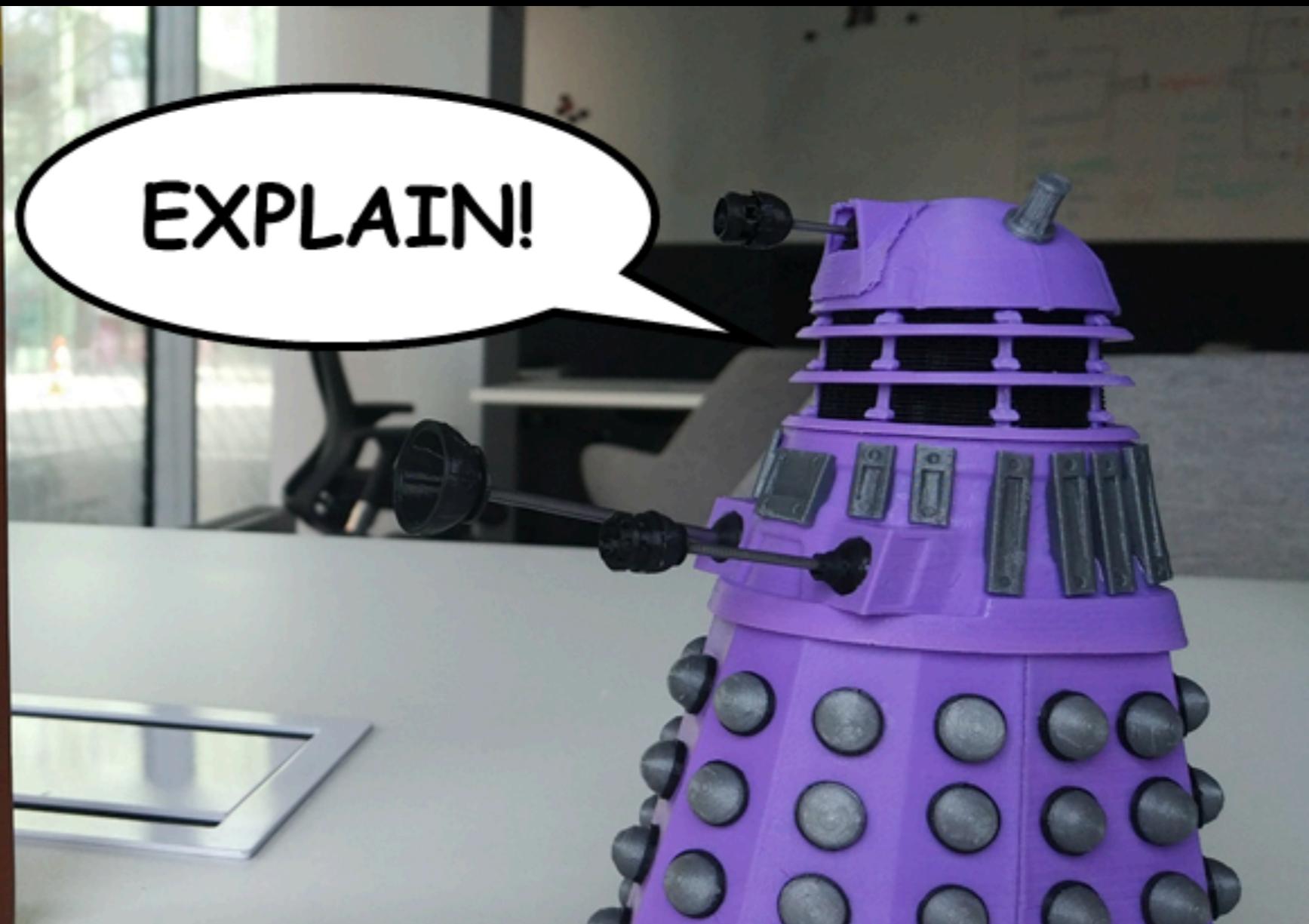
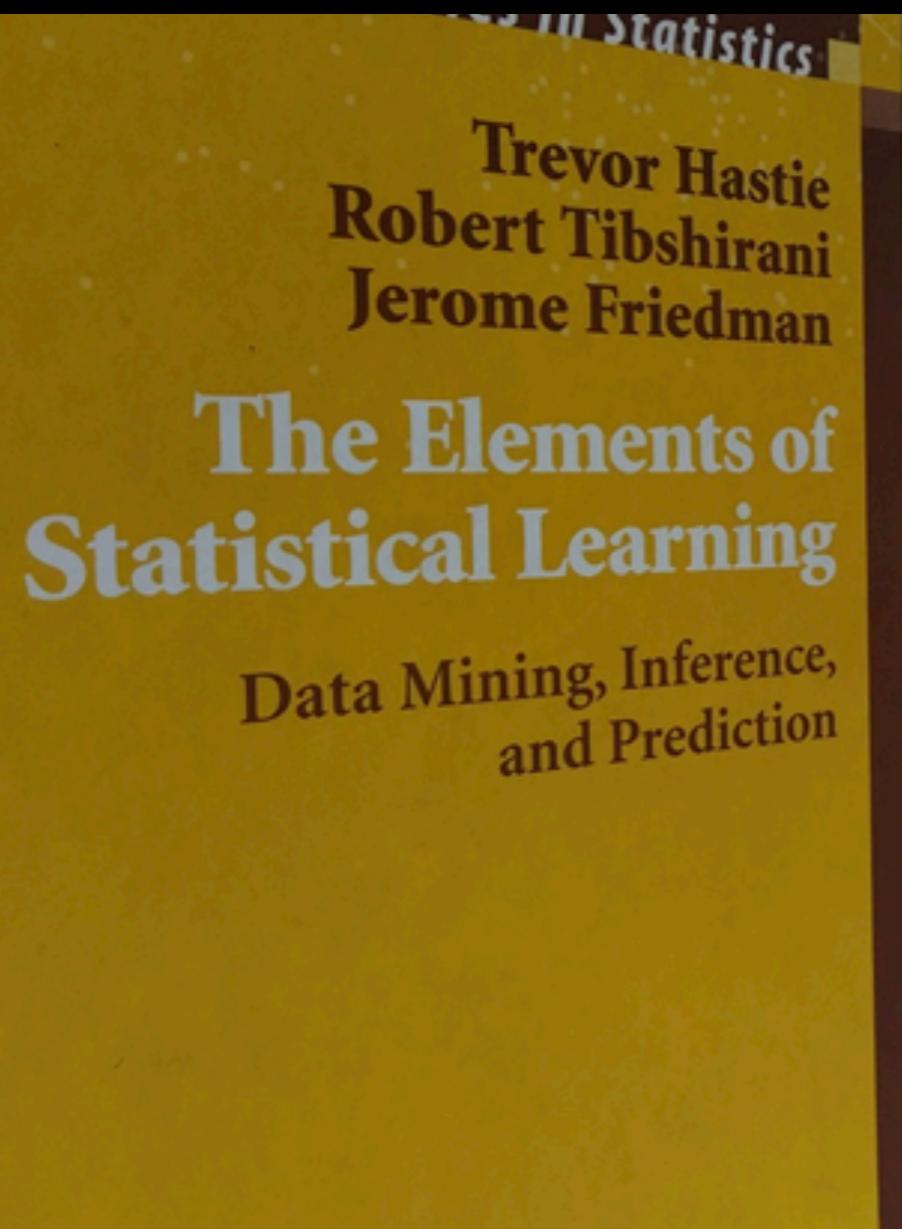


# DALEX: Descriptive mAchine Learning EXplanations



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15 years of experience in teaching,  
using, programming in R

Interested in DataVis, Explanations of  
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MSc student in Mathematics and  
Statistics @ University of Wrocław

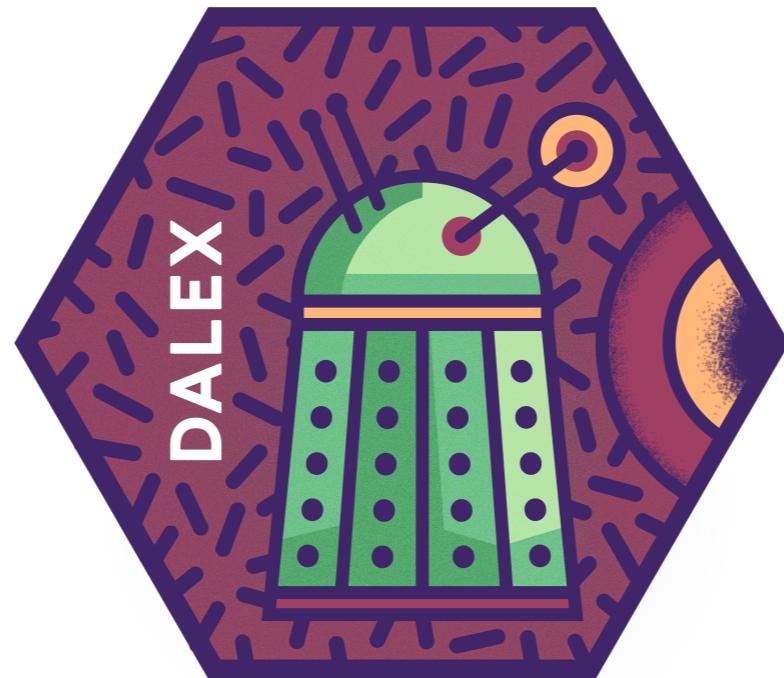
Fan of R programming

Working on machine learning  
interpretability.

<http://www.mstaniak.pl/>

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

How good is the predictive model?



Which variables are the most important in general?

How good is the model fit?

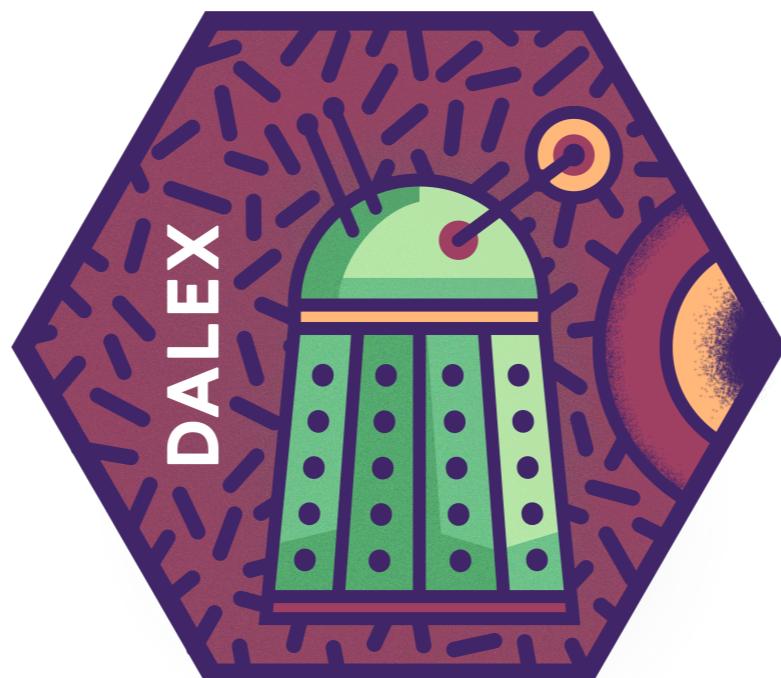
Which variables influence the single prediction?

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

Structure Explainers  
package: **randomForest**

Model Management  
package: **archivist**

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

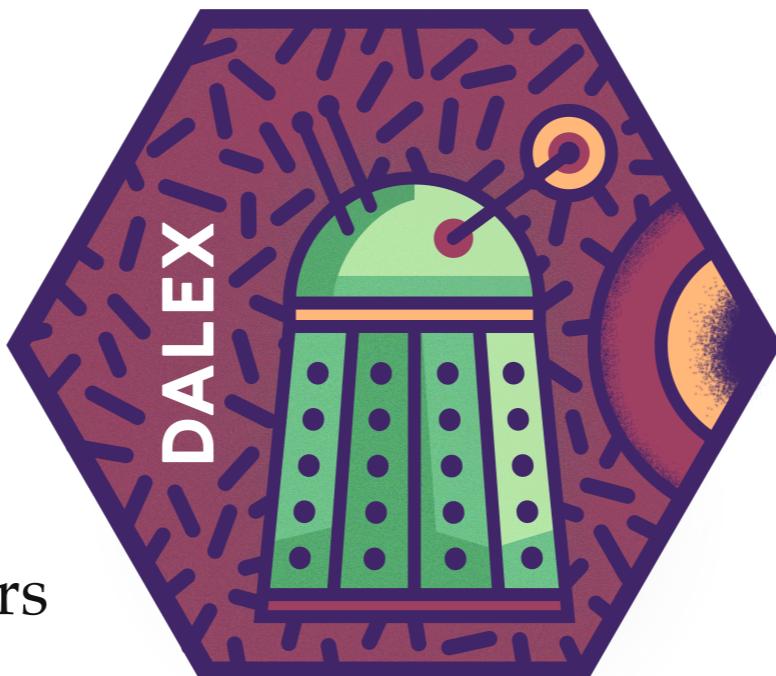


Model Performance Explainers  
package: **auditor**, **ROCR**, **caret**, **mlr**

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

# Today we will cover

1.  
Variable Explainers
2.  
Structure Explainers
3.  
Model Performance Explainers
4.  
Model Predictions Explainers



Lots of great  
applications for ML

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

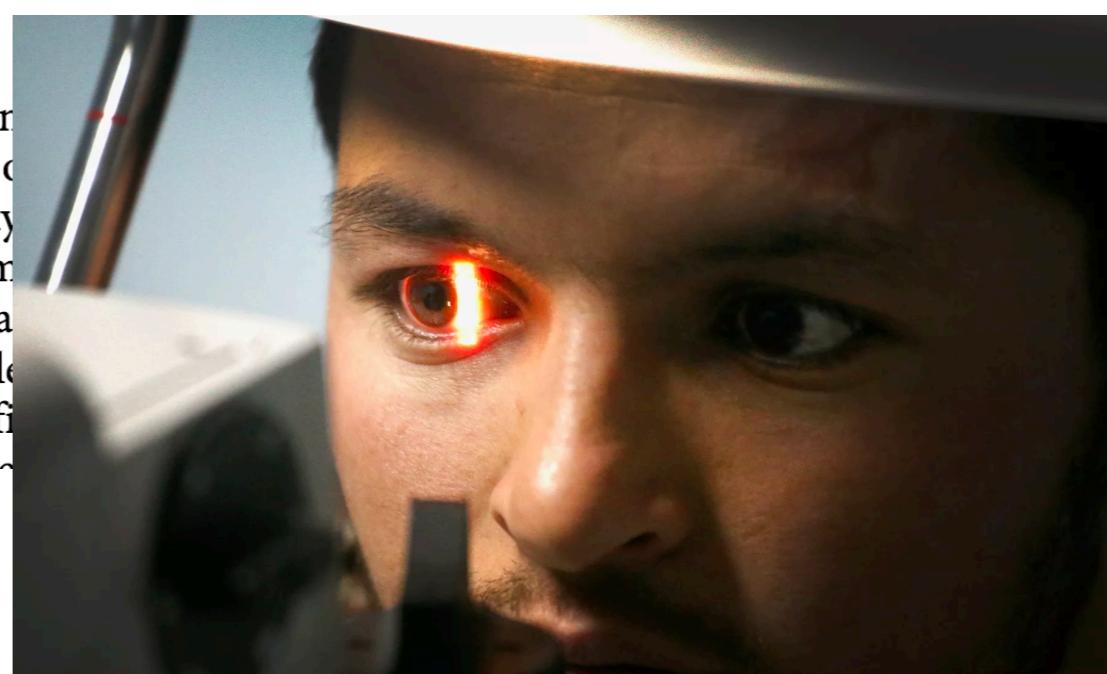
Ryan Poplin<sup>1,4</sup>, Avinash V. Varadarajan<sup>1,4</sup>, Katy Blumer<sup>1</sup>, Yun Liu<sup>1</sup>, Michael V. McConnell<sup>2,3</sup>, Greg S. Corrado<sup>1</sup>, Lily Peng<sup>1,4\*</sup> and Dale R. Webster<sup>1,4</sup>

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 the clinical utility of these models. In this work, we demonstrate that deep learning can predict cardiovascular risk factors from retinal fundus photographs.

Machine learning has the ability of classifying diseases based on





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>

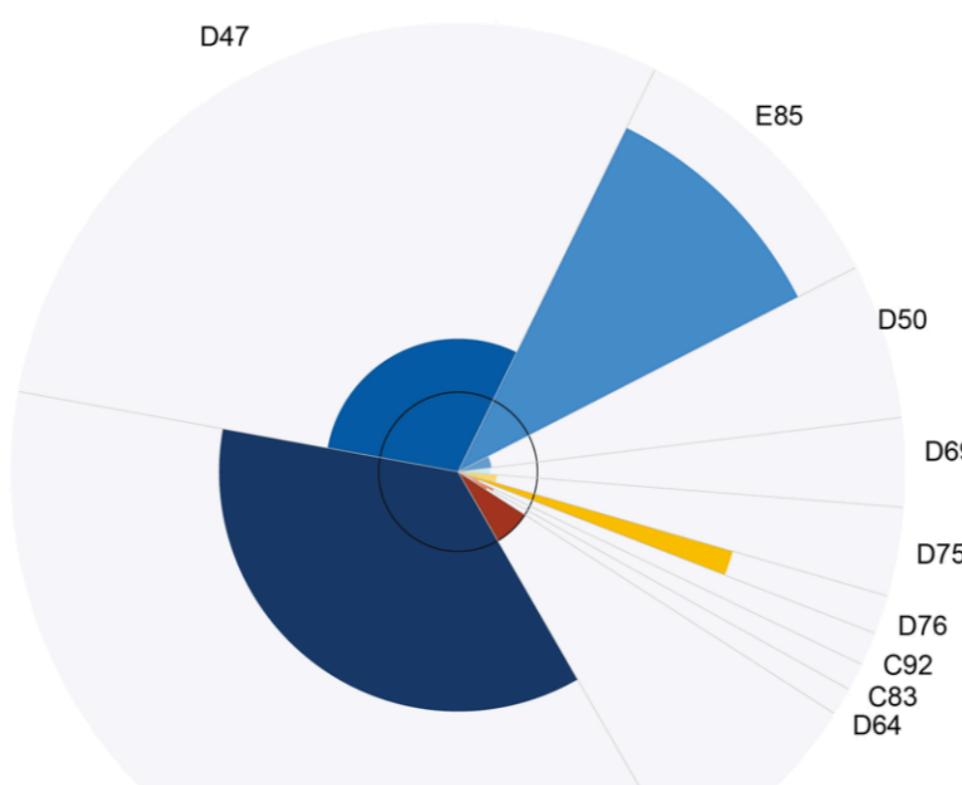
Received: 2 August 2017

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

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| 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   |

Imagine that these are predictions for  
you.  
Would you trust them?

Imagine that these are predictions for  
you.

Would you trust them?

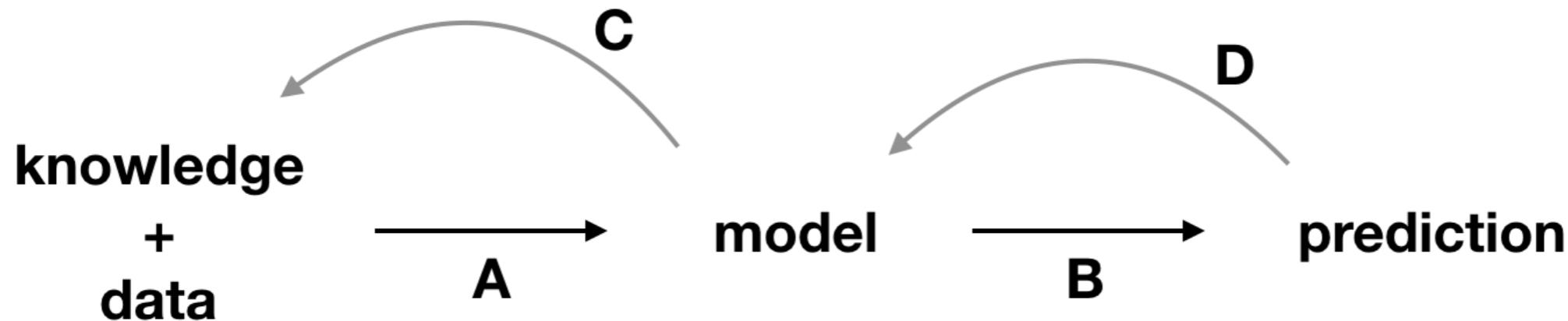
Having two black-box models with  
similar accuracy,  
which one would you trust?

# *Typical workflow in ML*



- A. Modelling is a process in which domain knowledge and data are turned into models.
- B. Models are used to generate predictions.

# *Typical workflow in ML*



- A. Modelling is a process in which domain knowledge and data are turned into models.
- B. Models are used to generate predictions.
- C. Understanding of model structure may increase our knowledge and in consequence leads to a better model. *DALEX helps here.*
- D. Understanding of drivers behind particular model predictions may help to correct wrong decisions and in consequence leads to a better model.  
*DALEX helps here.*

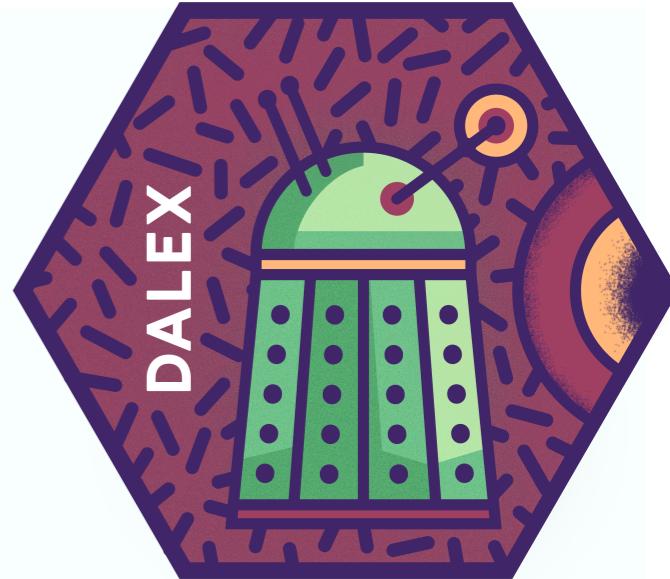
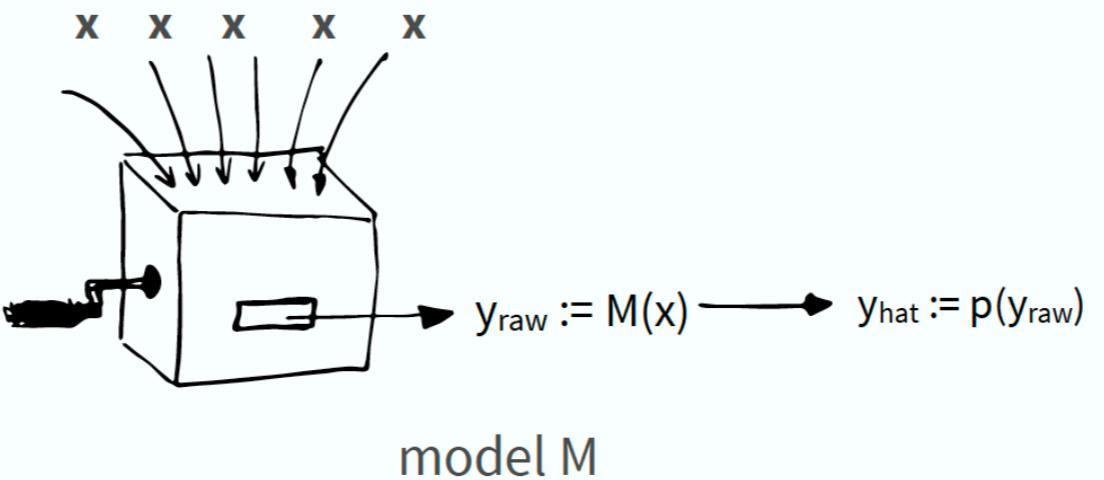


[http://www.warszawa.pl/biznes/panorama-warszawy/galeria/dzis\\_palac\\_kultury\\_i\\_nauki/](http://www.warszawa.pl/biznes/panorama-warszawy/galeria/dzis_palac_kultury_i_nauki/)



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

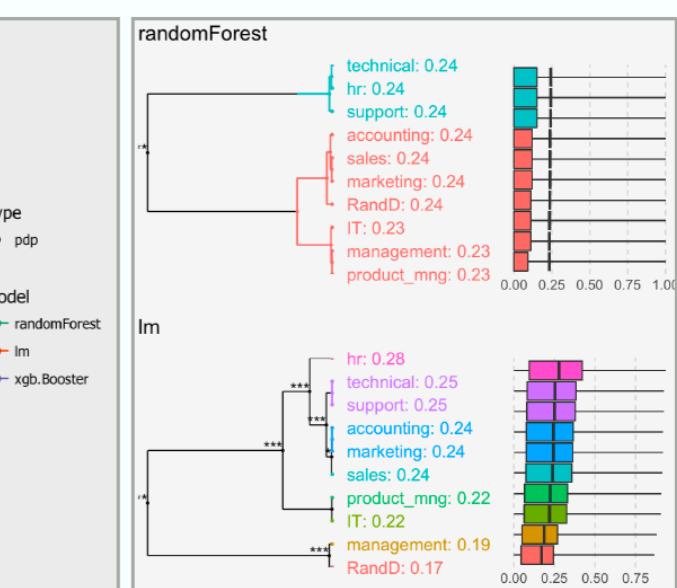
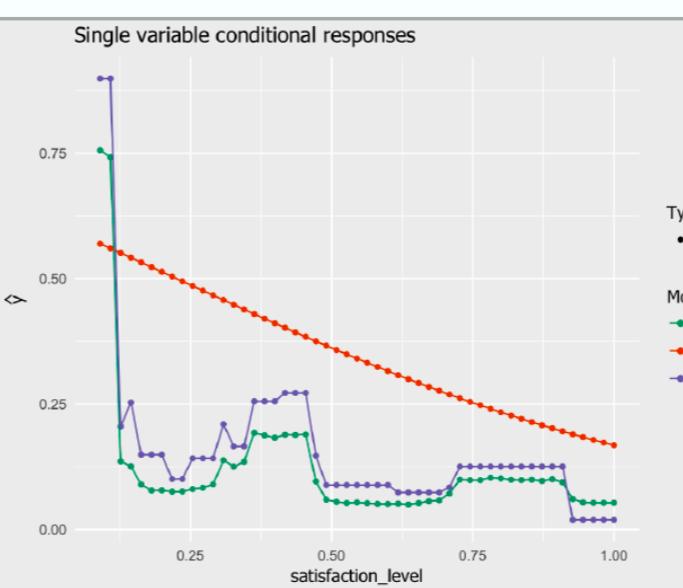
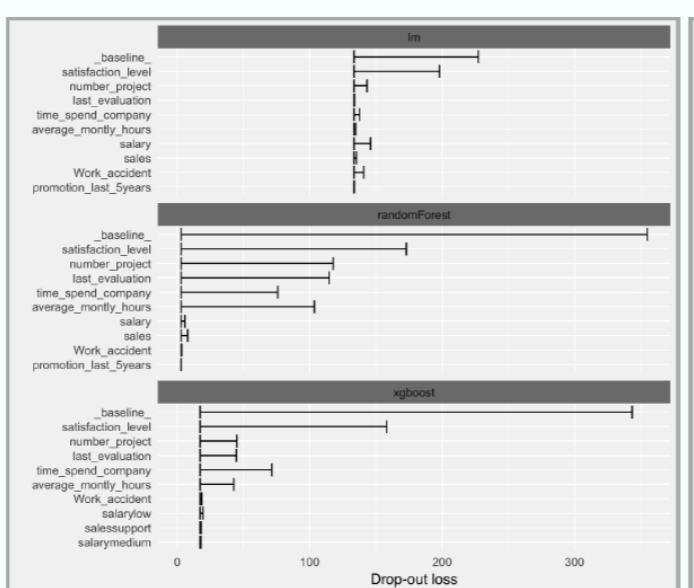
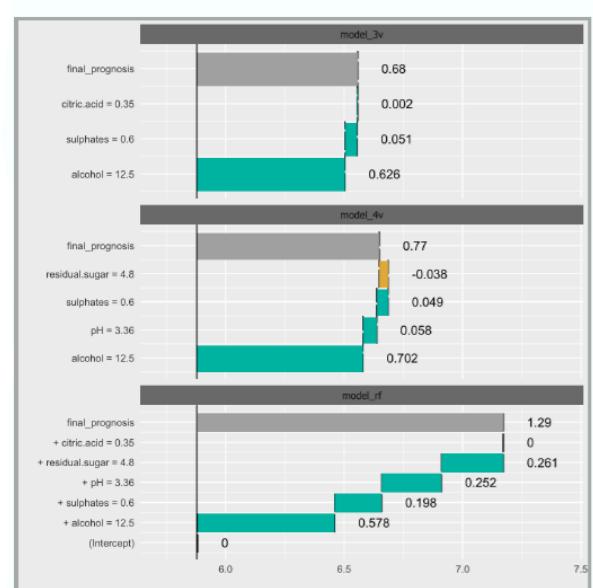
| m2.price | construction.year | surface | floor | no.rooms | district      |
|----------|-------------------|---------|-------|----------|---------------|
| 5897     | 1953              | 25      | 3     |          | 1 Śródmieście |
| 1818     | 1992              | 143     | 9     |          | 5 Bielany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

**A)****B)**

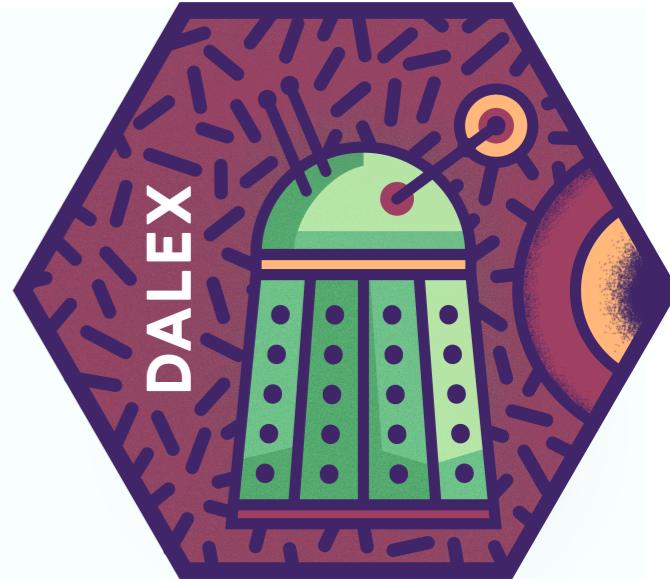
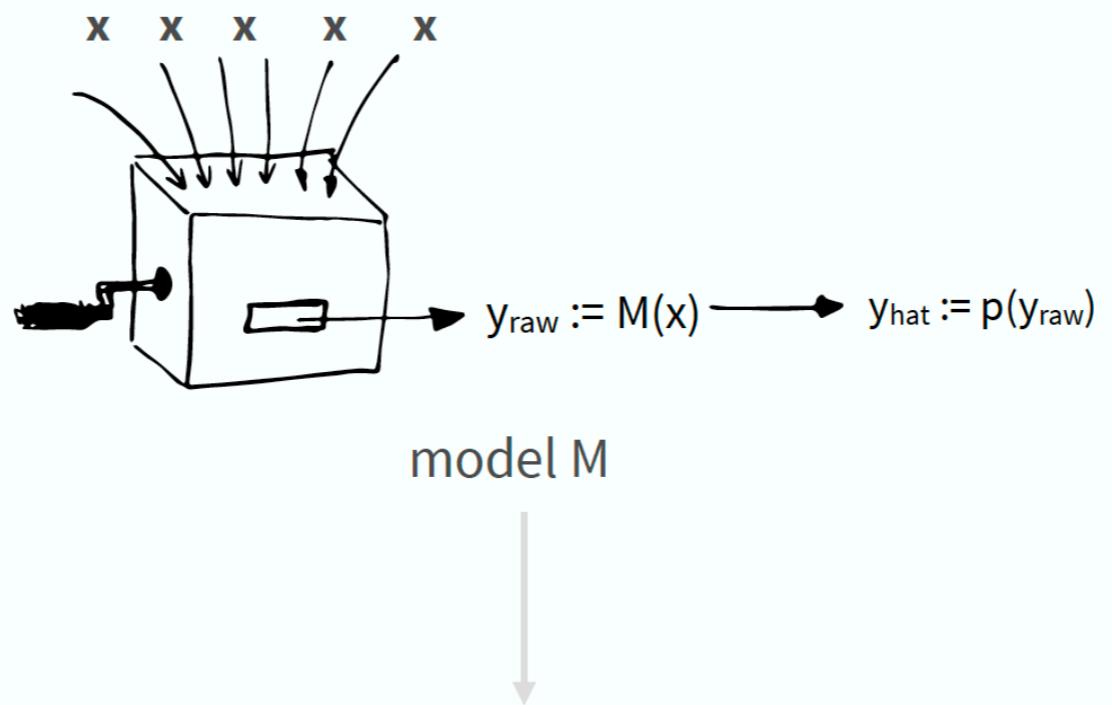
`explain(model; data; y; predict_function; trans)`

**C)**

`single_prediction(explainer, x)`   `variable_dropout(explainer)`   `single_variable(explainer, variable)`



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)

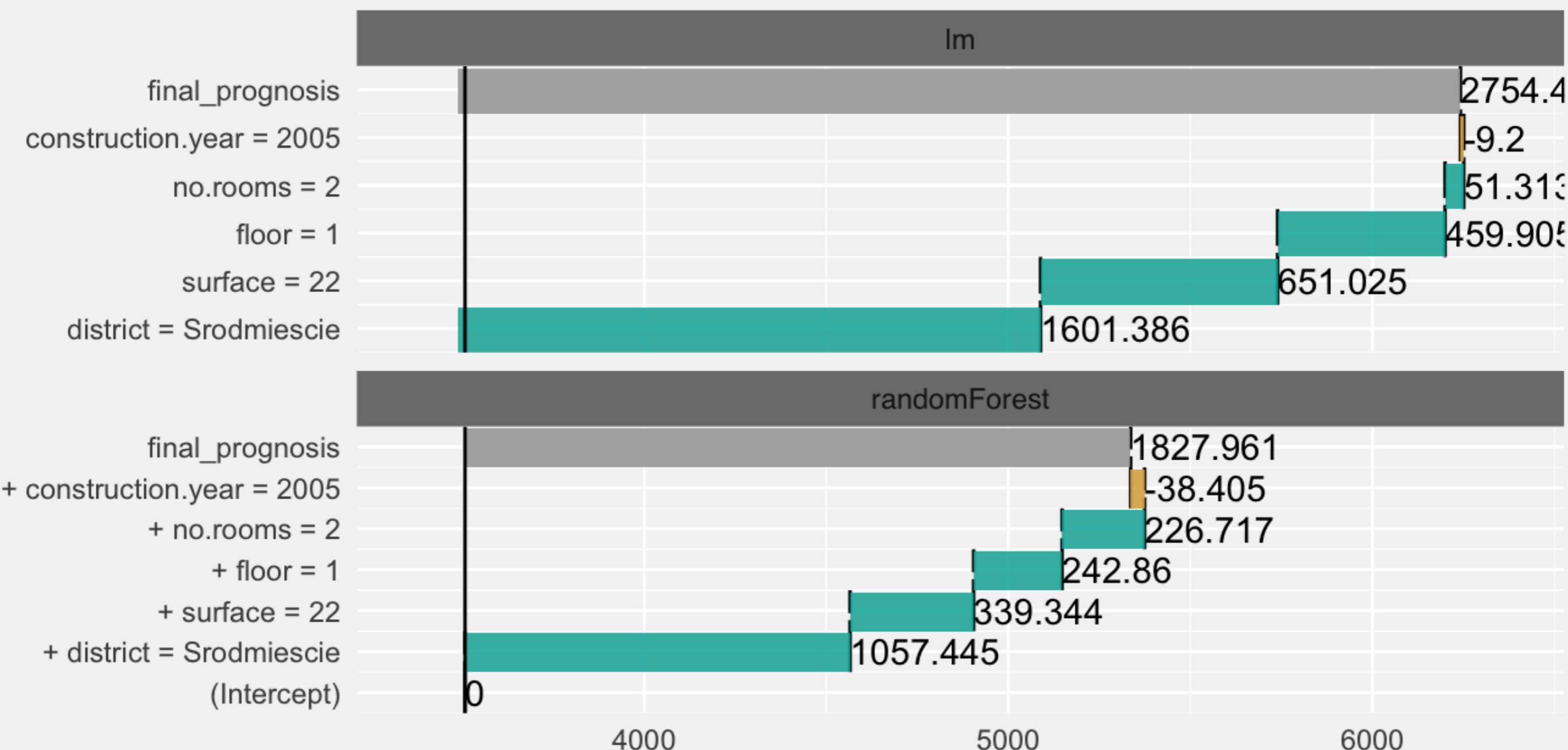
library("randomForest")
set.seed(59)
apartments_rf_model <- randomForest(m2.price ~ construction.year + surface + floor +
                                       no.rooms + district, data = apartments)

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

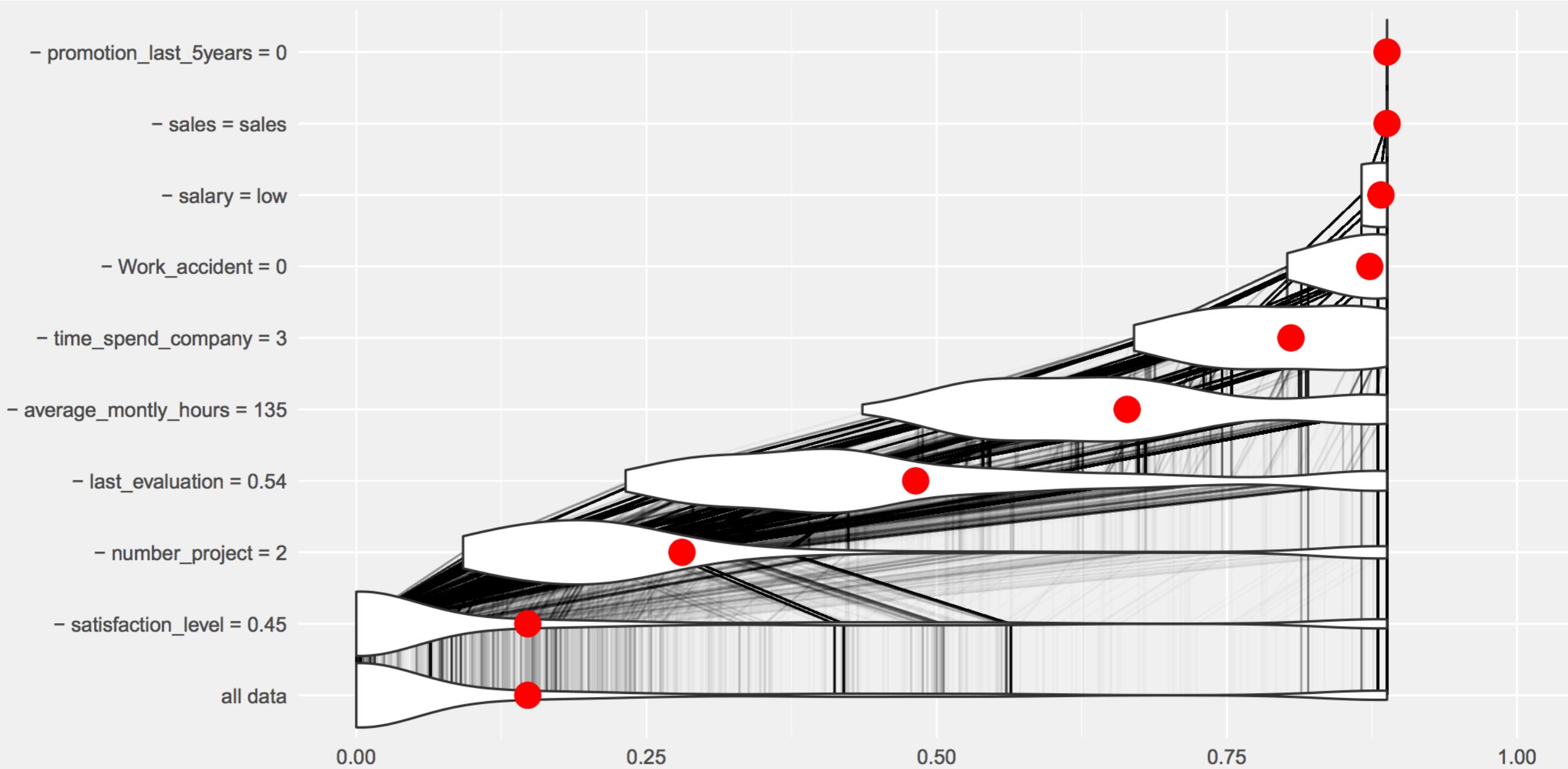
explainer_rf <- explain(apartments_rf_model,
                         data = apartmentsTest[,2:6], y = apartmentsTest$m2.price)
```

# 1. Prediction breakDown

# Which features influence a single prediction?



# Which features influence a single prediction?



# breakDown plots :: visual explanations for lm/glm models

## Linear model

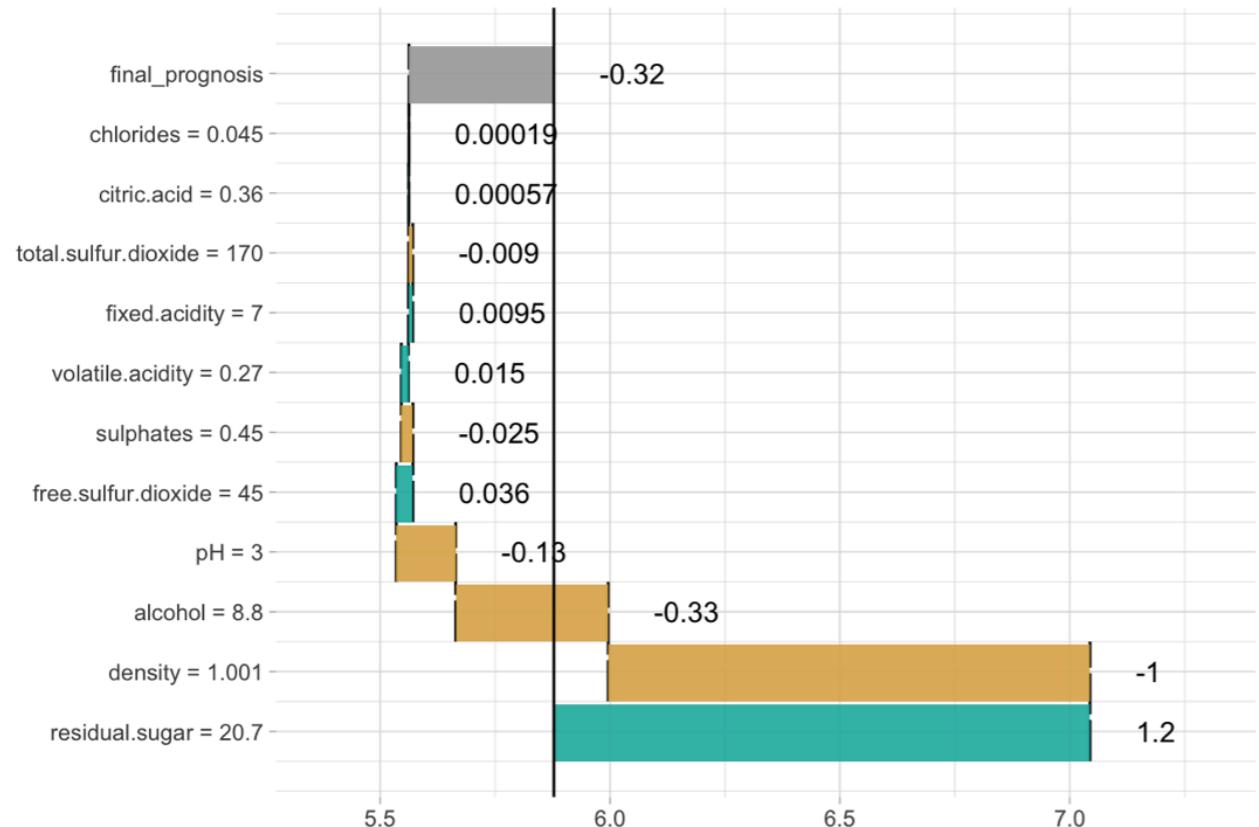
Linear models are widely used in predictive modeling. They have simple structure, which makes them easy to deploy or implement. But models with many variables are hard to understand.

The **breakDown** plot explains the relation between variables and model prediction for a new observation.

Explanations are generated in three steps:  
 1) create model with **lm()** function  
 2) break down model predictions with the **broken()** function  
 3) plot the graphical summary with the generic **plot()** function.

```
library(breakDown)
library(ggplot2)
model <- lm(quality ~ ., data = wineQuality)
br <- broken(model, wineQuality[1,],
              baseline = "Intercept")
br
#> contribution
#> residual.sugar = 20.7      1.20000
#> density = 1.001            -1.00000
#> alcohol = 8.8              -0.33000
#> pH = 3                   -0.13000
#> free.sulfur.dioxide = 45   0.03600
#> sulphates = 0.45          -0.02500
#> volatile.acidity = 0.27    0.01500
#> fixed.acidity = 7          0.00950
#> total.sulfur.dioxide = 170 -0.00900
#> citric.acid = 0.36         0.00057
#> chlorides = 0.045          0.00019
#> final_prognosis           -0.32000
#> baseline: 5.877909
plot(br)
```

breakDown plot for predicted quality of a wine



## Logistic regression

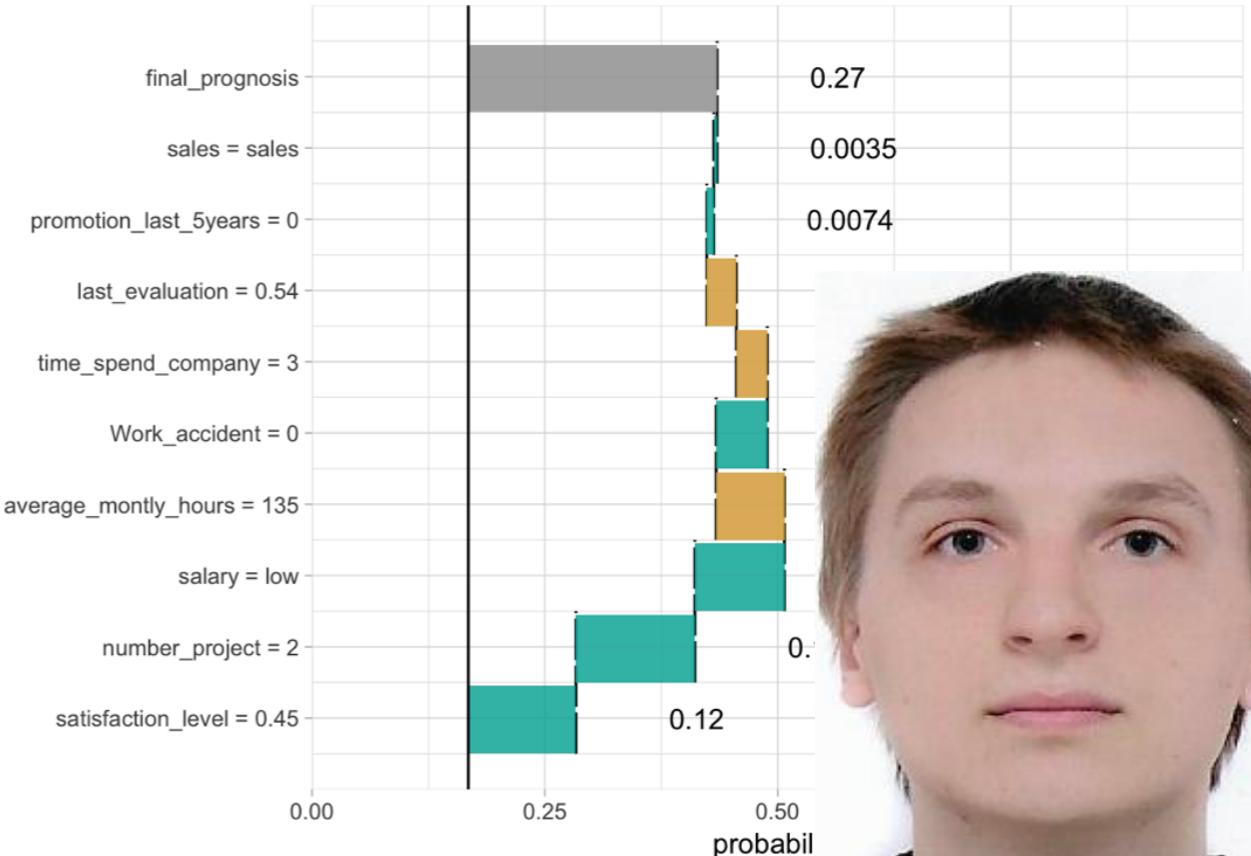
**breakDown** plots may be also used to explain predictions from the logistic regression model.

On the OX axis one may present linear predictions (default) or use probit/logit transformation to present contributions of variables from the model. Use the `trans`= argument to define the transformation.

The baseline is presented by the vertical black line in the plot. One may set the baseline to 0 or to population average (use the `baseline = "intercept"` argument).

```
library(breakDown)
library(ggplot2)
model <- glm(left~., data = HR_data,
              family = "binomial")
explain_1 <- broken(model, HR_data[11,],
                     baseline = "intercept")
explain_1
#> contribution
#> satisfaction_level = 0.45      0.670
#> number_project = 2             0.570
#> salary = low                  0.390
#> average_monthly_hours = 135   -0.290
#> Work_accident = 0              0.220
#> time_spend_company = 3        -0.130
#> last_evaluation = 0.54        -0.130
#> promotion_last_5years = 0     0.030
#> sales = sales                 0.014
#> final_prognosis               1.300
#> baseline: -1.601457
plot(explain_1, trans = function(x)
      exp(x)/(1+exp(x)))
```

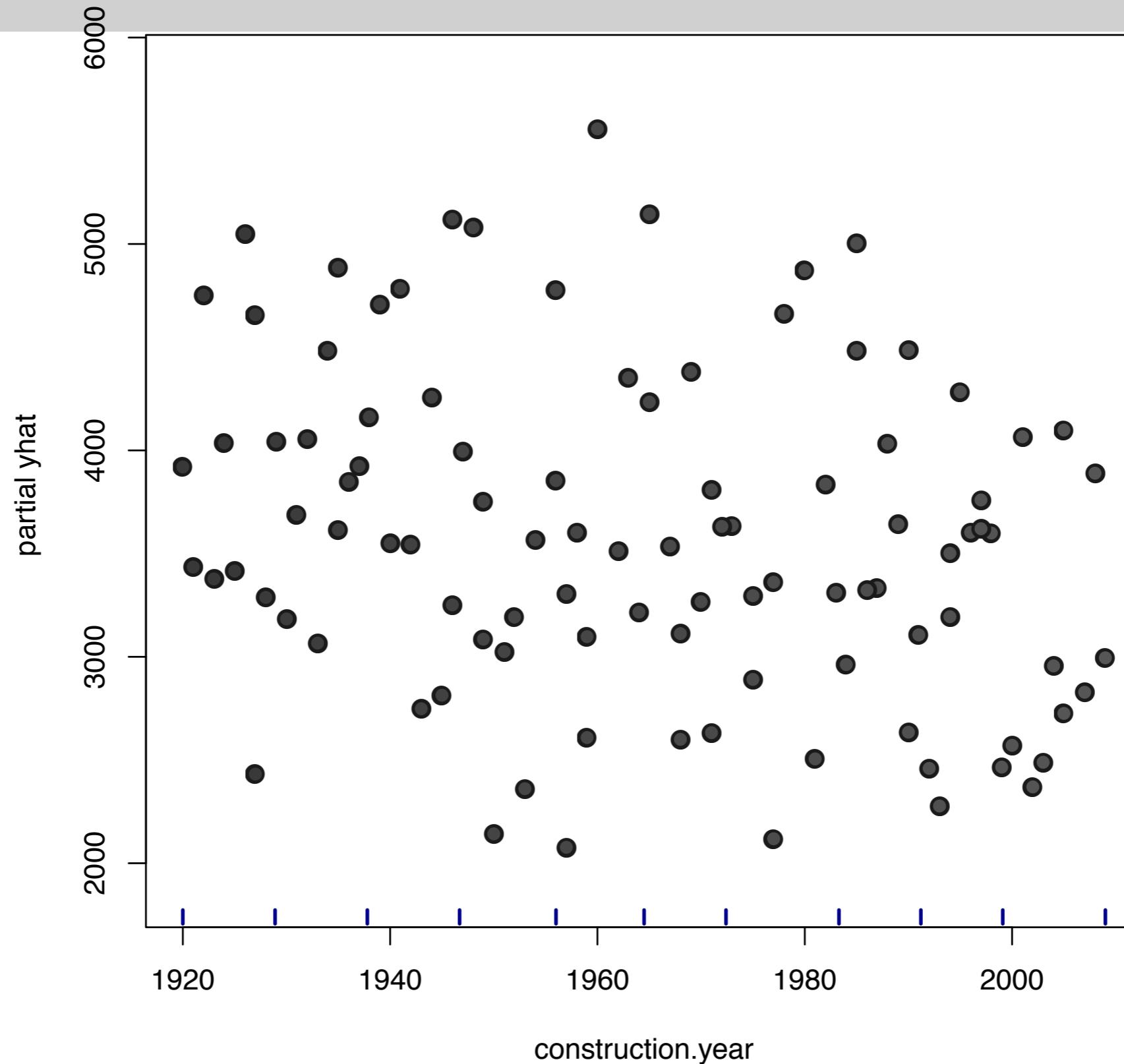
Predicted probability of leaving the company



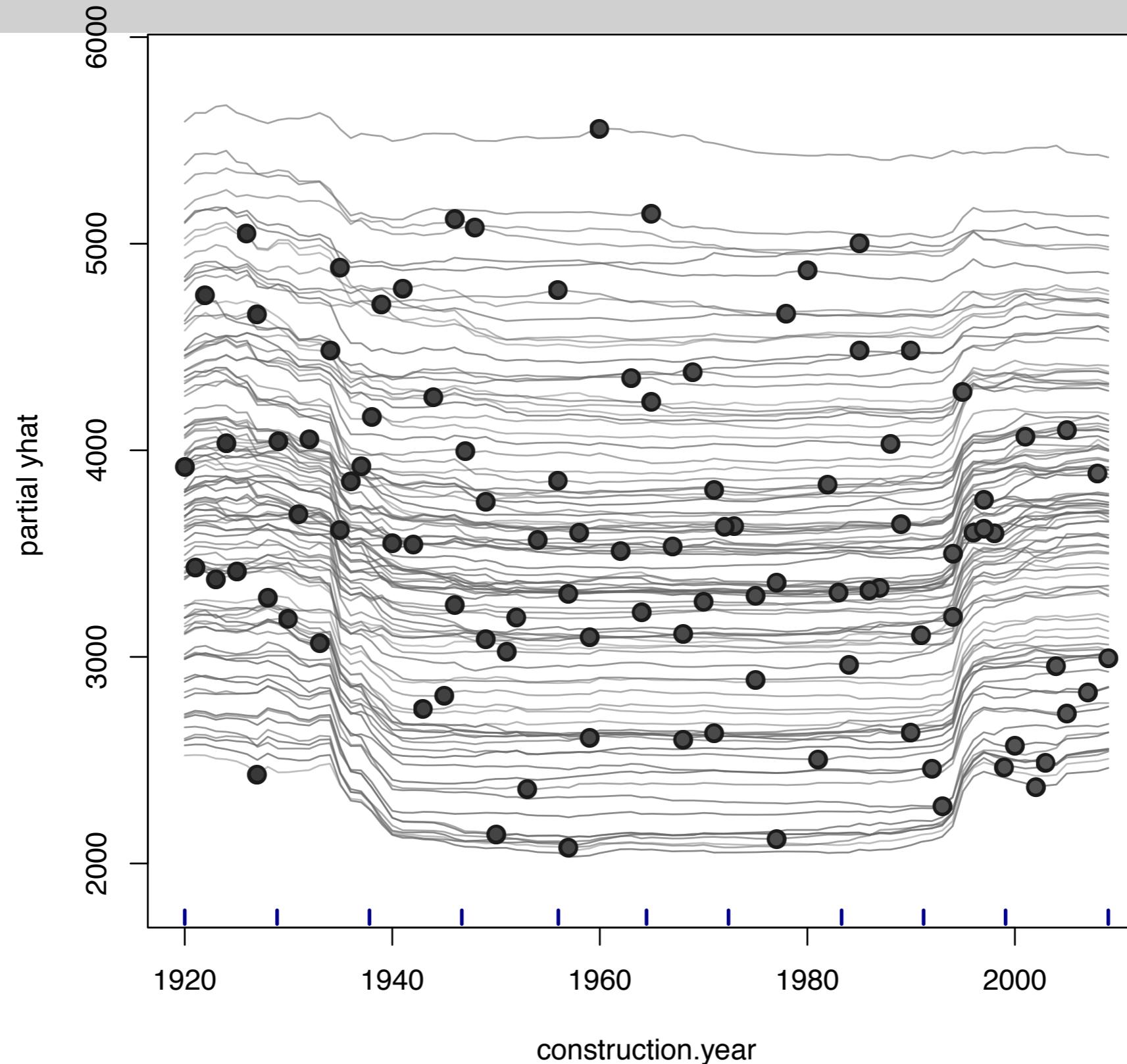
## 2. Variable response

How a single feature  
affects the model response?

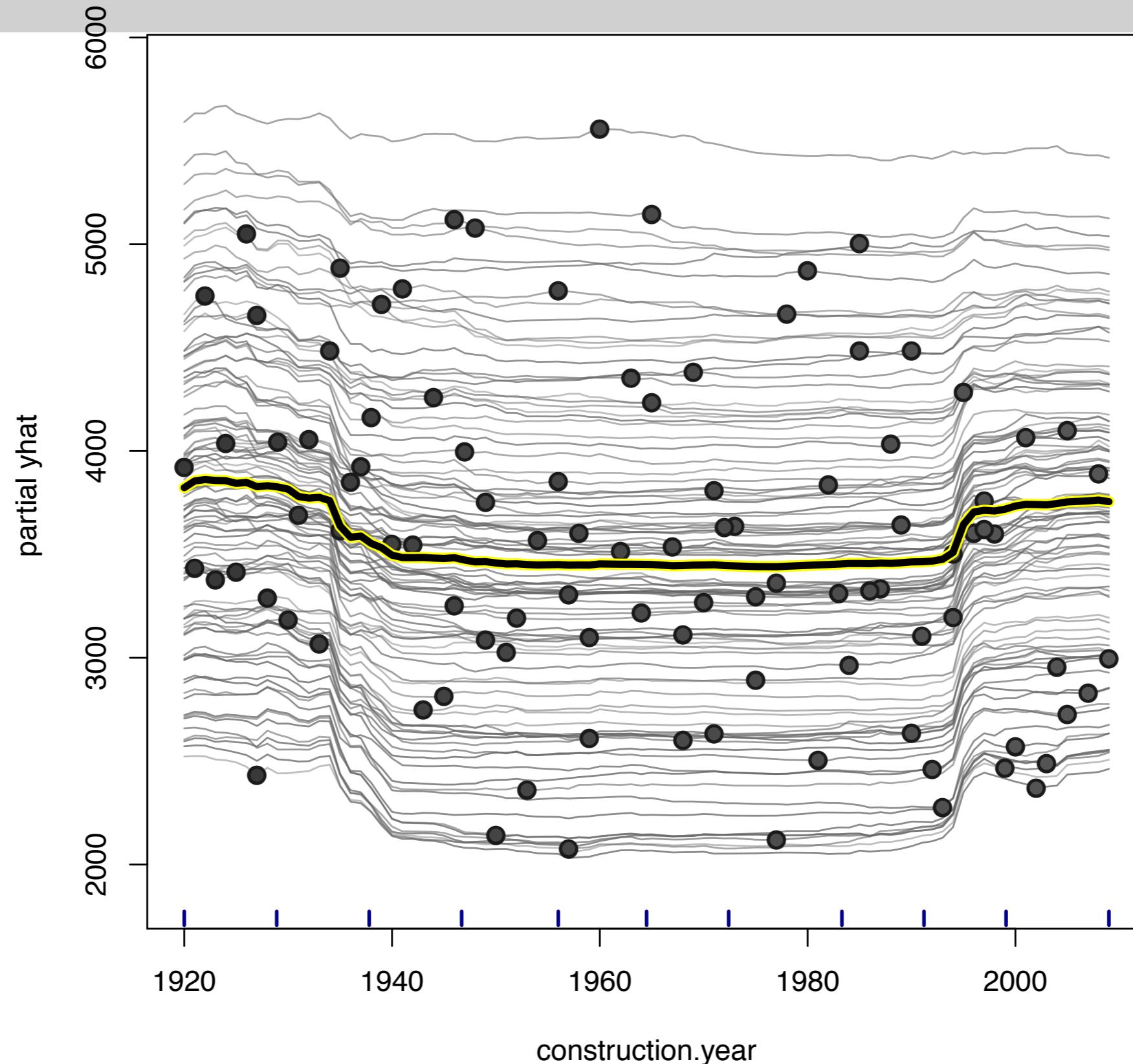
# How a single variable affect the response?



# How a single variable affect the response?



# How a single variable affect the response?



# 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>

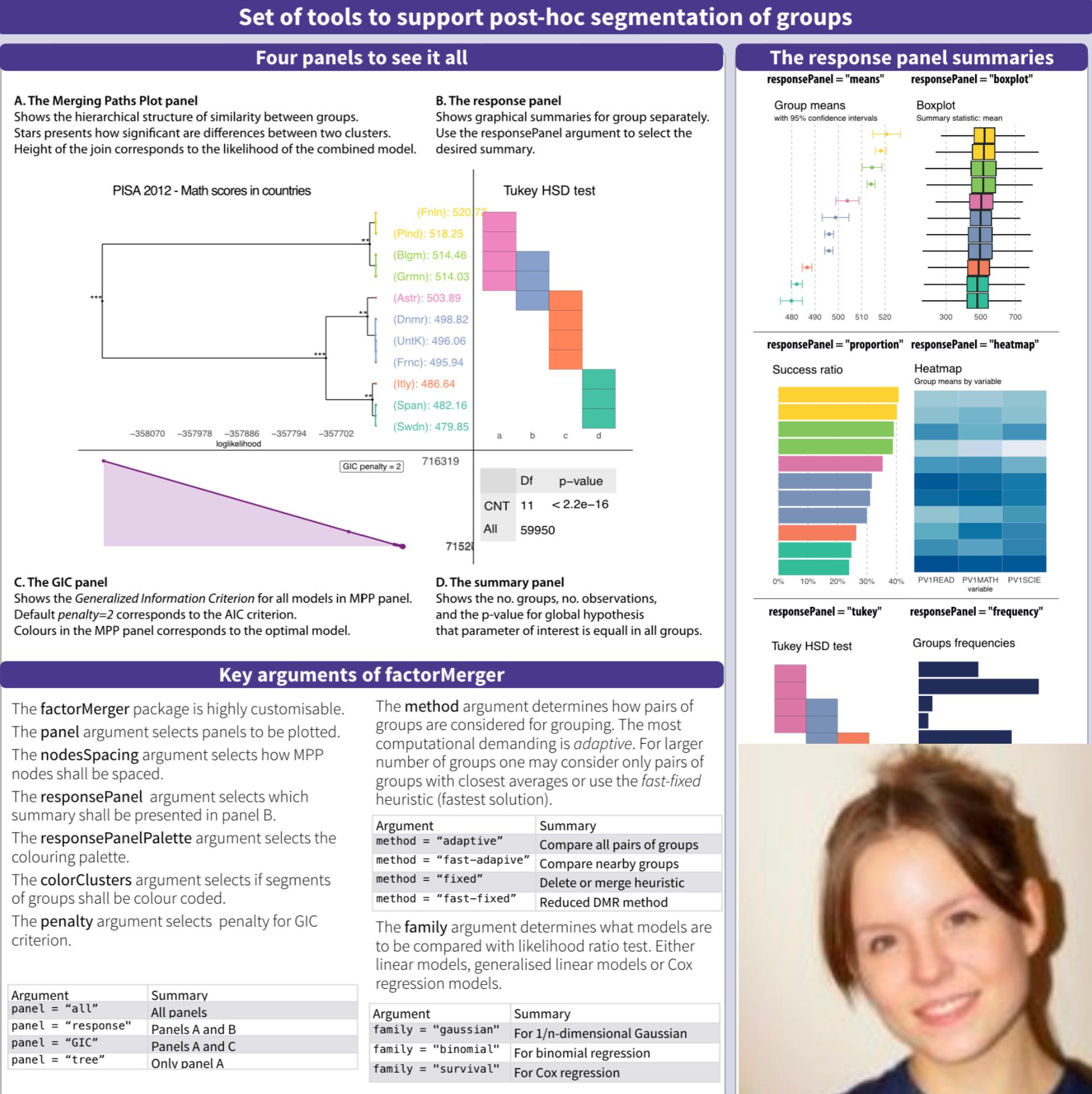
## Example

```
library(factorMerger)
```

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

```
print(fmAll)
```

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

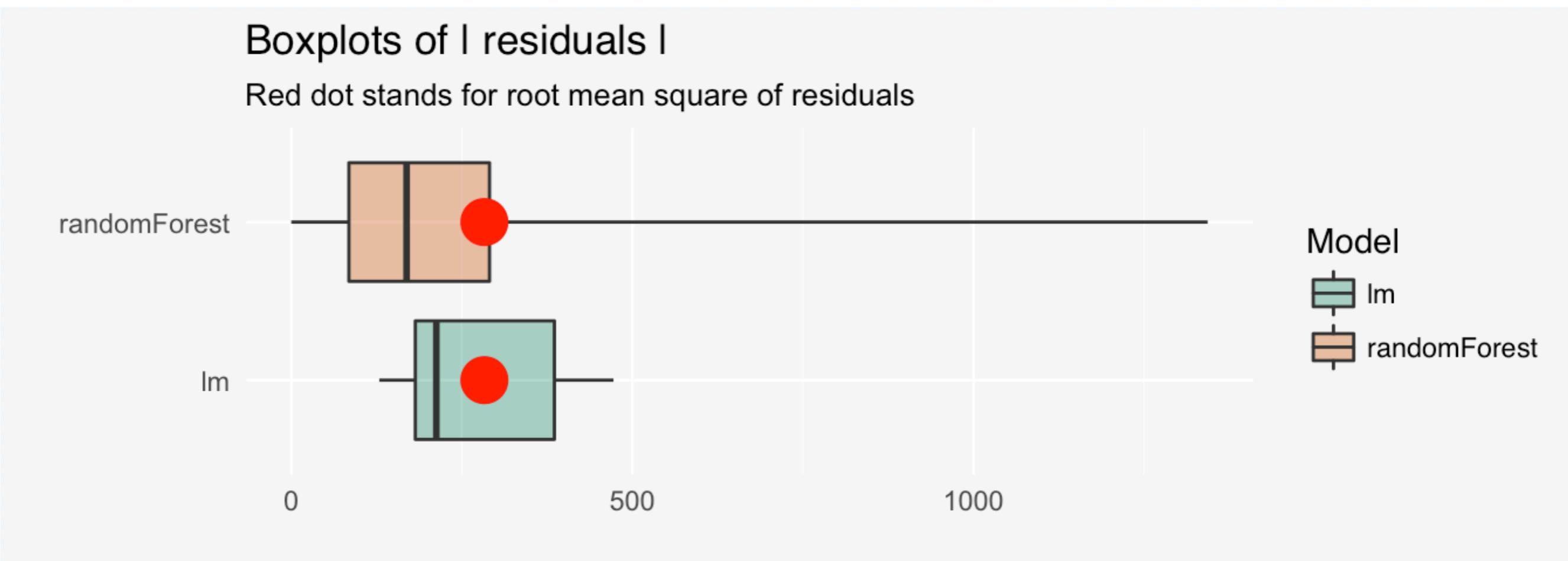


## 3. Model performance

How accurate is the model?

# Accuracy as a single number is not enough!

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



# 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

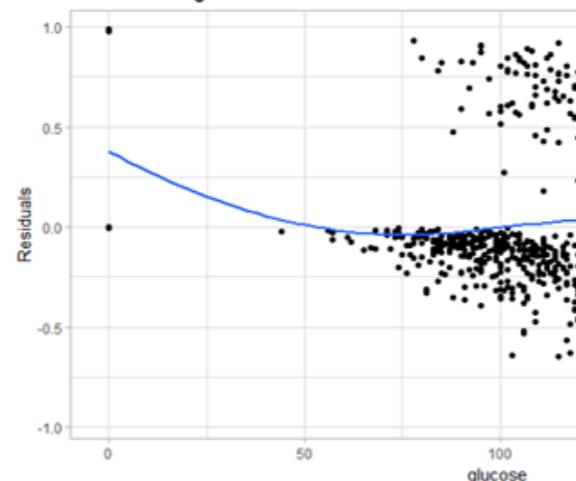
- Moral, R., Hinde, J., & Demétrio, C. (2017). Half-Normal Plots and Overdispersed Models in R: The *hnp* Package. *Journal of Statistical Software*, 81(10), 1 - 23.



## Basic plots

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

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



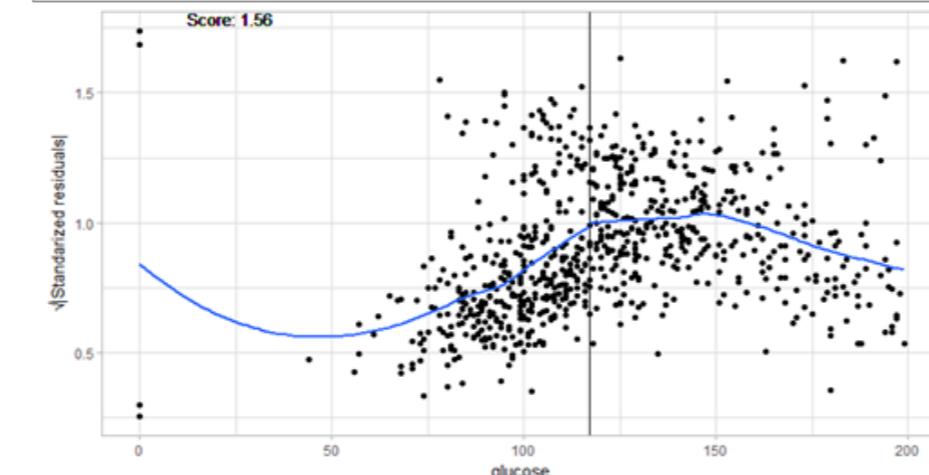
In the example above there were used response to provide any predict and residual function.

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'.

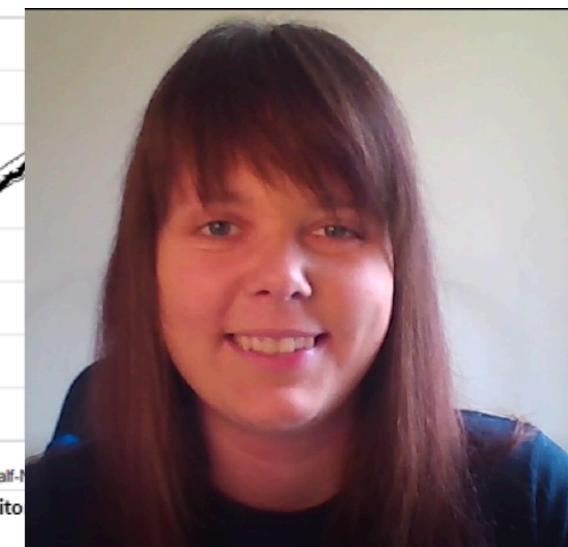
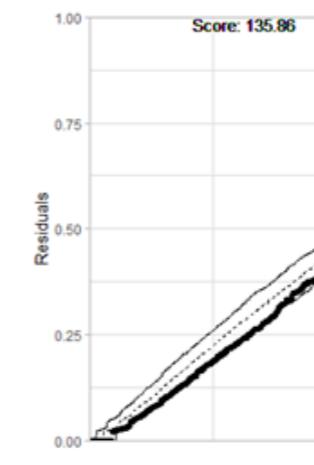
```
plot(audit_glm_dev, type="ScaleLocation",
      variable = "glucose")
```



Half-Normal plots 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.

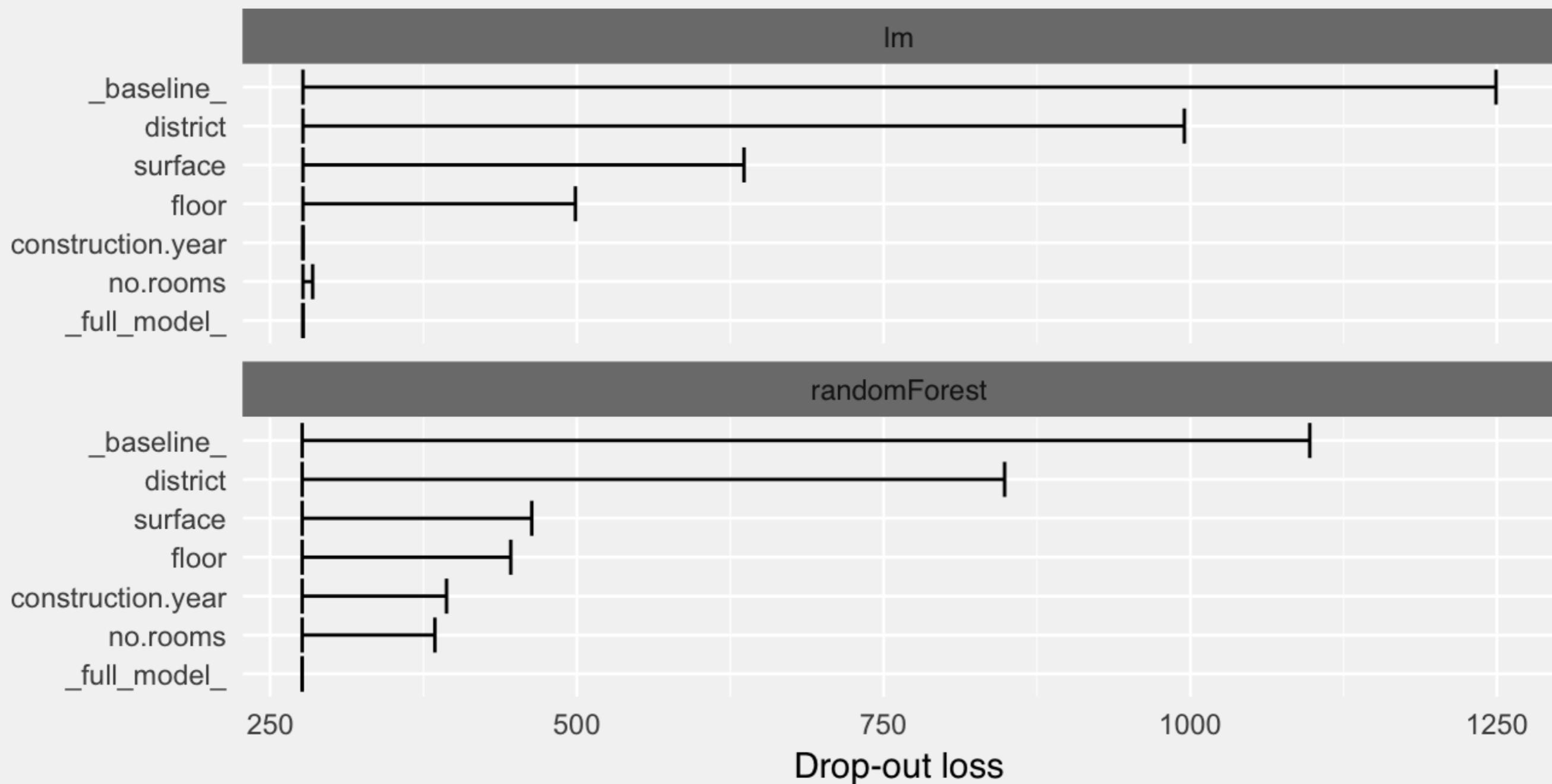
```
library(randomForest)
mod_rf <- randomForest(diabetes~.,
                        data=PimaIndiansDiabetes, ntree=100)
audit_rf <- audit(mod_rf)
plotHalfNormal(audit_rf)
```



## 4. Variable importance

Which variables are  
influential?

# Which variables are influential?



# Which variables are influential?

$$\hat{e}_{\text{orig}}(f) := \frac{1}{n} \sum_{i=1}^n L(f, \mathbf{Z}_{[i,\cdot]}) = \frac{1}{n} \sum_{i=1}^n L\{f, (\mathbf{y}_{[i]}, \mathbf{X}_{1[i,\cdot]}, \mathbf{X}_{2[i,\cdot]})\} = \hat{\mathbb{E}}L(f, Z),$$

$$\begin{aligned}\hat{e}_{\text{switch}}(f) &:= \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} h_f(\mathbf{Z}_{[i,\cdot]}, \mathbf{Z}_{[j,\cdot]}) \\ &= \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} L\{f, (\mathbf{y}_{[j]}, \mathbf{X}_{1[i,\cdot]}, \mathbf{X}_{2[j,\cdot]})\}.\end{aligned}$$

$$\text{Model Class Reliance} = \frac{\hat{e}_{\text{switch}}(f)}{\hat{e}_{\text{orig}}(f)},$$

Model Class Reliance: Variable Importance Measures for any Machine Learning Model Class, from the “Rashomon” Perspective

Aaron Fisher, Cynthia Rudin, Francesca Dominici

# DALEX::variable\_importance() - Explanations for Variable Importance



## Basics

Black-box models, like random forest or extreme gradient boosting machines, are commonly used due to their high performance. They are very flexible, what often results in high accuracy.

The problem is, that due to their complicated structure it is hard to understand which variables were the most influential for a particular model prediction

Variable Importance Explainers are designed to assess the influence of a single variable on the final model accuracy.

### How does it work?

The concept is straightforward, calculate how much we will loose on accuracy if a selected variable is perturbed.

For a selected loss function the model loss is calculated for the trained model applied to the original dataset against the original target. Then the drop in model loss is calculated for each variable in the dataset. It is calculated as the loss for a model applied to a dataset with selected column being permuted.

The variable importance plots shows the initial loss of the trained model, size of the additional losses that come from permutations of selected variables and the ‘baseline’ which is the loss for permuted model responses.

It is useful when different model are compared, since on a single plot we see the initial model performance and also drops that come from permutations of a single variable in the selected model.

### References

- Molnar, Christoph. 2018. *Interpretable Machine Learning*. <https://christophm.github.io/>
- Breiman, Leo. 2001. *Random Forests*. *Machine Learning* 45 (1). Springer: 5–32.
- Fisher, Aaron, Cynthia Rudin, and Francesca Dominici. 2018. *Model Class Reliance: Variable Importance Measures for any Machine Learning Model Class, from the ‘Rashomon’ Perspective*. <http://arxiv.org/abs/1801.01489>.

## 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>.

Here we are building a random forest model. The nice thing about this model is that it embeds some variable importance measure.

```
library("randomForest")
HR_rf_model <- randomForest(left~., data =
breakDown::HR_data, ntree = 100)
importance(HR_rf_model)
```

IncNodePurity

|                      |            |
|----------------------|------------|
| satisfaction_level   | 896.584411 |
| last_evaluation      | 294.195269 |
| number_project       | 496.397115 |
| average_montly_hours | 398.495343 |

So, now let's build an explainer and use it to calculate our model agnostic variable importance measure with **variable\_importance()** function.

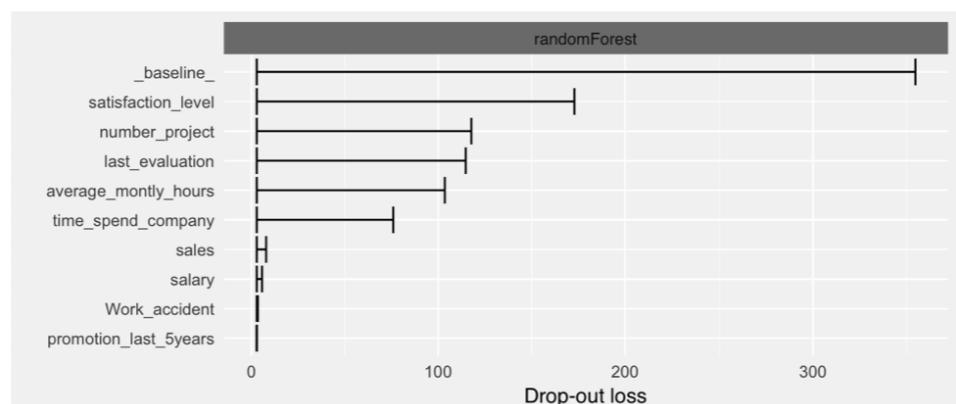
```
explainer_rf <- explain(HR_rf_model, data = HR_data,
y = HR_data$left)
vd_rf <- variable_importance(explainer_rf, type = "raw")
vd_rf
```

| variable           | dropout_loss | label        |
|--------------------|--------------|--------------|
| _baseline_         | 335.556063   | randomForest |
| satisfaction_level | 168.001733   | randomForest |
| last_evaluation    | 100.714534   | randomForest |
| number_project     | 100.568214   | randomForest |
| time_spend_company | 90.349207    | randomForest |

Values are different because different measures of importance are being calculated, but the order is more or less the same. Now we are ready to plot the variable importance with the generic **plot()** function.

Note that in addition to `type="raw"` one can also use “*difference*” or “*ratio*” as suggested in the Fisher et all 2018 article.

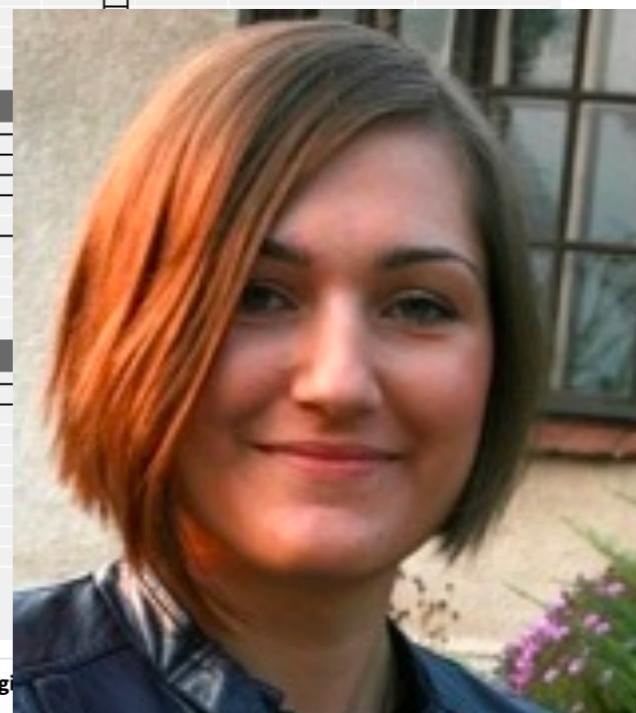
```
plot(vd_rf)
```



A very useful feature of the DALEX package is the capability to overlay responses from different models in a single plot. Below we present results for a Random Forest, GLM and XGBoost.

```
library("xgboost")
mm_train <- model.matrix(left~.-1, HR_data)
data_train <- xgb.DMatrix(model_matrix_train,
label = HR_data$left)
param <- list(max_depth = 2,
objective = "binary:logistic", eval_metric = "auc")
HR_xgb <- xgb.train(param, data_train, nrounds = 50)
ex_xgb <- explain(HR_xgb, data = mm_train,
y = HR_data$left, label = "xgboost")
vd_xgb <- variable_importance(ex_xgb, type = "raw")

HR_glm <- glm(left~., data=HR_data, family = "binomial")
ex_glm <- explain(HR_glm, data=HR_data, y = HR_data$left)
logit <- function(x) exp(x)/(1+exp(x))
vd_glm <- variable_importance(ex_glm, type = "raw")
plot(vd_rf, vd_glm, vd_xgb)
```

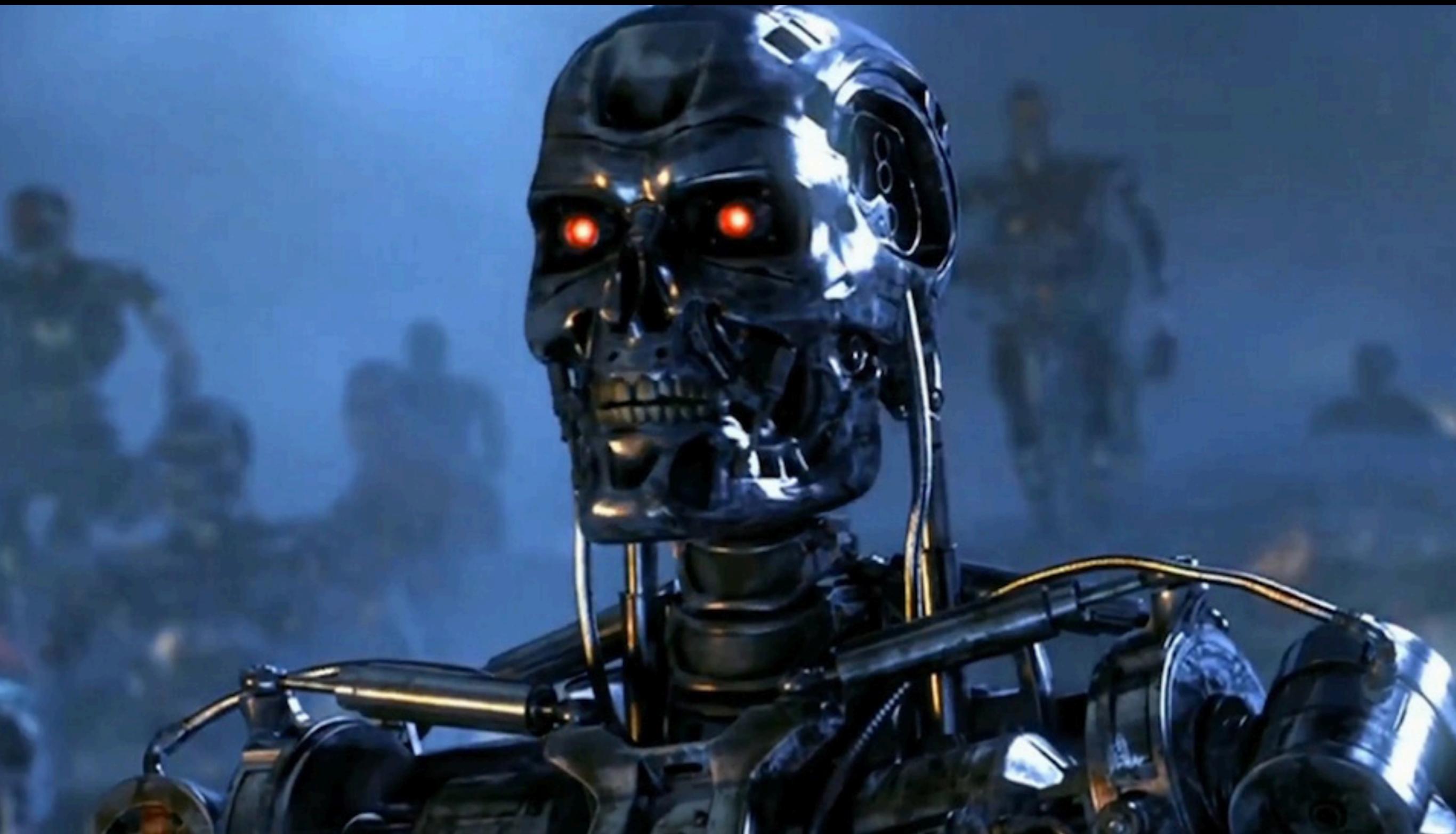


Model - Human interface

Hybrid AI + HI

How they will look like?

Machine Learning Models will replace humans



# Machine Learning Models will empower humans

