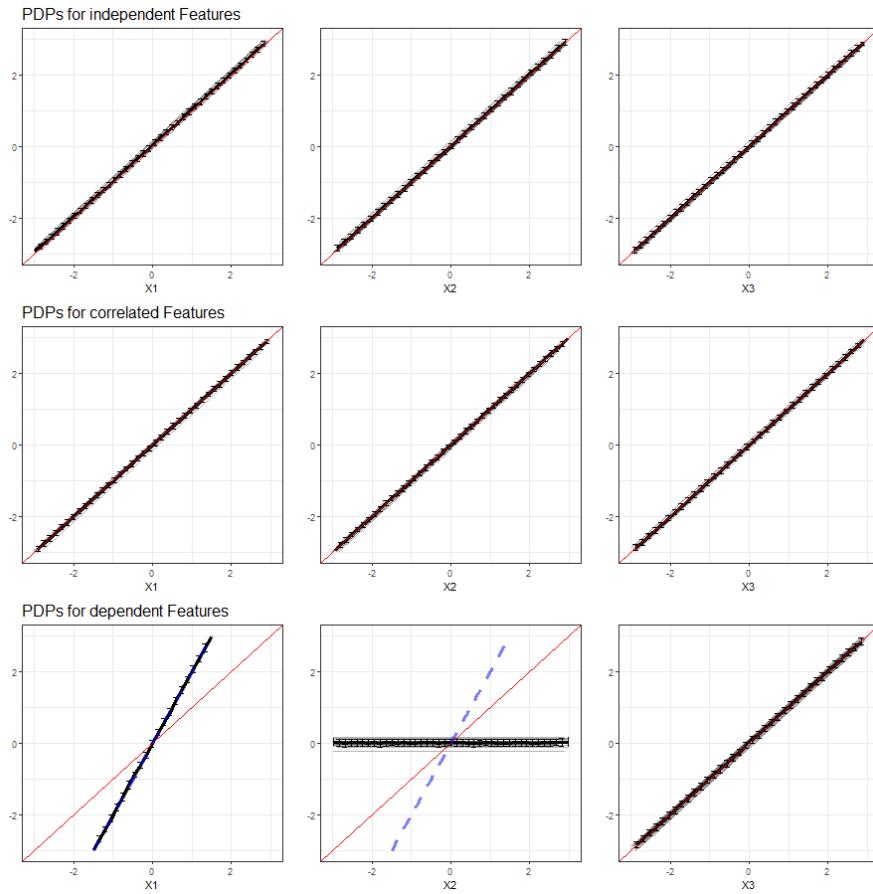


FIGURE 3.14: PDPs for features x_1 , x_2 and x_3 (left to right) in Setting 1, based on multiple simulations with Linear Model as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

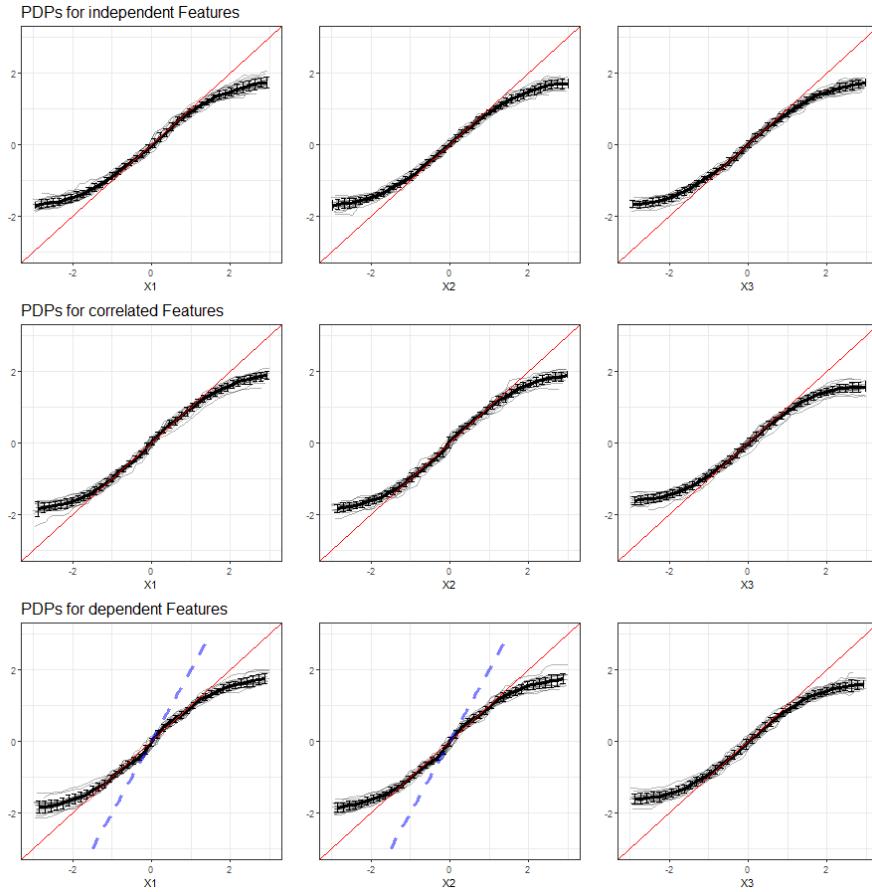


FIGURE 3.15: PDPs for features x_1 , x_2 and x_3 (left to right) in Setting 1, based on multiple simulations with Random Forest as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

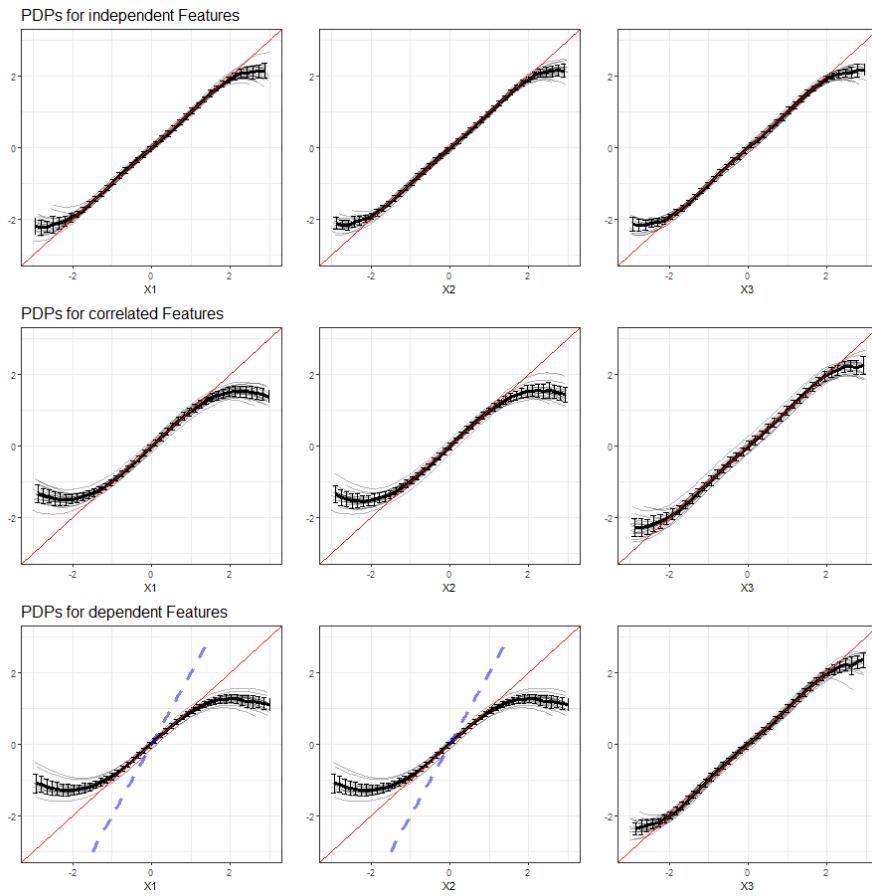


FIGURE 3.16: PDPs for features x_1 , x_2 and x_3 (left to right) in Setting 1, based on multiple simulations with Support Vector Machines as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

of the PDPs for the dependent features reveals the true common effect of x_1 and x_2 .

3.3.3 Simulation of Setting 2: Nonlinear Dependence

In simulation setting 2 we are looking at a DGP with a nonlinear relationship of x_1 and y and a linear impact of x_2 and x_3 . Due to the nonlinearity in one of the features, it is clear that the LM would not deliver accurate results. For this reason, in this chapter we will restrict our analysis to RF and SVM.

3.3.3.1 PDPs based on Random Forest

The results of our simulations in setting 2 based on Random Forest are shown in figure 3.17:

From the PDP of feature x_1 in the first row of figure 3.17 it is evident that Random Forest as a learner can retrace the nonlinear effect of the variable quite well, except for the margin areas of the feature distribution. The PDPs for feature x_2 and x_3 are equivalent to those in simulation setting (3.10).

With a simulated correlation between features x_1 and x_2 and a nonlinear relationship of x_1 and y , the ability of the respective PDPs to illustrate the feature's effect degrades with RF as learner. Both the nonlinear effect of x_1 and the linear effect of x_2 are distorted in the PDPs.

In the event of perfect multicollinearity, the PDPs for the involved feature variables fail even more. In contrast to the correlated case, we can observe that both curves take on a similar shape, which very roughly approximates the common effect.

3.3.3.2 PDPs based on Support Vector Machines

The results of our simulations in setting 2 based on SVM are shown in figure 3.18:

The findings derived from PDPs based on Random Forest are equivalently applicable to Support Vector Machines as machine learning algorithm. In the event of independent features, the PDPs can fairly well reveal the true feature effects, despite in the margins of the feature distributions. With strongly correlated or even dependent features, this ability vanishes and the PDPs of the affected features transform towards the variables' common effect.

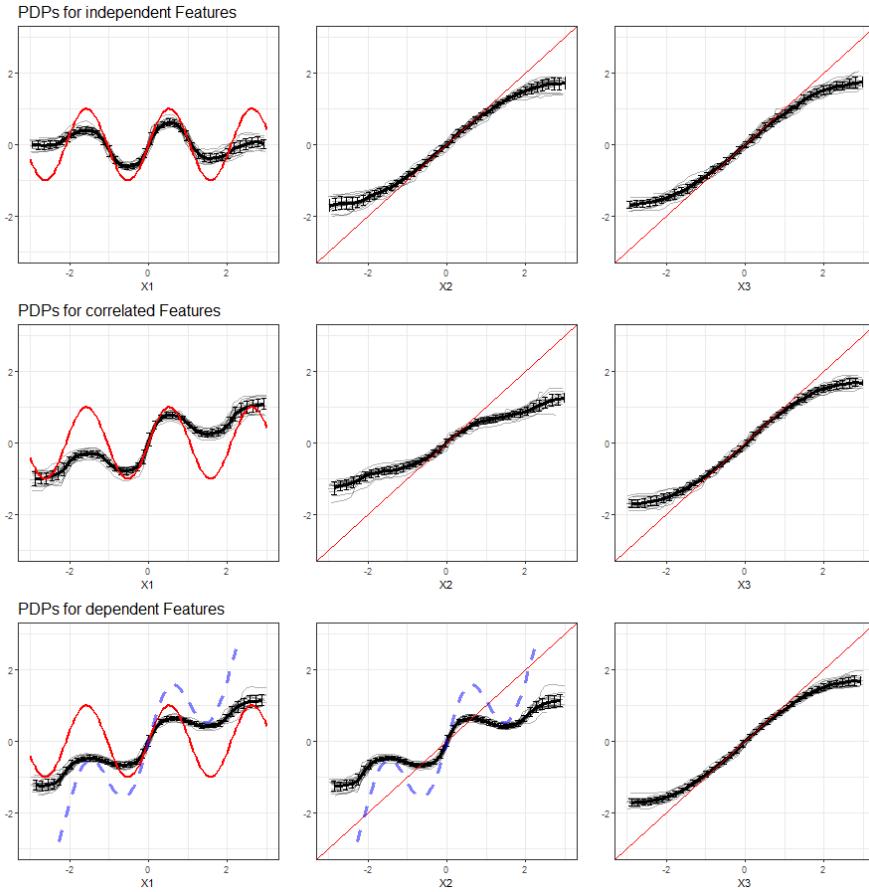


FIGURE 3.17: PDPs for features x_1 , x_2 and x_3 (left to right) in Setting 2, based on multiple simulations with Random Forest as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

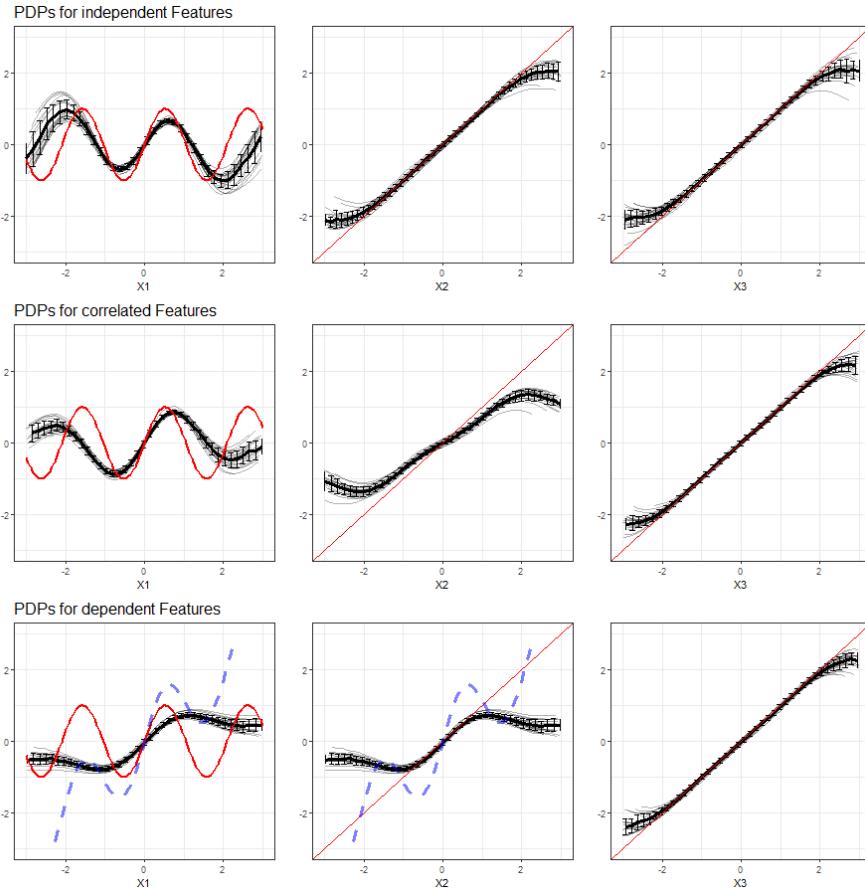


FIGURE 3.18: PDPs for features x_1 , x_2 and x_3 (left to right) in Setting 2, based on multiple simulations with SVM as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

3.3.4 Simulation of Setting 3: Missing informative feature x_3

In simulation setting 3, we assume that there are three variables with an impact on the data generating process of y . In the training process of the machine learning model, only two of those are considered. Consequently, when looking at the PDPs, we only compare the independent, the correlated and the dependent case for x_1 and x_2 respectively.

3.3.4.1 PDPs based on Linear Model

The results of our simulations in setting 3 based on the Linear Model are shown in figure 3.19:

Compared to the PDPs of independent features the Linear Model produced in setting (3.10), the variation in individual PDPs is slightly higher with missing information from x_3 . Overall, the learner can adequately reflect the linear feature effects of x_1 and x_2 .

The increase in variability between the individual PDPs is even more evident in the correlated case. On average, we still obtain the true linear effect of the correlated features, but there are some individual curves which do indicate a steeper or more moderate slope.

The PDPs drawn on basis of the Linear Model and dependent features indicate that for both individual features, the PDP consistently provides false effects on the predicted outcome. While both effects are actually linear with a slope of 1, the PDP for x_1 shows a steeper increase and x_2 fails completely. Nonetheless, the PDP for x_1 does reflect the common effect of both variables together.

3.3.4.2 PDPs based on Random Forest

The results of our simulations in setting 3 based on Random Forest are shown in figure 3.20:

Compared to setting (3.10), where all relevant feature variables were taken into account for the training of the model, the variation in PDP curves in setting (3.12) is larger. Between features x_1 and x_2 , which are independent, there is no systematic difference traceable from the PDPs.

Other than an increased variability between the individual PDP curves and a slightly tighter prediction interval, with correlated features and Random Forest as learner, there is no apparent deviation to the PDPs of independent features.

In accordance with the observations made in setting (3.10), the interval of predicted values for dependent features become even smaller while the PDP curves further deviate from the true effect. Neither the individual effect of each feature, nor their common effect are illustrated adequately.

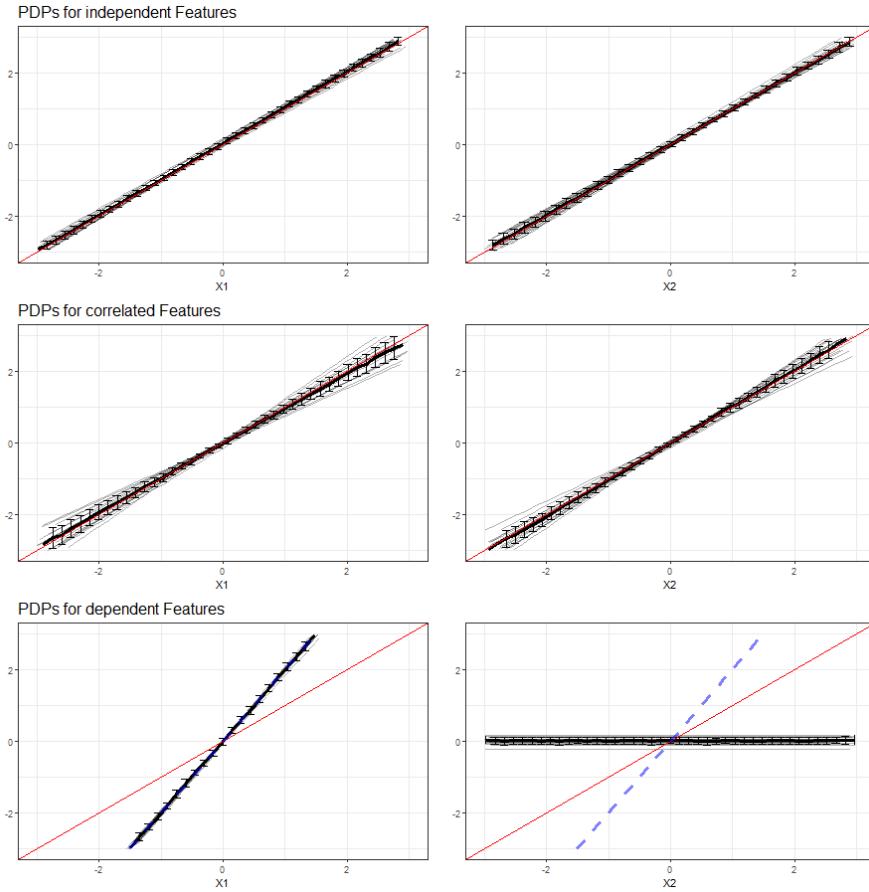


FIGURE 3.19: PDPs for features x_1 (left) and x_2 (right) in Setting 3, based on multiple simulations with LM as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

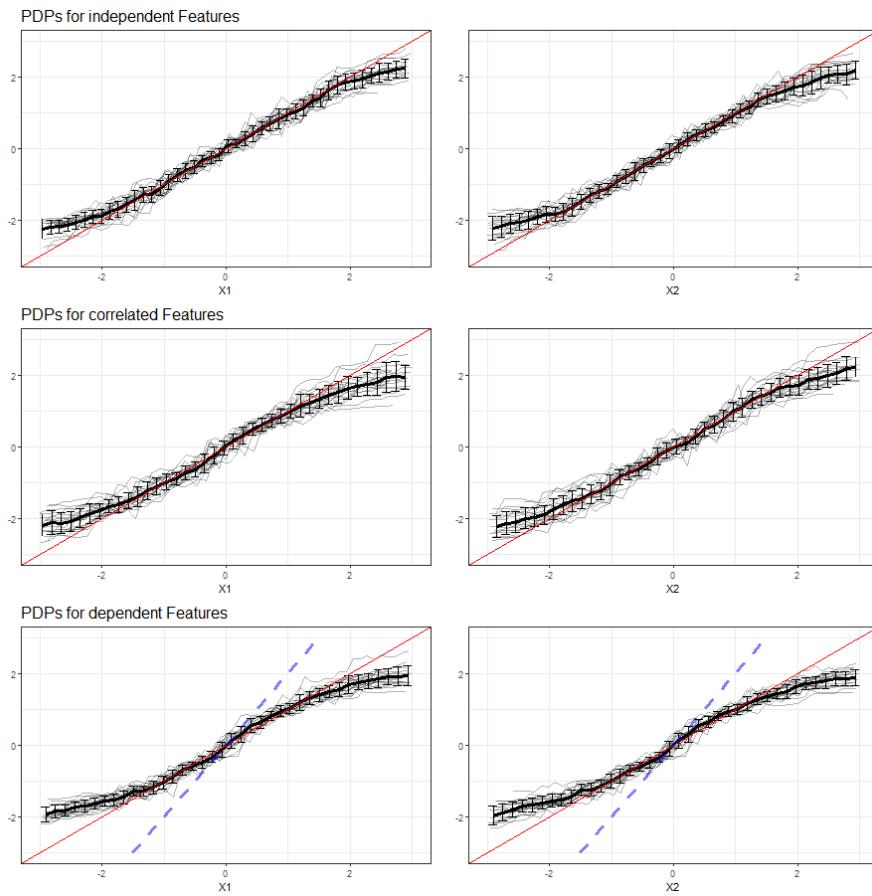


FIGURE 3.20: PDPs for features x_1 (left) and x_2 (right) in Setting 3, based on multiple simulations with RF as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

3.3.4.3 PDPs based on Support Vector Machines

The results of our simulations in setting 3 based on Support Vector Machines are shown in figure 3.21:

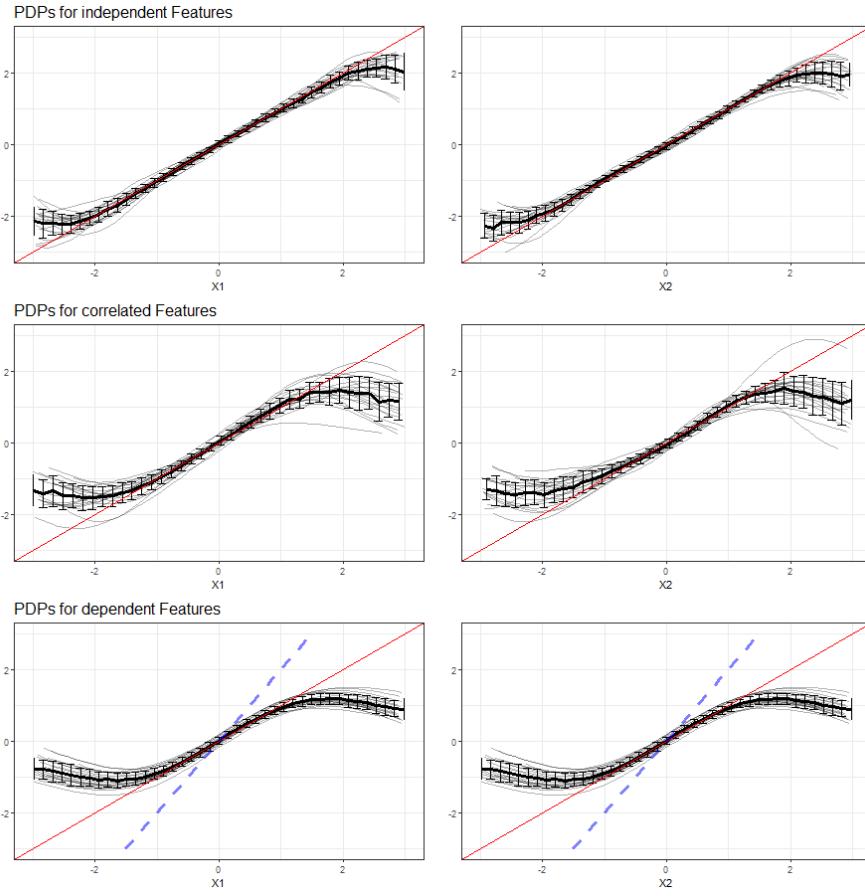


FIGURE 3.21: PDPs for features x_1 (left) and x_2 (right) in Setting 3, based on multiple simulations with SVM as learning algorithm. Top row shows independent case, second row the correlated case and bottom row the dependent case. The red line represents the true effect of the respective feature on y , the blue dashed line is the true common effect of x_1 and x_2 .

Similar to learning based on Random Forest, the SVM learner with missing feature variable x_3 produces a higher variability between the simulated PDP curves. The margin areas, where the PDPs cannot adequately reflect the linear dependence, are broader than in setting (3.10).

In the event of the two remaining features x_1 and x_2 being strongly correlated, the issue of larger variability between the individual simulations aggravates and the ability to reveal the linear effect ceases.

With a perfect multicollinearity of x_1 and x_2 , the variability of the individual PDP curves becomes smaller, but at the same time the models' ability to uncover the true linear effect vanishes. The interval of predicted values is remarkably smaller than in the independent case.

3.3.5 Simulation Settings: Categorical Features

In this chapter we want to investigate the impact of dependencies between two categorical and between a categorical and a numerical feature. For this purpose, we simulate data with a number of 1000 randomly drawn observations and three feature variables, where:

- x_1 categorical variable $\in \{0, 1\}$,
- x_2 categorical variable $\in \{A, B, C\}$,
- x_3 numerical variable with $x_3 \sim N(\mu, \sigma^2)$.

All features are characterized by their linear relationship with the target variable: $y = x_1 + x_2 + x_3 + \varepsilon$.

Again, in order to isolate the individual effects of two dependent features on their respective PDPs, we define three different simulation settings:

1. Independent Case: In this setting, the feature variables are drawn independently from each other, i.e. the observations are randomly sampled with the following parameters:

- $x_1 : P(x_1 = 1) = P(x_1 = 0) = 0.5$
- $x_2 : P(x_2 = A) = 0.475, P(x_2 = B) = 0.175, P(x_2 = C) = 0.35$
- $x_3 : P(x_3 \sim N(1, 1)) = 0.5, P(x_3 \sim N(20, 2)) = 0.5$

The association between x_1 and x_2 can be measured by the corrected contingency coefficient, which is rather low with a value of 0.10. In accordance with the approach in chapter 3.2.3, we calculate the association between x_1 and x_3 by means of the variance-explained measure. With a value of 0.01 we take the independence assumption as confirmed.

2. Dependency between two categorical features: In this setting, x_1 and x_2 are depending on each other, i.e. the observations are randomly sampled with the following parameters:

- $x_1 : P(x_1 = 1) = P(x_1 = 0) = 0.5$
- $x_2 : \begin{cases} P(x_2 = A) = 0.90, P(x_2 = B) = 0.10, P(x_2 = C) = 0, & \text{if } x_1 = 0, \\ P(x_2 = A) = 0.05, P(x_2 = B) = 0.25, P(x_2 = C) = 0.70, & \text{if } x_1 = 1 \end{cases}$
- $x_3 : P(x_3 \sim N(1, 1)) = 0.5, P(x_3 \sim N(20, 2)) = 0.5$

The corrected contingency coefficient of 0.94 confirms a strong association between features x_1 and x_2 .

3. Dependency between categorical and numerical features: In this setting, x_1 and x_3 are depending on each other, i.e. the observations are randomly sampled with the following parameters:

- $x_1 : P(x_1 = 1) = P(x_1 = 0) = 0.5$
- $x_2 : P(x_2 = A) = 0.475, P(x_2 = B) = 0.175, P(x_2 = C) = 0.35$
- $x_3 : \begin{cases} x_3 \sim N(1, 1), & \text{if } x_1 = 0 \\ x_3 \sim N(20, 2), & \text{if } x_1 = 1 \end{cases}$

With a value of 0.986, the variance-explained measure indicates a substantial degree of dependency between x_1 and x_3 .

3.3.5.1 PDPs based on Linear Model

Figure 3.22 shows the PDPs for all feature variables and all simulation settings based on the Linear Model.

Apparently, the Linear Model is robust against our simulated dependencies, since the PDPs of the correlated and dependent features do not differ significantly from those of independent features.

3.3.5.2 PDPs based on Random Forest

Figure 3.23 shows the PDPs for all feature variables and all simulation settings based on Random Forest.

Based on Random Forest, the partial dependence function seems to be impacted much stronger by our simulated dependencies, since the PDPs for dependent variables indicate feature effects which differ from those in the independent case. This is particularly true for a strong association between a categorical and a numerical variable (bottom row of figure 3.23).

3.3.5.3 PDPs based on Support Vector Machines

Figure 3.24 shows the PDPs for all feature variables and all simulation settings based on Support Vector Machines.

In accordance with our findings based on the Linear Model, the predicted effects based on SVM seem to be robust against our simulated dependencies, since the PDPs for the individual settings do not differ significantly from the independent case.

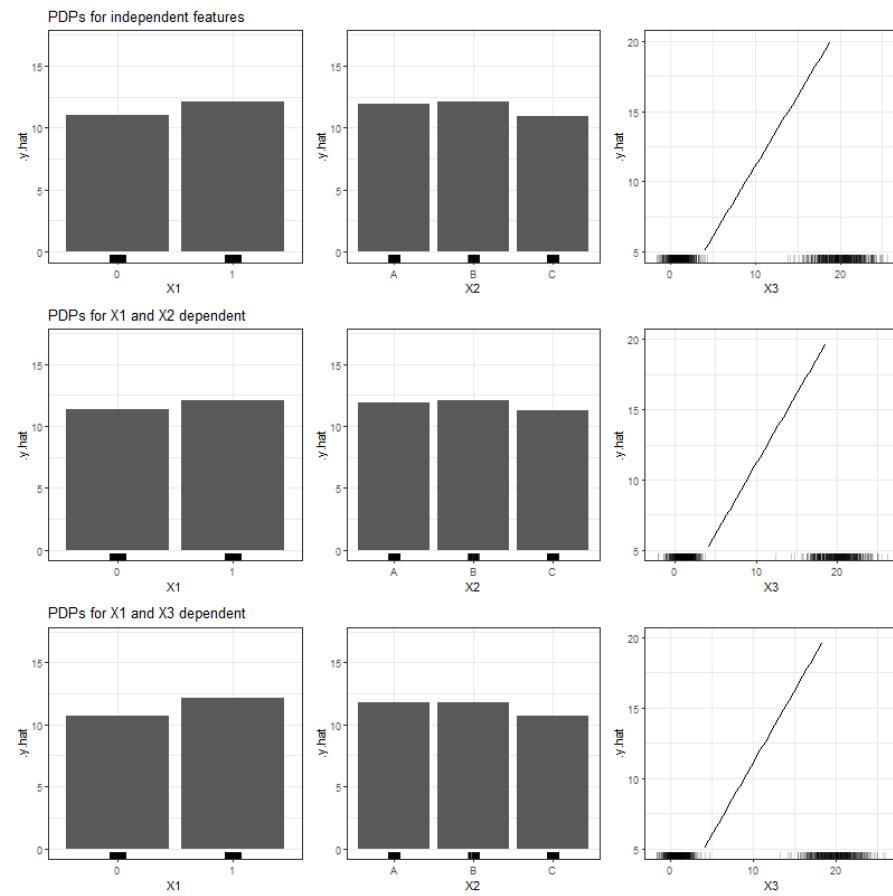


FIGURE 3.22: PDPs for categorical features x_1 , x_2 and numerical feature x_3 (left to right), based on simulated data and LM as learning algorithm. Top row shows independent case, second row the case of two dependent categorical features and the bottom row the case of a numerical feature depending on a categorical feature.

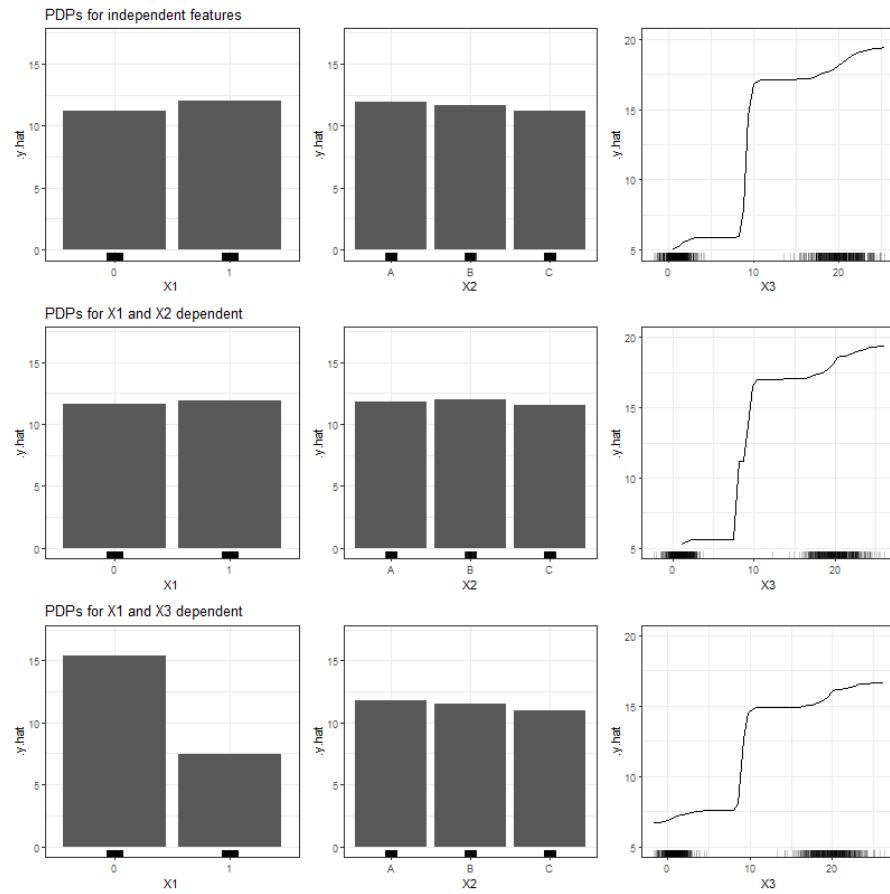


FIGURE 3.23: PDPs for categorical features x_1 , x_2 and numerical feature x_3 (left to right), based on simulated data and RF as learning algorithm. Top row shows independent case, second row the case of two dependent categorical features and the bottom row the case of a numerical feature depending on a categorical feature.

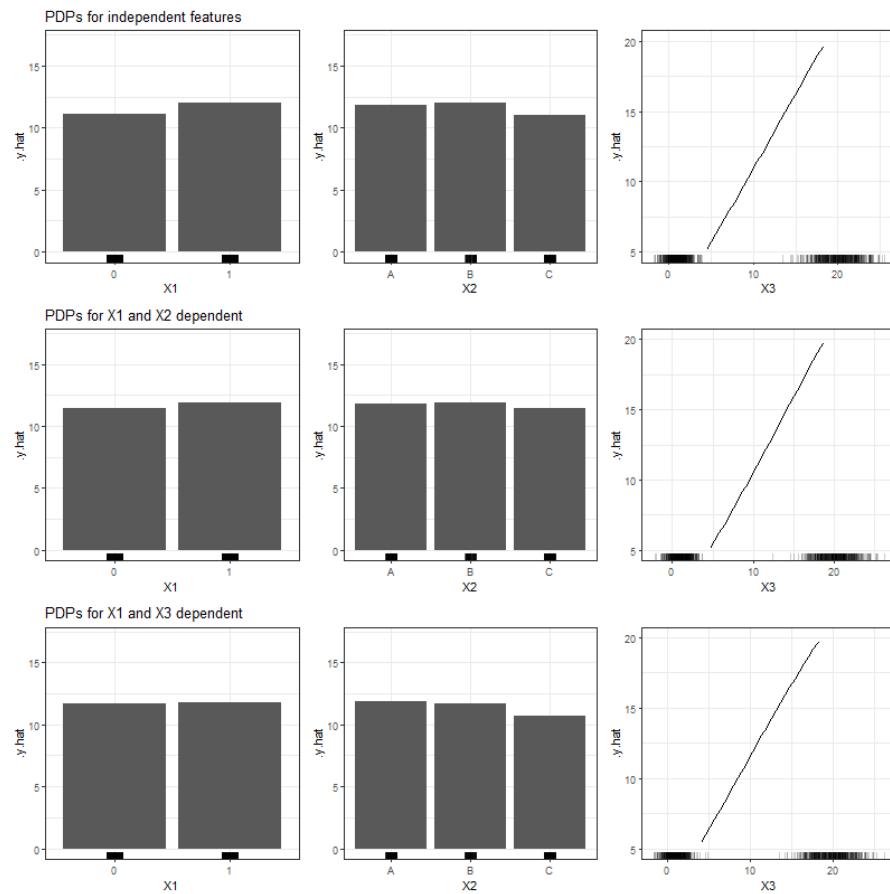


FIGURE 3.24: PDPs for categorical features x_1 , x_2 and numerical feature x_3 (left to right), based on simulated data and RF as learning algorithm. Top row shows independent case, second row the case of two dependent categorical features and the bottom row the case of a numerical feature depending on a categorical feature.

3.4 Extrapolation Problem: Simulation

3.4.1 Simulation based on established learners

In the problem description of this chapter we announced that, in addition to the issue with dependent features, we want to investigate the extrapolation problem and its implications for the computation of partial dependence plots. For this purpose, we use the dataset introduced in chapter 3.1, which was simulated once with x_1 and x_2 independent, and once with both features strongly correlated. Remember that in a next step, the observed data was manipulated by cutting out all observations with $x_1 \in [0, 1.5] \wedge x_2 \in [0, 1.5]$, and thus artificially producing an area with no observations (see figure 3.2).

Now we are looking at the PDPs resulting from these modifications. Figure 3.25 compares the PDP curves derived for both features based on the complete, uncorrelated dataset to its manipulated version with missing values.

The first row of PDPs in figure 3.25, computed on basis of the complete dataset of uncorrelated features, adequately reflects the true effects of x_1 and x_2 (red curves). In the presence of an extrapolation problem, the adequacy of the predicted effects decreases. Especially with the more complex, nonlinear effect of x_1 , extrapolation causes a clearly visible deviation between the partial dependence curves and the true feature effect, irrespective of the learner.

In figure 3.26 we do the same comparison, but this time based on the dataset with strongly correlated features.

From the first row of PDPs in figure 3.26, we again discover the difficulty to obtain reliable PDPs when features are dependent. The results in the bottom row of figure 3.26 are even more striking: with a combination of dependent features and extrapolation, the PDPs come up with estimated effects which are far from the true effects on the prediction. Those deviations seem to occur irrespective of the learning algorithm.

3.4.2 Simulation based on own prediction function

So far, all our analyses were based on the established learning algorithms LM, RF and SVM. We have seen that the choice of the learner does have an impact on the suitability of PDP curves. Obviously there is a countless number of other possibilities to come up with prediction functions other than the ones we have seen. PDPs are prone to fail when this prediction function is doing ‘weird’ stuff in areas outside the feature distribution. This can happen

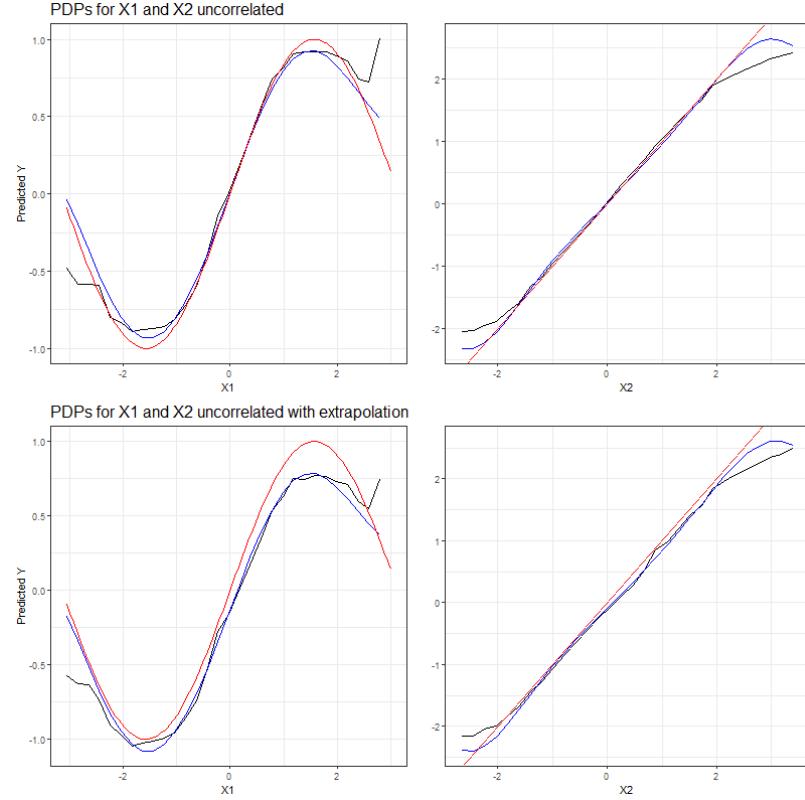


FIGURE 3.25: PDPs for uncorrelated features x_1 (left) and x_2 (right) based on complete simulated dataset (top row) and based on manipulated dataset with missing observations (bottom row). The red curve represents the true effect of the feature for which the PDP is drawn, while the PDPs derived from the machine learning models are represented by curves drawn in black (Random Forest) and blue (SVM).

due to the fact that the learner minimizes the loss based on training data while there is no penalization for extrapolation (Molnar, 2019).

Let's illustrate the issue with an example. Assume we want to predict the size of a potato (\hat{y}) by means of the share of maximum amount of soil (x_1) and the share of maximum amount of water (x_2) available during the process of growing the plant. The feature variables are dependent in the sense that when using a larger amount of soil, the farmer would also use a larger amount of water, i.e. x_1 and x_2 are positively correlated. Typically, the more resources the farmer invests, the larger the crops. The corresponding model is basically a simple linear regression which adds up the two components.

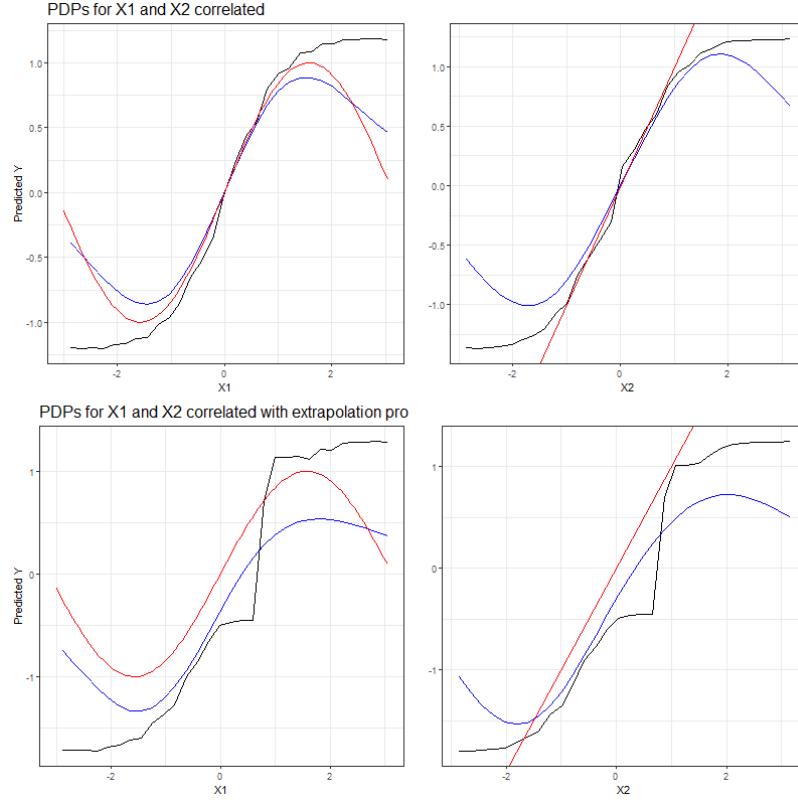


FIGURE 3.26: PDPs for correlated features x_1 (left) and x_2 (right) based on complete simulated dataset (top row) and based on manipulated dataset with missing observations (bottom row). The red curve represents the true effect of the feature for which the PDP is drawn, while the PDPs derived from the machine learning models are represented by curves drawn in black (Random Forest) and blue (SVM).

In the event of improper planting, meaning the usage of a too large amount of water in proportion to the soil (and vice versa), the plant would die and the result would be a potato of size 0. This is exactly what our self-constructed prediction function predicts. Luckily, all farmers in our dataset know how to grow potatoes, therefore there are no such zero cases in the underlying observations. Figure 3.27 illustrates our observations as points and the prediction function as shaded background colour.

In view of the observed data, one would expect to uncover a linear effect of both feature variables when looking at the corresponding PDPs. As we can see in figure 3.28, this is not necessarily the case. While the two-dimensional PDP perfectly depicts the prediction function, the individual PDPs for feature

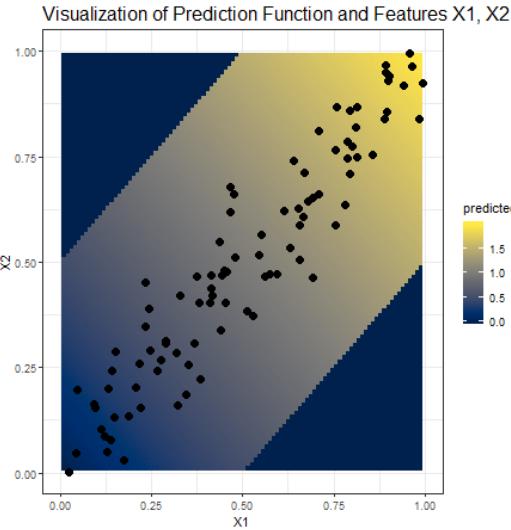


FIGURE 3.27: Visualization of the observed data points ($n=100$) and the self-constructed prediction function. Dark blue background colour indicates a predicted potato size of zero which increases with the brightness of the yellow shaded background colour.

x_1 and x_2 fail in the areas where the prediction function does ‘weird’ stuff compared to what has been observed.

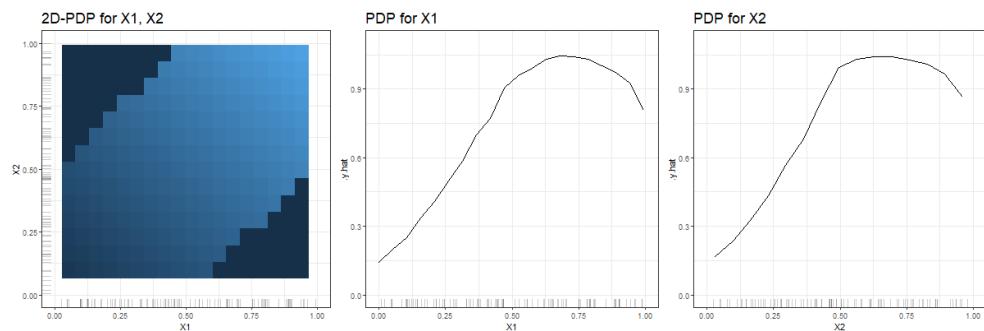


FIGURE 3.28: The first plot shows the two-dimensional PDP for features x_1 and x_2 . The darker the background colour, the smaller the predicted values. The other plots are the PDPs derived for feature x_1 and x_2 respectively. Up to a value of approximately 0.5 both partial dependence curves are mostly linear and bend at larger x_1 - / x_2 -values.

3.5 Summary

Our analysis of partial dependence plots in the context of dependent features and missing values has revealed that both a violation of the underlying independence assumption and the presence of areas with no observations can have a significant impact on the marginalized feature effects. As a consequence, there is a risk of misinterpretation of the effect of features in x_S . Hooker and Mentch (2019) propose to make use of local explanation methods in order to avoid extrapolation. ICE plots, as an example, can be restricted to values in line with the distribution of observed data. However, the authors also point out that this approach cannot serve as a global representation of the learned model (Hooker and Mentch, 2019).

In our simulations, we have also seen cases where the PDP (or the underlying machine learning algorithm) proved to be relatively robust against the dependency of features. Further to the independence assumption, there are also other parameters playing a role for the accuracy of PDPs, like the grid size, the number of observations, the learning algorithm, variance in the data, complexity of the data generating process, etc.

In practical applications it is recommended to analyse the variables used in the model, both by means of correlation and/or association measures and content-wise in liaison with experts having domain knowledge. Furthermore, data scientists can apply methods based on the conditional expectation, such as M-plots or ALE plots. The concept and limitations of the latter will be discussed in chapters 6-8 of this book.

4

PDP and Causal Interpretation

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4.1 Introduction

Machine learning methods excel at learning associations between features and the target. The supervised machine learning model estimates Y using the information provided in the feature set X . Partial dependence plots (PDPs) allow us to inspect the learned model. We can analyze how the model prediction changes given changes in the features.

The unexperienced user may be tempted to transfer this insight about the model into an insight in the real world. If our model's prediction changes given a change on some feature X_j , can we change the target variable Y in the real world by performing an intervention on X_j ?

Of course, this is not generally true. Without further assumptions we cannot interpret PDPs causally (like we cannot interpret coefficients of linear models causally). Curiously, certain assumption sets still allow for a causal interpretation.

In this Chapter we will elaborate on specific assumptions sets that allow causal interpretation and will empirically evaluate the resulting plots. We therefore assume certain data generating mechanisms, also referred to as structural equation models (SEMs), and use Judea Pearl's do-calculus framework to compute the true distributions under an intervention, allowing to e.g. compute the average causal effect. Graphs are used to visualize the underlying dependence structure. We will see scenarios in which the PDP gives the same result as an intervention and scenarios in which the limitations of the PDP as a tool for causal interpretation become clear.

To interpret causally means to interpret one state (the effect) to be the result of another (the cause), with the cause being (partly) responsible for the effect,

and the effect being partially dependent on the cause. (Zhao and Hastie, 2018) formulated three elements that are needed to ensure that the PDP coincides with the intervention effect:

1. A good predictive model which closely approximates the real relationship.
2. Domain knowledge to ensure the causal structure makes sense and the backdoor criterion, explained below, is met.
3. A visualization tool like a PDP (or an Individual Conditional Expectation plot)

The first condition is an important one, because there is a big difference between being able to causally interpret an effect for the *model* and using it as a causal interpretation for the real world. The second condition will make clear when PDPs are the same, and when they are different from interventions on the data. In this chapter we will systematically analyze a number of scenarios in order to see under which conditions PDPs can be causally interpreted or not.

4.2 Motivation

Before we have a look at various scenarios and settings involving interventions, let's look at an exemplary problem. Let's say we have a dataset containing data on the amount of ice-cream consumption per capita and the temperature outside. The temperature is causal for the ice-cream consumption: People eat more ice-cream when temperatures are high than when temperatures are low. Therefore, both quantities are dependent as well. A statistical model learns to use the information in one of the variables to predict the other, as is evident in the plots below.

While the dependence is learned correctly, it would be wrong to interpret the second plot causally. When more ice cream is consumed, it is likely that the temperature is higher. However, consuming more ice cream will not change the amount of ice cream that is being eaten.

This example illustrates the gap between predictive models and causal models. Without further assumptions we cannot interpret effects of changes in features on the model prediction as effects that would be present in the real world. In this simple scenario it is quite clear in which cases a causal interpretation is clear. However, in more complicated scenarios a more elaborate formalization of assumptions under which a causal interpretation is possible are helpful. We will analyze this theoretically in the next section and will empirically evaluate the theoretical findings.

It may be noted that other problems can occur when using PDPs for model

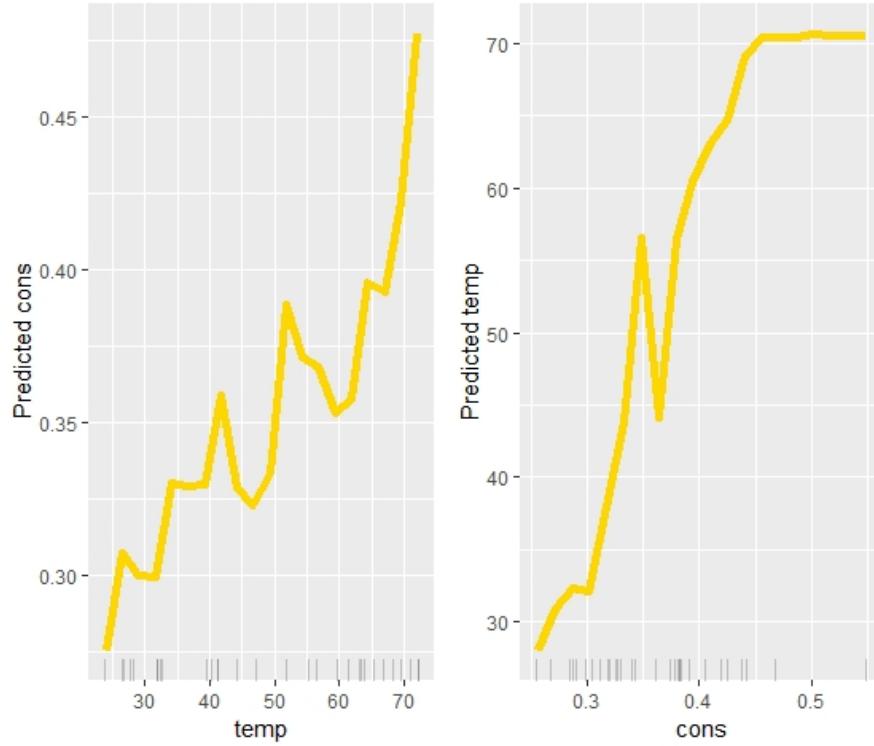


FIGURE 4.1: The PDP on the left shows temperature causing ice-cream consumption. The PDP on the right shows ice-cream consumption causing temperatures. Which one is correct?

interpretation. E.g. as shown by (Scholbeck, 2018), assume we have data that is distributed as follows:

$$Y \leftarrow X_1^2 - 15X_1X_2 + \epsilon \\ X_1 \sim \mathcal{U}(-1, 1), \quad X_2 \sim \mathcal{U}(-1, 1), \quad \epsilon \sim \mathcal{N}(0, 0.1), \quad N \leftarrow 1000$$

Training a Random Forest on this data leads to Figure 4.2 below. Looking at the PDP, one would assume that X_1 has virtually no impact on Y . The ICE curves, however, show that the averaging effect of the PDP completely obfuscates the true effect, which is highly positive for some observations while being highly negative for others. In this example too it would be misguided to simply interpret the PDP causally and state that X_1 does not have any impact on Y whatsoever. This may capture the average effect correctly, but evidently not true on the individual level.

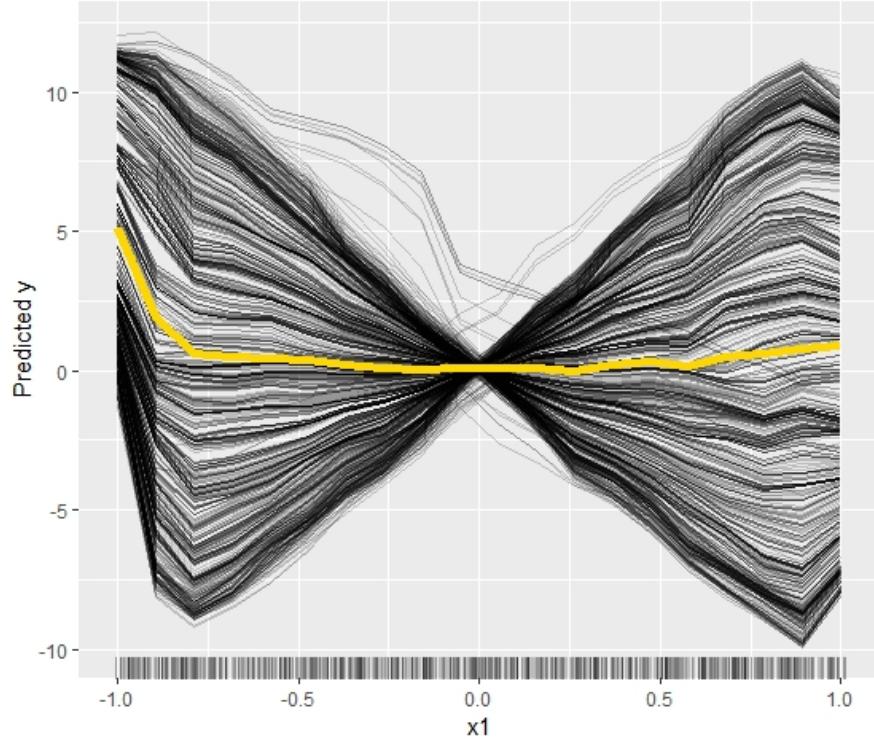


FIGURE 4.2: The average effect of the PDP (yellow line) hides the heterogeneity of the individual effects

4.3 Causal Interpretability: Interventions and Directed Acyclical Graphs

For the rest of the Chapter we will assume we know the structure of the mechanisms underlying our dataset to derive assumptions under which a causal interpretation is possible. With the help of Pearl's do-calculus (Pearl, 1993) we can compute the true causal effect of interventions. Pearl's do-calculus relies on an underlying Structural Equation Model, the structure of which can be visualized with causal graphs. In the structural equation model this is equivalent to removing all incoming dependencies for the intervened variable and fixing a specified value. As an effect, the distributions of variables that are caused by the intervened variable may change as well. For more details refer to (Pearl, 1993). It is important to recognize that an intervention is different

from conditioning on a variable. Therefore the difference between a variable X taking a value x naturally and having a fixed value $X = x$ is reflected in the notation. The latter is denoted by $do(X = x)$. As such, $P(Y = y|X = x)$ is the probability that $Y = y$ conditional on $X = x$. $P(Y = y|do(X = x))$ is then the population distribution of Y if the value of X was fixed at x for the entire population.

In order to avoid complex scenarios (dynamical models, equilibrium computation) we restrict ourselves to causal structures that can be visualized with Direct Acyclical Graphs. A DAG is a representation of relationships between variables in graphical form. Each variable is represented as a *node* and the lines between these nodes, or *edges*, show the direction of the causal relationship through arrowheads. In addition to being directed, these graphs are per definition acyclical. This means that a relationship $X \rightarrow Y \rightarrow Z \rightarrow X$ can not be represented as a DAG. Several examples of DAGs follow in the rest of the chapter, as each scenario starts with one. With regards to interventions, in a graphical sense this simply means removing edges from direct parents to the variable.

In order to know when a causal interpretation makes sense, more is needed than only a representation of a DAG and knowledge of how to do an intervention. An important formula introduced by (Pearl, 1993) addresses exactly this problem: The back-door adjustment formula. This formula stipulates that the causal effect of X_S on Y can be identified if the causal relationship between the variables can be visualized in a graph and X_C , the complementary set to X_S , adheres to what he called the back-door criterion. The back-door adjustment formula is:

$$P(Y|do(X_S = x_S)) = \int P(Y|X_S = x_S, X_C = x_C)dP(x_C)$$

As (Zhao and Hastie, 2018) pointed out, this formula is basically the same as the formula for the partial dependence of g on a subset of variables X_S given output $g(x)$:

$$g_S(x_S) = \mathbb{E}_{x_C}[g(x_S, X_C)] = \int g(x_S, x_C)dP(x_C)$$

If we take the expectation of Pearl's adjustment formula we get:

$$E[Y|do(X_S = x_S)] = \int E[Y|X_S = x_S, X_C = x_C]dP(x_C)$$

These last two formulas are the same, if C is the complement of S .

(Pearl, 1993) defined a back-door criterion that needs to be fulfilled in order for the adjustment formula to be valid. It states that:

1. No node in X_C can be a descendant of X_S in the DAG G .

2. Every “back-door” path between X_S and Y has to be blocked by X_C .

4.4 Scenarios

After these two introductory problems of PDPs, the rest of this chapter will look at PDPs through the causal framework of (Pearl, 1993). This means we will look at various causal scenarios visualized through DAGs and compare the PDPs created under this structure with the actual effect of interventions.

In each scenario nine settings will be simulated for PDP creation, consisting of three standard deviations for the error term (0.1, 0.3 and 0.5) and three magnitudes of observations (100, 1000, 10000). Furthermore, each setting for the PDP was simulated across twenty runs. Each of the nine plots will therefore show twenty PDPs in order to give a solid view of the relationship the PDPs capture for each setting. In addition to the plots of the PDPs, which will be the first three columns in each figure, the actual effect under intervention will be shown in a fourth column as a single yellow line. The true intervention effects (column 4) were all simulated with a thousand observations. Initial tests resulted in a large increase in computation time with a higher number of observations, but with results that hardly differed from those obtained with one thousand observations. For reasons of computational efficiency, we only use out of the box random forest models. In future work, other model classes and hyperparameter settings should be considered, e.g. by using approaches from automatic machine learning.

The process for obtaining the intervention curve was as follows: Let X be the predictor variable of interest with possible values x_1, x_2, x_n and Y the response variable of interest. for each unique $i \in \{1, 2, \dots, n\}$ do

- (1) make a copy of the data set
- (2) replace the original values of X with the value $X_{(i)}$ of X under intervention
- (3) recompute all variables dependent on X using the replacement values as input. This includes Y , but potentially also other features that rely on X for their value. Note that only X is replaced with X_i in the existing equations. Both the equations and error terms remain the same as before.
- (4) Compute the average Y_i in dataset i given X_i .
- (5) (X_i, Y_i) are a single point on the intervention curve.

Scenario 1:

In the first scenario, we have a chain DAG, seen in Figure 4.3. Our variable X is impacted by Z and has a direct effect on Y . Z , however, does not. X_C consists of Z , which is not a descendant of X . There is also no backdoor between

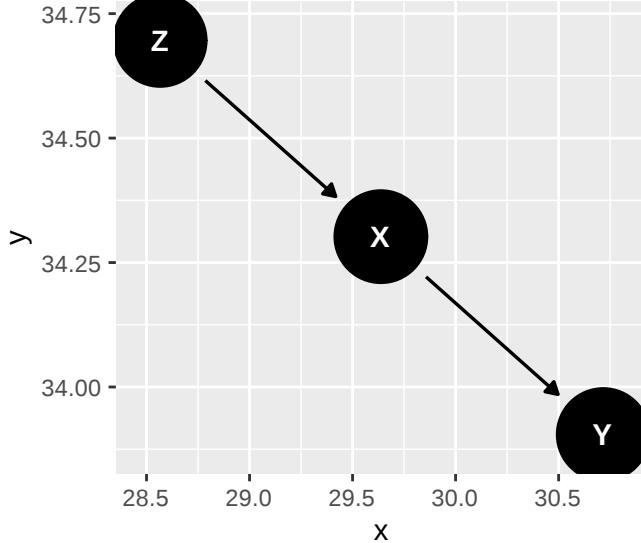


FIGURE 4.3: Chain DAG where X has a direct impact on Y , but is dependent on Z

X and Y . The backdoor criterion is met. In this scenario the expectation is thus that the PDPs should be overall equal to the true intervention. The initial simulation settings for this scenario are as follows:

$$\begin{aligned} Y &\leftarrow X + \epsilon_Y \\ \epsilon_X, \epsilon_Y &\sim \mathcal{N}(0, 0.1), \quad \epsilon_Z \sim \mathcal{U}(-1, 1), \quad Z \leftarrow \epsilon_Z, \quad X \leftarrow Z + \epsilon_X, \quad N \leftarrow 100 \end{aligned}$$

As will be done in all scenarios, both standard deviaton for ϵ and N were varied across 3 levels leading to 9 settings.

Overall the PDPs match the intervention curves fairly well. Outside of the extreme regions of X , where some curvature is present, the linear quality of the intervention curve is evident in the PDPs. Furthermore, the scale of \hat{Y} is comparable to the scale of $Y_{intervention}$ in most settings.

Scenario 2: Chain DAG

In this scenario the DAG again looks like a chain. X has an effect on Y through Z , but no direct relationship between X and Y exists. Note that since Z is a descendant of X , the PDP and intervention curve should not coincide. The initial simulation settings for this scenario are as follows:

$$\begin{aligned} Y &\leftarrow Z + \epsilon_Y \\ \epsilon_Y, \epsilon_Z &\sim \mathcal{N}(0, 0.1), \quad \epsilon_X \sim \mathcal{U}(-1, 1), \quad X \leftarrow \epsilon_X, \quad Z \leftarrow X + \epsilon_Z, \quad N \leftarrow 100 \end{aligned}$$

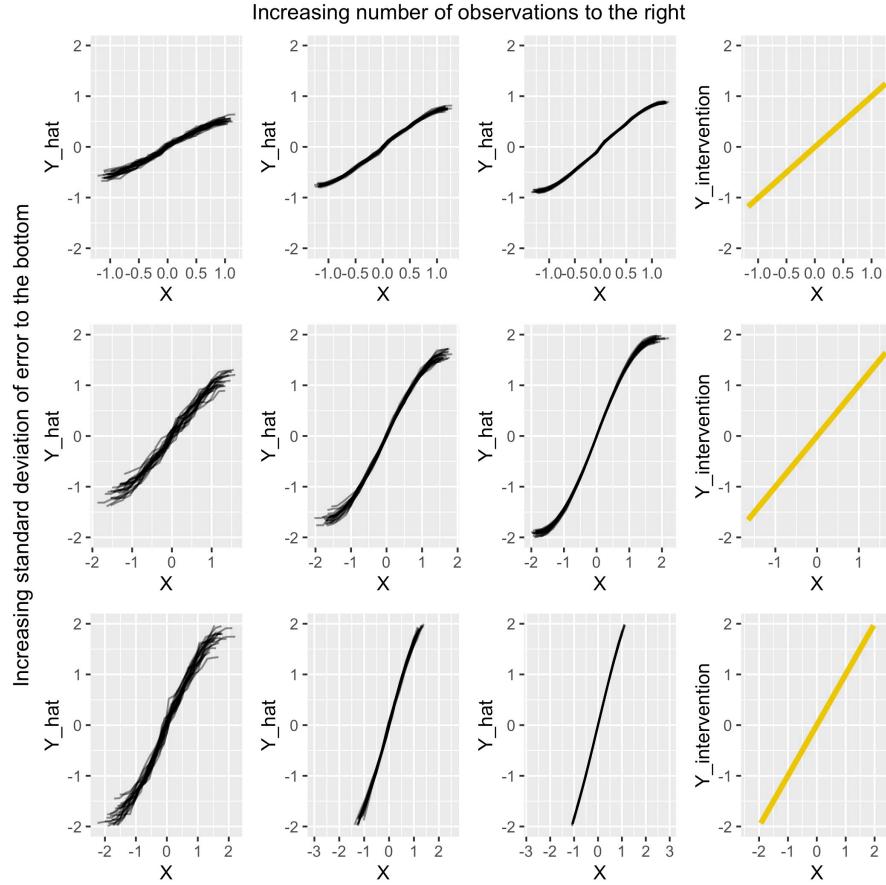


FIGURE 4.4: Comparison for scenario 1 of PDPs under various settings with the (yellow) intervention curve on the right

As can be seen from Figure 4.6, the PDP plots do not match the intervention plots well in several cases. The effect strength is a lot smaller and in fact, four out of nine settings show a negative slope for the relationship between X and Y in comparison to the overall positive slope for the true intervention. The first row performs best, as expected due to the relatively small error that is used. Interesting is also that in the second and third row, where the error has been increased, the PDP slope goes from positive to negative between the first and second column. PDP accuracy thus suffers in situations where the observation count is low. In theory, we would expect the slope to be zero. It remains to be investigated why we still see a trend, and why this trend is negative in some cases.

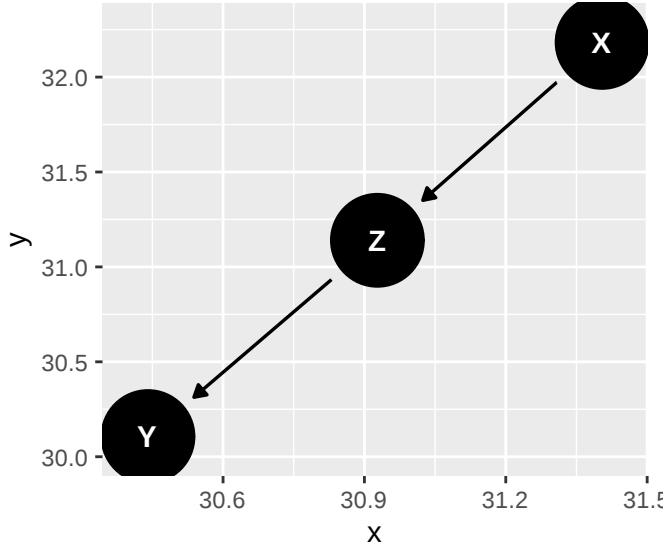


FIGURE 4.5: Chain DAG where X has no a direct impact on Y , but only indirectly through Z

Scenario 3

After two chains, we now have a scenario where X has an influence on both Z and Y directly, as well as Z having an impact on Y , as seen in Figure 4.7. X confounds $Z \rightarrow Y$ here. An example of a confounding variable in real life might be for instance the relationship between the *level of physical activity* and *weight gain*, which is confounded by *age*. *Age* affects both *weight gain* and the *level of physical activity* (on average), making it similar to the X in our scenario here. This scenario is similar to the previous one with only an edge between X and Y having been added. As can be seen from the DAG in 4.7, Z is still a descendant of X . As the backdoor criterion is not met, we cannot expect a causal interpretation to be valid.

The similarity to the previous scenario can also be noted in the simulation settings, where the only difference is the addition of X to the equation for Y .

$$Y \leftarrow Z + X + \epsilon_Y \\ \epsilon_Y, \epsilon_Z \sim \mathcal{N}(0, 0.1), \quad \epsilon_X \sim \mathcal{U}(-1, 1), \quad X \leftarrow \epsilon_X, \quad Z \leftarrow X + \epsilon_Z, \quad N \leftarrow 100$$

The expectation was that the PDP would not show the same results as the true intervention. On first glance in Figure 4.8, the PDPs do not seem to be as inaccurate as they were in scenario 2. An overall upward trend seen in the true intervention on the right is also captured by the PDPs in all settings.

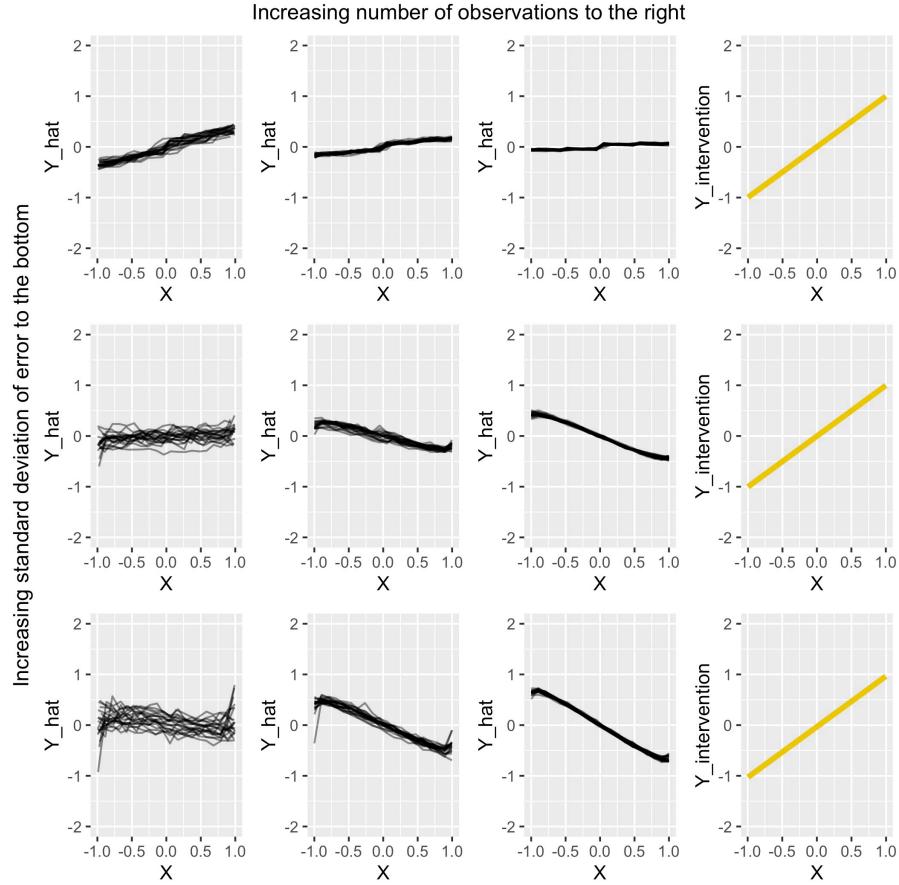


FIGURE 4.6: Comparison for scenario 2 of PDPs under various settings with the (yellow) intervention curve on the right

However, big differences do exist. First of all, the scale of \hat{Y} is off in every setting. This issue gets worse both when the standard deviation of the error increases and when the number of observations is increased. The worst setting is the bottom right, where $N = 10.000$ and the standard deviation of the error is 0.5. The range of \hat{Y} is very small compared to the true intervention next to it and the slope is not steep enough. In fact, the correct slope can only be seen in a very few points: In the top row plot 2 and 3 around $X = 0$ and on the second row plot 3, also around $X = 0$. Overall the result is not as poor as in scenario 2, but a causal interpretation of these plots would lead to a severe underestimation of the impact X has on Y .

Scenario 4

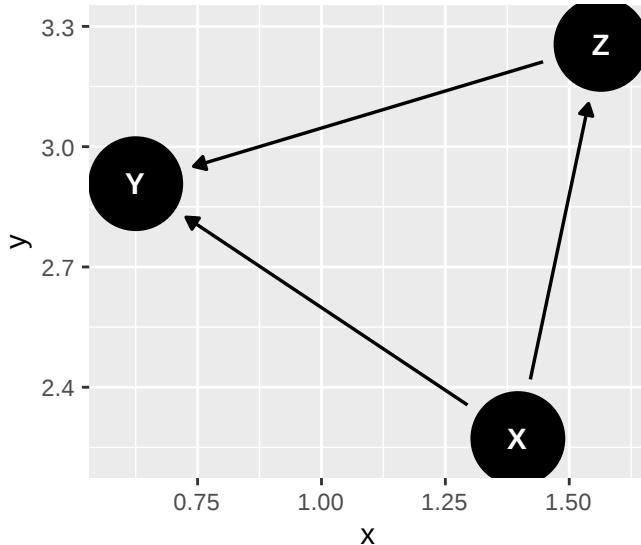


FIGURE 4.7: X is a confounding variable impacting both Z and Y

Scenario 4 consists of a direct effect of X on Y . Z meanwhile is unrelated to both X and Y . It is however included in the simulation and included in the model that is run to create the PDPs. In a non-simulated setting, Z can be seen as a variable that we assume might be related to Y and therefore include, but in actuality has nothing to do with the causal process and should not be included. We will see now how the PDP deals with this kind of variable in the mix.

For the simulation the initial settings look as follows, again increasing both the standard deviation of the error and the magnitude of observations from this starting point.

$$Y \leftarrow X + \epsilon_Y \\ \epsilon_Y \sim \mathcal{N}(0, 0.1), \quad \epsilon_X, \epsilon_Z \sim \mathcal{U}(-1, 1), \quad X \leftarrow \epsilon_X, \quad Z \leftarrow \epsilon_Z, \quad N \leftarrow 100$$

The PDPs in Figure 4.10 are able to capture the intervention curve well. Only in the cases where $N = 100$ is there slight curvature at the extreme ends of X . With this low number of observations the model is less accurate. In all other settings a consistent slope is present from $X = -1$ to $X = 1$, with the scale of \hat{Y} matching that of $Y_{intervention}$.

Scenario 5

In this scenario Z is a confounding variable. This is similar to scenario 3 where X was the confounder. Thinking back to the example of *age* being a confounding variable for *level of physical activity* and *weight gain*, in the previous example our X was comparable to the confounder *age*. In this scenario,

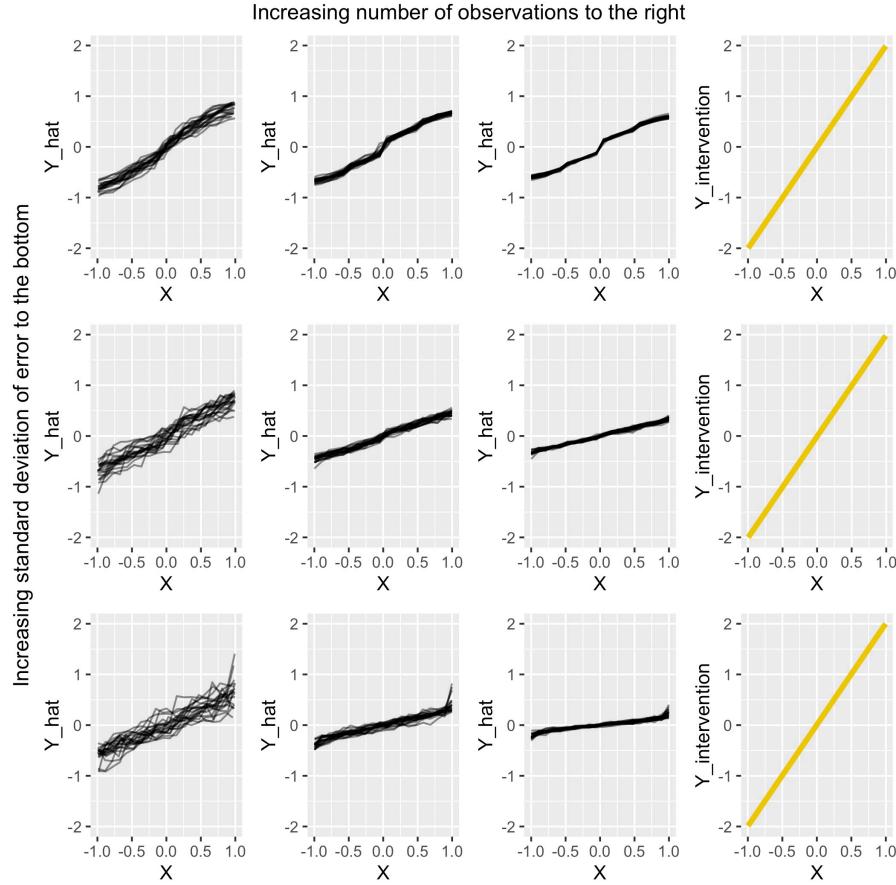


FIGURE 4.8: Comparison for scenario 3 of PDPs under various settings with the (yellow) intervention curve on the right

we can keep the same example, but say our variable X is now comparable to the variable *level of physical activity* that is being confounded. Since X has no descendants and there is no backdoor path, the expectation here is that the PDPs will be similar to the intervention curve.

The following simulation settings were used:

$$Y \leftarrow Z + X + \epsilon_Y \\ \epsilon_Y, \epsilon_X \sim \mathcal{N}(0, 0.1), \quad \epsilon_Z \sim \mathcal{U}(-1, 1), \quad Z \leftarrow \epsilon_Z, \quad X \leftarrow Z + \epsilon_X, \quad N \leftarrow 100$$

We can see in Figure 4.12 that aside from the extreme regions of X where the slope is flatter, the PDPs are fairly similar to the Intervention Curves on the

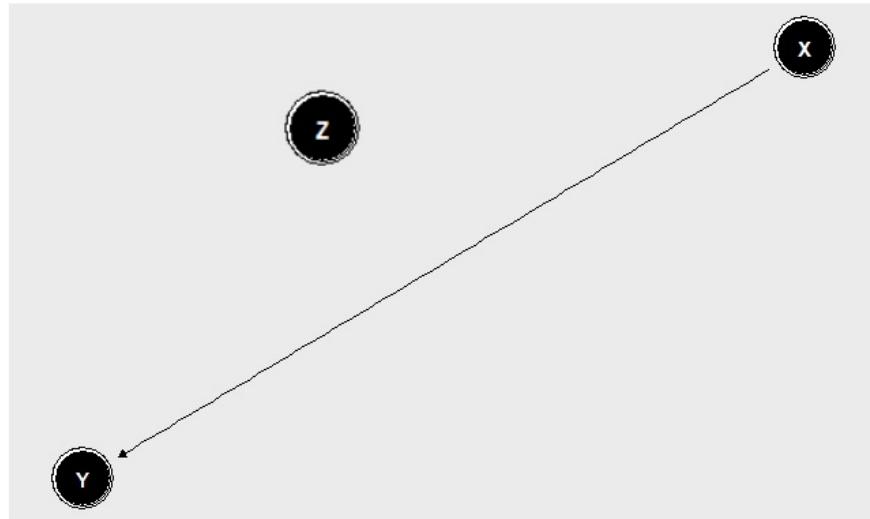


FIGURE 4.9: X directly impacts Y. Z is included in our model, but has no relationship to X or Y

right. We can see that as the standard deviations of the errors increase, so does the range of $Y_{\text{intervention}}$ from $(-1, 1)$ to $(-2, 2)$. This same trend can be observed in the PDPs. As could be expected, the PDPs with the highest number of observations are most accurate and have the lowest standard deviation of errors.

4.5 Conclusion

Causal interpretability of a PDP is dependent on several things: (1) The backdoor criterion being met. We have seen that if the backdoor criterion is met, meaning no variable in the complement set C is a descendant of our variable of interest, the PDP should be the same as the intervention curve. We say should, because in practice it will also depend on: (2) The model fit. Even when the backdoor criterion is met, the PDP might not fully capture the exact same relationship as the intervention curve. Especially in extreme regions, where data is potentially sparse, the PDP can be deceptive. Same in scenarios with a higher(er) error and low number of observations.

Point (2) can be estimated with the standard goodness of fit measures that

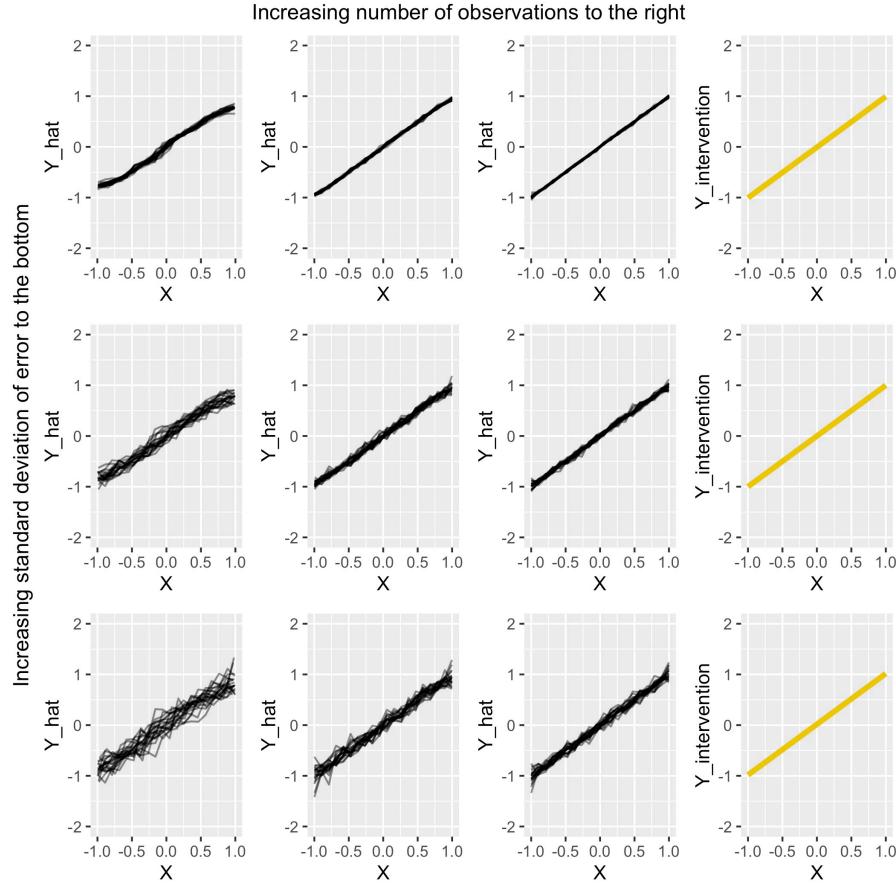


FIGURE 4.10: Comparison for scenario 4 of PDPs under various settings with the (yellow) intervention curve on the right

are pervasive in the statistics literature. It may be noted that models may show a good fit, but do not learn the patterns that we would expect them to learn from a theoretical point of view. Point (1) is even more difficult to verify, especially based on only the data. Here a certain amount of domain knowledge is needed to ensure the assumption is met. Still, it is a hard assumption to verify which could limit the confidence people have in a causal interpretation of a PDP. In the two variable case we may already have difficulty finding a causal interpretation. As we saw with the ice-cream example, the direction of the dependency already makes a large difference. In many cases, the necessary domain knowledge may be hard to attain.

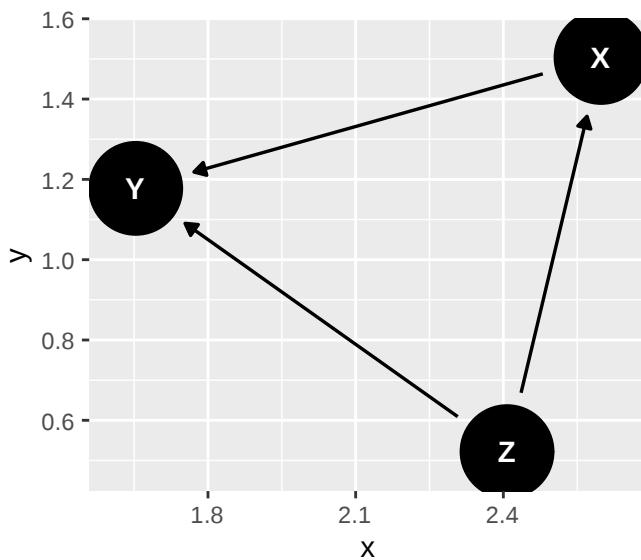


FIGURE 4.11: Z is a confounding variable impacting both X and Y

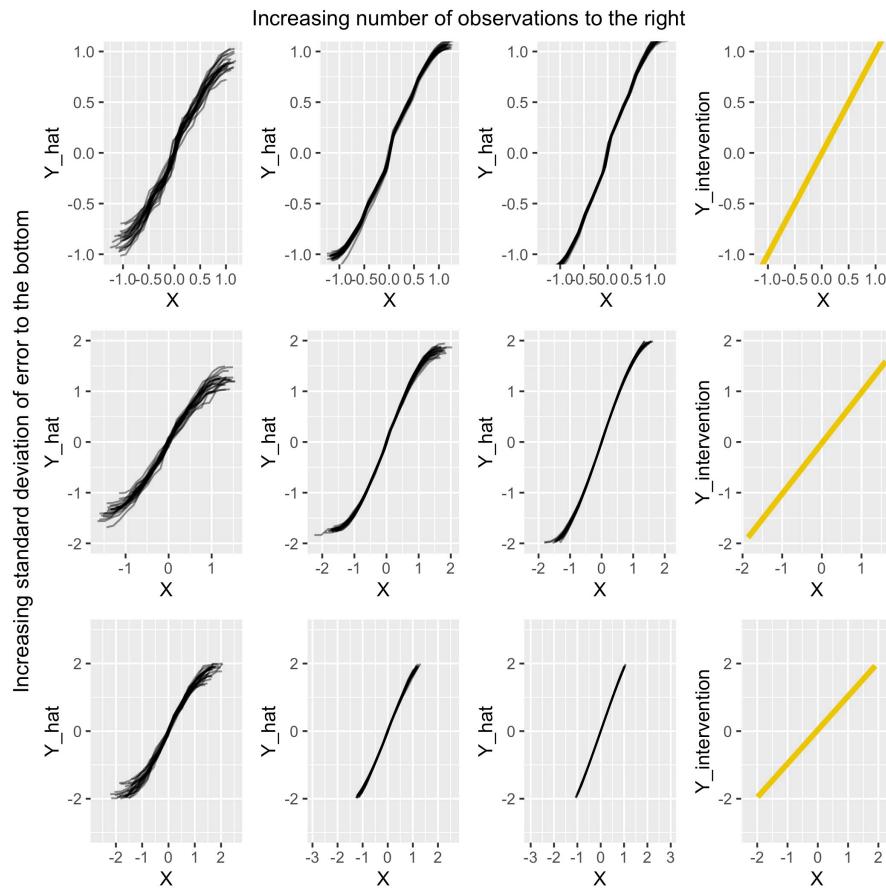


FIGURE 4.12: Comparison for scenario 5 of PDPs under various settings with the (yellow) intervention curve on the right

5

Introduction to Accumulated Local Effects (ALE)

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Supervisor: Christian Scholbeck

5.1 Motivation

As seen in section 2 PDPs don't work well as soon as two or more features are correlated. This gives rise to the definition of ALEs. Although their definition makes sense for high dimensional feature spaces including categorical features, within this section we only treat a space with two continuous features.

5.2 The Theoretical Formula

The uncentered ALE with respect to a starting point $z_{0,j}$ is defined by (Apley, 2016) as

$$\widetilde{ALE}_{\hat{f}, j}(x) = \hat{f}_{x_j, ALE}(x) = \int_{z_{0,j}}^x E_{X_c|X_j}[\hat{f}^j(X_j, X_c) | X_j = z_j] dz_j,$$

where \hat{f} is an arbitrary prediction function, as well as $\hat{f}^j(*, *)$ its j -th partial derivative. In this context X_j is the feature of interest while X_c represents the other features.

5.2.1 Centering

The ALE (centered ALE) is defined as

$$ALE_{\hat{f}, j}(x) = \widetilde{ALE}_{\hat{f}, j}(x) - E_{X_j}[\widetilde{ALE}_{\hat{f}, j}(X_j)]$$

The centering makes sense as it helps to interpret the ALE in a reasonable way. This will be explained in section 5.4.

5.3 Estimation Formula

Since this theoretical formula is of no use for a black box model with unknown or even non-existing gradients, an approximative approach will be used. The uncentered ALE can be approximated by the formula

$$\widehat{\widetilde{ALE}}_{\hat{f}, j}(x) = \int_{z_{0, j}}^x \sum_{k=1}^K \frac{1_{I_k}(x_j)}{n_j(k)} \sum_{i: x_j^{(i)} \in N_j(k)} \frac{[\hat{f}(z_{k, j}, x_{\setminus j}^{(i)}) - \hat{f}(z_{k-1, j}, x_{\setminus j}^{(i)})]}{z_{k, j} - z_{k-1, j}} dx_j .$$

In a first step the relevant dimension of the feature space is divided into K intervals beginning with the starting point $z_{0,j}$. As it is not clear how to exactly divide the feature space, section 3.x deals with that question. The upper boundary of the k-th interval is denoted by $z_{k, j}$ as well as the lower boundary by $z_{k-1, j}$. The half-open interval $]z_{k-1, j}, z_{k, j}]$ is defined as I_k . $N_j(k)$ denotes the k-th interval, i.e. $]z_{k-1, j}, z_{k, j}]$ and $n_j(k)$ the total number of observations having the j-value within this interval. $x_j^{(i)}$ is the j-value of the i-th observation and correspondingly $x_{\setminus j}^{(i)}$ the values of the other features. The term on the right approximates the expected partial derivative within each interval. Therefore each instance within an interval is shifted to the upper and lower limit of the interval and the total difference of the prediction is calculated. Divided by the length of the interval this is a reasonable approximation for the “local” effect on the prediction, if the feature of interest changes (cet. par.). By averaging these approximations over all observations within the k-th interval, we receive a rough estimator for the term $E_{X_c|X_j}[\hat{f}^j(X_j, X_c) | X_j \in N_j(k)]$, which we take as constant effect for the k-th interval. By integrating over this step function, which represents the locally estimated derivatives, the (local) changes are accumulated. That’s why the name Accumulated Local Effects is quite reasonable. The approximative formula for the centered ALE follows directly as

$$\widehat{ALE}_{\hat{f}, j}(x) = \widehat{\widetilde{ALE}}_{\hat{f}, j}(x) - \frac{1}{n} \sum_{i=1}^n \widehat{\widetilde{ALE}}_{\hat{f}, j}(x_j^{(i)}) .$$

5.3.1 Implementation Formula

As both the centered and the uncentered ALE estimations are piecewise linear functions (integration over a step function), one can first calculate the ALE at the interval boundaries and interpolate in a second step. Therefore the following formula proposed by (Apley, 2016, page 11) with slightly changed notation will be useful. The definitions of its components are as above. Additionally $k_j(x)$ is defined as the number of the interval that contains x , i.e. $x \in]z_{k_j(x)-1, j}, z_{k_j(x), j}].$

$$\widehat{\overbrace{ALE}}_{steps, \hat{f}, j}(x) = \sum_{k=1}^{k_j(x)} \frac{1}{n_j(k)} \sum_{i: x_j^{(i)} \in N_j(k)} [\hat{f}(z_{k, j}, x_{\setminus j}^{(i)}) - \hat{f}(z_{k-1, j}, x_{\setminus j}^{(i)})].$$

This formula returns a step function. The values in each interval are the accumulated values of the averaged total differences in each interval. To transfer this formula into the correct estimator of the uncentered ALE one has to linearly interpolate the points $(z_{k-1, j}, \widehat{\overbrace{ALE}}_{steps, \hat{f}, j}(z_{k-1, j}))$ with $(z_{k, j}, \widehat{\overbrace{ALE}}_{steps, \hat{f}, j}(z_{k, j}))$ for $k \in \{1, \dots, K\}$ and $\widehat{\overbrace{ALE}}_{steps, \hat{f}, j}(z_0, j) = 0$.

Since in this formula there is no integral, it is easier to implement.

5.4 Intuition and Interpretation

As the former sections introduced the theoretical basics for the ALE, this section shall provide an intuition as well for the calculation method as for the interpretation. As described above, the local behaviour of the model with respect to the variable of interest is estimated by moving the existing data points to the boundaries of their interval and evaluating the total difference of the prediction for the “new” data points. Figure 5.1 first offered by (Molnar, 2019) gives a good intuition for this procedure.

First one splits the total range of the variable of interest (in this case x_1) to intervals of suitable size.

For each interval the contained data points are moved to the interval boundaries. One gets twice as much “simulated” new data points as originally contained in each interval. The prediction function is now evaluated at these simulated points and the total difference of the prediction (for the given interval) is estimated as the mean change. Divided by the length of the interval one gets an estimation for the partial derivative within this interval. Theoretically one receives the uncentered ALE by integration over this step function.

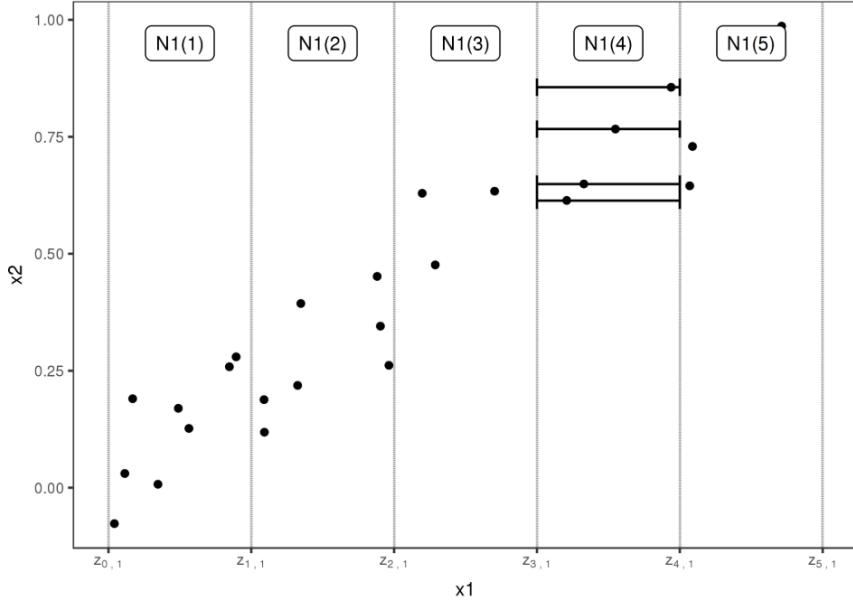


FIGURE 5.1: The data points within the 4-th interval are shifted to the interval boundaries $z_{3,1}$ and $z_{4,1}$.

Technically in a first step the total change per interval is accumulated. In a second step linear interpolation at the interval boundaries simulates a constant change within each interval. Both variants lead to the same result.

As the evaluation is ideally done on relatively small intervals, on the one hand the local behaviour of the model is estimated. On the other hand the covariance structure of the features is taken into account, as only “realistic” data points are simulated. This is in accordance with sampling from the conditional distribution.

In a last step the uncentered ALE is centered, i.e. shifted by a constant such that the expectation of the centered ALE is zero.

Figure 5.2 shows an example ALE which could match the data situation of Figure 5.1.

To understand the interpretation of the ALE it can be useful to first have a look at the intuition behind the uncentered ALE. If the value of the uncentered ALE at $x_1 = 2$ equals 1, this means that if one samples a data point from the joint distribution of both features but only knows that $x_1 = 2$, one would expect the prediction to be 1 higher than the average prediction for realistic data points at $x_1 = z_{0,1}$ (i.e. data points sampled from the conditional distribution at $x_1 = z_{0,1}$). This expectation strongly depends on the reference

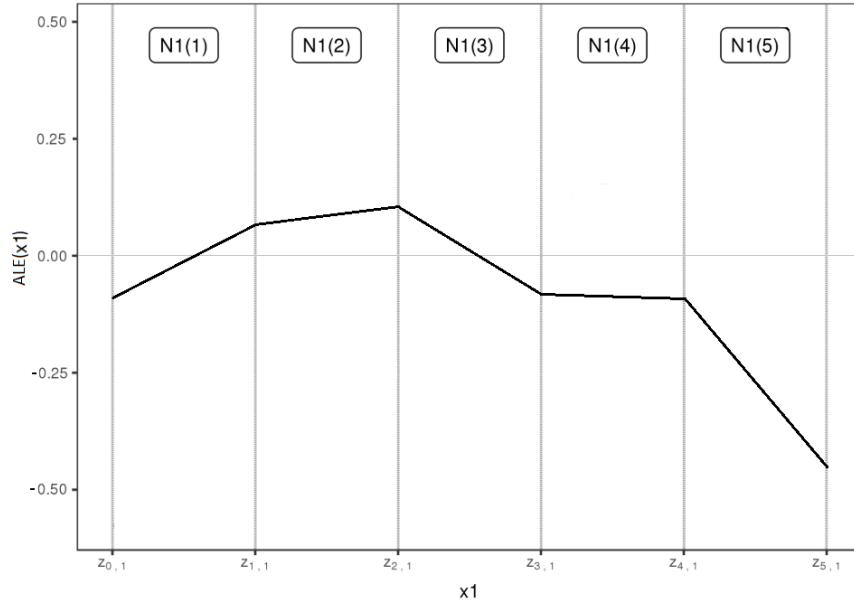


FIGURE 5.2: ALE on basis of 5 intervals

point $z_{0,1}$, which per definition is smaller than the smallest x_1 -value of the data. By subtracting the expectation of the uncentered ALE - which is the mean difference of the prediction of a data point from the joint distribution to the prediction of a realistic data point(i.e. from the conditional distribution) at $x_1 = z_{0,1}$ - the interpretation becomes a lot easier. If the value of the (centered) ALE at $x_1 = 2$ equals for example 2, this means that, if one samples a data point from the joint distribution of both features and x_1 equals 2, one would expect the 1st order effect of feature x_1 to be 2 higher than the average 1st order effect of this feature.

So far only the case of 2-dimensional feature spaces with one feature of interest was taken into account. In the following chapters methods and interpretation for ALE with two numeric features (second order effects) or one categorical feature will be in the focus. Furthermore we will have a look on the size of the intervals the data is evaluated on, which can be crucial for the expressiveness of the ALE.



6

Comparison of ALE and PDP

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This subchapter of ALE will focus on the comparison of ALE and PDP, especially on the influence of correlation in the underlying datasets. At first, the interpretation for the regular one dimensional (or 1D) ALE to the 1D PDP will be discussed. Thereafter two-dimensional ALEs will be introduced and their difference to PDPs will be explained. Additionally, a runtime comparison will be shown and to conclude this chapter a real-world example will be analyzed with ALE, PDP and ICE plots.

6.1 Comparison one feature

So far in this book, one could already see a few examples of the PDP for one feature and its limitations. The ALE is kind of the solution for the biggest issue with the PDP. The ALE can interpret models predicting on correlated variables correctly, while the PDP may fail in this case. Before the two methods will be compared, here comes a short reminder regarding the interpretation.

Given a value for the feature of interest ...

...the 1D PDP measures the expected prediction for this value by averaging over the prediction of all observations pretending the feature of interest is that value.

... the 1D ALE shows the expected and centered first order effect of this feature.

With these interpretations in mind, the first example with artificial data will be discussed.

6.1.1 Example 1: Multiplicative prediction function

The following Problem is constructed: There is a data set consisting of 150 observations with three features (x_1, x_2, x_3) and the target variable $y = x_1x_2x_3$. The features of each observation are sampled from the following distributions: $X_1 \sim \mathcal{U}(0, 0.5)$, $X_2 \sim \mathcal{N}(2, 2)$ and $X_3 | X_2, X_1 \sim \mathcal{N}(X_2, X_1)$.

So features one and two are independent of each other, while x_3 is strongly correlated with x_2 . It is also not independent from x_1 , although there is no influence of x_1 on the expected value of x_3 .

In this example (and in all other examples with artificial data in this chapter) the prediction function is not fitted but sets as the target variable, here $f(x_1, x_2, x_3) = y = x_1x_2x_3$. By setting the prediction function instead of fitting a learner on the data it is ensured that one can imagine how the ‘real’ influence of each feature would look like. This way one can see clearly if ALE or PDP are making mistakes in the interpretation. If one would fit a random forest one could never be sure if the ALE and PDP plots are making a mistake in explaining the fitted model or if the mistake is made by the learner and the explanation of the learner itself would be fine. This will become clear at the end of the chapter when the real-world example will be discussed.

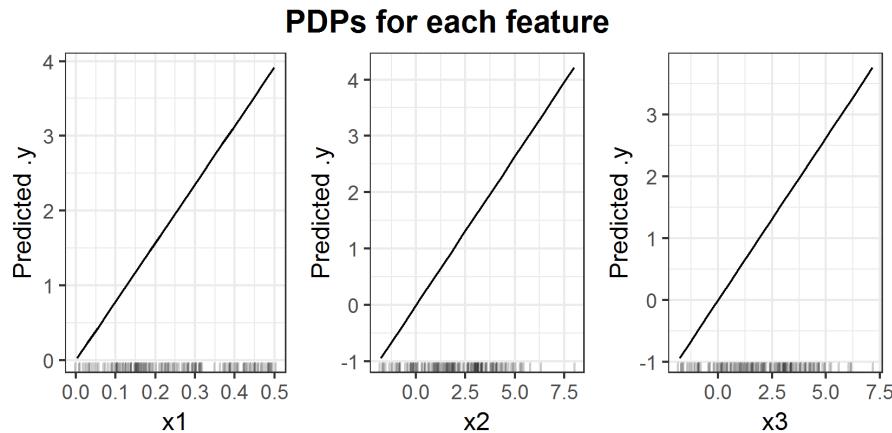


FIGURE 6.1: PDPs for prediction function $f(x_1, x_2, x_3) = x_1x_2x_3$.

Plot 6.1 shows the 1D PDP for each of the three features. One can see that the PDP detects a linear influence on the prediction for all 3 of the features.

On the other hand, the ALE (figure 6.2) attests the linear influence to the feature x_1 only. This plot exposes a weakness of the ALE compared to the PDP straight away. The ALE depends much more on the sampled data than the PDP does. The result is that the ALE can look a bit shaky. In this special case, it is that seriously one almost can’t see the linear influence. If there

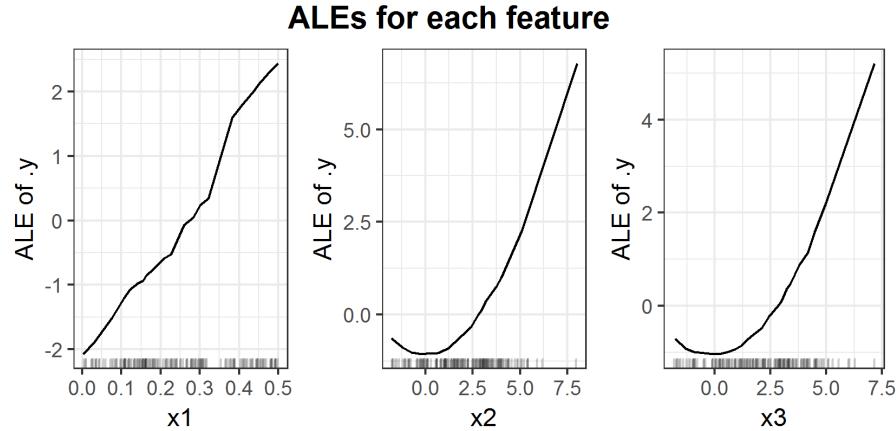


FIGURE 6.2: ALEs for prediction function $f(x_1, x_2, x_3) = x_1x_2x_3$.

would be more data or fewer intervals for the estimation, the plot would look more like the PDP for feature x_1 . The two other features seem to rather have a quadratic influence on the prediction. And this is the case indeed since it is the ‘true’ link between prediction and the correlated features. Feature x_3 has (in expectation) the same value as x_2 . Especially if feature x_1 has small values the variance of feature x_2 around x_3 becomes small as well. As consequence the last part of the prediction function ‘ x_2x_3 ’ can be approximated by ‘ x_2^2 ’ or ‘ x_3^2 ’. This explains the quadratic influence. By changing the prediction formula to $f(x_1, x_2, x_3) = y = x_1x_2^2$ the figures 6.3 and 6.4 for PDP and ALE plots are estimated.

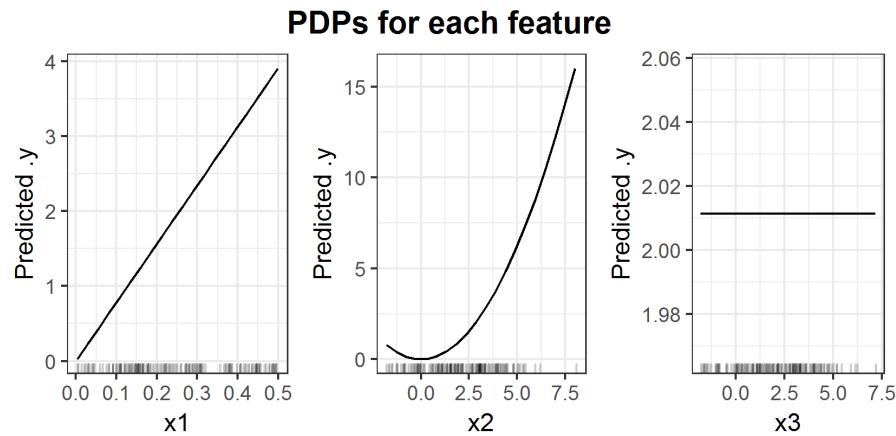


FIGURE 6.3: PDPs for prediction function $f(x_1, x_2, x_3) = x_1x_2^2$.

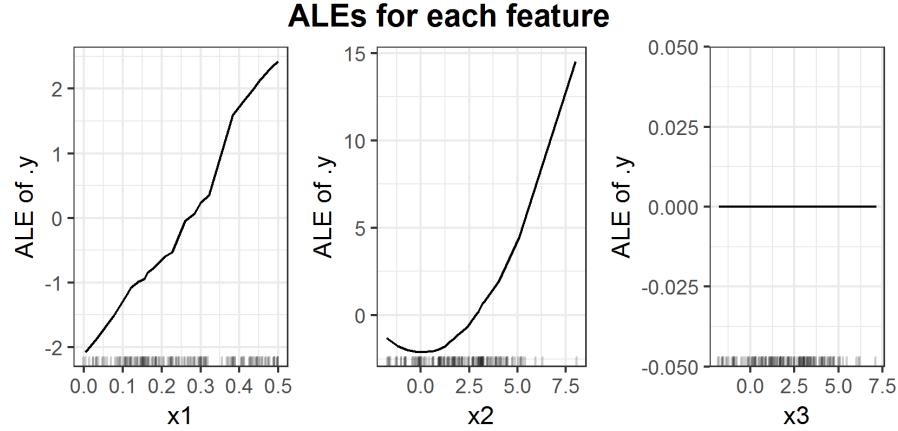


FIGURE 6.4: ALEs for prediction function $f(x_1, x_2, x_3) = x_1 x_2^2$.

Plots 6.3 and 6.4 clearly show the linear influence of x_1 again. Additionally this time both (ALE and PDP) attest a quadratic influence to feature x_2 on the prediction. Since x_3 does not have any influence on the prediction function, it is correct, that there is no influence detected. The reason for this behavior lies in the calculation method for the PDP. With the new prediction formula only depending on uncorrelated features x_1 and x_2 , the PDP works well. Since now the approach of PDP to calculate the mean effect is correct.

6.1.2 Example 2: Additive prediction function

In this example, PDP and ALE will be applied to an additive prediction function.

A data set consisting of three features (x_1, x_2, x_3) is constructed. In this case the target variable is $y = x_1 + x_2 - x_3$. Once again the prediction function is not learned but set to exactly the target variable, meaning $f(x_1, x_2, x_3) = x_1 + x_2 - x_3$. The distributions are similar to the ones from example 1 and again 150 observations are sampled. $X_1 \sim \mathcal{U}(0, 2)$, $X_2 \sim \mathcal{N}(2, 0.5)$ and $X_3 | X_2 \sim \mathcal{N}(X_2, 0.5)$

For this example one can see that the ALEs (6.6) and PDPs (6.5) are basically the same. Ignoring the centering both attest the same linear influence for all three features. And since it is an additive model this is actually correct. But neither the ALE nor the PDP recognize the strong correlation between the features x_2 and x_3 . The real influence of features x_2 and x_3 is in expectation zero, since it is $x_2 - x_3$ and $E[X_3 | X_2] = X_2$. So $E[X_2 - X_3 | X_2] = 0$.

This shows a few points one has to be aware of when working with these plots.

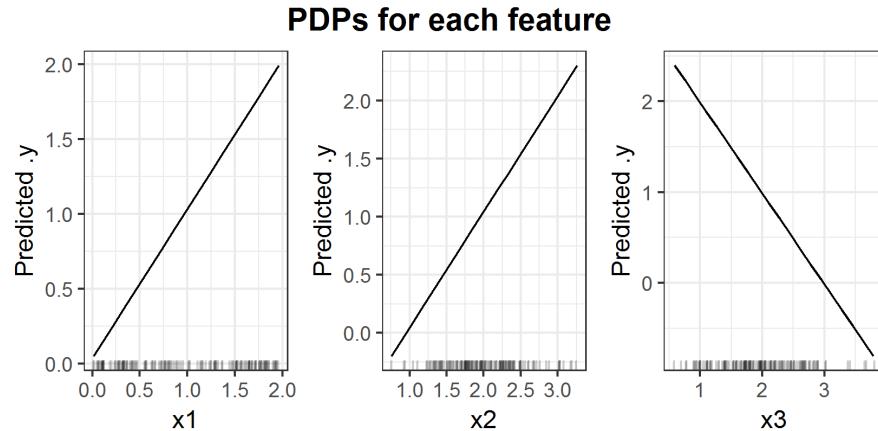


FIGURE 6.5: PDPs for prediction function $f(x_1, x_2, x_3) = x_1 + x_2 - x_3$.

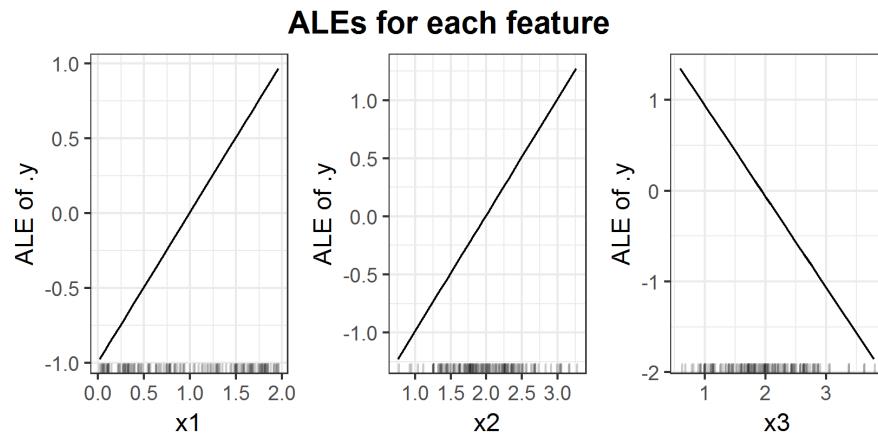


FIGURE 6.6: ALEs for prediction function $f(x_1, x_2, x_3) = x_1 + x_2 - x_3$.

In this example, if one uses the interpretation of the PDP for feature x_2 and states ‘If the value of feature x_2 is 2.5, then I expect the prediction to be 1.5’ it would be wrong. The problem here is the extrapolation in the estimation of the PDP. So it does not take into account any connection between the features but still works as good as the ALE in this example.

The general advantage of the ALE is the small chance of extrapolation in the estimation. But this does not mean it would recognize any correlation between the features in each scenario. And it is in general not possible to state something about the prediction with only one 1D ALE. The ALE is just showing the expected and centered main effect of the feature. In this

example an interpretation like ‘If feature x_2 has value 2.5 then in expectation the prediction will be 0.5 higher than the average prediction’ is wrong. If one needs a statement like that the other strongly correlated features have to be taken into account as well. One has to be aware of the higher order effects of the ALE, too.

To conclude the analysis of this example 2D ALEs are necessary. So it will be continued later this chapter.

6.2 Comparison two features

Before the 2D ALE and PDP will be applied to the same predictors, the 2D ALE has to be introduced. In the first place, the theoretical formula will be defined. Thereafter the estimation will be derived and then the comparison to the 2D PDP will be made.

6.2.1 The 2D ALE

6.2.1.1 Theoretical Formula 2D ALE

Similar to one variable of interest there is a theoretical formula for a 2-dimensional ALE. This ALE aims to visualize the 2nd order effect. Meaning one will just see the additional effect of interaction between those two features. The main effects of the features will not be shown in the 2D ALE.

To explain the formula it will be assumed that x_j and x_l are the two features of interest. The rest of the features is represented by x_c . So in the following variable x_c can be of higher dimension than 1. As for the 1D ALE, there is again a theoretical derivative for the fitted function \hat{f} . But this time it is the derivative in the direction of both features of interest. So in the following, this notation will hold:

$$\hat{f}^{(j, l)}(x_j, x_l, x_c) = \frac{\delta \hat{f}(x_j, x_l, x_c)}{\delta x_j \delta x_l}$$

The whole formula would be very long, so it is split into 3 parts (compare (Apley, 2016, page 8)):

1. The 2nd order effect (6.1)
2. 2nd order effect corrected for both main effects (6.2)

3. The 2D ALE; the corrected 2D ALE centered for its mean overall effect (6.3)

Equation (6.1) is the 2nd order effect with no correction for main effects of x_j and x_l . So this is not yet the pure 2nd order effect the 2D ALE is aiming for.

$$\begin{aligned} \widetilde{\widetilde{ALE}}_{\hat{f}, j, l}(x_j, x_l) = \\ \int_{z_{0,j}}^{x_j} \int_{z_{0,l}}^{x_l} E[\hat{f}^{(j, l)}(X_j, X_l, X_c) | X_j = z_j, X_l = z_l] dz_l dz_j \end{aligned} \quad (6.1)$$

Now from the uncorrected 2nd order effect, the two main effects of both features on the uncorrected 2D ALE are subtracted (see equation (6.2)). In this way the main effects of x_j and x_l on the final $ALE_{\hat{f}, j, l}(x_j, x_l)$ are both zero (Apley, 2016, page 9). But be careful, this is not centering by a constant as in the one-dimensional ALE. This is a correction for the also accumulated main effects which of course vary in the directions of the features.

$$\begin{aligned} \widetilde{ALE}_{\hat{f}, j, l}(x_j, x_l) &= \widetilde{\widetilde{ALE}}_{\hat{f}, j, l}(x_j, x_l) \\ &- \int_{z_{0,j}}^{x_j} E\left[\frac{\delta \widetilde{\widetilde{ALE}}_{\hat{f}, j, l}(X_j, X_l)}{\delta X_j} | X_j = z_j\right] dz_j \\ &- \int_{z_{0,l}}^{x_l} E\left[\frac{\delta \widetilde{\widetilde{ALE}}_{\hat{f}, j, l}(X_j, X_l)}{\delta X_l} | X_l = z_l\right] dz_l \end{aligned} \quad (6.2)$$

Equation (6.3) shows the final (centered) 2D ALE. The subtraction in the formula is now the real centering to shift the 2nd order effect (corrected for the main effects) to zero with respect to the marginal distribution of (X_j, X_l) .

$$ALE_{\hat{f}, j, l}(x_j, x_l) = \widetilde{ALE}_{\hat{f}, j, l}(x_j, x_l) - E[\widetilde{ALE}_{\hat{f}, j, l}(X_j, X_l)] \quad (6.3)$$

In the appendix 6.5.1 one can find the calculation of the theoretical ALE for Example 1.

6.2.1.2 Estimation 2D ALE

Analogously to the 1D ALE in most cases, it is not possible to calculate the 2D ALE. It has to be estimated. These estimation formulas are pretty long and might be confusing, especially the indices. But there will be an explanation including a visualization as well to clarify the estimation method.

First, all variables have to be defined. The two features of interest are x_j

and x_l . The prediction function is $\hat{f}(x_j, x_l, x_{\setminus\{j, l\}})$, while $x_{\setminus\{j, l\}}$ represents all the rest of the features, so it can be of higher dimension than 1. The areas including data for feature x_j and x_l are divided into the same number of intervals, namely K . The intervals in x_j direction are separated by $z_{k,j}$ for $k \in \{0, \dots, K\}$. $k_j(x_j)$ returns the interval number in which x_j lies. This holds for $z_{m,l}$ and $k_l(x_l)$ respectively in direction of x_l . $N_{\{j, l\}}(k, m)$ is the crossproduct of the k-th and m-th interval (in x_j and x_l direction), so it is defined as $(z_{k-1,j}, z_{k,j}] \times (z_{m-1,l}, z_{m,l}]$. $n_{\{j, l\}}(k, m)$ is the number of observations lying in this $N_{\{j, l\}}(k, m)$ cell. The parameter i represents the i-th observation (Apley, 2016). With these variables in mind, the definition of the 2D ALE estimation can begin.

The estimation equivalent to Formula (6.1) is:

$$\widehat{\overbrace{ALE}}_{\hat{f}, j, l}(x_j, x_l) = \sum_{k=1}^{k_j(x_j)} \sum_{m=1}^{k_l(x_l)} \frac{1}{n_{\{j, l\}}(k, m)} \sum_{i: x_{\setminus\{j, l\}}^{(i)} \in N_{\{j, l\}}(k, m)} \Delta_{\hat{f}}^{\{j, l\}, k, m}(x_{\setminus\{j, l\}}^{(i)}), \quad (6.4)$$

while the Δ function is:

$$\begin{aligned} \Delta_{\hat{f}}^{\{j, l\}, k, m}(x_{\setminus\{j, l\}}^{(i)}) &= \\ &[\hat{f}(z_{k, j}, z_m, l, x_{\setminus\{j, l\}}^{(i)}) - \hat{f}(z_{k-1, j}, z_m, l, x_{\setminus\{j, l\}}^{(i)})] \\ &- [\hat{f}(z_k, j, z_{m-1}, l, x_{\setminus\{j, l\}}^{(i)}) - \hat{f}(z_{k-1, j}, z_{m-1}, l, x_{\setminus\{j, l\}}^{(i)})] \end{aligned} \quad (6.5)$$

Now the correction for the main effects (equation (6.6) corresponding to theoretical formula (6.2)) is estimated:

$$\begin{aligned} \widehat{\overbrace{ALE}}_{\hat{f}, j, l}(x_j, x_l) &= \widehat{\overbrace{ALE}}_{\hat{f}, j, l}(x_j, x_l) \\ &- \sum_{k=1}^{k_j(x_j)} \frac{1}{n_j(k)} \sum_{m=1}^K n_{\{j, l\}}(k, m) [\widehat{\overbrace{ALE}}_{\hat{f}, j, l}(z_{k, j}, z_m, l) \\ &\quad - \widehat{\overbrace{ALE}}_{\hat{f}, j, l}(z_{k-1, j}, z_m, l)] \\ &- \sum_{k=1}^{k_l(x_l)} \frac{1}{n_l(k)} \sum_{m=1}^K n_{\{j, l\}}(k, m) [\widehat{\overbrace{ALE}}_{\hat{f}, j, l}(z_k, j, z_{m, l}) \\ &\quad - \widehat{\overbrace{ALE}}_{\hat{f}, j, l}(z_{k, j}, z_{m-1, l})] \end{aligned} \quad (6.6)$$

Equation (6.6) is the uncentered 2D ALE since it is just corrected for its main effects. And this is not a real centering in the sense of subtracting a constant value. Now it will be centered for its estimation $E[\widehat{ALE}_{\hat{f}, j, l}(X_j, X_l)]$ and this is a constant, so there will be no effect on the general shape of the ALE plot. Again this expected value has to be estimated, to complete the 2D ALE as is calculated in theoretical formula (6.3).

$$\begin{aligned} \widehat{ALE}_{\hat{f}, j, l}(x_j, x_l) = \\ \widehat{ALE}_{\hat{f}, j, l}(x_j, x_l) - \sum_{k=1}^K \sum_{m=1}^K n_{\{j, l\}}(k, m) \widehat{ALE}_{\hat{f}, j, l}(z_{k,j}, z_{m,l}) \end{aligned} \quad (6.7)$$

In contrast to the ALE for one feature of interest, the 2D ALE ((6.7)) is a two-dimensional step function, so there is no smoothing or something similar to make it a continuous function.

These formulas are pretty long, so to get an intuition of the estimation figure 6.7 will be helpful.

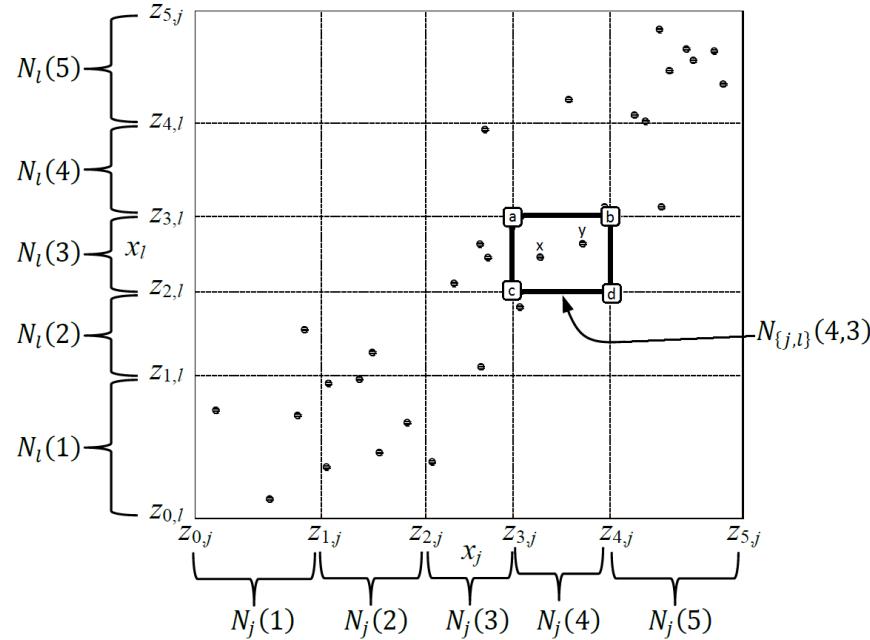


FIGURE 6.7: Visualization of the absolute differences for the 2nd order effect (Apley, 2016, page 13) and (Molnar, 2019).

To calculate the delta (6.5) for the uncorrected and uncentered ALE esti-

mation in each cell the predictions for the data points in that cell will be calculated pretending the x_l and x_j values are the corner values of the cell they are in. In the case of figure 6.7, these 2-dimensional corner values would be a, b, c, d. The delta for point x in this example would be calculated like this:

$$\begin{aligned}\Delta_{\hat{f}}^{\{j, l\}, 4, 3}(x_{\setminus\{j, l\}}) = & [\hat{f}(b, x_{\setminus\{j, l\}}) - \hat{f}(a, x_{\setminus\{j, l\}})] \\ & - [\hat{f}(d, x_{\setminus\{j, l\}}) - \hat{f}(c, x_{\setminus\{j, l\}})]\end{aligned}$$

The same would be done for point y. Thereafter the deltas would be averaged to get the mean delta for cell $N_{\{j, l\}}(4, 3)$. This would then be accumulated over all cells left or beneath this cell to get the uncorrected and uncentered ALE for the values in $N_{\{j, l\}}(4, 3)$.

The correction for the main effects extracts the pure 2nd order effect for the two features of interest by subtracting the main effect of the single features on the ALE (equation (6.6)). To stick with this example the correction for the main effect of feature x_j for values in $N_j(4)$ takes into account all cells in the first 4 columns and aggregates the first order effect. In cell $N_{\{j, l\}}(4, 3)$ this would look like this:

$$\overbrace{\overbrace{ALE}_{\hat{f}, j, l}(b)}^{} - \overbrace{\overbrace{ALE}_{\hat{f}, j, l}(a)}^{} \quad \quad$$

The correction for x_l looks pretty much the same just from the other direction. It takes into account the first 3 rows. So in cell $N_{\{j, l\}}(4, 3)$ the first order effect in direction of x_l would be

$$\overbrace{\overbrace{ALE}_{\hat{f}, j, l}(b)}^{} - \overbrace{\overbrace{ALE}_{\hat{f}, j, l}(d)}^{} \quad \quad$$

Thereafter the corrected ALE is centered for its mean (equation (6.7)), pretty much the same way as is done for one dimension. But this time the aggregation is not just over a line but over a grid.

There are a few questions that might arise.

First, how is the grid for the estimation defined? In the iml package, the cells are the cross products of the intervals used for the 1D estimation. It would be very hard to make a grid of rectangles which all include roughly the same amount of data points.

Another question is: How does the estimation treat empty cells, which include no data points? There are two options, they can either be ignored and greyed out or they receive the value of their nearest neighbor rectangle, which is determined using the center of the cells. The last method is implemented in the

iml package. This happens right after averaging over the $\Delta_{\hat{f}}^{\{j, l\}, k, m}(x_{\setminus \{j, l\}})$ s before the correction for the 1st order effects is done.

6.2.1.3 Example 1 continued - Theoretical and estimated 2D ALE

Before ALE and PDP will be compared for two features of interest, the analysis of example 1 will be continued in two dimensions, to get a first glance at the 2D ALE.

The data set is basically the same, just for sake of clearness in the 2D ALE example the distributions are a bit different. A data set consisting of 150 observations with three features (x_1, x_2, x_3) and the prediction function $f(x_1, x_2, x_3) = x_1 x_2 x_3$ is considered. But this time the three features are sampled from these distributions: $X_1 \sim \mathcal{U}(0, 0.5)$, $X_2 \sim \mathcal{N}(5, 1)$ and $X_3 | X_2, X_1 \sim \mathcal{N}(X_2, X_1)$. So feature x_2 is expected to be 5 and has a lower variance than it has in example 1. The rest stays the same.

With the formulas in the appendix 6.5.1 it is possible to calculate the theoretical 2D ALE.

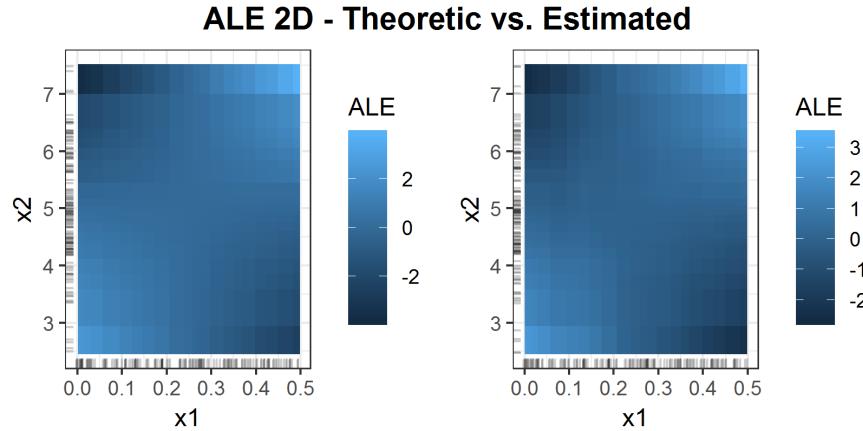


FIGURE 6.8: Theoretical 2D ALE (left) and estimated ALE (right).

Figure 6.8 shows the theoretical ALE compared to the estimated one. In this example, it looks pretty similar. The interpretation is a bit hard. Since one can only see the 2nd order effects, isolated from the 1st order effects, it is hardly possible to state something reasonable about the prediction with just this plot. But this problem will be discussed in the coming up chapter.

6.2.2 2D ALE vs 2D PDP

In this Chapter, only 2D plots for artificially constructed examples will be analyzed. To show the statement, that there are no main effects in the 2D ALE example 2 will be discussed again.

6.2.2.1 Example 2 - 2D comparison

Just a short reminder of example 2: the prediction function here is $f(x_1, x_2, x_3) = x_1 + x_2 - x_3$ and x_2 and x_3 are strongly positive correlated (they even share the same expected value).

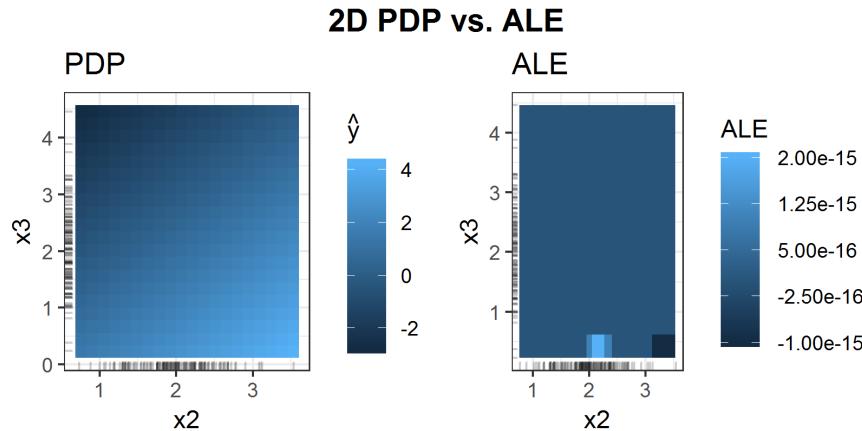


FIGURE 6.9: 2D PDP (left) vs. 2D ALE (right) for prediction function $f(x_1, x_2, x_3) = x_1 + x_2 - x_3$.

Figure 6.9 shows the direct comparison of 2D PDP and 2D ALE. The ALE is almost completely zero as expected. In this additive example, there are main effects only and since the 2D ALE is corrected for the main effects of the features, there is no pure 2nd order effect. The PDP in comparison shows the mean prediction. So, of course, there are the main effects estimated within the 2D PDP as well. Obviously, it is hard to compare those two interpretation algorithms just like this.

To get a better comparison the main effects (1D ALEs) of the two features of interest can be added to the 2D ALE.

Plot 6.10 shows the ALE added up with the corresponding 1st order effects of the features. And now it seems pretty much the same as the PDP in figure 6.9. On the right side, the same plot can be seen. This one additionally includes the underlying data points regarding features x_2 and x_3 . Furthermore these two features are independent of feature x_1 , so the PDP and ALE yield the

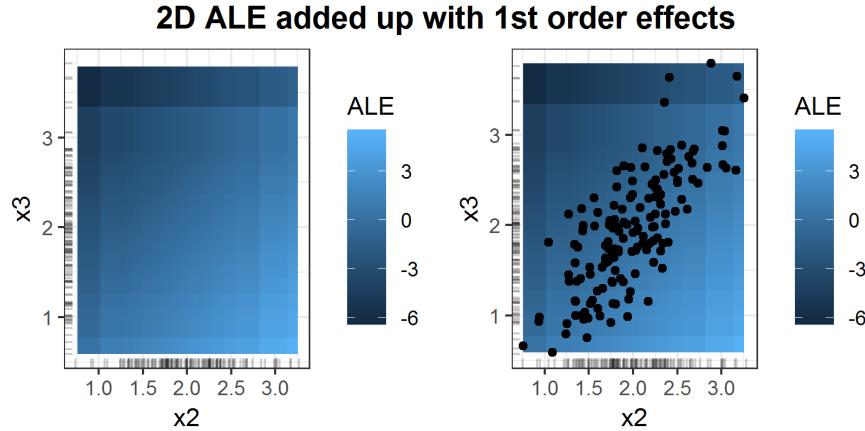


FIGURE 6.10: 2D ALE added up with 1st order effects of features x_2 and x_3 for prediction function $f(x_1, x_2, x_3) = x_1 + x_2 - x_3$. In the right plot the underlying 2 dimensional data points are included.

same correct interpretation, namely for realistic data points the influence of these two features is close to zero because of their strong positive correlation and their opposing first order effects (figures 6.6 and 6.5).

With this in mind, example 1 deserves another look regarding the 2nd order effect in comparison to the PDP.

6.2.2.2 Example 1 - 2D comparison

To be able to compare the 2D ALE from the last chapter for prediction function $f(x_1, x_2, x_3) = x_1 x_2 x_3$ with the 2D PDP one also should add up the 1st order effects to the 2D ALE.

This plot 6.11 shows exactly what happens in this case, when the 1st order effects of the ALE are added up to the 2nd order effects. One can see that although the connection between x_2 and x_3 has been detected by the 1st order ALEs (figure 6.2) and has not been by the 1D PDPs (figure 6.1), the comparable 2D plots look pretty much the same.

In these two examples, it seems like the 2D ALE is not that much better than the ALE. But making just a small change to the prediction function for unrealistic values (regarding the underlying data) exposes the sensitivity of the PDP estimation for extrapolation.

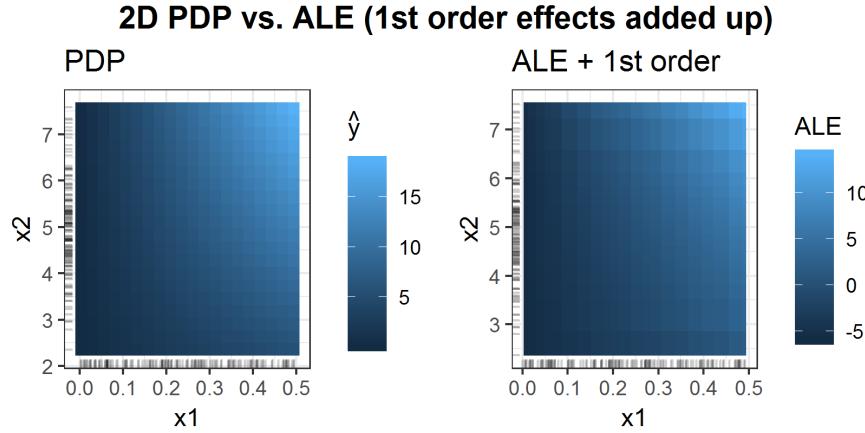


FIGURE 6.11: 2D PDP vs 2D ALE with added up 1st order effects of features x_1 and x_2 for prediction function $f(x_1, x_2, x_3) = x_1 x_2 x_3$.

6.2.2.3 Example 1 modified - 2D comparison

The setting of the problem stays basically the same. Just a small - for the real prediction actually irrelevant - change is made for the prediction function. It is not anymore $f(x_1, x_2, x_3) = x_1 x_2 x_3$ but

$$f(x_1, x_2, x_3) = \begin{cases} x_3^3, & \text{if } x_3 \geq 6, \quad x_2 \leq 4 \\ x_1 x_2 x_3, & \text{else} \end{cases}$$

This seems a bit unrealistic but especially tree-based predictors tend to do ‘strange’ things in areas without data.

The result of the 2D PDP compared to the ALE (figure 6.12) shows the problem. In the area where $x_2 < 4$ the values of the PDP are huge, since the big values for x_3^3 if $x_3 > 6$ increase the average drastically. These values are very unlikely for the underlying distribution but the PDP pretends them to be possible. This is the problem of the extrapolation in the PDP estimation. This is not a problem for the ALE. Here one can not recognise any difference to figure 6.11, where the prediction function is just $f(x_1, x_2, x_3) = x_1 x_2 x_3$.

One big advantage of the ALE in general over the PDP is, that it hardly extrapolates in the estimation, which is usually the case for the PDP with correlated features. And one can take a look at separated 1st and 2nd order effects, which can be very helpful, especially for real black-box models with complicated links. Furthermore, in the next chapter, the runtime will turn out to be a strong advocate for the ALE, especially for bigger datasets.

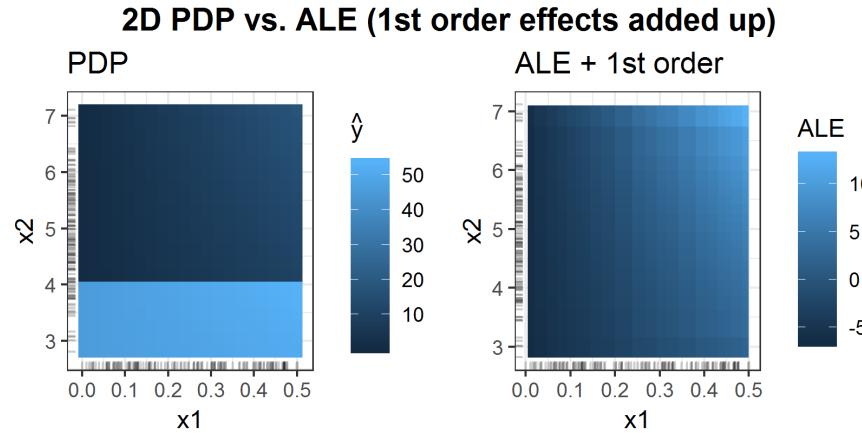


FIGURE 6.12: 2D PDP vs 2D ALE with added up 1st order effects of features x_1 and x_2 for stepwise prediction function.

6.3 Runtime comparison

In this chapter, the runtime of ALE and PDP will be compared. Therefore three general sizes of data sets have been sampled. One small with 100, a bigger one with 1,000 and the biggest with 10,000 observations. The number of features varies between 5 and 40, while there are always 2 categorial features and the others are numeric, as is the target variable. The predictor applied to these datasets is a regular SVM. It is way faster than the random forest, where the PDP estimation can easily take half a minute for just 1,000 observations.

To compare the runtime, the package ‘microbenchmark’ has been used. So the discussed results will all have the same structure, which will be explained with the first example. The comparison will cover the runtime for...

1. ...one numerical feature of interest
2. ...two numerical features of interest
3. ...one categorial feature of interest.

Each of these three will be compared for the different numbers of observations of course but also for different grid sizes (number of intervals the ALE and PDP are estimated on) and varying feature numbers.

	expr	min	1q	mean	median	uq	max
ale_one_numeric(svm.regr_100_5, grid.size = 20)	24.09772	25.10064	27.93897	25.61052	26.09577	50.07771	
ale_one_numeric(svm.regr_100_5, grid.size = 100)	24.34445	25.21641	26.49333	26.39217	27.42753	28.73137	
ale_one_numeric(svm.regr_100_20, grid.size = 20)	27.86269	28.64762	30.28864	29.21169	29.99293	39.79352	
ale_one_numeric(svm.regr_100_40, grid.size = 20)	31.33290	31.73933	32.28661	32.32987	32.74390	33.51898	
pdp_one_numeric(svm.regr_100_5, grid.size = 20)	33.32972	33.64870	34.82019	34.99196	35.50471	37.14067	
pdp_one_numeric(svm.regr_100_5, grid.size = 100)	150.27871	156.29749	180.45355	159.76052	165.38951	375.44635	
pdp_one_numeric(svm.regr_100_20, grid.size = 20)	46.15961	46.84192	50.44029	47.15494	53.05118	68.87754	
pdp_one_numeric(svm.regr_100_40, grid.size = 20)	59.72271	61.04831	64.69805	64.42924	67.95549	71.26888	

FIGURE 6.13: Runtime comparison ALE vs. PDP for one numeric feature. Differences for the number of features and grid size.

6.3.1 One numerical feature of interest

Figure 6.13 shows the runtimes for different configurations in milliseconds. The microbenchmark output shows the compared expressions (here the calculation of ALE and PDP) in the first column. The other columns are the measured runtime for 10 different runs. From left to right it is the minimum runtime, the lower quantile of the runtimes, the mean, the median, the upper quantile, and the maximal runtime. The main attention usually lies in the mean. In the expression, there are also configurations for the sampled dataset integrated. For example ‘ale_one_numeric(svm.regr_100_5, grid.size = 20)’ represents the following estimation: An ALE for one numeric feature of interest has been estimated. The prediction function was an SVM, fitted and evaluated on a sample of 100 observations with 5 features. The grid size, in this case, was 20, so the plots are estimated on 20 intervals.

Plot 6.13 shows the comparison for a change in grid size and number of features for one numeric feature of interest. It seems like the number of features does barely influence the runtime. Additionally for the ALE the grid size is not significantly changing the runtime.

That is completely different for the PDP. Here a factor 5 for the number of intervals increases the runtime by the same factor. This can be derived from the estimation. The ALE does the same number of predictions for any number of intervals, namely $\#observations \times 2$. It just averages more often for more intervals. But that happens without the prediction function and is just a simple mean calculation, so it barely needs time. The PDP, on the other hand, estimates the mean prediction for each interval border. So here $(\#intervals + 1) \times \#observations$ predictions have to be calculated. So the runtime grows linearly with the grid size and factor $\#observations$. This is also the explanation for the next comparison (figure 6.14). Here again, one can see a way faster increase of runtime for PDPs than for ALEs when increasing the number of observations

	expr	min	lq	mean	median	uq	max
ale_one_numeric(svm.regr_100_5, grid.size = 20)	24.97954	25.20369	25.60247	25.25007	25.93032	26.64875	
ale_one_numeric(svm.regr_1000_5, grid.size = 20)	57.18522	58.29160	58.56108	58.87333	58.96775	59.48748	
ale_one_numeric(svm.regr_10000_5, grid.size = 20)	589.31907	599.62174	608.06454	610.89367	613.74644	626.74178	
pdp_one_numeric(svm.regr_100_5, grid.size = 20)	34.61756	34.62782	37.87758	35.34091	41.60478	43.19682	
pdp_one_numeric(svm.regr_1000_5, grid.size = 20)	487.69353	491.54431	535.51957	491.91666	500.33992	706.10344	
pdp_one_numeric(svm.regr_10000_5, grid.size = 20)	7587.24507	7814.43991	7818.31926	7861.48914	7887.19573	7941.22643	

FIGURE 6.14: Runtime comparison ALE vs. PDP for one numeric feature. Differences for the number of observations.

	expr	min	lq	mean	median	uq	max
ale_two_numeric(svm.regr_100_5, grid.size = 20)	93.94821	94.71877	123.8936	96.28515	100.1743	363.1177	
ale_two_numeric(svm.regr_100_5, grid.size = 100)	143.62155	155.37914	183.5492	158.31669	171.4674	393.0446	
ale_two_numeric(svm.regr_100_20, grid.size = 20)	103.39030	103.99922	110.3022	107.97028	109.6629	137.5974	
ale_two_numeric(svm.regr_100_40, grid.size = 20)	108.09796	110.97372	117.8499	113.98701	124.4461	137.2846	
pdp_two_numeric(svm.regr_100_3, grid.size = 20)	605.95540	618.88628	693.3990	629.42459	844.9768	878.6817	
pdp_two_numeric(svm.regr_100_5, grid.size = 100)	30473.79668	34214.49919	36374.1959	35029.63392	37447.6418	45625.4264	
pdp_two_numeric(svm.regr_100_20, grid.size = 20)	876.51701	882.15318	926.3787	903.14791	916.8196	1146.8898	
pdp_two_numeric(svm.regr_100_40, grid.size = 20)	1206.08702	1219.19689	1272.5305	1258.11824	1271.9964	1400.6923	

FIGURE 6.15: Runtime comparison ALE vs. PDP for two numeric features. Differences for number of features and grid size.

6.3.2 Two numerical features of interest

In figure 6.15 the runtimes for different 2D ALE and PDP configurations can be seen. Again the number of features is not a great deal for both algorithms. The ALE has no huge increase in runtime when the grid size is higher but the PDP has. The issue here is that the estimation for 2D PDP requires $(grid.size + 1)^2 \times \#observations$ predictions, while the ALE just needs $4 \times \#observations$ predictions calculated for the estimation. This especially can be seen when increasing the number of observations.

	expr	min	lq	mean	median	uq	max
ale_two_numeric(svm.regr_100_5, grid.size = 20)	113.6278	113.6278	113.6278	113.6278	113.6278	113.6278	
ale_two_numeric(svm.regr_1000_5, grid.size = 20)	178.4526	178.4526	178.4526	178.4526	178.4526	178.4526	
ale_two_numeric(svm.regr_10000_5, grid.size = 20)	1272.1623	1272.1623	1272.1623	1272.1623	1272.1623	1272.1623	
pdp_two_numeric(svm.regr_100_5, grid.size = 20)	784.9901	784.9901	784.9901	784.9901	784.9901	784.9901	
pdp_two_numeric(svm.regr_1000_5, grid.size = 20)	11119.2517	11119.2517	11119.2517	11119.2517	11119.2517	11119.2517	
pdp_two_numeric(svm.regr_10000_5, grid.size = 20)	592522.9523	592522.9523	592522.9523	592522.9523	592522.9523	592522.9523	

FIGURE 6.16: Runtime comparison ALE vs. PDP for two numeric features. Differences for the number of observations.

Figure 6.16 shows such an increase in observations. One can see that factor 100 in observations becomes almost factor 1,000 for the runtime of PDP while it is just a bit more than 10 for ALE.

6.3.3 One categorial feature of interest

Lastly, a look at the estimation for 1D categorial PDP and ALE will be taken.

Figure 6.17 shows the runtimes of PDP and ALE for a categorial feature of interest. Analyzing categorial features does not require a grid size since the

	expr	min	1q	mean	median	uq	max
ale_one_cat(svm.regr_100_5)	94.54019	94.75531	99.60971	97.68650	105.80104	108.93051	
ale_one_cat(svm.regr_100_20)	347.35541	352.14670	362.91692	353.56057	376.75881	402.81558	
ale_one_cat(svm.regr_100_40)	681.78034	685.60607	701.45315	694.62070	719.30814	738.54682	
pdp_one_cat(svm.regr_100_5)	18.71033	20.22231	20.63243	20.39822	20.46206	24.62853	
pdp_one_cat(svm.regr_100_20)	24.77961	25.19753	25.83508	25.95311	26.31663	27.14796	
pdp_one_cat(svm.regr_100_40)	32.10757	32.87978	34.00759	33.04194	34.23248	40.10593	

FIGURE 6.17: Runtime comparison ALE vs. PDP for one categorial feature. Differences for number of features only, since there is no grid size for categorial features.

number of categories already defines the number of different evaluations. This time one recognizes that it is the other way around. The calculation time stays the same for the PDP with a growing number of features, while ALE shows a significant growth. This is clearly caused by the reordering of the features for their category (will be explained in the next chapter). The reordering is based on the kind of nearest neighbors (depends on implementation). The calculation of these neighbors takes longer the more features have to be taken into account.

	expr	min	1q	mean	median	uq	max
ale_one_cat(svm.regr_100_5)	92.98182	95.89084	104.20978	98.98172	107.26786	125.14276	
ale_one_cat(svm.regr_1000_5)	141.94946	143.49470	149.50597	144.26978	148.48264	189.87805	
ale_one_cat(svm.regr_10000_5)	884.31175	891.17992	902.50493	899.02002	903.75282	954.53049	
pdp_one_cat(svm.regr_100_5)	19.24196	19.93535	20.32778	20.32638	20.86151	21.42763	
pdp_one_cat(svm.regr_1000_5)	242.53307	243.51711	245.11559	244.56068	246.06815	249.78878	
pdp_one_cat(svm.regr_10000_5)	3545.40465	3554.96302	3566.24054	3559.92305	3578.69701	3607.40991	

FIGURE 6.18: Runtime comparison ALE vs. PDP for one categorical feature. Differences for the number of observations.

Figure 6.18 shows a similar picture as can be seen in figure 6.13. Just this time compared to the estimation for one numeric feature the ALE is way slower for the categorial feature, while the PDP is twice as fast as for the numeric feature. That might come from the fact that the grid size here (6.13) was 20 and in this case, there are just 10 classes for the feature of interest. Meaning that half as many calculations for the estimation are required. So it might be the same speed for the PDP from numeric to categorial (at least with comparable parameters). The ALE will always be slower for categorical features since the reordering of the categories is necessary.

In general, one can state that ALE is by far faster. For an SVM that might not be that much of a problem. But with ensemble predictors like a random forest it can be very slow to calculate a PDP for a high grid size and 10,000+ observations.

6.4 Comparison for unevenly distributed data - Example 4: Munich rents

To conclude this chapter a real-world problem with a fitted learner will be analyzed with ICE, PDP, and ALE, to see them in action.

This is an example with data for rents in Munich from 2003. The target variable ‘nm’ is the rent per month per flat. To predict the rent a random forest has been fitted. The features in this example are ‘wfl’ (size in square meters) and ‘rooms’ (number of rooms) of the flat. These two variables are clearly positively correlated since there will not be an apartment with 15 square meters and 5 rooms. The other features are not that strongly correlated as one can see in figure 6.19. To fit the random forest only ‘wfl’ and ‘rooms’ were used.

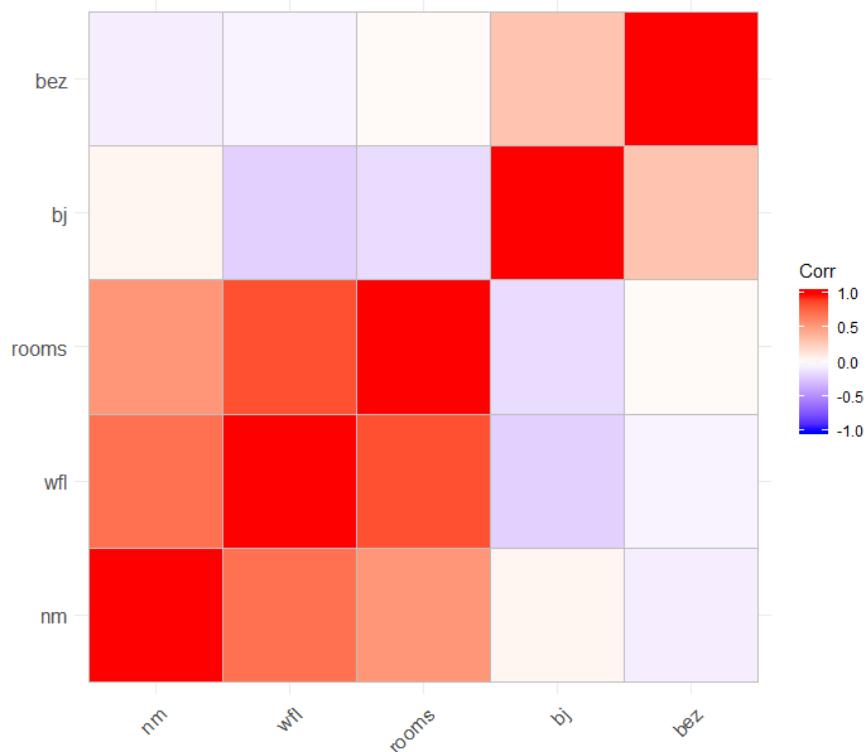


FIGURE 6.19: Correlation matrix for rents in Munich.

Figure 6.20 shows a more or less expected influence of space on the rent. The

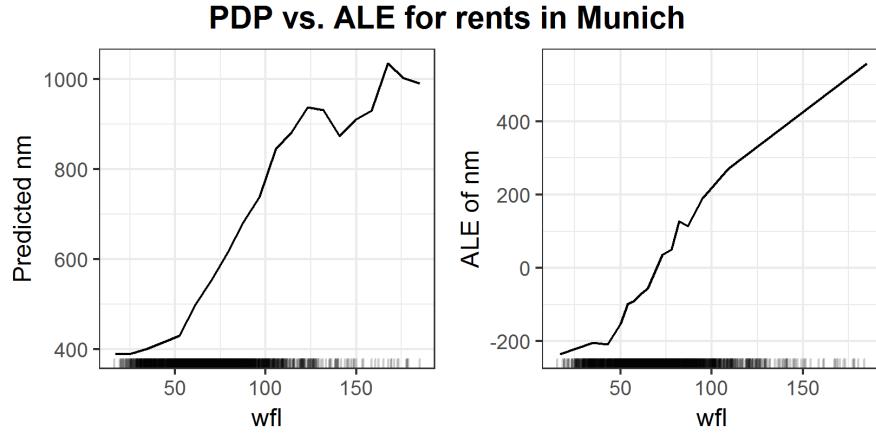


FIGURE 6.20: PDP and ALE plots for the influence of space on rents in Munich.

bigger the apartment the more expensive it is. In the area with a lot of data between 0 and 100, the PDP looks more smooth than the ALE which is a bit shaky. In the area with not that many observations, it is the other way around. The PDP suddenly breaks down what seems quite unrealistic, while the ALE has a pretty straight trend. Since the ALE shows a more expected behavior for the prediction of rents one could tend to state that the ALE outperforms the PDP. One could think that some unrealistic feature combinations in the estimation of the PDP caused this strange drop. But a look at the ICE plot reveals something else.

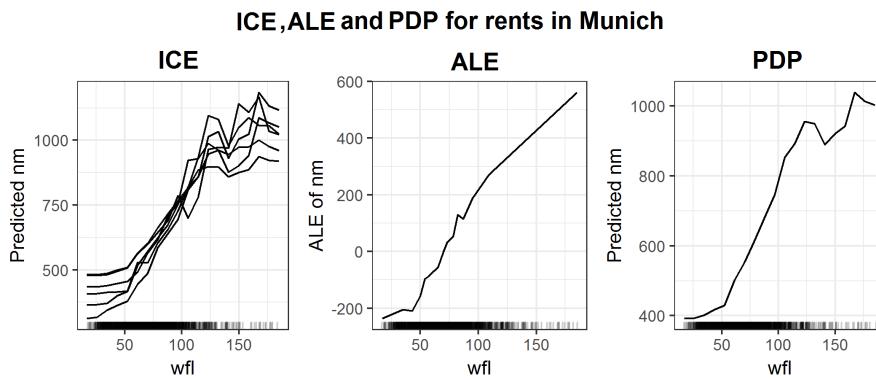


FIGURE 6.21: ICE, ALE and PDP plots for influence of space on rents in Munich.

Figure 6.21 additionally shows the ICE curves for this example. Since the only

other feature used for the fit was ‘rooms’ and in the data set are just flats with 6 or fewer rooms, there are just 6 graphs. Now one could argue, maybe the apartments with less than 4 rooms (which are way more in this data set than those with 4 or more rooms) somehow cause the strange drop for the PDP. But figure 6.22 shows that almost all rooms have this drop, especially the apartments with 4 and 5 rooms.

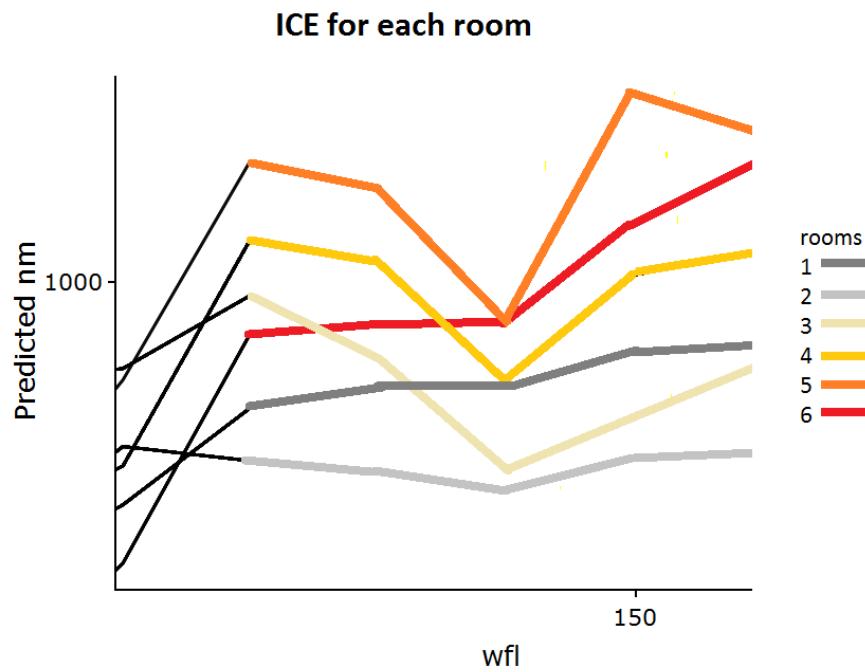


FIGURE 6.22: ICE for rents in Munich zoomed in for the critical area.

The issue here is that rooms don't have a strong influence on the prediction at all. In return, the PDP does not get problems with the correlation between the two features. And the PDP in the iml implementation generates an equidistant grid on the area with observations for feature ‘wfl’. On the other hand, the ALE divides this area aiming for equally many observations in each interval. This results in very small intervals for apartments with less than 109 square meters of space. But the flats with 109 or more square meters are evaluated in one interval only. This simply yields to this ALE plot, where it just ignores/skips this drop. And as one can see this can be dangerous when interpreting the prediction function. In this special situation, the ALE might get better the true link between the rent and the size of the apartments but that is not what one is interested in. The goal is always to interpret the predictor and not the data.

This example demonstrated a crucial weakness of the ALE regarding the size of the intervals, which will be discussed in the next chapter. It also shows that ICE and PDP might still be worth a look despite their issues with correlated features and runtime. In general, if one needs to get a deep understanding of the prediction function it might be clever to use as many interpretation algorithms as possible. By being aware of their strengths and weaknesses and combining the results of those algorithms one can get a detailed look at the influence of each variable which should also be reliable.

6.5 Appendix

6.5.1 Calculation of theoretical 2D ALE example

Features x_1 , x_2 , x_3 and the prediction function $\hat{f}(x_1, x_2, x_3) = x_1 x_2 x_3$ are given. The features are sampled from the these disrtibutions: $X_1 \sim \mathcal{U}(a, b)$, $X_2 \sim \mathcal{N}(\mu, \sigma)$ and $X_3 | X_2, X_1 \sim \mathcal{N}(X_2, X_1)$.

The theoretical 2D ALE for features x_1 and x_2 will be calculated.

First is the calculation of uncorrected and uncentered 2nd order effect:

$$\begin{aligned}
 \widetilde{\widetilde{ALE}}_{\hat{f}, 1, 2}(x_1, x_2) &= \\
 &= \int_{z_{0,1}}^{x_1} \int_{z_{0,2}}^{x_2} E[\hat{f}^{(1, 2)}(X_1, X_2, X_3) | X_1 = z_1, X_2 = z_2] dz_2 dz_1 \\
 &= \int_{z_{0,1}}^{x_1} \int_{z_{0,2}}^{x_2} E[X_3 | X_1 = z_1, X_2 = z_2] dz_2 dz_1 \\
 &= \int_{z_{0,1}}^{x_1} \int_{z_{0,2}}^{x_2} z_2 dz_2 dz_1 \\
 &= \int_{z_{0,1}}^{x_1} \frac{1}{2}(x_2^2 - z_{0,2}) dz_1 \\
 &= \frac{1}{2}(x_2^2 - z_{0,2})(x_1 - z_{0,1})
 \end{aligned} \tag{6.8}$$

Next is the calculation of the corrected pure 2nd order effect:

$$\begin{aligned}
\widetilde{ALE}_{\hat{f}, 1, 2}(x_1, x_2) &= \widetilde{\widetilde{ALE}}_{\hat{f}, 1, 2}(x_1, x_2) \\
&\quad - \int_{z_{0,1}}^{x_1} E\left[\frac{\delta \widetilde{\widetilde{ALE}}_{\hat{f}, 1, 2}(X_1, X_2)}{\delta X_1} \mid X_1 = z_1\right] dz_1 \\
&\quad - \int_{z_{0,2}}^{x_2} E\left[\frac{\delta \widetilde{\widetilde{ALE}}_{\hat{f}, 1, 2}(X_1, X_2)}{\delta X_2} \mid X_2 = z_2\right] dz_2 \quad (6.9)
\end{aligned}$$

The two terms which are correcting for the main effect of the two features will be calculated separately:

$$\begin{aligned}
\int_{z_{0,1}}^{x_1} E\left[\frac{\delta \widetilde{\widetilde{ALE}}_{\hat{f}, 1, 2}(X_1, X_2)}{\delta X_1} \mid X_1 = z_1\right] dz_1 &= \\
&= \int_{z_{0,1}}^{x_1} E\left[\frac{1}{2}(X_2^2 - z_{0,2}^2) \mid X_1 = z_1\right] dz_1 \\
&= \int_{z_{0,1}}^{x_1} \frac{1}{2}(\mu^2 + \sigma^2 - z_{0,2}^2) dz_1 \\
&= \frac{1}{2}(\mu^2 + \sigma^2 - z_{0,2}^2)(x_1 - z_{0,1}) \quad (6.10)
\end{aligned}$$

$$\begin{aligned}
\int_{z_{0,2}}^{x_2} E\left[\frac{\delta \widetilde{\widetilde{ALE}}_{\hat{f}, 1, 2}(X_1, X_2)}{\delta X_2} \mid X_2 = z_2\right] dz_2 &= \\
&= \int_{z_{0,2}}^{x_2} E[X_2(X_1 - z_{0,1}) \mid X_2 = z_2] dz_2 \\
&= \int_{z_{0,2}}^{x_2} z_2\left(\frac{a+b}{2} - z_{0,1}\right) dz_2 \\
&= \frac{1}{2}\left(\frac{a+b}{2} - z_{0,1}\right)(x_2^2 - z_{0,2}^2) \quad (6.11)
\end{aligned}$$

Combining (6.10) and (6.11) with (6.9) yields:

$$\begin{aligned}
\widetilde{ALE}_{\hat{f}, 1, 2}(x_1, x_2) &= \widetilde{\widetilde{ALE}}_{\hat{f}, 1, 2}(x_1, x_2) - \frac{1}{2}(\mu^2 + \sigma^2 - z_{0,2}^2)(x_1 - z_{0,1}) \\
&\quad - \frac{1}{2}\left(\frac{a+b}{2} - z_{0,1}\right)(x_2^2 - z_{0,2}^2) \\
&= x_2^2 x_1 + (x_1 - z_{0,1})(\mu^2 + \sigma^2) - \frac{a+b}{2}(x_2^2 - z_{0,2}^2) \quad (6.12)
\end{aligned}$$

The last part is the centering for the mean:

$$\begin{aligned}
ALE_{\hat{f}, 1, 2}(x_1, x_2) &= \widetilde{ALE}_{\hat{f}, 1, 2}(x_1, x_2) - E[\widetilde{ALE}_{\hat{f}, 1, 2}(X_1, X_2)] \\
&= \frac{1}{2}(x_2^2 x_1 + (x_1 - z_{0,1})(\mu^2 + \sigma^2) - \frac{a+b}{2}(x_2^2 - z_{0,2}^2) \\
&\quad - E[X_2^2 x_1 + (X_1 - z_{0,1})(\mu^2 + \sigma^2) - \frac{a+b}{2}(X_2^2 - z_{0,2}^2)]) \\
&= \frac{1}{2}[x_2^2 x_1 - (x_1 - z_{0,1})(\mu^2 + \sigma^2) - \frac{a+b}{2}(x_2^2 - z_{0,2}^2) \\
&\quad - (z_{0,1}(\mu^2 + \sigma^2) + z_{0,2}^2 \frac{a+b}{2} - (\mu^2 + \sigma^2) \frac{a+b}{2})] \\
&= \frac{1}{2}[x_2^2 x_1 - x_1(\mu^2 + \sigma^2) - x_2^2 \frac{a+b}{2} + (\mu^2 + \sigma^2) \frac{a+b}{2}]
\end{aligned} \tag{6.13}$$

This formula was used to calculate the theoretical plot in figure 6.8.

7

ALE Intervals, Piece-Wise Constant Models and Categorical Features

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As mentioned in the former section the choice of intervals and starting value $z_{0,j}$ have both a certain influence on the estimated ALE - curve. While the main influence of $z_{0,j}$ is canceled out by centering the ALE, the choice of intervals stays crucial. Therefore the next section is dedicated to this topic.

7.1 How to choose the number and/or length of the intervals

Before investigating the choice of intervals one should be clear about how far they influence the estimation. On the one hand for a given interval the ALE estimation will be linear due to the expected constant effect within this interval. Remember that within each interval the local effect within this interval was calculated by the mean total difference of the prediction when shifting the variable of interest from the lower interval boundary to the upper one. This leads by definition to a constant effect within this interval that results in a linear function when integrating over the interval.

It seems obvious that the ALE estimation (within a grid interval) can only be as good as a linear approximation for the “real” and usually unknown prediction function can be. Therefore it is crucial for a good estimation to have small enough intervals especially in regions where the prediction function is shaky or far from linear (i.e high second derivatives) with respect to the feature of interest. On the other hand, to get stable estimations for a grid interval it is important to have a sufficiently high number of data points within the interval. This means that the intervals shouldn’t become too small so that they would contain only a few data points. Note that this is only true if the other features have an influence on the local effect of the prediction function. If they don’t, any data point within the grid interval would lead to the same predictions

at the interval boundaries. That's why there is a natural trade-off between a small interval width and the number of the contained data points.

7.1.1 State of the art

So the question is how to optimally choose the grid intervals. Should they all be of the same width containing a different number of data points? Should they all contain the same or at least a similar number of data points, accepting different interval sizes. Or could there even be a better solution in between the two concepts?

Within the iml-package which is one of two implementations of ALE - plots the chosen method is the second one. The quantiles of the distribution of the feature are used as the grid that defines the intervals. That means the length of the intervals depends on the chosen grid size and the given feature distribution.

In the following section, some examples with artificial data sets are provided, that should help to get a better feeling for the different deterministic factors that influence the goodness of the ALE estimation. Within the whole chapter, the ALE estimation is conducted via the iml-package implementation.

7.1.2 ALE Approximations

In the following section, we only consider two-dimensional data sets, of continuous features x_1 and x_2 with a certain correlation. Furthermore, we use some exemplary prediction functions which are differentiable such that we can calculate the theoretical ALE (see section 5.2) and use it to evaluate the goodness of the estimated ALE - curve. As we want to isolate some of the above mentioned influential factors, we start with some easy examples adding step by step more complexity to the problem.

7.1.3 Example 1: additive feature effects

In the first example we assume a uniform distribution for the feature x_1 on the interval $[0, 10]$, i.e. $X_1 \sim U(0, 10)$. Furthermore we assume the conditional distribution of the feature x_2 given x_1 to be also uniform on the interval $[x_1 - 3, x_1 + 3]$, i.e. $X_2|X_1 = x_1 \sim U(x_1 - 3, x_1 + 3)$. Sampling 100 data points from this distribution yields the first dataset (see Figure 7.1).

Why we only made assumptions about the conditional distribution of X_2 and not on the joint distribution of (X_1, X_2) gets clearer once we take a look on the calculation of the theoretical ALE. Therefore we first assume the prediction function $\hat{f}_1(x_1, x_2) = (x_1 - 4)(x_1 - 5)(x_1 - 6) + x_2^3$. Due to the special structure

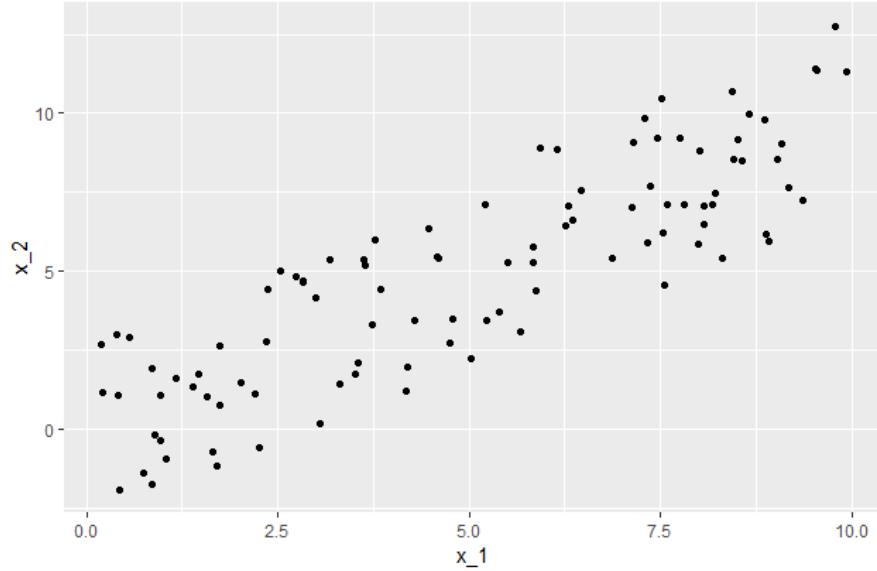


FIGURE 7.1: The correlation is clearly recognizable.

of f_1 the partial derivative with respect to x_1 is a polynomial of degree 2 which doesn't depend on x_2 , concretely $\hat{f}^1(x_1, x_2) = 3x_1^2 - 30x_1 + 74$ (Remember the unusual notation for the j-th partial derivative as f^j). Now we can calculate the theoretical (uncentered) ALE:

$$\begin{aligned}
 (1) \quad & \widetilde{ALE}_{\hat{f},1}(x) = \int_{z_{0,1}}^x E_{X_2|X_1=z_1}[\hat{f}^1(x_1, x_2)] dz = \\
 (2) \quad & \int_{z_{0,1}}^x \int p_{X_2|X_1=z}(x_2) \hat{f}^1(z, x_2) dx_2 dz = \\
 (3) \quad & \int_{z_{0,1}}^x \hat{f}^1(z, x_2) \int p_{X_2|X_1=z}(x_2) dx_2 dz = \\
 (4) \quad & \int_{z_{0,1}}^x \hat{f}^1(z, x_2) dz = \\
 (5) \quad & \int_{z_{0,1}}^x 3z^2 - 30z + 74 dz = \\
 (6) \quad & [z^3 - 15z^2 + 74z + c]_{z_{0,1}}^x = \\
 (7) \quad & x^3 - 15x^2 + 74x - z_{0,1}^3 + 15z_{0,1}^2 - 74z_{0,1}
 \end{aligned}$$

Here $p_{X_2|X_1=z}(x_2)$ notates the conditional density of $X_2|X_1$ for $x_1 = z$.

Step (3) makes use of the fact that $\hat{f}^1(x_1, x_2)$ doesn't depend on x_2 and in step (4) the integral over the density gives 1. To get the centered ALE we have to calculate:

$$(8) \quad ALE_{\hat{f},1}(x) = \widetilde{ALE}_{\hat{f},1}(x) - E[\widetilde{ALE}_{\hat{f},1}(X_1)] =$$

$$(9) \quad x^3 - 15x^2 + 74x - z_{0,1}^3 + 15z_{0,1}^2 - 74z_{0,1} -$$

$$E[X_1^3 - 15X_1^2 + 74X_1 - z_{0,1}^3 + 15z_{0,1}^2 - 74z_{0,1}] =$$

$$(10) \quad x^3 - 15x^2 + 74x - E[X_1^3 - 15X_1^2 + 74X_1] =$$

$$(11) \quad x^3 - 15x^2 + 74x - E[X_1^3] + 15E[X_1^2] - 74E[X_1] =$$

$$(12) \quad x^3 - 15x^2 + 74x - 250 + 15\left(\frac{100}{3}\right) - 74 * 5 =$$

$$(13) \quad x^3 - 15x^2 + 74x - 120 .$$

In Step (12) the formula for the k th - moment of the uniform distribution which is given by $m_k = \frac{1}{k+1} \sum_{i=0}^k a^i b^{k-i}$ was used. Knowing the theoretical ALE-curve we can have a look at the behavior of the estimated ALE for different grid sizes. Figure 7.2 shows the theoretical ALE and the estimations for grid sizes 2, 3, 5, and 10.

While the estimated ALE with grid size 2 only shows a linear effect over the whole data range, the estimated ALE with grid size 3 already gives a good approximation to the theoretical ALE in the second interval, where the theoretical ALE has a low curvature. With grid size 5 only the outer intervals show clearly recognizable deviations to the theoretical ALE and with grid size 10 the approximation looks quite reasonable. As the partial derivative of the prediction function was independent of x_2 , there was no risk of getting bad estimations due to too few data points within an interval. That's why we take a look at a second example.

7.1.4 Example 2: multiplicative feature effects

Now we assume the prediction function $\hat{f}_2(x_1, x_2) = (x_1 - 4)(x_1 - 5)(x_1 - 6)x_2^3$. In this case the partial derivative with respect to x_1 is a polynomial of degree 2 which clearly depends on x_2 , concretely $\hat{f}^1(x_1, x_2) = (3x_1^2 - 30x_1 + 74)x_2^3$. The new structure of the partial derivative yields a new calculation for the theoretical uncentered ALE:

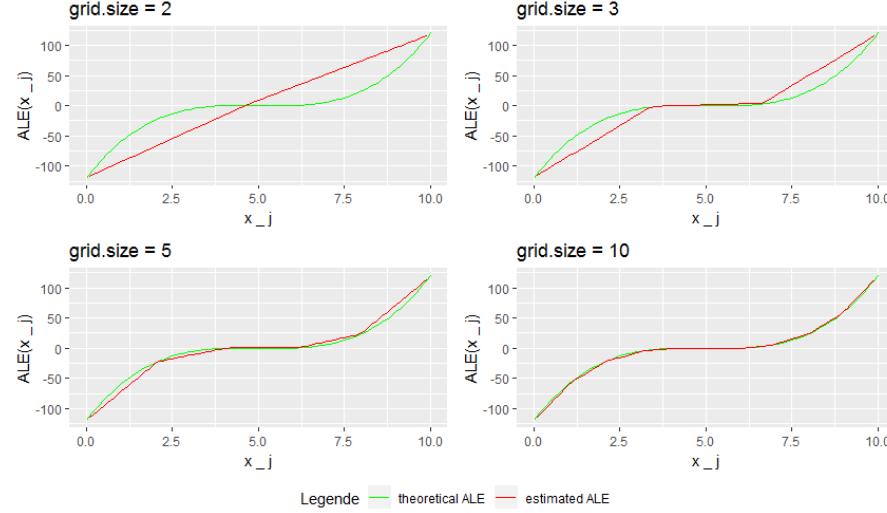


FIGURE 7.2: Theoretical vs estimated ALE

$$(1) \quad \widetilde{ALE}_{\hat{f},1}(x) = \int_{z_{0,1}}^x E_{X_2|X_1=z_1}[\hat{f}^1(x_1, x_2)] dz =$$

$$(2) \quad \int_{z_{0,1}}^x \int p_{X_2|X_1=z}(x_2) \hat{f}^1(z, x_2) dx_2 dz =$$

$$(3) \quad \int_{z_{0,1}}^x \int p_{X_2|X_1=z}(x_2) (3z^2 - 30z + 74)x_2^3 dx_2 dz =$$

$$(4) \quad \int_{z_{0,1}}^x (3z^2 - 30z + 74) \int p_{X_2|X_1=z}(x_2) x_2^3 dx_2 dz =$$

$$(5) \quad \int_{z_{0,1}}^x (3z^2 - 30z + 74) E_{X_2|X_1=z}[X_2^3] dz =$$

$$(6) \quad \int_{z_{0,1}}^x (3z^2 - 30z + 74) \left(\frac{1}{4} \sum_{i=0}^{k=3} (z-3)^i (z+3)^{k-i} \right) dz =$$

$$(7) \quad \int_{z_{0,1}}^x (3z^2 - 30z + 74)(z^3 + 9z) dz =$$

$$(8) \quad \int_{z_{0,1}}^x 3z^5 - 30z^4 + 101z^3 - 270z^2 + 666z dz =$$

$$(9) \quad \left[\frac{3}{6}z^6 - \frac{30}{5}z^5 + \frac{101}{4}z^4 - 90z^3 + 333z^2 \right]_{z_{0,1}}^x$$

Centering yields

$$(10) \quad ALE_{\hat{f},1}(x) = \frac{3}{6}x^6 - \frac{30}{5}x^5 + \frac{101}{4}x^4 - 90x^3 + 333x^2 -$$

$$E\left[\frac{3}{6}X_1^6 - \frac{30}{5}X_1^5 + \frac{101}{4}X_1^4 - 90X_1^3 + 333X_1^2\right]$$

Again using the formula for the moments of a uniform distribution we finally obtain

$$(11) \quad ALE_{f,1}(x) = \frac{3}{6}x^6 - \frac{30}{5}x^5 + \frac{101}{4}x^4 - 90x^3 + 333x^2 -$$

$$\left(\frac{3}{6}\frac{10^6}{7} - \frac{30}{5}\frac{10^5}{6} + \frac{101}{4}\frac{10^4}{5} - 90\frac{10^3}{4} + 333\frac{10^2}{3}\right) =$$

$$(12) \quad ALE_{f,1}(x) = \frac{3}{6}x^6 - \frac{30}{5}x^5 + \frac{101}{4}x^4 - 90x^3 + 333x^2 - 10528.57 .$$

Figure 7.3 shows the behavior of the ALE with different grid sizes in this setting.

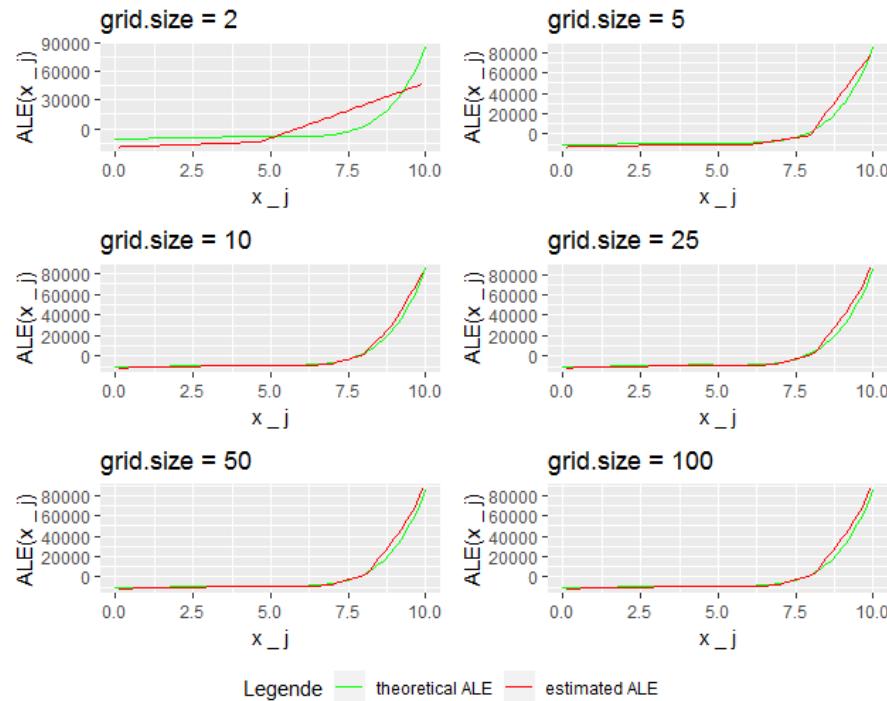


FIGURE 7.3: Theoretical vs estimated ALE for different grid sizes

While for grid size 5 and bigger the approximations for the region 0 to 7.5 seem quite reasonable it looks like for the region 7.5 to 10 the approximation is best for grid size 10 and gets worse with higher grid sizes. Zooming in for grid sizes 10 and 25 reveals this effect more clearly (Figure 7.4).

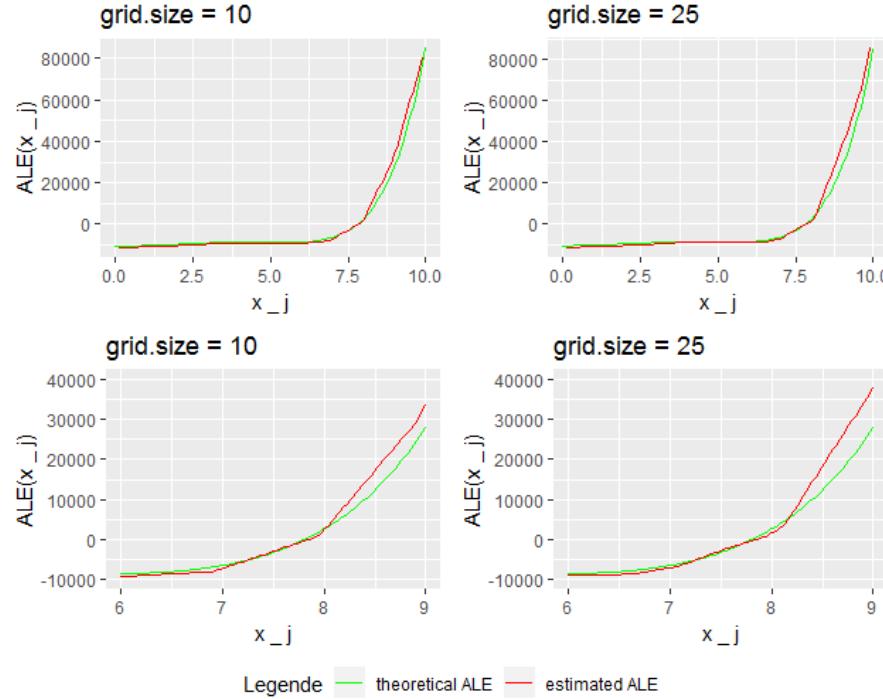


FIGURE 7.4: ALE-plots for grid sizes 10 and 25 (zoomed in)

Where does this come from? The structure of the prediction function leads to an increasing effect of x_2 on the total differences calculated for the series of intervals. Due to insufficient many datapoints within the intervals, there is a high probability of under or overestimating this effect. With grid size 25 only 4 data points are used for the estimation. Obviously, it's quite probable that the x_2 values of those data points are clearly above average in some intervals. If that happens for high x_1 - which implies due to the correlation structure high x_2 - the total difference will be clearly overestimated as the delta in x_1 is multiplied by the average x_2^3 . As the effect on the intervals is accumulated, the error persists for the whole ALE-curve from that point on.

To get a deeper insight into this dynamic, for the given context ALE - curves for 50 sampled datasets were estimated with grid sizes 10, 25, and 50. For each grid size at each value of x_1 the minimal and the maximal ALE estimation was taken as the boundary of the range of estimations. Figure 7.5 shows this range exemplarily for grid size 10.

The vertical lines indicate the absolute delta of the maximal and minimal ALE estimation at x. Plotting these deltas for the grid sizes 10, 25, and 50 yields Figure 7.6.

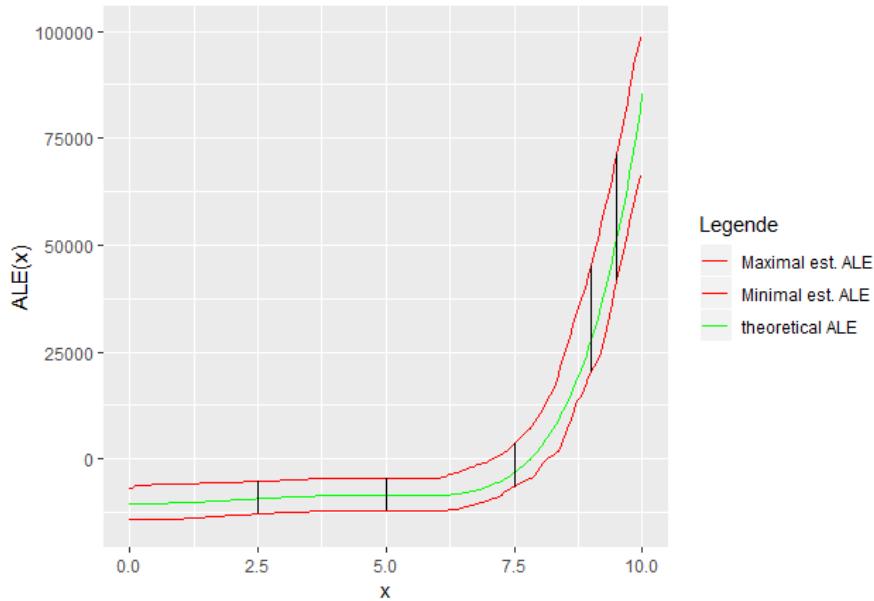


FIGURE 7.5: Maximum range of estimation

It is clearly recognizable that on the one hand for higher x the variance in the ALE estimation increases for all grid sizes. The expected higher variance of the estimations with higher grid sizes is in particular revealed in the region from $x_1 = 7$ to $x_1 = 10$, because the estimation is quite sensible to the absolute value of x_2 , which also increases with x_1 .

As the theoretical ALE in this example was quite smooth, grid size 10 gave reasonable estimations. The following example shows problems that occur once the prediction function is quite shaky especially in regions with only a few observations.

7.1.5 Example 3: Unbalanced datasets and shaky prediction functions

In the 3rd example we assume $X_1 \sim N(10, 3)$ as well as $X_2|X_1 = x_1 \sim U(x_1 - 3, x_1 + 3)$.

For this example the sample size was 1000 (see figure 7.7). As expected the correlation is clearly recognizable. This time only a few data points lay in the outer regions, i.e. between 0 and 2.5 and 17.5 and 20, while there is a high concentration of data around the mean at 10.

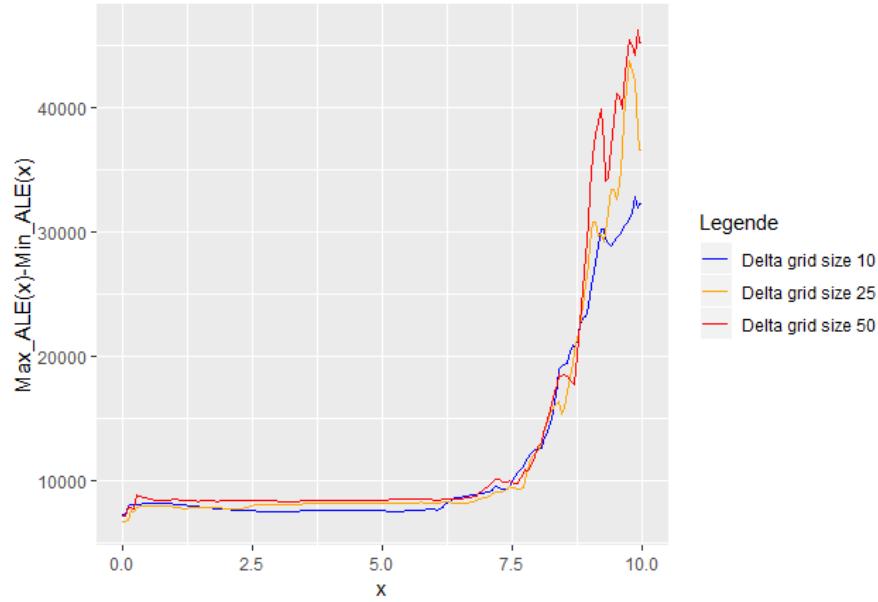


FIGURE 7.6: Delta of maximal and minimal estimated ALE for different grid sizes

Furthermore we look at the prediction function $\hat{f}_3(x_1, x_2) = \sin(10x_1)x_2$. The calculation of the theoretical uncentered ALE (as before) yields

$\widetilde{ALE}_{\hat{f},1}(x) = x \sin(x) + \frac{1}{10} \cos(10x)$. For centering the expectation of the uncentered ALE, i.e. $E[\widetilde{ALE}_{\hat{f},1}(X_1)]$, was estimated by Monte-Carlo integration to be almost zero. As well as the prediction function, the theoretical ALE has lots of extreme points. This leads to some troubles, especially for low grid sizes. Figure 7.8 shows the estimated and the theoretical ALE for three different grid sizes.

For grid size 20 the local behavior of the theoretical ALE is absolutely not recognizable. Only one peak left of the mean was estimated reasonable, which is due to the high data intensity in this region. For the rest of the plot, the grid intervals contain two or more peaks. Within each of them, the ALE is estimated linear and therefore the true effect smoothed out.

Increasing the grid size to 100 one nicely sees how the approximation becomes quite reasonable in the inner region, i.e. between 6 and 14, while in the outer region, where the intervals still are too long the ALE continues to be estimated wrong. The more one increases the grid size the wider the inner region of good estimation becomes. Anyway still at grid size 1000 which implies only one data point per interval, the estimations near the boundaries stay bad, as there are

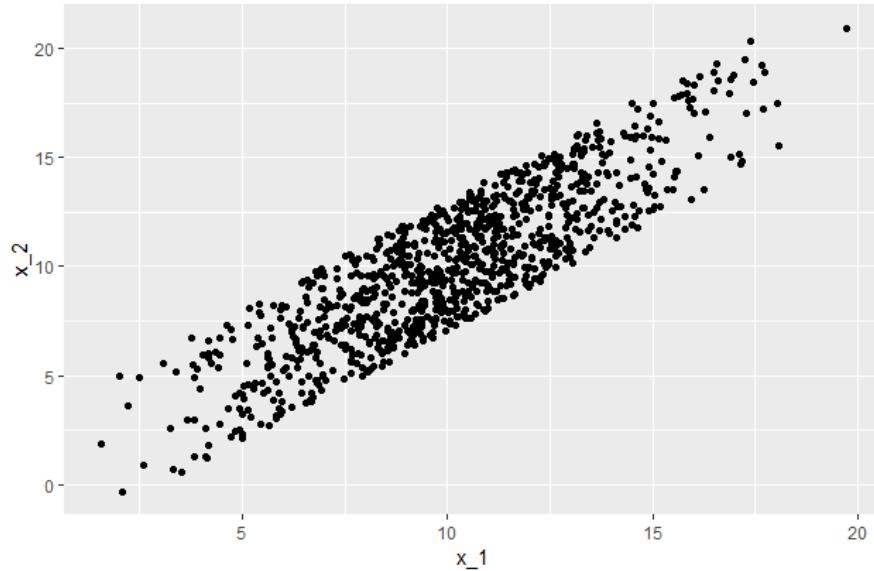


FIGURE 7.7: A mixture of normal and uniform distributed features

simply not sufficient observations to show the fine structure of the prediction function. As this was a constructed example, the latter shouldn't be overrated, as in real data situations it is quite improbable that a learner results in a that granular prediction function within regions with such few data points. While in figure 7.8 apparently both grid sizes (100 and 1000) result in equally good ALE estimations in the inner region, zooming in reveals that this isn't the case.

Figure 7.9 shows a very small part around the mean. As expected the estimations for grid size 100 are a little closer to the theoretical ALE as again the true effect of the second feature, which still affects the prediction, is better estimated within each interval (10 observations vs 1 observation).

At the end of this section, we have seen a good example of the natural trade-off between small intervals on the one hand and sufficient data to get a good and stable estimation on the other hand. The optimal choice of the number /size of intervals thereby highly depends on the given prediction function and the data. This can be taken as the main message of the section. The next section shall provide the reader with an understanding of how far additional problems can occur in the context of piece-wise constant models.

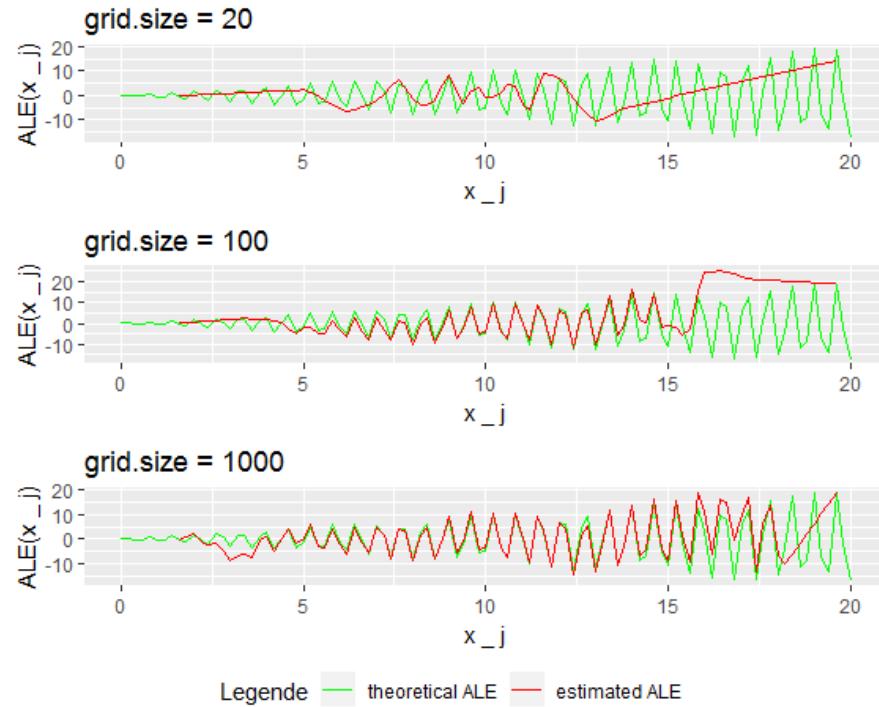


FIGURE 7.8: Theoretical vs. estimated ALE

7.2 Problems with piece-wise constant models

Piece-wise constant models such as for example decision trees and random forests don't have continuous prediction functions, which implies they are not differentiable. Thus the concept of theoretical ALE doesn't make any sense in this context as the partial derivative doesn't exist. Still, it is possible to estimate the ALE as the "jump" will result in a more or less steep linear part, depending on the interval size of the interval containing the step. It is intuitive that the goodness of the estimation highly depends on if one manages to place the intervals quite narrow around the steps. As the following examples will show, problems can occur due to "wrong" interval sizes or unlucky distributed data in the region of the steps.

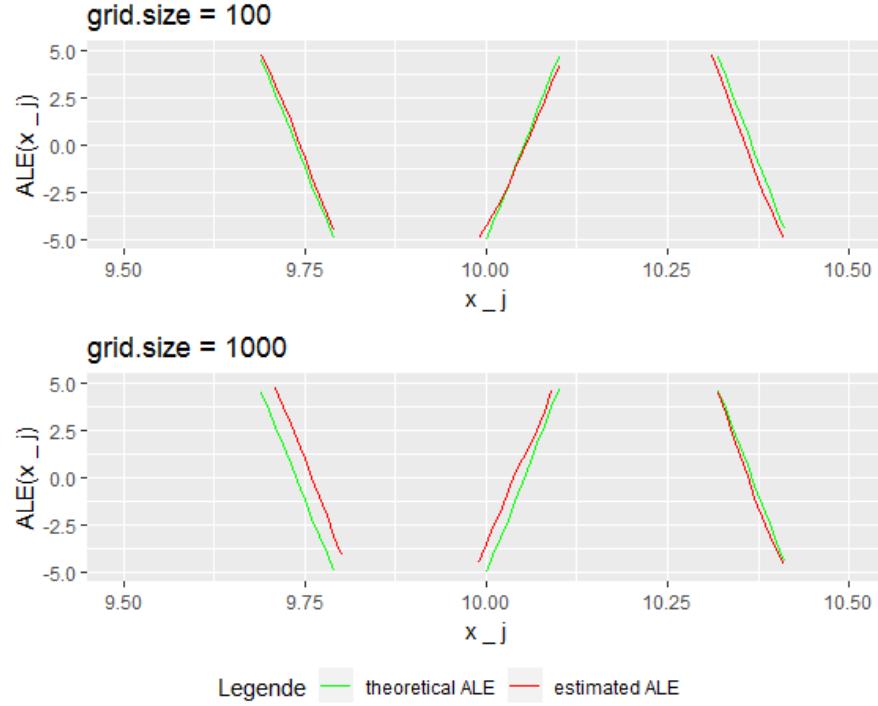


FIGURE 7.9: Zooming in reveals the bias for grid size 1000

7.2.1 Example 4: Simple step function

Throughout this section we assume X_1 to be uniformly distributed on the interval $[0, 10]$, i.e. $X_1 \sim U(0, 10)$ as well as X_2 given X_1 uniformly on the interval $[\max(x_1 - 3, 0), \min(x_1 + 3, 10)]$, i.e. $X_2|X_1 = x_1 \sim U(\max(x_1 - 3, 0), \min(x_1 + 3, 10))$. That means all the data is distributed within the 10 times 10 square. In the first example, we take a look at a simple prediction function to get a good understanding of the basic problem with piece-wise constant models. We assume a prediction function that independently of x_2 predicts 0, except if x_1 falls into a certain small interval around 5. In this case, it predicts 10. Concretely $f(x_1, x_2) = 1_{[4.9, 5.1]}(x_1) * 10$.

Figure 7.10 shows a sampled data set of 100 data points and a sketch of the prediction function.

As mentioned above a good estimation of the ALE would result in quite steep linear parts, one around 4.9 and a second inverse one around 5.1. The problem now is that the ALE estimation won't catch those jumps as long as both jumps lay within the same interval. The reason is that all the points within

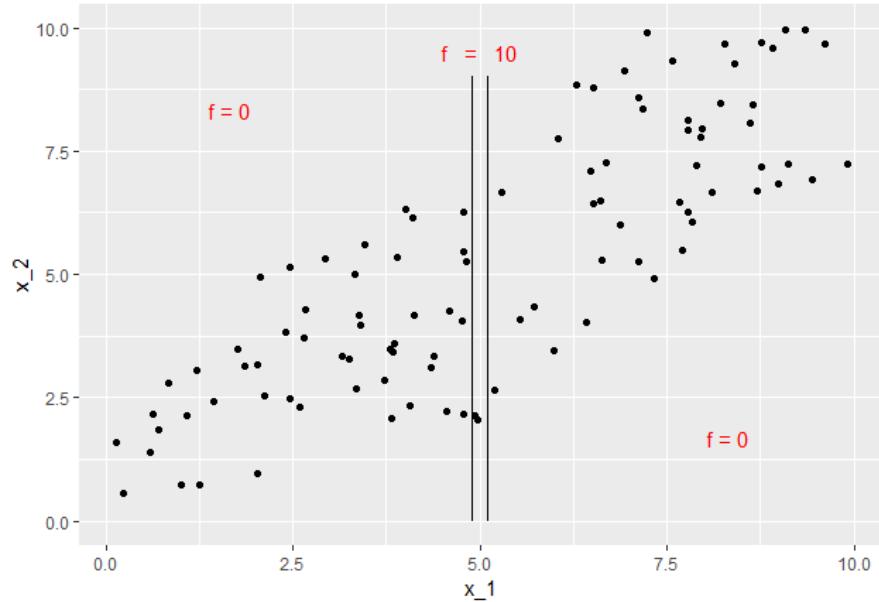


FIGURE 7.10: Prediction Function 1

this interval would be moved to the interval boundaries which lay outside the area, where the prediction function predicts 10. This leads to an estimation of the local effect as zero. Figure 7.11 shows the estimates for different grid sizes 20, 30, 50 and 100.

As expected the ALE estimations with grid size 20 and 30 are not sensitive to the effect. Increasing the grid size ensures that some interval boundaries fall into the interval [4.9, 5.1] which exposes the step of the prediction function. Having a second look at the data situation in this example, one notes that only 2 data points fall to the interval [4.9, 5.1]. Grid size 50 implies for 100 datapoints 2 data points per interval. That means that we even got lucky in this example that the 2 data points didn't fall into the same grid interval. Otherwise, the effect would have remained hidden even at grid size 50. The following example shows how unluckily distributed data points can lead to bad ALE estimations.

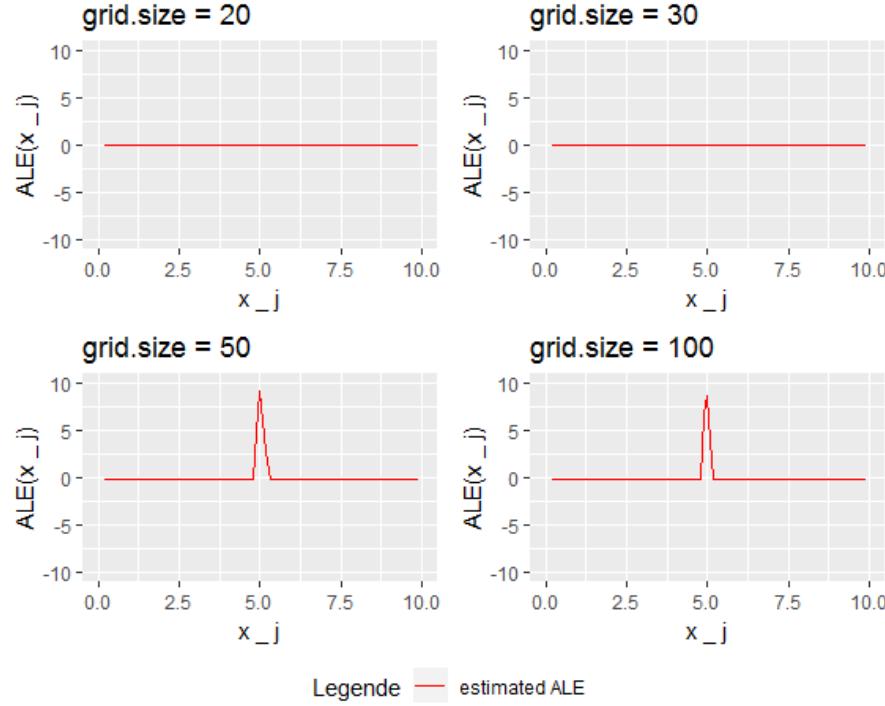


FIGURE 7.11: The behavior of ALE estimation with increasing grid size

7.2.2 Example 5: Two-dimensional step functions and unluckily distributed data

We assume the same data distribution as in the former example. Furthermore well take a look on two prediciton functions, one independent of x_2 defined as $f(x_1, x_2) = 1 + 1_{[0, \frac{10}{3}]}(x_1) + 1_{[\frac{10}{3}, \frac{20}{3}]}(x_1)$. The second also depends on x_2 and is defined as $f(x_1, x_2) = 3 (1_{[\frac{10}{3}, \frac{20}{3}]}(x_1) * 1_{[\frac{10}{3}, \frac{20}{3}]}(x_2)) + 2 (1_{[0, \frac{10}{3}]}(x_1) * (1_{[0, \frac{10}{3}]}(x_2) + 1_{[\frac{20}{3}, 10]}(x_2)) + (1_{[\frac{20}{3}, 10]}(x_1) * (1_{[0, \frac{10}{3}]}(x_2) + 1_{[\frac{20}{3}, 10]}(x_2)))$. Both on the first sight a little unhandy become quite easy to understand looking at the sketches below (see figures 7.12 and 7.13).

In the following, the ALE was estimated for increasing grid sizes. In figure 7.14 starting with grid size 5 on the left side we see the behavior of the first prediction function on the right side for the second one.

For grid size 5 both estimations recognize the step but estimate it relatively flat, which is not very surprising as the interval length should be around 2. For the first prediction function, we see a total increase within the second grid interval of 1 and a total decrease in the fourth one of 2. This reflects

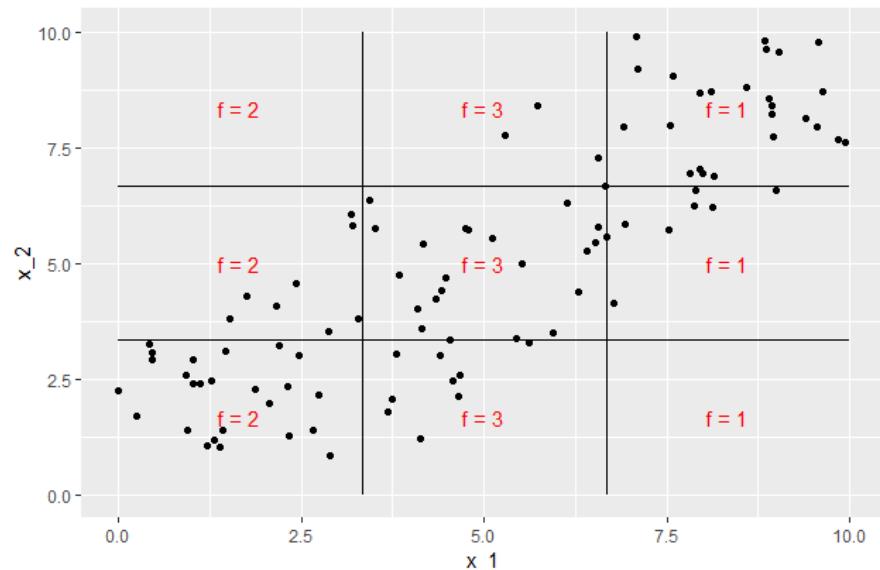


FIGURE 7.12: Prediction function 2

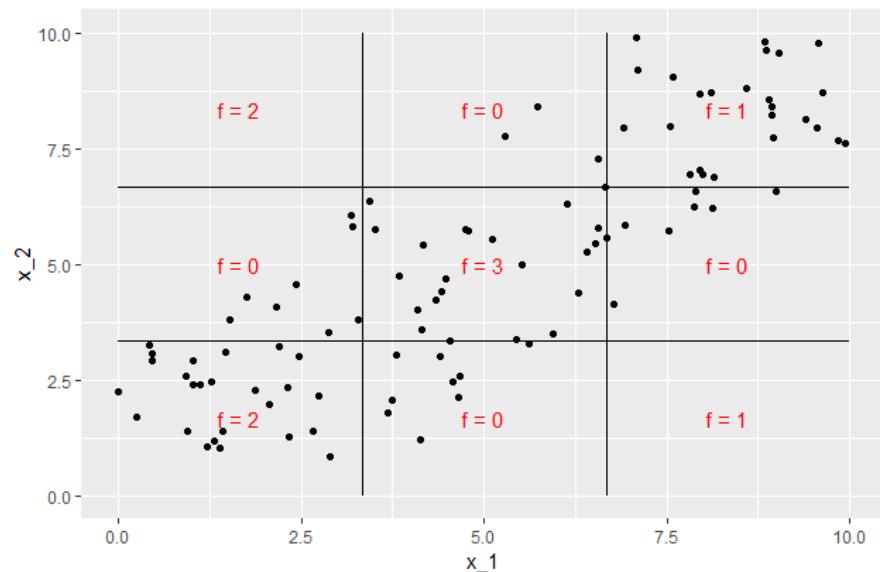


FIGURE 7.13: Prediction function 3

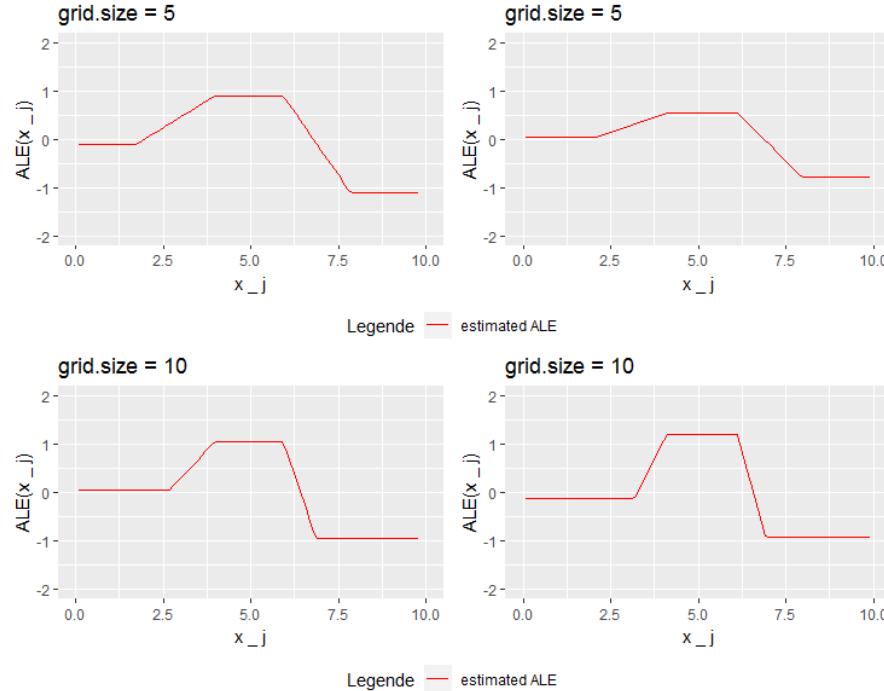


FIGURE 7.14: Behaviour of ALE estimations for prediction function 2 (left-side) and 3 (rightside)

the behavior of the prediction function, so the only problem is the low grid size. For the second prediction functions, the total changes are estimated to be much lower. This is due to the areas of 0 prediction which clearly influence the mean change in prediction, as some data points change from 0 to 3, but others from 2 to 0 within the second grid interval, as well as from 3 to 0 and from 0 to 1 within the fourth grid interval. So the absolute effect of x_1 is relativized by the influence of x_2 , which is intended by the concept of ALE. At grid size 10 the estimations for both prediction functions look quite similar. The steps become steeper as the grid intervals shrink to half their length. The estimated change in prediction for the second prediction function now is even bigger than for the first one. Due to the correlation, now more (relatively more) datapoints are shifted from prediction 0 to 3 and 3 to 0 respectively, which leads to the slightly higher estimation of the effect.

Increasing the grid size first to 20 and then to 50 reveals the whole danger of this situation. While prediction function 2 seems to be estimated quite stable (the absolute changes stay to be 1 and -2, while the steps become steeper and steeper), the estimation for prediction function 3 changes its behavior. At grid size 20 the left step grows to be 3, at grid size 50 the second step to be -3.

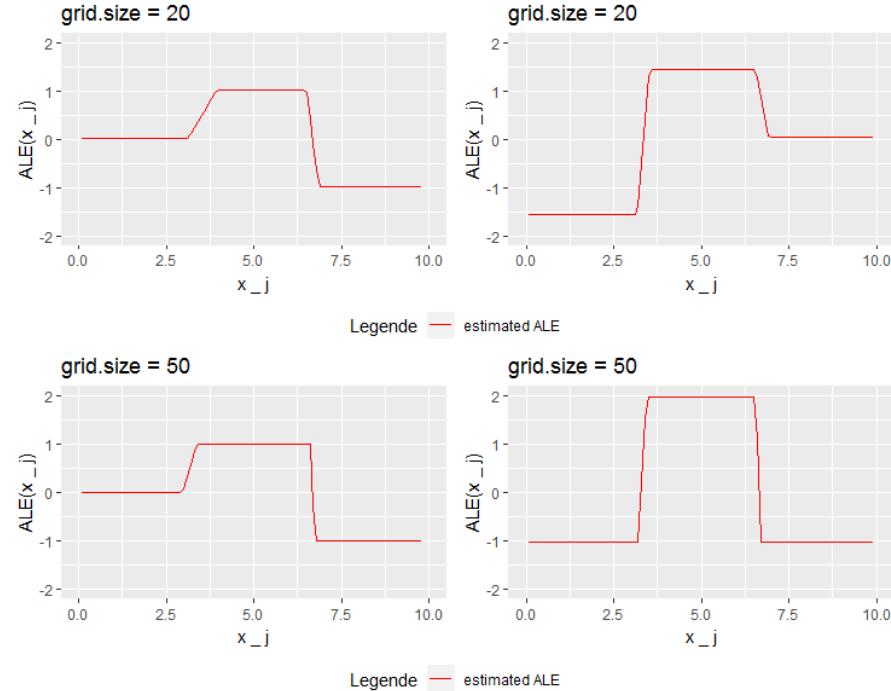
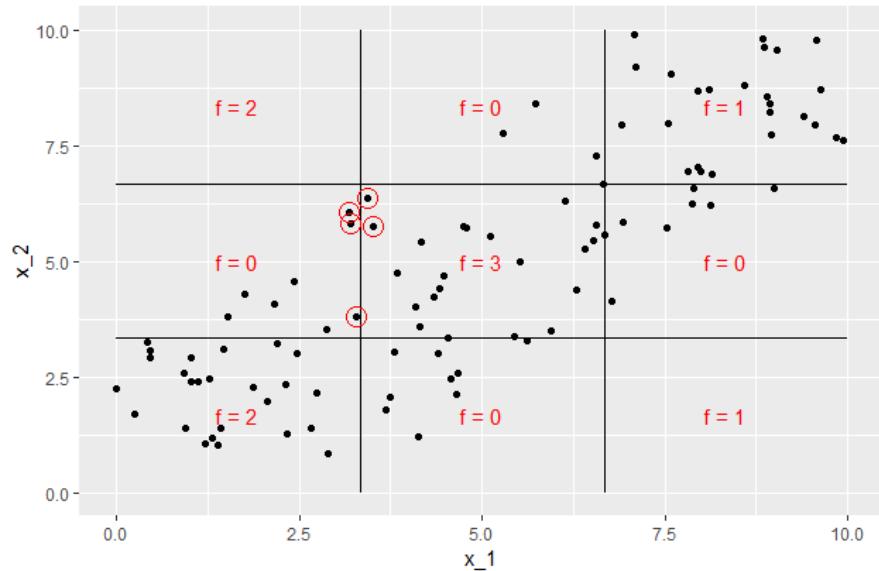
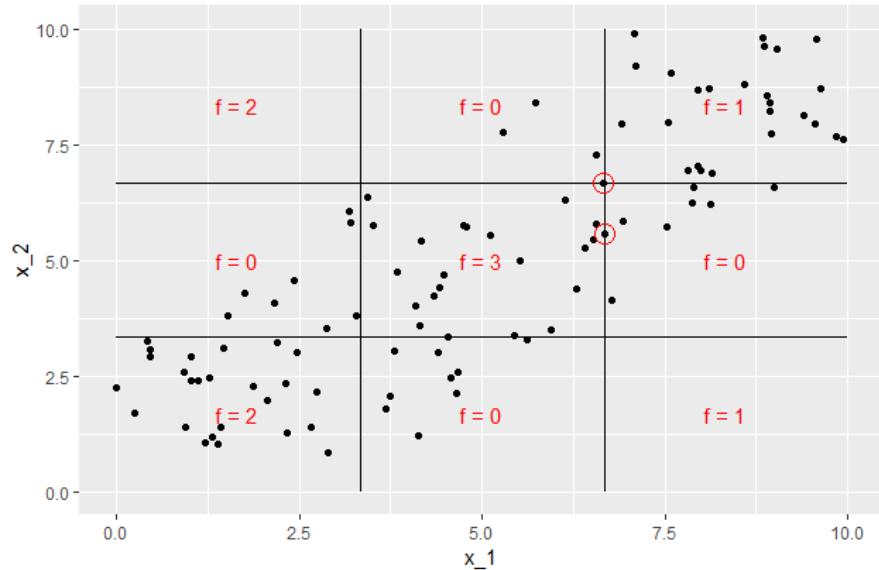


FIGURE 7.15: Behaviour of ALE estimations for prediction function 2 (leftside) and 3 (rightside)

Centering leads to quite radical upwards and downwards shifts of the whole plot. To understand this we'll have a look at the data points that are used to estimate the steps.

For grid size 20, 5 data points are used to estimate the total change in prediction. As figure 7.16 shows, coincidentally 5 data points with x_2 -values between $\frac{10}{3}$ and $\frac{20}{3}$ fall into the step interval. This is why the mean difference of the prediction is estimated to be 3.

Analogously for grid size 50, only two data points are used. As again both fall into the same x_2 - range, the estimation of the mean change of prediction in this grid interval is -3 now. Looking at figure 7.17 it becomes clear that only a little higher x_2 value of the upper data point would have lead to an estimation of -1 instead. This shows how sensitive the ALE estimation in the context of piece-wise constant models is. While there could be arguments for the height of the steps in the first 3 estimations, the last estimation clearly displays a false image. Here the interpretation would be that there is no main effect of feature 1 changing from less than $\frac{10}{3}$ to higher than $\frac{20}{3}$, which is obviously wrong.

**FIGURE 7.16:** Points that are used to estimate the step at grid size 20**FIGURE 7.17:** Points that are used to estimate the step at grid size 50

7.2.3 Outlook

We have seen that ALE estimations in the context of piece-wise constant models are even more critical due to sharp changes in the prediction at the steps. On the one hand, one needs the intervals to be within the steps to recognize them and at the same time quite narrow around them to catch the steepness of the step. Notice that in real-world examples one cannot know if there is a step or if the flat linear approximation is true. On the other hand, the data distribution around the steps has a strong influence on the ALE which leads to highly unstable estimations. In this context different methods of interval selection, maybe even adaptive, data-driven methods should be investigated.

7.3 Categorical Features

So far we were only interested in ALE-estimations for a numerical feature of interest. In real data situations, categorical features often play an important role. That's why it would be nice to expand the concept of ALE so that it can also be applied to categorical features. In the original paper by (Apley, 2016) this concept was not described but still, the first method implemented. (Molnar, 2019) adapted the method for the iml-package. The following section briefly describes the implemented method as well as the interpretation of ALE-plots for categorical features. It also shows some specific problems.

7.3.1 Ordering the features

One of the biggest and crucial differences of categorical and numerical features in the context of ALE is that categorical features usually don't have a natural order. As the concept of ALE is based on accumulating the local effects in a certain direction, an order of the feature is indispensable. Sometimes the categorical feature is an ordinal feature that comes with a natural order. In this case, the natural order should be used. If there is no natural order, the first essential step to calculate the ALE is to order the feature. Therefore different methods are conceivable. The iml-package implementation tries to order the feature with respect to the similarity of the other features. As we'll see in the next subsection for the estimation of the ALE the data points of a category will be shifted to the neighbor categories (neighbor categories only exist if the feature is ordered). To stay with the original idea of ALE and try to avoid extrapolation, ordering the feature with respect to the similarity of the other features seems reasonable. Within the iml-package, in a first step,

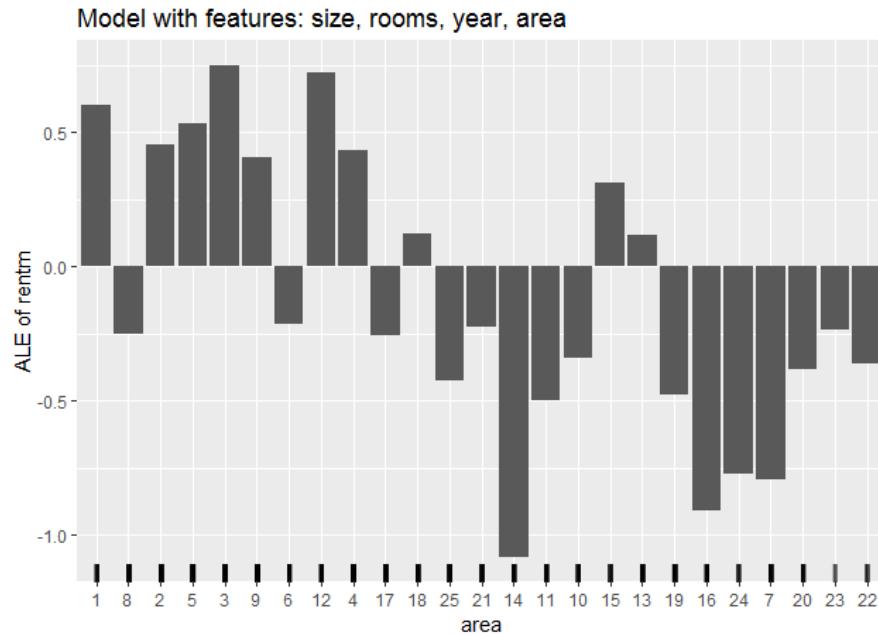
the distance of each pair of categories (of the feature of interest) is calculated with respect to every other feature. This results in $\frac{c(c-1)(f-1)}{2}$ distances, where f is the total number of features while c is the number of categories of the feature of interest. To calculate these distances for numerical features the Kolmogorov-Smirnov distance is used. It is defined as the maximal absolute difference of two distribution functions, which are estimated from the data within the two compared categories. For categorical features, one simply sums up the absolute differences of the relative frequencies of the categories. Finally, the distance between the two categories is calculated as the sum of their distances with respect to all features. Once the distance between all categories is calculated, multidimensional scaling is used to reduce the distance matrix to a one-dimensional distance measure (Molnar, 2019).

7.3.2 Estimation of the ALE

Once the features are ordered (no matter if as proposed by (Apley, 2016) and (Molnar, 2019) or in a different order) it's still not clear how to estimate the ALE. The partitioning of the axis into intervals doesn't make sense anymore as the categories themselves kind of partition the range of the feature in a natural manner. But there are no "values" in-between them and at the same time, the data points fall exactly on them. A continuous ALE wouldn't make sense at all, as there are no possibilities of changing the feature value if not from one category to another category. That's why the idea is to estimate exactly these expected changes in prediction if one category is changed to its neighbor category. Therefore for each pair of neighbor categories, the expected change is estimated by shifting the data from the lower to the upper category and vice versa and calculating the mean difference of the prediction. This mean difference is taken to be the expected effect between these two categories. How these changes are accumulated and how the ALE-plot looks, becomes clearer once looking at an example.

7.3.3 Example of ALE with categorical feature

For the following example the Munich rent dataset, which consists of a sample of 2053 apartments from the data collected for the preparation of the Munich rent index 2003, was used. For our purposes we restricted the data to the variables `rentm` (Net rent per square meter in EUR (numeric)), `size` (Floor area in square meters (numeric)), `rooms` (Number of rooms (numeric)), `year` (Year of construction (numeric)) and `area` (Urban district where the apartment is located (Factor with 25 levels)). In the first step, a model (Support Vector Machine for Regression) was fitted to predict the variable `rentm`. Now the ALE for the feature `area`, which is a categorical variable, was estimated with the `iml`-package. Figure 7.18 shows the result.



delta is not any longer the change of prediction between the two categories but the estimated change of prediction for shifting through all the categories in between in exactly the given order. The reason is that the estimated delta is not path independent. For example, the delta between categories 1 and 2 in the example above was calculated using data points of category 1, 8, and 2. If they were direct neighbors, the data points of category 8 wouldn't be involved in the estimation at all. This problem clearly grows the further two categories are ordered. Having this in mind the absolute values of the bars shouldn't be interpreted at all. Furthermore, this is another argument for ordering the categories in a reasonable manner, while it stays arguable what "reasonable" in this context means.

7.3.5 Changes of the ALE due to different orders

The last two graphics show how much the ALE for categorical features depends on the underlying order of the features. For the first one, the same learner was fitted on a restricted feature space containing only the variables year and area.

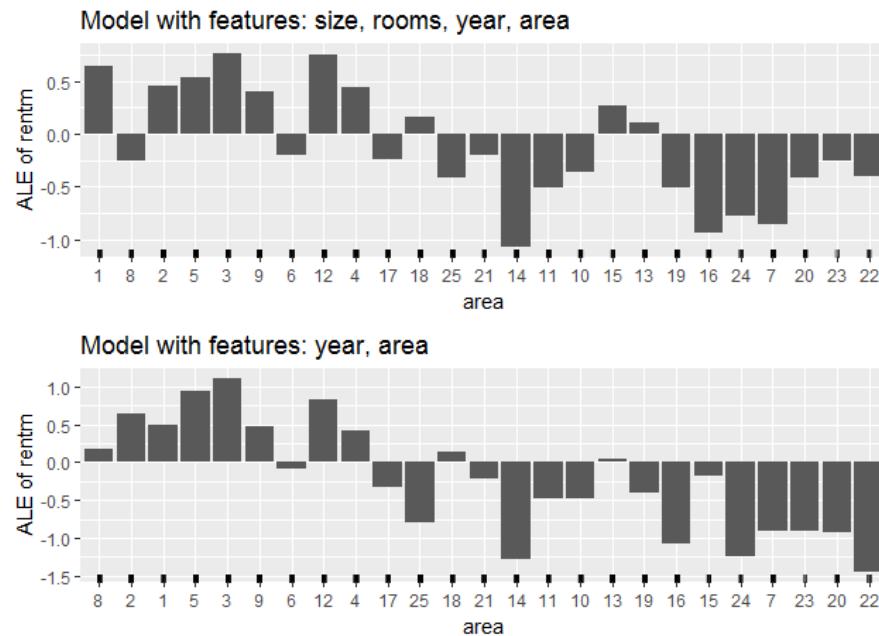


FIGURE 7.19: ALE-plot of the full model vs ALE-plot of the restricted model

As the comparison of the ALE-plots of figure 7.19 shows, the similarity-based order changes as it is only calculated on basis of the variable year (instead of

size, room, year). As the underlying model is now a different one, changes in the ALE are not surprising. Still, the comparison is quite difficult due to the new order.

The second ALE-plot of figure 7.20 is again based on the full model. This time the area was taken as an ordered factor, such that the similarity-based order wasn't calculated. The resulting ALE takes the district enumeration as order and proceeds accordingly.

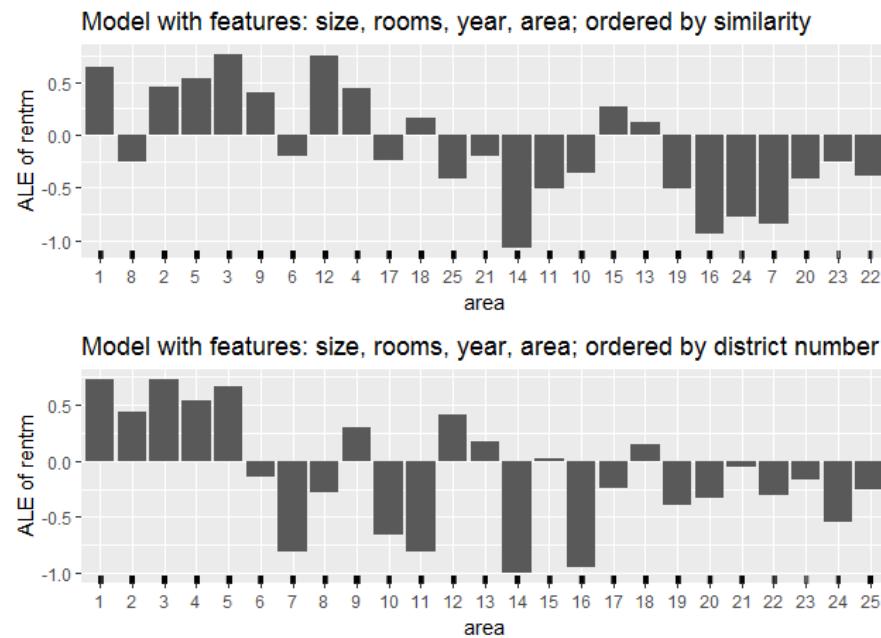


FIGURE 7.20: Two ALE-plots for different orders of the category area

Although the underlying model is the same, the ALE changes completely. Not only the order of the features changed but also the delta between some not adjacent categories. For example, we see a decrease from category 1 to 12 instead of an increase, as in the ALE-plot with similarity-based order. This underlines how careful one should be when interpreting ALE-plots for categorical features.

7.3.6 Conclusion

We have seen how sensitive the ALE (for categorical features) is for different orders of the category. Due to the lack of theoretical foundations concerning the

implemented order method, further investigations are highly recommended. The interpretation of the ALE should be done quite carefully.

8

Introduction to Feature Importance

Authors: Cord Dankers, Veronika Kroneder, Moritz Wagner *Supervisor:* Giuseppe Casalicchio

As in previous chapters already discussed, there exist a variety of methods that enable a better understanding of the relationship between features and the outcome variables, especially for complex machine learning models. For instance, Partial Dependence (PD) plots visualize the feature effects on a global, aggregated level, whereas Individual Conditional Expectation (ICE) plots unravel the average feature effect by analyzing individual observations. The latter allows to detect, if existing, any heterogeneous relationship. Yet, these methods do not provide any insights to what extent a feature contributes to the predictive power of a model - in the following defined as Feature Importance. This perspective becomes interesting when recalling that black-box machine learning models aim for predictive accuracy rather than for inference. Hence, it is persuasive to also establish agnostic-methods that focus on the performance dimension. In the following, the two most common approaches, Permutation Feature Importance (PFI) by Breiman (2001a) and Leave-One-Covariate-Out (LOCO) by Lei et al. (2018), for calculating and visualizing a Feature Importance metric, are introduced. At this point, it is worth to clarify that the concepts of feature effects and Feature Importance can by no means be ranked. Instead, they should be considered as mutual complements that enable interpretability from different angles. After introducing the concepts of PFI and LOCO, a brief discussion of their interpretability but also its non-negligible limitations will follow.

8.1 Permutation Feature Importance (PFI)

The concept of Permutation Feature Importance was first introduced by Breiman (2001a) and applied on a random forest model. The main principle is rather straightforward and easily implemented. The idea is as follows: When permuting the values of feature j , its explanatory power mitigates, as it breaks the association to the outcome variable y . Therefore, if the model

relied on the feature j , the prediction error $e = L(y, f(X))$ of the model f should increase when predicting with the “permuted feature” dataset X_{perm} instead of with the “initial feature” dataset X . The importance of feature j is then evaluated by the increase of the prediction error which can be either determined by taking the difference $e_{perm} - e_{orig}$ or taking the ratio e_{perm}/e_{orig} . Note, taking the ratio can be favorable when comparing the result across different models. A feature is considered less important, if the increase in the prediction error was comparably small and the opposite if the increase was large. Thereby, it is important to note that when calculating the prediction error based on the permuted features there is no need to retrain the model f . This property constitutes computational advantages, especially in case of complex models and large feature spaces. Below, a respective PFI algorithm based on Fisher et al. (2018) is outlined. Note however, that their original algorithm has a slightly different specification and was adjusted here for general purposes.

The Permutation Feature Importance algorithm based on Fisher, Rudin, and Dominici (2018):

Input: Trained model f , feature matrix X , target vector y , error measure $L(y, f(X))$

1. Estimate the original model error $e_{orig} = L(y, f(X))$ (e.g. mean squared error)
2. For each feature $j = 1, \dots, p$ do:
 - Generate feature matrix X_{perm} by permuting feature j in the data X
 - Estimate error $e_{perm} = L(y, f(X_{perm}))$ based on the predictions of the permuted data
 - Calculate permutation feature importance $PFI_j = e_{perm}/e_{orig}$. Alternatively, the difference can be used: $PFI_j = e_{perm} - e_{orig}$
3. Sort features by descending FI.

In Figure 8.1 it is illustrated, by a fictional example, how the permutation algorithm alters the original dataset. For each of the p features, the respectively permuted dataset is then used to first predict the outcomes and then calculate the prediction error.

To show, how the PFI for all features of a model can be visualized and thereby more conveniently compared, the PFI algorithm with a random forest model is applied on the dataset “Boston” (see Figure 8.2), which is available in R via the MASS package. To predict the house price, seven variables are included, whereby as the results show, the PFI varies substantially across the variables. In this case, the features Status of Population and Rooms should be inter-

	Original data set						Data set with permuted covariate x_1						
	x_1	x_2	\dots	x_p	y	\hat{y}		x_1	x_2	\dots	x_p	y	\hat{y}
1	2	0.2		female	1	1	1	14	0.2		female	1	0
2	8	0.6		male	0	0	2	11	0.6		male	0	1
3	7	0.5		male	1	0	3	2	0.5		male	1	1
4	3	1.1		female	0	0	4	7	1.1		female	0	1
5	14	0.8		female	1	1	5	3	0.8		female	1	0
...							...						
n	11	0.4		male	1	1	n	8	0.4		male	1	1

$$PFI_1 = L(y, f(X_{\text{perm},1})) - L(y, f(X))$$

	Original data set						Data set with permuted covariate x_p						
	x_1	x_2	\dots	x_p	y	\hat{y}		x_1	x_2	\dots	x_p	y	\hat{y}
1	2	0.2		female	1	1	1	2	0.2		male	1	1
2	8	0.6		male	0	0	2	8	0.6		female	0	0
3	7	0.5		male	1	0	3	7	0.5		male	1	0
4	3	1.1		female	0	0	4	3	1.1		male	0	1
5	14	0.8		female	1	1	5	14	0.8		female	1	1
...							...						
n	11	0.4		male	1	1	n	11	0.4		female	1	0

$$PFI_p = L(y, f(X_{\text{perm},p})) - L(y, f(X))$$

FIGURE 8.1: Example for Permutation Feature Importance. The tables illustrate the second step of the algorithm of PFI, in particular the permutation of the features x_1 and x_p . As shown, the respective columns in dark grey are the ones which were shuffled. This breaks the association between the feature of interest and the target value. Based on the formula underneath the tables, the PFI is calculated.

pretted as the most important ones for the model, whereas **Blacks** is considered as less important.

8.2 Leave-One-Covariate-Out (LOCO)

The concept of Leave-One-Covariate-Out (LOCO) follows the same objective as PFI, to gain insights on the importance of a specific feature for the prediction performance of a model. Although applications of LOCO exist, where comparable to PFI, the initial values of feature j are replaced by its mean, median or zero (see Hall et al., 2017), and hence, circumvent the disadvantage of re-training the model f , the common approach follows the idea to simply leave the respective feature out. The overall prediction error of the re-trained model f_{-j} is then compared to the prediction error resulted from the baseline model. However, re-training the model results in higher computational costs, which becomes more severe with an increasing feature space. Typically, one is interested in assessing the Feature Importance within a fixed model f . Applying LOCO might raise plausible concerns, as it compares the performance

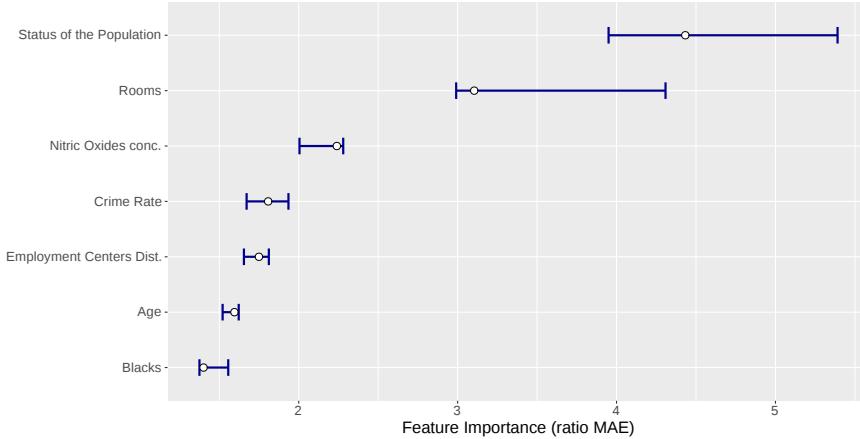


FIGURE 8.2: Visualization of Permutation Feature Importance with a random forest applied on Boston dataset. The depicted points correspond to the median PFI over all shuffling iterations of one feature and the boundaries of the bands illustrate the 0.05- and 0.95-quantiles, respectively (see `iml` package).

of a fixed model with the performance of a model f_{-j} which is merely fitted with a subset of the data (see Molnar, 2019). The pseudo-code shown below, illustrates the algorithm for the common case where the feature is left out (see Lei et al., 2018).

The Leave-One-Covariate-Out algorithm based on Lei et al. (2018):

Input: Trained model f , feature matrix X , target vector y , error measure $L(y, f(X))$

1. Estimate the original model error $e_{orig} = L(y, f(X))$ (e.g. mean squared error)
2. For each feature $j = 1, \dots, p$ do:
 - Generate feature matrix X_{-j} by removing feature j in the data X
 - Refit model f_{-j} with data X_{-j}
 - Estimate error $e_{-j} = L(y, f_{-j}(X_{-j}))$ based on the predictions of the reduced data
 - Calculate LOCO Feature Importance $FI_j = e_{-j}/e_{orig}$. Alternatively, the difference can be used: $FI_j = e_{-j} - e_{orig}$
3. Sort features by descending FI.

In Figure 8.3 it is shown, how the LOCO algorithm alters the original dataset, whereby it always differs, depending on the respective feature that is left out.

Note, that the qualitative and quantitative interpretations correspond to the ones from the PFI method. So do the visualization tools and therefore at this point it is refrained from providing the reader with an additional real data example.

Original data set							Data set without covariate x_1					
	x_1	x_2	\dots	x_p	y	\hat{y}		x_2	\dots	x_p	y	\hat{y}_{-1}
1	2	0.2		female	1	1		0.2		female	1	1
2	8	0.6		male	0	0		0.6		male	0	1
3	7	0.5		male	1	0		0.5		male	1	1
4	3	1.1		female	0	0		1.1		female	0	1
5	14	0.8		female	1	1		0.8		female	1	1
...												
n	11	0.4		male	1	1		0.4		male	1	0

$$L(y, f_{-1}(X_{-1})) - L(y, f(X)) = FI_1$$

Original data set							Data set without covariate x_p						
	x_1	x_2	\dots	x_p	y	\hat{y}		x_1	x_2	\dots	x_{p-1}	y	\hat{y}_{-p}
1	2	0.2		female	1	1		2	0.2			1	0
2	8	0.6		male	0	0		8	0.6			0	0
3	7	0.5		male	1	0		7	0.5			1	0
4	3	1.1		female	0	0		3	1.1			0	0
5	14	0.8		female	1	1		14	0.8			1	1
...													
n	11	0.4		male	1	1		11	0.4			1	0

$$L(y, f_{-p}(X_{-p})) - L(y, f(X)) = FI_p$$

FIGURE 8.3: Example for Leave-One-Covariate-Out Feature Importance. The tables illustrate the second step of the algorithm of LOCO in particular the drop of x_1 and x_p . The dark grey columns of the original dataset mark the variables that will be dropped and therefore ignored when refitting the model. This breaks the relationship between the feature of interest and the target value. Based on the formulae underneath the tables, the Feature Importance of LOCO is calculated.

8.3 Interpretability of Feature Importance and its Limitations

After both methods are presented, it will be now questioned to what extent these agnostic-methods can contribute to a more comprehensive interpretability of machine learning models. Reflecting upon these limitations will constitute the main focus in the following chapters. Conveniently, both methods are highly adaptable on whether using classification or regression models, as they are non-rigid towards the prediction error metric (e.g. Accuracy, Precision, Recall, AUC, Average Log Loss, Mean Absolute Error, Mean Squared

Error etc.). This allows to assess Feature Importance based on different performance measures. Besides, the interpretation can be conducted on a high-level, as both concepts do consider neither the shape of the relationship between the feature and outcome variable nor the direction of the feature effect. However, as illustrated in Figure 8.2, PFI and LOCO only return for each feature a single number and thereby neglect possible variations between subgroups in the data. Chapter 10 will focus on how this limitation can be, at least for PFI, circumvented and introduces the concepts of Partial Importance (PI) and Individual Conditional Importance (ICI) which both avail themselves on the conceptual ideas of PD and ICE (see Casalicchio et al., 2018). Besides, two general limitations appear when some features in the feature space are correlated. First, correlation makes an isolated analysis of the explanatory power of a feature complicated which results in an erroneous ranking in Feature Importance and hence, in incorrect conclusions. Second, if correlation exists and only in case of applying the PFI method, permuting a feature can result in unrealistic data instances so that the model performance is evaluated based on data which is never observed in reality. This makes comparisons of prediction errors complicated and therefore it should always be checked for this problem, if applying the PFI method. Chapter 9 will focus on this limitations by comparing the performance of PFI and LOCO for different models and different levels of correlation in the data. Beyond these limitations, it is evident to also question whether these agnostic-methods should be computed on training or test data. As answering that depends highly on the research question and data, it is refrained from going into more detail at this point but will be examined and further discussed in chapter 11.

9

PFI, LOCO and Correlated Features

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Supervisor: Giuseppe Casalicchio

The method of Feature Importance is a powerful tool in gaining insights into black box models under the assumption that there is no correlation between features of the given data set. However, this fundamental assumption can often be rejected in reality. As mentioned in chapter 3, PDPs may suffer in their interpretability, if this assumption is violated. Not only the interpretability of PDPs can be affected, but also the interpretability of Feature Importance can strongly depend on the correlations between the input features. In case of correlated features in the data, which are very likely to occur in reality, the results of the Feature Importance method do not reflect the individual true Feature Importance anymore. This can lead to a misleading importance ranking of the features and hence to incorrect interpretations of a feature's relevance in a model.

There are two main issues when it comes to correlated features, which will be illustrated in the following two examples. The first and most crucial issue is the misleading ranking of correlated features. Adding a correlated feature to the data set can lead to a decrease in Feature Importance. Imagine you want to predict the risk of a heart attack by looking at the weight of a person had yesterday as well as other uncorrelated features. For instance, you choose a random forest model and calculate the corresponding PFI. It is well known that overweight can have a significant influence on the likelihood of heart attacks. Thus, the PFI indicates that weight is the most important feature. What happens if you also add the weight of the person of today which is highly correlated to yesterday's weight of a person? Usually, one big advantage of a random forest model is the application and predictive accuracy of high dimensional data sets (Strobl et al., 2008). This also holds for cases of correlated features or interaction effects. Hence, adding a new component should cause no issues. Yet, some effects of the Feature Importance can make an interpretation more difficult. This is due to the fact that the PFI can now split between both features. During the training of the random forest some of the decision trees will choose the weight today, the weight yesterday, both or none of these as a split point. Eventually, both features will be selected

equally, because they are equally beneficial for the performance of the model. ([Molnar, 2019](#))

The second issue arises only when the PFI is conducted. During the shuffling step of a feature not only the association to the target variable gets broken, but also the association with the correlated features. So in case the features are correlated, unrealistic data points may occur. These new data points range from unlikely all the way up to completely impossible. The central question then becomes: Can we still trust the informative value of the PFI, if it is calculated with data instances that are not observed in reality and therefore biased ([Molnar, 2019](#))? Figure 9.1 illustrates an example with a possible outcome of unrealistic data instances.

	dteday	season	weekday	workingday	weathersit	temp	cnt
## 1	2011-01-01	SPRING	SAT	NO WORKING DAY	MISTY	8.175849	985
## 2	2011-01-02	SPRING	SUN	NO WORKING DAY	MISTY	9.083466	801
## 3	2011-01-03	SPRING	MON	WORKING DAY	GOOD	1.229108	1349
## 4	2011-01-04	SPRING	TUE	WORKING DAY	GOOD	1.400000	1562
## 5	2011-01-05	SPRING	WED	WORKING DAY	GOOD	2.666979	1600
## 6	2011-01-06	SPRING	THU	WORKING DAY	GOOD	1.604356	1606

	dteday	season	weekday	workingday	weathersit	temp	cnt
## 1	2011-01-01	SPRING	WED	NO WORKING DAY	MISTY	8.175849	985
## 2	2011-01-02	SPRING	FRI	NO WORKING DAY	MISTY	9.083466	801
## 3	2011-01-03	SPRING	SAT	WORKING DAY	GOOD	1.229108	1349
## 4	2011-01-04	SPRING	WED	WORKING DAY	GOOD	1.400000	1562
## 5	2011-01-05	SPRING	SAT	WORKING DAY	GOOD	2.666979	1600
## 6	2011-01-06	SPRING	SAT	WORKING DAY	GOOD	1.604356	1606

FIGURE 9.1: The two tables showing a subset of the bike sharing data set we already know from previous chapters. The one on top shows the first six rows of the original data set. The table below shows the first six rows of the data set where the feature ‘weekday’ is shuffled. As you can see, some of the new data points appear to make no sense. For example, in observation 1 Wednesday is claimed to be a no working day.

In this chapter, we want to shed light on some issues of correlated features with respect to Feature Importance and present possible reasons for the outcomes. Our purpose is not to list all possible effects, as this would go beyond the scope of this chapter. Rather than that we would like to increase the reader’s awareness of the problem itself, such that mistakes can be avoided in the future.

9.1 Effect on Feature Importance by Adding Correlated Features

A major part of this chapter will pay attention to the problem of interpreting Feature Importance when adding or observing correlated features in a given data set. Our focus lies on the behavior of Permutation Feature Importance by Breiman (2001a) as well as of the LOCO Feature Importance by Lei et al. (2018), which have been previously introduced. There will be a comparison of these measures applied on different learners namely the random forest, support vector machine (SVM) and linear model. Each of them will be trained on data sets with different correlation intensities between the features. The random forest and the SVM in this context are black box models (hard to interpret), whereas the linear model is a white box model (easy to interpret). These algorithms should show different behaviors. First, we have a look at simulated data sets and later on there is an application to a real data set Boston.

9.1.1 Simulation

A good way to visualize the effects of correlated features on the Feature Importance measures is to simulate some data with the desired dependencies of the features. This allows us to show the effects on the PFI and LOCO Feature Importance more precisely than looking on a real data set where additional dependencies between each features exist and may falsify the results. To filter out the real effect, it is necessary to hold the influence of other features as small as possible to prevent misinterpretations. For the complete R Code of these simulations please refer to the R file attached to this chapter. Our simulation design resembles the one from Strobl et al. (2008) or Archer and Kimes (2008).

In total, there will be three different scenario settings to investigate the influence of correlated features on the PFI and LOCO. The following setup is used as a general baseline for the scenarios:

$$y_i = x_{i1} + x_{i2} + x_{i3} + x_{i4} + \epsilon_i$$

The scenarios differ in the way they represent different dependencies of the features on the target variable. We investigate here a linear dependence as well as a non-linear one. To create a simple fictive data set with these dependencies, four features x_{i1}, \dots, x_{i4} were randomly drawn a thousand times out of a multivariate Gaussian distribution with a mean of 0: $X \sim MVN(0, \Sigma)$. The covariance Σ depends on the variance of all features, which were set equally to $\sigma_{j,j} = 1$, and the covariances $\sigma_{j,l}$. The covariance for feature $X1$ and $X2$ $\sigma_{1,2}$

were set to either $\rho = 0; 0.25; 0.5; 0.75$ or 0.99 depending on our correlation intensity of interest whereas the covariances of the other features were set to $\sigma_{j,l} = 0$ which means they are independent. Note: Here the correlation and the covariance are the same, because we set the variance to 1 such that the Pearson correlation coefficient $\rho = \frac{Cov(X_j, X_l)}{\sqrt{Var(X_j)}\sqrt{Var(X_l)}} = Cov(X_j, X_l)$. The reason behind setting $\rho = 0.99$ and not to $\rho = 1$ is to avoid issues when calculating with matrices. If ρ would be equal to 1, we would have perfect multicollinearity. Thus, the rank of the covariance matrix would not be full. Hence, setting ρ to 0.99 instead simplifies subsequent calculations, especially in terms of applying the linear model. The choice of the noise ϵ_i and its variance should be hold small in order to clarify the behavior we observe and avoid misinterpretation. In this case, we assume that the mean is zero and the standard deviation is only ten percent of the absolute value of the mean of $y_i = x_{i1} + x_{i2} + x_{i3} + x_{i4}$.

Furthermore, we will also include an uninformative feature "Uninf" randomly drawn out of a uniform distribution to the data set. This is our benchmark indicating us whether the importances of the features are higher than this random effect. As a consequence, we are eventually generating five data sets, each with five numerical features. Now we are able to run the learning algorithms on the data sets. For the random forest, we use the `randomForest` package ([original by Leo Breiman et al., 2018](#)) and for SVM the `ksvm()` function out of the `kernlab` package ([Karatzoglou et al., 2004](#)). For both functions the default settings for all the parameters were used.

How to compare PFI and LOCO?

As mentioned in the introduction to this chapter, for PFI as introduced by [Breiman \(2001a\)](#), one does not need to refit the model whereas for LOCO it is necessary to refit. In the `iml` package ([Molnar et al., 2018](#)), which we use throughout the entire book, the implementation uses Hold-out for performance evaluation. Typically, Hold-out is not ideal to evaluate the performance of a model unless the data set is sufficiently large. The variance of the performance value can get quite high which means that it can fluctuate a lot. To lower the variance of PFI, the values are calculated by repeatedly shuffling the features in the permutation step. However, Hold-out is definitely not suitable for LOCO, because reshuffling is not possible due to the fact that the interested feature is completely left out of consideration. Thus, the danger of high variance increases tremendously. In contrast to Hold-out, we can make use of Resampling methods which use the data more efficiently by repeatedly dividing the data into train and test data and finally aggregating the results. Therefore, in order to improve the comparability of two approaches, we decided to use Subsampling (repeated Hold-out) for measuring the performance for PFI. This also means that we use PFI on test data (see also chapter 12), so it is necessary to refit our model. In our case a Subsampling with a 20-80% split and 10 iterations were used. In principle we want to compare two models

in each iteration step, once without the permuted feature and once with the permuted feature. Therefore we should use the same train-test splits in each iteration. The following visualizations show the Feature Importance values as well as the importance ranks, which are both aggregated by the average over the 10 iterations of Subsampling. Furthermore, we calculate the Feature Importance by taking the ratio e_{perm}/e_{orig} for PFI or the the ratio e_{-j}/e_{orig} for LOCO (see chapter 9).

1) Linear Dependence:

In the first scenario setting the dependence of the features on the target value y is a linear one:

$$y_i = x_{i1} + x_{i2} + x_{i3} + x_{i4} + \epsilon_i$$

In order to get meaningful results, one has to first check, whether the underlying model was proved to be accurate. In case your model does not generalize accurately, the Feature Importance can vary greatly when rerunning the algorithms. Therefore, the resulting effects cannot be seen as significant (Parr et al., 2018). Figure 9.2 shows the benchmark result for the learning algorithms used on the simulated data sets with independence, medium and high correlation. As a performance measures we decided showing two. On the one hand, the mean squared error (MSE), since it is also used as a loss measure for evaluating the Feature Importance. On the other hand R^2 , because it is a common measure for linear models and we have a linear dependence of the features on the target value. $R^2 = 1$ implies that all residuals are zero, so a perfect prediction. Whereas $R^2 = 0$ means that we predict as badly as a constant. As you can see, all learning algorithms have very good up to perfect results, or in other words are accurate for our further investigations. The random forest is considered as the worst of the models at hand. That is not surprising as the random forest learns multiple step function trying to fit a linear prediction function. The linear model is by far the best model to predict this linear dependence on the target value.

Figure 9.3 shows the result of applying the PFI on the random forest model. The plot on the left-hand side shows the average importance values (in the graph shown as a dot). Moreover, it presents the 0.05- and 0.95-quantiles over the 10 subsampling iterations, respectively. In addition, the plot on the right-hand side shows the average importance rank based on the ten subsampling iterations. It is important to mention that typically the Feature Importance is interpreted in a rank order. One can see that, in case of independence, the PFI of all features are approximately the same except for the uninformative one. Since the uninformative indicated a complete random effect, one can suggest that all features have an influence on the performance of the model. Overall, the PFI of the correlated features X_1 and X_2 tend to increase more in comparison to the uncorrelated features as ρ increases. Moreover, the span of the quantile bands increases with higher ρ . This effect can also be seen

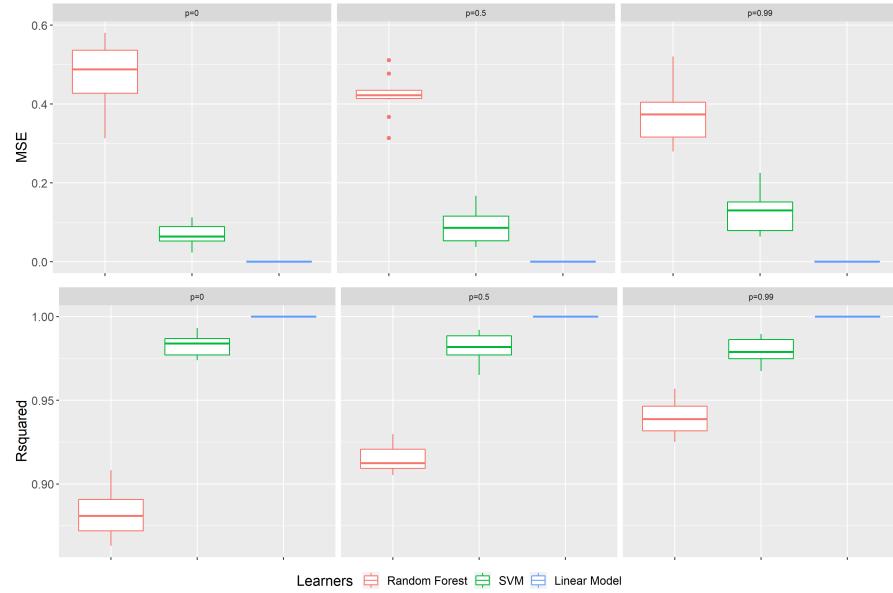


FIGURE 9.2: Benchmark results of scenario 1 for data sets with $p = 0$, $p = 0.5$ and $p = 0.99$ (from left to right). On top the performance measure is the MSE, at the bottom R^2 . The colour represents the learning algorithm. Red: Random Forest, green: SVM and blue: Linear Model.

in the right plot. For independence, all points are near the average rank of 2.5. The small fluctuations or deviations can be explained by the underlying stochastic. However, for a correlation higher than 0.5 we see a gap between the correlated features in red colour and the uncorrelated in green colour. The correlated features settle down at an average rank of about 1.5 and the uncorrelated ones at about 3.5. Although all features have the same influence on the target value, one can see that PFI can be misleading as it shows a higher PFI rank the higher the correlation between two features.

One possible explanation for this effect is given by Hooker and Mentch (2019). They state that the main reason behind this effect is caused by extrapolation which we already mentioned in the context of problems with PDPs. A small recap, extrapolation is the process of estimating beyond the distribution of our original data set. Figure 9.4 shows on the left the random forest applied on the simulated data set with independent features X_1 and X_2 . On the right it is applied on the data set where both are highly correlated. At first sight you cannot see a structure in the data distribution for the independent case. Furthermore, the data points fill out much more space in comparison to the correlated case. Here one can see a clear positive correlation between X_1 and X_2 . For instance, if you permute one observation of X_1 represented by the

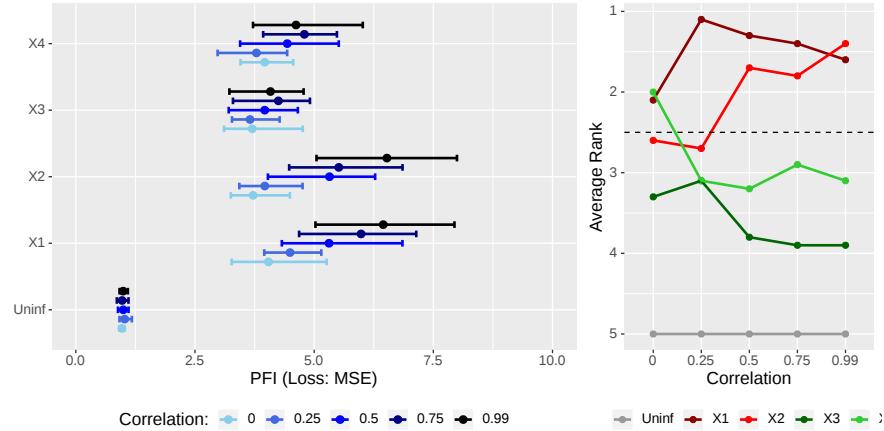


FIGURE 9.3: Scenario 1: PFI on the random forest models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line is used as an indicator of how far away certain features are from the true theoretical importance rank.

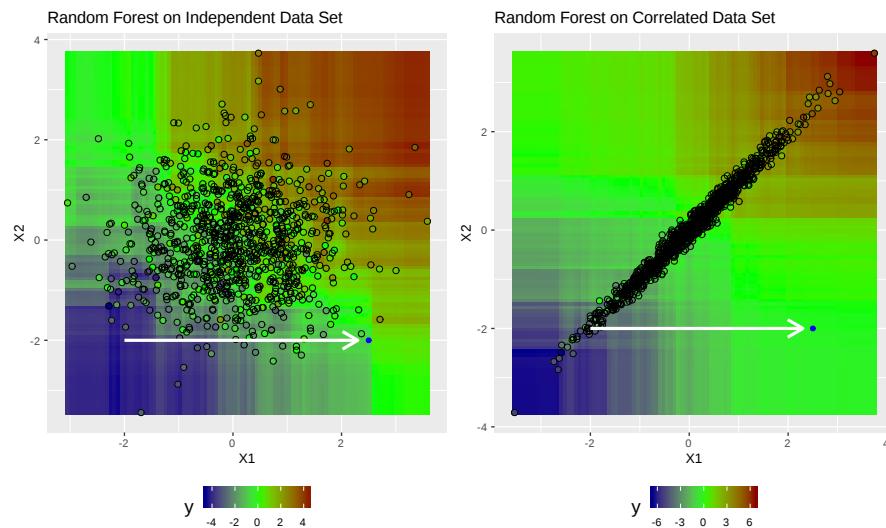


FIGURE 9.4: Extrapolation visualization. On the left, the prediction of the random forest on the simulated independent data set. On the right, the prediction of the random forest on the simulated high correlated data set. The arrow is indicating a permutation of one observation for feature X_1 .

white arrow, the permuted observation point is still near the data distribution in the independent case. However, in the correlated case there are no other data points nearby. The data distribution of the training data lies on the diagonal (bisector). The region outside of the point cloud was not learned well enough by the random forest which becomes evident through the less rectangle lines in this area. As a consequence of permuting, the random forest also evaluates points which are far away from training data. Thus, the prediction can be far away from the true value which leads to a large drop in performance. Although the feature is equally important in comparison to the others, it gets indicated as more important. The larger span of the quantile bands can be explained by the random permuting of the data points. If the observation is still close to the data distribution after permuting it, the error made is less severe as in the example shown in the plot. For example, the point is still in the blue shaded area. Hence, the change in error strongly depends on how far away the permuted data is from the real underlying data distribution. To sum up, the extrapolation problem of the random forest is associated with the correlation intensity.

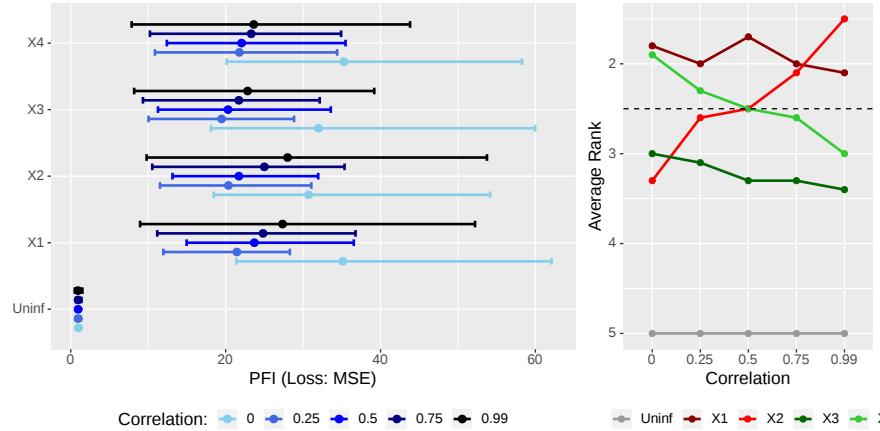


FIGURE 9.5: Scenario 1: PFI on the SVM models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line is used as an indicator of how far away certain features are from the true theoretical importance rank.

The next Figure 9.5 demonstrates the application of the support vector machines on the simulated data sets. Again, we have the same results for the independence case, because the importance values and quantile bands are similar to each other. This is underpinned by the average rank plot, which as

you can see fluctuates around the overall average rank. It seems like the importance values drop quite heavily when we are going from $\rho = 0$ to $\rho = 0.25$. It then rises again slightly the higher the correlation becomes. For the features X_1 and X_2 it seems like they are growing more in comparison to the independent ones. The average rank plot indicates the same, since for $\rho > 0.5$ there is a clear change in pattern towards that the highly correlated features being indicated as more important. Furthermore, the quantile bands for the highly correlated features X_1 and X_2 are getting larger in comparison to the independent ones. Thus, we recognize kind of similar effects like for random forest, where correlated features are indicated as more important. With the small deviation, that we do not exceed the initial importance value in case of independence and that the effect is less strong.

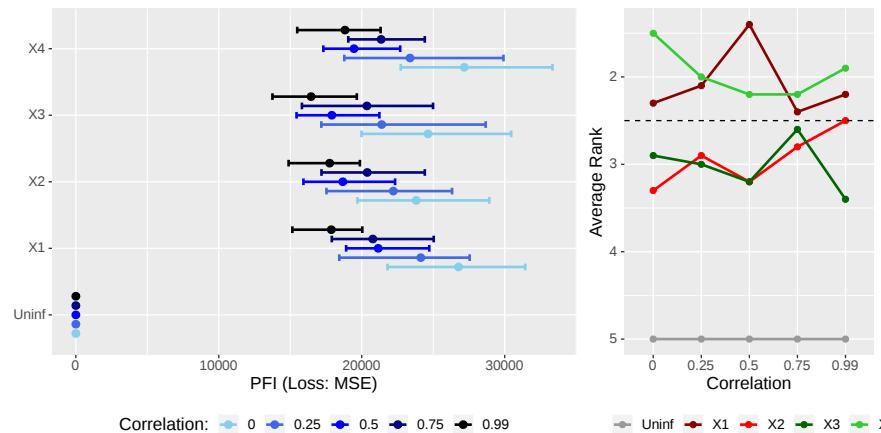


FIGURE 9.6: Scenario 1: PFI on the linear models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line is used as an indicator of how far away certain features are from the true theoretical importance rank.

When applying the linear model and calculating the PFI, the ranking of the features varies a lot. The underlying reason is that the importance values for each correlation intensity are very close to each other. The ranking seems to be very random and thus can be explained by stochastic. One interesting effect is that, the higher the correlation, the lower the Feature Importance values get. Figure 9.6 shows that the values of PFI are quite large. As mentioned before (see Figure 9.2), the MSE values of the linear model are close to zero. The linear model performs unsurprisingly very well. For the calculation of PFI we take the ratio e_{perm}/e_{orig} . Here the numerator's value is very small,

and the value of denominator is even smaller (close to zero) which results in a very large value for PFI. Increasing the error term ϵ_i would lower the PFI value, since the MSE would be higher. All in all, it looks like the PFI of a linear model is quite robust against changes in the correlation intensity. By assigning all features almost the same importance value, it reflects the true theoretical rank quite well.

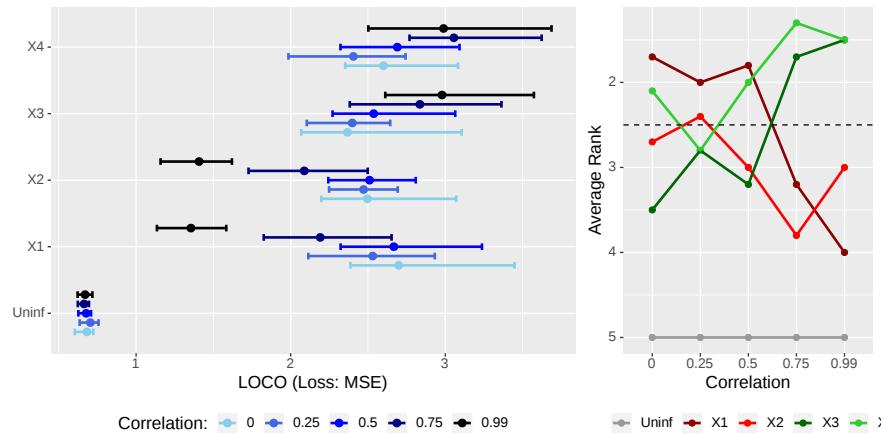


FIGURE 9.7: Scenario 1: LOCO on the random forest models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line is used as an indicator of how far away certain features are from the true theoretical importance rank.

In contrast to the PFI, there is a drop in LOCO Feature Importance of the two features X_1 and X_2 the higher the correlation. In particular for almost perfect multicollinearity, the outcome differs a lot from the theoretical true importance with the value dropping to almost 1. In terms of ratio comparison of the errors, this indicates that there is no influence on the performance prediction of the two features. Here we can see the downside of correlation in regards to LOCO. Both features should generally be considered as equally influential as X_3 and X_4 . However, in case of almost perfect multicollinearity, if you leave one of the features X_1 or X_2 out of consideration to calculate the LOCO Feature Importance, the other feature can kind of “pick up” the effect on the target variable. As a consequence, there is no change in accuracy which means that there is only a small, up to no, increase in the error (Parr et al., 2018). Another noteworthy result is a kind of a compensation effect. The importance values for X_3 and X_4 increase as the correlation of X_1 and X_2 rises. According to the right-hand side plot of Figure 9.7, the average rank

till $\rho = 0.5$ fluctuates a lot. For larger ρ values you can recognize a tendency towards higher average rank for uncorrelated features and a lower average rank for correlated features shown by the crossing over of the green and red lines. Basically, this is exactly the opposite to what we observe for PFI on the random forest model.

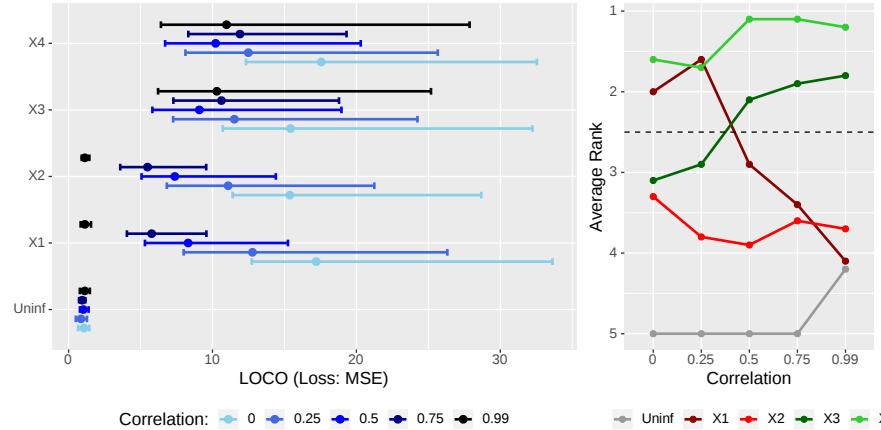


FIGURE 9.8: Scenario 1: LOCO on the SVM models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line is used as an indicator of how far away certain features are from the true theoretical importance rank.

Figure 9.8 presents the LOCO Feature Importance on the simulated data sets within the SVM model. Once again, we can observe a drop in importance of X_1 and X_2 the higher the correlation. In comparison to the random forest, you cannot recognize a compensation effect of the uncorrelated features. The plot on the left reveals that under independence the quantile bands for X_1 and X_2 are very large whereas under high correlation they are getting smaller and even hardly discernible. In addition to that, for $\rho = 0.99$ you can recognize that the average importance rank for the uninformative feature increases, because X_1 and X_2 are also considered as unimportant.

Apparently, the value of the average importance for LOCO is also very high if applying the linear model on the simulated data sets (Figure 9.9). The same phenomenon occurs for PFI on the linear model. Overall, one of the main similarities we can derive for the all three learning algorithms is that when perfectly multicollinearity is given the LOCO Feature Importance values are dropping to either 1 or 0 depending on whether you take the ratio or the difference of the estimated errors.

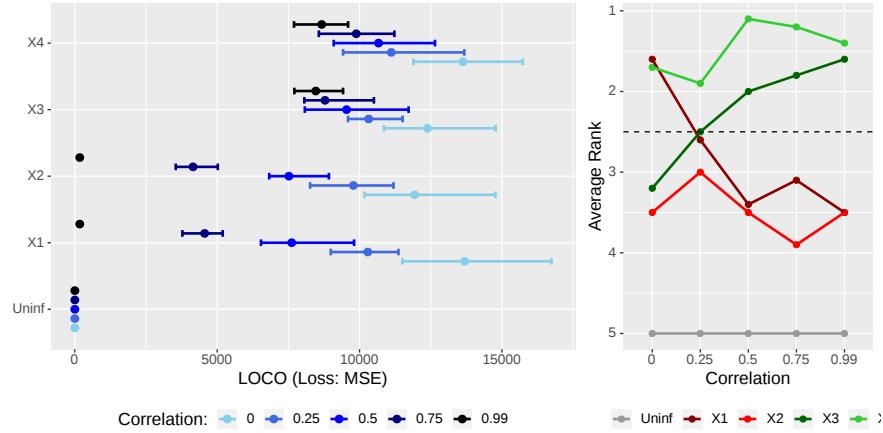


FIGURE 9.9: Scenario 1: LOCO on the linear models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line is used as an indicator of how far away certain features are from the true theoretical importance rank.

2) Linear Dependence with a larger coefficient for X_4 :

In the second scenario the dependence of the features on the target value y is also a linear one, yet with a small change in the coefficient of X_4 from 1 to 1.2. As a result, there is now a larger influence of this feature on the target y :

$$y_i = x_{i1} + x_{i2} + x_{i3} + 1.2x_{i4} + \epsilon_i$$

Figure 9.10 underlines the common problem of PFI and random forest in case of high correlation. As noted, X_4 has a higher impact on the target value i.e. a higher theoretical true importance in comparison to the other features. Nevertheless, one should notice the possibility that the PFI of X_1 and X_2 are considered as more important than X_4 . Consequently, there occurs a misleading importance ranking which can result in misinterpretations. This is also confirmed by the right-hand side plot. The average rank of X_4 represented by the light green line decreases and finally stays below the average rank of X_1 and X_2 pictured by the two red curves.

Figure 9.11 and Figure 9.12 depict that there are no misleading PFI ranking for the SVM as well as for the linear model with respect to X_4 . As expected, X_4 has a higher overall importance rank; the other features are more or less equally important. There is a clearly defined pattern in the average rank plots where the graph shows a plateau for feature X_4 at the average rank level

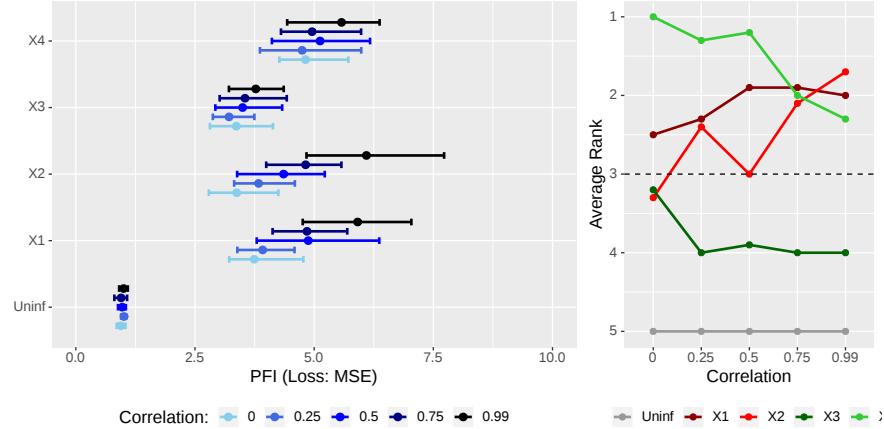


FIGURE 9.10: Scenario 2: PFI on the random forest models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_1 , X_2 and X_3 .

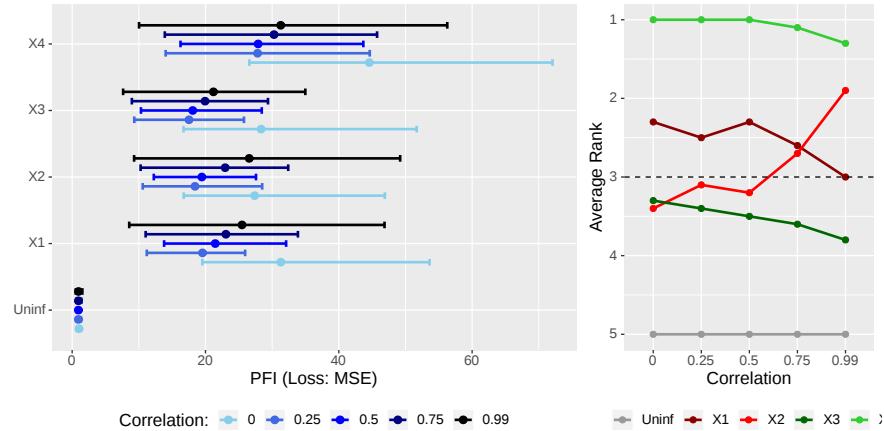


FIGURE 9.11: Scenario 2: PFI on the SVM models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_1 , X_2 and X_3 .

of 1. This can be taken as indication that PFI considers the true theoretical importance rank for feature X_4 . The main difference between SVM and LM is their typical appearance for PFI as described in scenario 1 before.

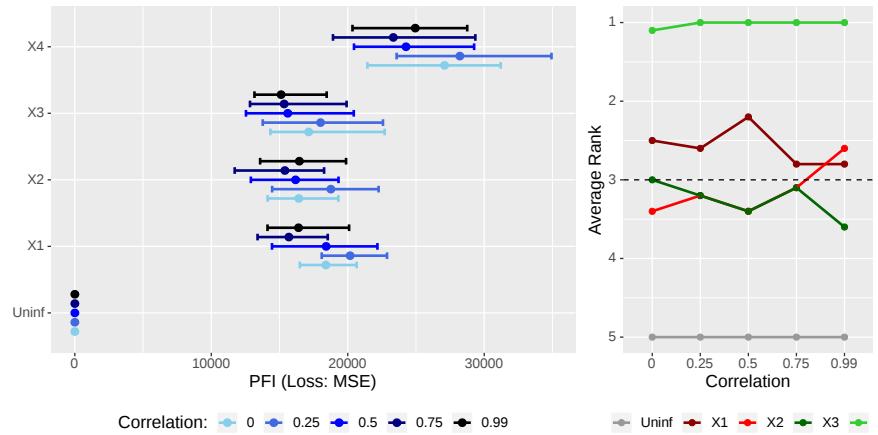


FIGURE 9.12: Scenario 2: PFI on the linear models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_1 , X_2 and X_3 .

As you can see in Figure 9.13 the LOCO Feature Importance remains unchanged throughout an increase of the X_4 coefficient. The PFI and LOCO again have opposite effects with regard to the random forest. Generally speaking, the plots show the same main issues of LOCO as we already seen before. A small exception is the higher importance rank for X_4 . This is depicted again by the plateau of the average importance rank for X_4 represented by the light green line. Furthermore, in case of high correlation the compensation effect also remains valid for X_4 .

The impact of LOCO on the SVM and the linear model are visualized in Figure 9.14 and 9.15. Both suggest that X_4 is more important compared to $X_1 - X_3$. Other than that, we can observe once more the typical behavior of LOCO in case of high correlation. At a correlation intensity of around $\rho = 0.5$ the two correlated features are incorrectly identified as less important than X_3 .

3) Nonlinear Dependence:

In the third scenario there is no pure linear relationship between the target value y and the features. The two feature X_1 and X_3 are plugged into the sine function:

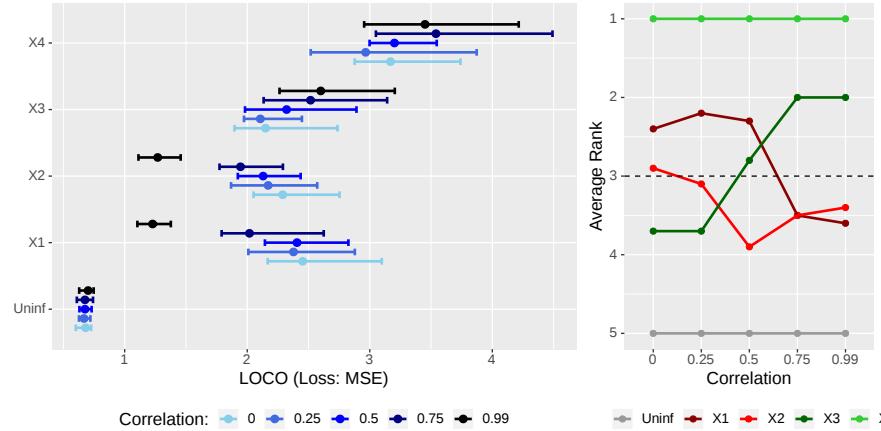


FIGURE 9.13: Scenario 2: LOCO on the random forest models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_1 , X_2 and X_3 .

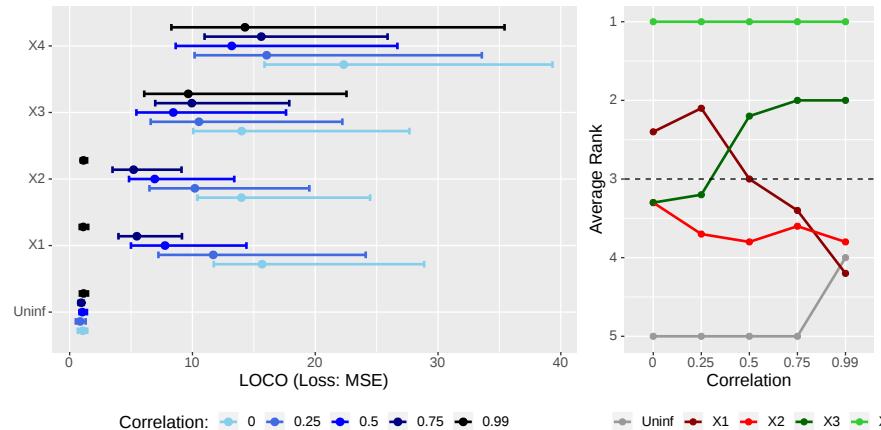


FIGURE 9.14: Scenario 2: LOCO on the SVM models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_1 , X_2 and X_3 .

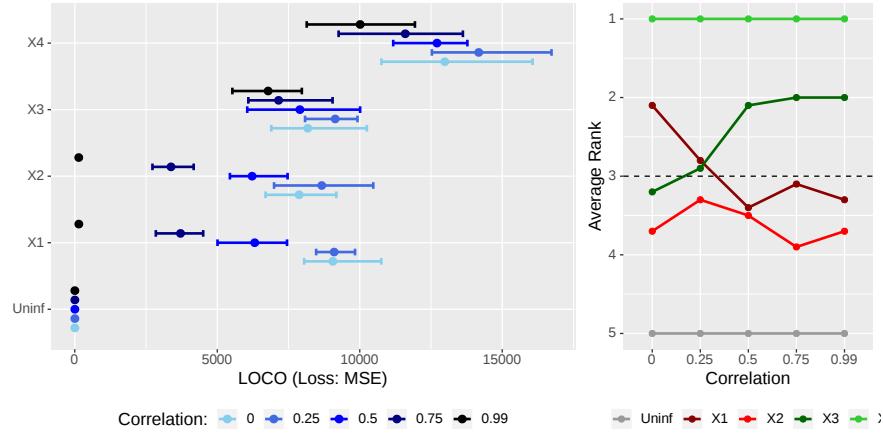


FIGURE 9.15: Scenario 2: LOCO on the linear models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_1 , X_2 and X_3 .

$$y_i = \sin(x_{i1}) + x_{i2} + \sin(x_{i3}) + x_{i4} + \epsilon_i$$

In Figure 9.16 the benchmark result of the third scenario is illustrated. Here we can observe that the linear connection to the target value is broken. Since, one consequence of this break is that the linear model is no longer identified as the best model. The benchmark results present the SVM as the best performing model instead. Still the random forest is performing worst in comparison to the others. All in all, we have accurate models at hand again. Hence, we can investigate this scenario with regards to correlation effects on the Feature Importance as well.

Figure 9.17 displays the effects of PFI for the application of the random forest on the simulated data sets of scenario 3. On first sight, comparing X_3 with X_4 , you can see that the features inside the sine function are ranked as less important than the linear ones. However, in case of high correlation feature X_1 gains drastically in importance. This even goes as far as X_1 having the same importance rank as those features with a linear dependence. This leads to the perception that the importance value of X_1 adapts to the value of X_2 . Once again the PFI assesses the importance rank incorrectly.

According to Figure 9.18, PFI shows its typical behavior on the SVM model. As in case of the random forest the features within the sine function are classified as less important than the linear ones. Similarly, it is interesting to

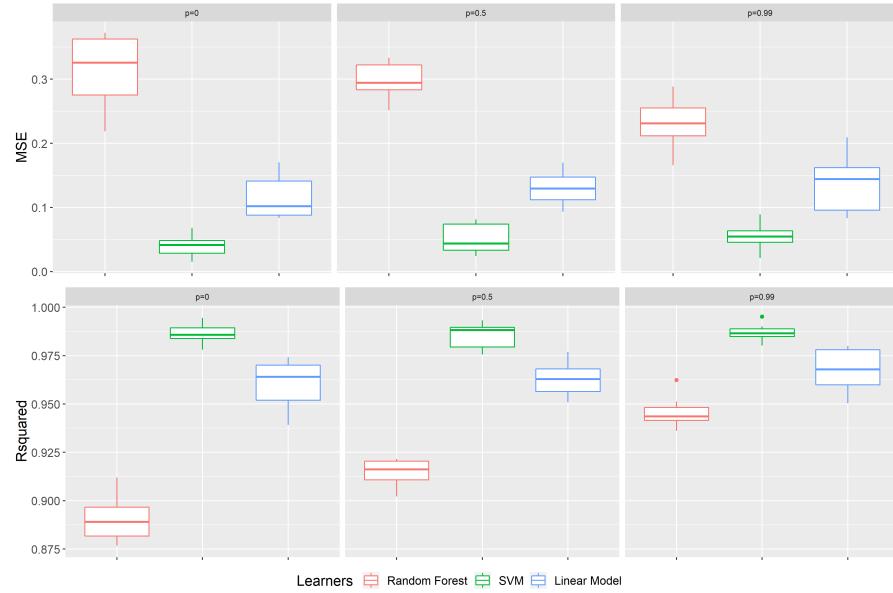


FIGURE 9.16: Benchmark results of scenario 3 for data sets with $p = 0$, $p = 0.5$ and $p = 0.99$ (from left to right). On top the performance measure is the MSE, at the bottom R^2 . The colour representing the learning algorithm. Red: Random Forest, green: SVM and blue: Linear Model.

see the adaption effect of feature X_1 . Yet, X_1 does not exceed the rank of X_2 . The PFI on the linear model, illustrated in Figure 9.19, has a very parallel looking appearance. Thus, one can conclude that it is kind of robust against correlation and shows the theoretical true importance rank.

The impacts of LOCO on the different models are visualized in Figure 9.20, 9.21 and 9.22 respectively. All of them suggest that the linear features are more important. The higher the correlation, the lower the feature importance for feature X_2 drops. Again, we can observe the typical behavior of LOCO in case of high correlation. At a certain correlation intensity in the range between $\rho = 0.75$ and $\rho = 0.99$ LOCO specifies X_3 as more important than X_2 . Other than that LOCO shows the same results for the various models as mentioned before.

9.1.2 Real Data

In order to illustrate the problems arising from correlated features on Feature Importance using a real data set, we will take a look at the “Boston” data set which is available in R via the MASS package. The data set was originally

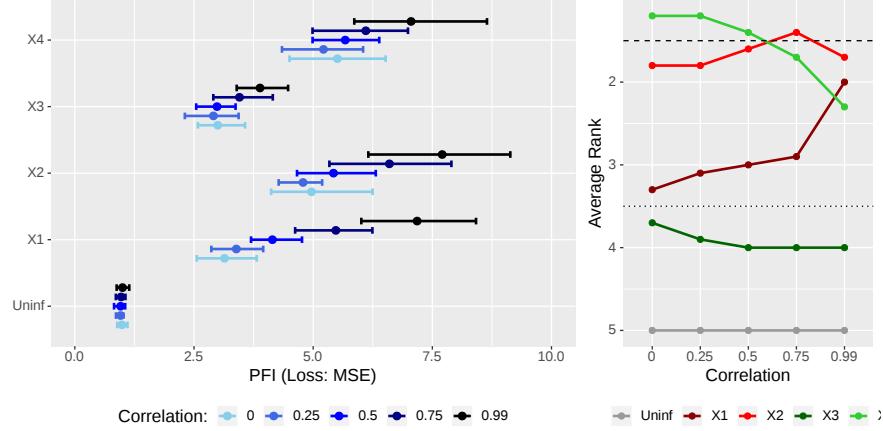


FIGURE 9.17: Scenario 3: PFI on the random forest models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_2 and X_4 , the dotted line of X_1 and X_3 .

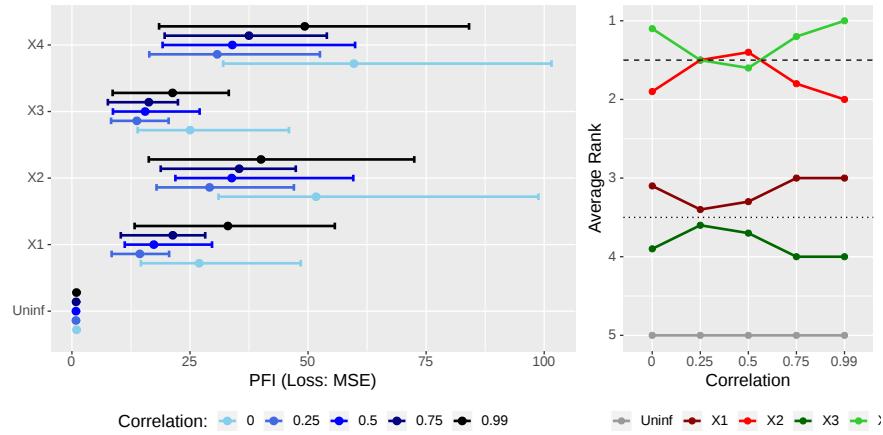


FIGURE 9.18: Scenario 3: PFI on the SVM models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_2 and X_4 , the dotted line of X_1 and X_3 .

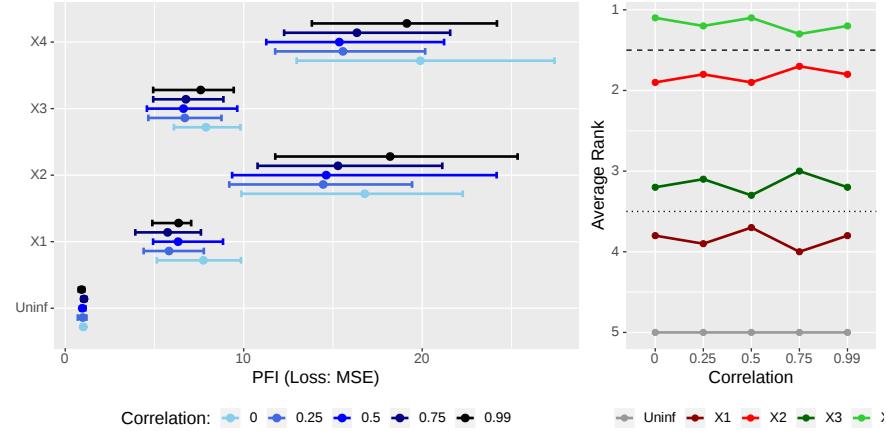


FIGURE 9.19: Scenario 3: PFI on the linear models with different correlations of features X_1 and X_2 . The left plot shows the PFI values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_2 and X_4 , the dotted line of X_1 and X_3 .

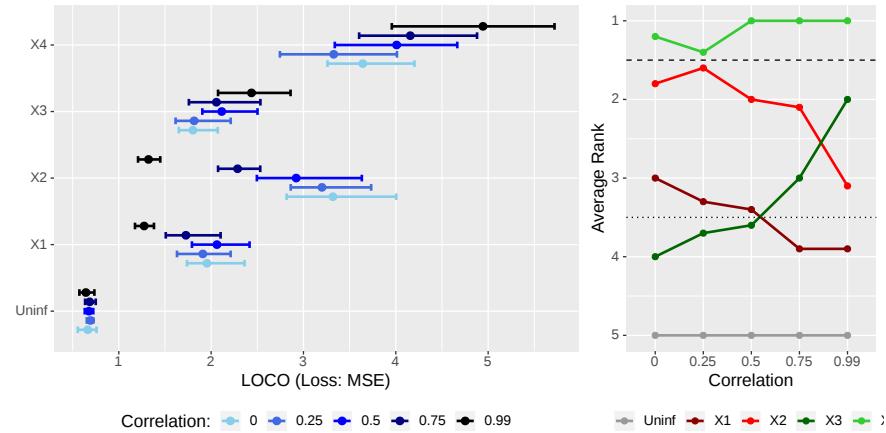


FIGURE 9.20: Scenario 3: LOCO on the random forest models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_2 and X_4 , the dotted line of X_1 and X_3 .

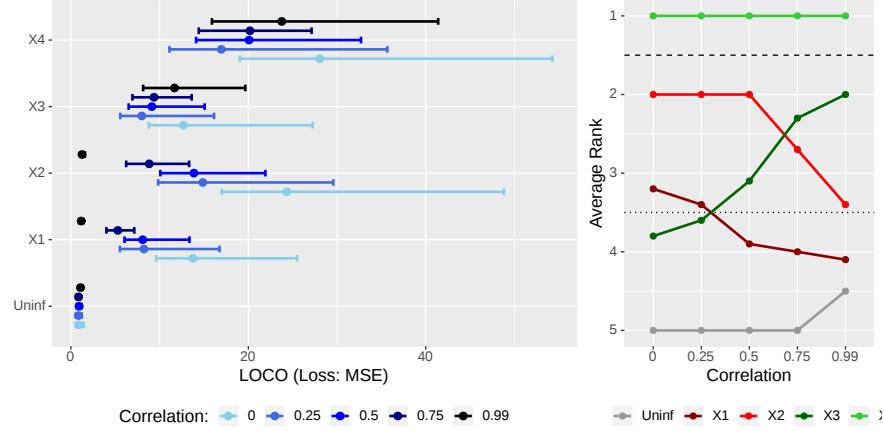


FIGURE 9.21: Scenario 3: LOCO on the SVM models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_2 and X_4 , the dotted line of X_1 and X_3 .

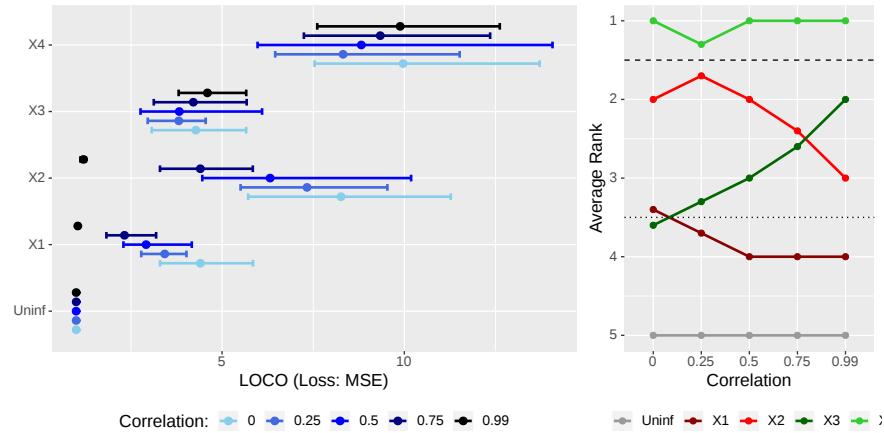


FIGURE 9.22: Scenario 3: LOCO on the SVM models with different correlations of features X_1 and X_2 . The left plot shows the LOCO values for different correlation intensities. The right plot represents the average rank of the features at a certain correlation intensity. The red lines mark the two correlated features and the green lines the independent ones. The dashed line illustrates the true theoretical importance rank of X_2 and X_4 , the dotted line of X_1 and X_3 .

published by [Harrison and Rubinfeld \(1978\)](#). To make the results a little bit more feasible and clear, we only look at a subset of the data. Out of the original 13 features we picked out 6. The objective is to predict the house prices with respect to the given features.

The following variables are considered part of the subset:

```
DIS - weighted distances to five Boston employment centres  
AGE - proportion of owner-occupied units built prior to 1940  
NOX - nitric oxides concentration (parts per 10 million)  
CRIM - per capita crime rate by town  
RM - average number of rooms per dwelling  
LSTAT - % lower status of the population  
  
MEDV - target: Median value of owner-occupied homes in $1000's
```

First of all, we want to have a look at the benchmark results illustrated in Figure 9.23 on the left-hand side. Here, the best result can be observed with respect to the MSE for the random forest. Since Features Importance was introduced to interpret black box models like the random forest, but has shown multiple complications in our simulations, our focus here is on the random forest model.

The following experiments are inspired by [Parr et al. \(2018\)](#). An easy way to create a feature with perfect multicollinearity in a data set is by duplicating one feature and adding it to the data set. As a result the correlation coefficient equals 1. To make the two features less correlated, we also present a case where instead of simply duplicating one, a noise constant is added to the duplicate. This should lower correlation to a certain amount. The noise constant was calculated so it fits the value range of the feature. In order to show meaningful results, the constant's standard deviation was set to 30 percent times the mean of the feature itself.

Evaluating the PFI on our given data set indicates the feature lower status of the population `lstat` as the most important feature with a value around 4.3 (see Figure 9.24). By duplicating the feature “`lstat`” and adding it to the data set as well as repeating PFI, one can see that `dup_lstat` and `lstat` are equally important. As a rule of thumb the PFI of both are kind of sharing the Feature Importance from the case before. Since now, the PFI values of `lstat` and `dup_lstat` dropping down to ca. 2.4. This makes sense as equally important features should be considered as a split with the same probability during the prediction process of random forest. As a consequence in this situation we have a 50-50 choice between `lstat` and `dup_lstat`. More importantly, the feature `lstat` is no longer ranked as the most important feature, instead the average number of rooms per dwelling `rm` moves to the leader board. Again, we show how correlation between features can lead to wrong interpretations.

When adding a noise variable to `dup_lstat` (`n_lstat`), the correlation should

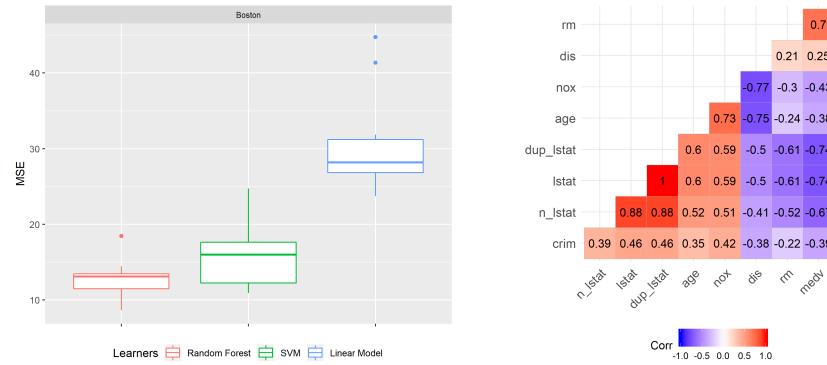


FIGURE 9.23: On the left-hand side the benchmark result for the random forest (red), the SVM (green) and the linear model (blue) on the basis of the Boston data set. The underlying performance measure is the MSE. On the right-hand side a Pearson correlation plot with the features of the Boston data set.

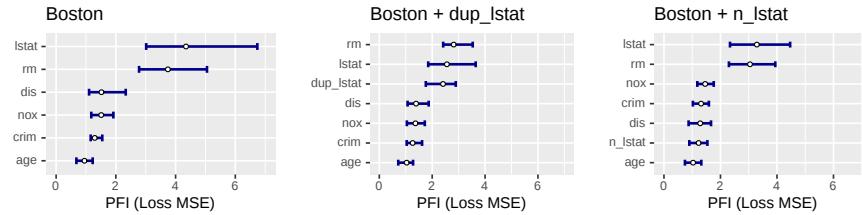


FIGURE 9.24: PFI on the original data set (left), on the data set including a duplicate of `lstat` (middle) and on data set with a noise added to the duplicate (right).

decrease. In fact, Figure 9.23 shows in the right-hand side plot, that this yields to a Pearson correlation coefficient of around 0.88. Now the initial importance value of around 4.3 is shared between `lstat` = 3.3 and `n_lstat` = 1.2 at a ratio of 3 to 1. In contrast to the case of multicollinearity, the importance values are moving away from each other. Now `lstat` is ranked most important, yet only by a very marginal amount and still being below the actual value of 4.3 as in the initial case. It seems that two correlated features are pulling each other down, with the extent and fraction depending on the correlation strength.

As a contrast to PFI, the LOCO Feature Importance specifies `rm` = 1.8 as the most important feature, closely followed by `lstat` = 1.75 (see Figure 9.25). Furthermore, there is a large overlap of the quantile bands of both features. In order to make this case easier to compare with PFI, we have another look at `lstat`. Adding the duplicate of `lstat` to the data and rerunning LOCO, one

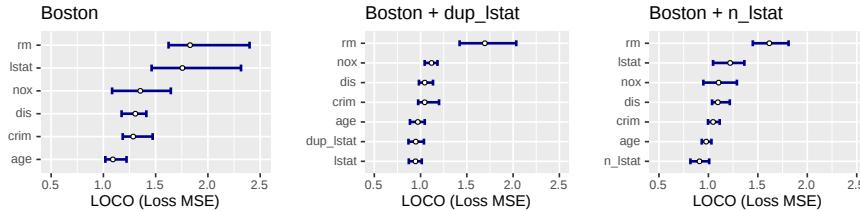


FIGURE 9.25: LOCO on the original data set (left), on the data set including a duplicate of `lstat` (middle) and on data set with a noise added to the duplicate (right).

can see that `lstat` disappears from the top ranking. This leads to the same effect as in previous simulations. Both highly correlated features `dup_lstat` and `lstat` are erroneously indicated as unimportant. Understanding the fact that LOCO Feature Importance measures the drop in performance of a model, one can easily come up with a reason for this. If you leave out one feature that is perfectly correlated to the other, the performance will be the same as before. Since the feature which is still in the data set contains exactly the same information as the one left out there is no alteration in performance. Adding a little bit of noise to the duplicate `dup_lstat` leads to an increase of LOCO Feature Importance for `lstat`. This trend increases with higher variance of the noise or, in other words, the lower the correlation of the two features.

From the examples given as well as by looking at the correlation in the data set (see Figure 9.23), one can conclude that there should be correlation effects even without intervening in the data set. For instance, `lstat` is correlated in multiple ways with other features. The extent of correlation with the other features never drops below the 0.5 mark. If you look at the correlation of the lower status of population and the average number of rooms per dwelling, this indicates a ρ of -0.61. This makes sense, because one can assume that a larger amount of rooms can only be financed by wealthy people. A possible conclusion could be that in case of PFI both features are overestimated and hence at the top of the ranking board. Moreover, both features show quite large quantile bands in comparison to others. These outcomes look kind of similar to the ones shown in the simulation section (compare with Figure 9.3). Obviously, correlation exists before adding any new feature to the data set. In these kinds of set-ups you cannot verify the true theoretical importance. The only option are assumptions about the underlying effects and guessing the true importance based on simulations as the ones presented here. This shows how unpleasant correlation can be in connection with Feature Importance.

9.2 Alternative Measures Dealing with Correlated Features

To sum up, we want to highlight that feature importance measures like LOCO or PFI can be strongly misleading when features of a given data set are correlated. Thus, a check for correlation between features before usage of these two methods is recommended or even necessary in order to have a credible interpretation. In the literature there are some suggestions on how to deal with collinearity with respect to Feature Importance. One suggestion which is related to the PFI seems kind of obvious. The PFI is usually calculated by permuting one specific feature. In case of strong correlation of, for example, two features, it is sensible to permute these together, meaning the building of a group such that the correlation is still present in the calculation of PFI ([Parr et al., 2018](#)). For illustration, let's look at the example of the bikesharing data set mentioned in the introduction (Figure 9.1). Since `weekday` and `working day` are highly correlated, they should be only permuted together. If this is done, a strange combination of data like Wednesday and no working day is not possible. This should also solve the severe problems with extrapolation, because we are not leaving the real data distribution.

Other alternative measures are focusing on the idea of permuting new values of a feature by taking the distribution conditional on the remaining features into consideration like the Conditional Feature Importance by [Strobl et al. \(2008\)](#). Despite the fact that the Conditional Feature Importance cannot completely solve the problem of overestimating correlated features as more important, it proves to be better at identifying the true important features of a model. Another approach is a mixture of a relearning PFI ([Mentch and Hooker, 2016](#)) and the Conditional Feature Importance. ([Hooker and Mentch, 2019](#))

To conclude, some of these approaches are quite easy to implement, others prove to be a bit more complicated. What most of them have in common are high computational costs. These either emerge from refitting the model or simulating from the conditional distribution ([Hooker and Mentch, 2019](#)). This makes an application in case of large data sets and feature spaces less favourable. Another possible idea is an indicator variable for the given data set that shows how much trust we can have in the outcome on the basis of feature correlation. In order to derive a suitable interpretation of the machine learning algorithm, we recommend to have a look at other model-agnostic tools like PDP, ICE, ALE or LIME as well.

9.3 Summary

Calculating Feature Importance for simple linear models is not strongly affected by correlation. However, the calculation of Feature Importance of black box models, like random forest, is susceptible to correlation effects. Overall, we cannot clearly define whether PFI or LOCO is the preferable Feature Importance measure. Both measures showed their pros and cons.

In the simulation section we demonstrated some interesting results regarding issues caused by correlation. For LOCO Feature Importance, the most remarkable problem was the huge drop in importance value or ranking number for highly correlated features. This even goes so far as features being erroneously identified as completely unimportant. This issue was observable throughout all models. In contrast to LOCO, the effect of PFI mostly depends on the learning algorithm. In case of the random forest, there was a clear trend towards highly correlated features i.e. they were declared as more important than the other features. The SVM showed similar results as for the random forest, but the effects were less strong. In contrast, the linear model was more or less robust against correlations. In the literature the random forest calculated by the out-of-bag observations or other learning algorithms, like neural networks, showed similar results (Hooker and Mentch, 2019). Furthermore, the real data application supported the theses, we saw in the simulation section. The results make us even more aware that the correlation intensity is critical for the importance ranking of the features.

Aside of the present simulations, further options are possible. For instance, we limited ourselves to numerical features and regression tasks. However, in reality you often have correlated categorical features and classification tasks as well. Even an adjustment of the hyperparameters of the models used here is an option. This goes to show that, despite all of the used methods in this chapter, there are even more interesting effects to discover when it comes to Feature Importance and correlation. Yet, this goes beyond the scope of this chapter and deviates from our aim to raise the reader's awareness of aforementioned issues with regards to correlation in order to avoid mistakes in the future.

All in all, PFI and LOCO can have misleading effects in case of correlated features. This holds especially true as evaluating the Feature Importance rank can be expensive and most of the time you are only looking at e.g. the top three important features (Molnar, 2019). In those cases a wrong importance rank can cause a lot of damage to the unobservant user. This leads to the conclusion that next time we use Feature Importance we should be aware of correlation effects as a limitation to methods' accuracy.

9.4 Note to the reader

For our analysis, we used R ([R Core Team, 2017](#)). For all the models and Feature Importance measures, we used the mlr package ([Bischl et al., 2020](#)) as well as the iml package ([Molnar et al., 2018](#)). All plots have been created using ggplot2 ([Wickham et al., 2019](#)).

10

Partial and Individual Permutation Feature Importance

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The introductory chapter discussed the relevance of PFI and LOCO for the interpretability of machine learning models. It was argued that for interpretation purposes, the concept of Feature Importance is an indispensable complement to analyzing Feature Effects. The Feature Importance quantifies the contribution of a specific feature to the prediction power of a model. Yet, it was also remarked that an aggregated, global measure of Feature Importance might be insufficient. It might be the case that within a feature, some single values or subgroups are more important for predictions than others. This heterogeneity, however, could not be captured by a single metric. Besides, it is trivial to understand that with increasing heterogeneity, the global PFI becomes less revealing. By implication, a complementary method that captures such heterogeneity becomes more decisive.

To identify whether such heterogeneity exists, an algorithm is required that calculates the Feature Importance for each value of the respective feature. Briefly, a measure that indicates the contribution of an individual value to the global Feature Importance. However, as the range of values can be rather large, a tabular description seems to be cluttered. Therefore, a visualization tool that allows gaining meaningful and concise insights on how the Feature Importance varies, should be derived. One would then plot the respective values of the feature against its local Feature Importance measures. In the case of heterogeneity, the plotted curve should then deviate from a constant shape.

Following the objective of visualization, one can make use of the concepts of Partial Dependence and Individual Conditional Expectation, as these methods allow us to detect heterogeneity in the context of Feature Effects. [Casalicchio et al. \(2018\)](#) avail themselves from these concepts and transfer them to the concept of Feature Importance, by introducing the metrics Partial Importance (PI) and Individual Conditional Importance (ICI) (see [Goldstein et al. \(2013\)](#)). They show that these methods enable to detect subgroups with differing levels

of Feature Importance and are, therefore when striving for a complete picture, non-negligible complements to the global PFI metric.

However, it might be of interest to not only reliably detect heterogeneity but to also better understand its drivers. In general, it can be distinguished between three different sources for heterogeneity. First, if the relationship between a feature and the response is non-linear. Secondly, if features are correlated and third if interaction effects between features are existent. In what follows, it will be focused on the latter as the first represents no actual concern and the second was already discussed in the previous chapter.

As will be seen, uncovering interaction effects is not as straightforward, as the structural relationship between covariates and the outcome variables is unknown. Hence, from first glance, it is unclear whether there is just a non-linear relationship or whether indeed interactions between covariates exist. But if the PI or ICI method does not enable us to distinguish between these sources, the applicant does not gain a better understanding. If heterogeneity is not understood, one can hardly interpret the results and if so, the methods failed to a certain extent.

Hence, the motivation is clear. If interaction effects between covariates are existent, it should be, for the sake of the interpretability of a machine learning model, of major interest to detect them. Detecting them is an indispensable objective to be enabled to then explain them. And only if they can be explained, the heterogeneity in Feature Importance can be understood and the results can be interpreted accordingly.

To answer the questions, formulated above, the remaining subchapters are structured as follows: In chapter 10.1, the concepts of Partial Importance (PI) and Individual Conditional Importance (ICI) are theoretically introduced. This shall provide the reader with an in-depth understanding of how the Feature Importance can be visualized, both on an aggregated, global and disentangled, local level. With these preliminaries, the reader is equipped with sufficient knowledge to understand the following simulations (see chapter 10.2) which are meant to cover two broader topics.

In the subchapter 10.2.1, it will be focussed on to what extent the PI and ICI plots can uncover interaction effects between features. To give this a new angle of perspective, a new method, called “derivative-ICI” (see chapter 10.2.1.2) will be introduced.

The subchapter 10.2.2 will then discuss the issue of actually explaining the detected interaction effects. Pursuing this objective, an additional method will be introduced which will predict the global Feature Importance of the feature of interest based on the remaining features in the model (see chapter 10.2.2.1). A significant relationship between the PFI and at least one feature would then not only confirm the conjecture of interaction effects but also explain between which features these interactions took place.

The simulation chapter will then be closed by bringing the results together. With that, one can then calculate the respective conditional Feature Importance (see chapter 10.2.2.2). Plotting this provides the user with an exhaustive understanding of why the local Feature Importance differs between subgroups. Further, it even allows quantifying the difference in Feature Importance. Yet, the focus here will lay on the visualization and not on the direct quantification. The latter was already discussed by Casalicchio et al. (2018).

The whole simulation chapter serves as a “cookbook” on how to still reach meaningful and interpretable results when heterogeneity is driven by unobserved interaction effects. After this is completed, the methods will be verified on real data (see chapter 10.3). Pursuing this, a brief analysis is conducted on the Boston Housing Data.

The chapter is then closed by a summary and discussion of the methods (see chapter 10.4). This will include a final evaluation of the PI and ICI plots and thereby answer the question of whether the methods are useful or not.

10.1 Preliminaries on Partial and Individual Conditional Importance

Once the concept of the global PFI is clear, it will be shown that deriving the Partial Importance as well as the Individual Conditional Importance is straightforward. To be able to comprehend that, one should briefly recall that the global PFI of a feature S is defined as

$$PFI_S = E(L(f(X_S, X_C), Y)) - E(L(f(X), Y)) \quad (1)$$

where the first term corresponds to the theoretical generalization error of the model, including the permuted feature x_S and the second term depicts the generalization error resulting from the original model. The difference then gives the global PFI of feature S . However, in the application, the joint distribution of X and Y is unknown so that the generalization error needs to be approximated by the empirical error. The first term of equation (1) is derived by the formula

$$\widehat{GE}_C(\hat{f}, D) = \frac{1}{n} \sum_{i=1}^n \frac{1}{n} \sum_{k=1}^n L(\hat{f}(X_S^{(k)}, X_C^{(i)}), y^{(i)}) \quad (2)$$

which states that the empirical losses for all observations $i \in \{i, \dots, n\}$ are calculated respectively for each permutation $k \in \{i, \dots, n\}$ of X_S and averaged over n . Here, $\widehat{GE}_C(\hat{f}, D)$ is subscripted with C as it shall indicate the generalization error when only predicting with the remaining feature subset X_C . Equivalently, the second term of equation (1) can be approximated by the formula

$$\widehat{GE}(f, D) = \frac{1}{n} \sum_{i=1}^n L(f(x^{(i)}, y^{(i)}) \quad (3)$$

In equations (2) and (3), \hat{f} corresponds respectively to the fitted supervised machine learning model and D is defined as the underlying test data, sampled from a *i.i.d* distribution P . Taking the difference of both approximations from equations (2) and (3) yields the formula for the global PFI_S which is defined as

$$\widehat{PFI}_S = \frac{1}{n^2} \sum_{i=1}^n \sum_{k=1}^n (L(\hat{f}(X_S^{(k)}, X_C^{(i)}), y^{(i)}) - L(f(x^{(i)}, y^{(i)})) \quad (4)$$

whereby calculating the global PFI becomes computationally expensive when

n is large as the iteration scales with $O(n^2)$. This issues becomes more apparent when considering the full set of possible permutations $(\tau_1, \dots, \tau_{n!})$, resulting in an equation equivalent to formula (5) where the algorithm iterates over all $n!$ permutations

$$\widehat{GE}_{C,perm}(\hat{f}, D) = \frac{1}{n} \sum_{i=1}^n \frac{1}{n!} \sum_{k=1}^{n!} L(f(x_S^{\tau_k^{(i)}}, x_C^{(i)}), y^{(i)}) \quad (5)$$

To circumvent the computational disadvantage, it is advisable to rather approximate $GE_C(f, D)$ by $GE_{C,approx}(f, D)$ which only entails a randomly selected set of m permutations, defined as

$$\widehat{GE}_{C,approx}(\hat{f}, D) = \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{k=1}^m L(f(x_S^{\tau_k^{(i)}}, x_C^{(i)}), y^{(i)}) \quad (6)$$

This results in an approximated global PFI defined as

$$PFI_{S,approx} = \frac{1}{n \cdot m} \sum_{i=1}^n \sum_{k=1}^m (L(f(x_S^{\tau_k^{(i)}}, x_C^{(i)}), y^{(i)}) - L(f(x^{(i)}, y^{(i)})) \quad (7)$$

From there, Individual Conditional Importance can be computed. One can calculate the change in performance for each i -th observation by taking the summands from equation (7) which is defined as

$$\Delta L^{(i)}(x_S) = L(\hat{f}(x_S, x_C^{(i)}), y^{(i)}) - L(\hat{f}(x^{(i)}), y^{(i)}) \quad (8)$$

and repeat that for all permutations m , resulting in m components $\Delta L^{(i)}(x_S^{(k)})$ for each observation i . Taking the average overall permutations yields the global PFI for observation i which can be interpreted as the individual contribution of the i -th observation to the global PFI metric.

In order to visualize the ICI, one can plot the pairs $\left\{(x_S^{(k)}, \Delta L^i(x_S^{(k)}))\right\}_{k=1}^n$. In the same manner, the partial importance (PI) which corresponds to the expected change in performance at a certain value of x_S . The estimated PI can be derived by taking the pointwise average over all ICI curves at the respective fixed points of x_S . This is equivalent to $\widehat{PI}_S(x_S) = \frac{1}{n} \sum_{i=1}^n \Delta L^{(i)}(x_S)$. Equivalent to above, the PI curve can be visualized by plotting the pairs $\left\{(x_S^{(k)}, \widehat{PI}_S(x_S^{(k)}))\right\}_{k=1}^n$.

The visualization of both, the ICI curves and the PI curves is illustrated in figure 10.1. The illustration corresponds to an artificial dataset with only three observations. The dashed lines correspond to the respective ICI curves and the

solid line illustrates the PI curve. The plot can be interpreted as follows. If the ICI curve takes the value 0, the original value of x_S was replaced by its original value and therefore, no change in performance occurred. Besides, it is also expected that if the distance between the original value and the replacing value increases, the difference in performance also increases. This is also confirmed by the shape of the ICI curves.

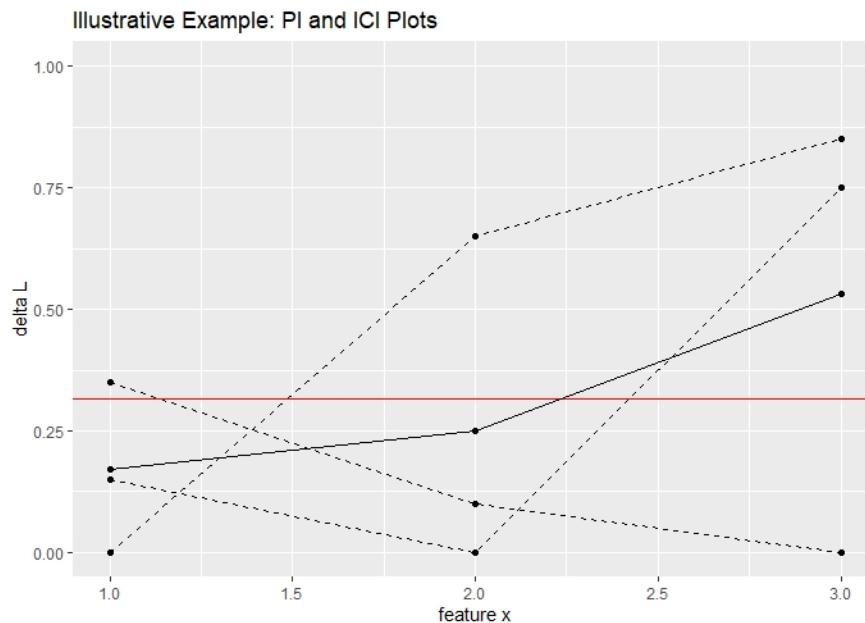


FIGURE 10.1: Visualization of PI and ICI plots based on an illustrative example. The visualization corresponds to three observations and a total of three permuted datasets. The dashed lines correspond to the ICI curves. The solid line corresponds to the PI curve.

As already theoretical described, averaging the ICI curves, yields the PI curve and taking the integral of the PI curve yields the global PFI of feature x_S . In figure 10.1, the red line corresponds to the global PFI.

Note, that the exchangeability between PFI, PI and ICI depicts a convenient property for further analyses. The PI allows detecting regions with a higher or lower Feature Importance, whereby the ICI allows us to analyze individual observations and its contribution to the global PFI.

10.2 Simulations: A cookbook for using with PI and ICI

Simulations are a convenient choice to check statistical models for their correctness and validity. The following simulations are meant to guide the reader through a proposed step-by-step procedure which first, shall detect, then explain and lastly visualize interaction effects and their impact on a feature's heterogeneity in importance. Even though each step is motivated by a limitation from its preceding method, they should be considered as mutual complements that aim to derive a complete picture.

10.2.1 Detect Interactions

In general, two kinds of relationships between two covariates exist. First, the most common one, they are correlated. Second, the covariates do interact. Detecting correlation can be obtained by calculating the correlation matrix between the features. If two features are independent, the correlation is 0. The reverse, however, is not necessarily true as correlation measures only linear dependence. In such cases, a concept of information theory could be used. The metric “mutual information” describes the amount of information about one feature that is obtained when observing the other feature. Briefly, it quantifies the amount of shared information between features and therefore, measures implicitly the dependence between them. If the mutual information is 0, the features are indeed independent. This allows to even quantify interactions between features.

Hence, methods exist which can detect and even quantify the dependence between variables, apart from correlation. Now, it is to be clarified whether PI or ICI plots do have a similar power.

10.2.1.1 Partial Importance and Individual Conditional Importance plots

Again, the goal is to assess whether visualizations can detect interaction effects. To gain a first visual understanding of PI and ICI plots, consider the following data-generating model.

$$y = 5x_1 + 5x_2 + x_3 + \epsilon \\ x_1 \stackrel{i.i.d}{\sim} \mathcal{N}(0, 1), x_2 \stackrel{i.i.d}{\sim} \mathcal{N}(0, 1) \text{ and } x_3 \stackrel{i.i.d}{\sim} B(1, 0.5), \epsilon \stackrel{i.i.d}{\sim} \mathcal{N}(0, 1)$$

The model is simulated with 1000 observations which are split into 80% training and 20% test data. On the training data, a Random Forest model is

fitted and based on the estimates, the Partial Importance and the Individual Conditional Importance are calculated on the test data. The latter is done as outlined in the preliminaries. In figure 10.2, the plots are visualized for feature w_2 .

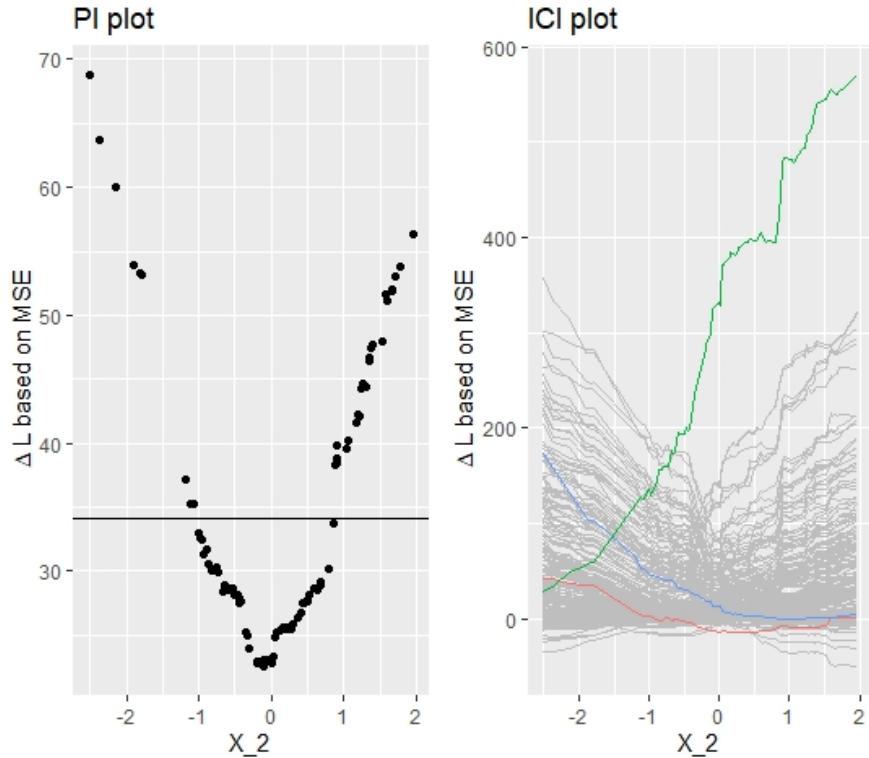


FIGURE 10.2: Simulated data (simulation 1): PI Plot and ICI Plot for feature x_2 . Introductory example with no interaction effect. Still, heterogeneity is observed.

The PI plot indicates already a heterogeneous relationship, where the Partial Importance becomes large for large absolute values. The minimum is reached at around $x_2 = 0$. The respective ICI plot provides even more insights. It shows that some observations have a low local Feature Importance for large negative values and a large local Feature Importance for large positive values and vice-versa. As the shape of the curves are in both directions similar and the minimum is around $x_2 = 0$, it can be concluded that the feature x_2 is equally distributed around its mean.

But how does this coincide with the fact that none of the above-discussed sources for heterogeneity are apparent in this simulation? As expected, no heterogeneity should be observed and yet the heterogeneity is considerable.

The observed heterogeneity is because inherently extreme input values are considered on average as more important. Extreme values are replaced by values that are on average further away from the original input value which in turn results in higher loss differences. This problem is getting worse when choosing loss functions that penalize large errors more extreme. Briefly, the heterogeneity should be higher with a L2-loss compared to a more robust L1-loss.

Hence, the plots might be misleading as it should not be concluded that large positive or large negative values are more important. Therefore, if features are normally distributed, the shape of the curves should be considered as a baseline plot whereby only deviations from there can be considered as a “true”, interpretable or meaningful heterogeneity. Yet, keeping that in mind, the PI and ICI plots do explain the heterogeneity to the full extent.

With these baseline insights, one can now evaluate to what extent PI and ICI plots can detect heterogeneity which evolved through interaction effects. Following this objective, the following data-generating model is considered:

$$y = x_1 + 5x_2 + 5x_2 \mathbf{1}_{x_2 > 2, x_3=0} + \epsilon$$

$$x_1 \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1), x_2 \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 4) \quad \text{and} \quad x_3 \stackrel{i.i.d.}{\sim} B(1, 0.5), \epsilon \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1)$$

Besides the comparable linear relationship between the covariates and the outcome variable, the model contains additionally an interaction effect between x_2 and x_3 . The model suggest that the feature x_2 should become more important for values $x_2 > 2$ and $x_3 = 0$. Hence, the plots should reveal large values in this area.

The respective PI and ICI plots (see figure 10.3) are at first glance quite similar to the plots, resulting from simulation 1. Yet, the above-mentioned differences can be observed. First, the PI plot reveals that the Feature Importance increases with a higher magnitude for large positive values, indicating that these observations are relatively more important. Looking at the ICI plot and highlighting the observations with the highest, the lowest and the median FI, yields some clearer insights. The blue curve corresponds to the observation with the largest contribution to the global PFI. Its initial value for x_2 is beyond the threshold of 10 and the corresponding x_3 takes the value 0. Hence, the interaction effect triggered and the feature became more important. The blue curve ascends decisively in the area around $x_2 = 2$. Once the threshold is reached, the fitted model does not trigger the interaction effect anymore and therefore, the predictions diverge increasingly. This observed property already indicates that an interaction effect is a major driver for heterogeneity.

Yet, the quite similar plots from simulation 1 and simulation 2 might cause problems to identify this interaction at first glance. Therefore, in what follows,

an additional method will be introduced which aims for less ambiguous results. Besides, it is important to note that these plots still do not explain which features drive the heterogeneity in Feature Importance.

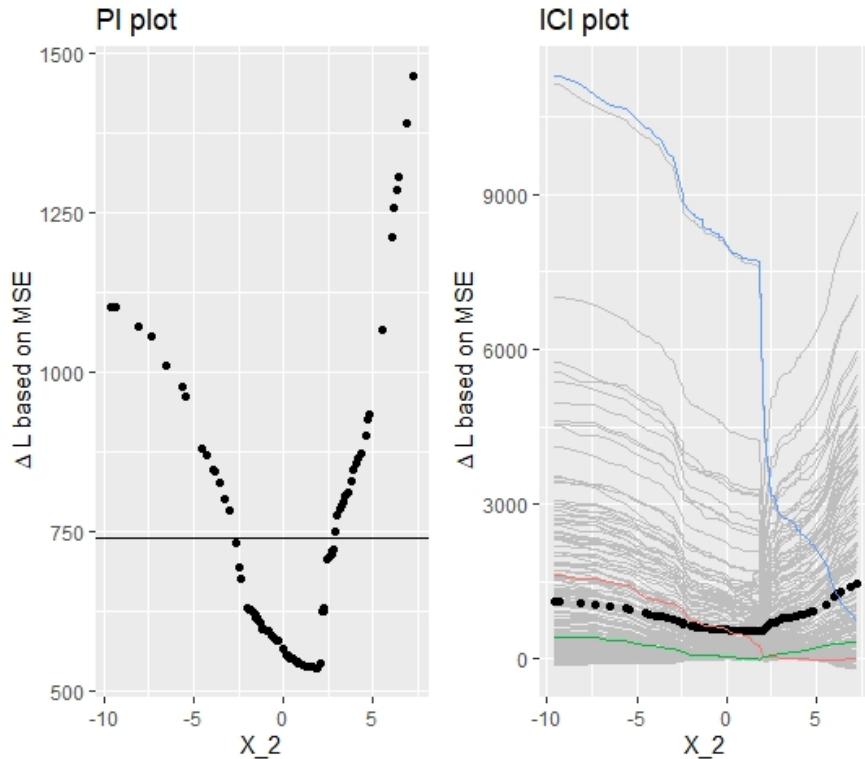


FIGURE 10.3: Simulated data (simulation 2): PI Plot and ICI Plot for feature x_2 . Visualizations correspond to data-generative model with interaction effect between x_2 and x_3 .

10.2.1.2 d-ICI (derivative Individual Conditional Importance)

To supplement the results, yielded from the PI and ICI plots, a method will be proposed that was introduced by Goldstein et al. (2013) with the purpose to detect interaction effects in the context of analyzing Feature Effects.

By calculating the numerical derivative for each ICE curve, they show that the respective derivative plots enable to detect interaction effects. They argue that the derivatives should be constant over the range of values if no interaction effects exist. In the case of interaction effects, the derivatives should show a larger positive or negative magnitude at the point where the interaction effect takes place.

Taking this, we can transfer the theoretical concept from Feature Effects to Feature Importance by calculating the derivatives of each ICI curve respectively. It was already observed that an interaction triggers an initially higher level of Feature Importance which was represented in a sudden increase or decrease of the ICI curves that were affected by the interaction. This should be perfectly captured by the derivatives.

Even though the conceptual transfer seems straightforward, the interpretation of the derivative plots should be adjusted slightly. First, one should not expect that the plots are constant in the case when no interaction is existent. Figure 10.4 shows for the model with no interaction effect that, there is also some altitude in the derivatives. However, this is approximately equally distributed over the feature's range of values and therefore, it is reasonable to assume that there is no interaction effect.

Secondly, by contrast to the derivative of the ICE curves, it is to be expected that the derivatives of the ICI curves are both, negative (descending curves) and positive (ascending curves). The respective d-ICI plot (see figure 10.5) for simulation 2 depicts a distinguished picture. Over the whole range of values, the derivatives are comparably low in magnitude, except for the derivatives at $x_2 = 2$.

Without going into further detail at this point, one can conclude that d-ICI plot seems to be a valid method to obtain a more robust indicator for interaction effects. Besides, the plots directly reveal where the interaction effect triggers which constitutes an important property when aiming for better interpretability.

However, even if the d-ICI plots are sometimes convenient choices to detect interaction effects, they are still only applicable if some properties hold. First, and that is the most crucial one, the interaction effects shall not be existent over the entire range of values of the considered feature. If so, one cannot identify a single spot within the range where the feature becomes initially more important. Hence, the d-ICI plot is expected to take a similar shape as if no interaction was existent.

Secondly, the d-ICI plot is only assumed to yield unambiguous results, if the interaction effect is strong enough. However, this must not necessarily be interpreted as a limitation. It merely shows that the second-order effect (interactions between two features) should not be decisively smaller than the first-order effect (main effect of the feature). If the second-order effect is too small, then it is open for discussion whether detecting this interaction effect is even decisive for interpreting the machine learning model.

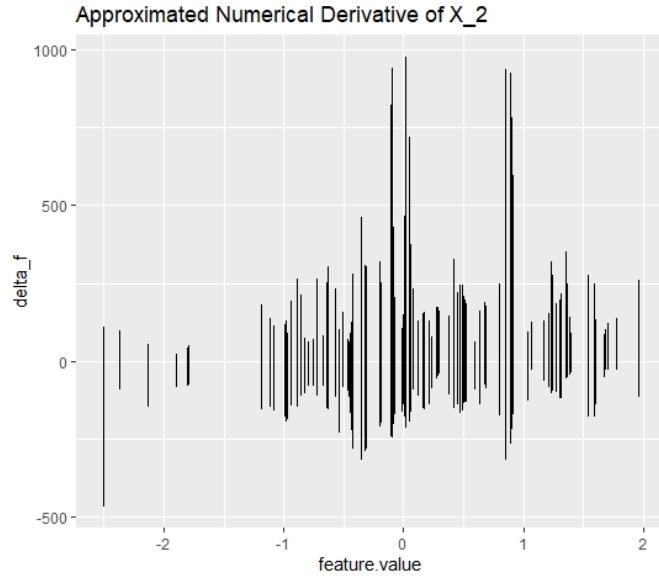


FIGURE 10.4: Simulated data (simulation 1): d-ICI plot for feature x_2 . The d-ICI plot shows a less clear structure of the derivatives. This corresponds to the case where the respective feature does not interact

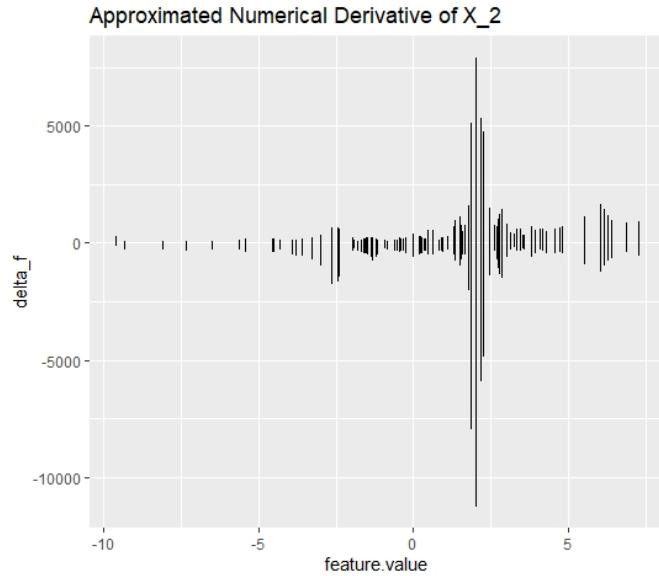


FIGURE 10.5: Simulated data (simulation 2): d-ICI plot for feature x_2 . The d-ICI plots shows a distinguished amplitude at $x_2 = 2$. This finding is in line with the interaction effect between x_2 and x_3 .

10.2.2 Explain Interactions

So far it is understood that PI and ICI plots do probably not provide the clearest insights on whether interaction effects exist or not. Yet, calculating the Individual Conditional Importance allows implementing d-ICI plots which provide better insights.

Still, it is not clarified between which features the interaction takes place. Enabling this would have a major impact on the interpretability of machine learning models. The following will introduce a reliable method that resolves the issue of a lack of explanatory power for interaction effects. These results will then be complemented by the insights from the previous simulations to obtain a full picture of the heterogeneity in Feature Importance.

10.2.2.1 Drivers for Heterogeneity in Feature Importance

Chapter 10.1 highlighted the fact the taking the integral of the Individual Conditional Importance yields the aggregated Feature Importance for each observation. This property can be used to predict the global Feature Importance for each observation concerning the remaining covariates. If interaction exists, for instance a d-ICI plot suggests, then a significant relationship with at least one other feature should be yielded.

Here, it is still not clarified which learner is the most suited. Ideally, one would like to yield sparse results where noise is not fitted. This would prevent that other independent features are included in the model. This property would hold for any regularized regression model. Yet, it would be additionally convenient if the learner would additionally output the threshold were the interaction takes place.

Both desired properties hold best when inducing a decision-tree with a tree-depth of 1. This configuration is quite robust against noise and the returned split point indicates the threshold for which the conditional Feature Importance should be calculated.

In conjunction with the results from the d-ICI plots, one obtains a complete understanding of the nature of the interaction effect. These insights can then be used to later calculate and visualize the conditional Feature Importance.

Figure 10.6 visualizes the fitted decision tree. The results show that the Feature Importance of x_2 is distinctly larger for values $x_3 < 0.5$. As x_3 is a binary variable, either taking the value 0 or 1, the results show that if and only if $x_3 = 0$, interaction takes place. In the case of only one interaction effect between two covariates, the decision tree should yield stable results.

However, there might be several interaction effects taking place so that a decision-tree with tree-depth = 1 is insufficient. Still, this poses no actual

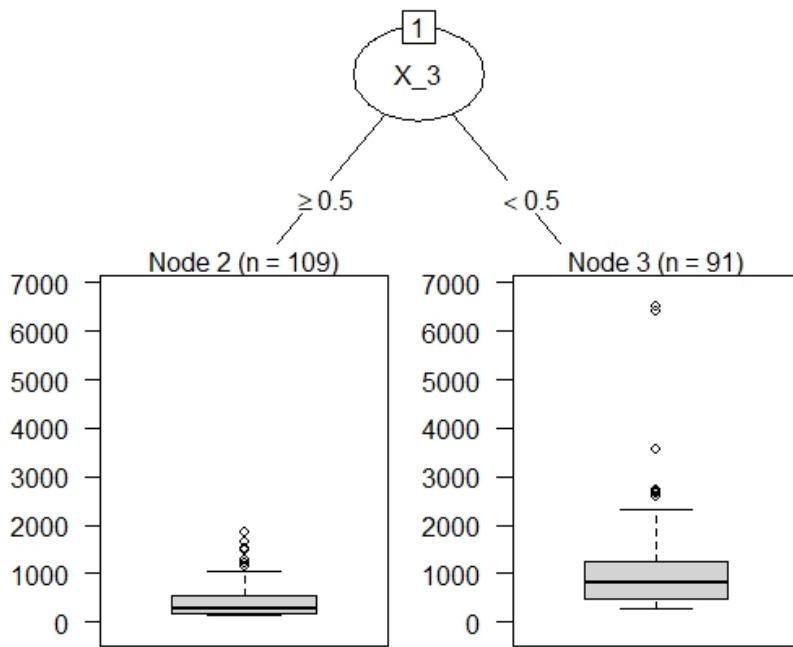


FIGURE 10.6: Simulated data (simulation 2): The decision stump reveals the interaction between x_2 and x_3 . The split node gives information about where the interaction takes place.

problem as this method is in general not restricted to a specific learner. However, it would be still advantageous to preserve the Importance dimension. Hence, fitting a random forest model would be a suitable method. As the main idea should be clear, it will be refrained from going more into detail at this point.

10.2.2.2 Conditional Importance plots

With results from above, one can now calculate the Conditional Individual Importance of the feature x_2 . Therefore, one just simply subdivides the Individual Conditional Importance into the respective groups. Meaning, calculate the PI for x_2 for all observations where $x_3 = 0$ and for all observations where $x_3 = 1$. As the plot below shows, the PI for the observations where the interaction triggered is above average and hence, the observations with $x_3 = 1$ are below average over the entire range.

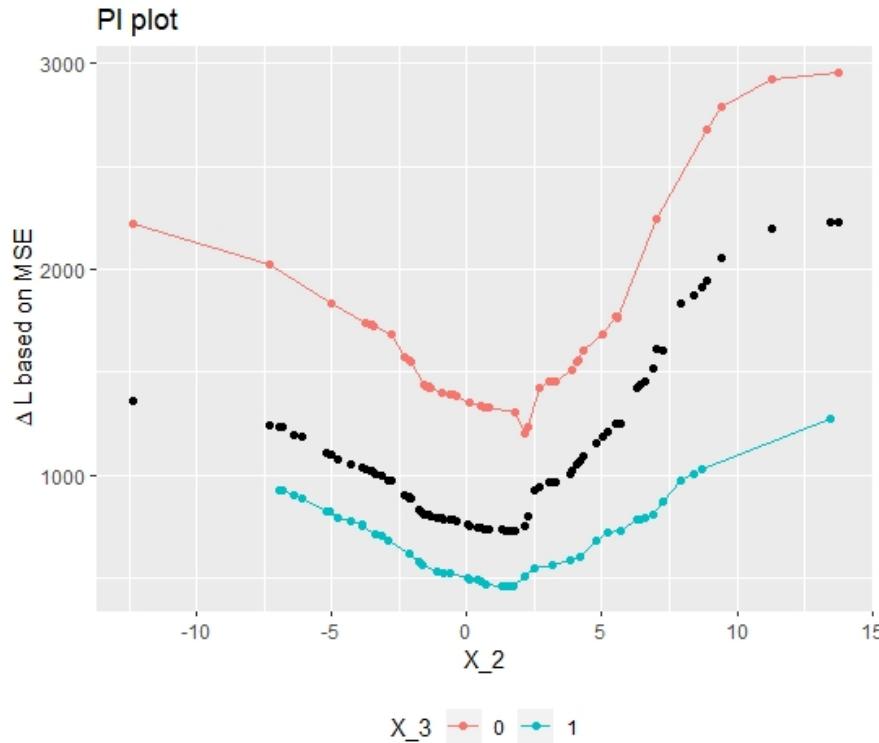


FIGURE 10.7: Simulated data (simulation 2): The conditional Feature Importance plot visualizes the impact of the interaction effect on the heterogeneity in Feature Importance.

Finally plotting the conditional Feature Importance (see figure 10.7) indeed confirms the interaction effect and its impact on the Feature Importance. Besides, to get there, some additional interesting insights were obtained. Now, it is known between which features and where in the feature's range of values the interaction effect takes place. With the conditional Feature Importance, one can even quantify the difference and therefore measure the impact of the interaction effect. Concluding, that the initially observed heterogeneity is understood to its full extent.

Applying this on a real data application would then allow a more meaningful, contextual interpretation.

10.2.3 Stress Methods in a Non-Linear Relationship Setting

When trying to detect interaction effects, it was already seen that the inherent heterogeneity diffuses a clear and unambiguous picture. However, with some background knowledge and the d-ICI plot, it was still possible to reliably detect the interaction effect.

Still, it seems reasonable to further validate the robustness of these methods within a data-generative model with a non-linear relationship. By doing so, it can be assessed whether the methods still detect interaction effects even though additional inherent heterogeneity is introduced. For this purpose, consider the following data-generative model:

$$y = x_1 - 5 * \sin(x_2) + x_3 + 5x_2 \mathbf{1}_{x_2 > 2, x_3 = 0} + \epsilon$$

$$x_1 \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1), x_2 \stackrel{i.i.d.}{\sim} \mathcal{N}(1, 4) \text{ and } x_3 \stackrel{i.i.d.}{\sim} B(1, 0.5), \epsilon \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1)$$

Inducing further heterogeneity by including the sinus function seems appropriate as heterogeneity is “uniformly” distributed over the feature’s range of values. The function values are bounded by -1 and 1, so that the heterogeneity is controlled and does not exceed extreme values.

The plotted PI curve (see figure 10.8) indicates that the Feature Importance for $x_2 > 5$ is above the average. Therefore, one might conclude that interaction which makes the feature more important takes place in this area. Disentangling the PI curve into its components yields a slightly different picture. It shows a steep descent of some curves at $x_2 = 2$ and descending but also ascending curves at $x_2 = 5$. Compared to the PI curves, the ICI curves allow a more detailed analysis of the heterogeneity. But, still it is not clarified whether interaction takes place at $x_2 = 2$ or $x_2 = 5$.

Hence, again the derivatives can be calculated and plotted as shown below (see figure 10.9).

Despite the additional heterogeneity, the d-ICI plots still disentangles the diffused picture and uniquely identifies the interaction effects. It can be seen that the largest descent of the ICI curves takes place at $x_2 = 2$. It further can be excluded that an interaction effect takes place at $x_2 = 5$.

Of course, as it is known that the feature is sinusoidally distributed, the steep ascent of the ICI curves at $x_2 = 5$ could have been explained. Having a closer look at the ICI plot it also reveals that the ascent is gradually increasing which does not hold for the ascent at $x_2 = 2$. But still, it can be concluded that within this setting, the PI and ICI plots are not very telling.

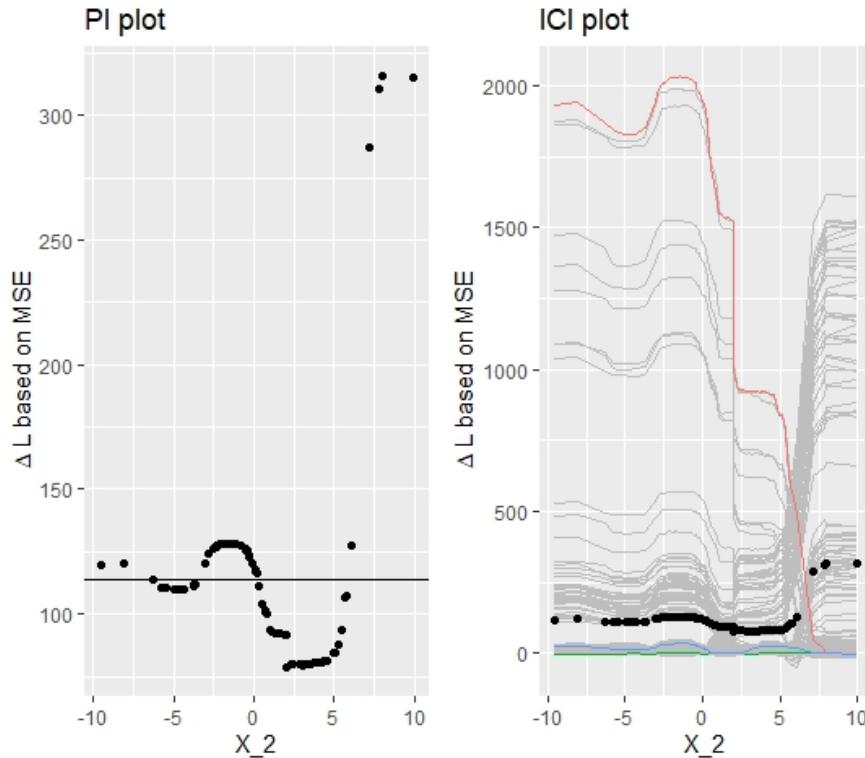


FIGURE 10.8: Simualated data (simulation 3): PI Plot and ICI Plot corresponding to the variable x_2 .

10.3 Real Data Application: Boston Housing

Before this chapter will be closed by a brief discussion and an outlook for further research, the introduced methods will be now applied to real data. Doing so is important for final validation. Only if it can be shown that these methods apply to real data, they can be assessed as useful.

Pursuing this objective, we will calculate the PFI, PI, and ICI for the predictors of the Boston Housing dataset. In this setting, it is of interest to predict and explain the “median value of owner-occupied homes in USD1,000\$. In a pre-analysis, the predictor variable `lstat` was chosen to conduct further analyses. Briefly, `lstat` measures the percentage share of lower status people in the population and from an economic perspective, it is assumed that there is a significant relationship between the predictor and the outcome variable.

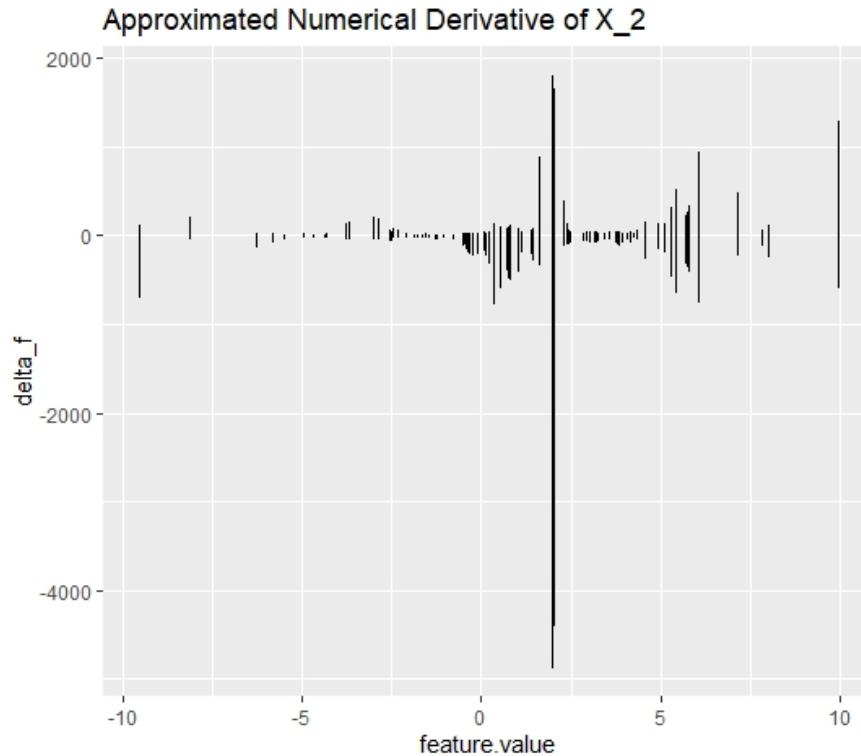


FIGURE 10.9: Simulated data (simulation 3): d-ICI plot for variable x_2 . Calculating and plotting the derivatives of the ICI curves, reveals the spot where interaction takes place.

As in the simulation analysis, the model is fitted equivalently by a random forest model and the calculation of the Importance metrics follows the same principle. The PI and ICI plots below, allow a first interpretation of the Feature Importance.

The PI plot reveals that on average the explanatory power of `lstat` becomes decisively larger for values below 10. Briefly, if the percentage of people with lower status is below 10%, the variable becomes a more important constitute of the predictive model. The ICI plot confirms this result and shows some additional heterogeneity in this area which, however, is hard to interpret within this visualization setting. Therefore, again, the derivatives of the ICI curves can be calculated to detect the heterogeneity more comprehensively.

The d-ICI plot for the feature `lstat` additionally confirms the heterogeneity, visible in the ICI plot. Especially at $lstat = 10$ a significant amplitude can be identified. This indicates that an interaction between `lstat` and another

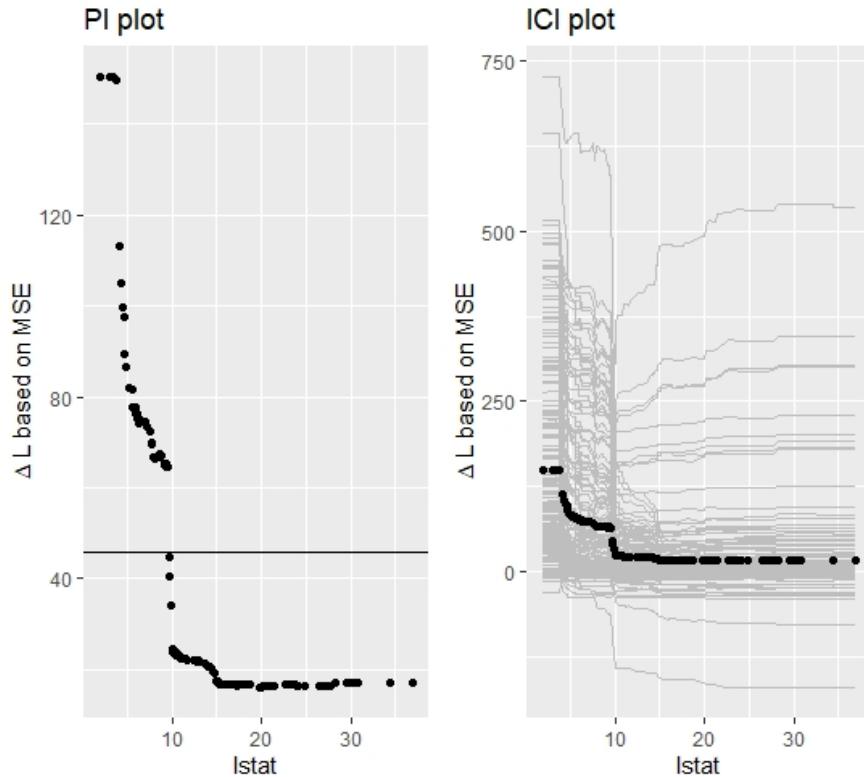


FIGURE 10.10: Boston Housing Data: PI and ICI plot for feature ‘lstat’. A clear and not uniformly distributed heterogeneity can be observed.

covariate takes place in the area around $lstat \leq 10$. Given this insight, it is now to be determined with which covariate the feature “lstat” interacts. Therefore, we again predict the integral of each observation’s Feature Importance concerning the remaining covariates.

At this point, one has gained a rather complete picture of why there is heterogeneity in the Feature Importance of the feature “lstat”. Therefore, one can now calculate the Conditional Feature Importance of `lstat` on the variable `dis`. Plotting the conditional curves (see figure 10.13), confirms the analysis of the previous results. Even though the results are not as distinguished as in the simulation settings, the interaction taking place is still clearly visible.

With the insights from the Real Data Application, one can conclude that the presented methods also work beyond the simulation setting and is, therefore, applicable for explaining heterogeneity in Feature Importance within a machine learning model. Yet, the heterogeneity problem was merely discussed

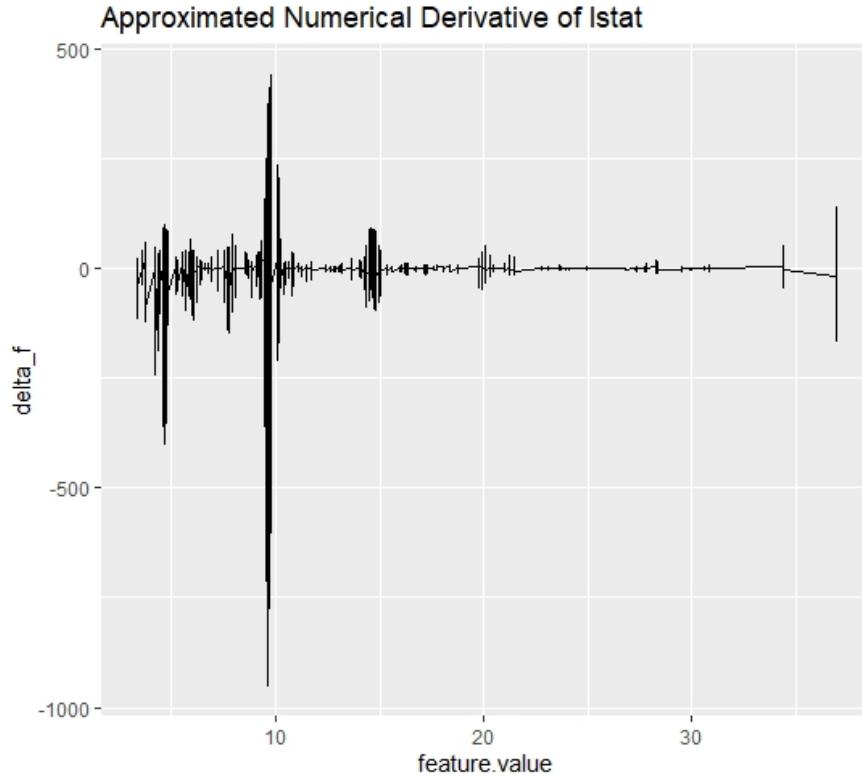


FIGURE 10.11: Boston Housing Data: d-ICI plot for feature ‘lstat’. The plot provides further insights on the initially observed heterogeneity.

in the context of interaction effects. It could be further discussed whether it might be even possible to identify the structural relationship between a feature and the response. Besides, it would be also interesting to investigate the PI and ICI plots in the context of correlated features.

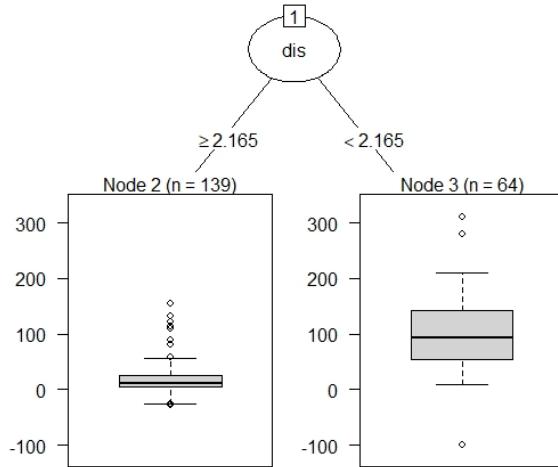


FIGURE 10.12: Boston Housing Data: Explain Interaction Effects for feature ‘lstat’. The decision stump identifies the interaction between feature ‘lstat’ and feature ‘dis’. Again the split point indicates where the interaction effect takes place.

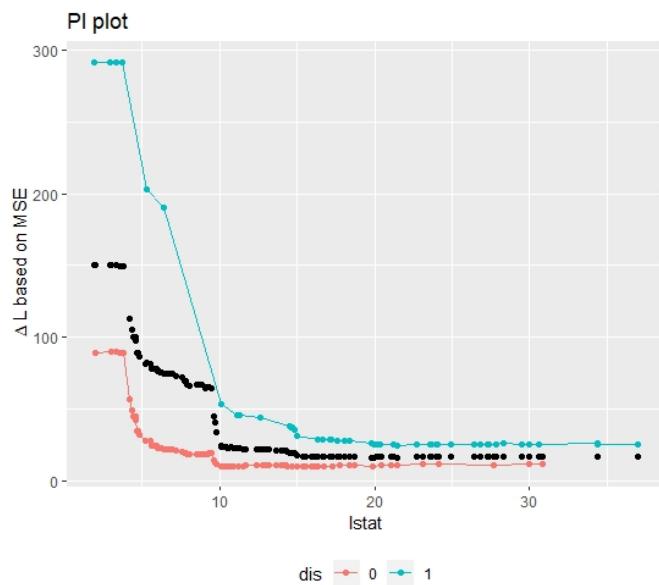


FIGURE 10.13: Boston Housing Data: Conditional Importance Plot. Importance of ‘lstat’ conditional on values of ‘dist’

10.4 Discussion

So far, it was stressed to what extent the PI and ICI plots are suitable tools to obtain a better interpretation of Feature Importance. To give this a final evaluation, the critical assessment is subdivided into two parts. The first part will summarize the capabilities of the visualization tools. The second part will explore the possibilities that have arisen through the data obtained.

The simulation chapter revealed that the ICI and PI plots are indeed able to visualize heterogeneity but both had its limitations when trying to detect interaction effects. First, even though no heterogeneity was expected, the PI and ICI plot still visualized heterogeneity. Even though it can be explained by the distributional properties of the feature, it can lead to confusion. One could circumvent the problem by weighting the local Feature Importance of each observation with its respective probability mass. This would “squash” the curves to a linear shape and merely only deviations from that could be interpreted as a proper heterogeneity. Second, when a non-linear relationship between response and the feature was induced, both methods did not yield robust and reliable results.

Further, it was argued that explaining interactions is as important as detecting interaction effects. Even if the ICI plots were able to detect interaction effects, it was not possible to explain them. Briefly, between which features and where did the interaction take place.

Concluding, the visualization of PI and ICI does indeed disentangle the global PFI metric but has its non-negligible limitations when interpreting the results properly.

Even though the PI and ICI plots themselves are very limited in its explanatory power, it was still possible with the underlying data to create a cookbook that enabled a full picture. The d-ICI plots represent a robust method for detecting interactions, even in a “messy” non-linear relationship. It turned out that calculating the approximated Feature Importance was easy to implement and therefore posed no major challenge. Further, as the Partial Importance was already calculated it was not difficult to implement a method which explains between which features interaction takes place. Solving that, one can calculate the conditional Feature Importance and therefore, finally visualize the actual effect of the interaction on Feature Importance.

Concluding, even though the PI and ICI plots have its limitations, the underlying data represents an exhaustive foundation for yielding a complete picture of the heterogeneity. Therefore, it can be stated that disentangling the global PFI into its components is a valid and insightful approach to better understand what exactly drives the predictions of a machine learning model.

11

PFI: Training vs. Test Data

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Supervisor: Florian Pfisterer

In this chapter we will deal with the question whether we should use test or training data to calculate permutation feature importance. First of all we'll give a short overview of the interesting components.

Permutation Feature Importance (PFI)

In order to calculate the impact of a *single* feature on the loss function (e.g. MSE), we shuffle the values for one feature to break the relationship between the feature and the outcome. Chapter 8 contains an introduction to permutation feature importance.

Dataset

In this chapter, we consider two partitions of a dataset D :

- D_{train} : Training data, used to set up the model. Overfitting and underfitting is possible
- D_{test} : Test data used to check if the trained model works well on unseen data.

In this chapter, we focus on answering the following three questions:

1. When should I use test or training data to compute feature importance?
2. How is the permutation feature importance of test or training data affected by over- and underfitting?
3. Does correlation influence the decision what kind of data to use?

11.1 Introduction to Test vs. Training Data

In addition to the question of how permutation feature importance should be used and interpreted, there is another question that has not yet been discussed in depth: Should the feature importance be calculated based on the test or the training data? This question is more of a philosophical one. To answer it you have to ask what feature importance really is (again a philosophical topic) and what goal you want to achieve with feature importance.

So what is the difference of calculating the permutation feature importance based on training or test data? To illustrate this question we will employ an example.

Imagine you have a data set with independent variables - so there is no correlation between the explanatory and the target variables. Therefore, the permutation feature importance for every variable should be around 1 (if we use ratios between losses). Differences from 1 stem only from random deviations. By shuffling the variable, no information is lost, since there is no information in the variable that helps to predict the target variable.

Let us look again at the permutation feature importance algorithm based on Fisher, Rudin, and Dominici (2018):

Input: Trained model f , feature matrix X , target vector y , error measure $L(y, f(X))$

1. Estimate the original model error $e_{orig} = L(y, f(X))$ (e.g mean squared error)
2. For each feature $j = 1, \dots, p$ do:
 - Generate feature matrix x_{perm} by permuting feature j in the data X
 - Estimate error $e_{perm} = L(y, f(X_{perm}))$ based on the predictions of the permuted data,
 - Calculate permutation feature importance $PFI_j = e_{perm}/e_{orig}$. Alternatively, the difference can be used: $PFI_j = e_{perm} - e_{orig}$
3. Sort features by descending FI.

The original model error calculated in step 1 is based on a variable that is totally random and independent of the target variable. Therefore, we would not expect a change in the model error calculated in step 2: $e_{orig} = E(e_{perm})$.

This results in a calculated permutation feature importance of 1 or 0 - depending on which calculation method from step 2 is used.

If we now have a model that overfits - so it “learns” any relationship, then we will observe an increase in the model error. The model has learned something based on overfitting - and this learned connection will now be destroyed by the shuffling. This will result in an increase of the permutation feature importance. So we would expect a higher PFI for training data than for test data.

After this brief review of the fundamentals of permutation feature importance, we now want to look in detail at what we expect when feature importance is calculated on training or test data. To do this, we distinguish different models and data situations, discuss them theoretically first and then look at the real application - both on a real data set as well as on self-created “laboratory” data.

11.2 Theoretical Discussion for Test and Training Data

When to use test or training data?

At the beginning, we will discuss the case for test data and for training data based on [Molnar \(2019\)](#).

Test data: First, we will focus on the more intuitive case for test data. One of the first things you learn about machine learning is, that one should not use the same data set on which the model was fitted for the evaluation of model quality. The reason is, that results are positively biased, which means that the model seems to work much better than it does in reality. Since the permutation feature importance is based on the model error we should evaluate the model based on the unseen test data. If the permutation feature importance is calculated on the training data instead, the impression is erroneously given that features are important for prediction. The model has only overfitted and the feature is actually unimportant.

Training data: After the quite common case for test data we now want to focus on the case for training data. If we calculate the permutation feature importance based on the training data, we get an impression of what features the model has learned to use. So, in the example mentioned above, a permutation feature importance higher than the expected 1 indicates that the model has learned to use this feature, even though there is no “real” connection between the explanatory variable and the target variable. Finally, based on the training data, the PFI tells us which variables the model uses to make predictions.

As you can see there are arguments for the calculation based on tests as well as training data - the decision which kind of data you want to use depends on the question you are interested in: How much does the model rely on the

respective variable to make predictions? This question leads to a calculation based on the training data. The second possible question is as follows: How much does the feature contribute to model performance on unknown data? In this case, the test data would be used.

11.3 Reaction to model behavior

What happens to the PFI when the model over/underfits?

In this section we want to deal with the PFIs behavior regarding over- and underfitting. The basic idea is that the PFI will change depending on the fit of the model.

In order to examine this thesis we have decided to proceed as follows:

1. Choose a model that is able to overfit and underfit
2. Perform a parameter tuning to get the desired fit
3. Run the model
4. Check for PFI on test and training data based on the aforementioned algorithm by Fisher, Rudin, and Dominici (2018)

We have chosen the gradient boosting machine as it is very easy to implement overfitting and underfitting.

In the following sub-chapter we will give a short overview of the gradient boosting machine.

11.3.1 Gradient Boosting Machines

Gradient boosting is a machine learning technique for regression and classification problems, which produces a prediction model in the form of an ensemble of weak prediction models, typically decision trees. It builds the model in a stage-wise fashion like other boosting methods do, and it generalizes them by allowing optimization of an arbitrary differentiable loss function.

How does a gradient boosting machine work?

Gradient boosting involves three elements:

1. A loss function to be optimized

- The loss function used depends on the type of problem being solved
 - Must be differentiable
2. A weak learner to make predictions
 - Decision trees are used as the weak learner
 - Constrain the weak learners in specific ways (maximum number of layers, nodes, splits or leaf nodes)
 3. An additive model to add weak learners to minimize the loss function
 - Trees are added one at a time, and existing trees in the model are not changed
 - A gradient descent procedure is used to minimize the loss when adding trees

To get an impression what a Gradient Boosting Machine does, we want to give a short (and naive) example in pseudocode:

1. Fit a model to the data: $F_1(x) = y$
2. Fit a model to the residuals: $h_1(x) = y - F_1(x)$
3. Create a new model: $F_2(x) = F_1(x) + h_1(x)$

Generalize this idea: $F(x) = F_1(x) \mapsto F_2(x) = F_1(x) + h_1(x) \dots \mapsto F_M(x) = F_{M-1}(x) + h_{M-1}(x)$

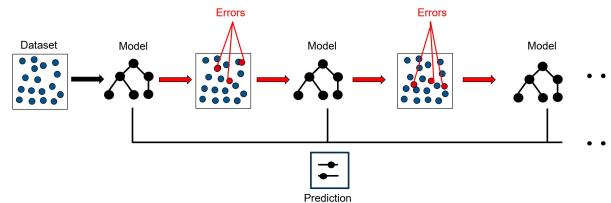


FIGURE 11.1: Simplified visualization of a gradient boosting machine. One trains a model based on the data. Then you fit a model to the resulting residuals. The result is then used to create a new model. This process is repeated until the desired result is achieved.

The over- and underfitting behavior of gradient boosting machines can be controlled via several *regularization* hyperparameters. An *overfitting* model can be trained by setting e.g. a high *max_depth*, i.e. the depth of trees fitted in each iteration, or a low *min_bucket*, i.e. a low minimum of samples that need to be present in each leaf in order to allow for further splitting. Vice-versa, an underfitting can be created by adjusting the hyper-parameters in the opposite direction. This results in a very flexible algorithm, that allows us to cover various situations between underfitting, good fit and overfitting.

11.3.2 Data sets used for calculations

As Mentioned above, we want to use two different data sets:

1. A self-created data set with pre-specified correlation structure.
2. A real data set to see if the observations made under “laboratory conditions” can also be observed in the real world.

Our self created data set looks as follows:

- Uncorrelated features which leads to a 0/1-classification
- x_1, x_2, x_3 and x_4 normally distributed with zero mean and standard deviation of 1
- Target variable based on linear function with a bias.
- Same data set with 2 highly correlated features x_1 and x_2 (correlation of 0.9)

The second data set is the IBM Watson Analytics Lab data for employee attrition:

- Uncover factors that lead to employee attrition
- Dataset contains 1470 rows

Used Features:

- Overtime
- Job Satisfaction
- Years at Company
- Age
- Gender
- Business Travel
- Monthly Income
- Distance from home
- Work-Life-Balance
- Education
- Years in current role

With these data sets, several models are fitted in order to generate over- and underfitting. The results are listed in the following section

11.3.3 Results

In this section we want to give an overview of the results of the comparison between the calculation of permutation feature importance based on the test and the training data.

We will start with the uncorrelated self created data set. Then the correlated self created data set and in the end we will have a look at the IBM Watson Employee Attrition data set.

Self created Data Set without Correlation

First, we will have the two permutation feature importance plots for a well tuned gradient boosting machine. We have four features, created based on the following formula:

$$z = 1 + 2 * x_1 + 3 * x_2 + x_3 + 4 * x_4$$

On the x-axis you can see the feature importance and on the y-axis the feature.

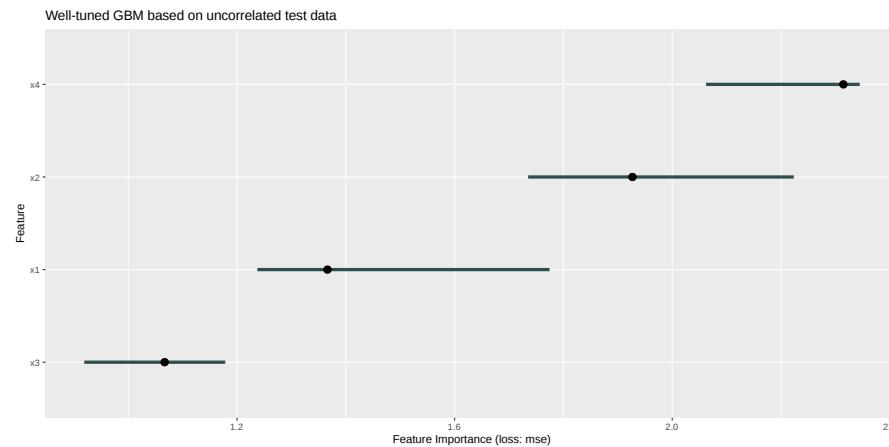


FIGURE 11.2: The used features are located on the x-axis. The corresponding permutation feature importance can be found on the y-axis. x_4 is the most important feature, followed by x_2 , x_1 and x_3

As you can see, both plots are quite similar. The order of test and training data is exactly the same. x_4 is the most important feature, followed by x_2 and x_1 . The least important feature is x_3 .

Furthermore, the range of the two plots is not the same - but comparable. The PFI-plot based on test data has a range from 1 to 2.4 and the PFI-plot based on training data from 1.1 to 4. This indicates still an overfit of the GBM.

Now, we used the same data set but an overfitting GBM. You can find the corresponding plots below:

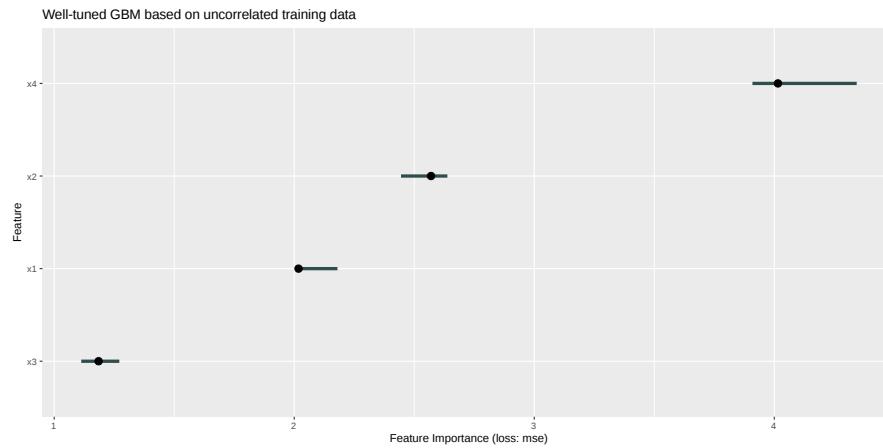


FIGURE 11.3: Again, x4 ist the most important feature, followed by x2, x1 and x3. The range of the PFI values differes from 1 - 4 and is therefore wider than the range regarding the test data

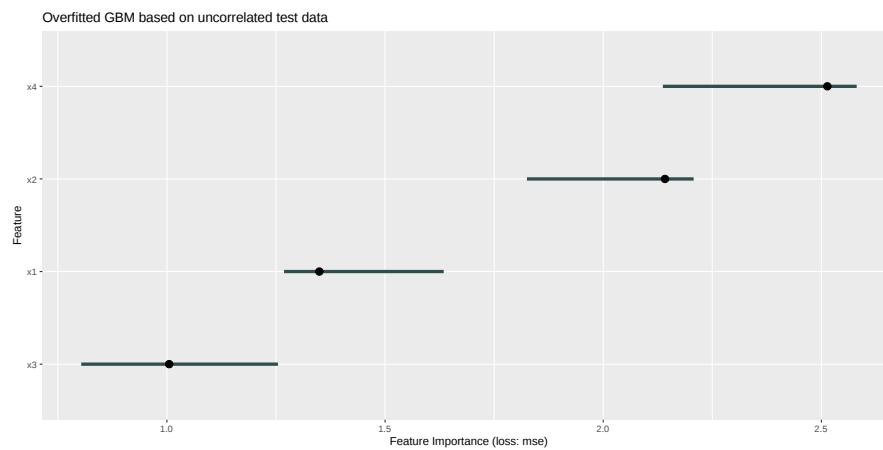
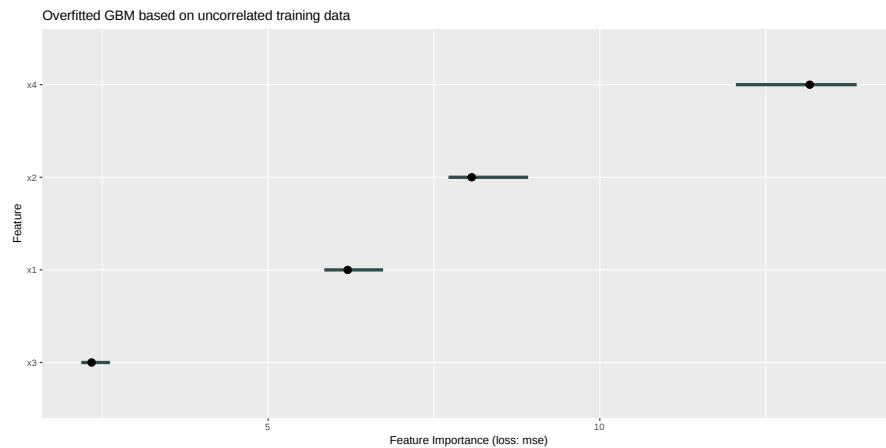


FIGURE 11.4: For an overfitting GBM the order for test data is the same as seen before in the well fitted case. The range of the test data is quite the same as before.



At first sight these two plots look very similar to the first two. The order of the features has remained the same and the relative distances to each other are also very similar. It is also noticeable that the plot regarding the test data has hardly changed - whereas the range of the permutation feature importance based on training data has become much wider. This is a typical behavior of overfitting in terms of feature importance, since the models learns to use a variable “better” than it actually is.

The last 2 plots for the uncorrelated data set are the ones of an underfitting GBM:

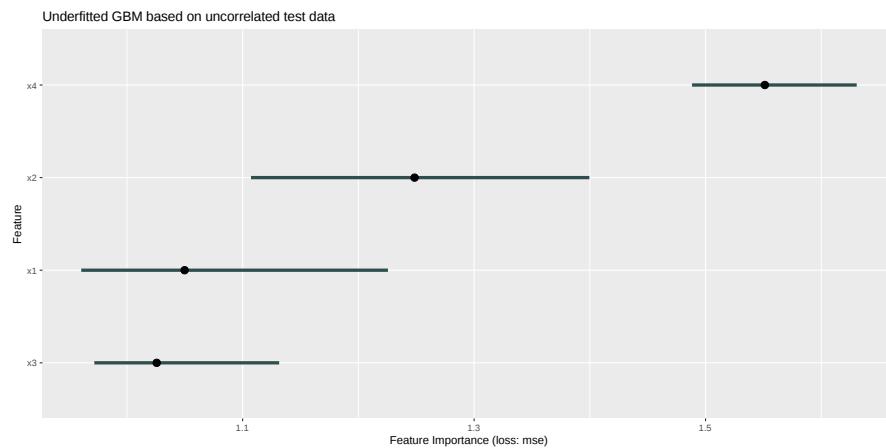
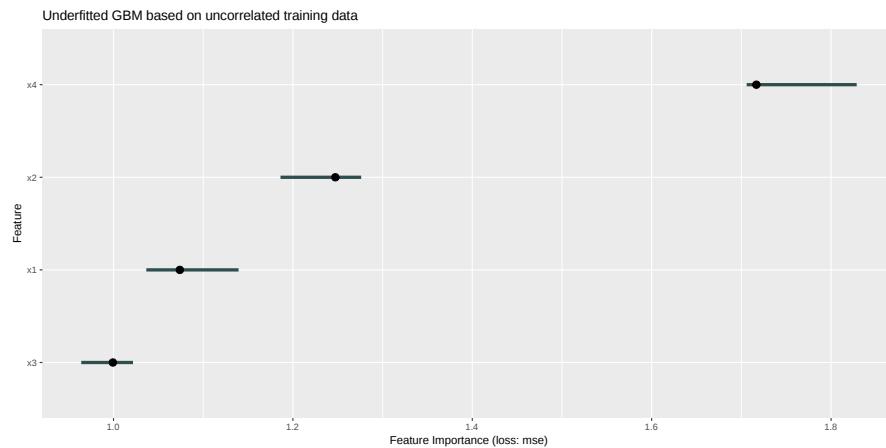


FIGURE 11.5: PFI plot of an underfitting GBM based on test data. The importance is now reduced with highest value at around 1.6 in contrast to 2.4 before. Furthermore, x1 is the least important feature now.



With the plots for an underfitting GBM it is noticeable that the range is almost the same - but at a low level (from 1-1.8 or 1-1.6). Most noticeable, however, is that the order has changed. Based on the test data, x_1 is now the least important variable. Overall, the feature importance decreases - and therefore a change in the positions becomes more probable.

Self created Data Set without Correlation

Now, we used the same data set but included 2 highly correlated features. The correlation between x_1 and x_2 is set to 0.9.

In the first plot the results for a well tuned GBM are compared for test and training data. The noteworthy areas are highlighted in red.

The order of the features has changed - but in the area of features that are close to 1 (i.e. unimportant features).

In the next plot, we want to compare test and training data permutation feature importance of an overfitting GBM:

The range for the training data set is much wider again - similar to the range for the uncorrelated data. In addition it is noticeable that the order has changed in the lower range - which is again due to the fact that the less important features are close to 1 (i.e. have no influence on the MSE).

The last plot for correlated data used an underfitting GBM:

It can be said that the order has remained the same - but x_1 x_2 and x_3 are very close to a feature importance of 1 (which means: no influence on the MSE). Furthermore, the range is very comparable.

IBM Watson Data of Employee Attrition

Finally, we will take a look at how test and training data behave outside laboratory conditions with real data. Here we looked at which variables contribute to an employee leaving the company.

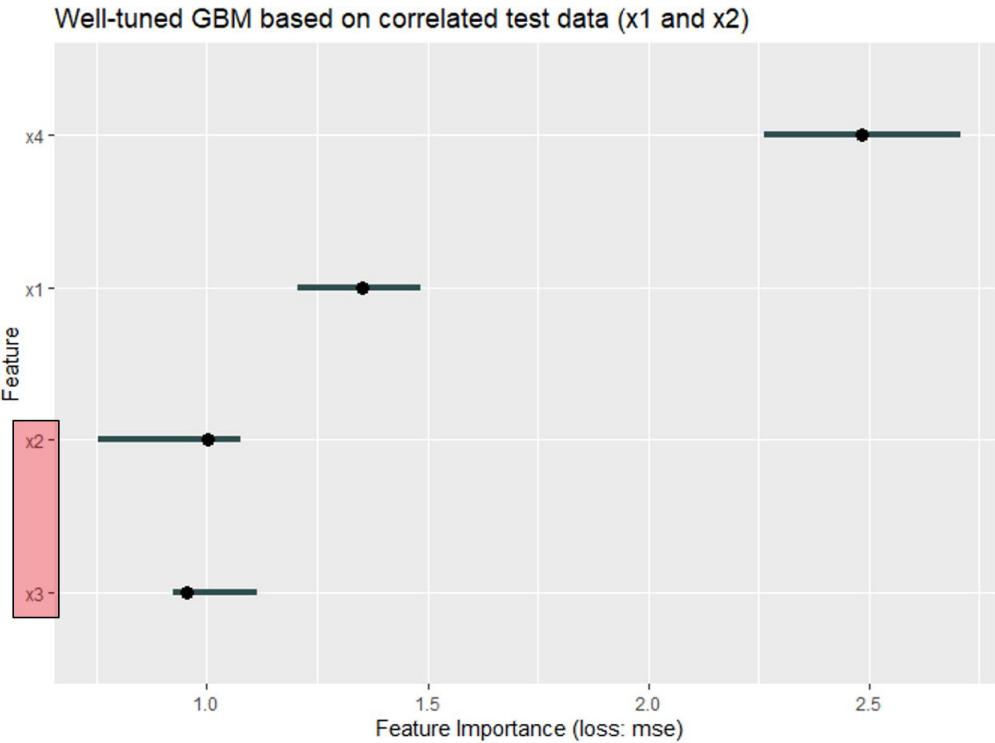


FIGURE 11.6: For the well fitted GBM at the correlated self created data set, the order differs. For the test data x4 ist the most important feature followed by x1, x2 and x3 whereas for the training data x2 and x3 changed places

Again, we compared the permutation feature importance of test and training data set.

The noticeable features are highlighted in green. As with the previous well fitted GBM, the range is very comparable - the order has also remained the same, at least in parts. (Overtime is the most important variable in both cases)

Also here we want to have a look at the behavior at over- and underfitting.

We start again with the plots for overfitting:

There's really a lot going on here. Both the range (as always with overfitting) and the order change a lot. The results are not comparable in any way.

Last but not least we will have a look at the underfitting GBM for the IBM Watson data set:

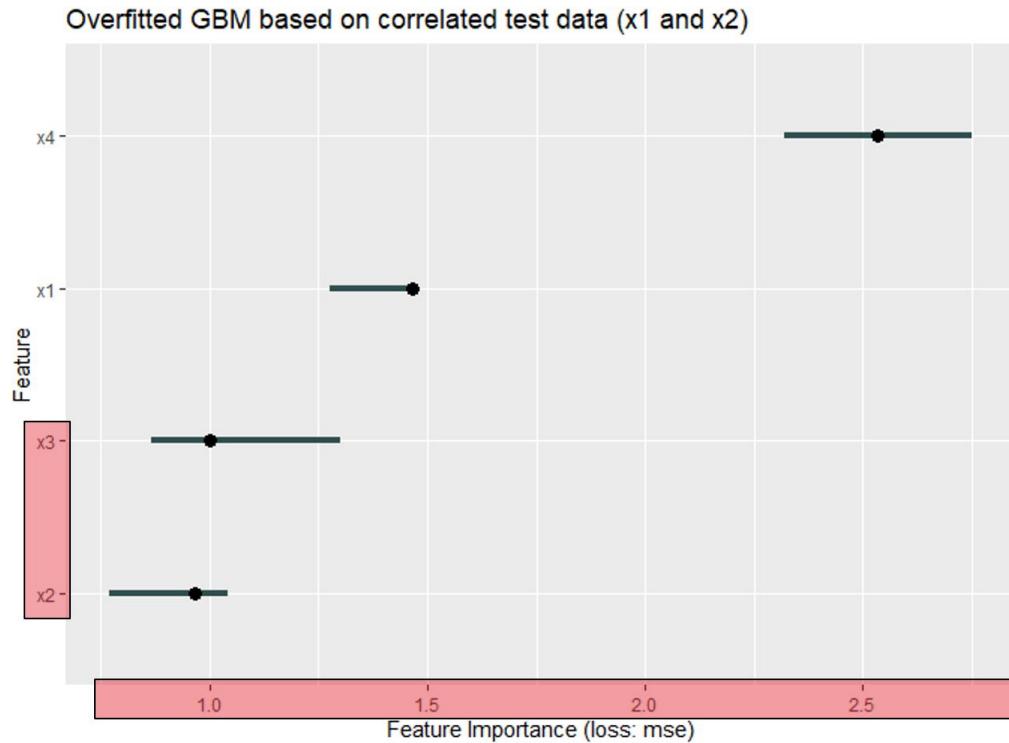


FIGURE 11.7: x4 is the most important feature in both plots. Followed by x1, x3 and x2 in descending order for the test data - and again x2 and x3 changed places for the training data. It has to be stated, that the range for training data is much wider.

The range is comparable - but very small (0.9 - 1.2). Again underfitting has a reducing effect on the feature importance. In addition, the order has changed extremely (work life balance has changed from the least important variable at the test data to the most important variable at the training data).

11.3.4 Interpretation of the results

At the end of this sub-chapter we want to answer the question how the permutation feature importance behaves with regard to over- and underfitting. First, it can be said that in the case of a well fit GBM there are only slight differences in feature importance. The results on test and training data are in any case comparable. But now we come to the problems regarding the meaningfulness of feature importance:

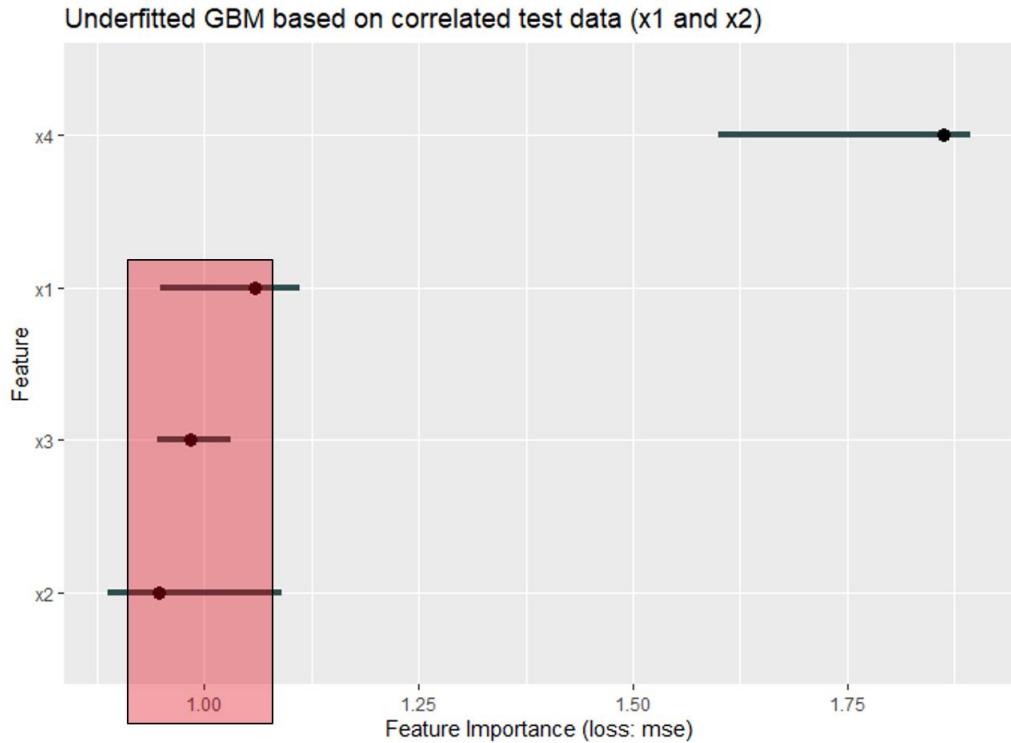


FIGURE 11.8: x4 is the most important feature in both plots. Followed by x1, x3 and x2 in descending order. Except x4 all permutation feature importance values are close to 1

Problems with overfitting:

- Overfitting results in a very strong effect on the MSE only on the training data
- Furthermore, the order differs a lot

Problems with underfitting:

- The effect on the MSE is low - the results are consistently lower
- As in the overfitting case the order differs a lot

Over- and underfitting has definitely an impact on feature importance

Our third question was, if correlation does effect the decision whether to use test or training data for calculating the permutation feature importance:

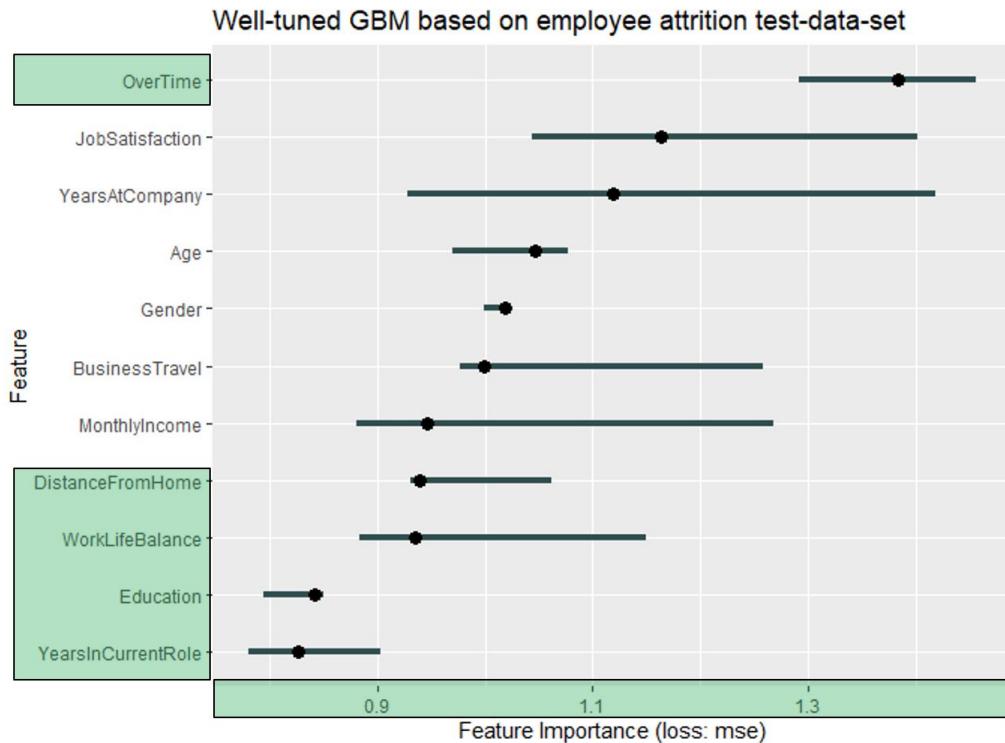


FIGURE 11.9: For both data sets Overtime is the most important feature. Furthermore, the 4 least important variables are the same - and in the same order (Dist from home, WorkLifeBalance, Education and YearsInCurrentRole)

11.4 Summary

The Question what data set you use for calculation of the permutation feature importance still depends on what you are interested in:

- Contribution to the performance on unknown data?
- or
- How much the model relies for prediction?

It was shown that PFI reacts strongly to over- and underfitting:

- PFI on both can be a proxy identifying over- or underfitting

Correlated features have a big influence on the results of feature importance,

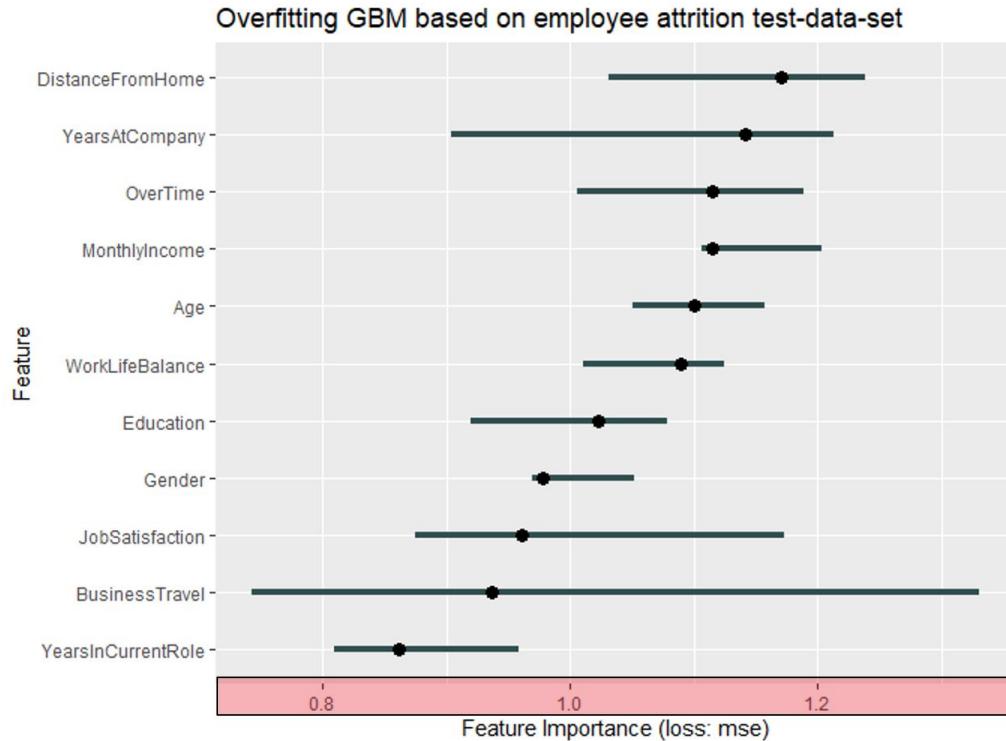


FIGURE 11.10: For the test data based on an overfitting GBM, DistanceFromHome is the most important variable. For the training data it is only the fourth most important one, whereas Overtime is most important. It can be stated that the order changed a lot

but not on the question whether to use test or training data - therefore they are negligible in this question. Nevertheless, correlations have been shown to lead to major feature importance problems, as discussed in previous chapters.

Basically it can be said that it has been shown that the model behavior (overfitting or underfitting) greatly distorts the interpretation of the feature importance. Therefore it is important to set up your model well, because it was shown that the differences for a well calibrated model are only small and the question of choice doesn't play a big role anymore.

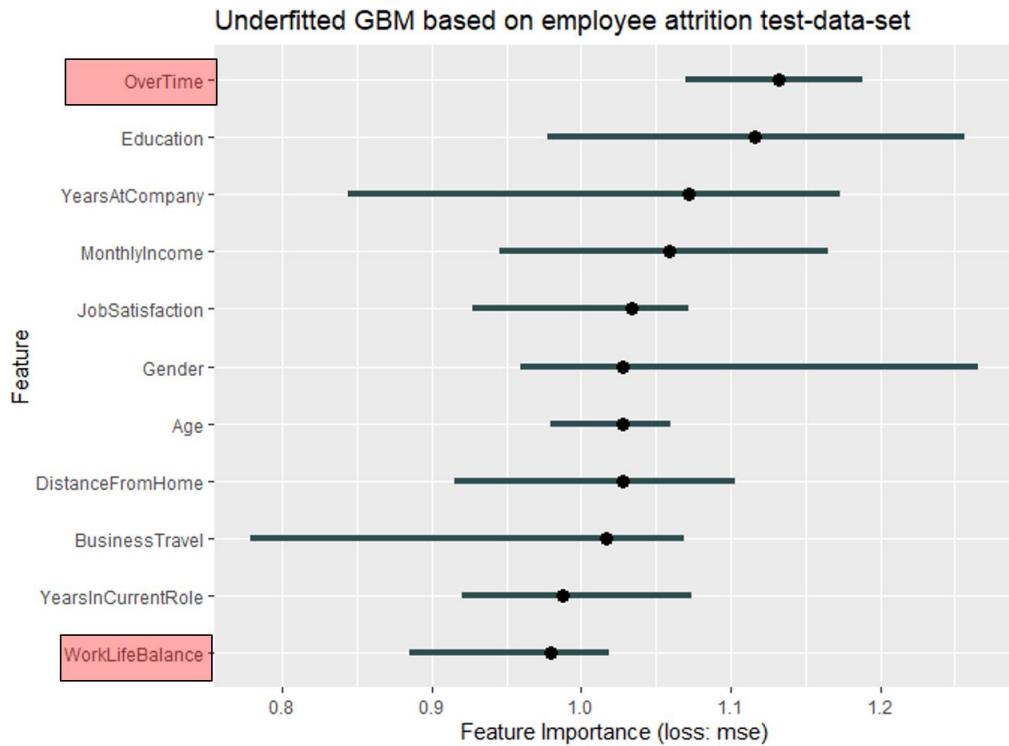


FIGURE 11.11: In this Figure it is quite interesting that the order changed completely. Overtime is the most important variable based on the test data and is only at place number 8 for the training data. Even more extreme is the case with WorkLifeBalance

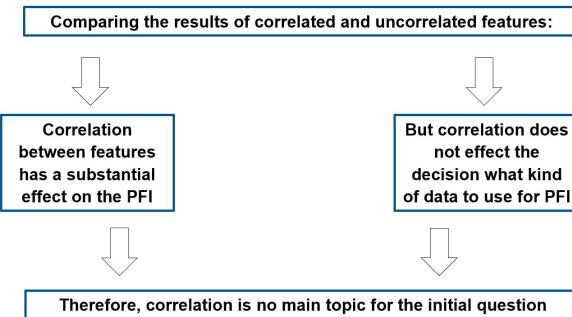


FIGURE 11.12: Visualisation of the impact of correlation on the feature importance. As you have seen above, correlation is a problem regarding permutation feature importance but does not effect the decision regarding test vs. training data

12

Introduction to Local Interpretable Model-Agnostic Explanations (LIME)

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Supervisor: Christoph Molnar

When doing machine learning we always build models. Models are simplifications of reality. Even if the predictive power of a model may be very strong, it will still only be a model. However, models with high predictive capacity do most of the time not seem simple to a human as seen throughout this book. In order to simplify a complex model we could use another model. These simplifying models are referred to as surrogate models. They imitate the black box prediction behaviour of a machine learning model subject to a specific and important constraint: surrogate models are interpretable. For example, we may use a neural network to solve a classification task. While a neural network is anything but interpretable, we may find that some of the decision boundaries are explained reasonably well by a logistic regression which in fact yields interpretable coefficients.

In general, there are two kinds of surrogate models: global and local surrogate models. In this chapter, we will focus on the latter ones.

12.1 Local Surrogate Models and LIME

The concept of local surrogate models is heavily tied to Ribeiro et al. (2016b), who propose local interpretable model-agnostic explanations (LIME). Different from global surrogate models, local ones aim to rather explain single predictions by interpretable models than the whole black box model at once. These surrogate models, also referred to as explainers, need to be easily interpretable (like linear regressions or decision trees) and thus may of course not have the adaptability and flexibility of the original black box model which they aim to explain. However, we actually don't care about a **global** fit in

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this case. We only want to have a very **local** fit of the surrogate model in the proximity of the instance whose prediction is explained.

A LIME explanation could be retrieved by the following algorithm:

1. Get instance x out of the data space for which we desire an explanation for its predicted target value.
2. *Perturb* your dataset X and receive a perturbed data set Z of increased size.
3. Retrieve predictions \hat{y}_Z for Z using the black box model f .
4. Weight Z w.r.t. the proximity/neighbourhood to x .
5. Train an explainable weighted model g on Z and the associated predictions \hat{y}_Z .

Return: An explanation for the interpretable model g .

The visualisation below nicely depicts the described algorithm for a two-dimensional classification problem based on simulated data. We start only with our data split into two classes: 1 and 0. Then, we fit a model that can perfectly distinguish between the two classes. This is indicated by the sinus-shaped function drawn as a black curve. We do not perturb the data in this case. (However, we may argue that our perturbation strategy is to use the original data. We will more formally discuss perturbation later on.) Now, we choose the data point, which we want an explanation for. It is coloured in yellow. With respect to this point, we weight our data by giving close observations higher weights. We illustrate this by the size of data points. Afterwards, we fit a classification model based on these weighted instances. This yields an interpretable linear decision boundary – depicted by the purple line. As we can see, this is indeed locally very similar to the black box decision boundary and seems to be a reasonable result.

This way we receive a single explanation. This one explanation can only help to understand and validate the corresponding prediction. However, the model as a whole can be examined and validated by multiple (representative) LIME explanations.

12.2 How LIME works in detail

So far so good. However, the previous outline was not very specific and leaves (at least) three questions. First, what does neighbourhood refer to? Second,

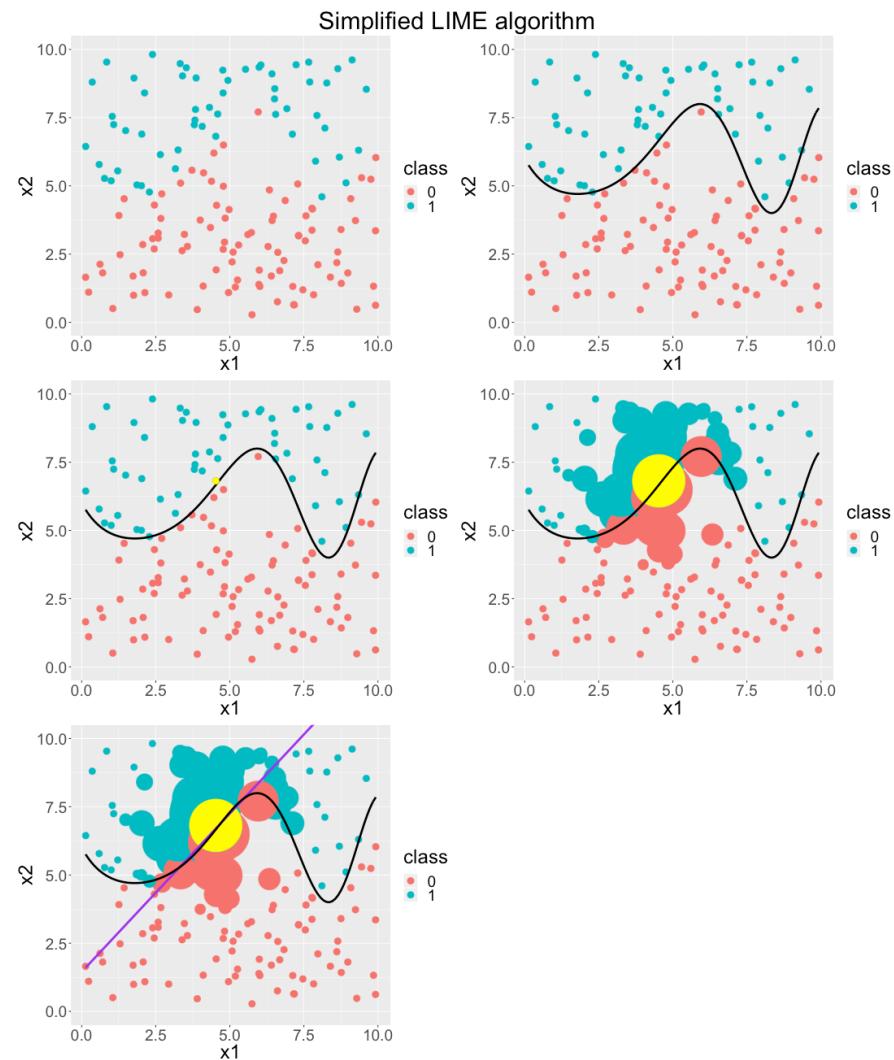


FIGURE 12.1: Simplified graphical representation of the LIME algorithm. Each single panel represents one step of the described algorithm. It reads from left to right.

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what properties should suitable explainers have? Third, what data do we use, why and how do we perturb this data?

To better assess these open questions it may be helpful to study the mathematical definition of *LIME*. The explanation for a datapoint x , which we aim to interpret, can be represented by the following formula:

$$\text{explanation}(x) = \arg \min_{g \in G} \mathcal{L}(f, g, \pi_x) + \Omega(g)$$

Let's decompose this compact, yet precise definition:

x can be an instance that is entirely new to us as long as it can be represented in the same way as the training data of the black box model. The final explanation for x results from the maximisation of the loss-like fidelity term $\mathcal{L}(f, g, \pi_x)$ and a complexity term $\Omega(g)$. f refers to the black box model we want to explain and g to the explainer. G represents the complete hypothesis space of a given interpretable learner. The explanation has to deal with two trade-off terms when minimising: The first term $\mathcal{L}(f, g, \pi_x)$ is responsible to deliver the optimal fit of g to the model f while a low *loss* is desirable indicating high (local) *fidelity*. The optimal fit is only found with respect to a proximity measure $\pi_x(z)$ in the neighbourhood of x .

12.2.1 Neighbourhood

This leads us to the first open question: What does neighbourhood refer to? Neighbourhood is a very vague term. This is for good reason because a priori it is not clear how to specify a neighbourhood properly. Technically, there are many different options to deal with this issue. Weighting the observations w.r.t. their distance to the observation being explained seems like a good idea. This may be implemented as an arbitrarily parametrised kernel. However, this leaves in total many scientific degrees of freedom which makes the neighbourhood definition somewhat problematic. This neighbourhood issue will be discussed in more detail in the next chapter.

12.2.2 What makes a good explainer?

We already answered the second open question – what properties suitable explainers should have – in parts. We mentioned the interpretability property and outlined generalised linear models or decision trees as examples. However, we did not discuss further desired properties of these models. Since they have strong assumptions, it is unlikely that they are capable of maintaining an optimal fit to the original black box model. Recall our formula. As we want local optimal fit subjected to a certain (low) degree of explainer complexity – in order to allow interpretation – our formula needs to facilitate this aspect.

$\Omega(g)$ is our complexity measure and responsible to choose the model with the lowest complexity. For example, for decision trees, tree depth may describe the complexity. In the case of linear regression, the L_1 norm may indicate how simple the interpretation has to be. The resulting LASSO model allows us to focus only on the most important features.

12.2.3 Sampling and perturbation

Having answered the first two open question we still have the last question related to the data and the perturbation unresolved. Besides the tabular data case, we can also interpret models trained on more complex data, like text data or image data. However, some data representations (e.g. word embeddings) are not human-interpretable and must be replaced by interpretable variants (e.g. one-hot-encoded word vectors) for LIME to yield interpretable results. The function modeled by the black box model operates in the complete feature space. It can even yield predictions for instances not seen in the training data. This means that the original data does not sufficiently explore the feature space. Hence, we want to create a more complete *grid* of the data and fill the feature space with new observations so that we can better study the behaviour of the black box model. Still, the data for the explainer should be related to the original data. Otherwise the explainer may be ill-placed in space having nothing in common with the original problem anymore. This is why we perturb the original data. But how does perturbation work? This is a priori not clear at all. For categorical features, perturbation may be realised by randomly changing the categories of a random amount of features, or even recombining all possible levels of these. Numerical features may be drawn from a properly parametrised (normal) distribution. The perturbed data set, which is used to train the explainer, should be much larger than the original one and supposed to better represent the (possible) feature space, giving the surrogate model more anchor points – especially in sparse areas. Further details on this topic will be studied in the next chapters.

12.3 Example

A fully implemented example of LIME can be seen in the following code block with its resulting plot. In the latter we can observe how much each feature contributes to the surrogate model's prediction and to what extend this prediction offers a good fit on the black box model ('Explanation Fit' between 0 and 1).

```

library(lime)

##
## Attaching package: 'lime'
## The following object is masked from 'package:dplyr':
##
##     explain

library(mlr)

# separate data point we want to explain
to_explain = iris[ 1, 1:4]
train_set   = iris[-1, ]

# create task and calculate black box model
task_iris   = makeClassifTask(data = train_set,
                               target = "Species")
learner     = makeLearner("classif.randomForest",
                           ntree = 200, predict.type = "prob")
black_box   = train(learner, task_iris)

# use lime to explain new data point
explainer   = lime(train_set[, 1:4], black_box)
explanation = explain(to_explain,
                       explainer,
                       n_labels = 1,
                       n_features = 4)

plot_features(explanation)

```

12.4 Outlook

The definition of LIME still seems after all very rough and vague. This leaves us many scientific degrees of freedom when implementing it – for the good and for the bad. For example, we see that the model f can be any machine learning model that exists. This gives us the opportunity to drastically change the underlying predictive model while keeping the same explainer g with the same complexity constraints.

On the other hand, LIME being a very generic approach also means that many “hyperparameters”, like the neighbourhood definition or the sam-

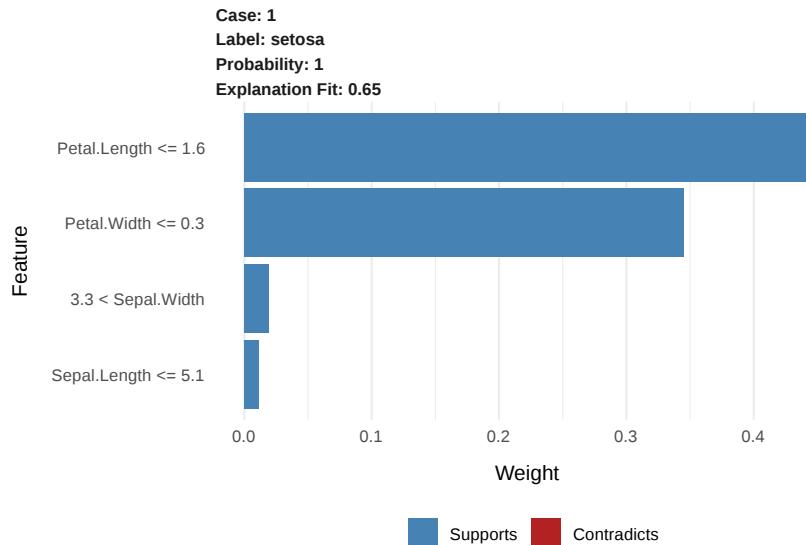


FIGURE 12.2: Basic example of a LIME application. We create a black box model on the iris dataset without the first data point and then explain the prediction of this point with LIME.

pling/perturbation strategy, are arbitrary. Hence, it is likely that in some use cases LIME explanations heavily depend on changing the hyperparameters. In these cases, the explanations can hardly be trusted and should be treated with great care.

The following two chapters will focus on two very significant hyperparameters: the neighbourhood definition and the sampling strategy. They will investigate how these affect the results of the method and their interpretability. We will emphasise the coefficient stability of LIME explainers in order to illustrate the trustworthiness of the results.



13

LIME and Neighborhood

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Supervisor: Christoph Molnar

This section will discuss the effect of the neighborhood on LIME’s explanations. This is in particular critical for tabular data. Hence, we will limit ourselves to the analysis of tabular data for the remainder of this chapter.

As described in the previous chapter, LIME aims to create local surrogate models – one for each observation to be explained. These local models operate in the proximity or *neighborhood* of the instance to be explained. They are fitted based on weights which indicate their proximity to the observation to be explained. The weights are typically determined using kernels that transform the proximity measure.

The proper parametrization of the kernel is obviously important. However, this is true for any approach that uses kernels, such as kernel density estimations. Figure 13.1 illustrates kernel densities from a standard normal distribution. We applied different kernel widths for the curve estimation.

One can easily see that the left panel seems to be appropriate while the right one is too granular. The proper definition of the neighborhood is very crucial in this case. However, with no prior information, this definition is arbitrary.¹ We can only judge on the proper definition of the neighborhood from our experience and our expectations. This may work in low dimensional problems and descriptive statistics. However, machine learning models operate in multivariate space and mostly tackle complex associations. Thus, it seems much harder to argue on the proper neighborhood definition when working with LIME.

This chapter reviews the neighborhood issue of the LIME algorithm critically. The objective of this chapter is rather to outline this particular issue and not to suggest solutions for it. First of all, it describes the neighborhood definition abstractly in greater detail (section 13.1). Then, it illustrates how problematic the neighborhood definition can be in a simple one-dimensional example in section 13.2. Furthermore, we study the effect of altering the kernel size more systematically in more complex contexts in the next section (13.3). This

¹Note that heuristics exist, though.

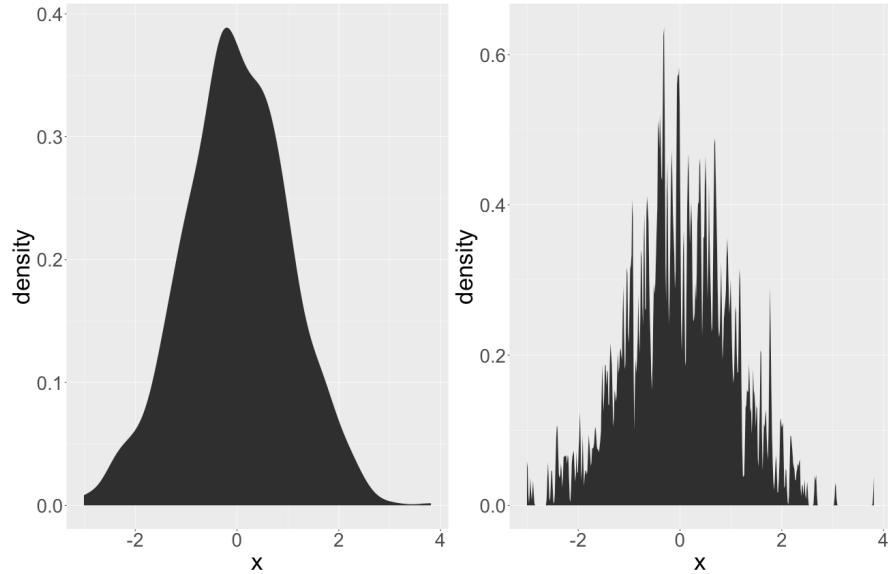


FIGURE 13.1: In(appropriate) kernel widths for kernel density estimations. The left panel illustrates an appropriate kernel width. The right one features an inappropriate one.

section deals with both, simulated (13.3.1) and real (13.3.2) data. The first subsection of the simulation (13.3.1.1) investigates multivariate globally linear relationships. The second one (13.3.1.2) researches local coefficients. The third one (13.3.1.3) studies non-linear effects. Section 13.3.2 uses the Washington D.C. bicycle data set to study LIME’s neighborhood in a real-world application. Afterwards, in section 13.4, we discuss the results and contextualize them with the existing literature. After concluding, we explain how LIME was used and why in section 13.5.

13.1 The Neighborhood in LIME in more detail

When obtaining explanations with LIME, the neighborhood of an observation is determined when fitting the model by applying weights to the data. These weights are chosen w.r.t. the proximity to the observation to be explained. However, there is no natural law stating that local models have to be found this way. Alternatively, Craven and Shavlik (1996) show that increasing the density of observations around the instance of interest is very helpful to achieve locally

fidele models. Hence, locality could be obtained in many more different ways than weighting observations combined with global sampling as it is in LIME. After sampling, the data points are weighted w.r.t. their proximity to the observation to be explained. One possible alternative to this procedure might be to combine steps 2 (sampling) and 4 (weighting) of the LIME algorithm² to a local sampling. This way we would increase the density around the instance already by proper sampling. In fact, Laugel et al. (2018) claim that this way should be preferred over the way LIME samples. In this chapter, however, we focus on the explicit implementation of LIME and analyze how the weighting strategy *ceteris paribus* affects surrogate model accuracy and stability.

When working with LIME, the weighting of instances is performed using a kernel function over the distances of all other observations to the observation of interest. This leaves us *arbitrary* (in fact, they may not be *that* arbitrary) choices on two parameters: the distance and the kernel function. Typical distance functions applicable to statistical data analysis are based on the L0, L1 and L2 norms. For numerical features, one tends to use either Manhattan distance (L1) or Euclidean distance (L2). For categorical features, one would classically apply Hamming distance (L0). For mixed data (data with both categorical and numerical features), one usually combines distances for numerical and categorical features. So does Gower's distance (Gower (1971)) or the distance proposed by Huang (1998):

$$d_H(x_i, x_j) = d_{euc}(x_i, x_j) + \lambda d_{ham}(x_i, x_j)$$

with d_{euc} referring to the Euclidean distance and d_{ham} to the Hamming distance. d_{euc} is only computed for numerical and d_{ham} only for categorical ones. λ steers the importance of categorical features relative to numerical ones. Huang (1998) recommends setting λ equal to the average standard deviation of the numerical features. For scaled numerical features (standard deviation is one) this metric is equivalent to the Euclidean distance. It is important to note that despite these existing measures it may be challenging to properly determine distances for mixed data. For text data, Ribeiro et al. (2016b) recommend using cosine distance and Euclidean distance for images.

For the kernel function itself, there are two parameters to be set. First of all, the type of kernel. Second, the kernel width. By default, the R implementation uses an exponential kernel where the kernel width equals the square root of the number of features.

The choice of the distance measure seems least arbitrary. Furthermore, the choice of the kernel function is not expected to have the most crucial impact on the neighborhood definition. Thus, we focus on the **kernel width** in our experimental study.

²Refer to the previous chapter.

13.2 The problem in a one-dimensional setting

How crucial the proper setting of the kernel width can be, is illustrated by a very simple example. We simulate data with one target and two features. One feature is pure noise and the other one has a non-linear sinus-like effect on the target. If we plot the influential feature on the x-axis and the target on the y-axis, we can observe this pattern in figure 13.2.

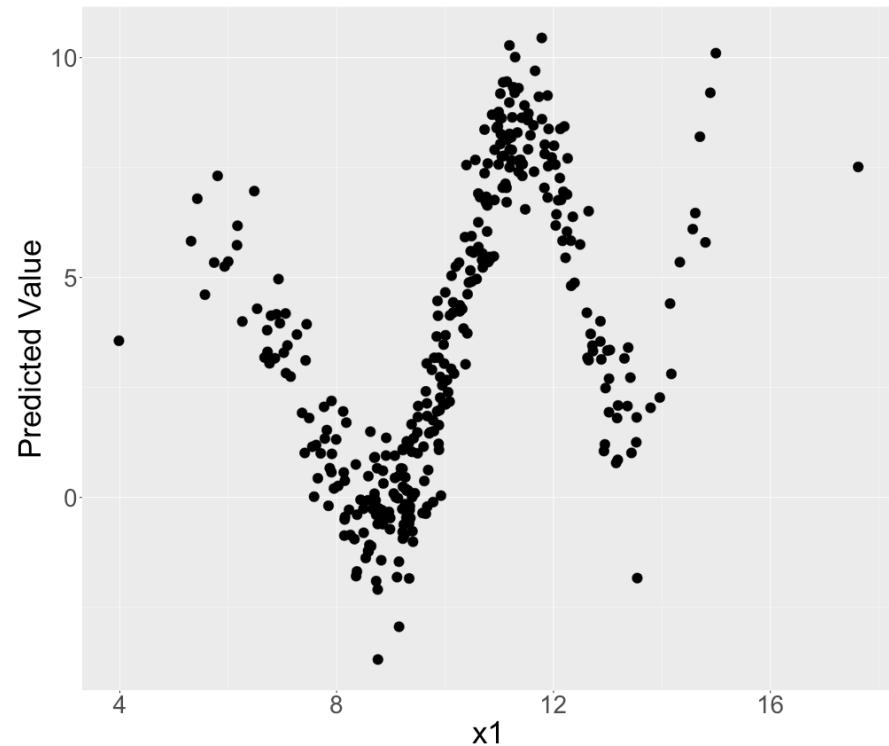


FIGURE 13.2: Simulated data: The non-linear relationship between the feature and the target.

Now we fit a random forest on this data situation which should be able to detect the non-linearity and incorporate it into its predictive surface. We observe that the predictions of the random forest look very accurate in figure 13.3. Only on the edges of the covariate (where the density is lower) the random forest turns out to extrapolate not optimally.

LIME could now be used to explain this random forest locally. “Good” local models would look very different w.r.t. the value of the feature, x_1 . For exam-

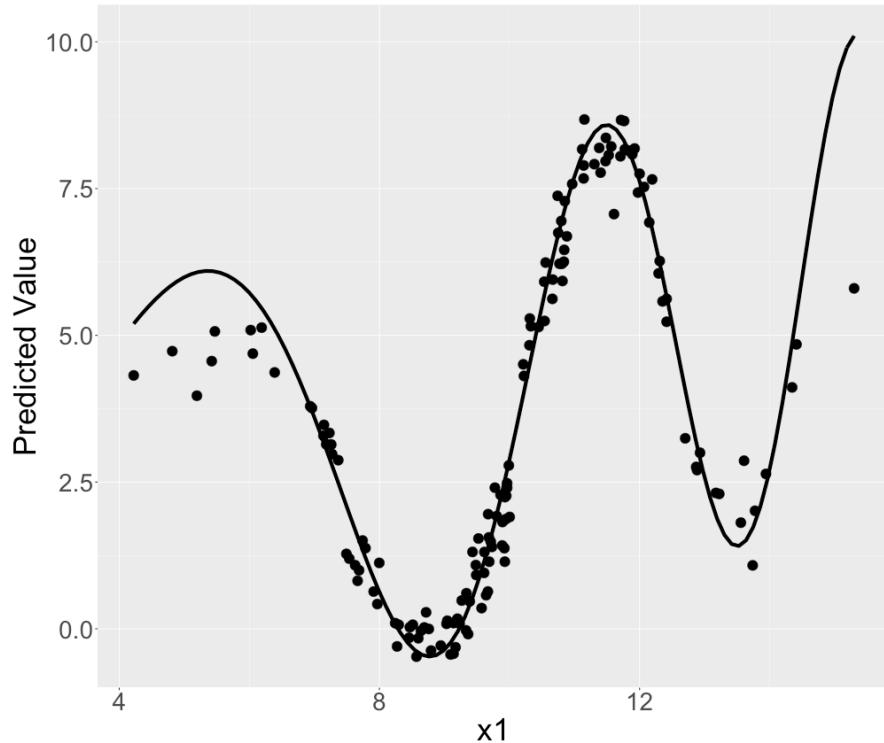


FIGURE 13.3: Simulated data: Random forest predictions for non-linear univariate relationship. The solid line represents the true predictive surface.

ple, we could describe the predictions locally well by piece-wise linear models. This is depicted in figure 13.4.

LIME should be able to find these *good* local explanations – given the right kernel size. Let's select one instance which we want an explanation for. We illustrate this instance by the green point in figure 13.5. This particular instance can be approximately linearly described by a linear regression with intercept 60 and slope -4.5 . If we set the kernel width to 0.08, we fit this local model. This is indicated by the red line in figure 13.5. However, if we increased the kernel width to 2, the coefficients change to -2.84 (intercept) and 0.64 (slope) (on average) which seems drastically distorted as observed by the yellow line in figure 13.5. The yellow line does not seem to fit a local linear model but rather a global one.

As a next step, we review explanations resulting from altering the kernel size in figure 13.6 more systematically. We average over many different models to achieve more robust local models. We do that because we observe some coefficient variations resulting from the (random) sampling in the LIME algorithm.

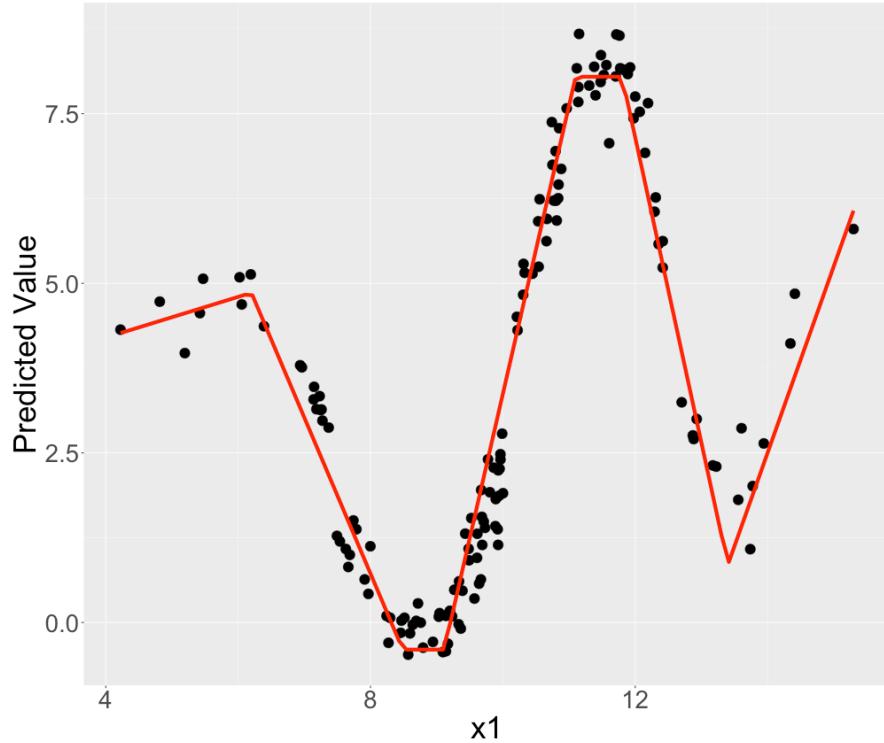


FIGURE 13.4: Simulated data: Non-linear univariate relationship explained by a piece-wise linear model.

In figure 13.6 (upper panel) we see these averaged models for different kernel sizes. We observe that the larger we set the kernel size, the more we converge to a linear model that operates globally. The largest three kernel sizes (0.5, 1 and 2) appear very global while 0.05 and 0.1 seem to fit good local models. 0.25 and 0.3 are neither global nor very local. This is very intuitive and complies with the idea of a weighted local regression.

Additionally, we analyze the same alteration of the kernel size for an observation where a good local approximation would be a linear model with a positive slope in the lower panel of figure 13.6. We observe a similar behavior.

This behavior is not necessarily a problem but only a property of LIME. However, it can be problematic that the appropriate kernel size is not a priori clear. Additionally, there is no straight forward way to determine a good kernel width for a given observation to be explained. The only generic goodness-of-fit criterion of LIME, model fidelity, is not necessarily representative: If we set the kernel size extremely small there will be many models with an extremely good local fit as local refers only to a single observation. In our examples, it looks

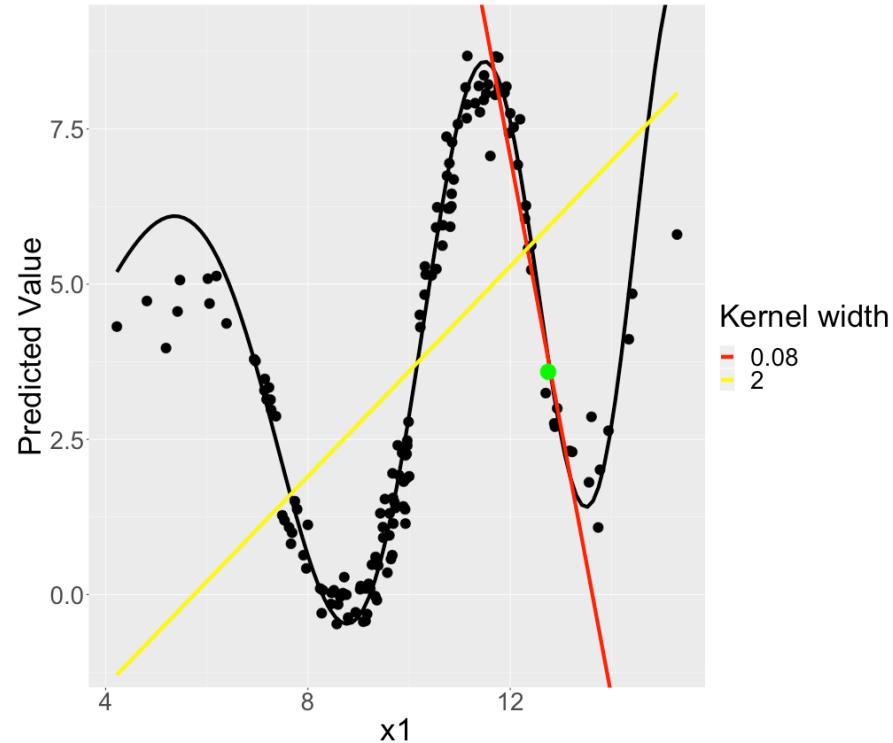


FIGURE 13.5: Simulated data: Possible local (LIME) models for the non-linear univariate relationship.

as if a very small kernel size should be preferred. A small kernel width indeed grants local fit. But what a small kernel width means, also strongly depends on the dimensionality and complexity of the problem.

13.3 The problem in more complex settings

The previous setting was trivial for LIME. The problem was univariate and we could visualize the predictive surface in the first place. This means that interpretability was mostly given. We will study our problem in more complex – non-trivial – settings to show that it persists. We will do so by examining simulated and real data.

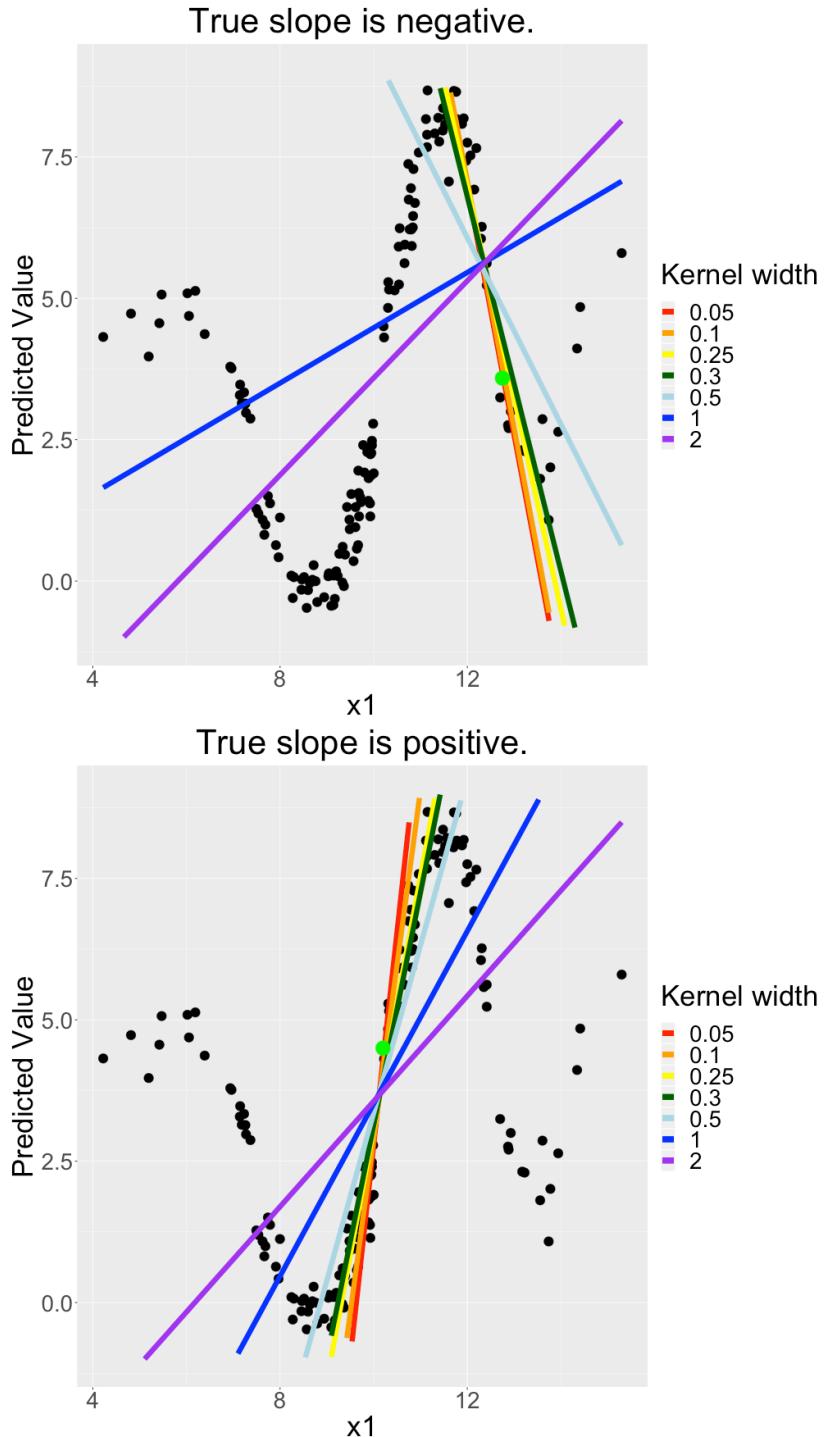


FIGURE 13.6: Simulated data: Local (LIME) models for non-linear univariate relationship with different kernel sizes for different observations.

13.3.1 Simulated data

We simulate data with multiple numeric features and a numeric target. We assume the features to originate from a multivariate normal distribution where all features are moderately correlated. We simulate three different data sets. In the first one, the true associations are linear (globally linear). In the second one, the true associations are linear but only affect the target within a subinterval of the feature domain (locally linear). ³ In the third one, we simulate globally non-linear associations. For all three data sets, we expect the kernel width to have an impact on the resulting explainer. However, for the global linear relationships, we expect the weakest dependency because the true local model and the true global model are identical. Details on the simulation can be obtained in our R code and section 13.3.1.1.

13.3.1.1 Global Linear Relationships

We simulate data where the true predictive surface is a hyperplane. *Good* machine learning models should be able to approximate this hyperplane. This case is – again – somewhat trivial for LIME. The most suitable model for this data would be linear regression which is interpretable in the first place. Thus, LIME can be easily tested in this controlled environment. We know the true local coefficients as they are equal to the global ones. We can evaluate the suitability of the kernel width appropriately.

The simulated data looks as follows: The feature space consists of three features (x_1, x_2, x_3). All originate from a multivariate Gaussian distribution with mean μ and covariance Σ . μ is set to be 5 for all features and Σ incorporates moderate correlation. The true relationship of the features on the target y is described by:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

We set the true coefficients to be $\beta_1 = 4, \beta_2 = -3, \beta_3 = 5$.

We use linear regression (the true model) as a black-box model. Using cross-validation, we confirm that the model has a high predictive capacity – approaching the Bayes error. Not surprisingly, the linear model describes the association very well.

We choose random observations and compute the local LIME model for each one of them w.r.t. different kernel sizes. We expect that the kernel size may be infinitely large as the global model should equal good local models. However, if the kernel width is set too small we may fit too much noise. Hence, in this case, we may find no good local models.

³This should examine LIME's ability to assess local features.

The figures below (all four panels of figure 13.7) indicate the local parameters for one of the selected observations for different kernel sizes which have been determined by LIME. The three vertical lines indicate the true global coefficients. This behavior is representative of all observations.

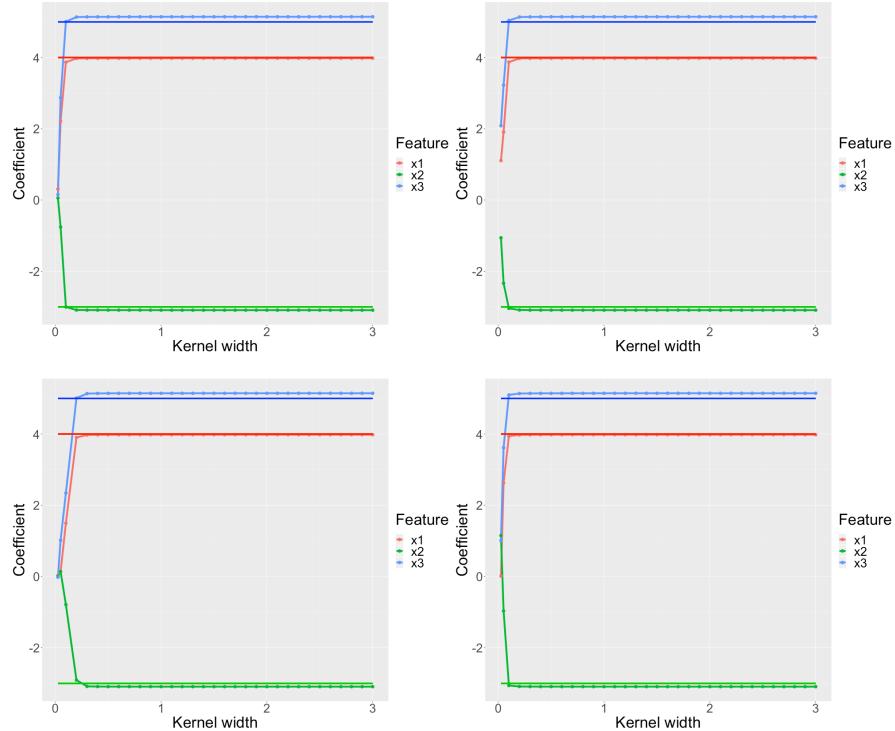


FIGURE 13.7: Simulated data: Each panel represents a single (representative) observation. For each observation we analyze the LIME coefficients for different kernel widths. The underlying ground truth model is a linear model. Each feature is depicted in a different color. The solid vertical lines represent the true coefficient of the LIME explanation.

We observe that too small kernel widths are not able to reproduce the global predictive surface at all. However, provided the kernel width is not too small, all kinds of kernel widths from small size to very large kernels fit very similar models which are all very close to the *true* model.

These results allow concluding that for explaining linear models the kernel width is a non-critical parameter. However, this case may be seen as trivial and tautological for most users of LIME. Still, this result is valuable as it shows that LIME works as expected.

13.3.1.2 Local Linear Relationships

For non-linear relationships, we have already seen that the kernel width is more crucial. Thus, we aim to study the behavior of the explanations w.r.t. the kernel size where the true associations are non-linear or *locally* different.

We may induce non-linearity by different means. However, first of all it seems interesting to study how the kernel width affects LIME explanations in a very simple form of non-linearity: The features only affect the target locally linearly, as expressed by:

$$y = \beta_0 + \beta_1 x_1 1_{x_1 < c_1} + \beta_2 x_2 + \beta_3 x_3 + \epsilon + \gamma_0 1_{x_1 > c_1} + \epsilon_i$$

where x_1 only affects y within the given interval. γ_0 corrects the predictive surface by another intercept to avoid discontinuities. This time, we fit a MARS (multivariate adaptive regression splines) model (Friedman et al. (1991)) which can deal with this property of local features. In theory, MARS can reproduce the data generating process perfectly and hence is our first choice. Using cross-validation we confirm that the model has a high predictive capacity. However, note that all of our results would be *qualitatively* (MARS turns out to feature clearer results.) identical between MARS and random forest. Given an appropriate kernel, LIME should succeed in recovering the local predictive surface.

We set $\beta_1 = 5$, $\beta_2 = -4$, $\beta_3 = 3$ and $c_1 = 5$. This means that the slope of β_1 equals to 5 until $x_1 = 5$ and to 0 afterwards. This results in an average slope of 2.5 over the whole domain.

We investigate *representative* observations, i.e. belonging to each *bin* of the predictive surface to check if LIME recovers all local coefficients.

Hence, representative means that we should investigate observations with the following properties:

1. $x_1 < 5$
2. $x_1 > 5$

We think these observations are best explained in areas with reasonable margin to $x_1 = 5$.

Below in figure 13.8, we depict the coefficient paths for four representative observations, two belonging to each bin (upper panels: $x_1 < 5$, lower panels: $x_1 > 5$). The true local coefficients are displayed by solid vertical lines.

We can see that in this case, we **cannot** simply set an arbitrary kernel width. The true local coefficient for x_1 is only approximated well within a limited interval of the kernel width. In our scenario, good kernel widths are between

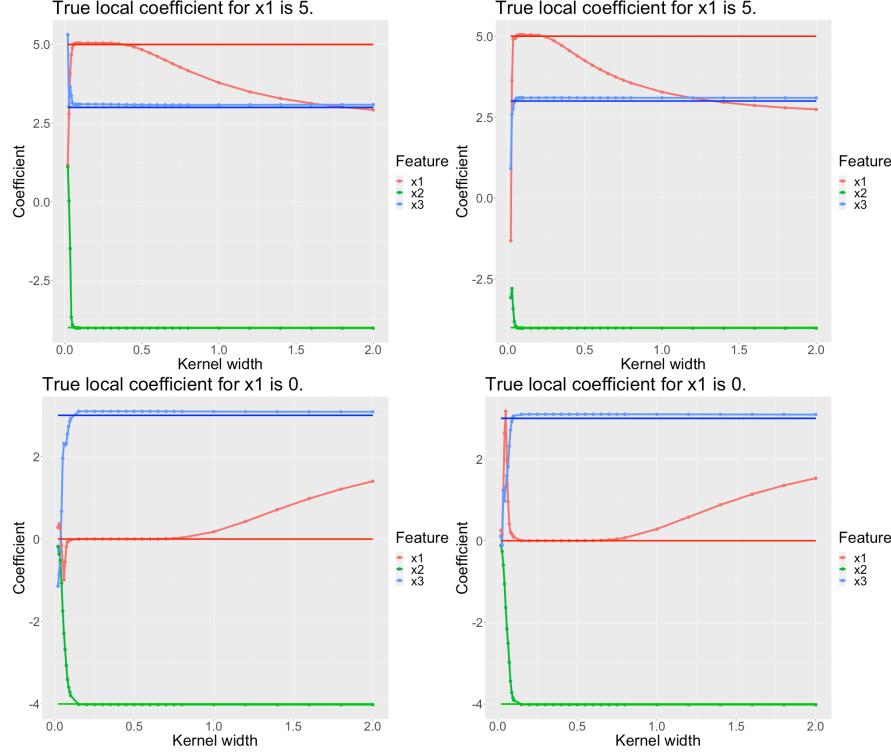


FIGURE 13.8: Simulated data: Each panel represents a single (representative) observation. For each observation we analyze the LIME coefficients for different kernel widths. The underlying ground truth model is a linear model where x_1 only has a local coefficient. Each feature is depicted in a different color. The solid vertical lines represent the true coefficient of the LIME explanation.

0.1 and 0.7 (while the upper bound varies for the observations). As before, we observe that a too-small kernel width (< 0.1) produces non-meaningful coefficients. On the other hand, for large kernel widths (> 0.7) the true coefficient is not approximated, but rather the global (average) linear coefficient: For x_1 a large kernel width results in a linear model that averages the local slopes. More formally, one could describe this sort of explanation as a global surrogate model. Additionally, we observe that for smaller kernel widths, the local models are rather volatile. More systematically, Alvarez-Melis and Jaakkola (2018) investigate this volatility and find that LIME is prone to finding unstable explanations.

This motivates us to further research the volatility. We display the mean and the confidence intervals of the coefficients of 100 different models for

different kernel sizes in figure 13.9 for x_1 . The black lines interpolate averaged coefficient estimates for different kernel sizes. The solid black line indicates the true local coefficient. The grey shaded area represents the (capped) 95% confidence intervals. For very low kernel widths we observe massive volatility. The volatility decreases to an acceptable level only after 0.1 for all covariates.

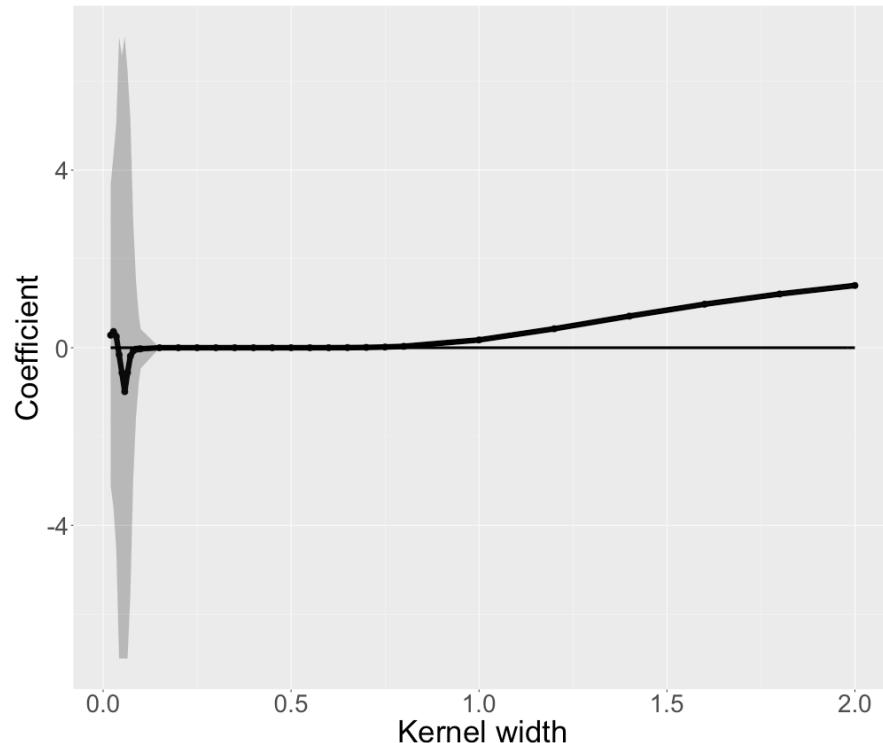


FIGURE 13.9: Simulated data: For one observation we display the local coefficient and confidence intervals for different kernel widths. The underlying ground truth model is a linear model where x_1 only has a local coefficient. Hence, we only investigate x_1 .

Note that we obtain the same picture for every covariate and other representative observations. We observe that there is a trade-off between stable coefficients and locality (expressed by a small kernel width). Our analysis suggests the following: Too large kernel sizes result in explanations biased towards a global surrogate. At the same time, the kernel width must result in stable coefficients. This means we cannot set it infinitesimally small. The resulting trade-off suggests choosing the minimal kernel size with stable coefficients as an optimal solution. Mathematically speaking, we aim minimal kernel size which still satisfies a volatility condition.

13.3.1.3 Global Non-Linearity

We further generalize the approach from the previous section and simulate data with the underlying data generating mechanism:

$$y = \beta_0 + \beta_1 x_1 + \beta_{2,1} x_2 \mathbf{1}_{x_2 < c_1} + \beta_{2,2} x_2 \mathbf{1}_{c_1 < x_2 < c_2} + \beta_{2,3} x_2 \mathbf{1}_{c_2 < x_2} + \beta_3 x_3 + \epsilon$$

where the slope β_2 is piece-wise linear and changes over the whole domain of x_2 . We set $\beta_1 = 5$, $\beta_{2,1} = -4$, $\beta_{2,2} = 3$, $\beta_{2,3} = -3$, $\beta_3 = 3$, $c_1 = 4$ and $c_2 = 6$.

We omitted the support intercepts $\gamma_0 \mathbf{1}_{c_1 < x_1 < c_2} + \gamma_0 \mathbf{1}_{x_1 > c_2}$ in the equation above (which guarantee continuity).

We study three *representative* observations complying with:

1. $x_2 < 4$
2. $4 < x_2 < 6$
3. $6 < x_2$

As before, we use a MARS model as our black box. When explaining the black box with LIME, we observe the same pattern as before. Figures 13.10 and 13.11 look very similar to the corresponding figures of the previous section. However, the intervals of “good” solutions are – naturally – much smaller. The more complex the true associations become, the more we observe this trend of decreasing solution intervals. It seems as if the more complex the predictive surface is, the harder it is for LIME to even find a good local model.

For globally non-linear associations, we also find that we prefer a small kernel which however also produces stable coefficients.

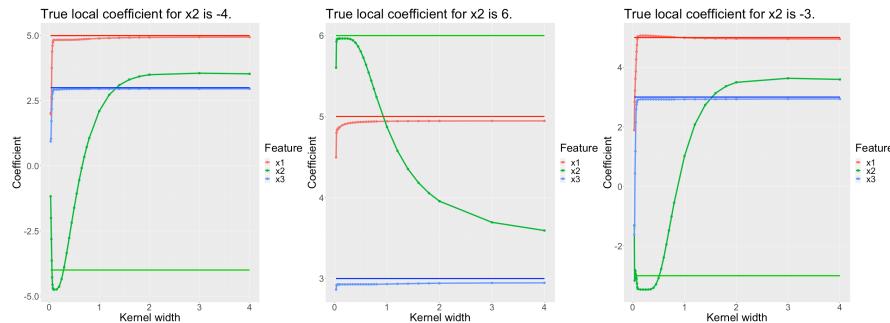


FIGURE 13.10: Simulated data: Local coefficients for different kernel widths explaining non-linear relationship (for x_2).

Having investigated simulated data where we knew the ground truth, gave us

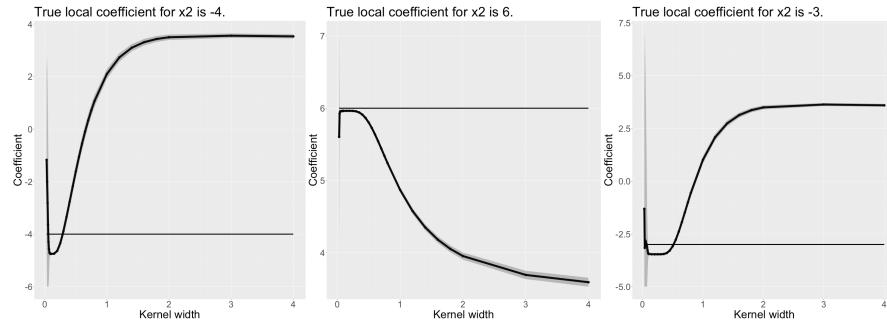


FIGURE 13.11: Simulated data: Local coefficients and confidence intervals for different kernel widths explaining non-linear relationship (for x_2).

a good intuition on how the kernel size affects the resulting explainer model. The neighborhood problem can be described briefly by the following. A (too) small kernel width creates unstable coefficients whilst a too large kernel width fits a global surrogate model. An optimal kernel size should balance these effects. We may formulate the problem as a minimization problem w.r.t. the kernel size. However, the minimization needs to consider the constraint that coefficients need to be stable.

13.3.2 Real data

Leaving the controlled environment may make things more difficult. Relevant challenges include:

1. High-dimensional data may be an issue for the computation of the kernel width. LIME computes dissimilarities. It is well-known that (some) dissimilarities get increasingly less meaningful as the feature space expands. This is one consequence of the curse of dimensionality.
2. Computing some dissimilarities (e.g. Manhattan or Euclidean) also comes with the problem that the cardinality of the features mainly steers this measure. Thus, LIME should always apply scaling.
3. When working with real data sets with many features, we typically want a sparse explanation. To achieve this, we should let LIME perform feature selection.

Luckily, the latter two are featured in the Python and R implementations.

Within this section, we study whether we can confirm our simulated data findings for real-world data. We will work with the well-known Washington

D.C. bicycle rental data set. This dataset contains daily bicycle hire counts of a Washington D.C. based rental company. The data has been made openly available by the company itself (Capital-Bikeshare). Fanaee-T and Gama (2014) added supplementary information on the weather data and season associated with each day. For details on the data set please refer to Molnar (2019) (<https://christophm.github.io/interpretable-ml-book/bike-data.html>). We select this data set because it is well-known in the machine learning community and this regression problem is easily accessible to most people. Furthermore, it has a reasonable feature space making it not highly prone to the curse of dimensionality of the distance measures. We only make use of a subset of all possible features as some are somewhat collinear.

Using this data we aim to use a random forest to predict the number of daily bicycle hires. We use LIME to explain the black box.

When working with LIME in practice, we want to obtain stable explanations. An explanation is stable if the surrogate model does not change much when altering the randomly drawn samples. We evaluate this property with the aid of a modified version of stability paths (Meinshausen and Bühlmann (2010)). Stability paths are used for sparse (regularised) models and indicate how likely each covariate is part of the model – w.r.t. a given degree of regularisation. Normally, they analyze the association of the regularisation strength and inclusion probabilities of features. On the x-axis, one depicts the regularisation strength and on the y-axis the inclusion probabilities (for all covariates). The probabilities for different regularisations are grouped by feature.

However, for LIME we rather aim to study how likely a covariate is part of the (sparse) model over a grid of kernel widths. Our motivation to use stability paths is that they are easier to interpret compared to coefficients paths (or similar evaluation methods) in our setting.

Over a grid of kernel widths (from almost 0 to 20), we compute multiple sparse explanations for the same kernel width. Sparse means that we limit our explainer to only the three most influential local features. We count how frequently each covariate has been part of the explanation model (out of all iterations). We divide by the total number of iterations and achieve estimates for the sampling probability for a given observation, a given number of features and a given kernel width. We search the full (predefined) grid of kernel widths. We can repeat this procedure for any other observation.

Our *pseudo* stability paths are stable in areas where we have extreme probabilities, i.e. either probabilities close to 1 or close to 0. Furthermore, they should not change extremely when the kernel width slightly changes.

Figure 13.12 displays ideal stability paths with the three distinct areas observed earlier:

1. High variability for small kernels.

2. Local stability for *optimal* kernels.
3. Convergence to a global surrogate for large kernels.

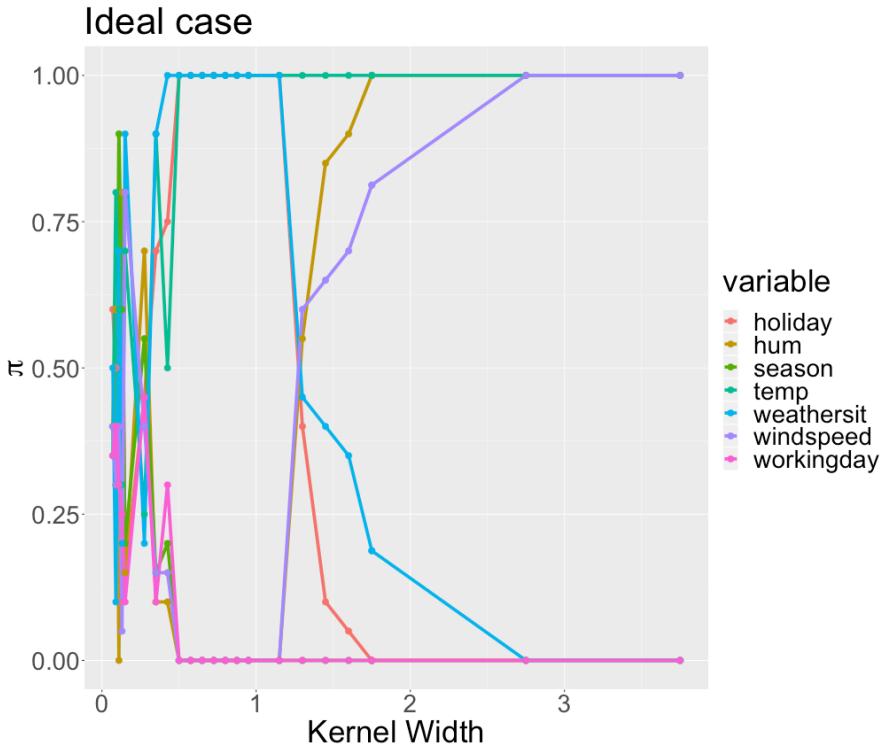


FIGURE 13.12: Real data: Example for ideal stability paths with three distinct areas. The x-axis displays different kernel widths. The y-axis indicates the respective inclusion probability of each variable. The variables are grouped by color.

The (toy example) stability paths suggest that temperature, weather situation and holiday are the local features while temperature, humidity and wind speed are deemed as the global ones.

This figure would help us to clearly identify a stable local model. However, in real life, things mostly are more complex. In figure 13.13, we display the stability paths for different selected observations for our random forest.

We observe that stability paths converge to a set of covariates if we set the kernel width large. These are the global features. There is one interesting observation about this. Different observations sometimes converge to different global surrogate models. The covariates humidity and temperature are always selected. Then, either the windspeed (e.g. only observation 1) or the season

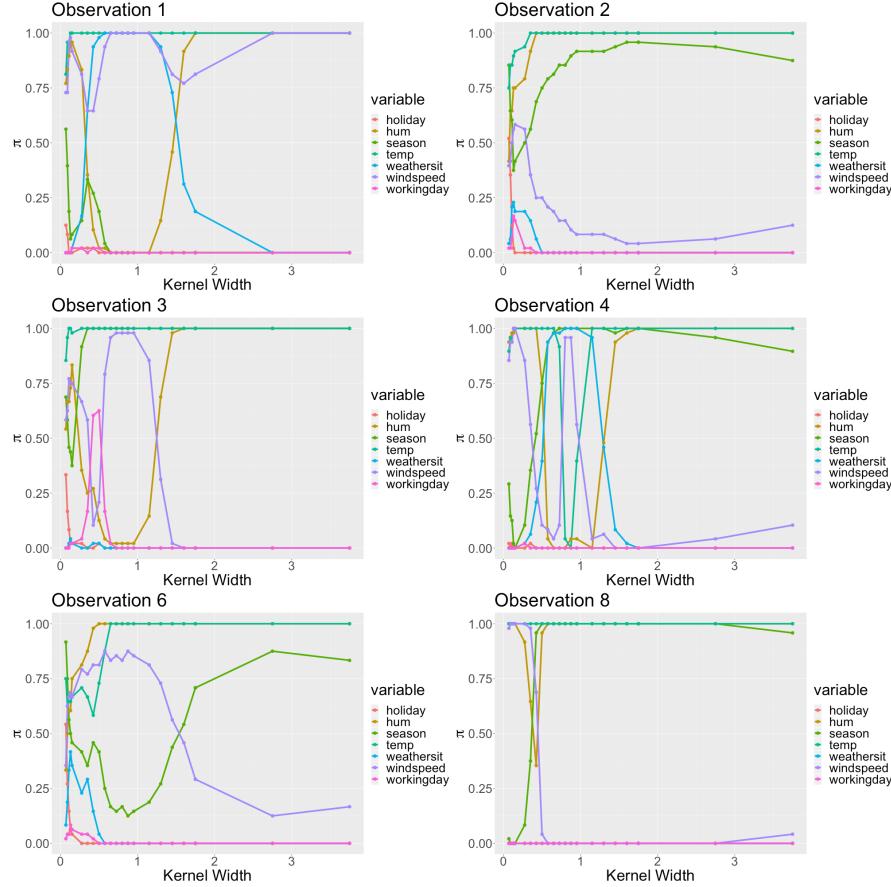


FIGURE 13.13: Real data: Stability paths for different observations from the bycicle data set explaining a random forest.

(the remainder observations) is selected as global feature. We believe that this is because both covariates are similarly strong on the global scope. Globally evaluating the feature importance of the random forest suggests that in fact temperature, season, humidity and wind speed are the most relevant features.

Furthermore, we observe that for small values of the kernel width, we have – like in our simulation – high variation. Here, this variation is expressed by intersecting paths where most covariates are (almost) equally likely to be sampled.

For some observations, there seems to be a narrow range where there are stable and local explanations. For instance, consider observations 1 and 3. Here, the local models seem quite clear. For observation 1, between kernel widths of 0.5 and 1 it seems as if the temperature, the wind speed, and the weather

situation are most influential. For observation 3, the selected local features are temperature, wind speed and season. For other observations, such as observations 4 and 8, we may argue that there are local and stable explanations, too. These are, however, by far less convincing than the previous ones. Additionally, we are struggling to identify stable local models for many observations, like observation 2 and 6. For those observations, there is only instability for small kernel widths which transforms immediately to the global surrogate once stabilized. The reasons for this variation of behavior can be manifold. However, not knowing the ground truth, it is hard to evaluate what is going on here in particular.

So even though we may find meaningful explanations from case to case, there is too much clutter to be finally sure about the explanations' goodness. Furthermore, "local" explanations still seem quite global as they seem quite similar for many different observations. Considering our explanations, the sparse models were highly correlated consisting of similar features for different observations. The only truly stable explanations remain essentially global ones with large kernel width. It seems as if the predictive surface is too complex to facilitate local and stable surrogate models properly. The curse of dimensionality affects locality very strongly. As distances in higher-dimensional Euclidean space are increasingly less meaningful, the definition of locality is very poor with an increasing number of features.

Summarising, we observe both effects being described in the literature also for our real data example: instability ([Alvarez-Melis and Jaakkola \(2018\)](#)) for small kernel widths and global surrogates ([Laugel et al. \(2018\)](#)) for large ones. For simulated data, we can observe these effects as well. At the same time, we can identify local and stable explanations in this controlled environment. For real data, however, it is hard to locate the area which we identified for simulated data where we find a stable **and** local model.

13.4 Discussion and outlook

LIME is capable of finding local models. We show this using simulated data. The specification of a proper kernel width is crucial to achieving this. A proper locality is expressed by the minimal kernel width producing stable coefficients. However, we see that it is difficult to find these models in practice. We are unable to detect explanations that were both, stable and local, for our real data application – at least with certainty. We largely observe the pattern described by [Laugel et al. \(2018\)](#) who claim that LIME explanations are strongly biased towards global features. At the same time, our study agrees with [Alvarez-Melis and Jaakkola \(2018\)](#) who find that local explanations are highly unstable. We

confirm these findings using the bicycle rental data set. Additionally, also for simulated data, it becomes harder to detect a good locality if the predictive surface becomes more complex.

Similar results can be obtained for alternative data sets. For the practitioner using LIME (for tabular data), this means that LIME should be used with great care. Furthermore, we suggest analyzing the resulting explanations' stability when making use of LIME.

We think that the global sampling of LIME is responsible for many of the pitfalls identified. Hence, we propose that LIME should be altered in the way proposed by [Laugel et al. \(2018\)](#) to LIME-K. Local sampling should replace global sampling to better control for the locality.

Even though having said this, we think that LIME is one of the most promising recent contributions to the Interpretable Machine Learning community. The problems described in this chapter are mainly associated with tabular data. Domains where LIME has been applied successfully include image data and text data. Within these domains, LIME works differently from tabular data. For example, LIME's sampling for text data is already very local. It only creates perturbations based on the instance to be explained.

13.5 Note to the reader

13.5.1 Packages used

For our analysis, we used R ([R Core Team \(2017\)](#)). For all black-box models, we used the mlr package ([Bischl et al. \(2020\)](#)) and the lime package ([Pedersen and Benesty \(2019\)](#)) for the LIME explanations. All plots have been created using ggplot2 ([Wickham et al. \(2019\)](#)).

13.5.2 How we used the lime R package and why

Using the lime package we heavily deviated from the default package options. We strongly recommend to not bin numerical features. The next chapter will outline in detail why this is not a good idea. In the first place, the main argument for binning has been enhanced interpretability. We suggest, though, that the same interpretability can be obtained by the **absolute contribution** of the feature to the prediction. This means, instead of the local coefficient, LIME should rather print the local coefficient times the feature value within

its explanation. This argument makes binning – provided that there is no additional benefit except interpretability (Refer to the next chapter.) – obsolete.

While we think Gower distance is an interesting approach to deal with mixed data, we explicitly promote not to use it. In the current (July 2019) R implementation, when working with Gower distance there is **no** kernel applied. Explanations do not correspond to altering the kernel width. As we have seen, a proper kernel width may look very different depending on the associated problem. So it is highly unlikely that a one-size-fits-all implicit kernel width always results in a proper result. In figure 13.14 we analyze this statement by comparing the Gower distance's local coefficient to the true coefficient and the local estimates of the non-linear data simulation from section 13.3.1.3.

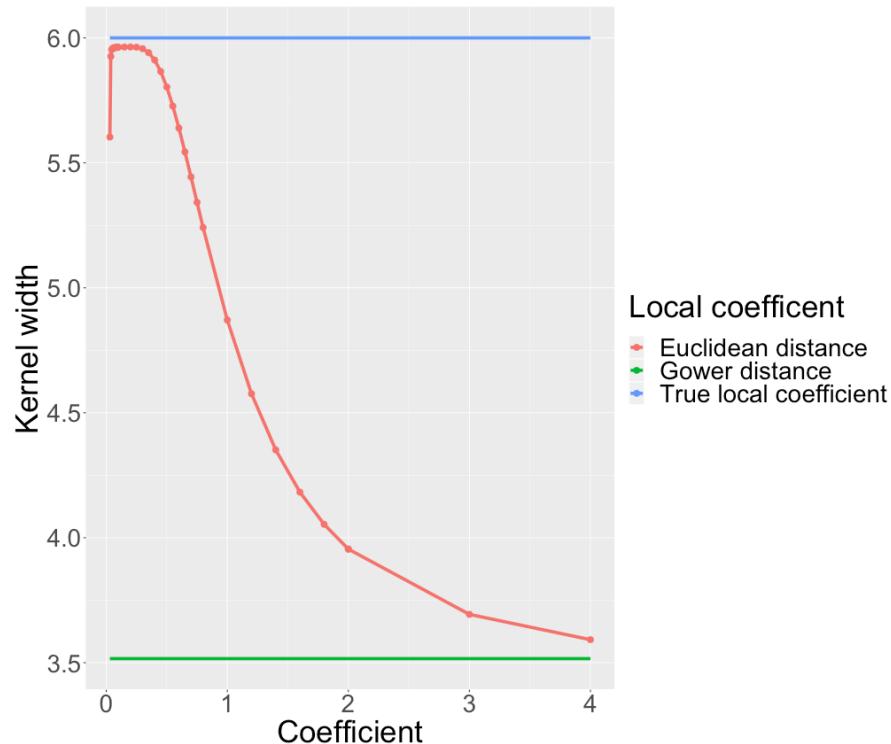


FIGURE 13.14: Simulated data: Gower distance vs. Euclidean distance (non-linear relationship). The blue line is the true coefficient. The interpolated curve represents the LIME coefficient estimates for different kernel widths when using Euclidean distance. The green line represents the estimate resulting from LIME when using Gower distance.

We see that our argument is valid. Gower distance is not able to recover the true coefficients and acts as a global surrogate.

Even though we think that Gower distance may result in some cases in good local models, its (currently) lacking flexibility most likely causes either instable or global explanations.

Usually, LASSO is the preferred option for variable selection as it is less seed dependent than, let's say, step-wise forward selection. However, we do not use LASSO but step-wise forward selection because the current implementation of LASSO has shortcomings and does not deliver results suitable for our analysis.

All in all, we strongly discourage the user of the lime R package to use the default settings.

14

LIME and Sampling

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Supervisor: Christoph Molnar

This chapter will deal with the sampling step in LIME and the resulting side effects in terms of feature weight stability of the surrogate model. Due to the randomness of sampling, the resulting feature weights may suffer from high discrepancies between repeated evaluations. As a consequence, trust in the explanation offered by LIME is impacted negatively.

14.1 Understanding sampling in LIME

In this section, we will discuss the fundamentals of LIME from a slightly different angle to receive a further understanding of what enables sampling and to have a look at how basic results look like.

14.1.1 Formula

If we do some small changes of notations compared to the introduction chapter, the task of calculating the LIME explainer can be seen as

$$g^* = \arg \min_{g \in G} \sum_{i=1}^{n'} \pi_{\tilde{x}}(x^{(i)}) L(f(x^{(i)}), g(x^{(i)})) + \Omega(g)$$

with $\mathcal{L}(f, g, \pi_{\tilde{x}}) := \sum_{i=1}^{n'} \pi_{\tilde{x}}(x^{(i)}) \times L(f(x^{(i)}), g(x^{(i)}))$ further expressed more in detail as in the introduction and \tilde{x} as our desired point to explain ([Peltola \(2018\)](#)). This change of notation allows us to spot the enabling property for sampling. Namely, the original target variable y is replaced by the response $f(x^{(i)})$ of the black box model. This means nothing more besides that we minimize this problem without accessing the original target. The great thing

about this is, that f can be evaluated for any value in the feature space, giving us – theoretically – an arbitrarily amount n' of non-stochastic observations compared to before. This may sound great at first, but we still need the values of our feature space for evaluation. And this is where problems arise on the horizon. At this point, one may ask why even try to receive new values of the feature space? Is our real dataset not enough? The ground truth for our surrogate model is a function of an infinite domain (assuming at least one numeric variable is present), so the more information we gather about this function, the better our approximation is going to be. So, if we can get more data, we will simply take it. One issue here is the definition of the feature space. We need a new dataset to receive the responses of f . However, a priori, it is not clear how this new data may look like. Our original dataset is a finite sample of infinite space in the numerical case, or of finite space exponentially growing with its dimension in the categorical case. As a consequence, we cannot assume producing a dataset equal to the size of our feature space – we need strategies to receive the best possible representation concerning our task.

14.1.2 Sampling strategies

Originally, sampling in LIME was meant as a perturbation of the original data, to stay as close as possible to the real data distribution ([Ribeiro et al. \(2016b\)](#)). Though, the implementations of LIME in R and Python ([Pedersen \(2019\)](#) and [Ribeiro \(2019\)](#)) took a different path and decided to estimate a univariate distribution for each feature and then draw samples out of that. The consequence of this approach is the total loss of the covariance structure, as our estimated distribution for the whole feature space is simply a product of several univariate distributions. This way, we may receive samples that lie outside the space of our real data generation process. Because almost all machine learning models are well defined on the whole input space, evaluating unrealistic values leads to no problems at first. But in theory, issues could occur, if a lot of unrealistic evaluations lied close to our point for explanation and influenced greatly the fit of the surrogate model. In that case, we would not be able to trust the results of LIME anymore, even though we got told the local fit is a very decent approximation. On the other hand, an issue like this was not encountered during the preparation of this work as most used learners are well regularized in space of low data denseness.

14.1.2.1 Categorical features

Categorical features are handled more straight forward than numerical ones due to finite space. The R LIME package ([Pedersen \(2019\)](#)) will sample with probabilities of the frequency of each category appearing in the original dataset. The case when this goes wrong is if one category is very infrequent

and then – due to bad luck – simply not drawn. Since the original data is thrown away after sampling, no information is leftover about this category for the fitting process. Additionally, by ignoring feature combinations, we may sample points that are impossible in the real world and add no value to our fit, or may even distort it.

14.1.2.2 Numerical features

Numerical features rise the challenge higher. While categorical features make it possible for at least very low dimensions to gather a dataset with all possible values, numerical features are theoretically of infinite size. There are currently three different options implemented in the R LIME package ([Pedersen \(2019\)](#)) for sampling numerical features. The first – and default – one uses a fixed amount of bins. The limits of these bins are picked by the quantiles of the original dataset. In the sampling step, one of these bins will be randomly picked and after that, a value is uniformly sampled between the lower and upper limit of that bin. The small benefit here is being allowed to fine-tune the number of bins, leading to a rougher or more detailed sample representation of the original feature. The downside is that the order of the bins is ignored, as a consequence risking the loss of a global fit as each bin receives its own weight. Additionally, bins have a lower and upper limit, i.e. the new point for explanation may lie outside of all bins. The current implementation handles this by discretizing the explanation with each bin as a category class, making it possible to assign values to the lowest (or highest) bin even if it lies below (or above) that bin. Another option would be to approximate the original feature through a normal distribution and then sample out of that one. This is relatively straight forward, but one may ask if the assumption of normally distributed features is correct. A lack of denseness of the training data for the surrogate model may be a result of a wrong assumption. Additionally, it is not possible to change options for each feature, so by choosing this distribution, all your features will be handled as normally distributed with their individual mean and variance. The last option for numerical features is approximating the real feature distribution through a kernel density estimation. Any downsides besides slightly increased computational effort have not been encountered with this option. Thus – and after gathering empirical evidence supporting this –, we choose to not use binning, but rather kernel density estimation for most of our trials following down.

14.1.3 Visualization of a basic example

To give more substance to the introduction, in figure 14.1 one can see two LIME results of a simple numerical example. Both use the same settings except one uses a different sample seed than the other. The black-box model in blue

is tried to be explained by the surrogate model as the red line. The black dots are the sampled values dealing as training data set for the surrogate model, which tries to explain our target point, the dot in yellow. The vertical bars are an indicator of the kernel width. This color scheme is kept from now on in all further graphics.

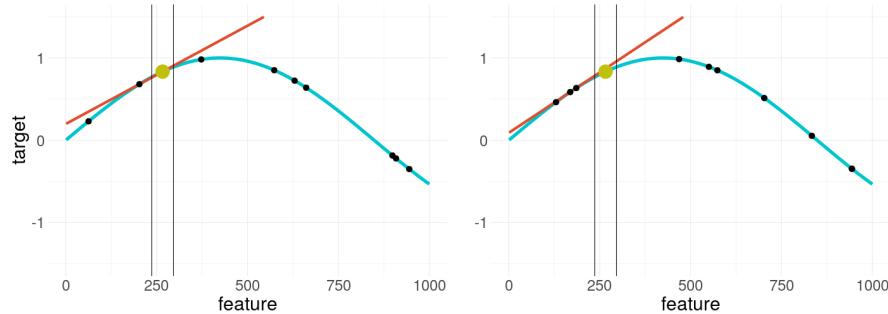


FIGURE 14.1: Visualization of LIME applied on a non-linear function - the right plot uses the same settings but is resampled

As can be seen the results in both cases are very similar, as one would wish. But this may not always be the case. The surrogate models depend only on randomly generated samples, that lie closer or further spread across the feature space. This raises the following questions. How much influence has a new sample of the explanation? What is the average confidence of certain weights? Do certain settings influence these and is there a tendency?

14.2 Sketching Problems of Sampling

To give an idea of the potential problems, a few artificial showcases are presented in the following. In figure 14.2 a sinus shaped black-box model is tried to be explained twice again with a different seed.

The two LIME explanations of the same scenario and with the same settings hold totally different results. This indicates how untrustworthy single explanations could be. So, what can we do here?

The most obvious step is increasing the sample size. As it is depicted in figure 14.3, this indeed shrinks the problem to irrelevancy, restoring some of the lost trust in our explanation. But the problem with this solution is its heavy computational burden, so it would be good to know in which cases the additional computational effort is necessary.

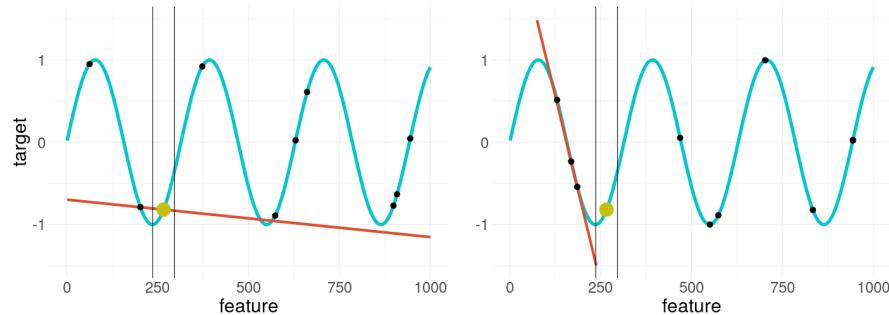


FIGURE 14.2: LIME applied on a non-convex function - again, the right plot uses the same settings but is resampled

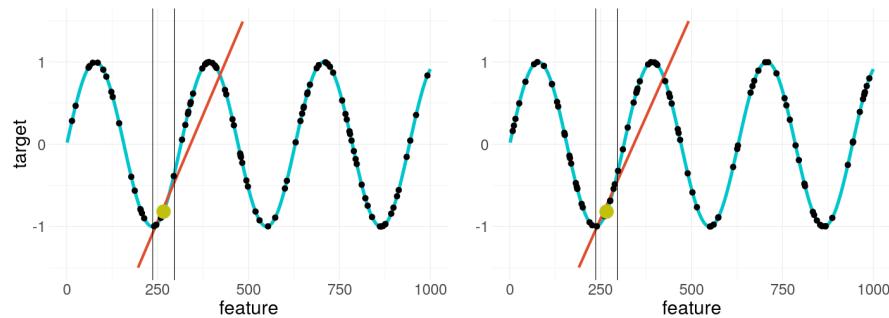


FIGURE 14.3: LIME applied twice on a non-convex function with increased sample size but different sample seed

Another possible step would be to increase the kernel width as seen in figure 14.4, making the explanations again more similar, but also greatly losing the locality of the explanation. Since chapter 13 already gave a thorough overview of this and because we assume we do not want to lose any locality, we focus on the default kernel width in the following and investigate the influence of further options on the weight stability of the LIME explanations.

14.3 Real World Problems with LIME

So far, only artificial problems have been shown for demonstration purposes, but how does LIME behave applied to real-world problems? We are using real datasets in the following to show weight stability associated with different circumstances.

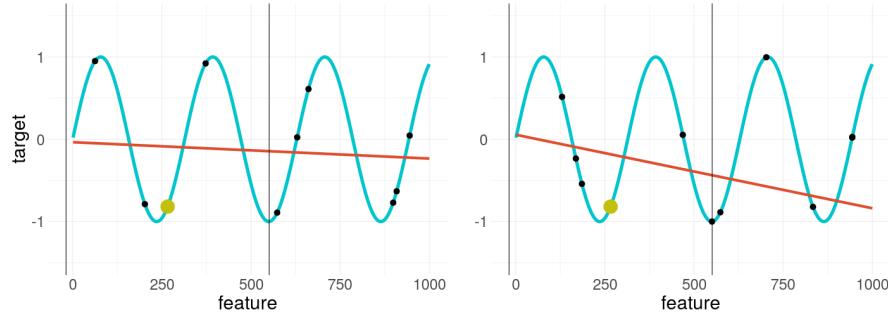


FIGURE 14.4: LIME applied on a non-convex function with increased kernel width and two different sample seeds in each plot

14.3.1 Boston Housing Data

Boston Housing dataset is a well-known data set, so a deeper description of its properties is skipped here. It is offering a good amount of numerical features ($p = 12$) and can be seen as a typical case of a numerical regression task. A quick overview of each of its features versus the target – the median housing price – is depicted in figure 14.5.

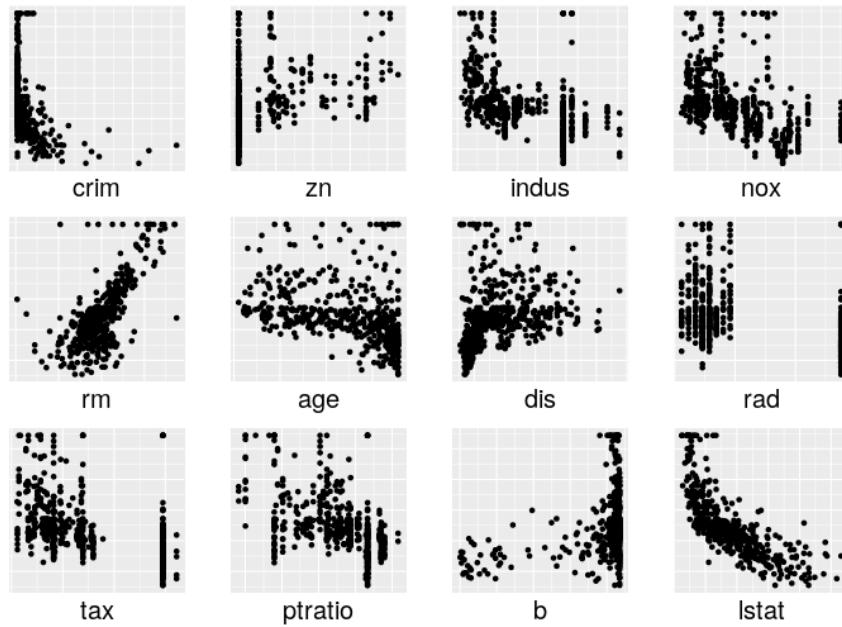


FIGURE 14.5: Overview of the normalized numerical features compared to the target 'medv' in the Boston Housing dataset

In the following, weight stability is explored by resampling an explanation 100 times for a specific setting. Of the 100 weights of each feature in the explanations, the mean and the empirical 2.5% and 97.5% quantiles are calculated and depicted in the figures. Based on the quantiles we then plot the empirical 95% confidence interval. As the black-box model, a random forest model with default parameters is used. The reasoning here is, that random forests are very common in practice and their default parameters usually perform well without tuning. For the sampling, we choose to use kernel density estimation. The reason is the results of later experiments, showing kernel density estimation as a benefactor for weight stability compared to the other methods. The target point to explain is the mean of the original dataset. In each of the following scenarios, only one of the above-described settings is changed. Not all possible scenarios are shown, but only a cherry-picked selection supposed to spark interest in the experiments further down.

14.3.1.1 Mean point versus outlying point

In the first showcase, the mean data point is compared with an extreme outlier (having the maximum appearing value of each feature). As we can see in figure 14.6, the outlier has larger confidence intervals as the mean point. This suggests that either the model is behaving roughly in its area, or, more likely, the sample size in the neighborhood has a significant influence on our stability, as our original features have higher density mass around the mean with the kernel density estimation copying that approximately.

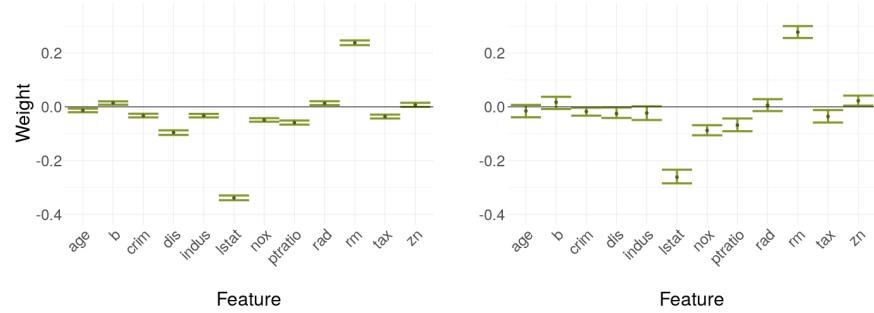


FIGURE 14.6: Weight coefficients of LIME applied to the mean data point in the left plot and an extreme outlier on the right plot – errorbars indicating the empirical 95% confidence interval across repeated runs

14.3.1.2 Decision tree versus linear regression model

This scenario compares two different black-box models. The left plot in figure 14.7 shows the weights explaining a decision tree, while the right one shows

the case for a linear regression model. It is kind of expected of the linear model to have very stable weights, but the differences to the decision tree are still striking, suggesting the black-box model could have a huge influence on weight stability.

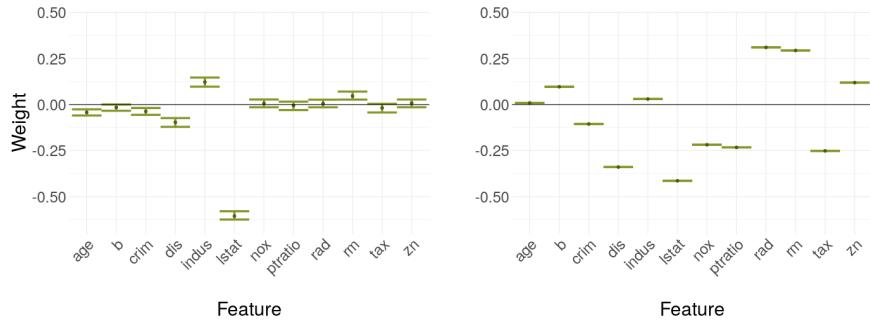


FIGURE 14.7: LIME weights of a decision tree as black-box model versus a linear regression model

14.3.1.3 Kernel density estimation versus binning

In this case, we compare two different sampling options. Binning is the default setting in the R LIME package (Pedersen (2019)). Due to sampling via normal distribution acting very similar to the kernel density estimation in the experiments further down, this option is left out here. The differences in figure 14.8 are clearly visible, leading to the question if there are strict ranks of the sampling options concerning weight stability.

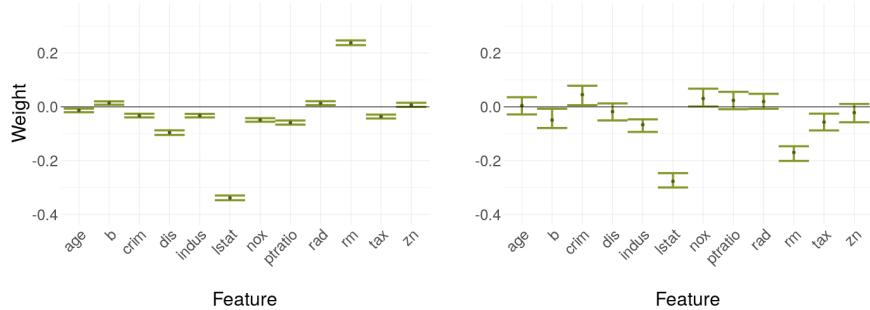


FIGURE 14.8: LIME weights of the mean data point with kernel density estimation as sampling strategy versus binning

14.3.2 Rental Bikes Data

So far, we only used numerical features. To also cover the categorical case, we are using the Rental Bikes dataset with only categorical features here. Originally, the data also contained a few numerical features, but these have been manually categorized by creating classes based on their 25%--, 50%--, and 75%-quantiles. In figure 14.9, boxplots of the classes in each feature with respect to the target ‘cnt’ – the count of bikes rented a day – is shown to give a quick overview. This means we are forced to use the Gower distance (Gower (1971)), a binary distance measure for the categorical case. The purpose of this short section is: Do we get similar results as for numerical features?

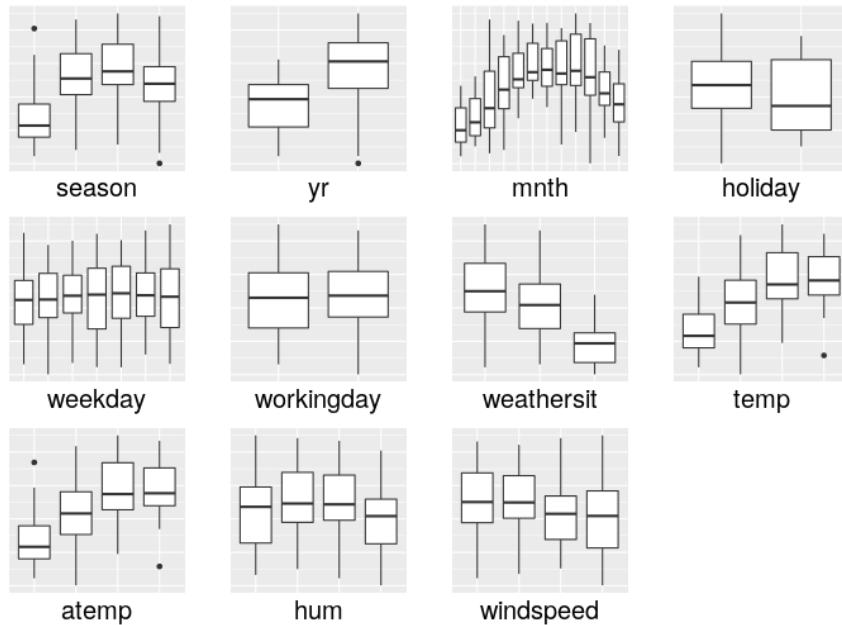


FIGURE 14.9: Overview of the categorical features compared to the target ‘cnt’ in the Rental Bikes dataset

We compare the same scenarios under the same settings as in the case of the Boston Housing data, except the sampling option, as we only have one (the class frequency of each feature). As we cannot calculate the mean and maximum of a categorical variable, we switch to the majority and minority point – the point having the most, and analogous the least frequent class in each feature respectively.

14.3.2.1 Majority data point versus minority data point

In figure 14.10, the majority data point is compared to the minority data point. The differences are a lot more subtle than in the Boston Housing case, almost not visible.

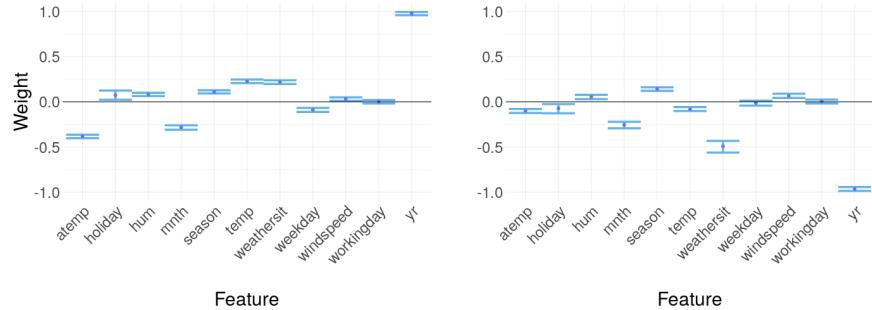


FIGURE 14.10: Weight coefficients of LIME applied to the majority data point versus the minority data point

14.3.2.2 Decision tree versus linear regression model

Again, we are comparing a decision tree with a linear regression model as the black-box model in figure 14.11. The differences are visible, but by far not as much as in the numerical case. This suggests we include this categorical data set in our experiments further down but expect the results will not be as clear cut as in the numerical case.

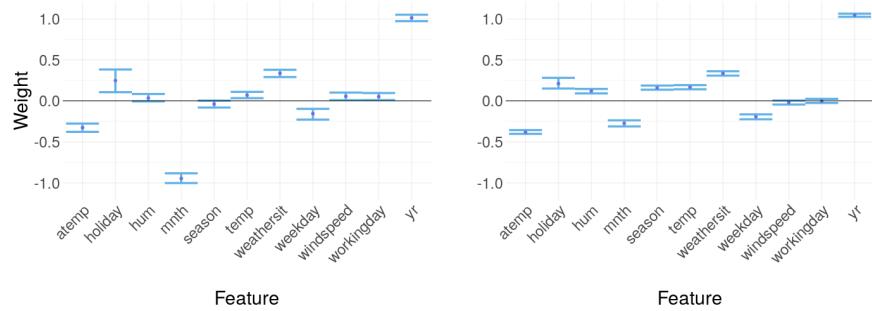


FIGURE 14.11: LIME weights of a decision tree as black-box model versus a linear regression model

14.4 Experiments regarding Sampling stability

All the different scenarios we have encountered so far show more or less discrepancy in weight stability between certain settings. We have observed:

- a target point in an area with higher sample denseness is more stable than an extreme outlier
- different black-box models have highly different stableness
- different sampling options and numerical features compared to categorical ones also show different behavior

Based on these findings, we construct several experiments to investigate each point and to see, if we receive results showing a clear, monotonous tendency for weight stability concerning available parameters.

14.4.1 Influence of feature dimension

The first and most obvious question regarding sampling, that was not showable for a fixed dataset, is if an increasing number of features also increases weight instability. The curse of dimensionality is a known problem in Machine Learning and to uncover its hidden influence on our case, we run the following experiment regarding feature dimension.

14.4.1.1 Feature dimension - setup

The experiment is designed as given by this algorithm:

- 1) Start with only two features of the original data as the training data.
- 2) Train a black-box model (random forest with default parameters).
- 3) Ten randomly sampled data points of the original data set are explained repeatedly ten times.
- 4) The standard deviation of the ten weights of each feature and each explained point is calculated, and then all the standard deviations are averaged to a single value.
- 5) If there are unused features left, add a new feature to the existing feature set and continue from step 2), else stop.

14.4.1.2 Feature dimension - results

This procedure is executed for all the sampling options possible for the Boston Housing and the Rental Bikes dataset. The results are shown in figure 14.12 and as can be seen, it is hard to spot a clear tendency. If the curse of dimensionality would apply for our case, we definitely would not expect improving stability by adding new features. Thus, a curse of dimensionality can not be identified in our case and a high feature amount should not necessarily concern the user. As a further thought, since LIME models the black-box and not the original data, dimensionality in the dataset has only an indirect impact as what matters is how the model fits interactions between features.

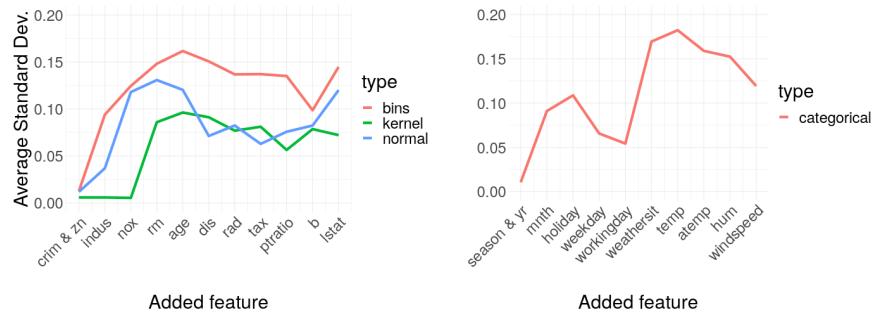


FIGURE 14.12: Average standard deviation of the resulting LIME weights regarding the feature dimension of the Boston Housing and Rental Bikes dataset. Each line shows a different sampling option.

14.4.1.3 Amount of features selected - setup

In the R LIME package (Pedersen (2019)), an option is available to only explain a fixed amount of features with the highest weight. This may sound interesting as a small side experiment to the general amount of features. Maybe this selection offers better stability in the results? For this, we use the full dataset instead of iterating over the number of features, but iterate over increasing parameter values of '*n_features*' in the explainer function.

14.4.1.4 Amount of features selected - results

As can be seen in figure 14.13, weight stability is remarkably constant for a low amount of features and suddenly becomes very jumpy for a higher amount of selected features. If the experiment was only evaluated for small amounts of selected features, a clear recommendation of sticking to less explained features could be given, but unfortunately, no real rule of thumb can be suggested in

this case. The inverted ‘U’ shape of the graph may result due to globally linear predictions for the least important features.

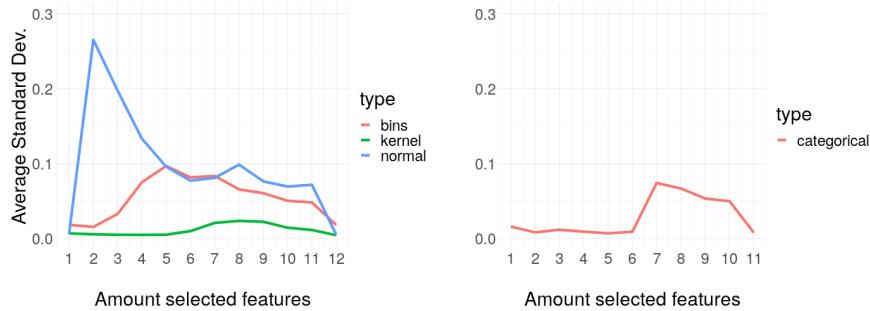


FIGURE 14.13: Average standard deviation with the same settings as before but with full feature size. The x-axis plots the number of features selected for the explainer.

14.4.2 Influence of sample size

The next experiment is about the influence of the sample size. The difference between an explained point in a high-density region compared to one sitting in a low-density area was easily recognizable in figure 14.6. The question is how this relates to an increased global sampling size, which we try to answer in the following. Here, the setup is basically the same as in the case for the experiment about the number of features selected, except we iterate over different sample sizes.

14.4.2.1 Sample size – results

Again, we run the modified algorithm of the experiment for all the possible sampling options at the Boston Housing and Rental Bike dataset. As a result, we receive the averaged standard deviation of all weights per sample size and sampling option. These are depicted in figure 14.14 and show a clear and monotonous trend of more samples having a huge positive impact on the stability. Additionally, binning seems to be consistently dominated by other sampling options.

We have seen before in figure 14.12 feature dimension being relatively unrelated to weight stability, while the sample size is the total opposite – does this make sense? After all if not the feature dimension, what else may cause a high sample requirement? As we have already seen in figure 14.7 the black-box model may be the phantom we are hunting. This motivates the last two experiments in this chapter.

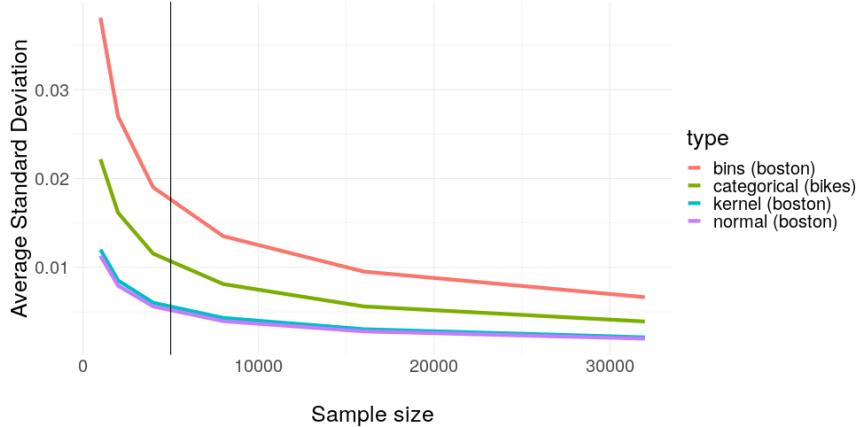


FIGURE 14.14: Average standard deviation with the same settings as before but increasing sample size. A clear trend can be seen here: Increasing the amount of samples (which is acting as train data for our surrogate model) has remarkable influence on weight stability.

14.4.3 Influence of black-box

The simulations already presented in figure 14.1 and figure 14.2 suggest more volatility and less smoothness of the prediction surface may influence weight stability. Demonstrating the problem through a slightly adjusted real case problem, we are using sampled Boston Housing data of sample size 20, and modeling only $medv \sim lstat$. Because LIME does not know the original data, the resulting black-box fit seems like an impossible task to approximate linearly in an appropriate manner with only small samples as seen in figure 14.15.

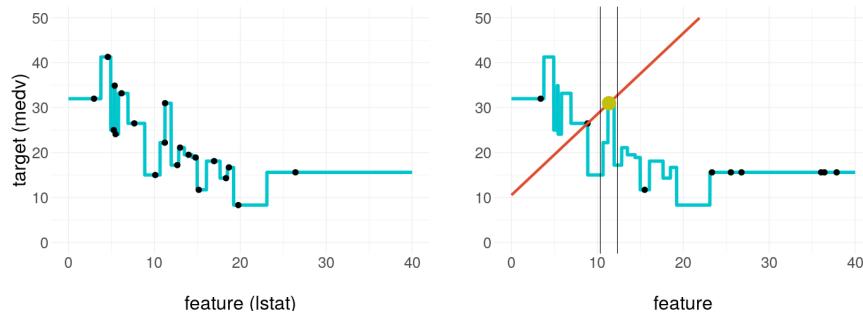


FIGURE 14.15: LIME trying to explain an extremely volatily prediction surface. The prediction surface is an extreme overfit of a small subset of the Boston Housing data.

14.4.3.1 Black-box – setup

To receive meaningful results, we need comparable models. For this, we choose to pick a random forest as the model class and iterate over the two parameters being the most responsible for a smooth fit. These are the tree amount and the minimum node size. A higher tree amount gives the prediction surface more smoothness (by reducing the average step size of each step in the prediction function), while a higher minimum node size reduces overfitting (by making predictions dependent on more train data points) and as consequence reducing the volatility of the prediction surface. Here is a slightly modified algorithm as the framework for our experiment:

- 1) Start with a tree amount of one and a minimum node size of one.
- 2) Train a random forest with these parameters on the full data.
- 3) Ten randomly sampled data points of the original data set are explained ten times repeatedly.
- 4) The standard deviation of the ten weights of each feature and each explained points is calculated, and then all the standard
- 5) If we have not reached ten iterations, increment the tree amount by ten and the minimum node size by one, and continue from step 2), else stop.

14.4.3.2 Black-box – results

The results in figure 14.16 are unambiguous: It is shown clearly how important the smoothness of the model is for weight stability. Keep in mind the model was fitted on two very specific datasets, which means if we would pick more complex data, the line could take much longer to flatten out, and vice versa for less complex data. As a small sidenote, binning is again consistently inferior.

We have just seen how important the smoothness is, but this would mean we can expect the inverted effect for more overfitting. After all, our data case could be misleading as there are more complicated tasks in the real world requiring a much more volatile fit. A certain level of smoothness is then often not given, so it would be nice to know of how much worse the stability can get in the case of extreme overfitting. This leads us to the last experiment.

14.4.3.3 Black-box overfit – setup

Before, we started with a very unsMOOTH model and gradually added more regularisation (more trees and higher minimum node size). But now, we are doing the opposite with a model class being able to fit an arbitrarily complex

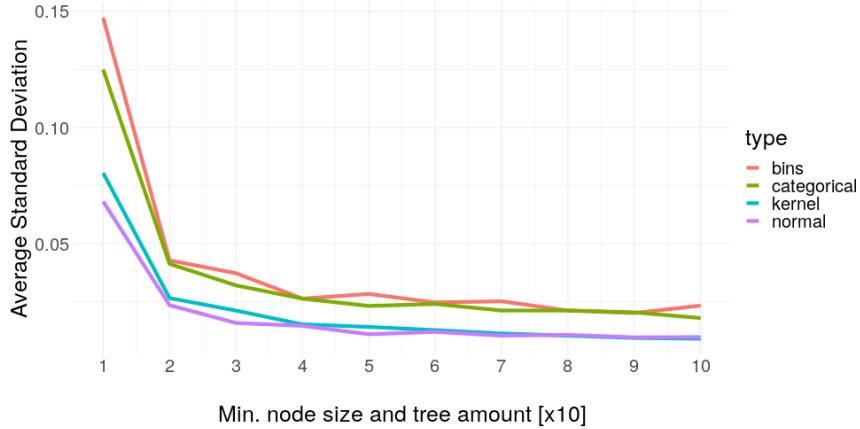


FIGURE 14.16: Average standard deviation of the same settings as before versus the black-box model smoothness. As the black-box model class, a random forest was used with increasing parameters per iteration. The last tick in this graph is corresponding to a random forest with 91 trees and a minimum node size of 10.

data structure by increasing only a single hyperparameter: Extreme Gradient Boosting ([Chen and Guestrin \(2016\)](#)). For this, we start with only two trees and double the amount with each iteration. All the other settings and the algorithm for receiving the results are kept the same. Additionally, we are also interested in the training error as it is a good indicator of when our boosting algorithm stops overfitting more (due to its nature of fitting residuals the test error cannot get worse after the training data is fitted perfectly).

14.4.3.4 Black-box overfit – results

As we can see in figure 14.17, as long as the XGBoost learner is able to reduce the training error, the weight stability gets consistently worse, but not any longer. Let's try to dissect why this is happening in such a dependent fashion: What makes the training error get smaller? Reducing the residuals. What consequence has reducing the residuals on the prediction surface assuming a certain level of Gaussian noise? It becomes more volatile. And this volatility kills our weight stability.

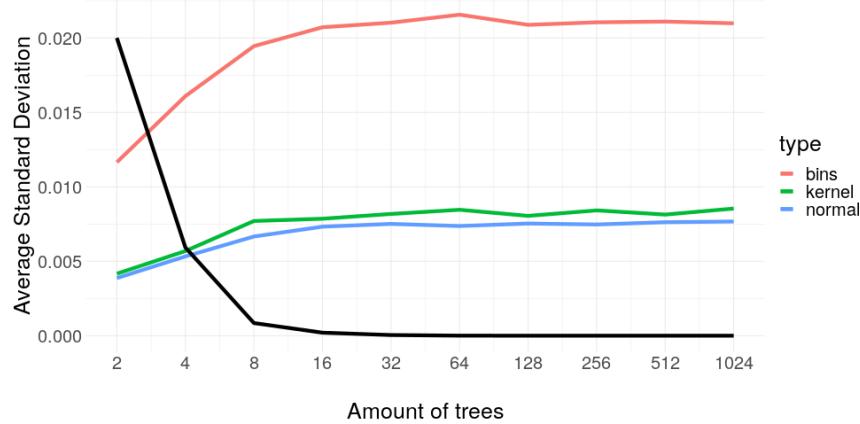


FIGURE 14.17: Average standard deviation with the same settings as before versus the tree amount of the XGBoost model used as black-box predictor. The black line indicates the train error rescaled linearly to fit between the plot boundaries.

14.5 Outlook

So far all the sampling methods have been about drawing out of a distribution representing the whole space of each feature. This global sampling disregards the covariance structure and results in a lot of samples drawn in areas so far away in distance from the point to explain, that their weight for the fitting process is essentially zero. (Just to not spark any confusion: ‘Weight’ in this subchapter refers to the weights in the loss function and not the weights of the explanation, as we have used so far.) These samples are a huge computational burden while having almost no influence at all on the fit. A solution to this problem is not implemented in the R and Python LIME packages ([Pedersen \(2019\)](#) and [Ribeiro \(2019\)](#)) but [Laugel et al. \(2018\)](#) gives a thorough overview of how local sampling tackles exactly that for the classification case. In short, the weighting based on a distance measure can be removed while we only sample in the area around the point to explain. Thus, points having a higher distance are sampled less likely or not at all, making the weights redundant and hugely increasing sampling efficiency. Because we only focused on regression tasks in our work so far, the figure 14.18 will also only show this case – for more details about classification please have a look into [Laugel et al. \(2018\)](#).

In practice the increase in sampling efficiency would not improve our computational burden since the sample size was a strictly monotonous benefactor for explanation stability and thus should not be reduced. But in the end, under

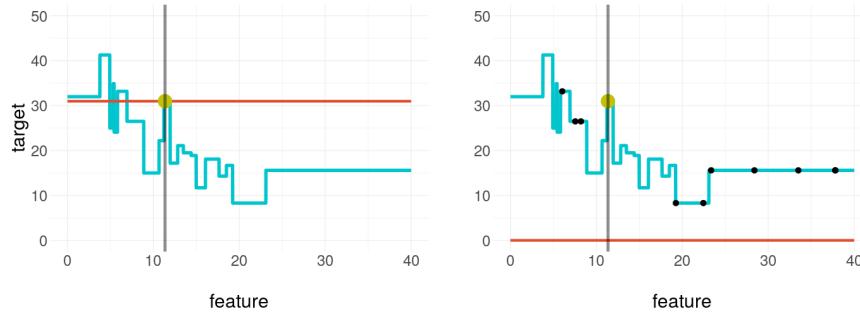


FIGURE 14.18: By sampling locally around our target point we can catch the plateau the point sits on as seen on the left plot. Indeed, the samples are too close to the explained point to be visible. As a local sampling strategy, a normal distribution was used with variance equal to the kernel width of the distance measure in the usual procedure. Achieving the same with global sampling in the right plot is a game of luck since the plateau is very narrow and hard to hit. In this case, our explanation even fails drastically as all the samples receive zero weight due to the small kernel width.

the same settings, we simply draw more in the area of relevance, drastically increasing the sample size in the neighborhood of our explained point, making our results more stable and trustworthy. Due to the absence of implementation in the R LIME package ([Pedersen \(2019\)](#)), this new ambitious procedure could not be part of the experiments to reinforce the assertions just made, but further research is strongly recommended.

14.6 Conclusion

In all cases of categorical and numerical data we investigated, weight stability issues can be found easily. But LIME explanations for numerical data can be stabilized a lot by simply changing the default option of binning as the sampling strategy to kernel density estimation. The advantage of binning lies in a purely pragmatic way: By using bins, numerical features are handled as categoricals and the effects of classes occupied are a lot easier to explain to the layman than the slope of a regression line. In a more general way, we would ask ourselves in the end, what makes us have trust in a single explanation? Weight stability is almost independent of the weight size, so high weights are very trustworthy. Additionally, picking a very high sample size increases stability in our experiments. This should be done whenever possible as the only disadvantage is a longer runtime. Furthermore, what makes us have less

trust in the LIME result? When we know the data set is very complex with a curvy/wavy fit almost surely going to happen, then we should be very careful. The same is suggested by our empirical findings if the model we are using is capable of extreme overfitting. In this case, the less regularisation we put onto it, the less stable our LIME explanations are going to be. If we are unsure about the trustworthiness of our explanation, it is always beneficial to rerun the same explanation a few times and average the results – this has a similar effect than a higher sample size, but this way we can actually use already computed results and we can also calculate a confidence interval, giving good indication of how much variance the results have.



15

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The most important contributions are from the students themselves. The success of such projects highly depends on the students. And this book is a success, so thanks a lot to all the authors! The other important role is the supervisor. Thanks to all the supervisors who participated! Special thanks to Bernd Bischl¹ who enabled us to conduct the seminar in such an experimental way, supported us and gave valuable feedback for the seminar structure. Thanks a lot as well to the entire Department of Statistics² and the LMU Munich³ for the infrastructure.

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¹<https://www.compstat.statistik.uni-muenchen.de/people/bischl/>

²<https://www.statistik.uni-muenchen.de/>

³<http://www.en.uni-muenchen.de/index.html>



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