

Predictive Models: Visualisation, Exploration and Explanation

With examples in R and Python

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Contents

Chapter 1

Introduction

Predictive models are used to automatically guess (statisticians would say: estimate) one interesting variable based on other variables. Think about prediction of sales based on historical data, prediction of risk of heart disease based on patient characteristics, prediction of political attitudes based on facebook comments.

Predictive models were constructed through the whole human history. Think about Flooding of the Nile for example. More rigorous approach to model construction may be attributed to the method of least squares, published by Legendre in 1805, and by Gauss in 1809, more than two centuries ago. Number of applications in economy, medicine, biology, agriculture was growing. The term *regression* was coined by Francis Galton in 1886, initially was referring to biological applications, today is used for various models that predict continues variable. Prediction of nominal variables is called *classification*, and its beginning may be attributed to works of Ronald Fisher in 1936.

During the last century we observed lot of developments in predictive models like linear models, generalized models, regression and classification trees, rule based models and many others. Developments in mathematical foundations of predictive models were boosted by increasing computational power of personal computers and availability of large datasets. So called the era of big data.

Increasing demand on predictive models favour models that are elastic, able to perform internally some feature engineering and leads to high precision of predictions. Robust models are now created with ensembles of models. Techniques like bagging, boosting or model stacking gather hundreds or thousands of small model into a one super model. Large deep neural models have over bilion of parameters.

There is a cost of this progress. Large models are opaque, obscure, they act like black boxes. On one hand, human is unable to understand how thousands of coefficients affect the model response, one the another hand the model itself may be treated as a trade secret. And the worst part of this is that these models are not as good as we wish them to be.

Deceived by model performance, big names of model producer we tend to believe that these black boxes are unerring oracles. The truth is that they are not. And we have more and more examples that model performance deteriorate with time or is biased in some sense.

An overview of real problems with large black box models may be found in an excellent book of Cathy O'Neil (?) on in her TED Talk „*The era of blind faith in big data must end*“. Various examples show how models that are opaque and unregulated lead to higher discrimination of inequality. And there are more examples of such problems, see „*Google and the flu: how big data will help us make gigantic mistakes*“, „*Report: IBM Watson delivered 'unsafe and inaccurate' cancer recommendations*“.

Today the true bottleneck for predictive modelling is not the lack of data, nor lack of computational power, nor lack of elastic models. It's lack of tools for model validation, explorations and explanations of model decisions.

In this book we present collection of methods that may be used for this purpose. It is a very active area of research and for sure more methods will be developed in this area. However here we present the mind-set, key problems and methods that are used in model exploration.

This book is about

- We show how to determine features that affect model response for a selected observation. In this book you will find theory and examples that explains prediction level methods like break down plots, ceteris paribus profiles, Local model approximations or Shapley values.
- We present techniques to examine fully trained Machine Learning models as a whole. In this book you will find theory and examples that explains model globally like Partial Dependency Plots, Variable Importance Plots and others.
- We present charts that are used to present key information in a quick way.
- We present tools and methods for model comparison.
- We present example code snippets for R and python that show how to use described methods.

This book is NOT about.

- We do not focus on any specific model. Presented techniques are model agnostic and do not have any assumptions related to model structure.
- We do not focus on the data exploration. There are very good books and techniques related to this, like R for Data Science <http://r4ds.had.co.nz/> or TODO
- We do not focus on the process of model building. There are also very good books about this, see An Introduction to Statistical Learning by Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani <http://www-bcf.usc.edu/~gareth/ISL/> or TODO
- We do not focus on particular tools for model building, see Applied Predictive Modeling By Max Kuhn and Kjell Johnson <http://appliedpredictivemodeling.com/>

This book has following structure

- In the Section 1 we introduce notation and vocabulary that will be used in this book. Same concepts have often different names in statistics and different in machine learning, thus show how to translate between these two worlds. In this section we also set expectations.
- In the part *Prediction level explainers* we present techniques for exploration and explanations single model predictions.
- In the part *Model level explainers* we present techniques for exploration and explanations model as a whole.

Every method for model exploration is described in a separate section. In each such section you will find.

- Subsection *Introduction*, that explains the goal of the method and the general idea behind this method.
- Subsection *The Algorithms*, that shows mathematical or computational details related to this methods. You can skip this section if you are not interested in details.
- Subsection *Example*, that show an example application of this method with discussion of results.
- Subsection *Pros and Cons*, that summarize pros and cons of this method and also give some guides when to use this method.
- Subsection *Code snippets*, that show how to use this method in R and python. You can skip this section if you are not interested in implementation.

1.1 White-box models vs Black-box models

In this book we focus on black box models, i.e. models with complex structure, high number of coefficients that are hard to trace and understand by humans.

The opposite are white box models, that have structure easy to understand even for non specialist. Two most common classes of white box models are decision or regression trees (see an example in Figure ??) or models with additive structure, like this model for relative risk.

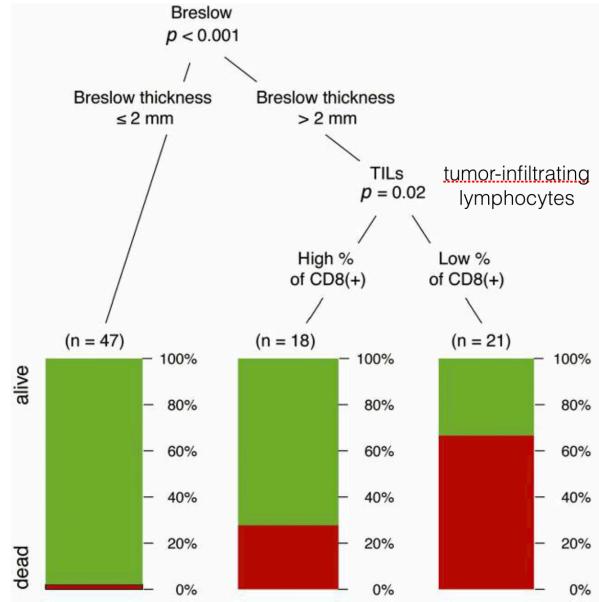


Figure 1.1: (fig:BILLCD8) Example tree model for melanoma risk

$$\text{RelativeRisk} = 1 + 3.6 * [\text{Breslow} > 2] - 2 * [\text{TILs} > 0]$$

For white box models it is easy to understand how they are working from the model structure. It may be complicated to build the model, collect necessary data, do model validation, but once the model is derived the understanding is easy.

Understanding of the model structure gives us few benefits

- For any model prediction we can easily link model prediction with variables
- We see which variables are used in the model and which are not, thus we may question the model, which variable X is not included.
- We may challenge the model against the domain knowledge. As we see how each variable influence the model prediction we may verify if it's along domain knowledge.

Note, that being a white box model is not only about the structure, but also about the number of parameters. A classification tree with 100s of nodes is hard to understand, linear model with 100s of parameters is hard to understand.

Things that are natural for white box models are hard for black box models. For complex models we may not understand how and which features influence the model decision, is the model consistent with the domain knowledge. Tools presented in this book help to extract such information even from complex models.

1.2 Model agnostic vs Model specific

Some classes of models attract higher interest than others or are developed for longer period of time. Thus some classes of models are quipped with very good tools for model exploration or visualisation. Just to mention some of them:

- Linear models have lots of tools for model diagnostic and validation of model assumptions. Assumptions are defined in a strict way (normality, linear structure, homogenous variance) and can be validated

with normality tests or plots (qq plot), diagnostic plots, tests for model structure (RESET test), tools for identification of outliers etc.

- More complex models with additive structure, like proportional hazards models have tools that verifies model assumptions.
- Random Forest model is equipped with out of bag method of evaluation of performance and few tools for measuring variable importance (?). Some tools were developed to extract information about possible interactions from the model structure (?). Similar tools are developed to other ensembles of trees, like xgboost models (?).
- Neural Networks have large collection of dedicated explainers that use Layer-wise Relevance Propagation technique (?) or Saliency Maps technique (?) or a mixed approach.

List of model classes is much longer, and for every class there is a collection of tools to use. But this variety of approaches leads to problems. (1) One cannot easily compare explanations for two models with different structures. (2) Every time when a new architecture of new ensemble of models is proposed, we need to look for new methods of model exploration. (3) For some new models we may not have yet any tool for model explanation.

This book is focused on model agnostic techniques. Thus we do not assume anything about model structure. The model will be treated as a black box and the only operation that we will be able to perform is evaluation of a model in a selected point.

However, even if we do not assume anything about the model, we have some assumptions about data. We assume that the model is a function of a form

$$f : R^p \rightarrow R$$

i.e. operates on a vector of p values. This assumption is most suited with tabular data, is held for images, text data video and so on. It may not be suited to models with states, or models with memory as there the model output depends not only on model inputs.

Note also that if p is high dimensional then techniques described here may not be enough to fully understand models with such large number of degrees of freedom.

1.3 Why do we need model explainers?

Machine Learning models have a wide range of applications in classification or regression problems. Due to the increasing computational power of computers and complexity of data sources, ML models are becoming more and more sophisticated. Models created with the use of techniques such as boosting or bagging of neural networks are parametrized by thousands of coefficients. They are obscure; it is hard to trace the link between input variables and model outcomes - in fact they are treated as black boxes. They are used because of their elasticity and high performance, but their deficiency in interpretability is one of their weakest sides.

In many applications we need to know, understand or prove how the input variables are used in the model. We need to know the impact of particular variables on the final model predictions. Thus we need tools that extract useful information from thousands of model parameters.

Tools for model exploration and model understanding have many applications. They may be useful during every phase of a model lifecycle.

Below we summaries how such tools will be useful during the model development, model deployment or model maintenance.

Model development

Model building or model development is a phase in which one is looking for best available model.

In the Section ?? we present tools for extraction of relations between features and target variable. Such methods may be used for feature engineering (assisted learning in which elastic black box model is used to learn features for the white box model). Learning from ML models may lead to model improvement.

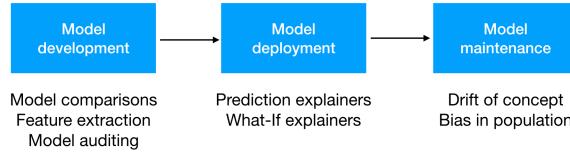


Figure 1.2: (fig:modelLifetime) Example applications of explainers in different phases of model lifetime

In the Section ?? we present tools that helps to compare models.

In the Section ?? we present tools that help to validate model, audit model residuals, identify potential strange behaviors.

If for some observations we observe lack of fit, then through tools introduced in the Section ?? we may verify which variables do and which do not influence model decisions. This may help to identify some problem in the model fit and in the end will help to correct the model.

Since the AutoML methods are being more and more popular, model explainers may actually help to understand how the model identified by AutoML method is working.

If we identify cases on which model is not working properly, then model explainers will help in model debugging. See an examples in the Section TODO.

Model deployment

Model deployment is a phase in which one wants final use trust in model decisions, understand these decisions and act accordingly. In some areas complex models are not being adopted because people do not understand nor trust them. Model explainers can change this and increase rate of aquisition of new models

Since most people would not trust in recommendations, that they do not understand, the key element here is to increase understanding related to features that affect model decisions.

In the Section ?? we introduce tools that identify key features that drive model decisions.

In the Section ?? we introduce tools for what-if analysis of model decisions.

In some areas there may be legal expectations or regulations that requires that model predictions are explainable (see the right to explanation). See (?) or (?) for example methods that identify bias in the data.

Model maintenance

Model maintenance is a phase in which one wants to make sure that model is still valid and suited to the new data. Due to concept drift or similar problems that may happen after some time, we need to monitor the model performance.

In the section ?? we present tools that may compare how thw model response behaves on the new dataset. This helps to detect flaws in model assumptions and biases in the data.

1.4 How model exploration is different from data exploration?

Exploration and visualization of models is not that known as exploration and visualization of data. As we will see in following chapters in both cases we may use similar charts and similar way to express ideas. This is because many people are already familiar with techniques for data visualization and when we do model visualization we want to take advantage of this knowledge.

Both in data visualization and in model visualization we use graphical representation to deliver some messages quicker in a form that is easier to digest. Despite all similarites we need to keep in mind few key differences between these two wrds.

- Data is generated by some unknown phenomena and with data exploration and visualization we want to understand this phenomena. Models are created based on the data but in most cases we do not know how close are these models to unknown phenomena. So we do model exploration to validate if the model is correct. If the model is valid. In most cases we do not validate data if they are correct. So we are more skeptical about models than about data.
- Data comes from some population; we treat data as a random sample, and there is some inherited randomness related to the sampling. On the opposite, models are just functions. Most models are not stochastic (or at least some models are not stochastic) and the randomness (if any) come from the fitting procedure not from the sampling.
- Models may be inaccurate or biased. When we ask question like „How the model is working?” we also ask „Is the model accurate, can I trust it, does it behave well, how much I can trust it?”. Similar question related to data do not question the data but question our understanding of the data.

To summaries. We may use similar techniques. But they are used to answer different questions.

1.5 Glossary / Notation

Let $f_M(x) : \mathcal{R}^d \rightarrow \mathcal{R}$ denote a predictive model, i.e. function that takes d dimensional vector and calculate numerical score. Dimensions of the vector x refer to different variables (aka features).

In section in which we work with larger number of models we use subscript M to index models. But to simplify notation, this subscript is omitted if profiles for only one model are considered.

Symbol $x \in \mathcal{R}^d$ refers to a point in the feature space. We use subscript x_i to refer to a different data points and superscript x^j to refer to specific dimensions. Additionally, let x^{-j} denote all coordinates except j -th and let $x|_j = z$ denote a data point x^* with all coordinates equal to x except coordinate j equal to value z . I.e. $\forall_{i \neq j} x^i = x^{*,i}$ and $x^j = z$. In other words $x|_j = z$ denote a x with j th coordinate changed to z .

- *Black-box model* is a model with structure that is hard to understand for humans. Usually it refers to the number of model parameters. As different humans may be better in understanding more or less complex models, there is no strict threshold that makes model a black-box. But in practice for most humans this threshold is closed to 10 rather than 100.
- *White-box model*, opposite to Black-box model, is a model that is easy to understand to human. Maybe not for every human. Consider small linear models and small CART trees as white box models.
- *Feature* or *Variable*, part of the model input space. Without large loss of generality we can assume that one feature is a single dimension in the input space. There are exceptions (among them: polynomials, interactions between variables, nominal variables), but they do not change the intuition.
- *Continuous variable*, a variable that can be presented as a number and the ordering makes some sense (zip codes or phone numbers are not considered as continuous variables). It does not need to be continuous in a mathematical sense. Counting variables (number of floors, steps) counts here as well.
- *Nominal variable*, opposite to *Continuous variables*, finite set of values that will not be threaded as a numeric

1.6 Acknowledgements

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Prediction level explanations

Chapter 2

Introduction

Prediction level explainers help to understand how the model works for a single prediction. This is the main difference from the model level explainers that were focused on the model in general. Prediction level explainers are always in context of a single observation.

Think about following use-cases

- One wants to attribute effects of variables to a model predictions. Think about model for heart attack. Having a final score for a patient one wants to understand how much of this score come from smoking or age or gender.
- One wants to understand how the model response would change if some inputs are changed. Think about model for heart attack. How the model response would change if a patient cuts the number of smoked cigarettes by half.
- Model is not working correctly for a particular point and one wants to understand why predictions for this point are wrong.

2.1 Variable attribution vs What-if analysis

TODO: variable attribution is not sparse, no reason for them to be like that

TODO: Three approaches: variable attribution, local model,

TODO: condvis (?)

Enslaving the Algorithm: From a ‘Right to an Explanation’ to a ‘Right to Better Decisions’? (?)

TODO: Sparse model approximation / variable selection / feature ranking

There are many different tools that may be used to explore model around a single data point and in following sections we will describe the most popular approaches. They can be divided into two classes.

- Analysis of the model curvature. Here we treat the model as a function and we are interested in the curvature of this function around the point of interest (see Figure ??). In the Section ?? we present the LIME method that approximates the black-box model in a point of interest while in section ?? we present Ceteris Paribus profiles that are more focused on conditional changes of model response given only one coordinate is modified.
- Analysis of the probabilistic behavior of the model. Here we are interested in decomposition of the model response to parts that can be attributed to particular features.

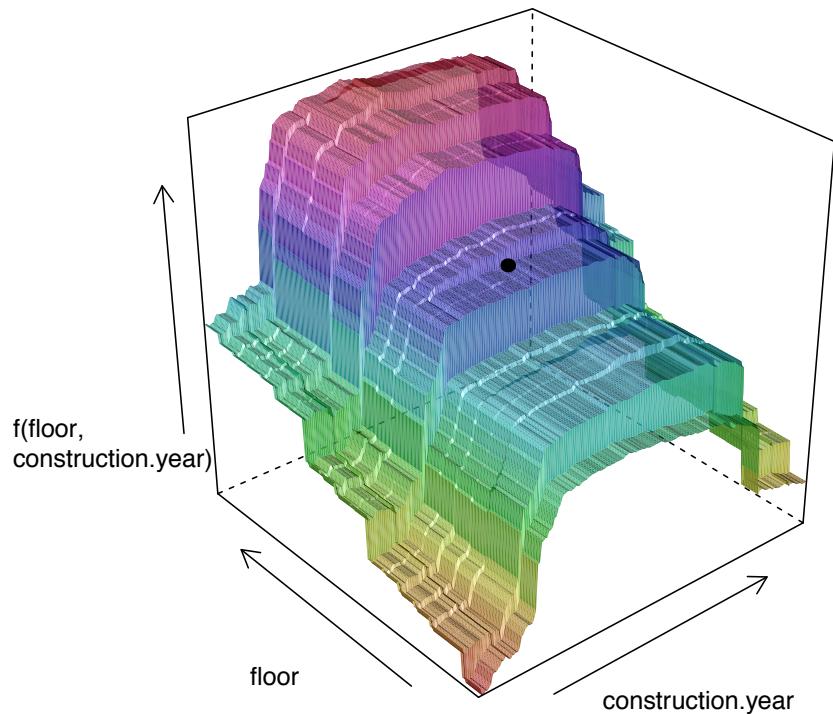


Figure 2.1: (fig:modelResponseCurve) Model response surface. We are interested in understanding the model behavior in a single point

2.2 When to use?

There are several use-cases for such explainers. Think about following.

- Model improvement. If model works particular bad for a selected observation (the residual is very high) then investigation of model responses for miss fitted points may give some hints how to improve the model. For individual predictions it is easier to notice that selected variable should have different effect.
- Additional domain specific validation. Understanding which factors are important for model predictions helps to be critical about model response. If model contributions are against domain knowledge then we may be more skeptical and willing to try another model. On the other hand, if the model response is aligned with domain knowledge we may trust more in these responses. Such trust is important in decisions that may lead to serious consequences like predictive models in medicine.
- Model selection. Having multiple candidate models one may select the final response based on model explanations. Even if one model is better in terms of global model performance it may happen that locally other model is better fitted. This moves us towards model consultations that identify different options and allow human to select one of them.

2.3 A bit of philosophy: Three Laws for Prediction Level Explanations

76 years ago Isaac Asimov devised Three Laws of Robotics: 1) a robot may not injure a human being, 2) a robot must obey the orders given it by human beings and 3) A robot must protect its own existence. These laws impact discussion around Ethics of AI. Today's robots, like cleaning robots, robotic pets or autonomous cars are far from being conscious enough to be under Asimov's ethics.

Today we are surrounded by complex predictive algorithms used for decision making. Machine learning models are used in health care, politics, education, judiciary and many other areas. Black box predictive models have far larger influence on our lives than physical robots. Yet, applications of such models are left unregulated despite many examples of their potential harmfulness. See *Weapons of Math Destruction* by Cathy O'Neil for an excellent overview of potential problems.

It's clear that we need to control algorithms that may affect us. Such control is in our civic rights. Here we propose three requirements that any predictive model should fulfill.

- **Prediction's justifications.** For every prediction of a model one should be able to understand which variables affect the prediction and how strongly. Variable attribution to final prediction.
- **Prediction's speculations.** For every prediction of a model one should be able to understand how the model prediction would change if input variables were changed. Hypothesizing about what-if scenarios.
- **Prediction's validations** For every prediction of a model one should be able to verify how strong are evidences that confirm this particular prediction.

There are two ways to comply with these requirements. One is to use only models that fulfill these conditions by design. White-box models like linear regression or decision trees. In many cases the price for transparency is lower performance. The other way is to use approximated explainers – techniques that find only approximated answers, but work for any black box model. Here we present such techniques.

Chapter 3

Introduction to variable attribution methods

In this section we introduce method for additive decomposition of predictions. The main goal for these tools is to help understand how model output may be attributed to input variables or sets of variables.

Presented explainers are linked with the first law introduced in Section ??, i.e. law for prediction's justifications. Note that there are more tools for variable attribution, some of them will be presented in next sections.

Think of following use cases:

- Think about a model for heart attack. A patient wants to know which factors have highest impact on the final heart risk score.
- Think about a model for apartment prices. An investor wants to know how much of the final price may be attributed to the location of an apartment.
- Think about a model for credit scoring. A customer wants to know if factors like gender, age or number of kids influence model decisions.

In the section ?? we will introduce key concepts and intuitions beyond variable attribution based on linear models. This approach may be easily applied to additive models and generalized linear models. In sections ?? and ?? we will present model agnostic extenstions of this concept.

3.1 Variable attribution for linear models

Linear model with coefficients $\beta = (\beta_0, \beta_1, \dots, \beta_p)$ has following form.

$$f(x) = \beta_0 + x_1\beta_1 + \dots + x_p\beta_p.$$

In other words, model response is the sum of weighted elements of $x = (x_1, x_2, \dots, x_p)$.

From a global perspective of a model, we are usually interested in questions like, how good is the model, which variables are significant or how accurate are model predictions.

But in this chapter we are focuses in a local perspective, i.e. for a single observation x^* how to measure the contribution of a variable x_i on model prediction $f(x^*)$.

Let $v(f, x^*, i)$ stands for the contribution of variable x_i on prediction of model $f()$ in point x^* . For linear models it is easy to define such contribution as

$$v(f, x^*, i) = f(x^*) - E[f(x)|x_{-1} = x_{-1}^*] = \beta_i x_i^* - E\beta_i X_i$$

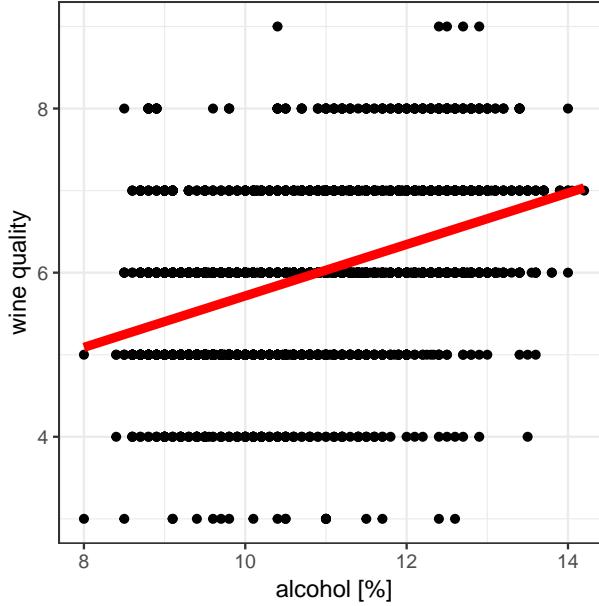


Figure 3.1: (fig:attribution1) Relation between wine quality and concentration of alcohol assessed with linear model

where the expected value can be estimated from the data

$$v(f, x^*, i) = \beta_i x_i^* - \beta_i \bar{x}_i = \beta_i (x_i^* - \bar{x}_i)$$

The logic behind the attribution is the following. Contribution of variable x_i is the difference between model response for value x_i^* minus the average model response.

3.1.1 Wine quality example

It may be a surprise, that the attribution for variable x_i is not the $\beta_i x_i$. But, please consider following example. Figure ?? shows the relation between alcohol and wine quality, based on the wine dataset (?). The corresponding linear model is

$$\text{quality}(\text{alcohol}) = 2.5820 + 0.3135 * \text{alcohol}$$

The weakest wine in this dataset has 8% of alcohol, average alcohol concentration is 10.51, so the contribution of alcohol to the model prediction is $0.3135 * (8 - 10.51) = -0.786885$. It means that low value of alcohol for this wine (8%) lower the prediction of quality by -0.786885 .

Note, that it would be confusing to forget about normalisation and say, that for the alcohol contribution on quality is $0.3135 * 8 = 2.508$ as this is high positive value.

Note that the linear model ma be rewritten in a following way

$$f(x) = \text{baseline} + (x_1 - \bar{x}_1)\beta_1 + \dots + (x_p - \bar{x}_p)\beta_p$$

where

$$\text{baseline} = \mu + \bar{x}_1\beta_1 + \dots + \bar{x}_p\beta_p.$$

Here *baseline* is an average model response and variable contributions show how prediction for particular x^* is different from the average response.

** NOTE for careful readers **

There is a gap between expected value of X_i and average calculated on some dataset \bar{x}_i . The latter depends on the data used for calculation of averages. For the sake of simplicity we do not emphasise these differences. To live with this just assume that we have access to a very large validation data that allows us to calculate \bar{x}_i very accurately.

3.2 Model agnostic approaches

In the Section ?? we introduced a method for calculation of variable attributions for linear models. This method is accurate, based directly on the structure of the model. But for most popular machine learning models we cannot assume that they are linear nor even additive.

In next sections we introduce a model agnostic approach. Note that even if the model itself is not additive, the model attribution will be additive.

Again, let $v(f, x^*, i)$ stands for the contribution of variable x_i on prediction of model $f()$ in point x^* .

We expect that such contribution will sum up to the model prediction in a given point (property called *local accuracy*), so

$$f(x^*) = \text{baseline} + \sum_{i=1}^p v(f, x^*, i)$$

where *baseline* stands for average model response.

Note that the equation above may be rewritten as

$$E[f(X)|X_1 = x_1^*, \dots, X_p = x_p^*] = E[f(X)] + \sum_{i=1}^p v(f, x^*, i)$$

what leads to quite natural proposition for $v(f, x_i^*, i)$, such as

$$v(f, x_i^*, i) = E[f(X)|X_1 = x_1^*, \dots, X_i = x_i^*] - E[f(X)|X_1 = x_1^*, \dots, X_{i-1} = x_{i-1}^*]$$

In other words the contribution of variable i is the difference between expected model response conditioned on first i variables minus the model response conditioned on first $i-1$ variables.

Such proposition fulfills the *local accuracy* condition, but unfortunately variable contributions depends on the ordering of variables.

See for example Figure ???. In the first ordering the contribution of variable `age` is calculated as 0.01, while in the second the contribution is calculated as 0.13. Such differences are related to the lack of additivity of the model $f()$. Propositions presented in next two sections present different solutions for this problem.

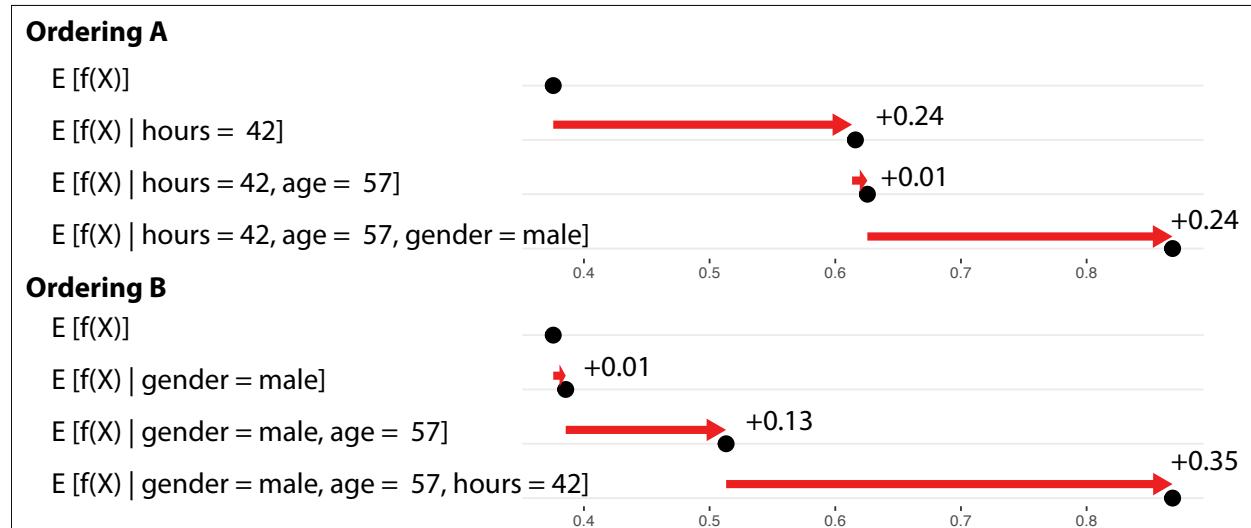


Figure 3.2: (fig:ordering) Two different paths between average model prediction and the model prediction for a selected observation. Black dots stand for conditional average, red arrows stands for changes between conditional averages.

Chapter 4

Break Down Attributions

The approach for variable attribution presented in the Section ?? has the property of *local accuracy*, but variable contributions depends on the variable ordering.

The Break Down method solves this problem by using two-step procedure. In the first step variables are ordered and in the second step the consecutive conditioning is applied to ordered variables.

4.1 The Algorithm

First step of this algorithm is to determine the order of variables for conditioning. It seems to be reasonable to include first variables that are likely to be most important, leaving the noise variables at the end. This leads to order based on following scores

$$score(f, x^*, i) = |E[f(X)] - E[f(X)|X_i = x_i^*]|$$

Note, that the absolute value is needed as variable contributions can be both positive and negative.

Once the ordering is determined in the second step variable contributions are calculated as

$$v(f, x_i^*, i) = E[f(X)|X_{I \cup \{i\}} = x_{I \cup \{i\}}^*] - E[f(X)|X_I = x_I^*]$$

where I is the set of variables that have scores smaller than score for variable i .

$$I = \{j : score(f, x^*, j) < score(f, x^*, i)\}$$

The time complexity of the first step is $O(p)$ where p is the number of variables and the time complexity of the second step is also $O(p)$.

4.2 HR dataset: Hire or Fire?

Let us consider a random forest model created for HR data. The average model response is $\bar{f}(x) = 0.385586$. For a selected observation x^* the table below presents scores for particular variables.

	Ei f(X)	scorei
hours	0.616200	0.230614
salary	0.225528	0.160058

	Ei f(X)	scorei
evaluation	0.430994	0.045408
age	0.364258	0.021328
gender	0.391060	0.005474

Once we determine the order we can calculate sequential contributions

variable	cumulative	contribution
(Intercept)	0.385586	0.385586
hours = 42	0.616200	0.230614
salary = 2	0.400206	-0.215994
evaluation = 2	0.405776	0.005570
age = 58	0.497314	0.091538
gender = male	0.778000	0.280686
final_prognosis	0.778000	0.778000

4.3 Break Down Plots

Once we calculated variable attributions we may plot them in an intuitive form. This intuition behind Break Down Plots is described in Figure ??.

The variable ordering determined in the first step of Break Down Algorithm is reflected by the ordering of variables in rows of the plot.

The last row of a plot shows the *baseline*, i.e. an average model prediction. The next row corresponds to average model prediction for observations with variable `surface` fixed to value 35. The next row corresponds to average model prediction with variables `surface` set to 35 and `floor` set to 1, and so on. The first row corresponds to model response for x^* .

In panels A and B violines show distribution of model predictions for selected points, while red dots stands for averages.

The most minimal form that shows important information is presented in the panel C. Positive values are presented with green bars while negative differences are marked with yellow bar. They sum up to final model prediction, which is denoted by a grey bar in this example.

4.4 Pros and cons

Break Down approach is model agnostic, can be applied to any predictive model that returns a single number. It leads to additive variable attribution. Below we summarize key strengths and weaknesses of this approach.

Pros

- Break Down Plots are easy to understand and decipher.
- Break Down Plots are compact; many variables may be presented in a small space.
- Break Down Plots are model agnostic yet they reduce to intuitive interpretation for linear Gaussian and generalized models.
- Complexity of Break Down Algorithm is linear in respect to the number of variables.

Cons

- If the model is non-additive then showing only additive contributions may be misleading.

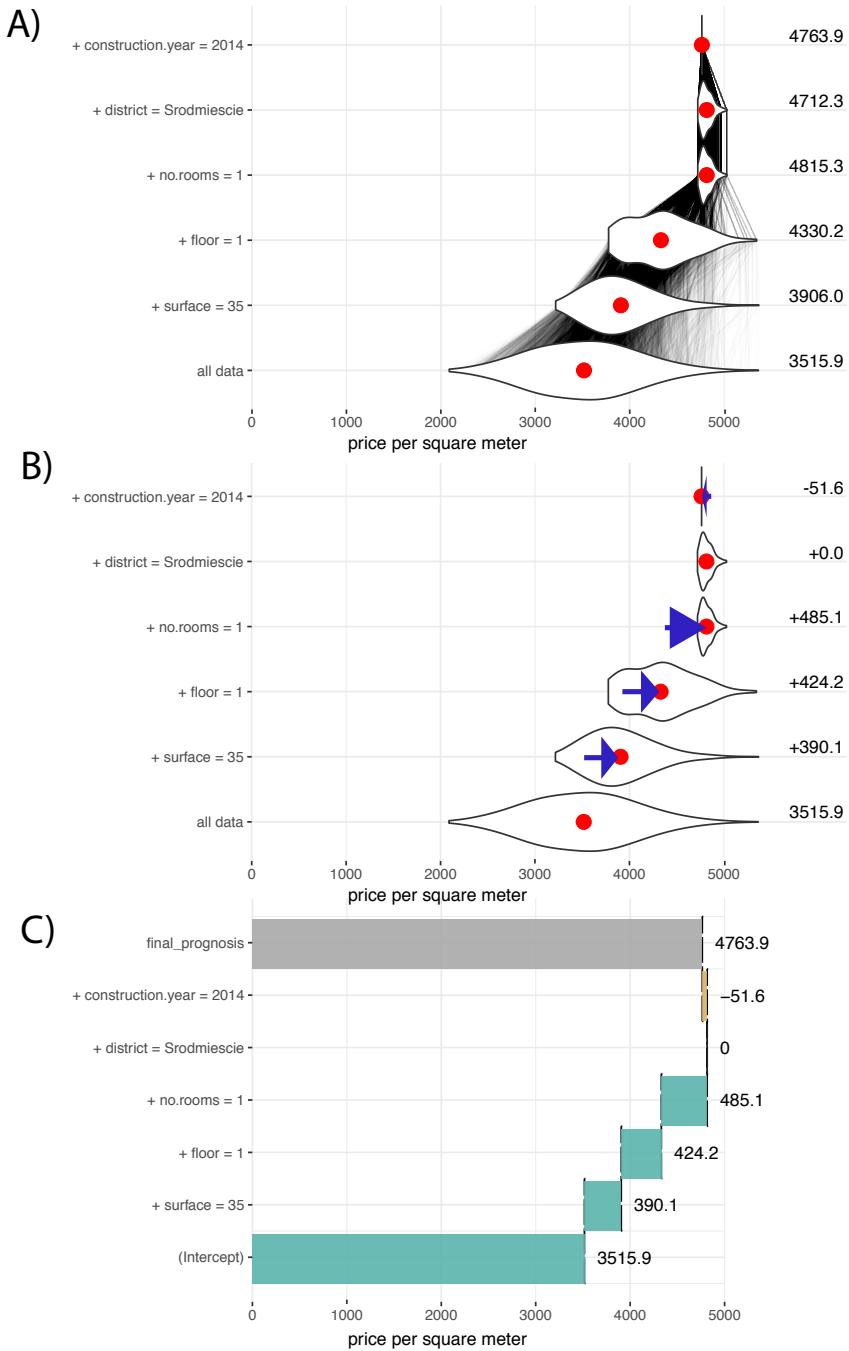


Figure 4.1: (fig:BDPrice4) Break Down Plots show how variables move the model prediction from population average to the model prognosis for a single observation. A) The last row shows distribution of model predictions. Next rows show conditional distributions, every row a new variable is added to conditioning. The first row shows model prediction for a single point. Red dots stand for averages. B) Blue arrows shows how the average conditional response change, these values are variables contributions. C) Only variable contributions are presented.

- Selection of the ordering based on scores is subjective. Different orderings may lead to different contributions.
- For large number of variables the Break Down Plot may be messy with many variables having small contributions.

4.5 Code snippets for R

In this section we present key features of the `breakDown` package for R (?). This package covers all features presented in this chapter. It is available on CRAN and GitHub. Find more examples at the website of this package <https://pbiecek.github.io/breakDown/>.

Model preparation

In this section we will present an example based on the `HR` dataset and Random Forest model (?). See the Section ?? for more details.

```
library("DALEX")
library("randomForest")
model <- randomForest(status ~ gender + age + hours + evaluation + salary, data = HR)
model

##
## Call:
## randomForest(formula = status ~ gender + age + hours + evaluation +      salary, data = HR)
##           Type of random forest: classification
##                   Number of trees: 500
## No. of variables tried at each split: 2
##
##          OOB estimate of  error rate: 27.41%
## Confusion matrix:
##             fired   ok promoted class.error
## fired     2277   380      198    0.2024518
## ok        531  1243      447    0.4403422
## promoted   199   396     2176    0.2147239
```

Model exploration with the `breakDown` package is performed in three steps.

1. Create an explainer - wrapper around model and validation data.

Since all other functions work in a model agnostic fashion, first we need to define a wrapper around the model. Here we are using the `explain()` function from `DALEX` package (?).

```
explainer_rf_fired <- explain(model,
                                 data = HR,
                                 y = HR$status == "fired",
                                 predict_function = function(m,x) predict(m,x, type = "prob")[,1],
                                 label = "fired")
```

2. Select an observation of interest.

Break Down Plots decompose model prediction around a single observation. Let's construct a data frame with corresponding values.

```
new_observation <- data.frame(gender = factor("male", levels = c("male", "female")),
                               age = 57.7,
                               hours = 42.3,
                               evaluation = 2,
                               salary = 2)
```

```
predict(model, new_observation, type = "prob")
```

```
##   fired      ok promoted
## 1  0.8 0.196    0.004
## attr(,"class")
## [1] "matrix" "votes"
```

3. Calculate Break Down decomposition

The `break_down()` function calculates Break Down contributions for a selected model around a selected observation.

The result from `break_down()` function is a data frame with variable attributions.

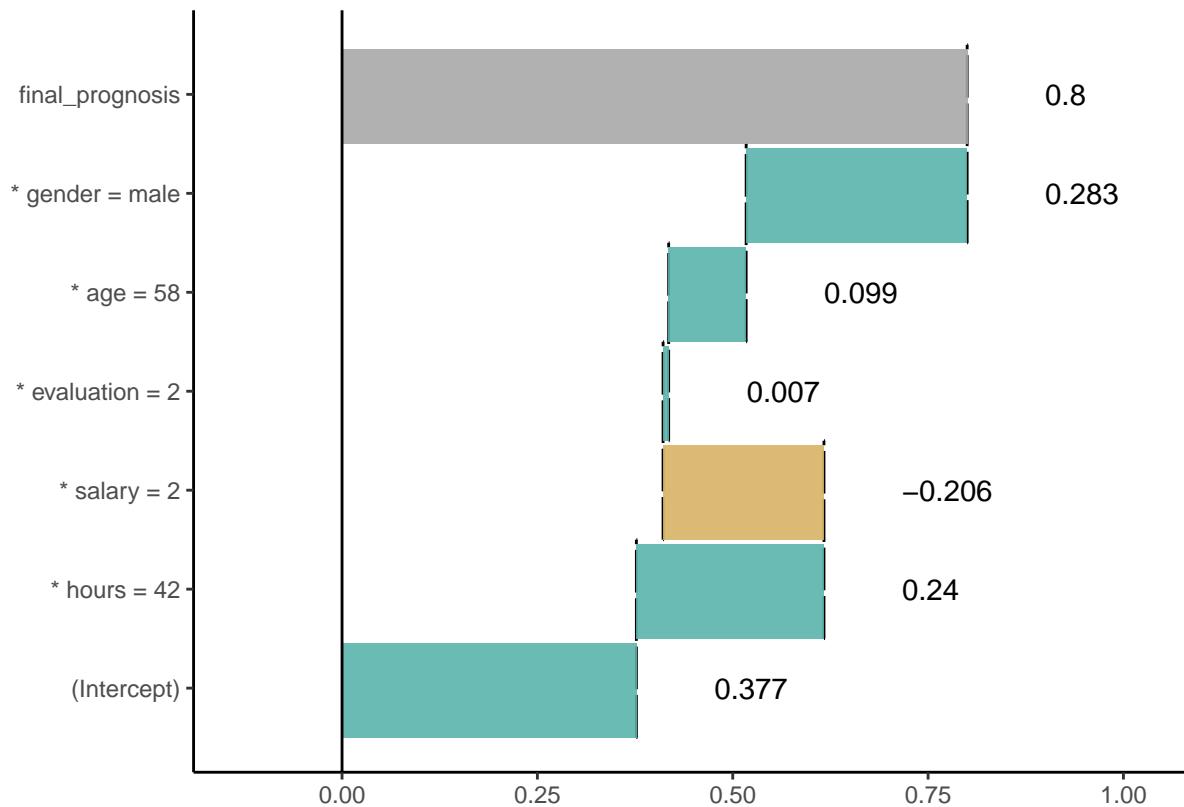
```
library("breakDown")
bd_rf <- break_down(explainer_rf_fired,
                     new_observation,
                     check_interactions = FALSE,
                     keep_distributions = TRUE)
```

```
bd_rf
```

	contribution
## (Intercept)	0.377
## * hours = 42	0.240
## * salary = 2	-0.206
## * evaluation = 2	0.007
## * age = 58	0.099
## * gender = male	0.283
## final_prognosis	0.800
## baseline:	0

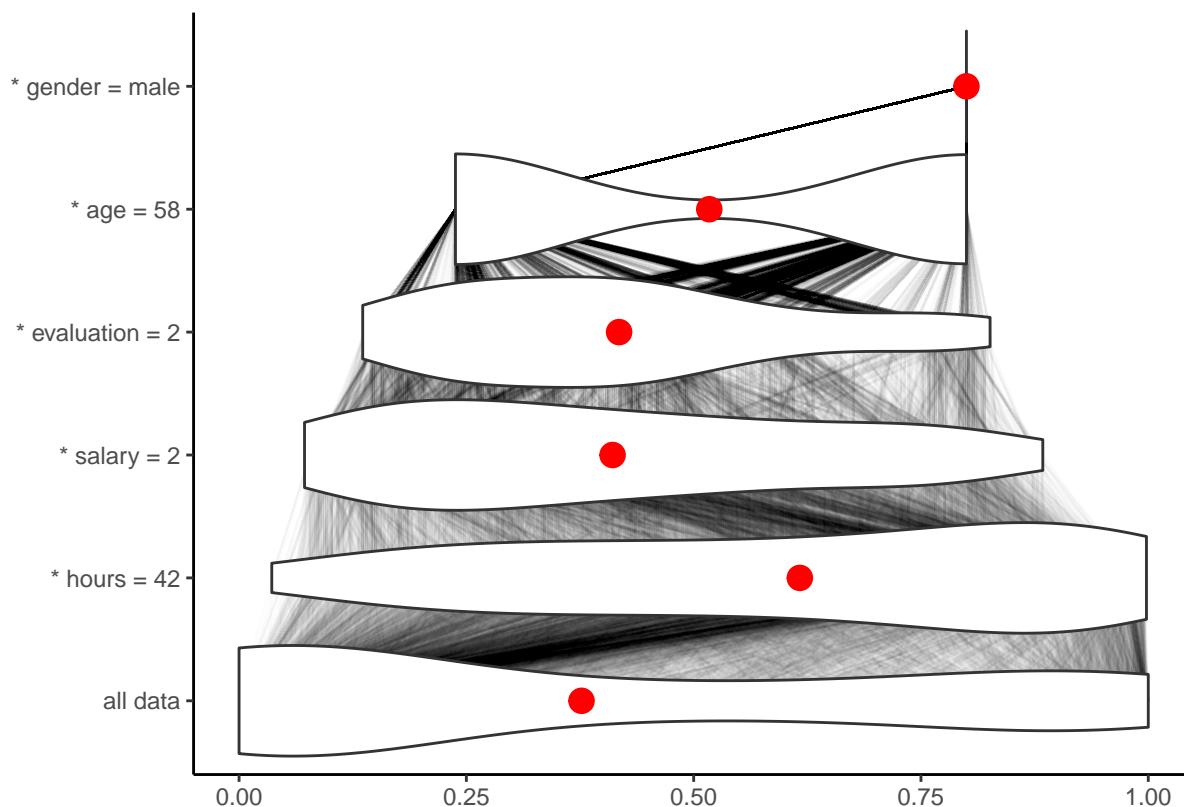
The generic `plot()` function creates a Break Down plots.

```
plot(bd_rf)
```



Add the `plot_distributions = TRUE` argument to enrich model response with additional information.

```
plot(bd_rf, plot_distributions = TRUE)
```



Chapter 5

Break Down for Interactions

In the Section ?? we presented model agnostic approach for additive decomposition of a model prediction for a single observation.

For non-additive models the variables contributions depend on values of other variables.

In this section we present an algorithm that identifies interactions between pairs of variables and include such interactions in variable decomposition plots. Here we present an algorithm for pairs of variables, but it can be easily generalized to larger number of variables.

5.1 The Algorithm

This algorithm is also composed out of two steps. In the first step variables and pairs of variables are ordered in terms of their importance, while in the second step the consecutive conditioning is applied to ordered variables.

To determine an importance of variables and pairs of variables following scores are being calculated.

For a single variable

$$score_1(f, x^*, i) = |E[f(X)|X_i = x_i^*] - E[f(X)]|$$

For pairs of variables

$$score_2(f, x^*, (i, j)) = |E[f(X)|X_i = x_i^*, X_j = x_j^*] - E[f(X)|X_i = x_i^*] - E[f(X)|X_j = x_j^*] + E[f(X)]|$$

Note that this is equivalent to

$$score_2(f, x^*, (i, j)) = |E[f(X)|X_i = x_i^*, X_j = x_j^*] - score_1(f, x^*, i) - score_1(f, x^*, j) + baseline|$$

In other words the $score_1(f, x^*, i)$ measures how much the average model response changes if variable x_i is set to x_i^* , which is some index of local variable importance. On the other hand the $score_2(f, x^*, (i, j))$ measures how much the change is different than additive composition of changes for x_i and x_j , which is some index of local interaction importance.

Note, that for additive models $score_2(f, x^*, (i, j))$ shall be close to zero. So the larger is this value the larger deviation from additivity.

The second step of the algorithm is the sequential conditioning. In this version in every new step we condition on a single variable or pair of variables in an order determined by $score_1$ and $score_2$.

The complexity of the first step is $O(p^2)$ where p stands for the number of variables. The complexity of the second step is $O(p)$.

5.2 HR dataset: Hire or Fire?

Again, let us consider a HR dataset. The table below shows $score_1$ and $score_2$ calculated for consecutive variables.

	Ei f(X)	score1	score2
hours	0.616200	0.230614	
salary	0.225528	-0.160058	
age:gender	0.516392		0.146660
salary:age	0.266226		0.062026
salary:hours	0.400206		-0.055936
evaluation	0.430994	0.045408	
hours:age	0.635662		0.040790
salary:evaluation	0.238126		-0.032810
age	0.364258	-0.021328	
evaluation:hours	0.677798		0.016190
salary:gender	0.223292		-0.007710
evaluation:age	0.415688		0.006022
gender	0.391060	0.005474	
hours:gender	0.626478		0.004804
evaluation:gender	0.433814		-0.002654

Once we determined the order, we can calculate sequential conditionings. In the first step we condition over variable `hours`, then over `salary`. The third position is occupied by interaction between `age:gender` thus we add both variables to the conditioning

	variable	cumulative	contribution
(Intercept)		0.385586	0.385586
hours = 42		0.616200	0.230614
salary = 2		0.400206	-0.215994
age:gender = 58:male		0.796856	0.396650
evaluation = 2		0.778000	-0.018856
final_prognosis		0.778000	0.778000

5.3 Break Down Plots

Break Down Plots for interactions are similar in structure as plots for single variables. The only difference is that in some rows pair of variable is listed in a single row. See an example in Figure ??.

5.4 Pros and cons

Break Down for interactions shares many features of Break Down for single variables. Below we summarize unique strengths and weaknesses of this approach.

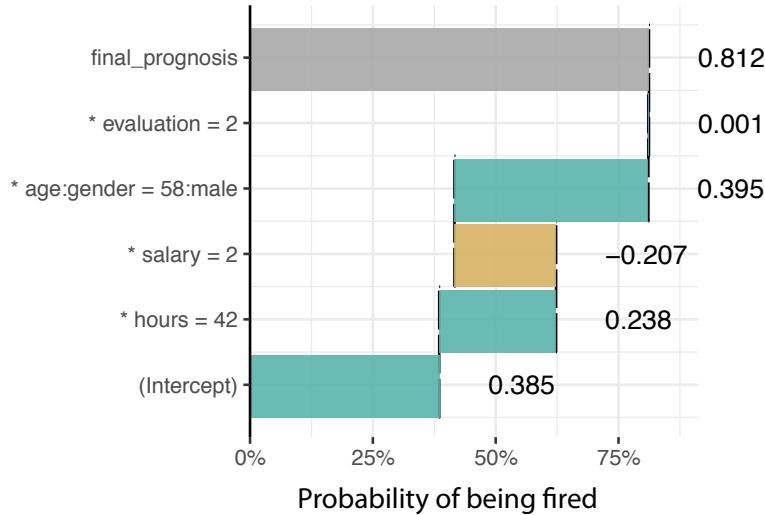


Figure 5.1: (fig:bdInter1) Break Down Plot for variable attribution with interactions

Pros

- If interactions are present in the model, then additive contributions may be misleading. In such case the identification of interactions leads to better explanations.
- Complexity of Break Down Algorithm is quadratic, what is not that bad if number of features is small or moderate.

Cons

- For large number of variables, the consideration of all interactions is both time consuming and sensitive to noise as the number of $score_2$ scores grow faster than number of $score_1$.

5.5 Code snippets for R

The algorithm for Break Down for Interactions is also implemented in the `break_down` function from `breakDown` package.

It is enough to set argument `check_interactions = TRUE` to identify interactions.

Model preparation

First a model needs to be trained.

```
library("DALEX")
library("randomForest")
model <- randomForest(status ~ gender + age + hours + evaluation + salary, data = HR)
model

##
## Call:
## randomForest(formula = status ~ gender + age + hours + evaluation +      salary, data = HR)
##           Type of random forest: classification
##                   Number of trees: 500
## No. of variables tried at each split: 2
##
##       OOB estimate of  error rate: 27.35%
```

```
## Confusion matrix:
##          fired   ok promoted class.error
## fired      2275   379     201    0.2031524
## ok         534   1242     445    0.4407924
## promoted   204   383     2184    0.2118369
```

Model exploration with the `breakDown` package is performed in three steps.

1. Create an explainer - wrapper around model and validation data.

Since all other functions work in a model agnostic fashion, first we need to define a wrapper around the model. Here we are using the `explain()` function from DALEX package.

```
explainer_rf_fired <- explain(model,
                                data = HR,
                                y = HR$status == "fired",
                                predict_function = function(m,x) predict(m,x, type = "prob")[,1],
                                label = "fired")
```

2. Select an observation of interest.

Break Down Plots decompose model prediction around a single observation. Let's construct a data frame with corresponding values.

```
new_observation <- data.frame(gender = factor("male", levels = c("male", "female")),
                               age = 57.7,
                               hours = 42.3,
                               evaluation = 2,
                               salary = 2)

predict(model, new_observation, type = "prob")
```

```
##    fired   ok promoted
## 1 0.774 0.224    0.002
## attr(,"class")
## [1] "matrix" "votes"
```

3. Calculate Break Down decomposition

The `break_down()` function calculates Break Down contributions for a selected model around a selected observation.

Note that `check_interactions = TRUE` is needed to identify interactions.

The result from `break_down()` function is a data frame with variable attributions.

```
library("breakDown")
bd_rf <- break_down(explainer_rf_fired,
                      new_observation,
                      check_interactions = TRUE)

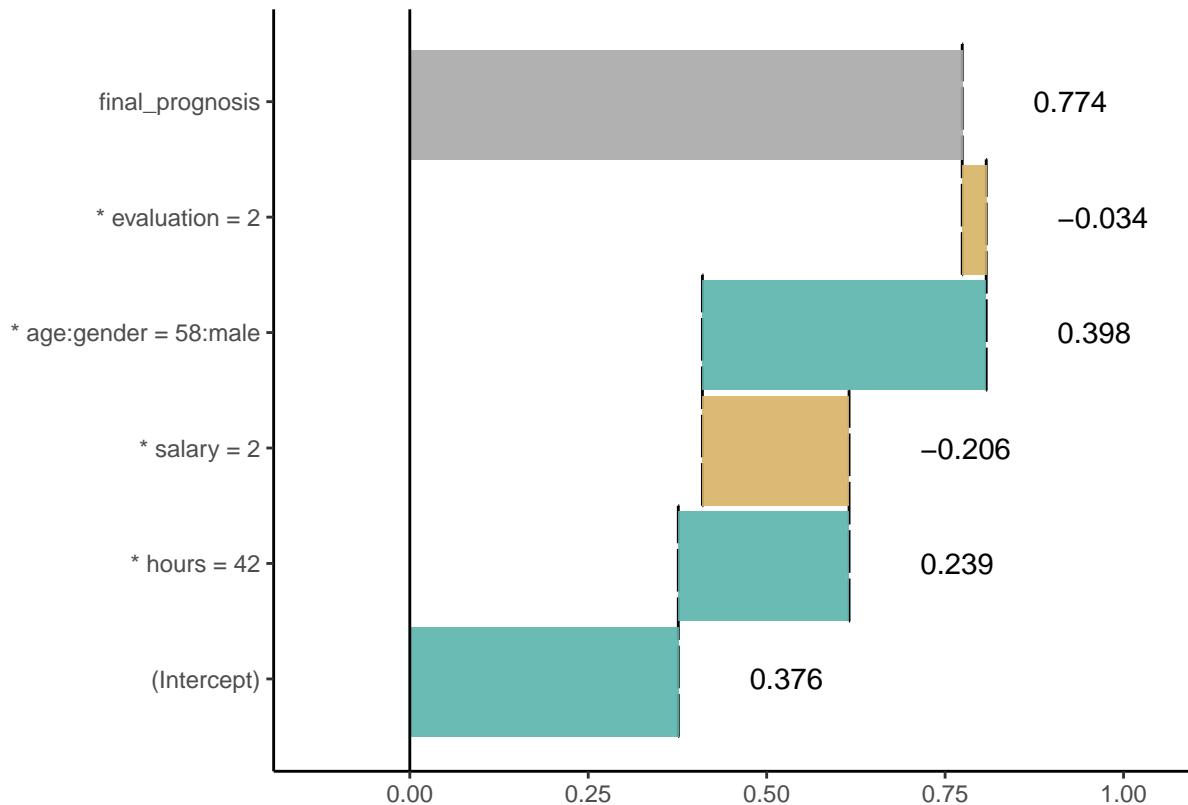
bd_rf
```

	contribution
## (Intercept)	0.376
## * hours = 42	0.239
## * salary = 2	-0.206
## * age:gender = 58:male	0.398
## * evaluation = 2	-0.034
## final_prognosis	0.774

```
## baseline: 0
```

The generic `plot()` function creates a Break Down plots.

```
plot(bd_rf)
```



Chapter 6

Shapley Attributions

In the Section ?? we show the problem related to the ordering of variables. In the Section ?? we show an approach in which the ordering was determined based on single step assessment of variable importance.

In this section we introduce other, very popular approach for additive variable attribution. The problem of contributions that depends on the variable ordering is solved by averaging over all possible orderings.

This method is motivated with results in cooperative game theory and was first introduced in (?). Wide adoption of this method comes with a NIPS 2017 paper (?) and python library SHAP <https://github.com/slundberg/shap>. Authors of the SHAP method introduced also efficient algorithm for tree-based models, see (?).

6.1 The Algorithm

The name *Shapley Values* comes from the solution in cooperative game theory attributed to Lloyd Shapley. The original problem was to assess how important is each player to the overall cooperation, and what payoff can he or she reasonably expect from the coalition? (?)

In the context of model interpretability the payoff is the average model response while the players are the variables in the conditioning. Then Formula for variable contributions is following.

$$v(f, x^*, i) = \frac{1}{|P|} \sum_{S \subseteq P \setminus \{i\}} \binom{|P|-1}{|S|}^{-1} \left(E[f(X)|X_{S \cup \{i\}} = x_{S \cup \{i\}}^*] - E[f(X)|X_S = x_S^*] \right)$$

where $P = \{1, \dots, p\}$ is the set of all variables. The intuition beyond this contribution is following. We consider all possible orderings of variables (yes, there is 2^p of them) and calculate the contribution of variable i as an average from contributions calculated in particular orderings.

The part $E[f(X)|X_{S \cup \{i\}} = x_{S \cup \{i\}}^*] - E[f(X)|X_S = x_S^*]$ is the contribution of variable i which is introduced after variables from S .

Time complexity of this method is $O(2^p)$ where p stands for the number of variables. Such complexity makes this method impractical for most cases. Fortunately it is enough to assess this value. (?) proposed to use sampling. (?) proposed fast implementations for tree based ensembles.

6.2 Code snippets for R

In this section we will present an example based on the HR dataset and Random Forest model (?). See the Section ?? for more details.

```
library("DALEX")
library("randomForest")
model_rf <- randomForest(status ~ gender + age + hours + evaluation + salary, data = HR)
```

Here we use the iml package, see more examples in (?).

```
library("iml")
explainer_rf = Predictor$new(model_rf, data = HR, type="prob")
```

Explanations for a new observation.

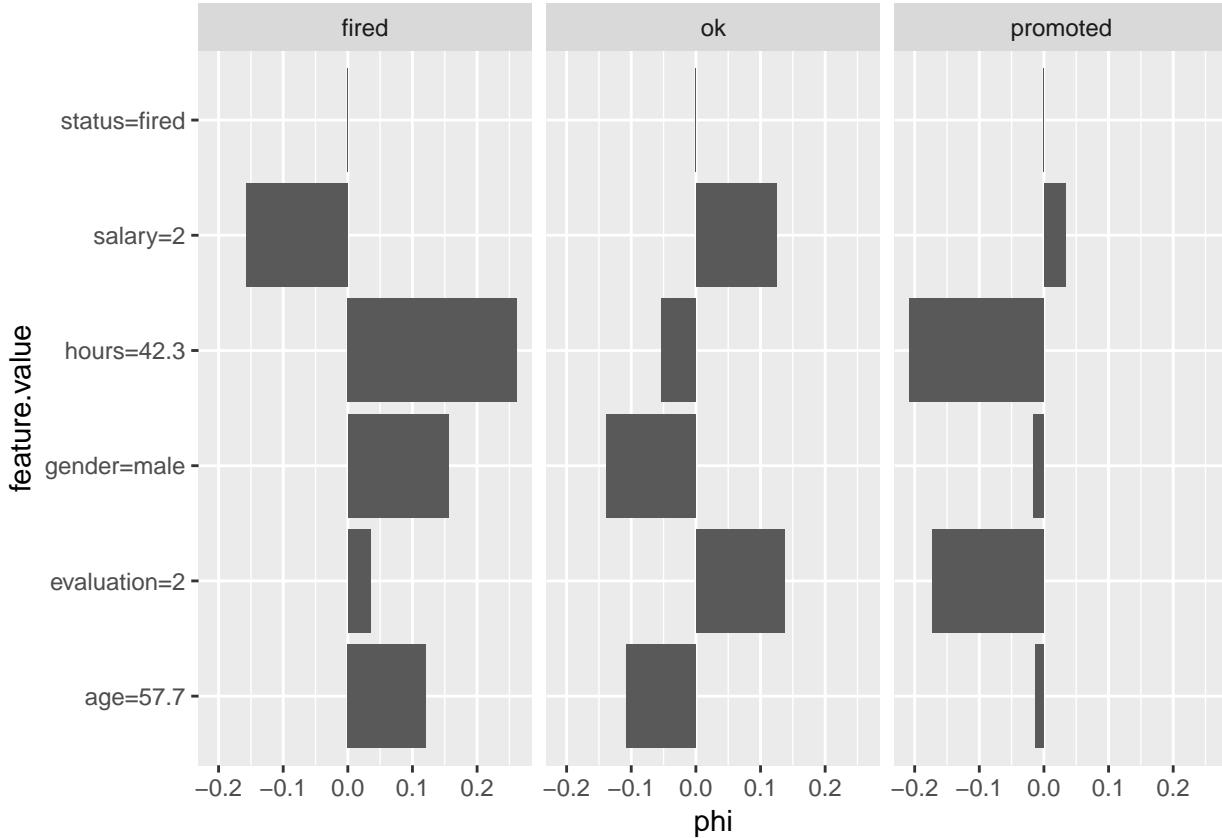
```
new_observation <- data.frame(gender = factor("male", levels = c("male", "female")),
                               age = 57.7,
                               hours = 42.3,
                               evaluation = 2,
                               salary = 2,
                               status = factor("fired"))

shapley = Shapley$new(explainer_rf, x.interest = new_observation)
shapley
```

```
## Interpretation method: Shapley
## Predicted value: 0.798000, Average prediction: 0.376094 (diff = 0.421906) Predicted value: 0.200000, Average prediction: 0.197900 (diff = 0.002100)
## Analysed predictor:
## Prediction task: unknown
##
## Analysed data:
## Sampling from data.frame with 7847 rows and 6 columns.
##
## Head of results:
##      feature class      phi    phi.var feature.value
## 1   gender fired  0.15600  0.09186570   gender=male
## 2     age fired  0.12082  0.08383548      age=57.7
## 3   hours fired  0.26154  0.10200605    hours=42.3
## 4 evaluation fired  0.03508  0.01745337 evaluation=2
## 5   salary fired -0.15776  0.04906184    salary=2
## 6   status fired  0.00000  0.00000000  status=fired
```

And the plot with Shapley attributions.

```
plot(shapley)
```



See more examples for `iml` package in the (?) book.

6.3 Pros and cons

Shapley Values give a uniform approach to decompose model prediction into parts that can be attributed additively to variables. Below we summarize key strengths and weaknesses of this approach.

Pros

- There is a nice theory based on cooperative games.
- (?) shows that this method unifies different approaches to additive features attribution.
- There is efficient implementation available for Python.
- (?) shows more desired properties of this method, like symmetry or additivity.

Cons

- The exact calculation of Shapley values is time consuming.
- If the model is not additive, then the Shapley scores may be misleading. And there is no way to determine if model is far from additiveness.

Note that fully additive model solutions presented in sections ??, ?? and ?? lead to same variable contributions.

Chapter 7

Local approximations with white-box model

A different approach to explanations of a single observations is through surrogate models. Models that easy to understand and are similar to black box model around the point of interest.

Variable attribution methods, that were presented in the Section ?? are not interested in the local curvature of the model. They rather compare model prediction against average model prediction and they use probability structure of the dataset.

The complementary approach would be to directly explore information about model curvature around point of interest. In the section ?? we introduced Ceteris Paribus tool for such what-if analysis. But the limitation of ceteris Paribus pltos is that they explore changes along single dimension or pairs of dimensions.

In this section we describe an another approach based on local approximations with white-box models. This approach will also investigate local curvature of the model but indirectly, through surrogate white-box models.

The most known method from this class if LIME (Local Interpretable Model-Agnostic Explanations), introduced in the paper *Why Should I Trust You?: Explaining the Predictions of Any Classifier* (?). This methods and it's clones are now implemented in various R and python packages, see for example (?), (?) or (?).

7.1 The Algorithm

The LIME method, and its clones, has following properties:

- *model-agnostic*, they do not imply any assumptions on model structure,
- *interpretable representation*, model input is transformed into a feature space that is easier to understand. One of applications comes from image data, single pixels are not easy to interpret, thus the LIME method decompose image into a series of super pixels, that are easier to interpret to humans,
- *local fidelity* means that the explanations shall be locally well fitted to the black-box model.

Therefore the objective is to find a local model M^L that approximates the black box model f in the point x^* . As a solution the penalized loss function is used. The white-box model that is used for explanations satisfies following condition.

$$M^L(x^*) = \arg \min_{g \in G} L(f, g, \Pi_{x^*}) + \Omega(g)$$

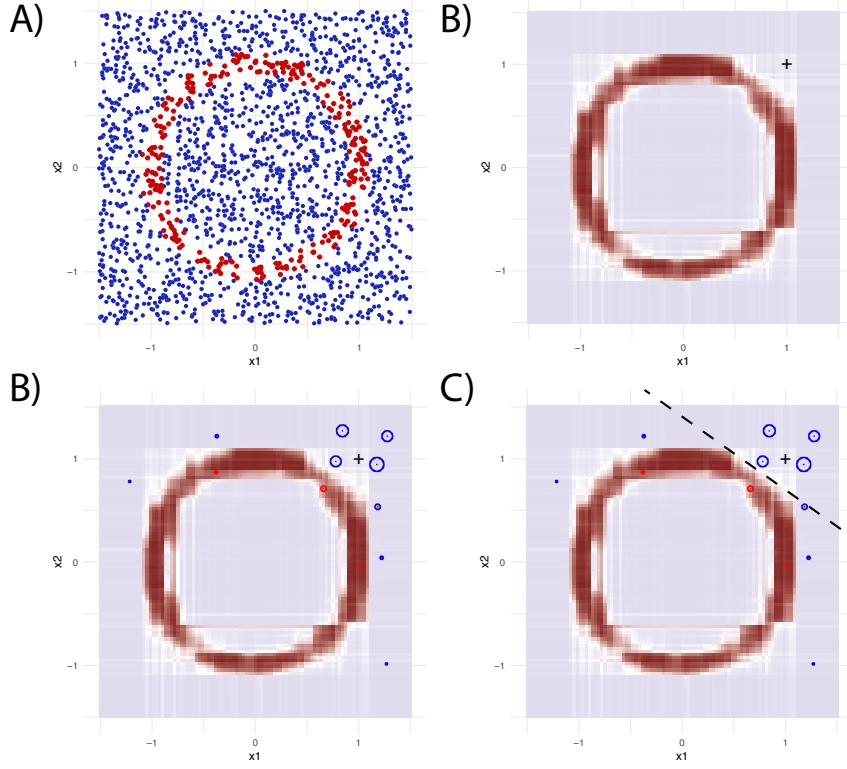


Figure 7.1: (fig:LIME1) A schematic idea behind local model approximations. Panel A shows training data, colors correspond to classes. Panel B shows results from the Random Forest model, this is where the algorithm starts. Panel C shows new data sampled around the point of interest. Their color correspond to model response. Panel D shows fitted linear model that approximated the random forest model around point of interest

where G is a family of white box models (e.g. linear models), Π_{x^*} is neighbourhood of x^* and Ω stands for model complexity.

The algorithm is composed from three steps:

- Identification of interpretable data representations,
- Local sampling around the point of interest,
- Fitting a white box model in this neighbourhood

Identification of interpretable data representations

For image data, single pixel is not an interpretable feature. In this step the input space of the model is transformed to input space that is easier to understand for human. The image may be decomposed into parts and represented as presence/absence of some part of an image.

Local sampling around the point of interest

Once the interpretable data representation is identified, then the neighbourhood around point of interest needs to be explored.

Fitting a white box model in this neighbourhood

Any model that is easy to interpret may be fitted to this data, like decision tree or rule based system. However in practice the most common family of models are linear models.

7.2 HR dataset: Hire or Fire?

7.3 Pros and cons

Local approximations are model agnostic, can be applied to any predictive model. Below we summarize key strengths and weaknesses of this approach.

Pros

- This method is highly adopted in text analysis and image analysis, in part thanks to the interpretable data representations.
- The intuition behind the model is straightforward
- Model explanations are sparse, thus only small number of features is used

Cons

- For continuous variables and tabular data it is not that easy to find interpretable representations
- The black-box model approximated the data and the white box model approximates the black box model. We do not have control over the quality of local fit of the white box model, thus the surrogate model may be misleading.
- Due to the *curse of dimensionality*, for high dimensional space points are sparse.

7.4 Code snippets for R

In this section we present example application of `lime` (?) and `lime` (?) packages. Note that this method is also implemented in `iml` (?) and other packages. These pacakages differ in some details and also results in different explanations.

Model preparation

In this section we will present examples based on the `HR` dataset. See the Section ?? for more details.

```
library("DALEX")
head(HR)
```

```
##   gender     age   hours evaluation salary   status
## 1 male 32.58267 41.88626      3     1 fired
## 2 female 41.21104 36.34339      2     5 fired
## 3 male 37.70516 36.81718      3     0 fired
## 4 female 30.06051 38.96032      3     2 fired
## 5 male 21.10283 62.15464      5     3 promoted
## 6 male 40.11812 69.53973      2     0 fired
```

The problem here is to predict average price for square meter for an apartment. Let's build a random forest model with `randomForest` package (?).

```
library("randomForest")
rf_model <- randomForest(status ~ gender + age + hours + evaluation + salary, data = HR)
rf_model

##
## Call:
##  randomForest(formula = status ~ gender + age + hours + evaluation + salary, data = HR)
##              Type of random forest: classification
##                      Number of trees: 500
## No. of variables tried at each split: 2
```

```

##          OOB estimate of  error rate: 27.39%
## Confusion matrix:
##             fired   ok promoted class.error
## fired      2284   377     194    0.2000000
## ok         533   1239     449    0.4421432
## promoted    209   387     2175   0.2150848

new_observation <- data.frame(gender = factor("male", levels = c("male", "female")),
                                age = 57.7,
                                hours = 42.3,
                                evaluation = 2,
                                salary = 2)

predict(rf_model, new_observation, type = "prob")

##    fired   ok promoted
## 1 0.802 0.198      0
## attr(,"class")
## [1] "matrix" "votes"

```

7.4.1 The lime pacakge

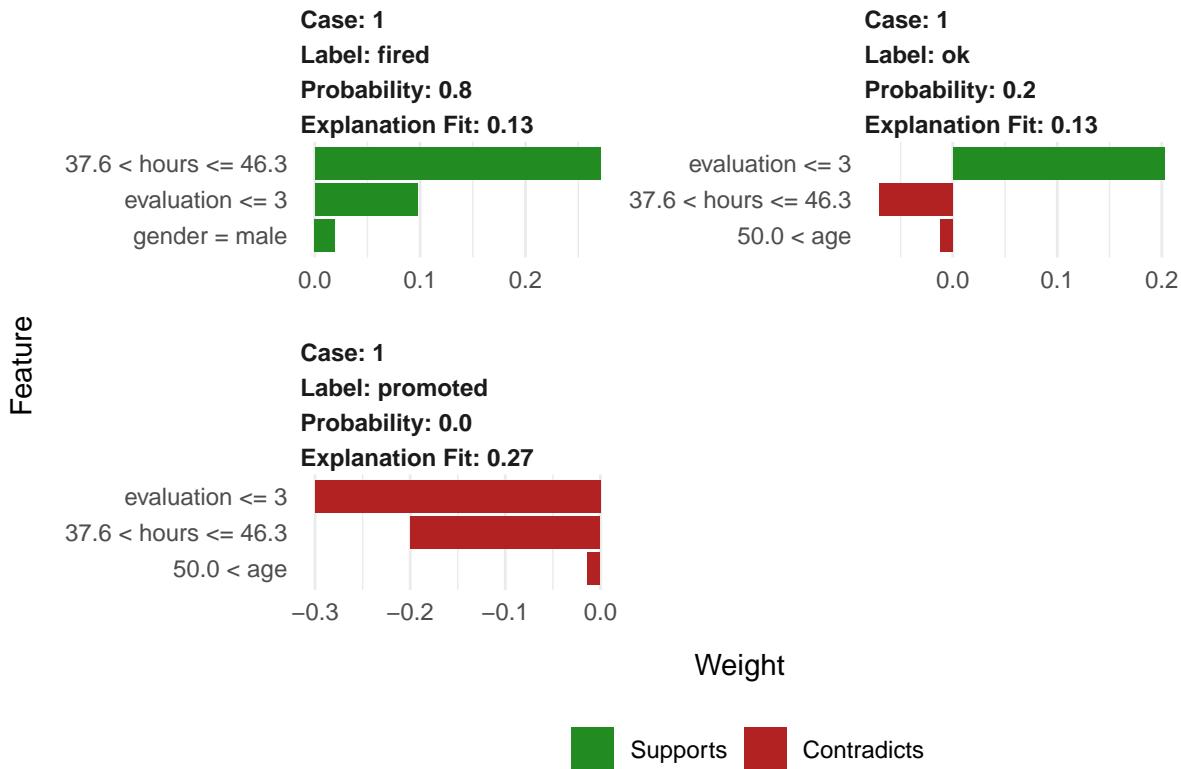
```

library("lime")
model_type.randomForest <- function(x, ...) "classification"
lime_rf <- lime(HR[,1:5], rf_model)
explanations <- lime:::explain(new_observation[,1:5], lime_rf, n_labels = 3, n_features = 3)
explanations

##      model_type case   label label_prob  model_r2 model_intercept
## 1 classification 1     fired  0.802 0.1326693  0.2601045
## 2 classification 1     fired  0.802 0.1326693  0.2601045
## 3 classification 1     fired  0.802 0.1326693  0.2601045
## 4 classification 1       ok  0.198 0.1328936  0.2201385
## 5 classification 1       ok  0.198 0.1328936  0.2201385
## 6 classification 1       ok  0.198 0.1328936  0.2201385
## 7 classification 1 promoted 0.000 0.2663979  0.5158718
## 8 classification 1 promoted 0.000 0.2663979  0.5158718
## 9 classification 1 promoted 0.000 0.2663979  0.5158718
##      model_prediction feature feature_value feature_weight
## 1           0.647513838 gender        2.0  0.01900717
## 2           0.647513838 hours       42.3  0.27104112
## 3           0.647513838 evaluation     2.0  0.09736102
## 4           0.340315741 age        57.7 -0.01174598
## 5           0.340315741 evaluation     2.0  0.20265622
## 6           0.340315741 hours       42.3 -0.07073304
## 7           0.002286556 age        57.7 -0.01355935
## 8           0.002286556 evaluation     2.0 -0.30029087
## 9           0.002286556 hours       42.3 -0.19973507
##      feature_desc                      data      prediction
## 1 gender = male 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
## 2 37.6 < hours <= 46.3 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
## 3 evaluation <= 3 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
## 4 50.0 < age 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000

```

```
## 5      evaluation <= 3 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
## 6 37.6 < hours <= 46.3 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
## 7      50.0 < age 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
## 8      evaluation <= 3 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
## 9 37.6 < hours <= 46.3 2.0, 57.7, 42.3, 2.0, 2.0 0.802, 0.198, 0.000
plot_features(explanations)
```



7.4.2 The live package

```
library("live")

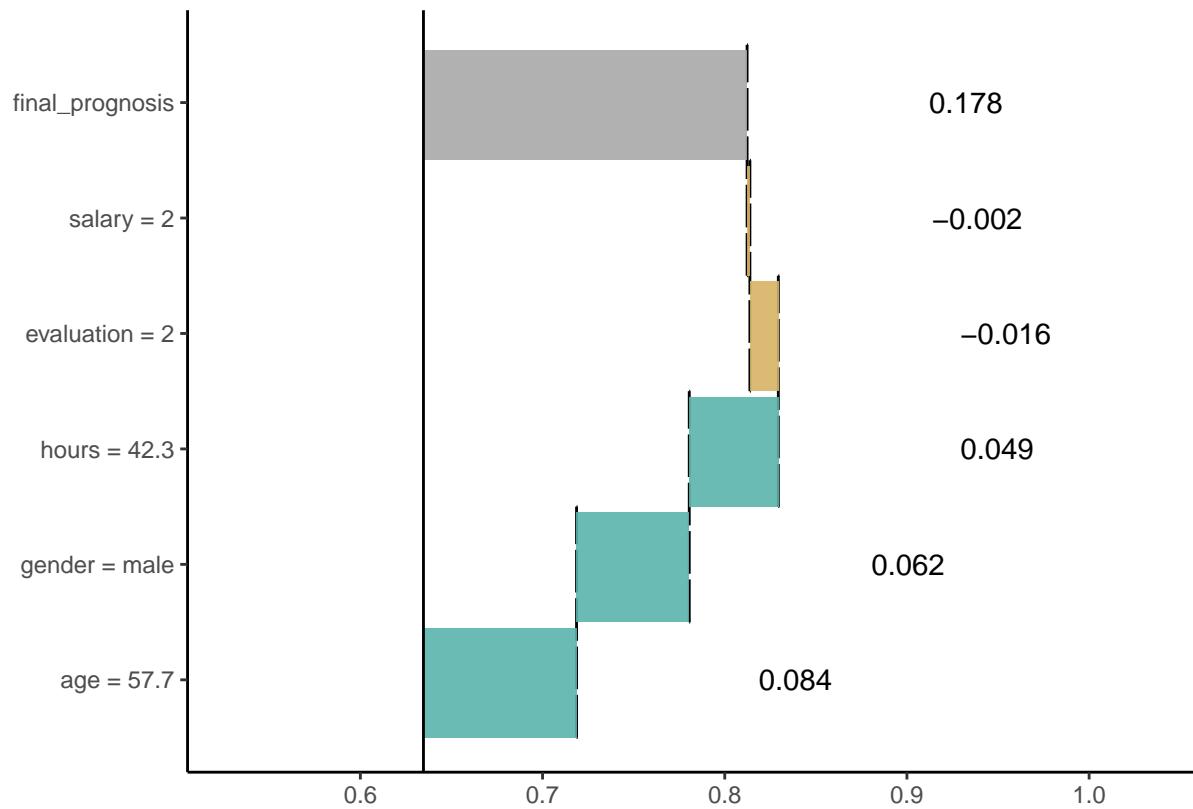
new_observation$status <- "fired"
explainer_rf_fired <- explain(rf_model,
  data = HR,
  y = HR$status == "fired",
  predict_function = function(m,x) predict(m,x, type = "prob")[,1],
  label = "fired")

local_model <- local_approximation(explainer_rf_fired, new_observation,
  target_variable_name = "status", n_new_obs = 500)

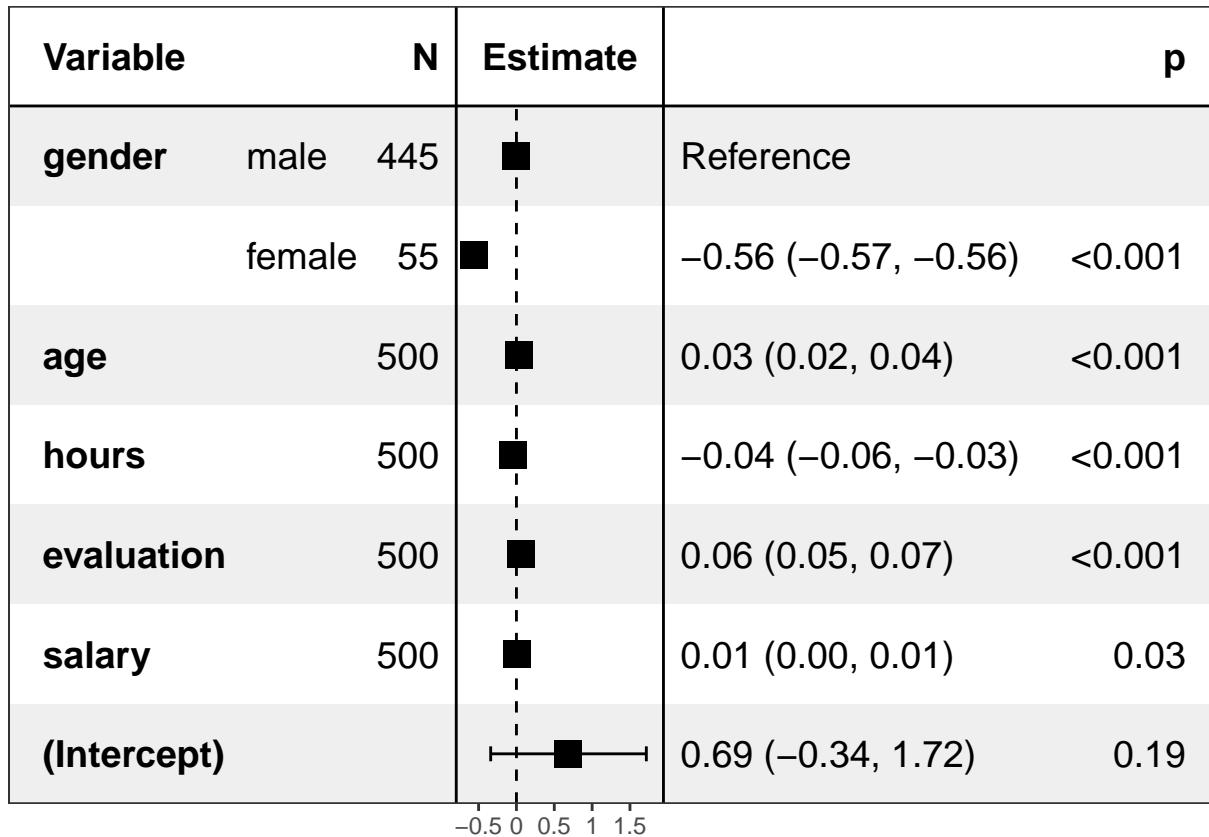
local_model

## Dataset:
## Observations: 500
## Variables: 6
## Response variable: status
## Explanation model:
```

```
##  Name:  regr.lm
##  Variable selection wasn't performed
##  Weights present in the explanation model
##  R-squared: 0.9834
plot(local_model)
```



```
plot(local_model, type = "forest")
```



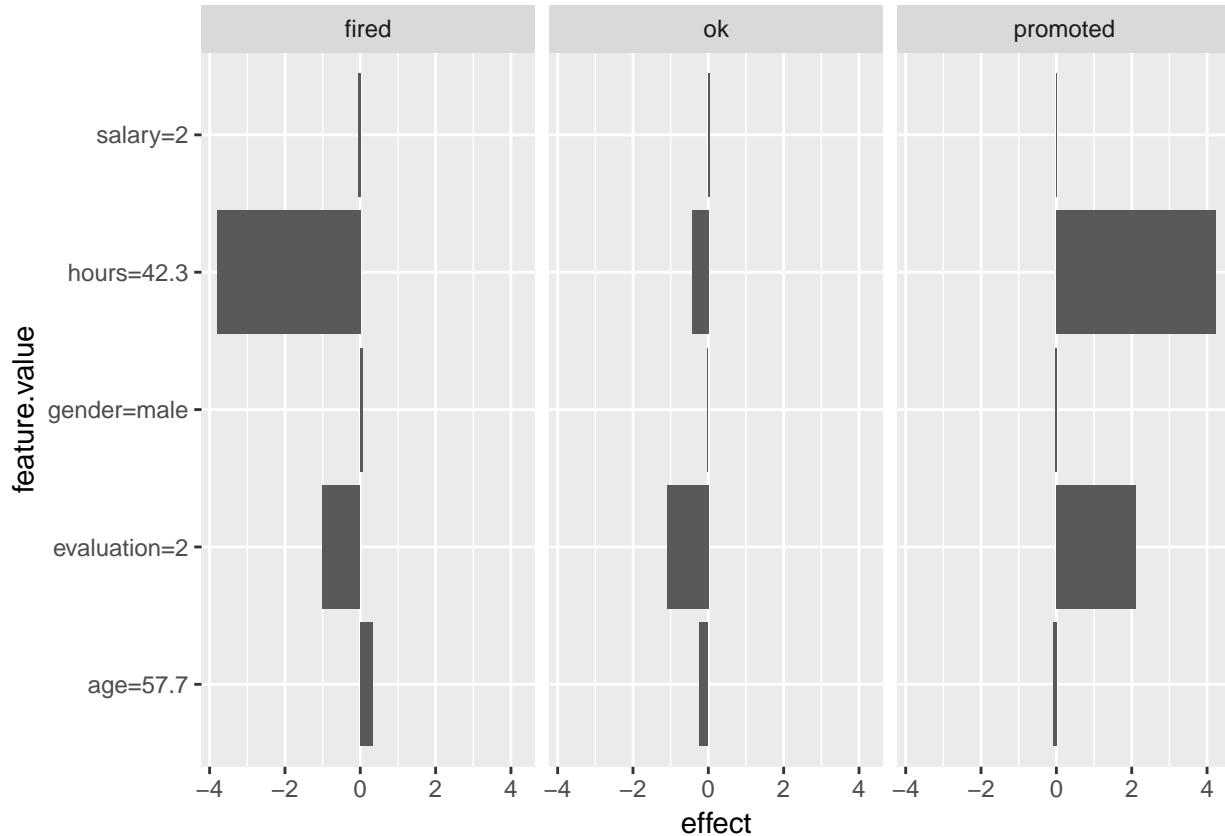
7.4.3 The iml package

```
library("iml")

explainer_rf = Predictor$new(rf_model, data = HR[,1:5])
white_box = LocalModel$new(explainer_rf, x.interest = new_observation[,1:5], k = 5)
white_box

## Interpretation method: LocalModel
##
## 
## Analysed predictor:
## Prediction task: unknown
## 
## 
## Analysed data:
## Sampling from data.frame with 7847 rows and 5 columns.
## 
## Head of results:
##           beta x.recoded      effect x.original      feature feature.value
## 1  0.065049360        1.0  0.06504936      male gender=male   gender=male
## 2  0.005639541       57.7  0.32540150     57.7       age    age=57.7
## 3 -0.090095457      42.3 -3.81103781     42.3      hours   hours=42.3
## 4 -0.504226839       2.0 -1.00845368      2 evaluation evaluation=2
## 5 -0.033152006       2.0 -0.06630401      2   salary    salary=2
## 6 -0.018448882       1.0 -0.01844888     male gender=male   gender=male
```

```
##   .class
## 1  fired
## 2  fired
## 3  fired
## 4  fired
## 5  fired
## 6      ok
plot(white_box)
```



Chapter 8

Ceteris Paribus Principle

In this section we introduce tools based on Ceteris Paribus principle. The main goal for these tools is to help understand how changes in model input affect changes in model output.

Presented explainers are linked with the second law introduced in Section ??, i.e. law for prediction's speculations. This is why these explainers are also known as *What-If model analysis* or *Individual Conditional EXpectations* (?). It turns out that it is easier to understand how black-box model is working if we can play with it by changing variable by variable.

Think of following usecases:

- Think about a model for heart attack. How the model response would change if a patient cuts the number of smoked cigarettes by half or increase physical activity.
- Think about a model for credit scoring. A customer gets a low score and is asking what he needs to change to increase this score to a certain level, to pass the bank criteria.
- Think about a model for apartment prices. An investor wants to know how much the price may increase if apartment standard is upgraded.

8.1 Introduction

Ceteris paribus is a Latin phrase meaning “other things held constant” or “all else unchanged”. Using this principle we examine input variable per variable separately, assuming that effects of all other variables are unchanged. See Figure ??

Similar to the LIME method introduced in the section ??, Ceteris Paribus profiles examine curvature of a model response function. The difference between these two methods is that LIME approximates the model curvature with a simpler white-box model that is easier to present. Usually the LIME model is sparse, thus our attention may be limited to smaller number of dimensions. In contrast, the CP plots show conditional model response for every variable. In the last subsection we discuss pros and cons of this approach.

8.2 1D profiles

Let $f_M(x) : \mathcal{R}^d \rightarrow \mathcal{R}$ denote a predictive model, i.e. function that takes d dimensional vector and calculate numerical score. Symbol $x \in \mathcal{R}^d$ refers to a point in the feature space. We use subscript x_i to refer to a different data points and superscript x^j to refer to specific dimensions. Additionally, let x^{-j} denote all coordinates except j -th and let $x|_j = z$ denote a data point x^* with all coordinates equal to x except coordinate j equal to value z . I.e. $\forall_{i \neq j} x^i = x^{*,i}$ and $x^j = z$. In other words $x|_j = z$ denote a x with j th coordinate changed to z .

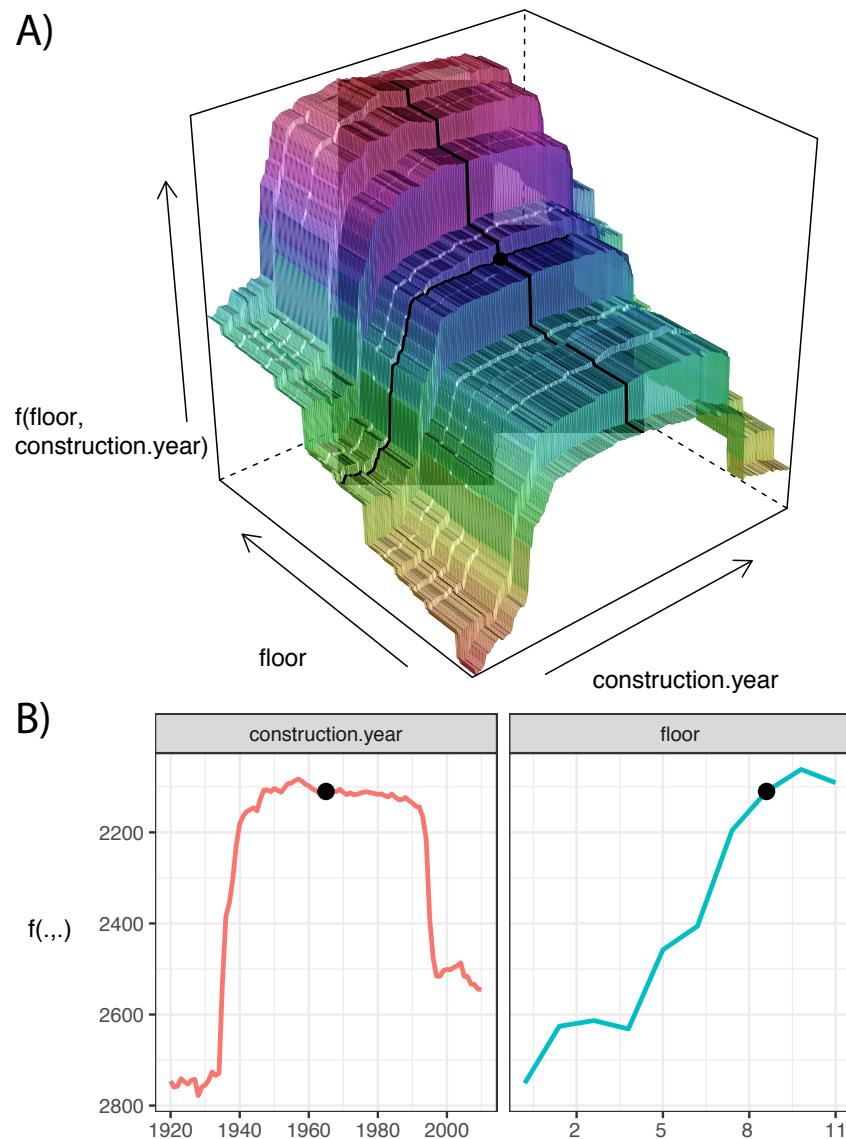


Figure 8.1: (fig:modelResponseCurveLine) A) Model response surface. Ceteris Paribus profiles marked with black curves helps to understand the curvature of the model response by updating only a single variable. B) CP profiles are individual conditional model responses

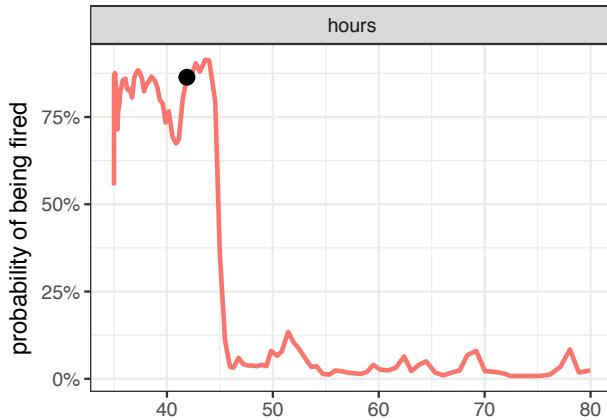


Figure 8.2: (fig:HRCPHiredHours) Ceteris Paribus profile for Random Forest model that assess the probability of being fired in call center as a function of average number of working hours

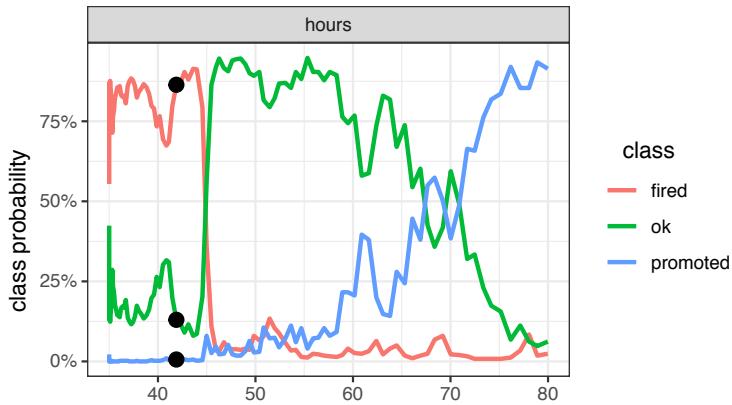


Figure 8.3: (fig:HCPAllHours) Ceteris Paribus profiles for three classes predicted by the Random Forest model as a function of average number of working hours

Now we can define uni-dimensional Ceteris Paribus Profile for model f , variable j and point x as

$$CP^{f,j,x}(z) := f(x|j = z).$$

I.e. CP profile is a model response obtained for observations created based on x with coordinate j changed and all other coordinates kept unchanged.

A natural way to visualise CP profiles is to use a profile plot as in Figure ??.

Figure ?? shows an example of Ceteris Paribus profile. The black dot stands for prediction for a single observation. Grey line show how the model response would change if in this single observation coordinate `hours` will be changed to selected value. One thing that we can read is that the model response is not smooth and there is some variability along the profile. Second thing is that for this particular observation the model response would drop significantly if the variable `hours` will be higher than 45.

Since in the example dataset we are struggling with model for three classes, one can plot CP profiles for each class in the same panel. See an example in the Figure ??.

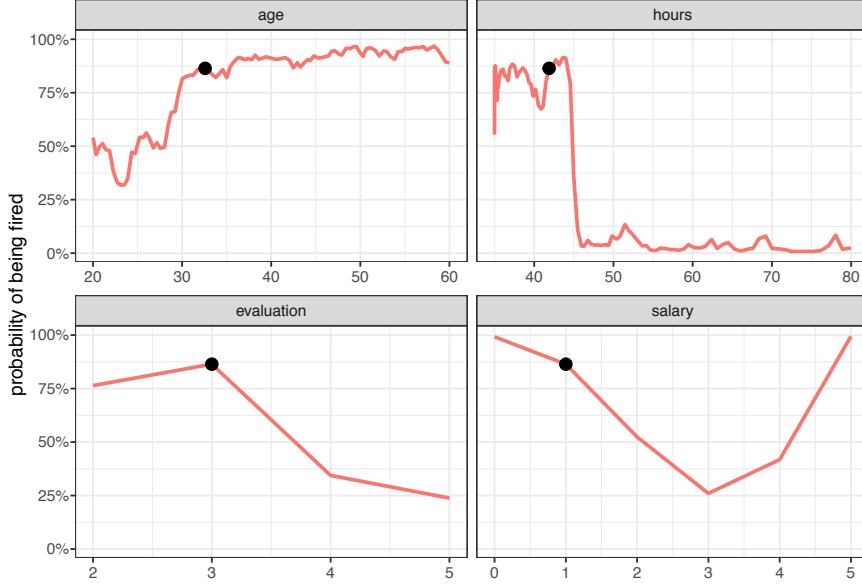


Figure 8.4: (fig:HRCPFiredAll) Ceteris Paribus profiles for all continuous variables

Usually model input consist many variables, then it is beneficial to show more variables at the same time. The easiest way to do so is to plot consecutive variables on separate panels. See an example in Figure ??.

8.3 Profile oscillations

Visual examination of variables is insightful, but for large number of variables we end up with large number of panels, most of which are flat. This is why we want to asses variable importance and show only profiles for important variables. The advantage of CP profiles is that they lead to a very natural and intuitive way of assessing the variable importance for a single prediction. The intuition is: the more important variable the larger are changes along the CP profile. If variable is not important then model response will barely change. If variable is important the CP profile change a lot for different values of a variable.

Let's write it down in a more formal way.

Let $vip_j^{CP}(x)$ denotes variable importance calculated based on CP profiles in point x for variable j .

$$vip_j^{CP}(x) = \int_{-\infty}^{\infty} |CP^{f,j,x}(z) - f(x)| dz$$

So it's an absolute deviation from $f(x)$. Note that one can consider different modification of this coefficient:

1. Deviations can be calculated not as a distance from $f(x)$ but from average $\bar{CP}^{f,j,x}(z)$.
2. The integral may be weighted based on the density of variable x^j .
3. Instead of absolute deviations one may use root from average squares.

TODO: we need to verify which approach is better. Anna Kozak is working on this

The straightforward estimator for $vip_j^{CP}(x)$ is

$$\widehat{vip}_j^{CP}(x) = \frac{1}{n} \sum_{i=1}^n |CP^{f,j,x}(x_i) - f(x)|.$$

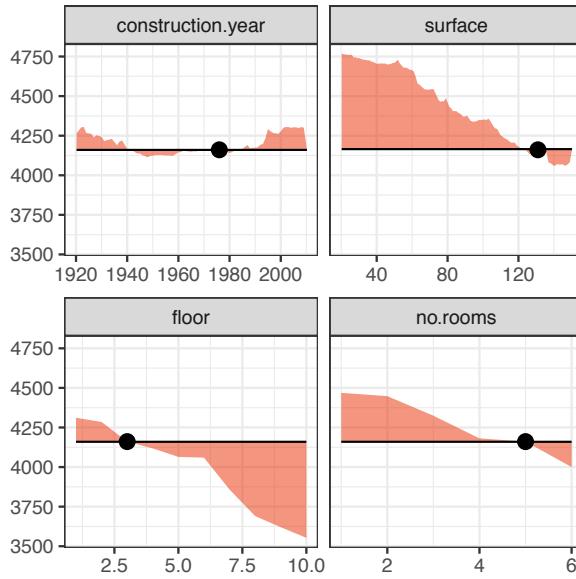


Figure 8.5: (fig:CPVIPprofiles) CP oscillations are average deviations between CP profiles and the model response

Figure ?? shows the idea behind measuring oscillations. The larger the highlighted area the more important is the variable.

Figure ?? summarizes variable oscillations. Such visuals help to quickly grasp how large are model oscillations around a specific point.

NOTE

Variable importance for single prediction may be very different than variable importance for the full model.

For example, consider a model

$$f(x_1, x_2) = x_1 * x_2$$

where variables x_1 and x_2 takes values in $[0, 1]$.

From the global perspective both variables are equally important.

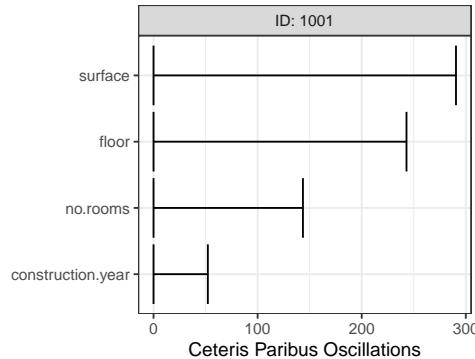


Figure 8.6: (fig:CPVIP1) Variable importance plots calculated for Ceteris Paribus profiles for observation ID: 1001

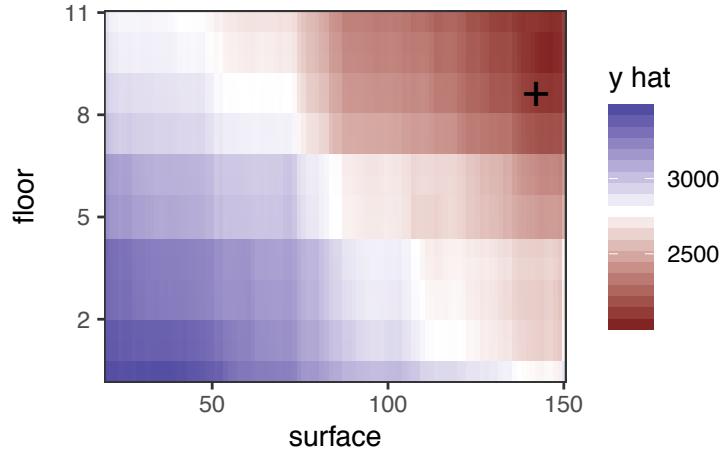


Figure 8.7: (fig:CP2Dsurflor) Ceteris Paribus plot for a pair of variables. Black cross marks coordinates for the observation of interest. Presented model estimates price of an apartment

But local variable importance is very different. Around point $x = (0, 1)$ the importance of x_1 is much larger than x_2 . This is because profile for $f(z, 1)$ have larger oscillations than $f(0, z)$.

8.4 2D profiles

The definition of ceteris paribus profiles given in section ?? may be easily extended to two and more variables. Also definition of CP oscillations ?? have straight forward generalization for larger number of dimensions. Such generalisations are usefull when model is non additive. Presence of pairwise interactions may be detected with 2D Ceteris Paribus plots.

Let's define two-dimensional Ceteris Paribus Profile for model f , variables j and k and point x as

$$CP^{f,(j,k),x}(z_1, z_2) := f(x|^{(j,k)} = (z_1, z_2)).$$

I.e. CP profile is a model response obtained for observations created based on x with j and k coordinates changed to (z_1, z_2) and all other coordinates kept unchanged.

A natural way to visualise 2D CP profiles is to use a level plot as in Figure ??.

If number of variables is small or moderate then it is possible to present all pairs of variables. See an example in Figure ??.

8.5 Local model fidelity

Ceteris Paribus profiles are also a useful tool to validate local model fidelity. It may happen that global performance of the model is good, while for some points the local fit is very bad. Local fidelity helps to understand how good is the model fit around point of interest.

How does it work?

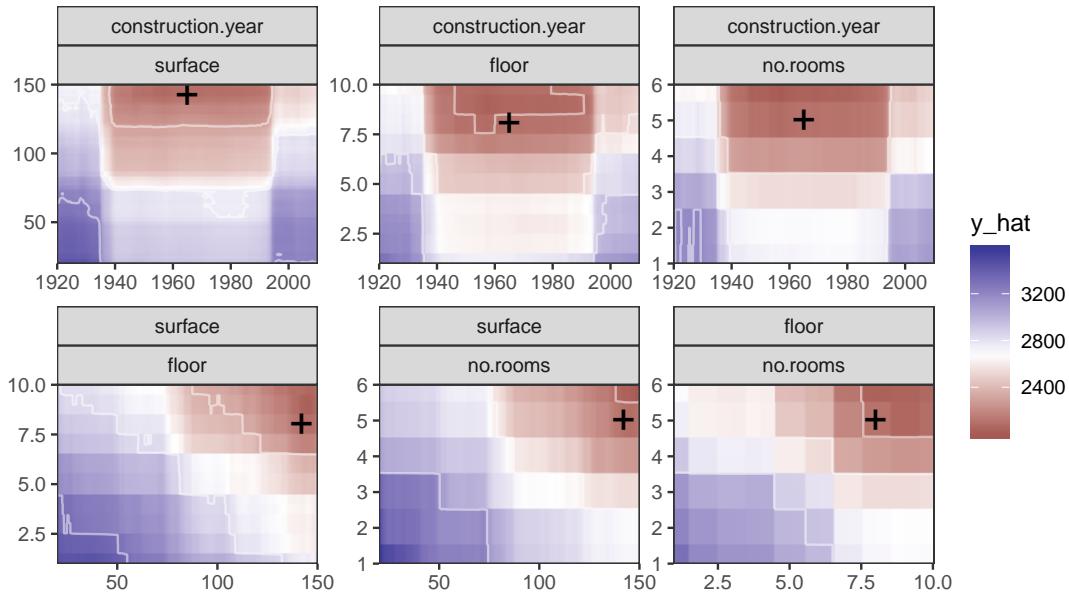


Figure 8.8: (fig:CP2Dall) Ceteris Paribus plot for all pairs of variables.

The idea behind fidelity plots is to select some number of points from the validation dataset that are close to the point of interest. It's a similar approach as in k nearest neighbours. Then for these neighbours we may plot Ceteris Paribus Profiles and check how stable they are.

Also, if we know true target values for points from the validation dataset we may plot residuals to show how large are residuals.

An example fidelity plot is presented in Figure ???. Black line shows the CP profiles for the point of interest, while grey lines show CP profiles for neighbors. Red intervals stand for residuals and in this example it looks like residuals for neighbors are all negative. Thus maybe model is biased around the point of interest.

This observation may be confirmed by plots that compare distribution of all residuals against distribution of residuals for neighbors.

See Figure ?? for an example. Here residuals for neighbors are shifted towards highest values. This suggests that the model response is biased around the observation of interest.

8.6 Pros and cons

Ceteris Paribus principle gives a uniform and extendable approach to model exploration. Below we summarize key strengths and weaknesses of this approach.

Pros

- Graphical representation of Ceteris Paribus profile is easy to understand.
- Ceteris Paribus profiles are compact and it is easy to fit many models or many variables in a small space.
- Ceteris Paribus profiles helps to understand how model response would change and how stable it is
- Oscillations calculated for CP profiles helps to select the most important variables.
- 2D Ceteris Paribus profiles help to identify pairwise interactions between variables.

Cons

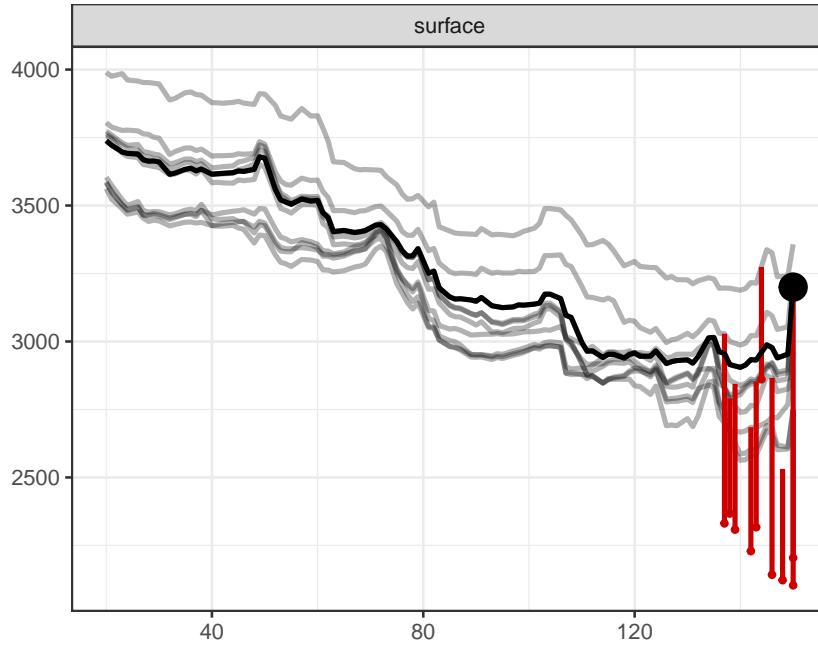


Figure 8.9: (fig;CPfidelity1) Local fidelity plots. Black line shows the CP profile for the point of interest. Grey lines show CP profiles for nearest neighbors. Red intervals correspond to residuals. Each red interval starts in a model prediction for a selected neighbor and ends in its true value of target variable.

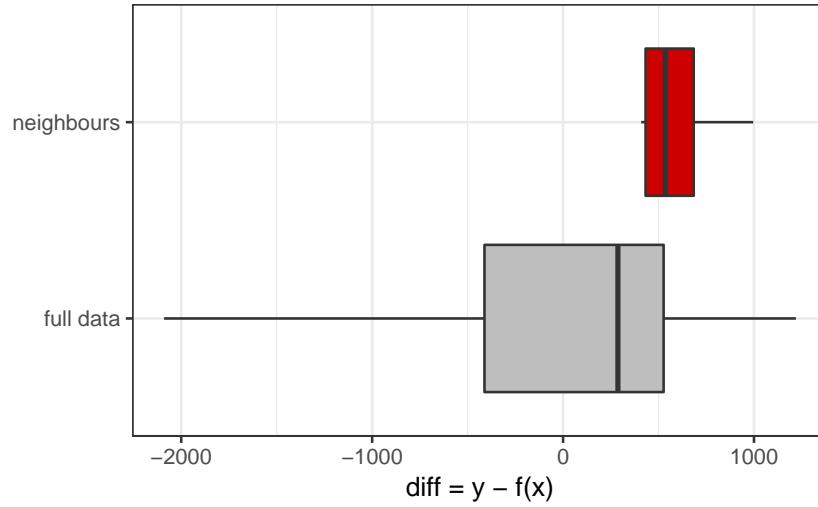


Figure 8.10: (fig;CPfidelityBoxplot) Distribution of residuals for whole validation data (grey boxplot) and for selected closes 15 neighbors (red boxplot).

- If variables are correlated (like surface and number of rooms) then the ‘*everything else kept unchanged*’ approach leads to unrealistic settings.
- Interactions between variables are not visible in 1D plots.
- This tool is not suited for very wide data, like hundreds or thousands of variables.
- Visualization of categorical variables is non trivial.

8.7 Code snippets for R

In this section we present key features of the `ceterisParibus` package for R (?). This package covers all features presented in this chapter. It is available on CRAN and GitHub. Find more examples at the website of this package <https://pbiecek.github.io/ceterisParibus/>.

Model preparation

In this section we will present examples based on the `apartments` dataset. See section TODO for more details.

```
library("DALEX")
head(apartments)
```

```
##   m2.price construction.year surface floor no.rooms    district
## 1      5897           1953     25     3       1 Srodmiescie
## 2      1818           1992    143     9       5     Bielany
## 3      3643           1937     56     1       2       Praga
## 4      3517           1995     93     7       3      Ochota
## 5      3013           1992    144     6       5      Mokotow
## 6      5795           1926     61     6       2 Srodmiescie
```

The problem here is to predict average price for square meter for an apartment. Let’s build a random forest model with `randomForest` package (?).

```
library("randomForest")
rf_model <- randomForest(m2.price ~ construction.year + surface + floor +
                           no.rooms, data = apartments)
rf_model

##
## Call:
## randomForest(formula = m2.price ~ construction.year + surface +      floor + no.rooms, data = apartments)
##                 Type of random forest: regression
##                         Number of trees: 500
## No. of variables tried at each split: 1
##
##                 Mean of squared residuals: 485220.9
##                               % Var explained: 40.92
```

Model exploration with `ceterisParibus` package is performed in four steps.

1. Create an explainer - wrapper around model and validation data.

Since all other functions work in a model agnostic fashion, first we need to define a wrapper around the model. Here we are using the `explain()` function from `DALEX` package (?).

```
library("DALEX")
explainer_rf <- explain(rf_model,
                        data = apartmentsTest, y = apartmentsTest$m2.price)
explainer_rf
```

```
## Model label: randomForest
## Model class: randomForest.formula,randomForest
## Data head :
##   m2.price construction.year surface floor no.rooms   district
## 1 1001      4644             1976     131      3       5 Srodmiescie
## 2 1002      3082             1978     112      9       4      Mokotow
```

2. Define point of interest.

Ceteris Paribus profiles explore model around a single point.

```
new_apartment <- data.frame(construction.year = 1965, no.rooms = 5, surface = 142, floor = 8)
new_apartment
```

```
##   construction.year no.rooms surface floor
## 1             1965         5     142     8
predict(rf_model, new_apartment)
```

```
##           1
## 2341.515
```

3. Calculate CP profiles

The `ceteris_paribus()` function calculates CP profiles for selected model around selected observation.

By default CP profiles are calculated for all numerical variables. Use the `variables` argument to select subset of interesting variables. The result from `ceteris_paribus()` function is a data frame with model predictions for modified points around the point of interest.

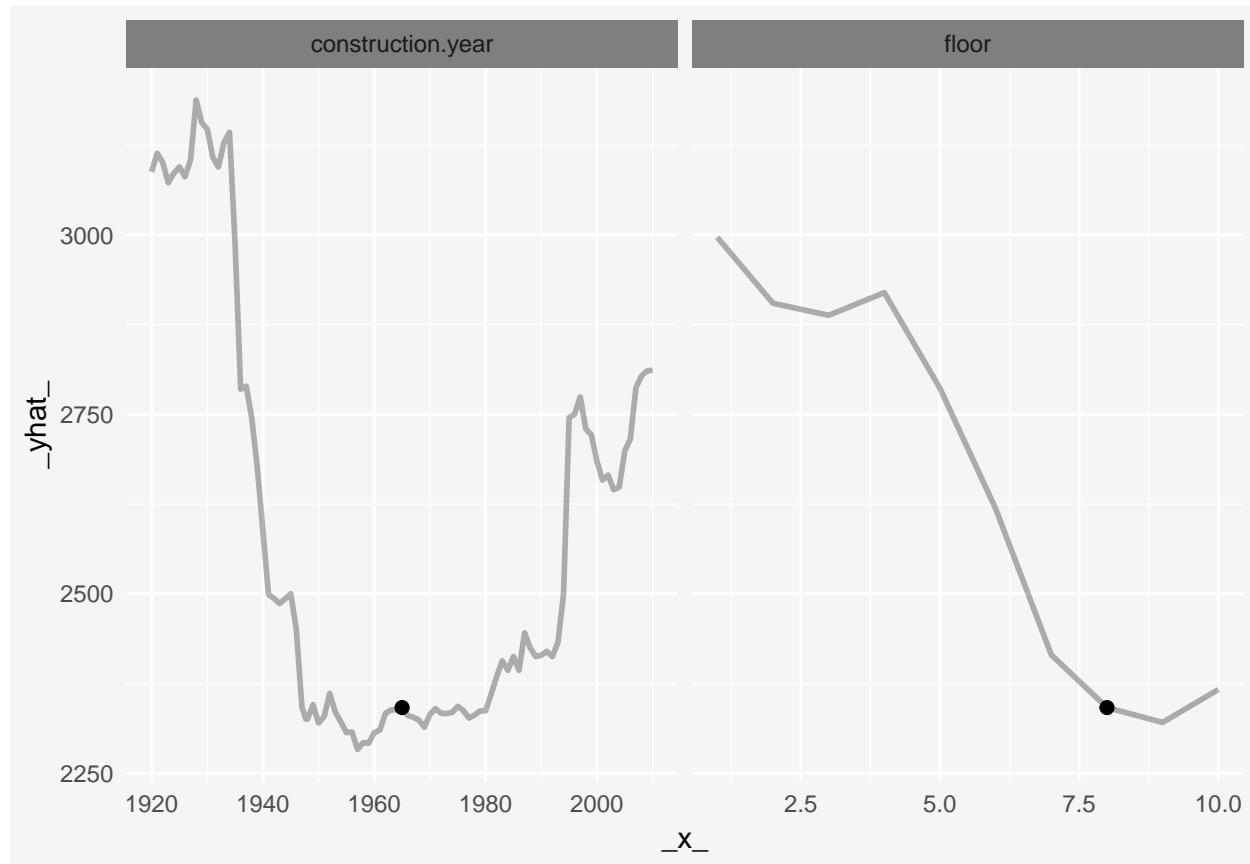
```
library("ceterisParibus")
cp_rf <- ceteris_paribus(explainer_rf, new_apartment,
                           variables = c("construction.year", "floor"))
cp_rf
```

```
## Top profiles    :
##   construction.year no.rooms surface floor   _yhat_      _vname_
## 1             1920         5     142     8 3087.961 construction.year
## 1.1            1921         5     142     8 3113.750 construction.year
## 1.2            1922         5     142     8 3100.954 construction.year
## 1.3            1923         5     142     8 3072.724 construction.year
## 1.4            1923         5     142     8 3072.724 construction.year
## 1.5            1924         5     142     8 3086.026 construction.year
##   _ids_      _label_
## 1      1 randomForest
## 1.1    1 randomForest
## 1.2    1 randomForest
## 1.3    1 randomForest
## 1.4    1 randomForest
## 1.5    1 randomForest
##
##
## Top observations:
##   construction.year no.rooms surface floor   _yhat_      _label_
## 1             1965         5     142     8 2341.515 randomForest
```

4. Plot CP profiles.

Generic `plot()` function plot CP profiles. It returns a `ggplot2` object that can be polished if needed. Use additional arguments of this function to select colors and sizes for elements visible in the plot.

```
plot(cp_rf)
```



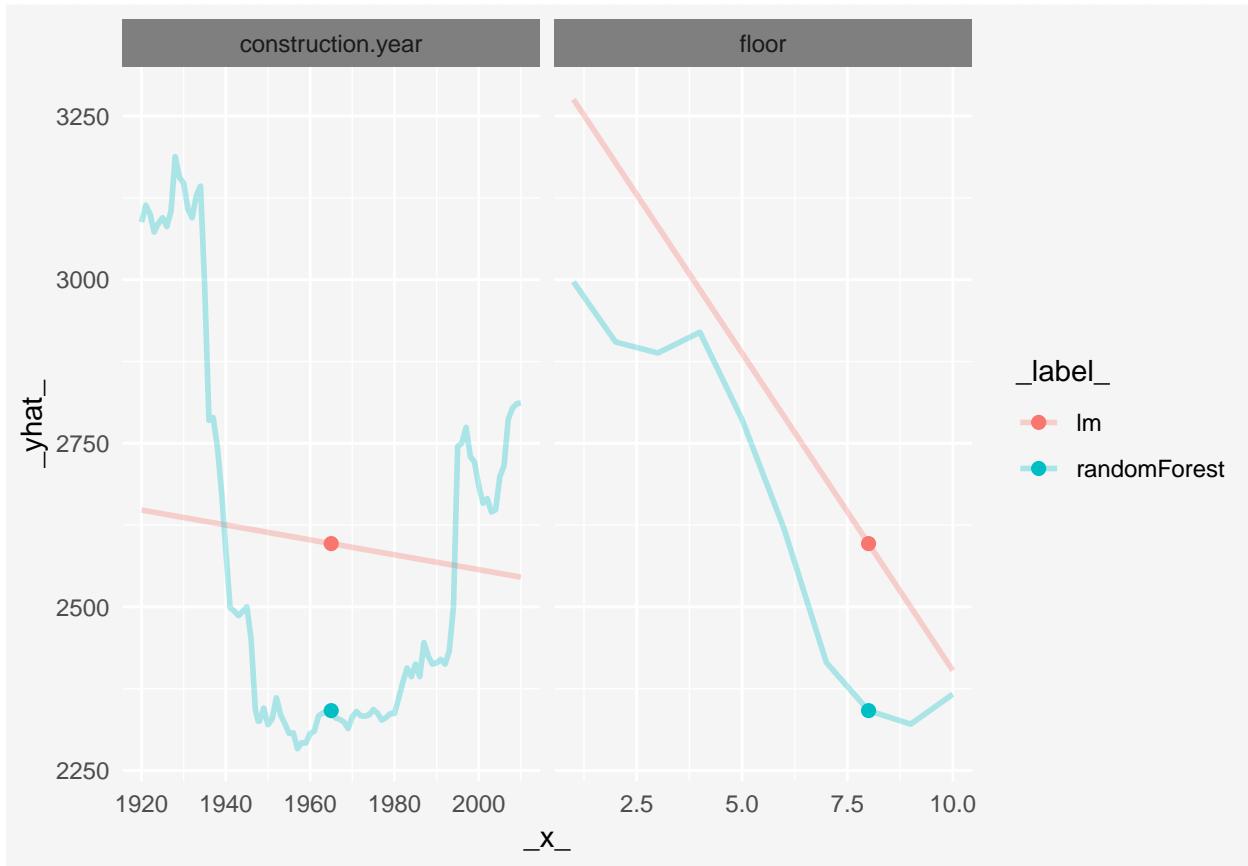
One of very useful features of `ceterisParibus` explainers is that profiles for two or more models may be superimposed in a single plot. This helps in model comparisons.

Let's create a linear model for this dataset and repeat steps 1-3 for the lm model.

```
lm_model <- lm(m2.price ~ construction.year + surface + floor +
  no.rooms, data = apartments)
explainer_lm <- explain(lm_model,
  data = apartmentsTest, y = apartmentsTest$m2.price)
cp_lm <- ceteris_paribus(explainer_lm, new_apartment,
  variables = c("construction.year", "floor"))
```

Now we can use function `plot()` to compare both models in a single chart. Additional argument `color = "_label_"` set color as a key for model.

```
plot(cp_rf, cp_lm, color = "_label_")
```

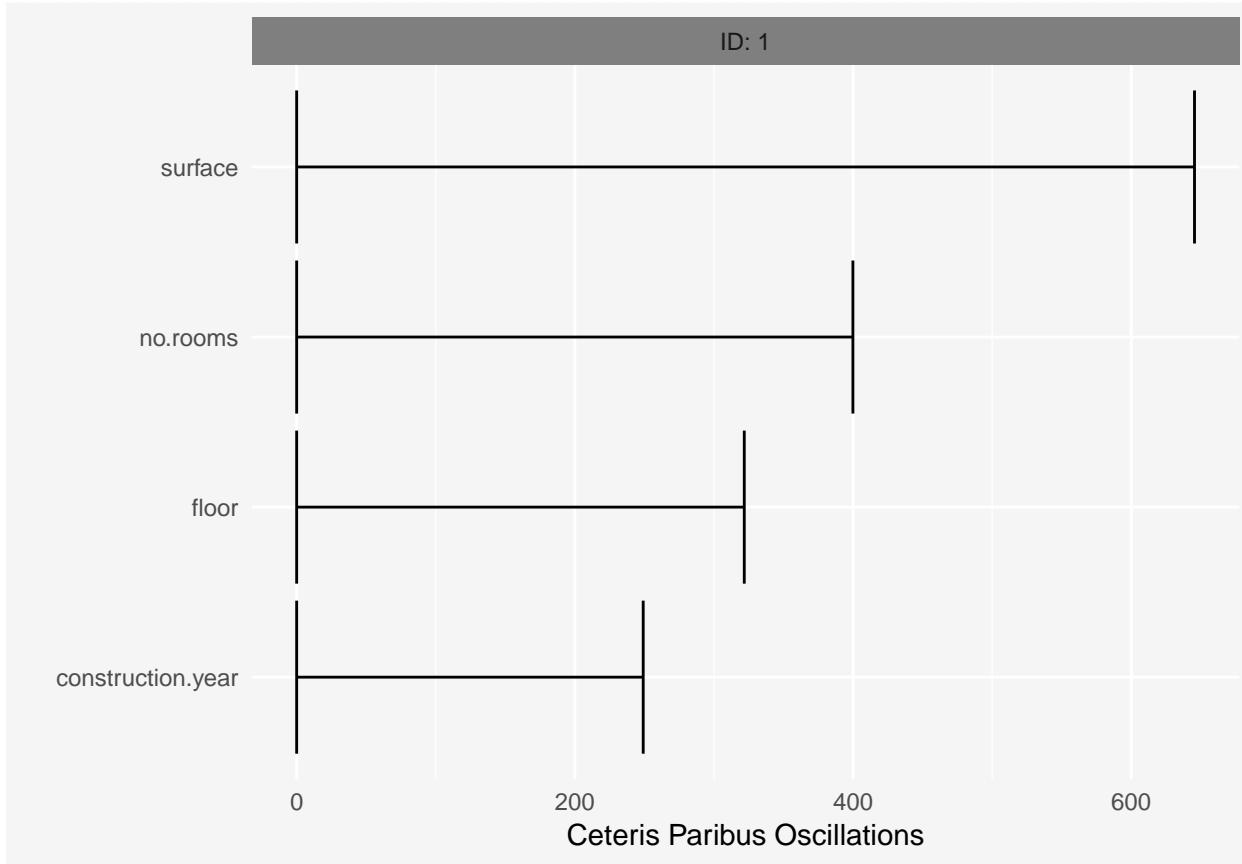


Oscillations

The `calculate_oscillations()` function calculates oscillations for CP profiles.

```
cp_rf_all <- ceteris_paribus(explainer_rf, new_apartment)
co_rf_all <- calculate_oscillations(cp_rf_all)
co_rf_all
```

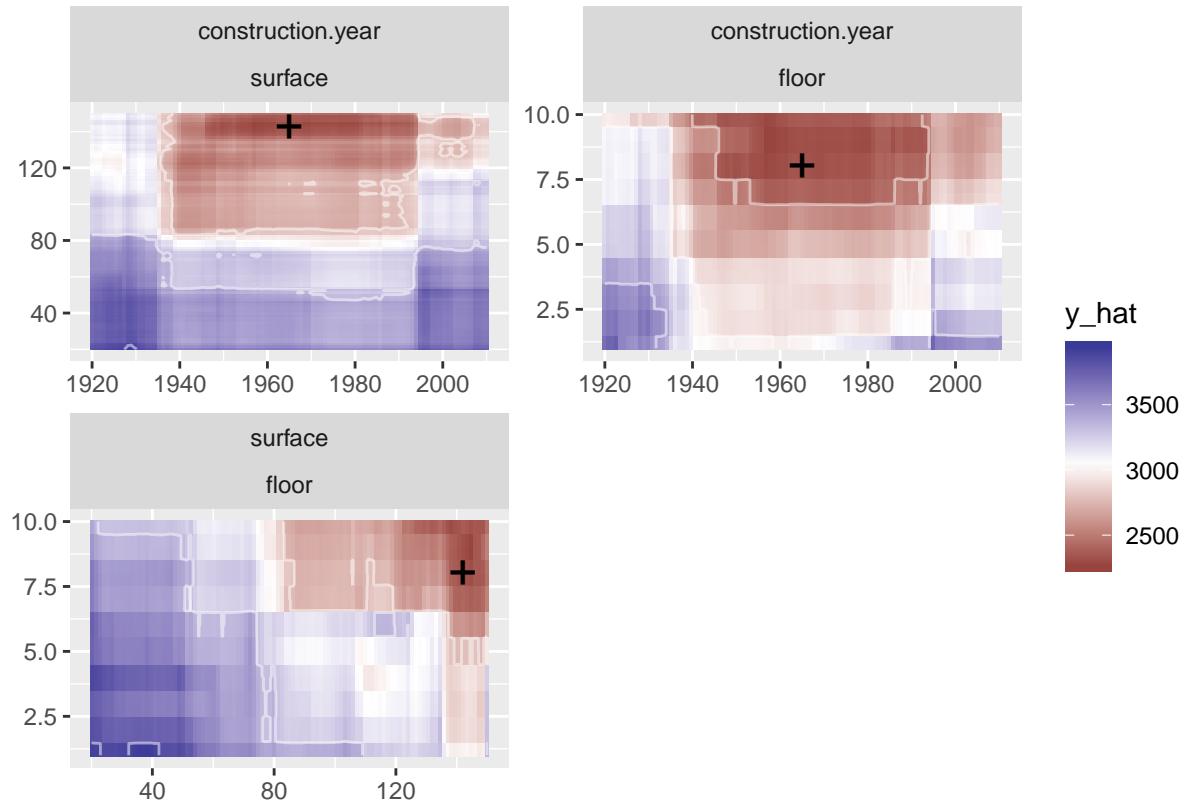
```
##          _vname_ _ids_ oscillations
## 2        surface    1     645.4397
## 4      no.rooms    1     399.8738
## 3         floor    1     321.7802
## 1 construction.year    1     249.1199
plot(co_rf_all)
```



2D Ceteris Paribus profiles

And the `what_if_2d()` function calculates 2D CP profiles.

```
wi_rf_2d <- what_if_2d(explainer_rf, observation = new_apartment,
                         selected_variables = c("surface", "floor", "construction.year"))
plot(wi_rf_2d, split_ncol = 2)
```



Model level explanations

Chapter 9

Introduction

9.1 A bit of philosophy

Rights:

1. audit model residuals
2. variable importance
3. partial dependency plot

9.2 Example: Price prediction

(?)

(?)

(?)

```
library("factorMerger")
```

In this chapter we show examples for three predictive models trained on `apartments` dataset from the `DALEX` package. Random Forest model (elastic but biased), Support Vector Machines model (large variance on boundaries) and Linear Model (stable but not very elastic). Presented examples are for regression (prediction of square meter price), but the CP profiles may be used in the same way for classification.

```
library("DALEX")
# Linear model trained on apartments data
model_lm <- lm(m2.price ~ construction.year + surface + floor +
                 no.rooms + district, data = apartments)

library("randomForest")
set.seed(59)
# Random Forest model trained on apartments data
model_rf <- randomForest(m2.price ~ construction.year + surface + floor +
                           no.rooms + district, data = apartments)

library("e1071")
# Support Vector Machinesr model trained on apartments data
model_svm <- svm(m2.price ~ construction.year + surface + floor +
                  no.rooms + district, data = apartments)
```

For these models we use DALEX explainers created with `explain()` function. There explainers wrap models, predict functions and validation data.

```
explainer_lm <- explain(model_lm,
                         data = apartmentsTest[,2:6], y = apartmentsTest$m2.price)
explainer_rf <- explain(model_rf,
                         data = apartmentsTest[,2:6], y = apartmentsTest$m2.price)
explainer_svm <- explain(model_svm,
                         data = apartmentsTest[,2:6], y = apartmentsTest$m2.price)
```

Examples presented in this chapter are generated with the `ceterisParibus` package in version 0.3.1.

```
library("ceterisParibus")
```

Chapter 10

Variable Importance

Feature selection

(?) (?) - variable importance

(?)

Beware Default Random Forest Importances

Terence Parr, Kerem Turgutlu, Christopher Csiszar, and Jeremy Howard March 26, 2018.

<http://explained.ai/rf-importance/index.html>

Chapter 11

Marginal Response

Feature extraction

11.1 Partial Dependency Plots

Accumulated Local Effects (ALE) Plots

(?) (?)

```
library(ALEPlot)
```

(?)

Interactions - extraction

11.2 Merging Path Plots

(?)

```
library(factorMerger)
```


Chapter 12

Performance Diagnostic

Model selection

Chapter 13

Residual Diagnostic

Model validation

(?)

```
library(auditor)
```


Chapter 14

Other topics

(?) (?) (?)

```
library(randomForestExplainer)
library(ICEbox)
library(ALEPlot)
```

(?)

```
library(modelDown)
```


Appendices

Chapter 15

Data Sets

15.1 Hire or Fire? HR in Call Center

In this chapter we present an artificial dataset from Human Resources department in a Call Center to present pros and cons for different techniques of prediction level explainers.

The dataset is available in the `DALEX` package (?). Each row corresponds to a single employee of a call center. Features like gender, age, average number of working hours per week, grade from the last evaluation and level of salary are used as predictive features.

The problem here is to first build a model, that will determine when to fires and when to promote an employer, so it's a classification problem with three classes. But having a model we will use prediction level explainers to better understand how the model works for selected cases.

```
library("DALEX")
head(HR)

##   gender     age   hours evaluation salary   status
## 1 male 32.58267 41.88626      3      1    fired
## 2 female 41.21104 36.34339      2      5    fired
## 3 male 37.70516 36.81718      3      0    fired
## 4 female 30.06051 38.96032      3      2    fired
## 5 male 21.10283 62.15464      5      3 promoted
## 6 male 40.11812 69.53973      2      0    fired
```

In this book we are focused on model exploration rather than model building, thus for sake of simplicity we will use two default models created with random forest (?) and generalized linear model (?).

```
set.seed(59)
library("randomForest")
model_rf <- randomForest(status ~ gender + age + hours + evaluation + salary, data = HR)

library("nnet")
model_glm <- multinom(status ~ gender + age + hours + evaluation + salary, data = HR)

## # weights:  21 (12 variable)
## initial value 8620.810629
## iter  10 value 7002.127738
## iter  20 value 6239.478146
## iter  20 value 6239.478126
## iter  20 value 6239.478124
```

```
## final value 6239.478124
## converged
```

15.2 How much does it cost? Price prediction for a square meter

In this chapter we present an artificial dataset related to prediction of prices for appartments in Warsaw. This dataset wil be used to discuss pros and cons for different techniques of model level explainers.

The dataset is available in the DALEX package (?). Each row corresponds to a single apartment. Features like surface, number of rooms, district or floor are used as predictive features.

The problem here is to predict price of a square meter for an appartment, so it's a regression problem with continouse outcome.

```
library("DALEX")
head(Apartments)
```

```
##   m2.price construction.year surface floor no.rooms   district
## 1      5897            1953     25    3       1 Srodmiescie
## 2      1818            1992    143    9       5     Bielany
## 3      3643            1937     56    1       2       Praga
## 4      3517            1995     93    7       3     Ochota
## 5      3013            1992    144    6       5     Mokotow
## 6      5795            1926     61    6       2 Srodmiescie
```

The problem here is to predict average price for square meter for an apartment. Let's build a random forest model with randomForest package (?).

```
library("randomForest")
model_rf <- randomForest(m2.price ~ construction.year + surface + floor + no.rooms + district, data = Apartments)
model_rf
```

```
##
## Call:
## randomForest(formula = m2.price ~ construction.year + surface +
##                 floor + no.rooms + district, data = Apartments)
##               Type of random forest: regression
##                   Number of trees: 500
## No. of variables tried at each split: 1
##
##           Mean of squared residuals: 82079.37
##                           % Var explained: 90.01
```

And a linear model.

```
model_lm <- lm(m2.price ~ construction.year + surface + floor + no.rooms + district, data = Apartments)
model_lm
```

```
##
## Call:
## lm(formula = m2.price ~ construction.year + surface + floor +
##     no.rooms + district, data = Apartments)
##
## Coefficients:
## (Intercept)  construction.year          surface
##             5020.139                  -0.229        -10.238
##             floor                  no.rooms      districtBielany
##             -99.482                 -37.730                  17.214
```

```
##      districtMokotow      districtOchota      districtPraga
##            918.380           926.254          -37.105
## districtSrodmiescie      districtUrsus      districtUrsynow
##           2080.611            29.942          -18.865
##      districtWola      districtZoliborz
##            -16.891            889.973
```