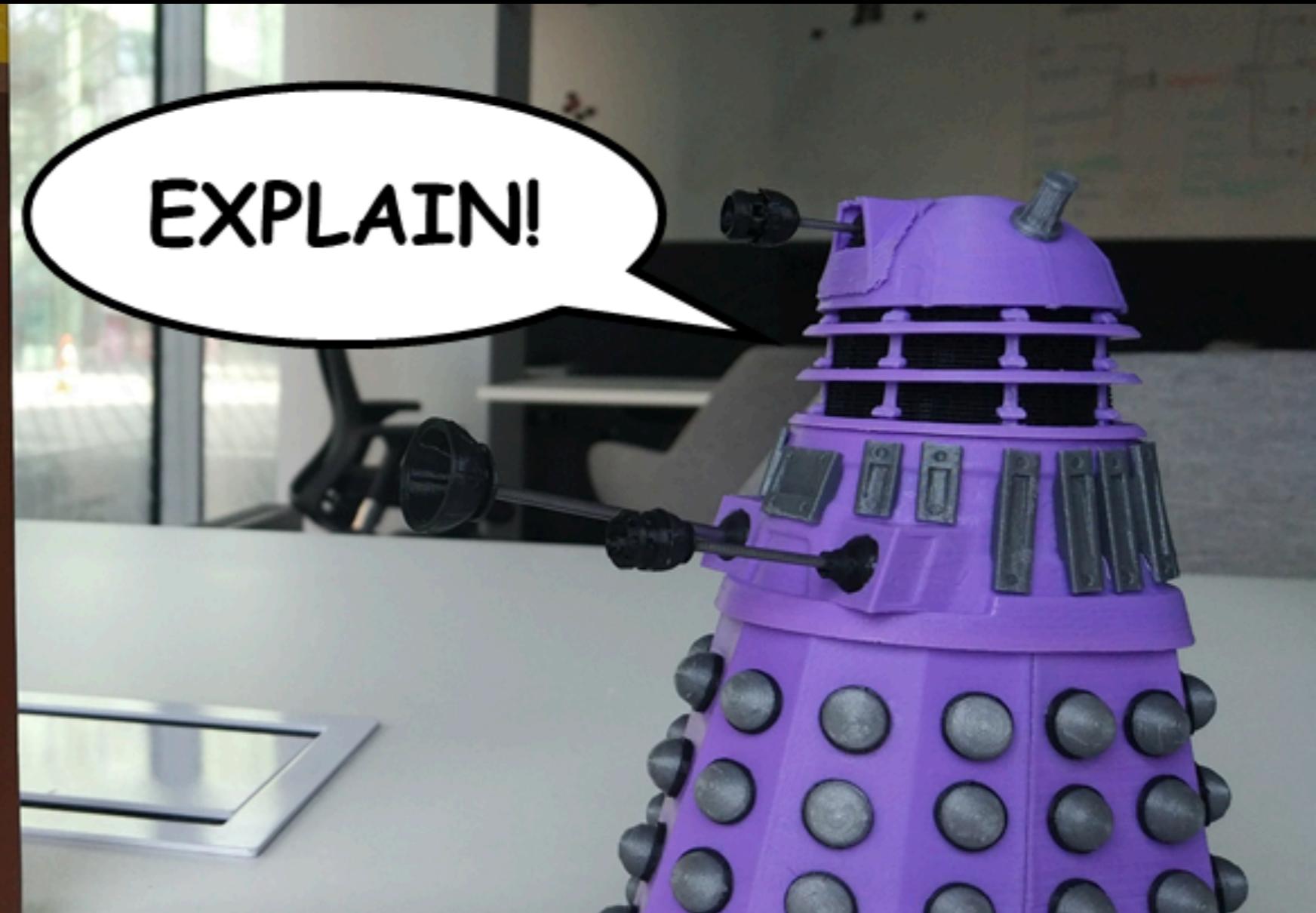
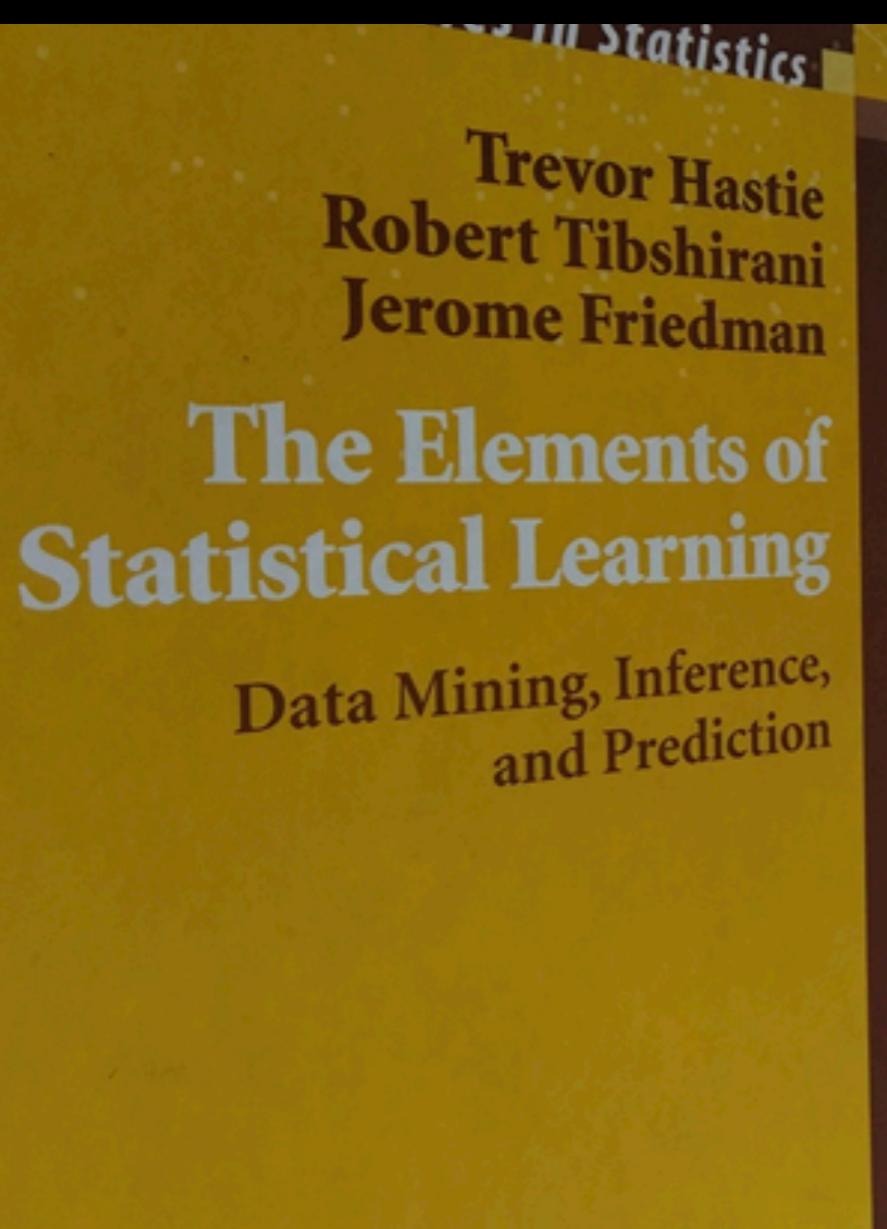
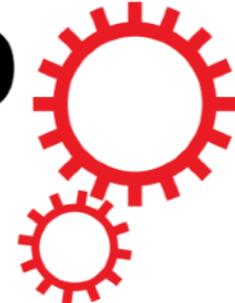


# explain! explain! explain!



Przemysław Biecek

The Good, the Bad  
and the Ugly



OPEN

# An application of machine learning to haematological diagnosis

Gregor Gunčar<sup>1</sup>, Matjaž Kukar<sup>1</sup>, Mateja Notar<sup>1</sup>, Miran Brvar<sup>2</sup>, Peter Černelč<sup>3</sup>, Manca Notar<sup>1</sup> & Marko Notar<sup>1</sup>

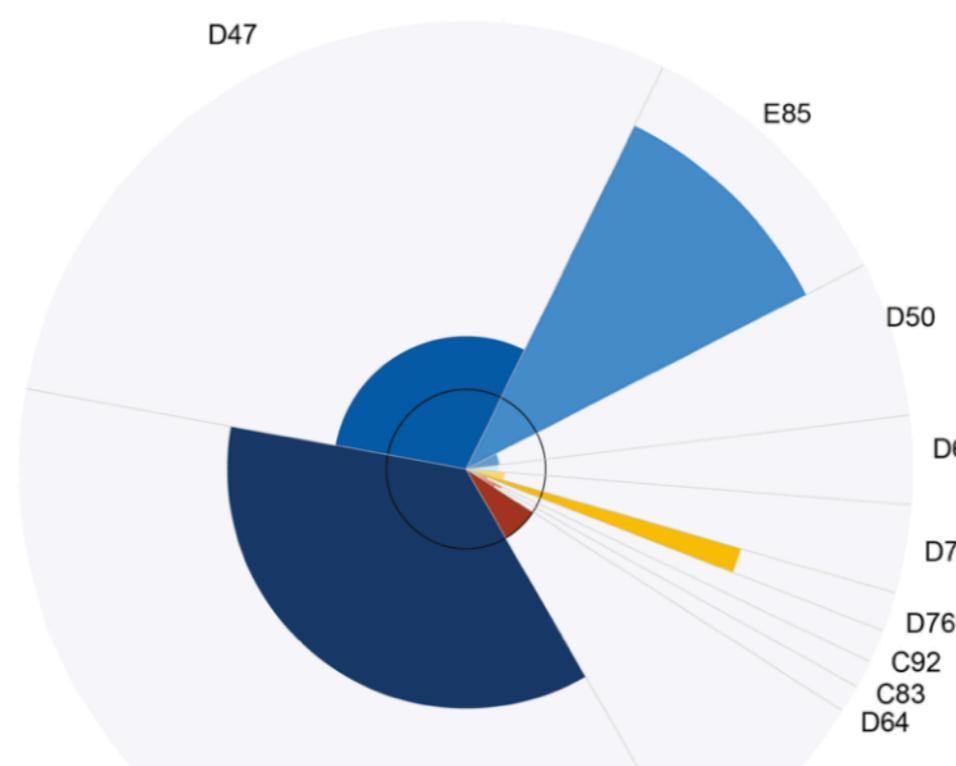
Received: 2 August 2017

Accepted: 14 December 2017

Published online: 11 January 2018

Quick and accurate medical diagnoses are crucial for the successful treatment of diseases. Using machine learning algorithms and based on laboratory blood test results, we have built two models to predict a haematologic disease. One predictive model used all the available blood test parameters and the other used only a reduced set that is usually measured upon patient admittance. Both models produced good results, obtaining prediction accuracies of 0.88 and 0.86 when considering the list of five most likely diseases and 0.59 and 0.57 when considering only the most likely disease. The models did not do well at distinguishing between diseases with similar symptoms.

"fingerprints" of diseases can be found in the blood. These "fingerprints" can be used to predict diseases based on laboratory blood test results. Machine learning can be used to build predictive models that can quickly and accurately predict diseases. These models can be used to support clinical decision-making. In this study, we used machine learning to predict haematological diseases based on laboratory blood test results. We built two predictive models: one that used all the available blood test parameters and another that used only a reduced set of parameters that are usually measured upon patient admittance. Both models produced good results, obtaining prediction accuracies of 0.88 and 0.86 when considering the list of five most likely diseases and 0.59 and 0.57 when considering only the most likely disease. The models did not do well at distinguishing between diseases with similar symptoms.



ICD code	Prediction	Information score	Disease category
C90	36.20%	2.01	Multiple myeloma and malignant plasma cell neoplasms
D47	29.40%	0.67	Other neoplasms of uncertain or unknown behaviour of lymphoid, haematopoietic and related tissue
E85	10.20%	3.81	Amyloidosis
D50	5.60%	-1.37	Iron deficiency anaemia
D69	3.20%	-1.50	Purpura and other haemorrhagic conditions
D75	3.20%	-1.05	Other diseases of blood and blood-forming organs
D76	1.40%	2.60	Certain diseases involving lymphoreticular tissue and reticulohistiocytic system
C92	1.20%	-2.55	Myeloid leukaemia
C83	1.00%	-1.01	Diffuse non-Hodgkin lymphoma
D64	1.00%	-1.41	Other anaemias

# Prediction of cardiovascular risk factors from retinal fundus photographs via deep learning

Ryan Poplin<sup>1,4</sup>, Avinash V. Varadarajan<sup>1,4</sup>, Katy Blumer<sup>1</sup>, Yun Liu<sup>1</sup>, Michael V. McConnell<sup>2,3</sup>, Greg S. Corrado<sup>1</sup>, Lily Peng<sup>1,4\*</sup> and Dale R. Webster<sup>1,4</sup>

Traditionally, medical discoveries are made by observing associations, making hypotheses from them and then designing and running experiments to test the hypotheses. However, with medical images, observing and quantifying associations can often be difficult because of the wide variety of features, patterns, colours, values and shapes that are present in real data. Here, we show that deep learning can extract new knowledge from retinal fundus images. Using deep-learning models trained on data from 284,335 patients and validated on two independent datasets of 12,026 and 999 patients, we predicted cardiovascular risk factors not previously thought to be present or quantifiable in retinal images, such as age (mean absolute error within 3.26 years), gender (area under the receiver operating characteristic curve (AUC) = 0.97), smoking status (AUC = 0.71), systolic blood pressure (mean absolute error within 11.23 mmHg) and major adverse cardiac events (AUC = 0.70). We also show that the trained deep-learning models used anatomical features, such as the optic disc or blood vessels, to generate each prediction.

Risk stratification is central to identifying and managing groups at risk for cardiovascular disease, which remains the leading cause of death globally<sup>1</sup>. Although the availability of cardiovascular disease risk calculators, such as the Pooled Cohort equations<sup>2</sup>, Framingham<sup>3–5</sup> and Systematic Coronary Risk Evaluation (SCORE)<sup>6,7</sup>, is widespread, there are many efforts to improve risk predictions. Phenotypic information, particularly of vascular health, may further refine or reclassify risk prediction on an

changes<sup>22,23</sup> and temic health clinical utility work, we dem cardiovascula Machine le ety of classifi of eye disease



# Prediction of cardiovascular risk factors from retinal fundus photographs via deep learning

Ryan P...  
Greg S.  
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risk factor  
years), ge  
blood pres  
the trained

Imagine that these are predictions for you.

Would you trust them?

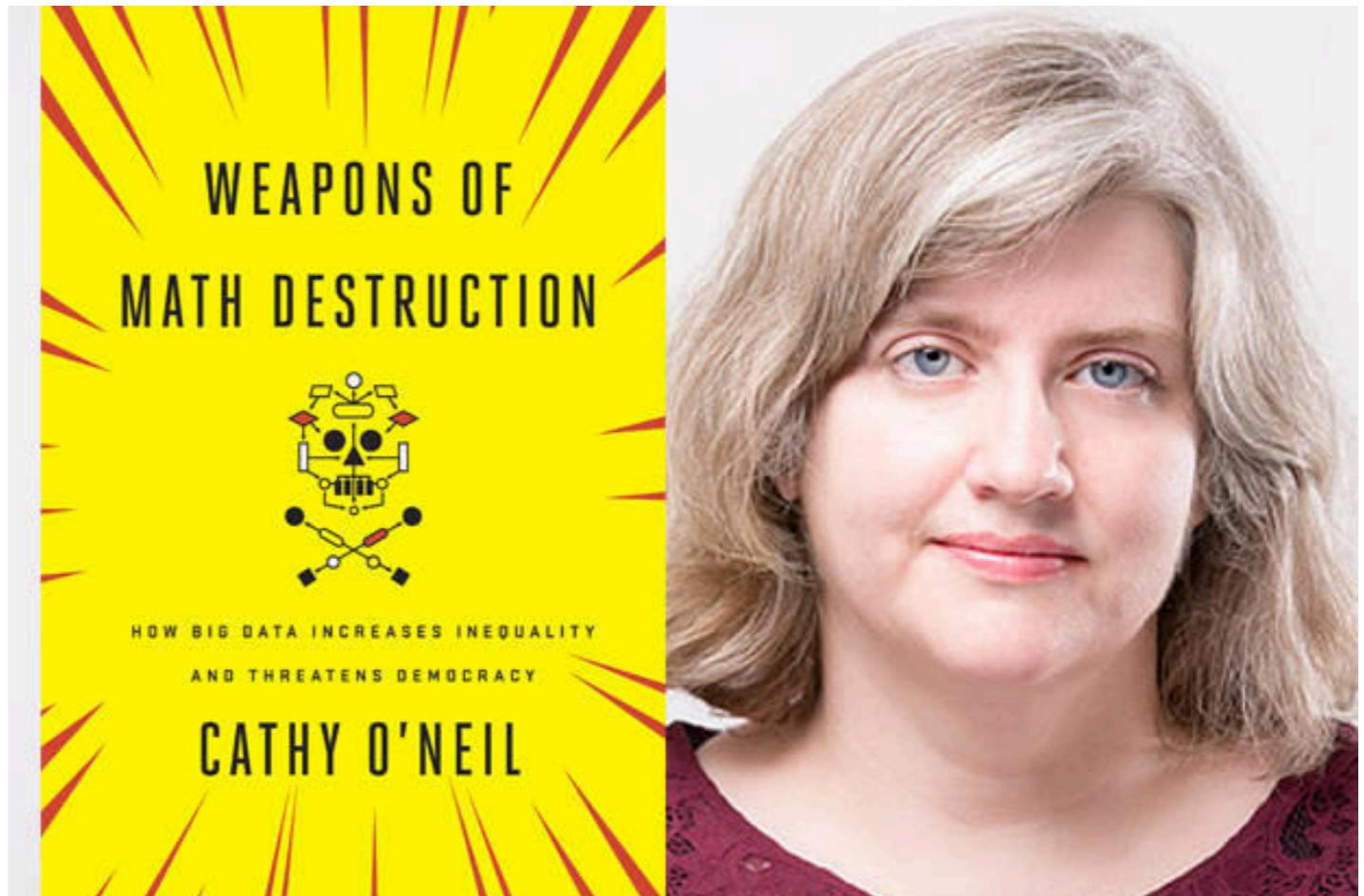
Risk str at risk for cardiovascular disease, which remains the leading cause of death globally<sup>1</sup>. Although the availability of cardiovascular disease risk calculators, such as the Pooled Cohort equations<sup>2</sup>, Framingham<sup>3-5</sup> and Systematic COronary Risk Evaluation SCORE)<sup>6,7</sup>, is widespread, there are many efforts to improve risk predictions. Phenotypic information, particularly of vascular health, may further refine or reclassify risk prediction on an

epidemiologic level by reflecting the systemic health of the cardiovascular system as well as future risk. The clinical utility of such features still requires further study. In this work, we demonstrate the extraction and quantification of multiple cardiovascular risk factors from retinal images using deep learning.

Machine learning has been leveraged for many years for a variety of classification tasks, including the automated classification of eye disease. However, much of the work has focused on 'feature

# Why do we need explanations for complex models?

**Cathy O'Neil:**  
**The era of blind faith**  
machine learning  
~~in big data must end~~



- “You don’t see a lot of skepticism,” she says. “The algorithms are like shiny new toys that we can’t resist using. We trust them so much that we project meaning on to them.”
- Ultimately algorithms, according to O’Neil, reinforce discrimination and widen inequality, “using people’s fear and trust of mathematics to prevent them from asking questions”.

<https://www.theguardian.com/books/2016/oct/27/cathy-oneil-weapons-of-math-destruction-algorithms-big-data>

# Why do we need explanations for complex models?

## Right to explanation

From Wikipedia, the free encyclopedia

In the [regulation of algorithms](#), particularly [artificial intelligence](#) and its subfield of [machine learning](#), a **right to explanation** (or **right to an explanation**) is a [right](#) to be given an [explanation](#) for an output of the algorithm. Such rights primarily refer to [individual rights](#) to be given an explanation for decisions that significantly affect an individual, particularly legally or financially. For example, a person who applies for a loan and is denied may ask for an explanation, which could be "Credit bureau X reports that you declared bankruptcy last year; this is the main factor in considering you too likely to default, and thus we will not give you the loan you applied for."

Some such [legal rights](#) already exist, while the scope of a general "right to explanation" is a matter of ongoing debate.

### Contents [\[hide\]](#)

- 1 [Examples](#)
  - 1.1 [Credit score in the United States](#)
  - 1.2 [European Union](#)
  - 1.3 [France](#)
- 2 [Criticism](#)
- 3 [See also](#)
- 4 [References](#)
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# Why do we need explanations for complex models?

## European Union [ edit ]

The European Union [General Data Protection Regulation](#) (enacted 2016, taking effect 2018), extends the automated decision-making rights in the 1995 [Data Protection Directive](#) to provide a legally disputed form of a right to an explanation, stated as such in [Recital 71](#): "[the data subject should have] the right ... to obtain an explanation of the decision reached". In full:

The data subject should have the right not to be subject to a decision, which may include a measure, evaluating personal aspects relating to him or her which is based solely on automated processing and which produces legal effects concerning him or her or similarly significantly affects him or her, such as automatic refusal of an online credit application or e-recruiting practices without any human intervention.

...

In any case, such processing should be subject to suitable safeguards, which should include specific information to the data subject and the right to obtain human intervention, to express his or her point of view, to obtain an explanation of the decision reached after such assessment and to challenge the decision.

However, the extent to which the regulations themselves provide a "right to explanation" is heavily debated.<sup>[4][5]</sup> There are two main strands of criticism. There are significant legal issues with the right as found in Article 22 — as recitals are not binding, and the right to an explanation is not mentioned in the binding articles of the text, having been removed during the legislative process.<sup>[6]</sup> In addition, there are significant restrictions on the types of automated decisions that are covered — which must be both "solely" based on automated processing, and have legal or similarly significant effect — which limits their applicability in many of the cases of algorithmic controversy that have been picked up in the media.<sup>[7]</sup>

# Single prediction explainers

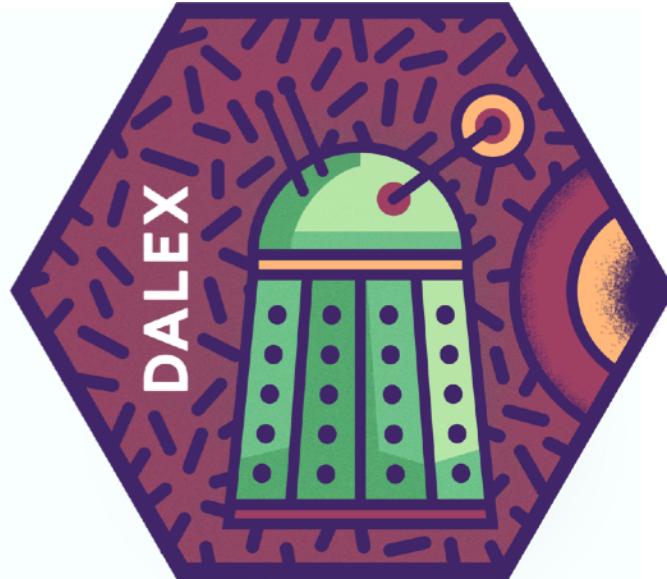
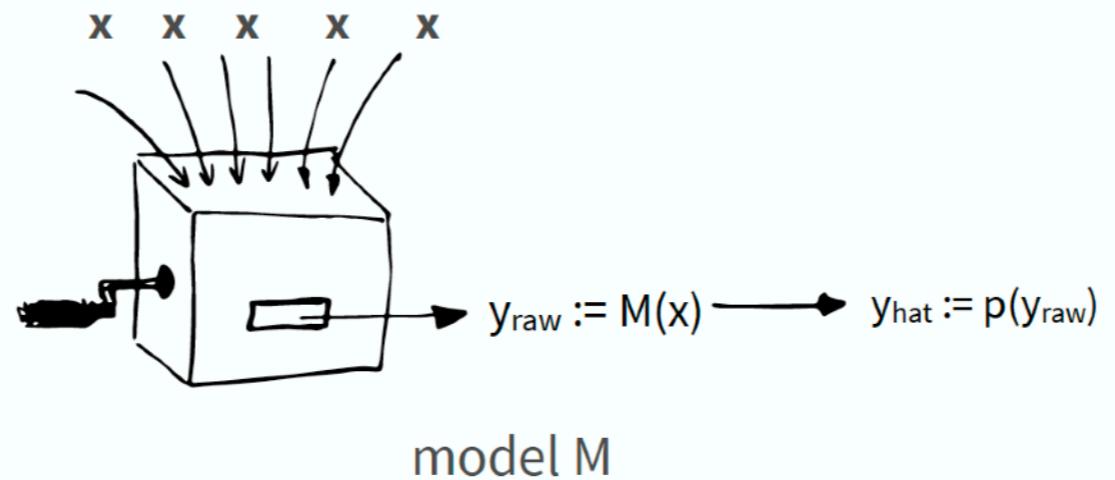




```
library("DALEX")
head(apartments)
```

m2.price	construction.year	surface	floor	no.rooms	district
5897	1953	25	3		1 Śródmieście
1818	1992	143	9		5 Bielany
3643	1937	56	1		2 Praga
3517	1995	93	7		3 Ochota
3013	1992 <sup>11</sup>	144	6		5 Mokotów

A)



B)

```
explain(model; data; y; predict_function; trans)
```

```
library("DALEX")
apartments_lm_model <- lm(m2.price ~ construction.year + surface + floor +
                           no.rooms + district, data = apartments)

library("randomForest")
set.seed(59)
apartments_rf_model <- randomForest(m2.price ~ construction.year + surface + floor +
                                       no.rooms + district, data = apartments)

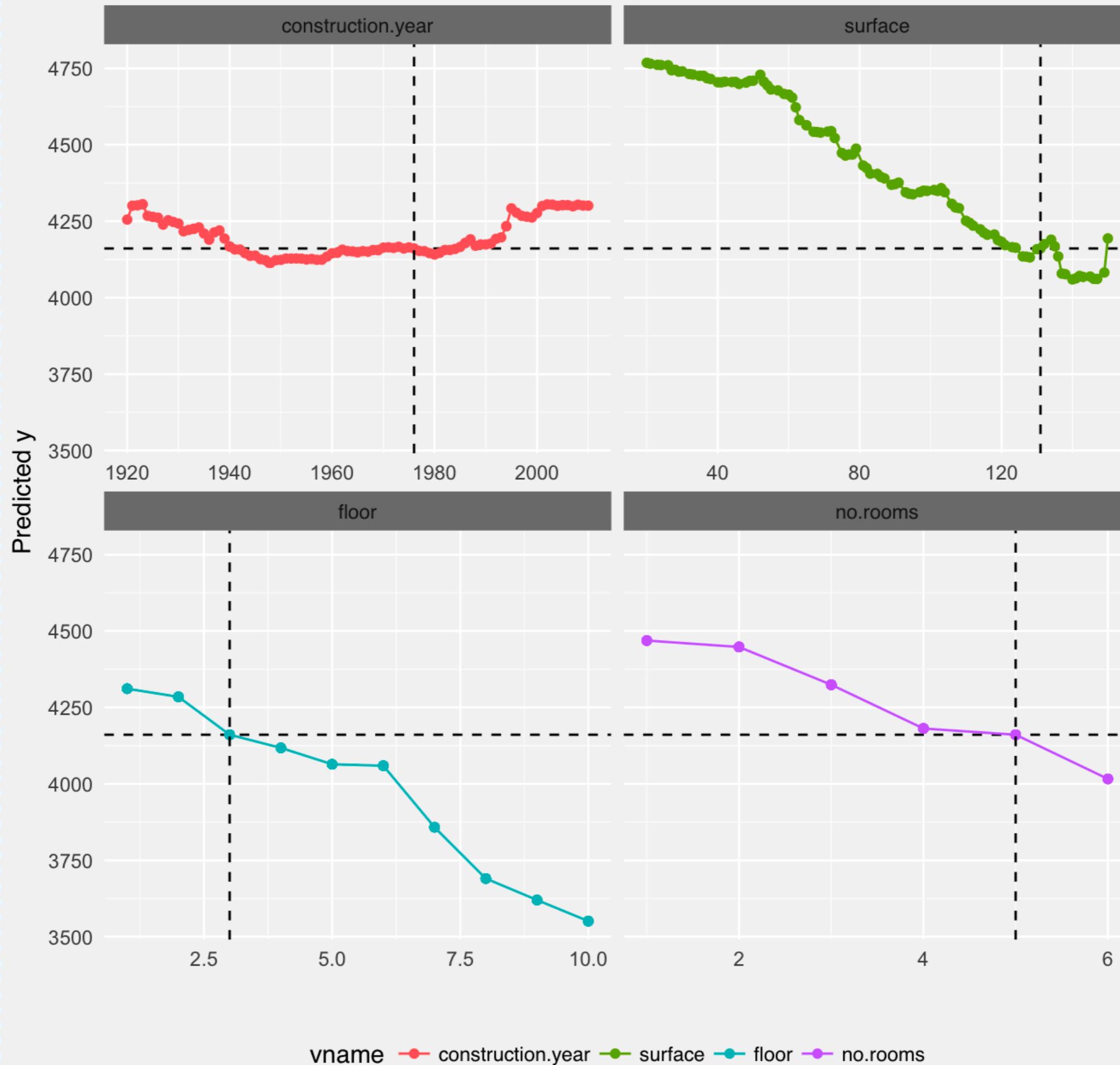
explainer_lm <- explain(apartments_lm_model,
                         data = apartmentsTest[,2:6], y = apartmentsTest$m2.price)

explainer_rf <- explain(apartments_rf_model,
                         data = apartmentsTest[,2:6], y = apartmentsTest$m2.price)
```

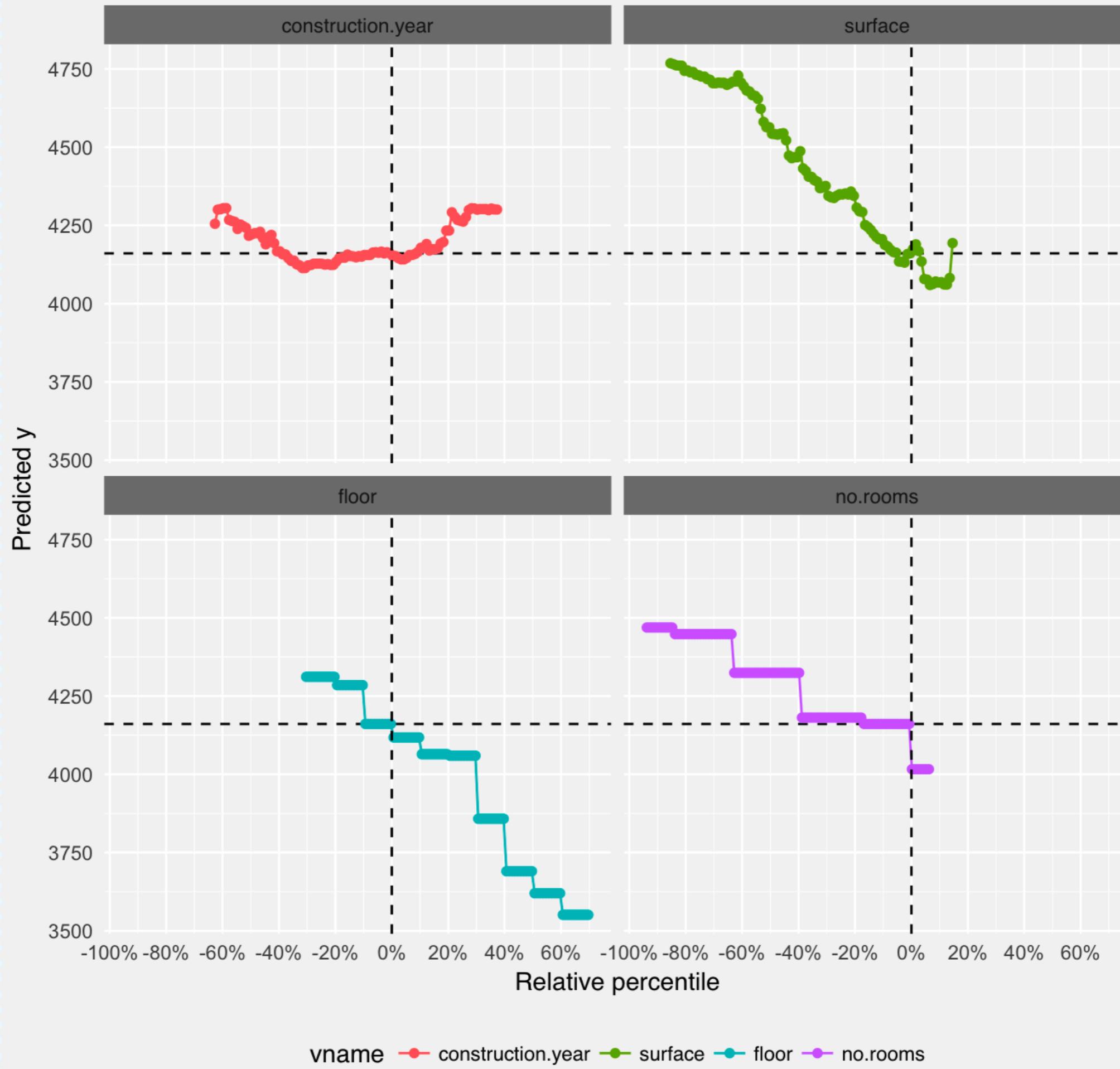
Case:  
large (130 m<sup>2</sup>) flat, 5 rooms, 3 rd floor  
from 1970

Prediction:  
4200 E/m<sup>2</sup>

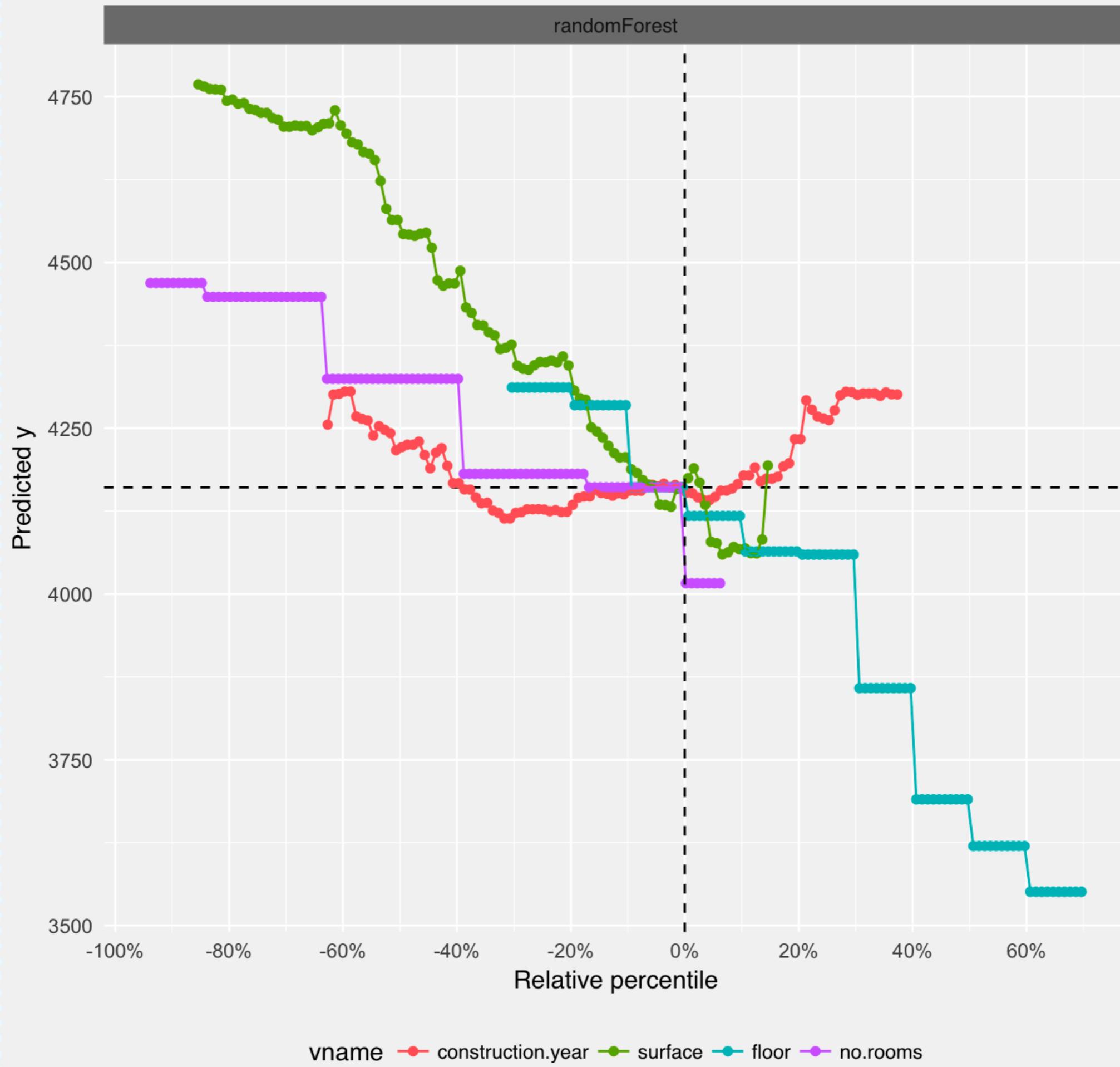
# Ceteris Paribus Plot



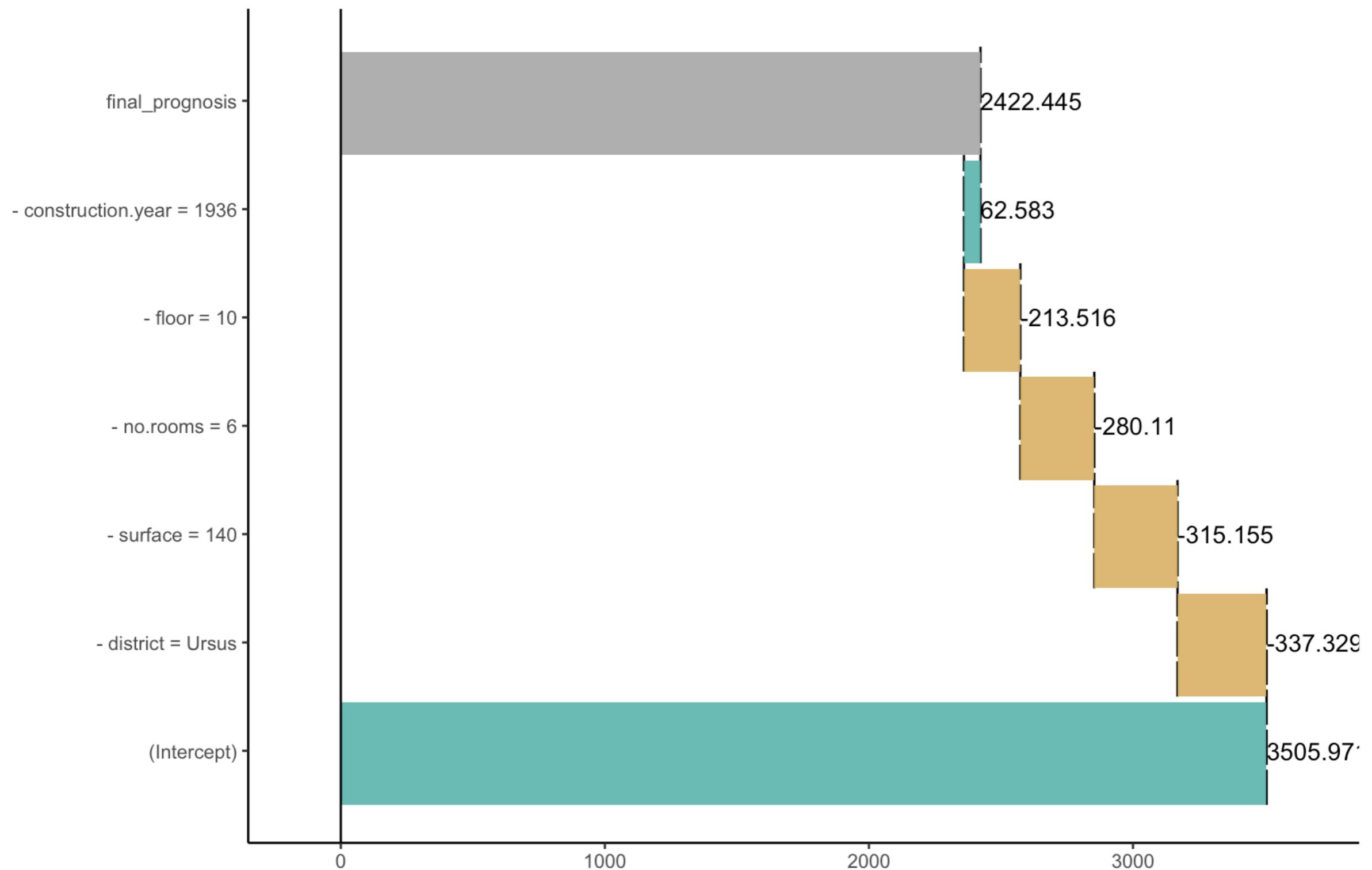
# Ceteris Paribus Plot



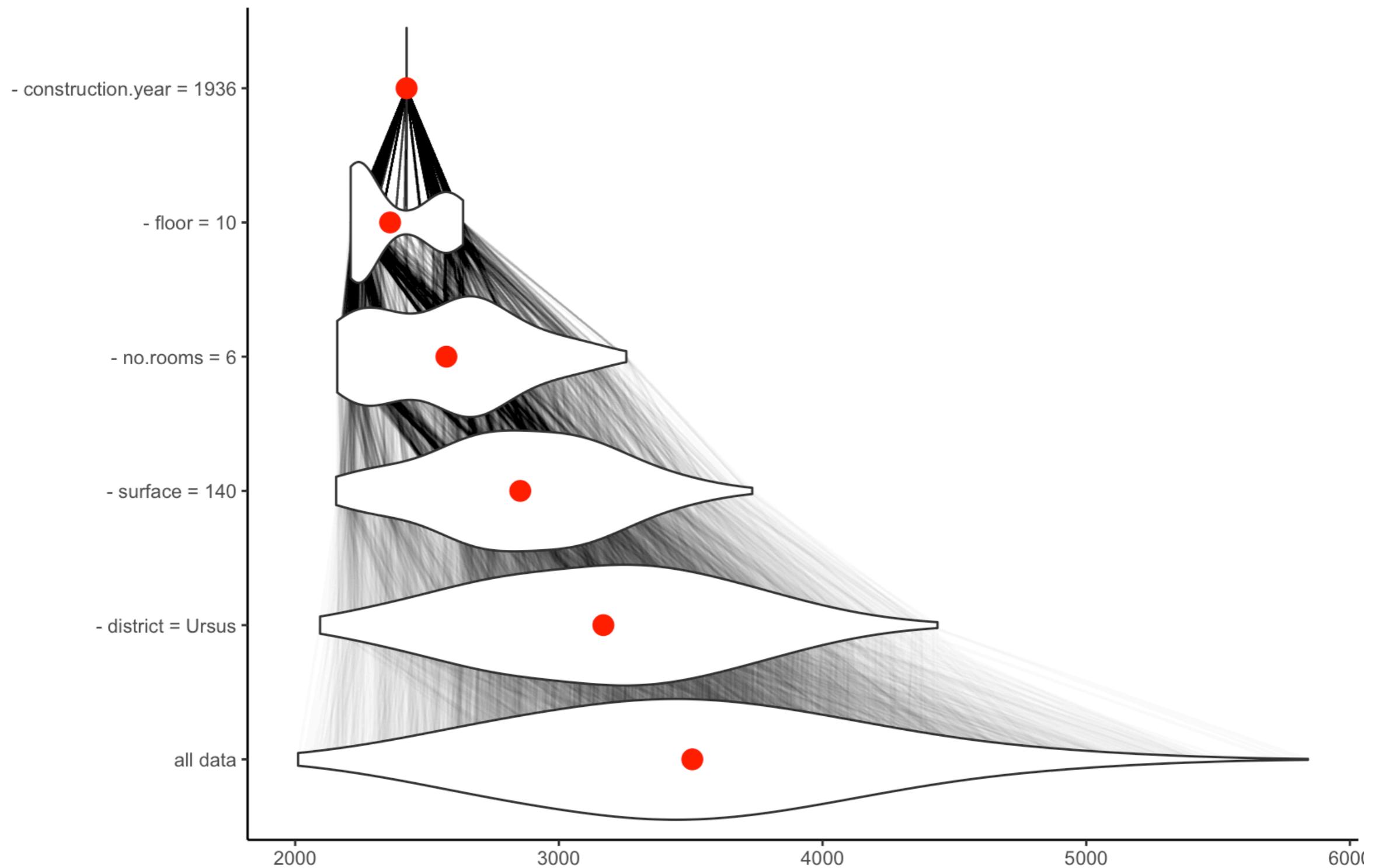
# Ceteris Paribus Plot



# Break Down Plots



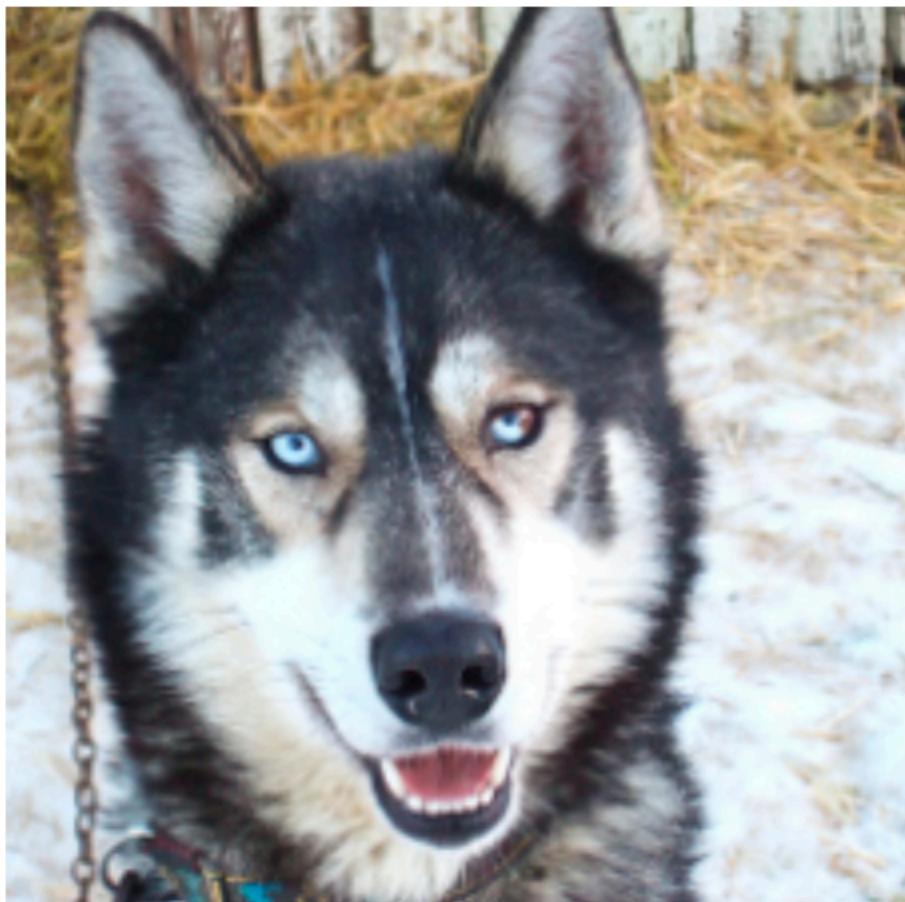
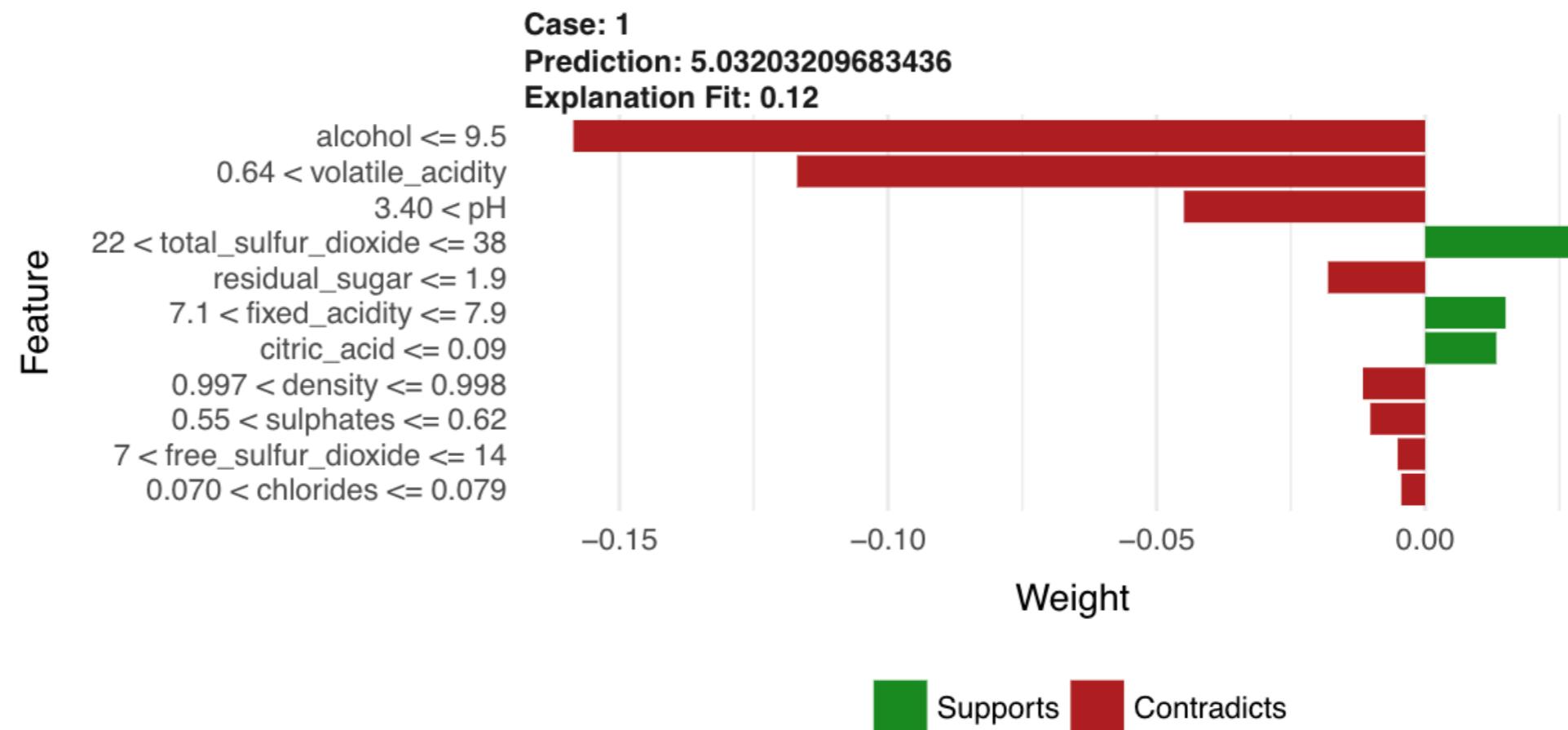
# Break Down Plots



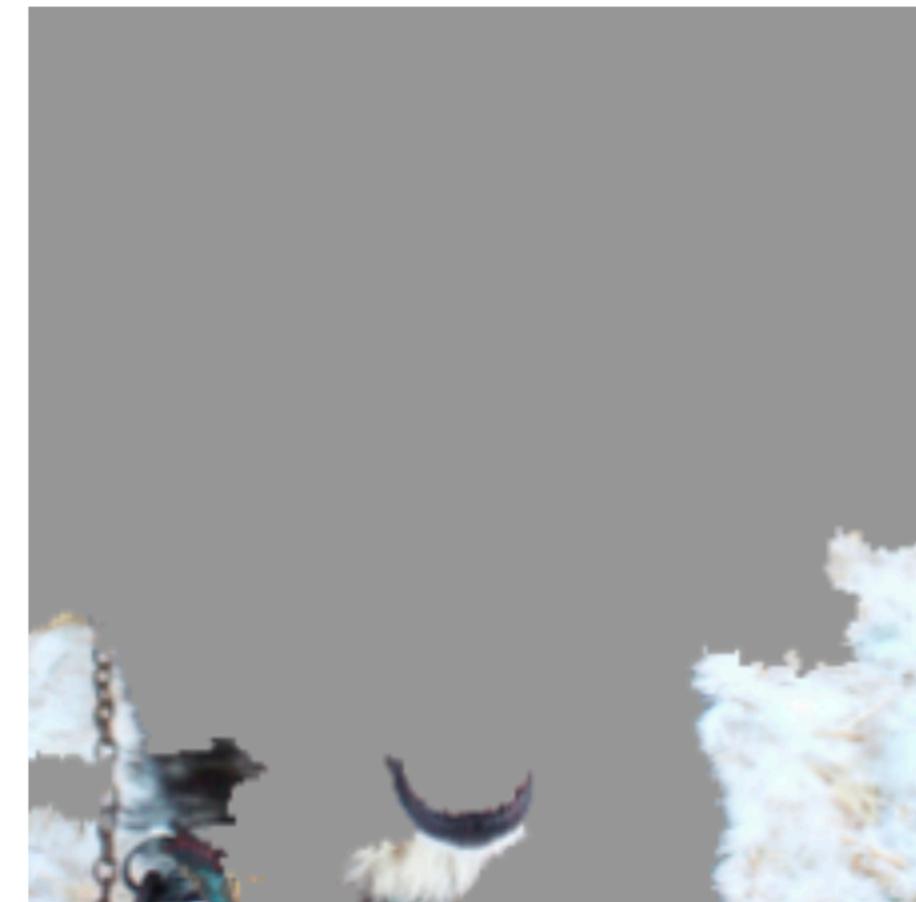
# LIME

VS

# breakDown



(a) Husky classified as wolf



(b) Explanation

# live :: Local Interpretable (Model-agnostic) Visual Explanations

## Basics

Black-box models, like random forest or extreme gradient boosting, are commonly used due to their high performance. They are very accurate on average on the test set. The problem is, that these models cannot justify nor explain predictions. So why shall you trust their predictions?

The **live** package helps to understand the local behaviour of a black-box model. The idea behind comes from the LIME method [Ribeiro 2016] and is adopted to models based on a mixed data.

### How does it work?

1. Sample a set of points (adjacency) that are close to the instance to be explained.
2. Use the original black-box model to calculate predictions for adjacency.
3. Fit a white-box model to the predictions generated for adjacency.
4. Present the white-model.

### Extra features

- Variable selection.
- Tools for model visualization.
- Focus on interpretable white-boxes

### References

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- Max Gordon and Thomas Lumley, forestplot: Advanced forest plot using 'grid' graphics, 2017
- Brandon Greenwell, pdp: An R Package for Constructing Partial Dependence Plots, The R Journal 9(2017), no. 1
- S. Lundberg and S.-I. Lee A unified approach to interpreting model predictions, ArXiv e-prints (2017)
- Carolin Strobl, Anne-Laure Boulesteix, Thomas Kneib, Thomas Augustin, and Achim Zeileis, Conditional variable importance for random forests, BMC Bioinformatics 9(2008)
- M. Tulio Ribeiro, S. Singh, and C. Guestrin: Model-Agnostic Interpretability of Machine Learning, ArXiv e-prints (2016)

## Use-Case

*Why are our best and most experienced employees leaving prematurely?* Let's see with a dataset from Kaggle Human Resources competition <https://www.kaggle.com/ludobenistant/hr-analytics/data>.

First, let's create a black-box model for prediction. Here we are using randomForest

```
library(live)
library(randomForest)

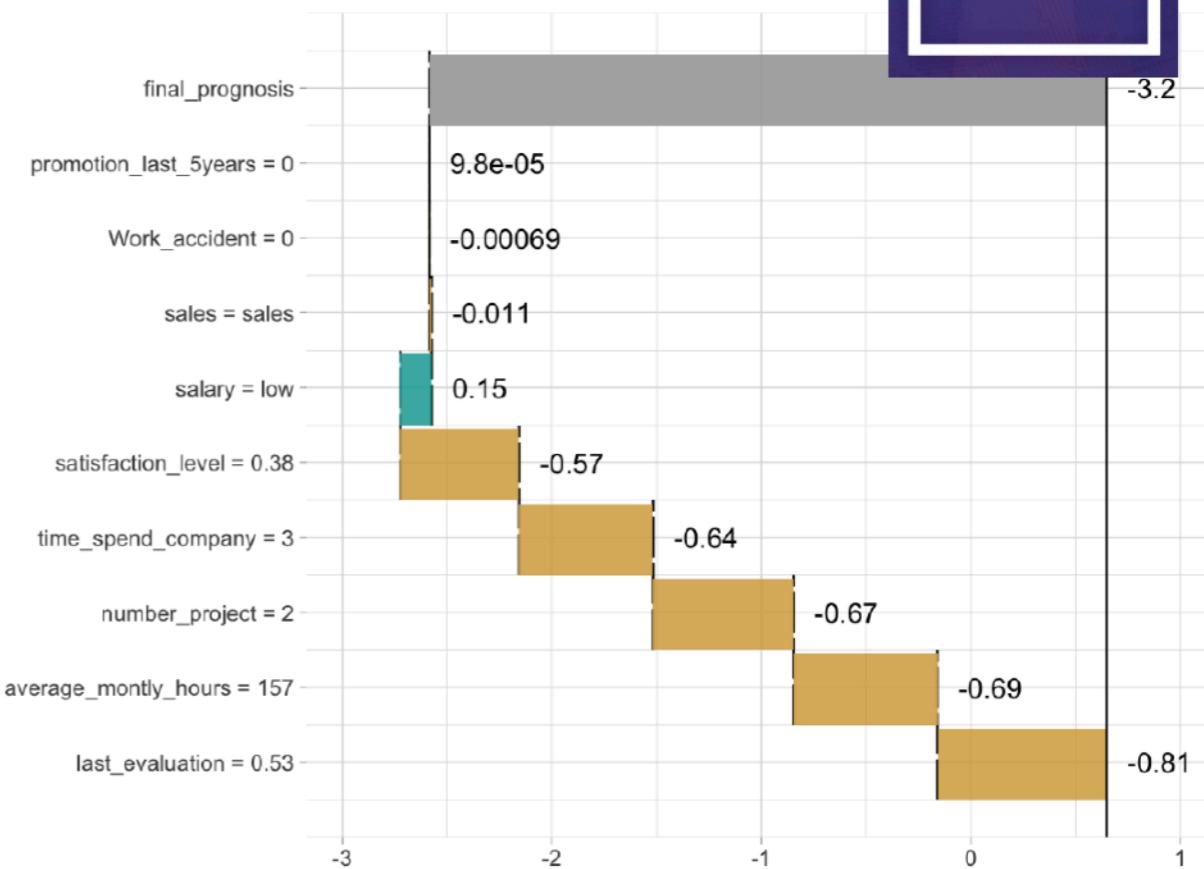
head(HR_data, 2)
#>   satisfaction_level last_evaluation
#> 1                 0.38             0.53
#>   number_project average_montly_hours
#> 1                   2                  157
#>   time_spend_company Work_accident left
#> 1                   3                  0     1
#>   promotion_last_5years sales salary
#> 1                   0 sales low
trees <- randomForest(left~, data = HR_data,
                      ntree=1000)
Type of random forest: classification
Number of trees: 1000
No. of variables tried at each split: 3

OOB estimate of  error rate: 0.69%
Confusion matrix:
      0    1 class.error
0 11412  16  0.00140007
1    88 3483  0.02464296
```

Then 1) create the adjacency (function **sample\_locally**), 2) fit the white box (function **fit\_explanations**) and 3) plot the white box.

For linear models one can use forest plots or breakDown plots, for classification trees one can use the core package.

```
similar <- sample_locally(data = HR_data,
                           explained_instance = HR_data[2,],
                           explained_var = "left",
                           size = 2000)
trained <- fit_explanation(
  live_object = similar,
  white_box = "regr.lm",
  selection = FALSE)
plot_explanation(trained, "waterfallplot",
  explained_instance = HR_data[1,])
plot_explanation(trained, "forestplot",
  explained_instance = HR_data[1,])
```



Variable	Observed	Estimate	Lower	Upper
time_spend_company	3	0.23	0.23	0.24
last_evaluation	0.53	2.58	2.5	2.66
average_montly_hours	157	0.01	0.01	0.01
satisfaction_level	0.38	1.41	1.35	1.48
number_project	2	0.23	0.22	0.24
salarylow		0.15	0.08	0.22
salessales		-0.13	-0.21	-0.05
Work_accident	0	0.06	0.01	0.12
salesmanagement		-0.05	-0.16	0.06
promotion_last_5years	0	-0.07	-0.22	0.09
salesIT		-0.04	-0.14	0.07
salesRandD		-0.02	-0.13	0.09
salestechnical		0.02	-0.08	0.11
salarymedium		-0.01	-0.07	0.06
salesproduct_mng		0.01	-0.1	0.12
salesmarketing		0.01	-0.1	0.11
saleshr		-0.01	-0.13	0.11
salessupport	0	-0.1	0.09	

DALEX is a set of tools that helps to understand the way complex predictive models work

Variable Explainers  
package: pdp, ALEPlot, **factorMerger**

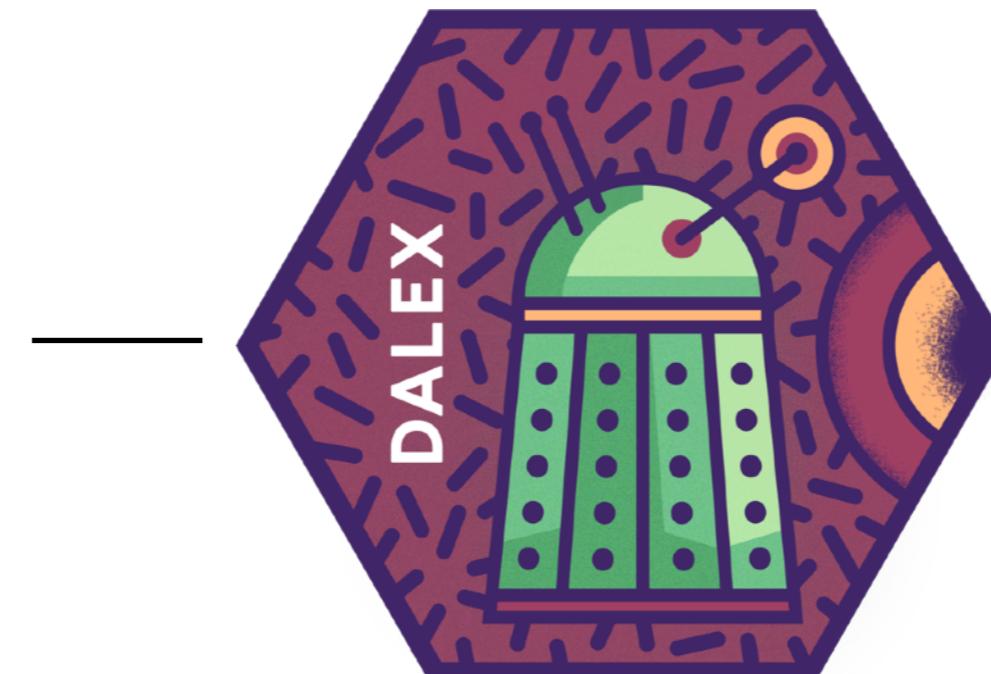
Model Management  
package: **archivist**

Model Performance Explainers  
package: **auditor**, ROCR, caret, mlr

Structure Explainers  
package: randomForest

Model Diagnostic Tools  
package: **auditor**, ggfortify

Model Predictions Explainers  
package: **breakDown**, live, shapleyr, lime



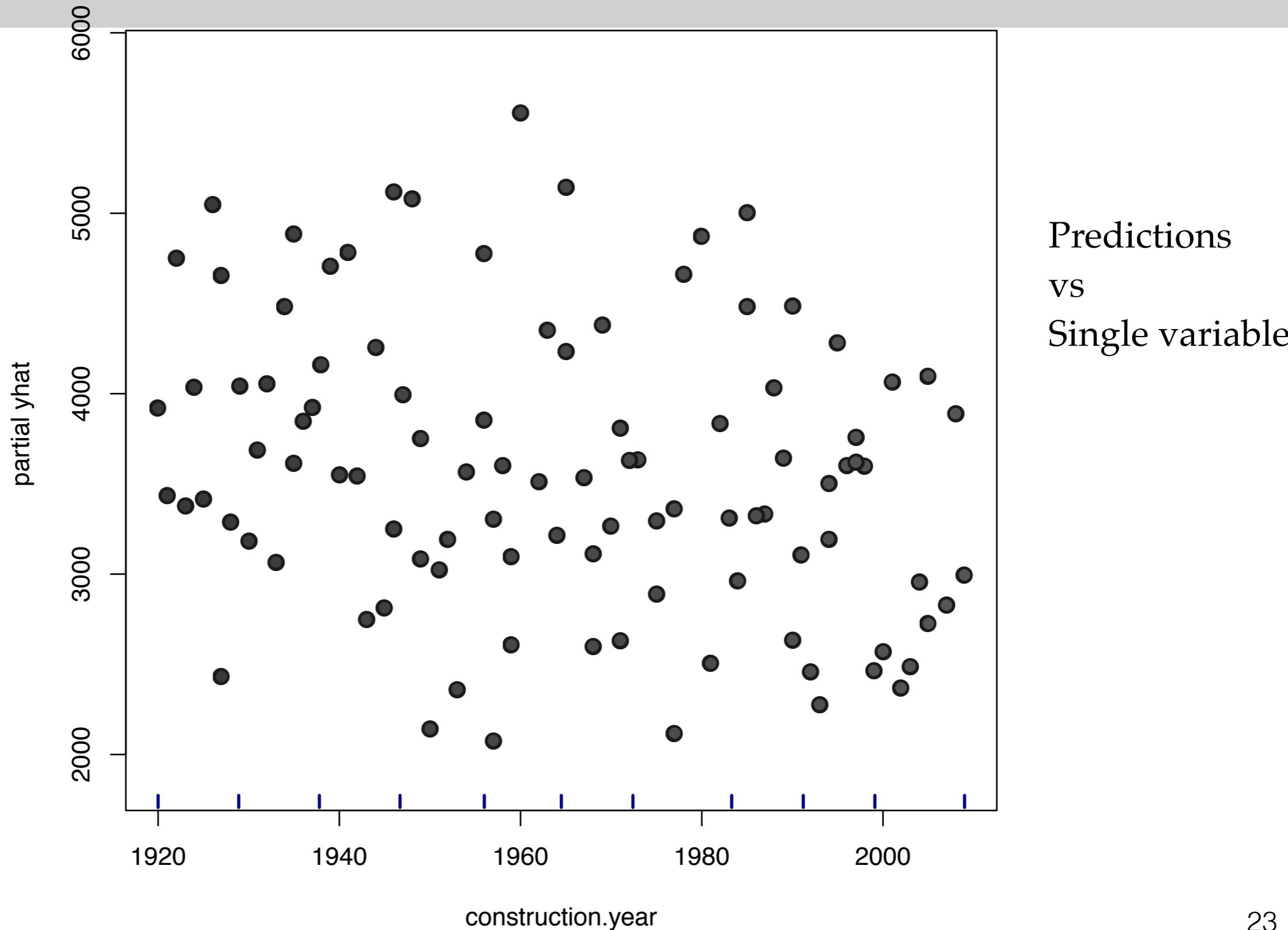
# A Tale of Two Models

Accuracy as a single number is not enough!

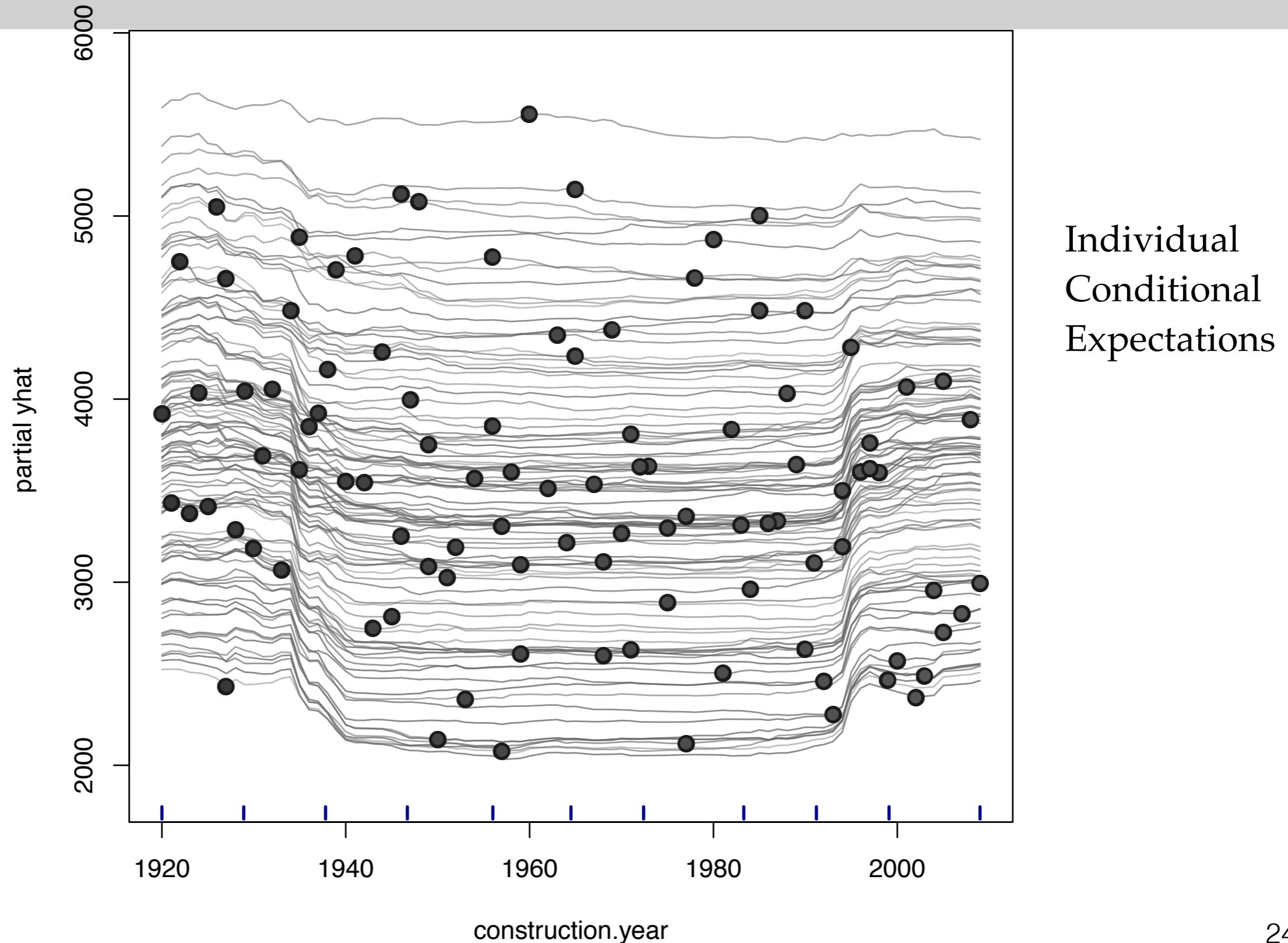
```
# root mean square
predicted_mi2_lm <- predict(apartments_lm_model, apartmentsTest)
sqrt(mean((predicted_mi2_lm - apartmentsTest$m2.price)^2))
## [1] 283.0865

# root mean square
predicted_mi2_rf <- predict(apartments_rf_model, apartmentsTest)
sqrt(mean((predicted_mi2_rf - apartmentsTest$m2.price)^2))
## [1] 283.3479
```

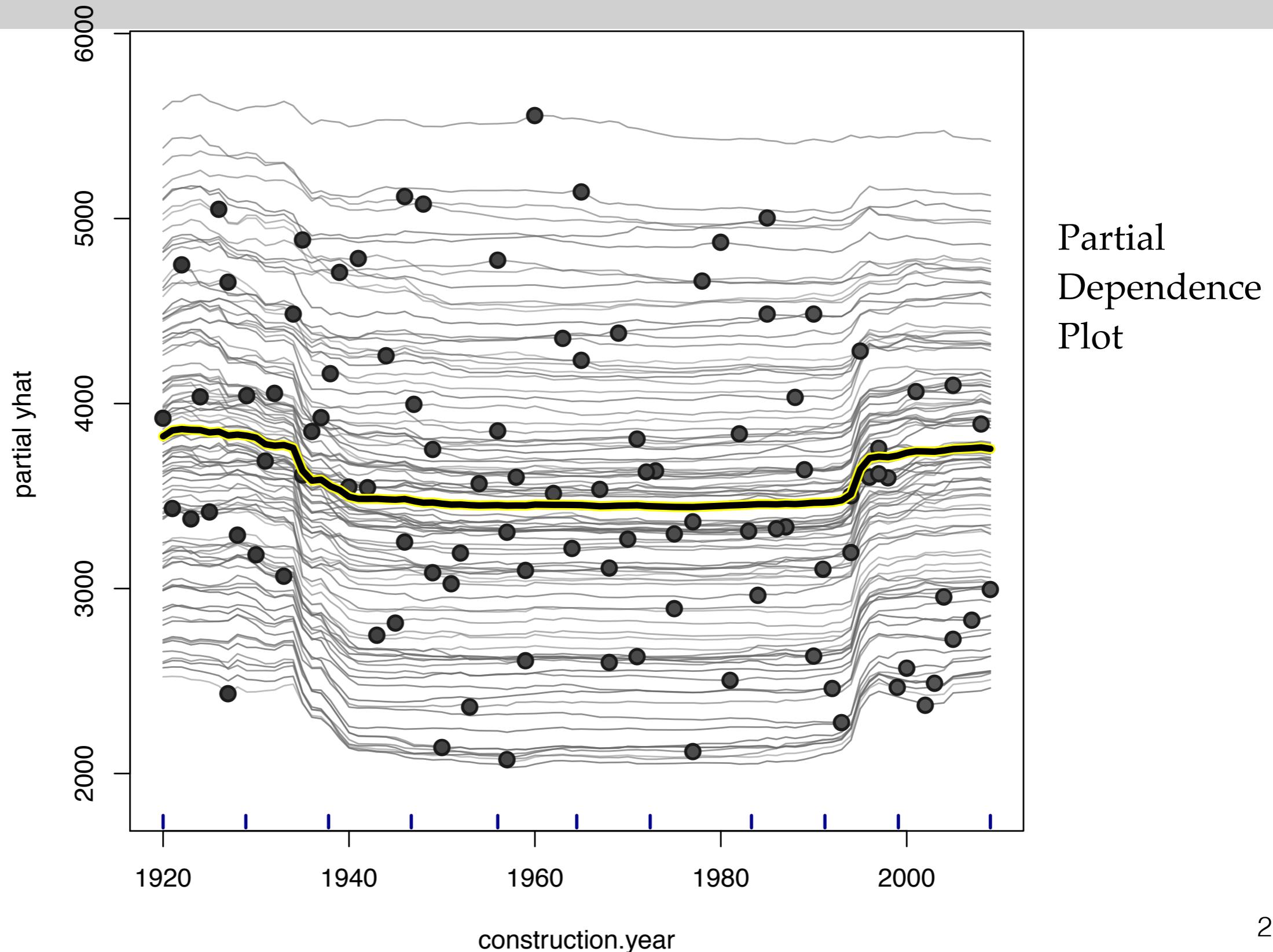
# How a single variable affects the response?



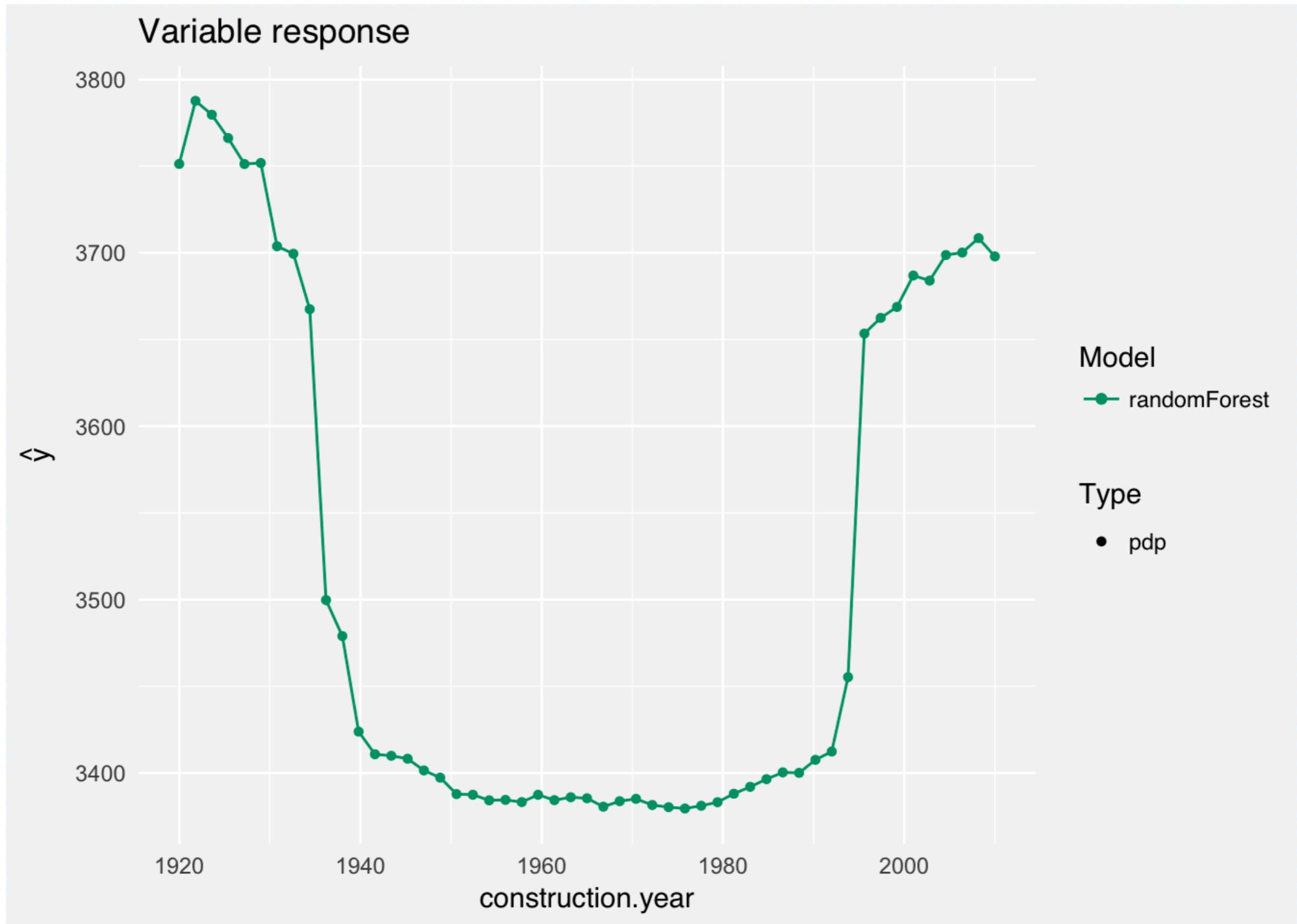
# How a single variable affects the response?



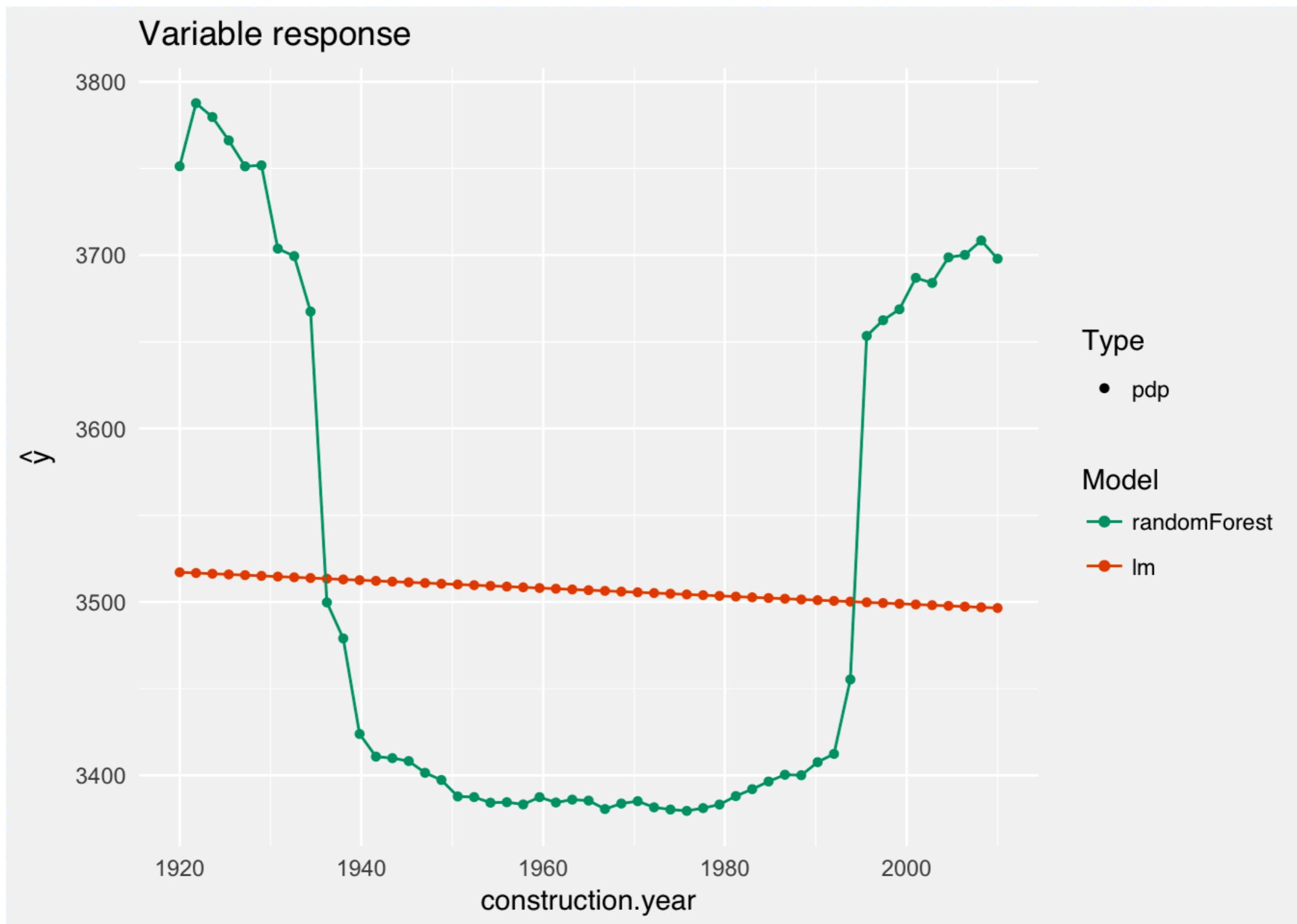
# How a single variable affects the response?



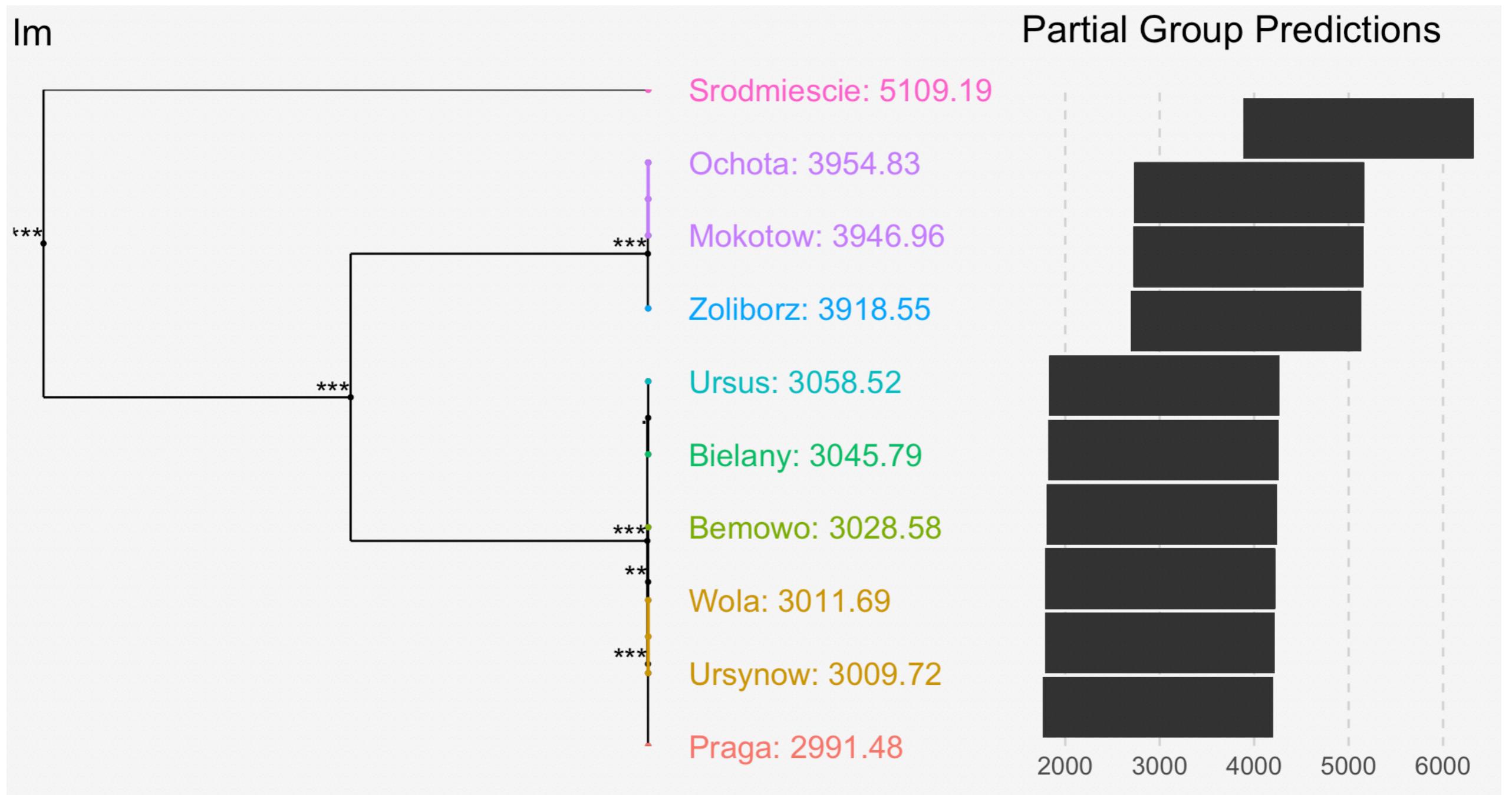
```
sv_rf <- single_variable(explainer_rf, variable = "construction.year", type = "pdp")
plot(sv_rf)
```



```
sv_lm <- single_variable(explainer_lm, variable = "construction.year", type = "pdp")  
  
plot(sv_rf, sv_lm)
```



```
svd_lm <- single_variable(explainer_lm, variable = "district", type = "factor")  
  
plot(svd_lm)
```



# factorMerger

## Cheat Sheet

Agnieszka Sitko [aut, cre]  
 Przemysław Biecek [aut, ths]  
 University of Warsaw



## Introduction

How to check if averages are different among k groups? Use **ANOVA**!

How to visualise how these groups are different? Use **factorMerger**!

The aim of **factorMerger** is to provide informative and easy to understand visualisations of *post-hoc* comparisons. It gives consistent and non-overlapping adaptive fusing of groups based on likelihood ratio test (LRT). The package **factorMerger** works for wide spectrum of families like Gaussian, binomial or survival.

Results from the adaptive fusing are presented with the *Merging Paths Plots* - a hierarchical representation of LRT-based distances among groups.

In addition, the *Generalized Information Criterion* (GIC) is presented for fused models. This criterion may be used to choose the optimal segmentation of groups.

Graphical summary of the variable of interest in each group is presented in the right panel.

Find more in <https://arxiv.org/abs/1709.04412>

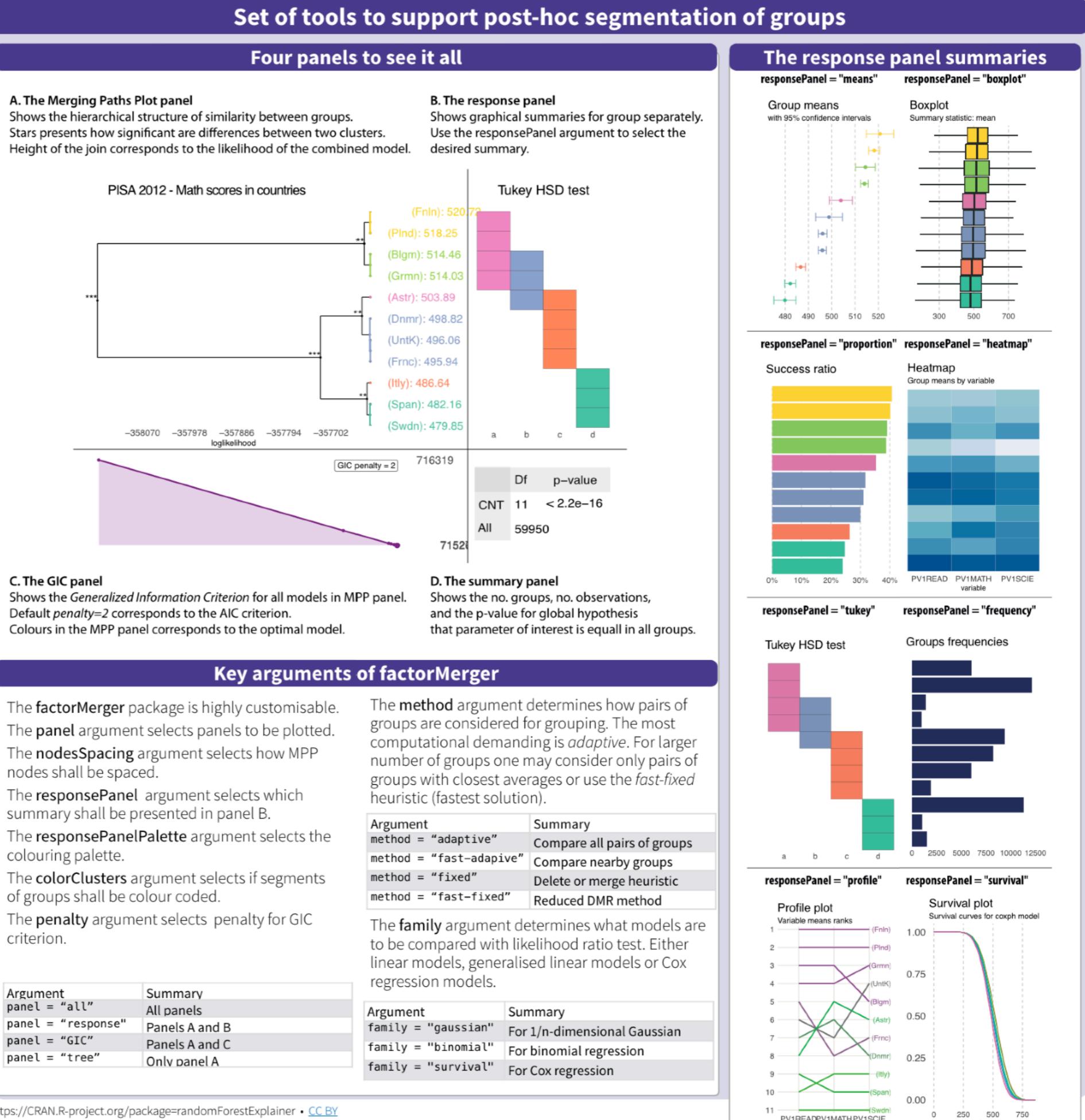
## Example

```
library(factorMerger)
```

```
fmAll <- mergeFactors(
  response = pisaEuro$math,
  factor = pisaEuro$country,
  method = "fast-adaptive",
  family = "gaussian")
```

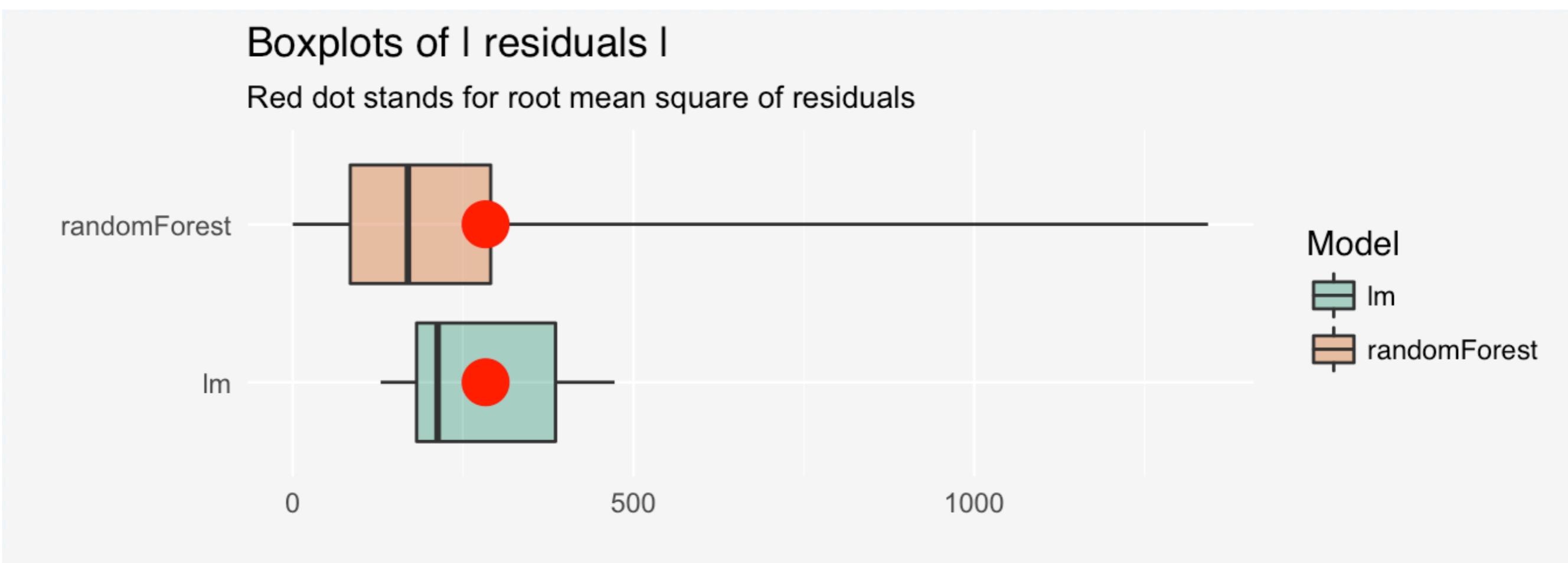
```
print(fmAll)
```

```
plot(fmAll,
  panel = "all",
  responsePanel = "tukey")
```

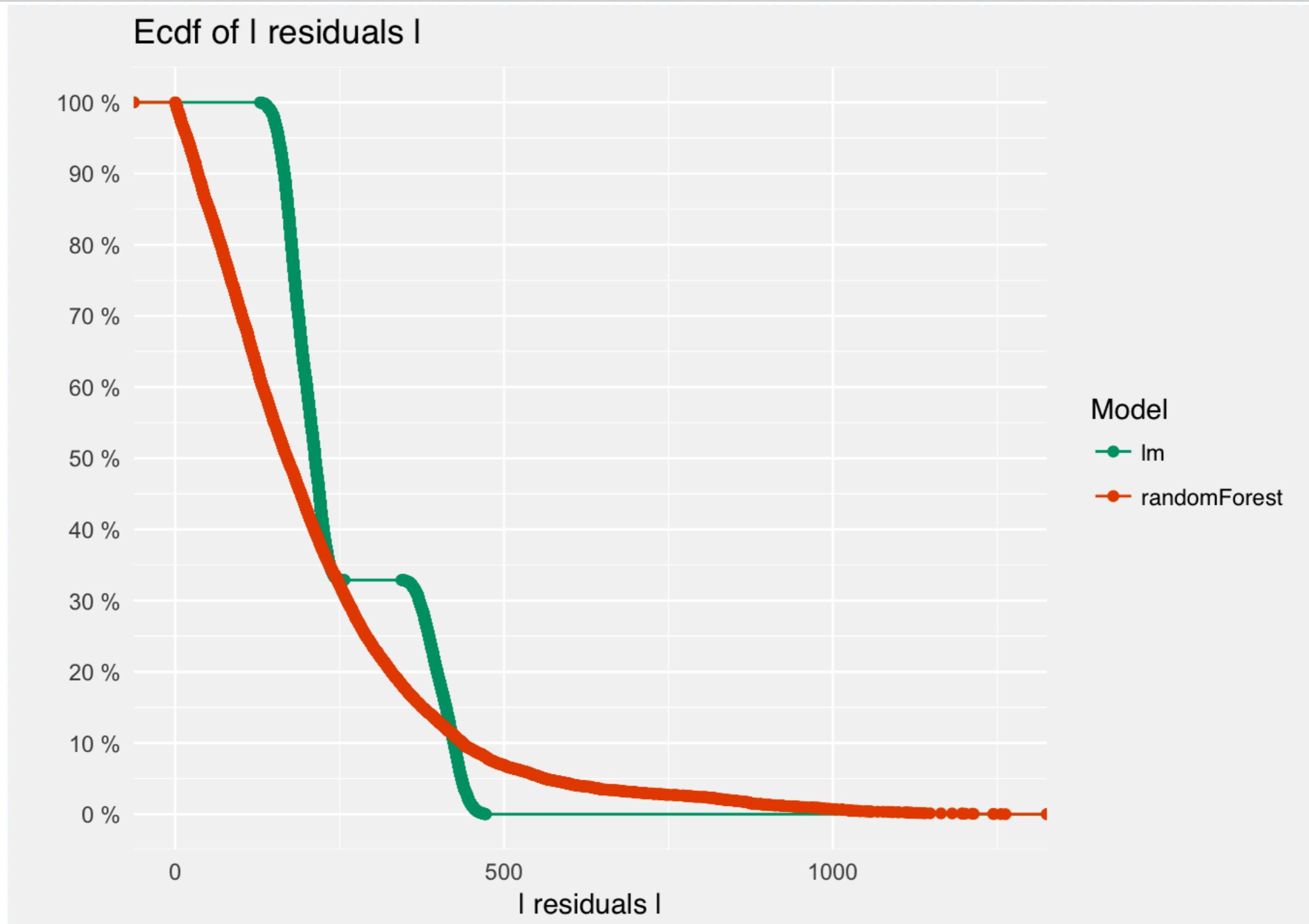


# Accuracy as a single number is not enough!

```
plot(mp_lm, mp_rf, geom = "boxplot")
```



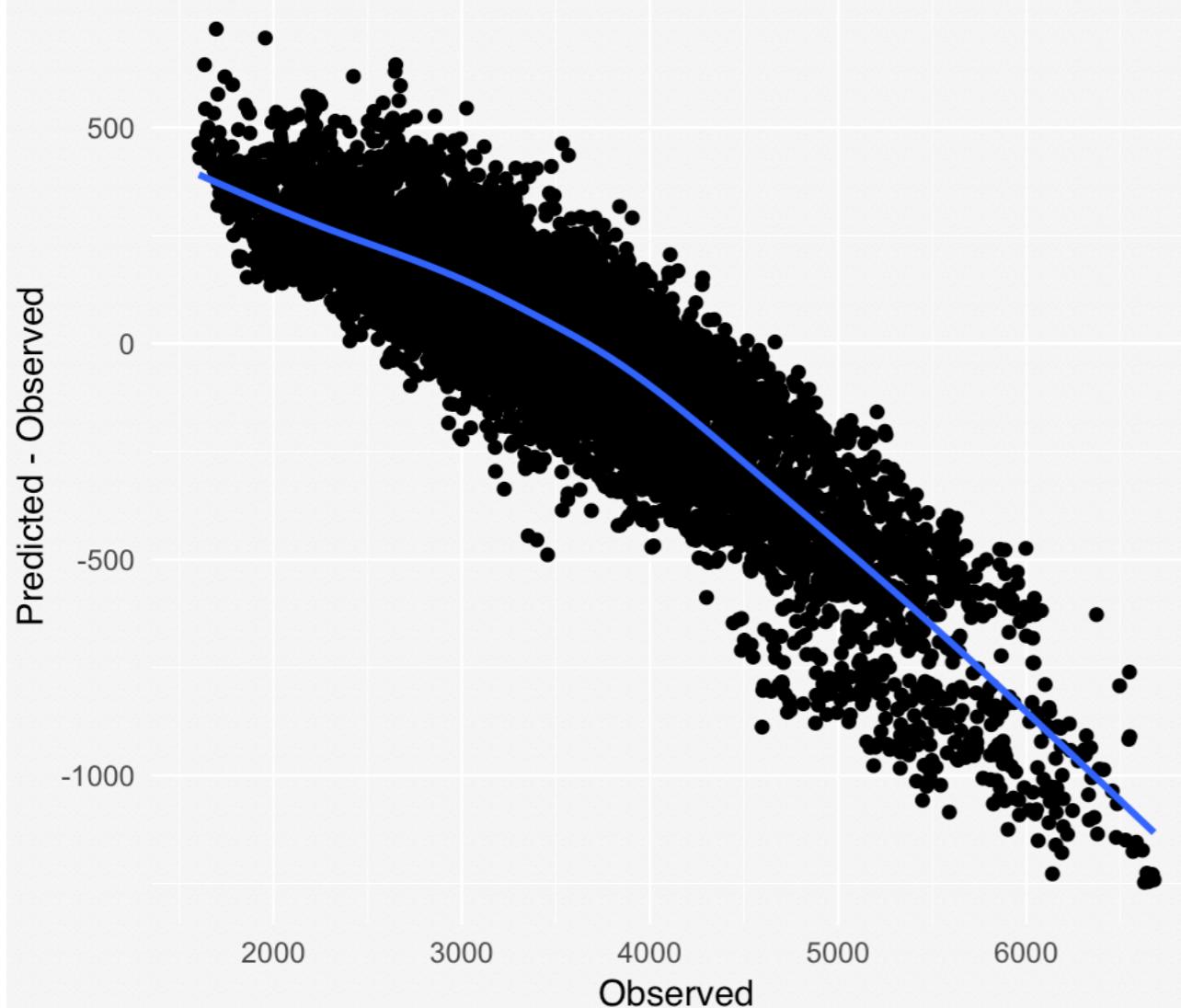
# Accuracy as a single number is not enough!



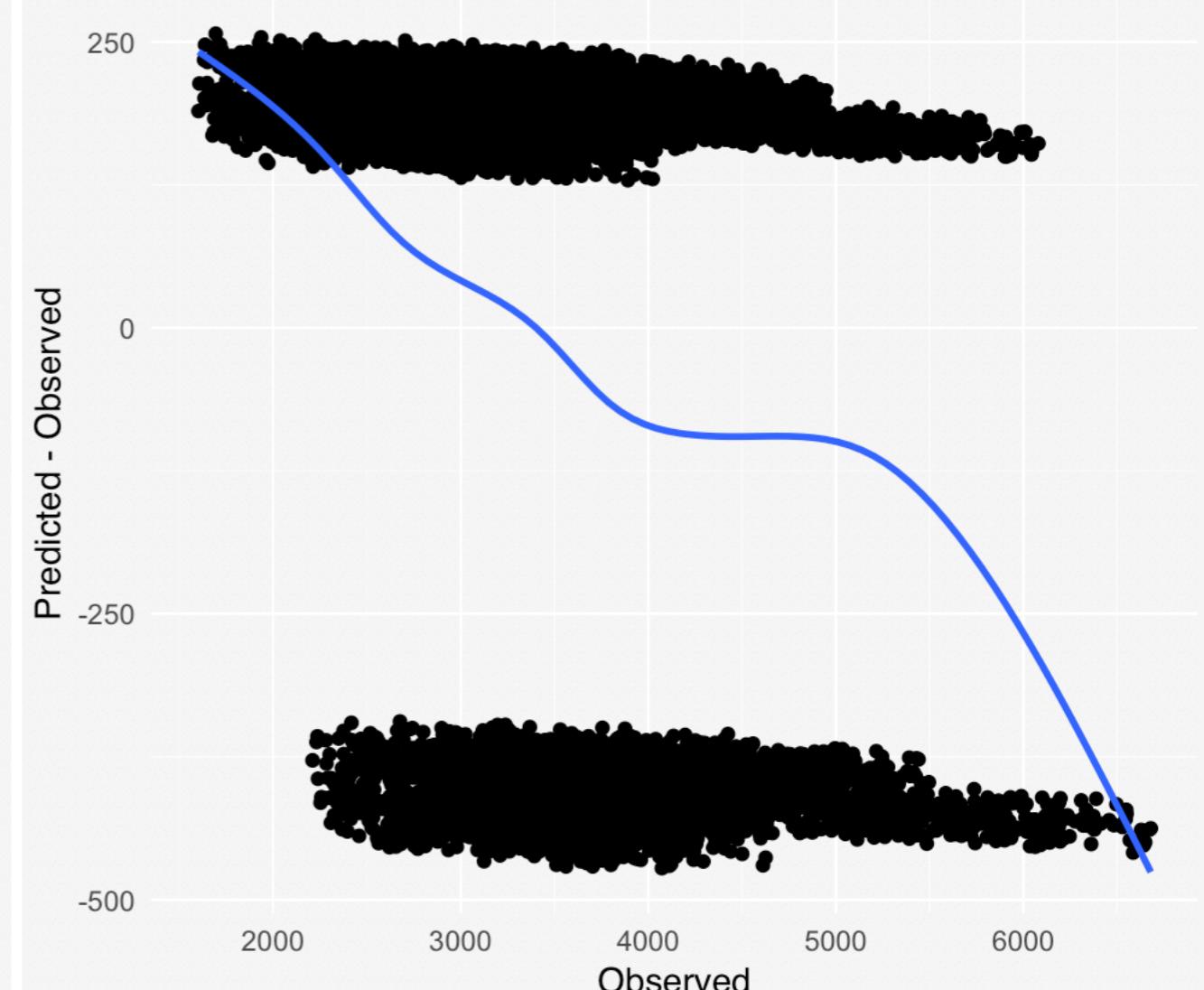
# Accuracy as a single number is not enough!

## Always validate your model!

Diagnostic plot for the random forest model



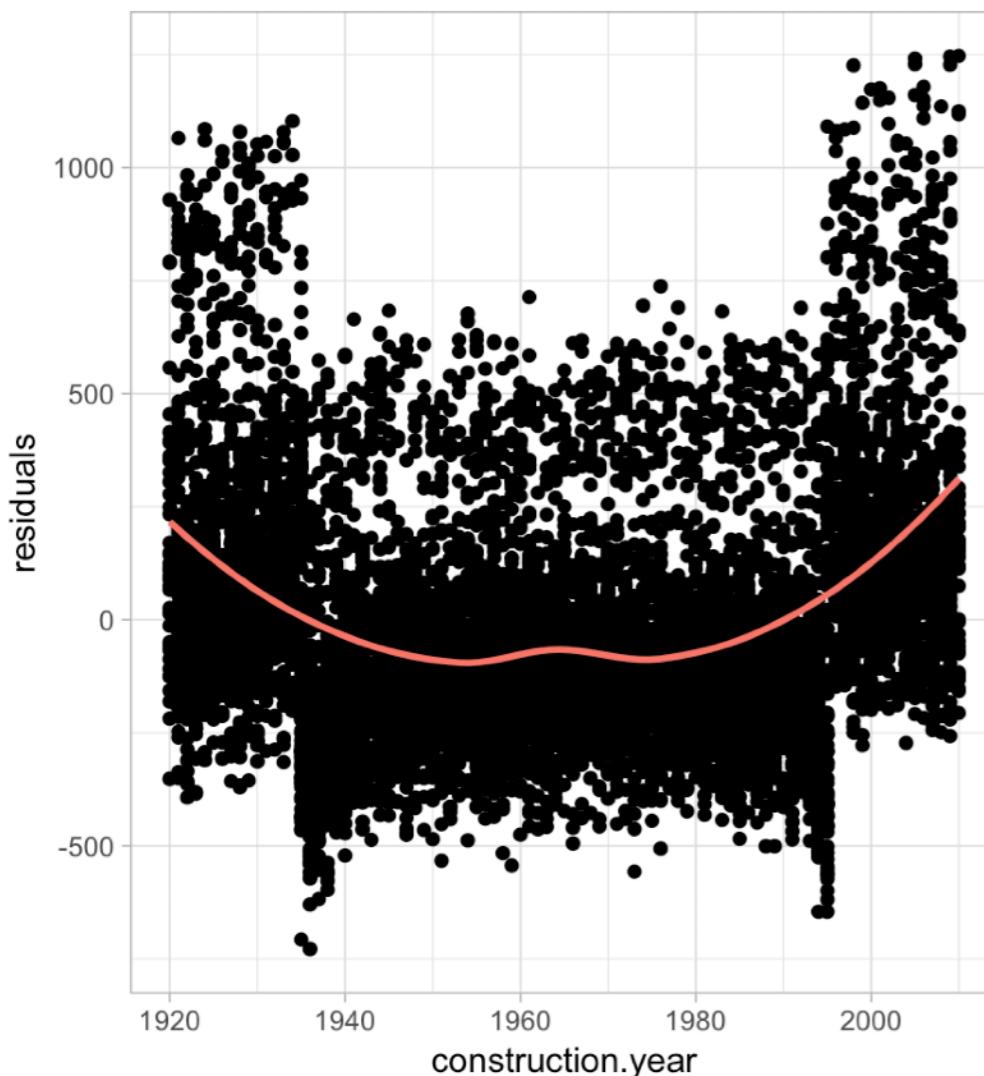
Diagnostic plot for the linear model



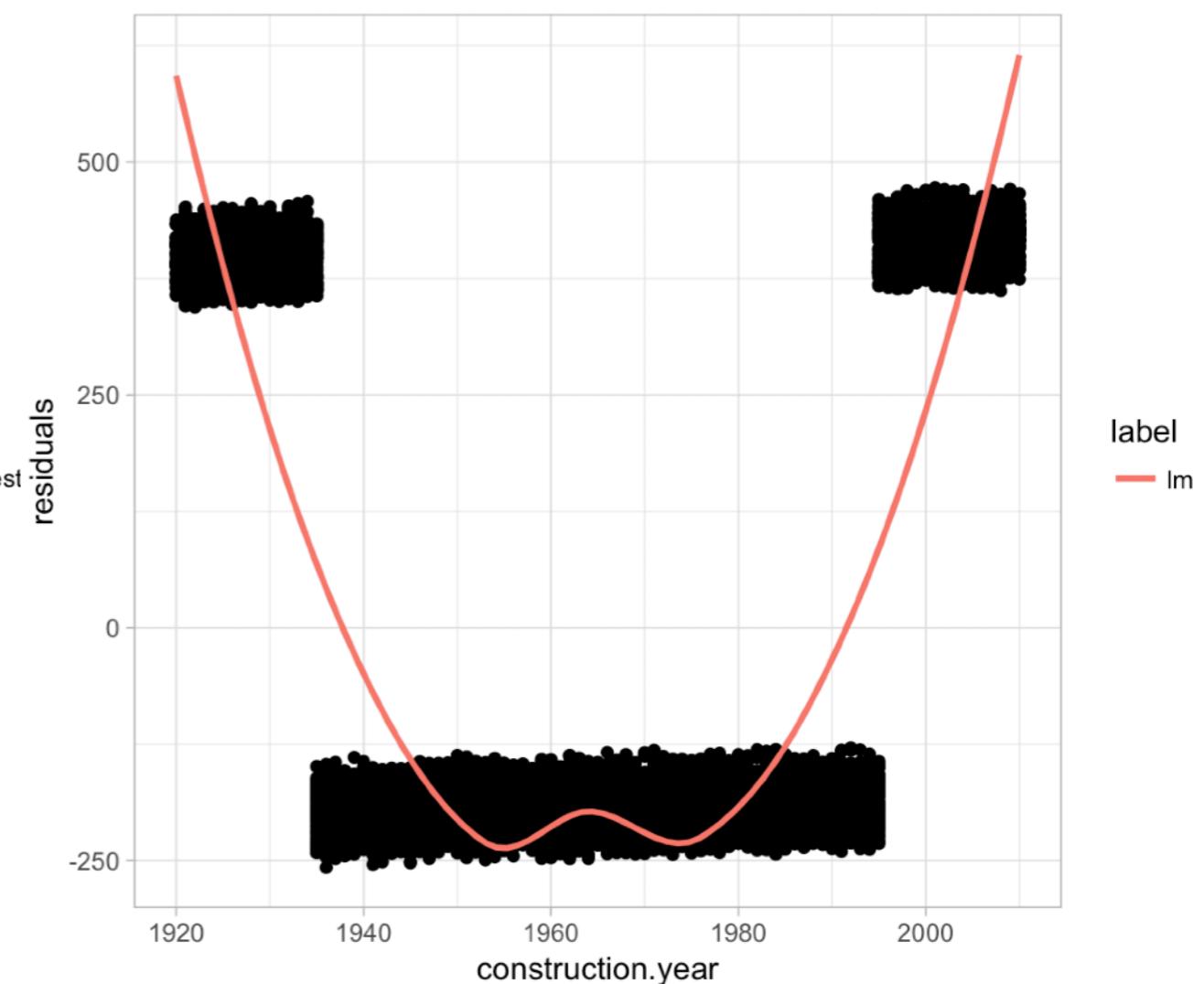
```
library(auditor)
audit_rf <- audit(explainer_rf)
plotResidual(audit_rf, variable = "construction.year")
```

```
audit_lm <- audit(explainer_lm)
plotResidual(audit_lm, variable = "construction.year")
```

Residuals vs construction.year



Residuals vs construction.year



# Error analysis with auditor :: CHEAT SHEET

## Basics

Package **auditor** provides several methods for model verification and validation by error analysis. This includes both, graphical methods and scores, which can be useful for comparison of models performance.

Residual analysis is widely used for linear and generalized linear models, so there are many statistical tools to evaluate the goodness of fit. However, these methods are not suitable for each machine learning model. In particular, it is difficult to apply them to black box models such as random forest, due to the lack of information about the error distribution.

The tools included in auditor can be used to assess the fit of many types of models, including black boxes.

## MODEL PREPARATION

We will show the use of a package for a logistic regression model.

The example uses the *Pima Indian Diabetes* data set.

```
library(mlbench)
data("PimaIndiansDiabetes")

mod_glm <- glm(diabetes~.,
                 family=binomial,
                 data=PimaIndiansDiabetes)
```

In order to analyse the model residuals, we need to convert model into a uniform structure readable by the auditor package.

```
library(auditor)
audit_glm <- audit(mod_glm)
```

An object created with the **audit()** function can be used to draw different diagnostic plots. We will show some of them in this cheatsheet.

More detailed description and additional functionalities are presented in the package vignettes which can be found on the auditor website:  
<https://mi2-warsaw.github.io/auditor>

## REFERENCES

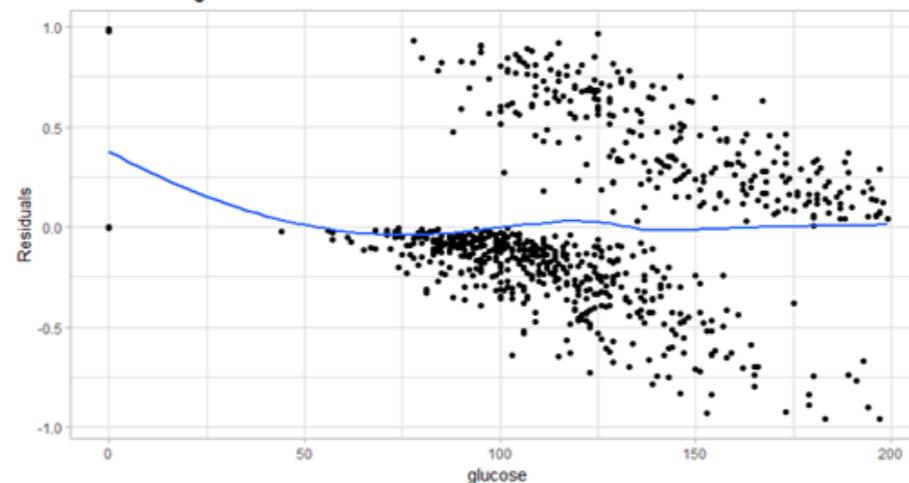
- Moral, R., Hinde, J., & Demétrio, C. (2017). Half-Normal Plots and Overdispersed Models in R: The *hnp* Package. *Journal of Statistical Software*, 81(10), 1 - 23.



## Basic plots

The **plot()** function can be used to draw several different graphs. By default it is drawn *Residuals vs variable plot*.

```
plot(audit_glm, variable = "glucose")
```



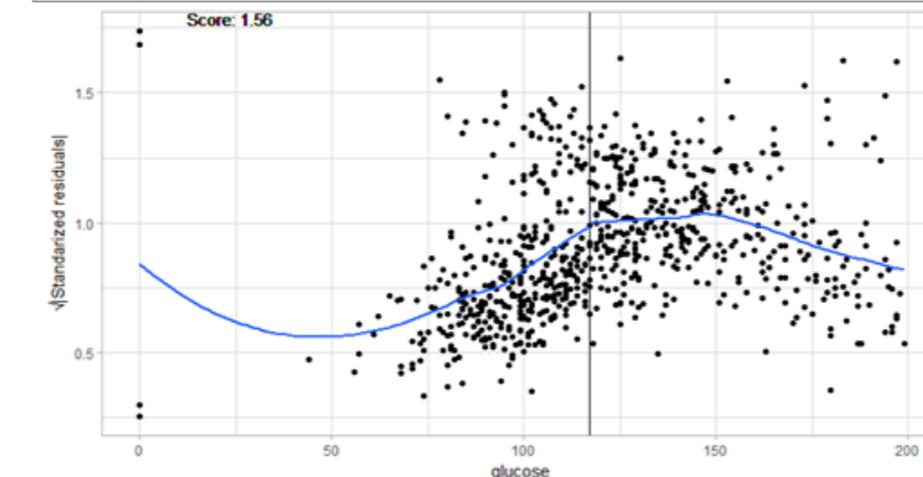
In the example above there were used response residuals, but it is possible to provide any predict and residual function.

To use non-defaulted functions to calculate the residuals and model prediction, you can use arguments **residual.function** and **predict.function** while using an audit function.

```
p.fun <- function(model, data){
  predict(model, data, type="link")
}
r.fun <- function(model,y){residuals(model)}
audit_glm_dev <- audit(mod_glm,
                       predict.function = p.fun,
                       residual.function = r.fun)
```

Use **type=plot name** to draw different types of diagnostic plots. The available parameter values are 'ACF', 'Autocorrelation', 'Cook', 'HalfNormal', 'Residuals' and 'ScaleLocation'.

```
plot(audit_glm_dev, type="ScaleLocation",
      variable = "glucose")
```

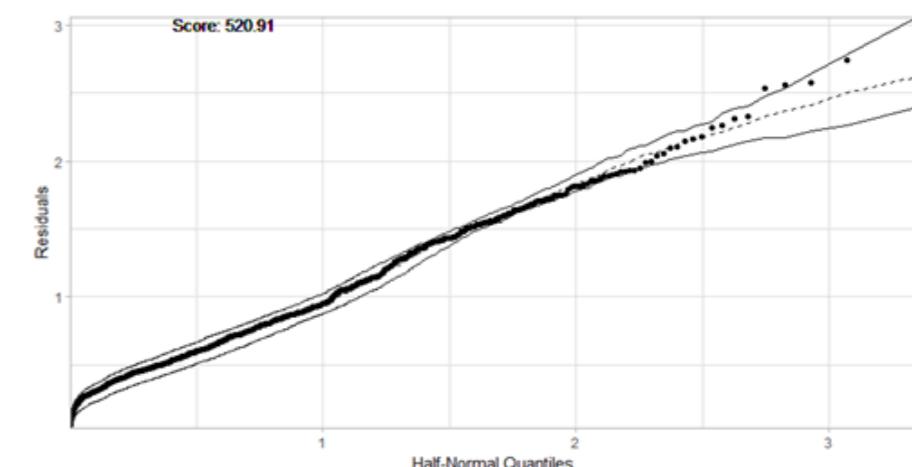


## Half-Normal plots

The half-normal plot is a graphical method for comparing two probability distributions by plotting their quantiles against each other. Points on the plot correspond to ordered absolute values of model residuals plotted against theoretical order statistics from a half-normal distribution.

If residuals are from the normal distribution, they are close to a straight line. However, if they don't come from a normal distribution, they still show a certain trend. Simulated envelopes can be used to help verify the correctness of this trend. For a well-fitted model, residuals should lay within the envelope.

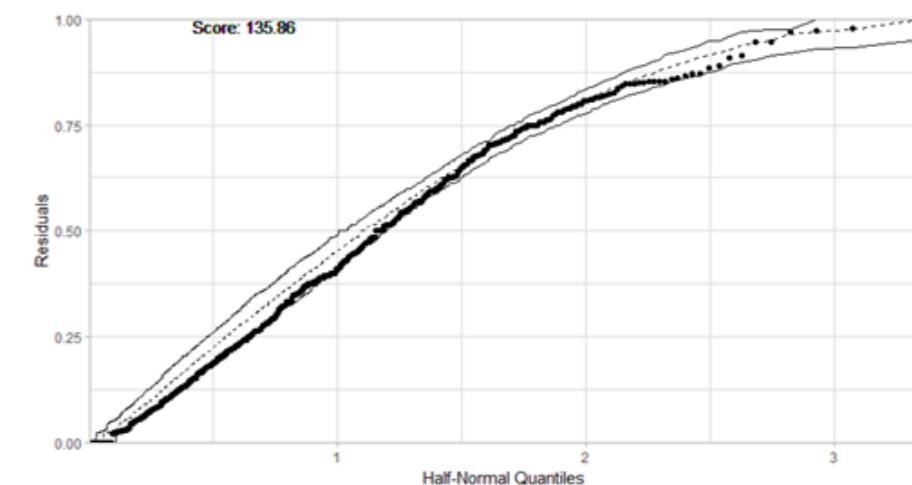
```
plotHalfNormal(audit_glm_dev, resid.type="response")
```



Half-Normal plots allow to check the model fit but comparing two models may be difficult.

A useful tool to compare goodness-of-fit of two models is score displayed on the plot. Score is a sum of logarithms of estimated PDF at each point. It is calculated on the basis of simulated data, so it may differ between function calls.

```
library(randomForest)
mod_rf <- randomForest(diabetes~.,
                        data=PimaIndiansDiabetes, ntree=100)
audit_rf <- audit(mod_rf)
plotHalfNormal(audit_rf)
```

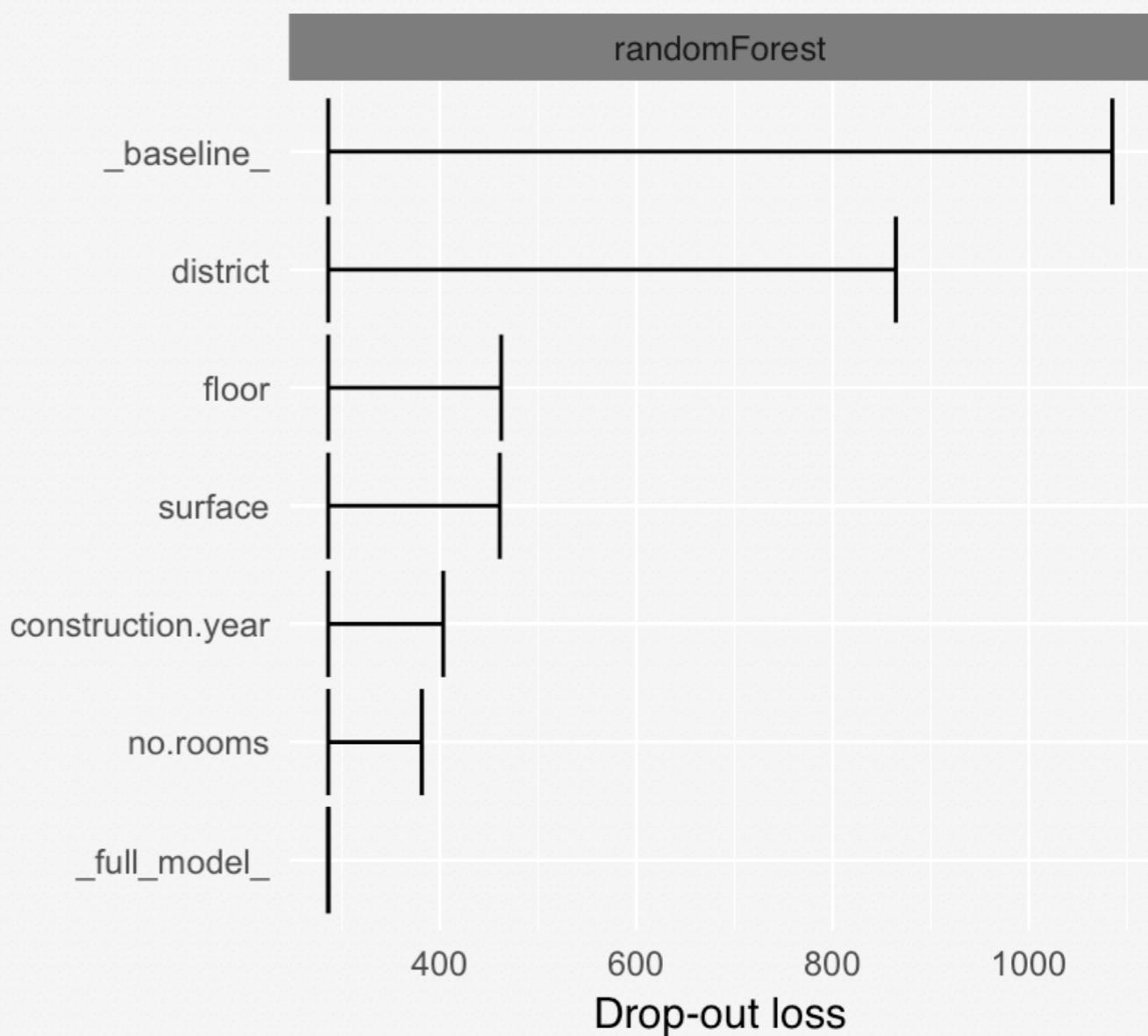


# Which variables are influential for RF?

> vi\_rf <- variable\_importance(explainer\_rf, loss\_function = loss\_root\_mean\_square)  
> vi\_rf

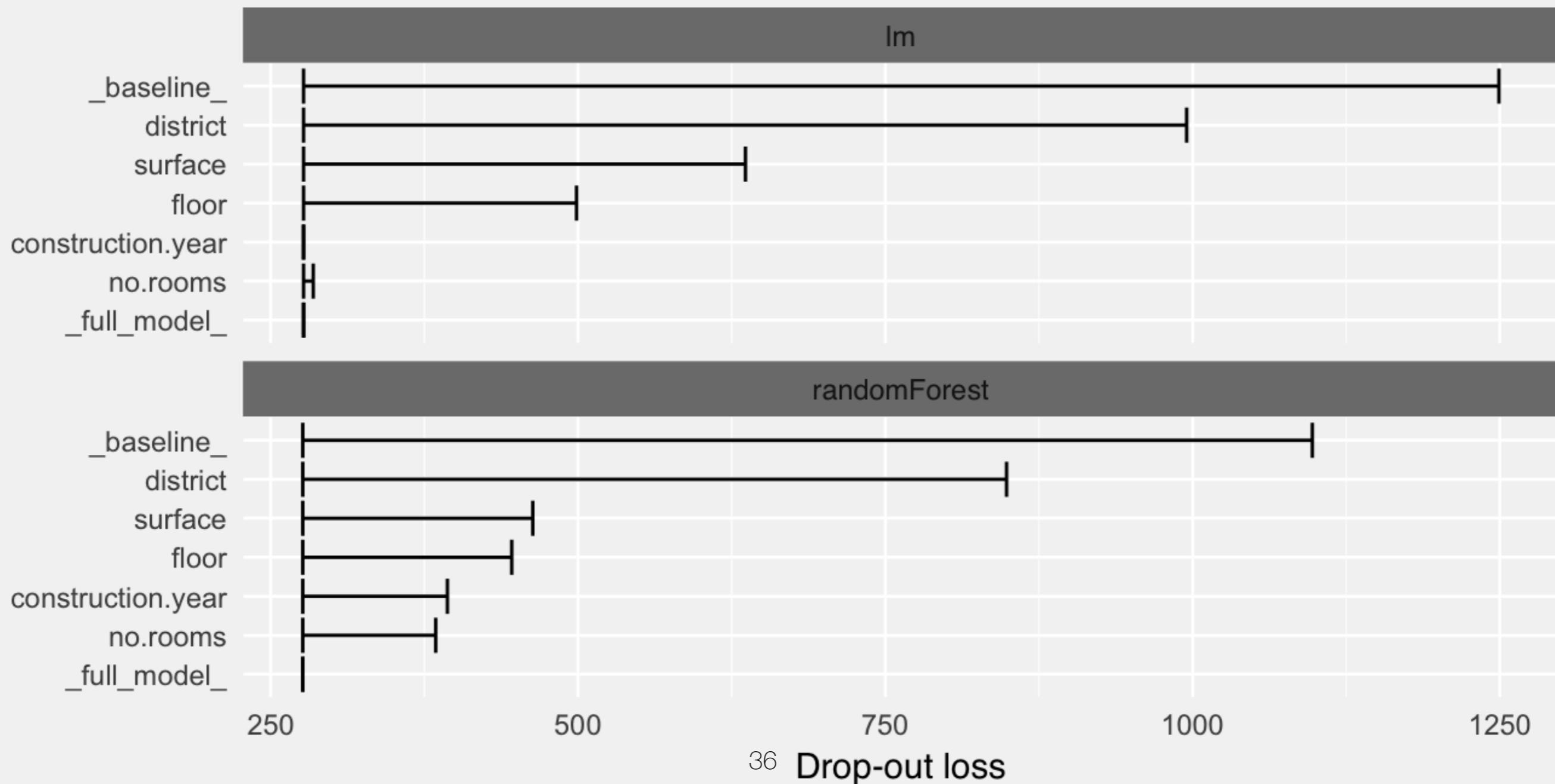
	variable	dropout_loss	label
1	_full_model_	286.2676	randomForest
2	no.rooms	381.5975	randomForest
3	construction.year	403.4376	randomForest
4	surface	461.0018	randomForest
5	floor	462.3999	randomForest
6	district	864.4315	randomForest
7	_baseline_	1084.9218	randomForest

>  
> plot(vi\_rf)



# Find 5 differences!

Such statistics may be directly compared across variables and across models!



# randomForestExplainer

## What's in the forest?

Aleksandra Paluszynska [aut, cre]  
Przemysław Biecek [aut, ths]  
University of Warsaw



### Basics

The aim of the **randomForestExplainer** package is to support structure exploration and visualisation for a random forest model.

Once you have a model created with the **randomForest** package, use following functions to examine its structure.

```
library(randomForest)
library(randomForestExplainer)

forest <- randomForest(PV1MATH~.,
data = pisa2015, localImp = TRUE)
```

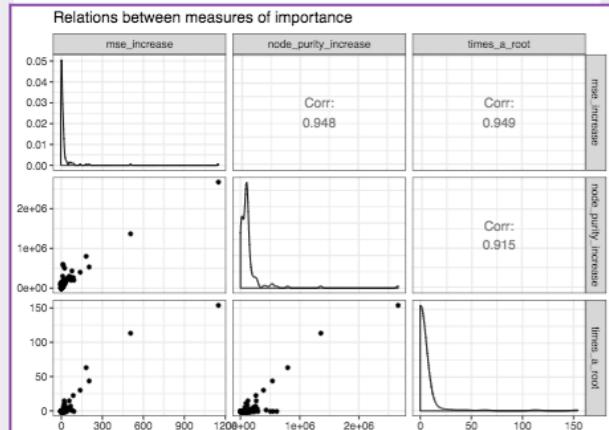
### Variable Importance

The **measure\_importance()** function calculates different measures of importance for variables presented in the forest. Note that different variables are available for classification forests and regression forests.

Use the **plot\_importance\_ggpairs()** function to plot examine relations between selected measures.

```
forest_stats <-
measure_importance(forest, measures =
c("mse_increase",
"node_purity_increase",
"times_a_root"))

plot_importance_ggpairs(forest_stats)
```



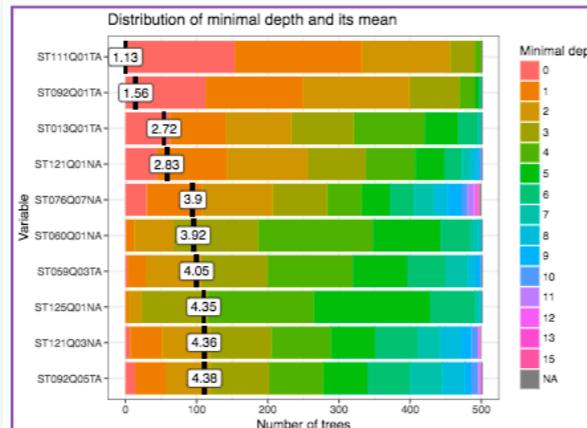
## randomForestExplainer - Structure mining and visualisation for Random Forests

### Variable Depth

The **min\_depth\_distribution()** function calculates distribution of minimal depth of given variable in all trees. Use the **plot\_min\_depth\_distribution()** function to plot this distribution along with mean depths for variables. In general, the higher are variables the more influential they are.

```
forest_frame <-
min_depth_distribution(forest)

plot_min_depth_distribution(forest_frame)
```

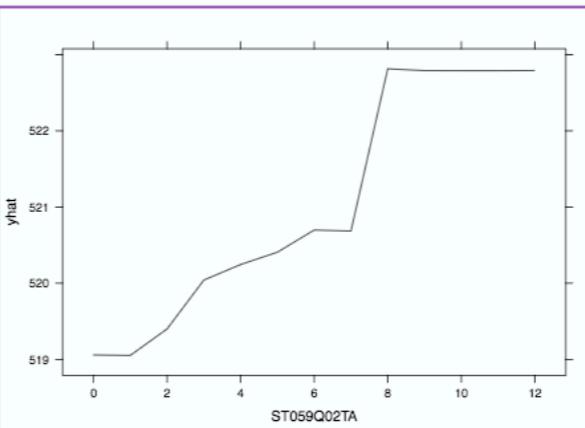


### Partial Dependence Plots

The **partial()** function from the **pdp** package calculates marginal relation between target variable and selected one or two independent variables. The relation can be noted with **lattice** graphical system with the **plotPartial()** function or with **ggplot2** system with the **autoplot()** function.

```
library(pdp)

pdp1 <- partial(forest, "ST059Q02TA")
plotPartial(pdp1)
```

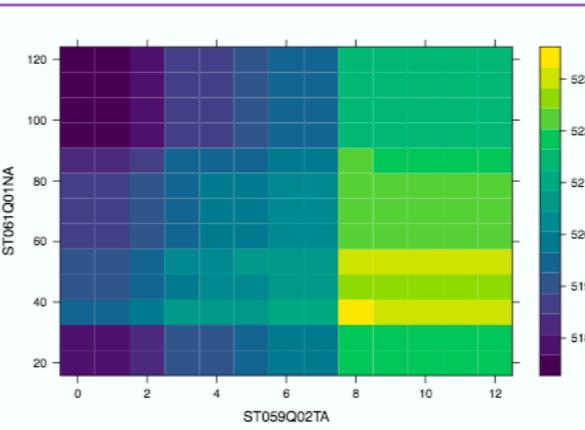


### Local Approximations

Based on LIME

Variable depth and variable importance functions are useful in identification which variable/variables are worth watching, while the **pdp** plots are useful to understand the nature of the relation between target variable and variable/s of interest.

```
pdp2 <- partial(forest, c("ST059Q02TA",
"ST061Q01NA"))
plotPartial(pdp2)
```



### Literature

**ggRandomForests**: Random Forests for Regression. John Ehrlinger (2016)

**pdp**: An R Package for Constructing Partial Dependence Plots. Brandon M. Greenwell (2017)

**forestFloor**: Forest Floor Visualizations of Random Forests. Soeren Welling, Hanne Refsgaard, Per Brockhoff, Line Clemmensen (2016)

# Language for Human-Model Interaction

