Interpretable Features for Explaining Machine Learning Models

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Joint work with Przemysław Biecek

Leuven, 15 VII 2019

The need for interpretability

Before

5 years of web logs + ML

=

proved to be a more useful and timely indicator [of flu] than government statistics with their natural reporting lags

- Viktor Mayer-Schönberger and Kenneth Cukier ,
Big Data: A Revolution That Will Transform How We Live, Work and Think

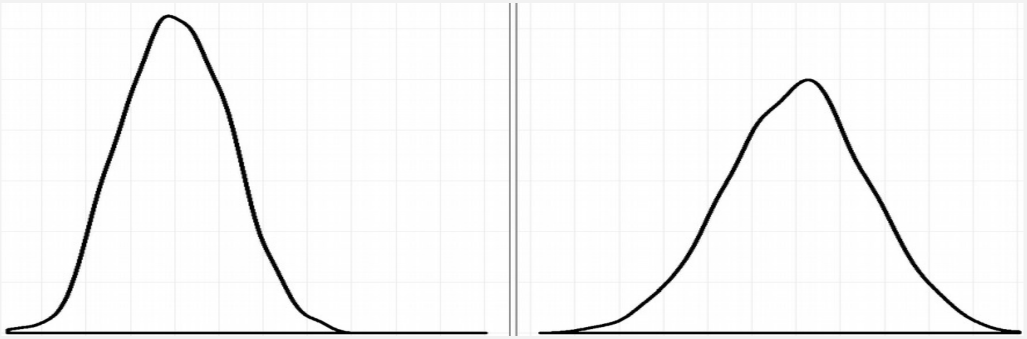
After

wired.com/2015/10/can-learn-epic-failure-google-flu-trends/

Machine Learning models are vulnerable to:

- Biased training (and other data quality issues),
- Concept drift,
- Unmeasurable objectives (Fairness, Lawfulness).

Females vs Male frequencies



Training data vs validation data

Amazon scraps secret AI recruiting tool that 'didn't like women'

- Amazon ended job recruiting service that was reportedly biased against women
- It was created by Amazon's Edinburgh team in 2014 to automatically sort CVs
- The AI taught itself to downgrade resumes that included words like 'women's'

Types of Explanations

Intrinsic vs post-hoc

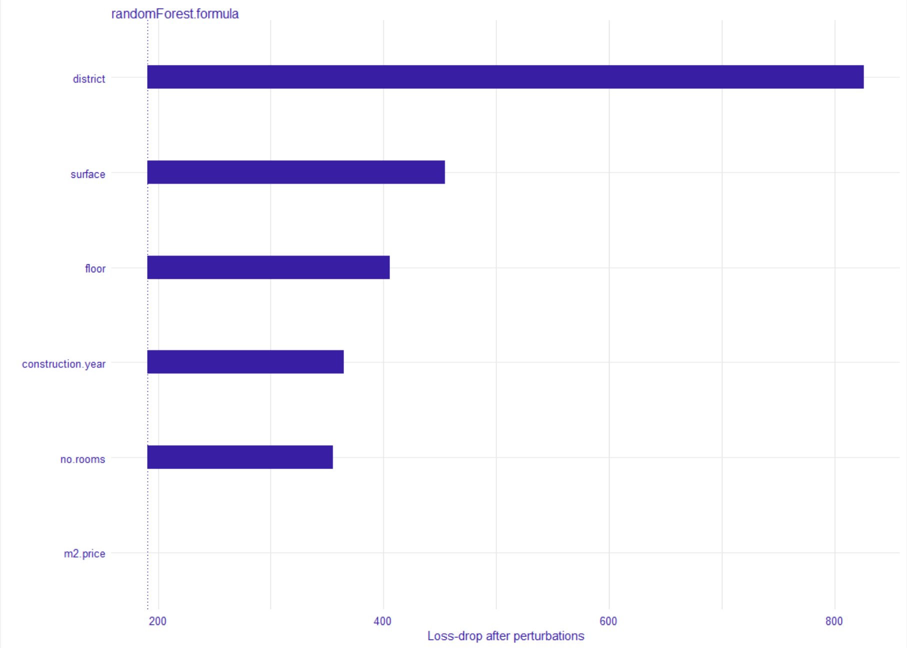
- Intrinsic explanations are based on specific algorithm design
  (model form, training explanations and model jointly).

- Post-hoc explanations are concerned with an already trained model
  (model is never re-fitted, only predictions are used).

```
lm(formula = m2.price ~ ., data = apartments)

Residuals:
   Min     1Q Median     3Q    Max
-247.5 -202.8 -172.8  381.4  469.0

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)        5020.1391   682.8721   7.352 4.11e-13 ***
construction.year    -0.2290     0.3483  -0.657   0.5110
surface             -10.2378     0.5778 -17.720  < 2e-16 ***
floor               -99.4820     3.0874 -32.222  < 2e-16 ***
no.rooms            -37.7299    15.8440  -2.381   0.0174 *
districtBielany      17.2144    40.4502   0.426   0.6705
districtMokotow     918.3802    39.4386  23.286  < 2e-16 ***
districtOchota      926.2540    40.5279  22.855  < 2e-16 ***
districtPraga       -37.1047    40.8930  -0.907   0.3644
districtSrodmiescie 2080.6110   40.0149  51.996  < 2e-16 ***
districtUrsus        29.9419    39.7249   0.754   0.4512
districtUrsynow     -18.8651    39.7565  -0.475   0.6352
districtWola        -16.8912    39.6283  -0.426   0.6700
districtZoliborz    889.9735    40.4099  22.024  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```



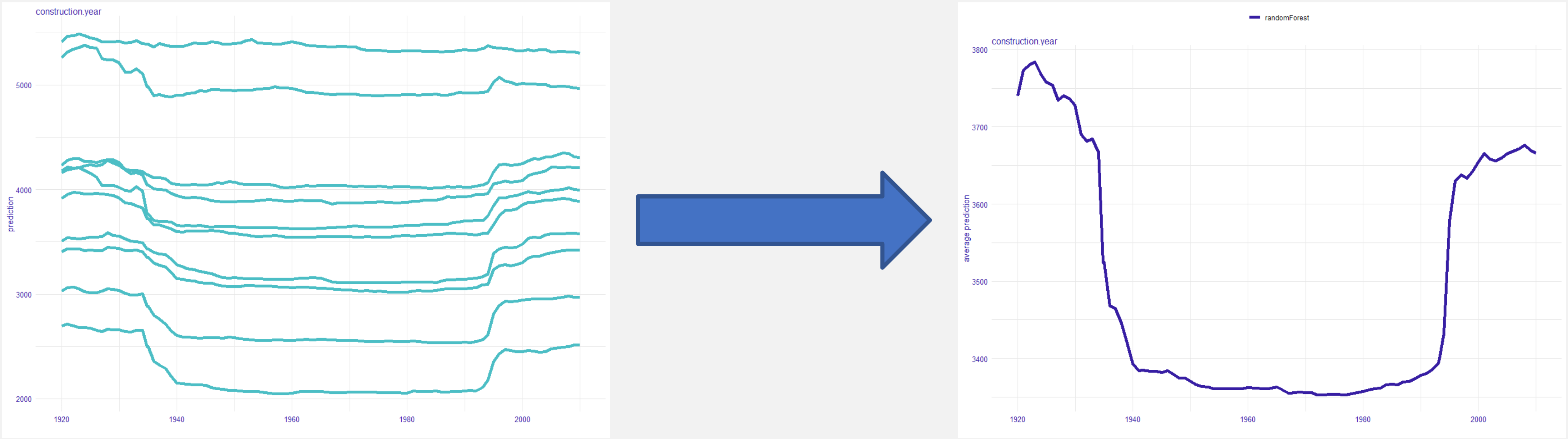
Model-agnostic Approach

	Definition	Example	Comments
Model-agnostic explanations	Do not use knowledge about the specific algorithm	Permutation-based variable importance	Do not require model re-fitting
Model-specific explanations	Assume that a specific algorithm was used to fit the model	Average minimum depth in a random forest	Can be more accurate

Local vs Global Explanations

- Local explanations are concerned with a single observation and its prediction.
- Global explanations are concerned with the model as a whole.

  Global explanations are often aggregation of local explanations (e.g. mean).

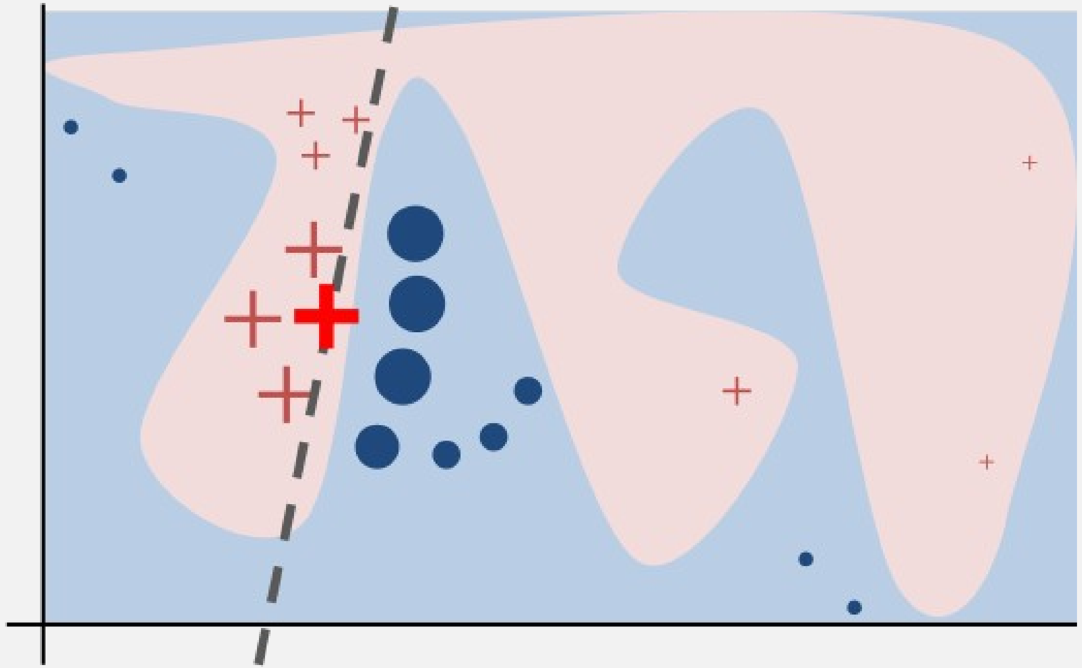


Local Explanations

Approaches to Local Explanations

- What-If analysis (marginal response of the model when changing a single variable for a single observation):
  - Ceteris Paribus profiles (Individual Conditional Expectation).
- Local surrogate models (fitting an interpretable model locally – original paper: LIME, 2016):
  - LIME and its modifications (aLIME, k-LIME, localSurrogate),
  - **LIVE and localModel (versions of LIME developed at MI2 Data Lab).**
- Example-based explanations
  - Contrastive explanations
  - Prototypes and criticism
- Prediction decomposition (attributing additive scores to features).
  - EXPLAIN,
  - Shapley Values,
  - **Break Down and iBreakDown (methods connected to Shapley Values developed at MI2 Data Lab)**

Local Interpretable Model-agnostic Explanations



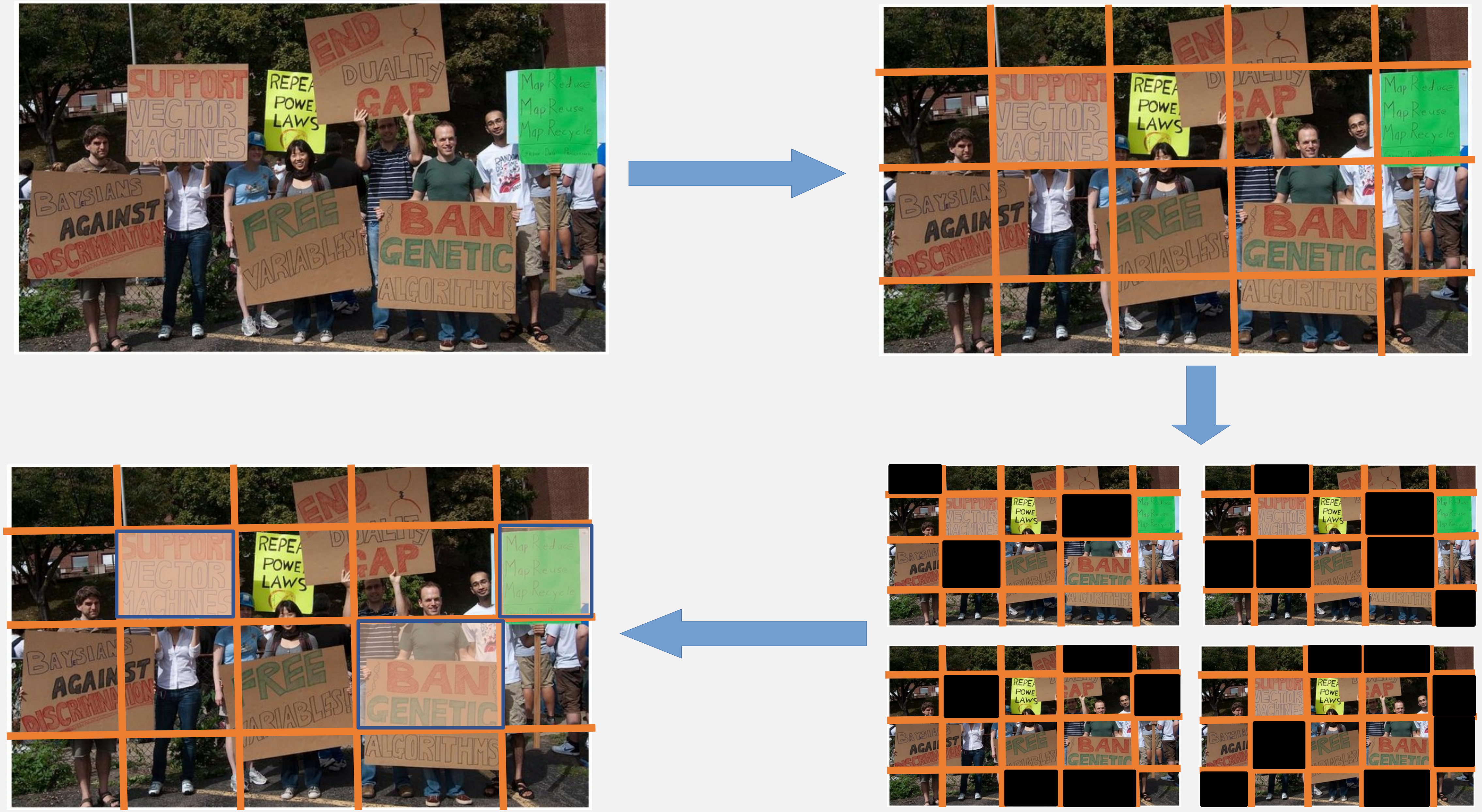
[1]

M. T. Ribeiro, S. Singh, C. Guestrin, „«Why Should I Trust You?»: Explaining the Predictions of Any Classifier", *Proceedings of the 22Nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 2016

- Optimization problem:

$$\mathcal{L}(f, g, \pi_x) = \sum_{z, z' \in \mathcal{Z}} \pi_x(z) \left(f(z) - g(z')\right)^2$$

  - f is the explained model,
  - g is the explanation model,
  - z is a interpretable representation of x,
  - π is a distance measure (a kernel).


SUPPORT VECTOR MACHINES
REPEA POWE LAWS
END DUALITY GAP
Map Reduce
Map Reuse
Map Recycle
BAYSIANS AGAINST DISCRIMINATION
FREE VARIABLES!
BAN GENETIC ALGORITHMS

LIME explanations

https://github.com/marcotcr/lime

X_1	...	X_p
M	...	0.11
F	...	-0.25
...	...	...
U	...	0.887

f(x)

y
0.87
0.14
...
0.54

1)

Z_1	...	Z_p
X_1 = M	...	$X_p < 0.2$
X_1 = F, U	...	$X_p < 0.2$
...	...	...
X_1 = F, U	...	$X_p > 0.2$

X_1 = F, U	...	$X_p < 0.2$

2)

X_1 = F, U	…	$X_p < 0.2$

X_1 = M	…	$X_p < 0.2$
X_1 = F, U	…	$X_p > 0.2$
X_1 = M	…	$X_p > 0.2$

…

X_1 = F, U	…	$X_p < 0.2$

Z_1	…	Z_p
X_1 = M	…	$X_p < 0.2$
X_1 = F, U	…	$X_p > 0.2$
X_1 = M	…	$X_p > 0.2$
…	…	…
X_1 = F, U	…	$X_p < 0.2$

3)

Z_1	…	Z_p
X_1 = M	…	$X_p < 0.2$
X_1 = F, U	…	$X_p > 0.2$
X_1 = M	…	$X_p > 0.2$
…	…	…
X_1 = F, U	…	$X_p < 0.2$

X_1	…	X_p
M	…	0.111
F	…	1.27
M	…	0.887
…	…	…
F	…	-0.2

4)

f(x)

f(x)
0.93
0.77
0.122
…
0.64

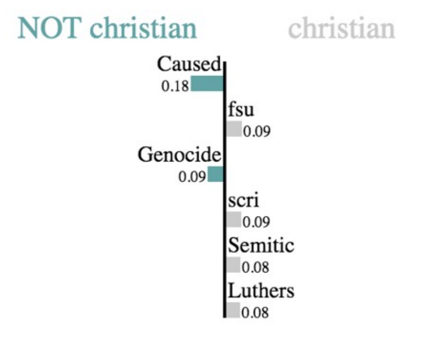
5)

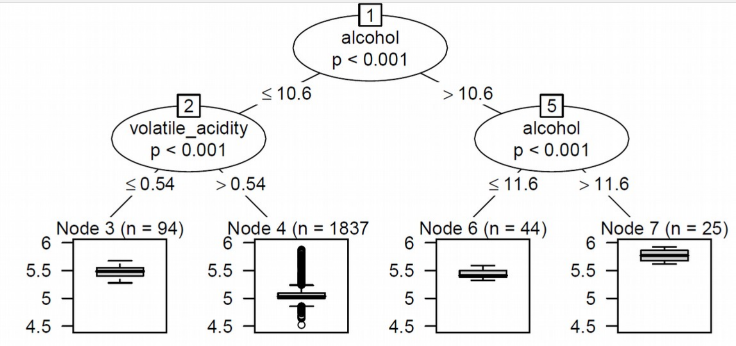
Z_1	…	Z_p	f(x)
X_1 = M	…	X_p < 0.2	0.93
X_1 = F, U	…	X_p > 0.2	0.77
X_1 = M	…	X_p > 0.2	0.122
…	…	…	…
X_1 = F, U	…	X_p < 0.2	0.64

g(z) →

g(z)
0.90
0.81
0.07
…
0.641

6) g(z) →





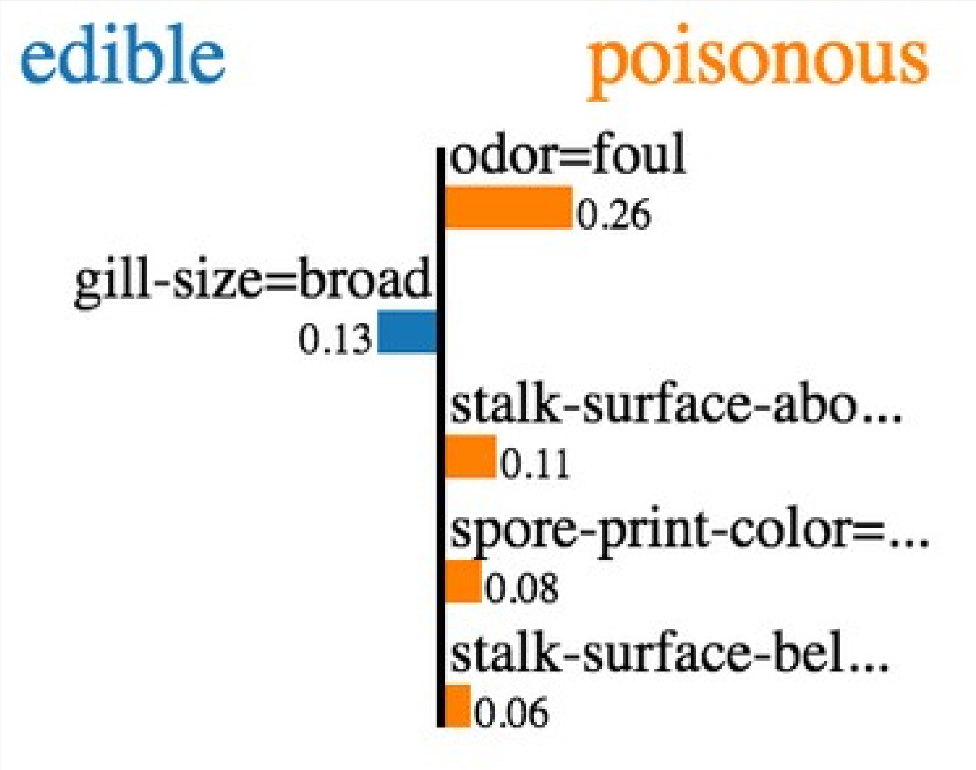
Some remarks on LIME for tabular data

- Most of the work so far focused on step **2)** – the sampling:
  - Laugel et al. 2018: the neighbourhood must include the decision boundary,
  - Adhikari et a. 2018: the neighbourhood must include enough data points from both classes,
  - Tan et al. 2019: sampling introduces significant uncertainty.
- For image or text step **3)** is trivial, but for tabular data and non-trivial interpretable input spaces, the inverse transformation is a problem.
- For tabular data, step **1)** is important, but often features are not transformed. It is not clear, what should be considered an interpretable feature.

Existing Approaches for Tabular Data

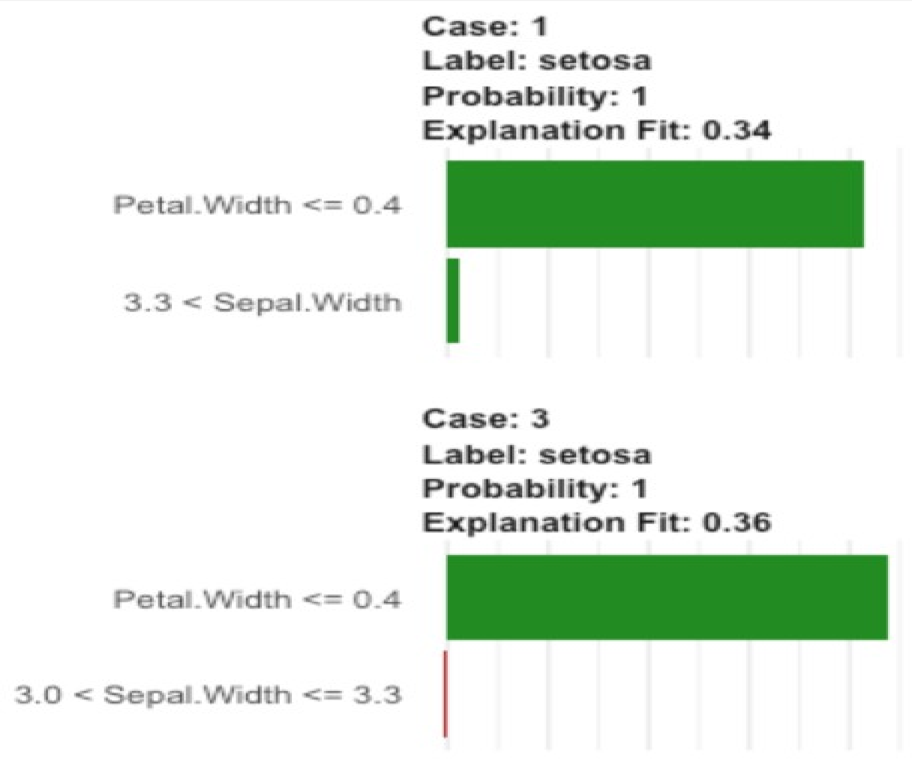
Discretized features

- lime library (Python)
  – Marco Tulio Ribeiro



https://github.com/marcotcr/lime

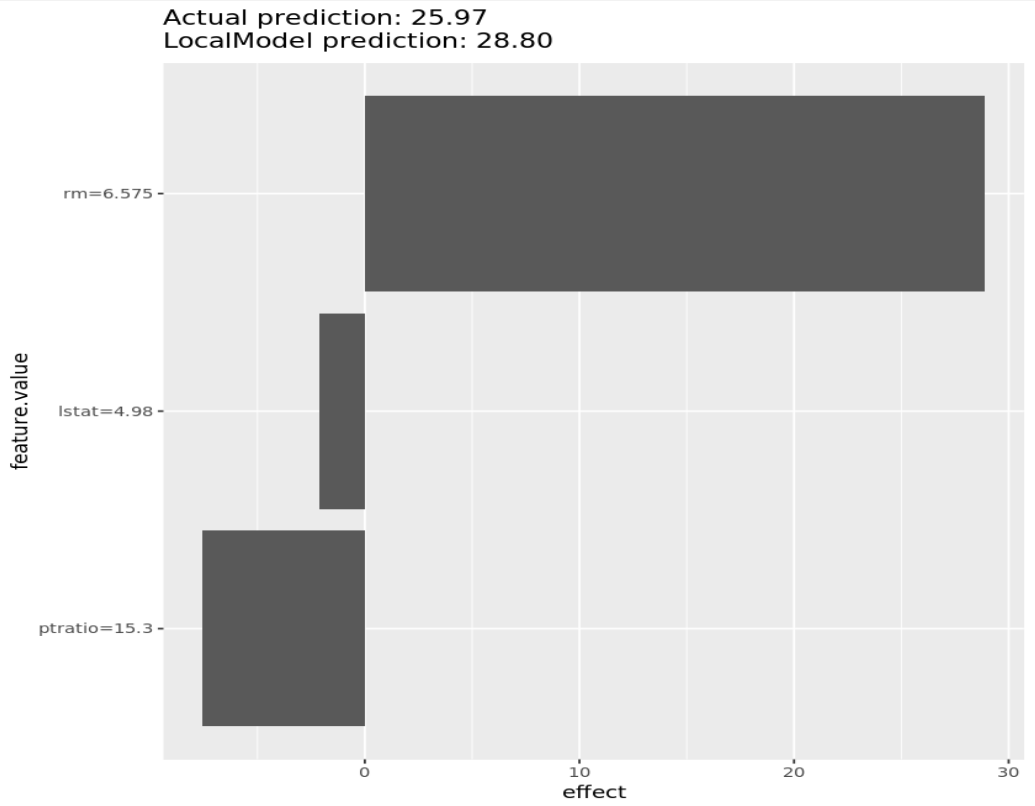
- lime package (R)
  – Thomas Lin Pedersen



https://github.com/thomasp85/lime

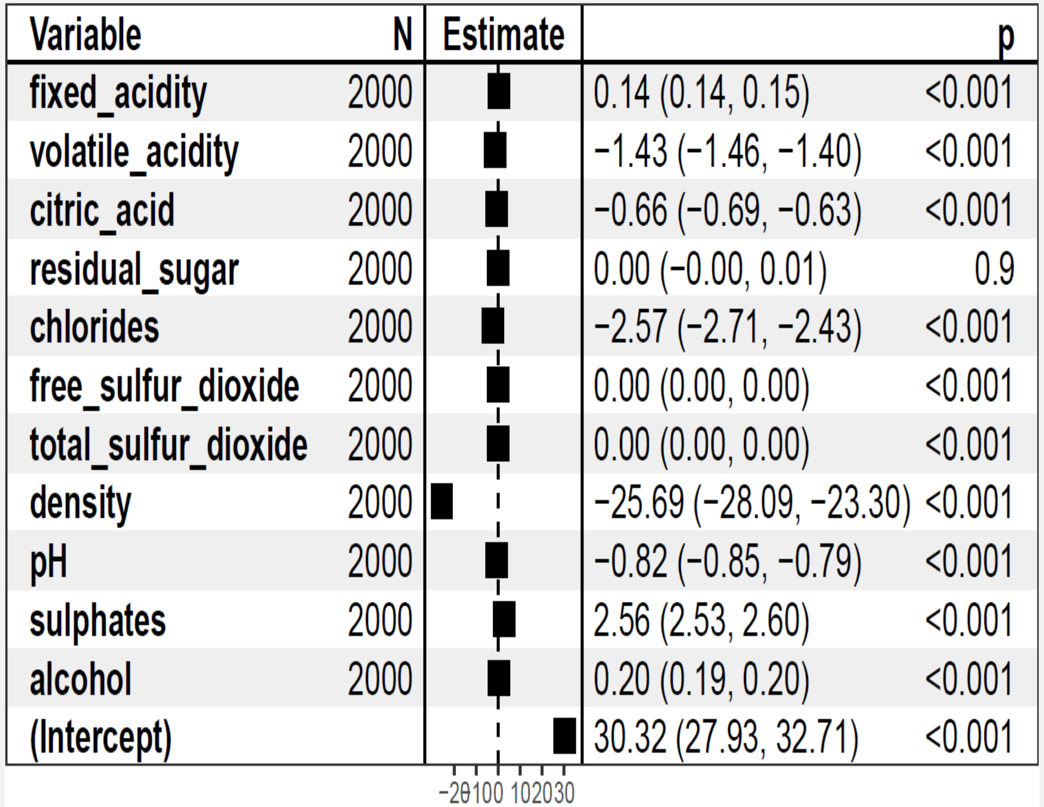
Continuous features

- iml package (R) – Christoph Molnar (JOSS, 2018)



https://github.com/christophM/iml

- live package (R) – Mateusz Staniak (R Journal, 2018)



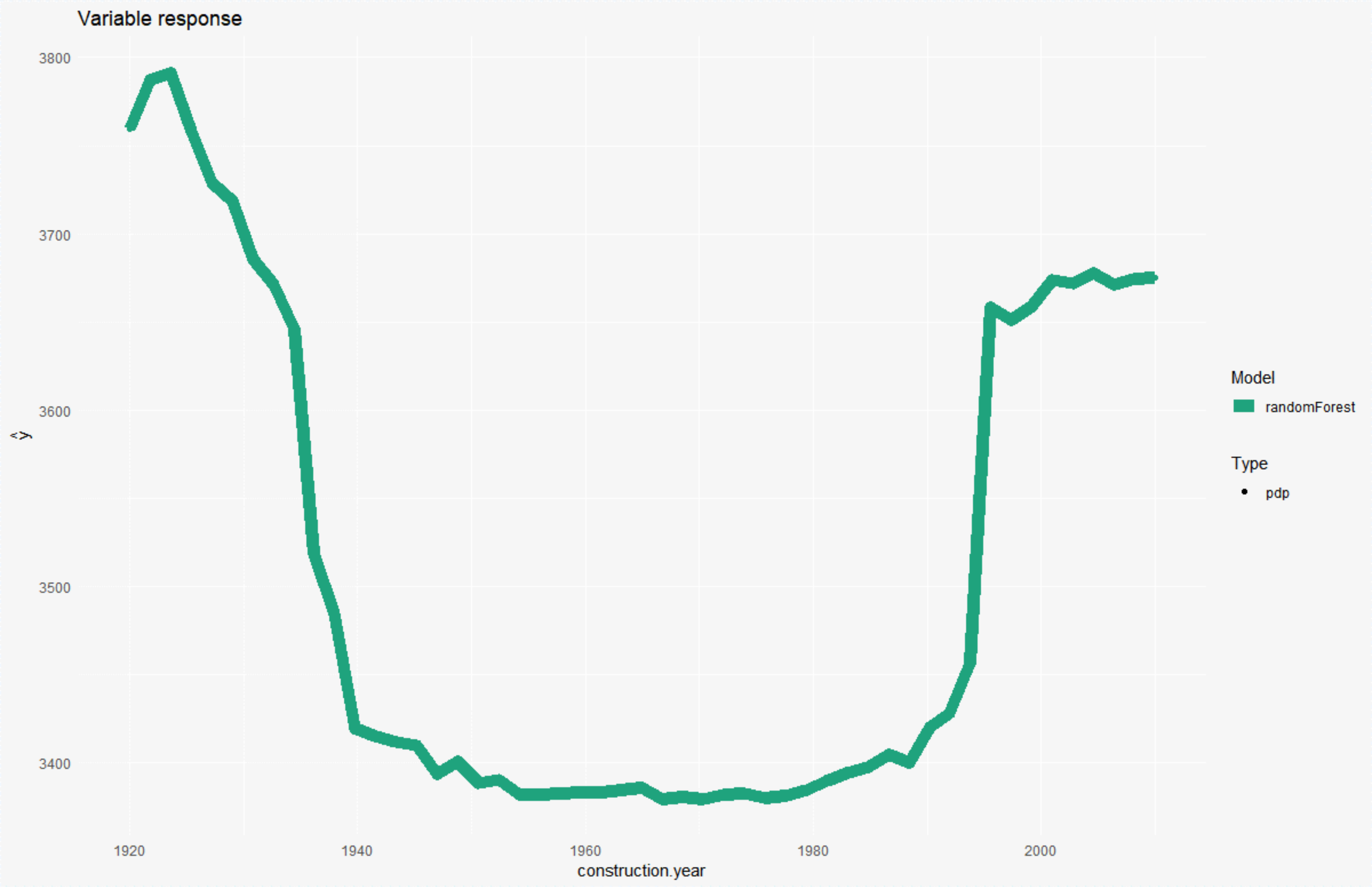
Variable	N	Estimate		p
fixed_acidity	2000		0.14 (0.14, 0.15)	<0.001
volatile_acidity	2000		−1.43 (−1.46, −1.40)	<0.001
citric_acid	2000		−0.66 (−0.69, −0.63)	<0.001
residual_sugar	2000		0.00 (−0.00, 0.01)	0.9
chlorides	2000		−2.57 (−2.71, −2.43)	<0.001
free_sulfur_dioxide	2000		0.00 (0.00, 0.00)	<0.001
total_sulfur_dioxide	2000		0.00 (0.00, 0.00)	<0.001
density	2000		−25.69 (−28.09, −23.30)	<0.001
pH	2000		−0.82 (−0.85, −0.79)	<0.001
sulphates	2000		2.56 (2.53, 2.60)	<0.001
alcohol	2000		0.20 (0.19, 0.20)	<0.001
(Intercept)			30.32 (27.93, 32.71)	<0.001

https://github.com/MI2DataLab/live

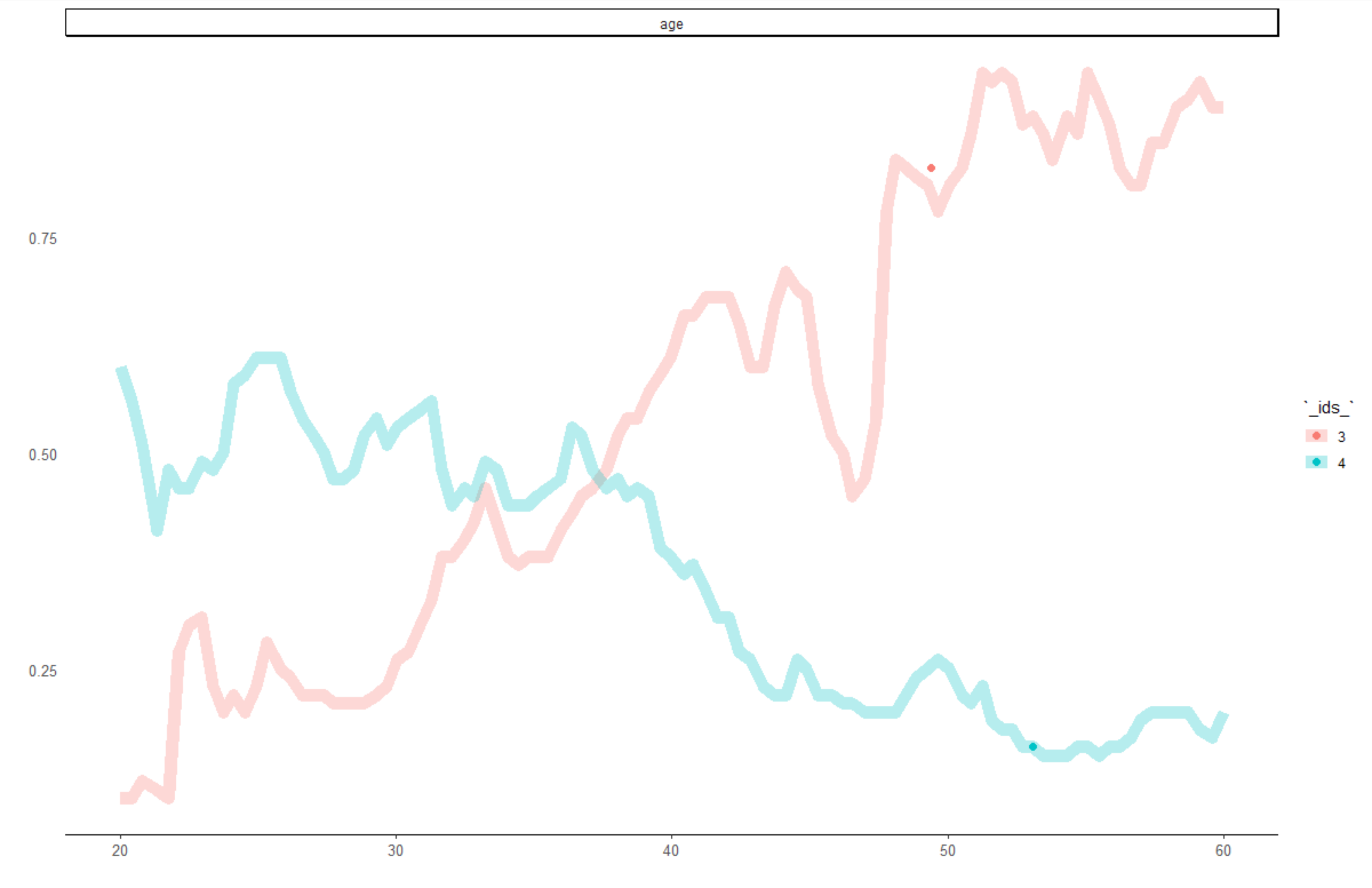
A New Approach:

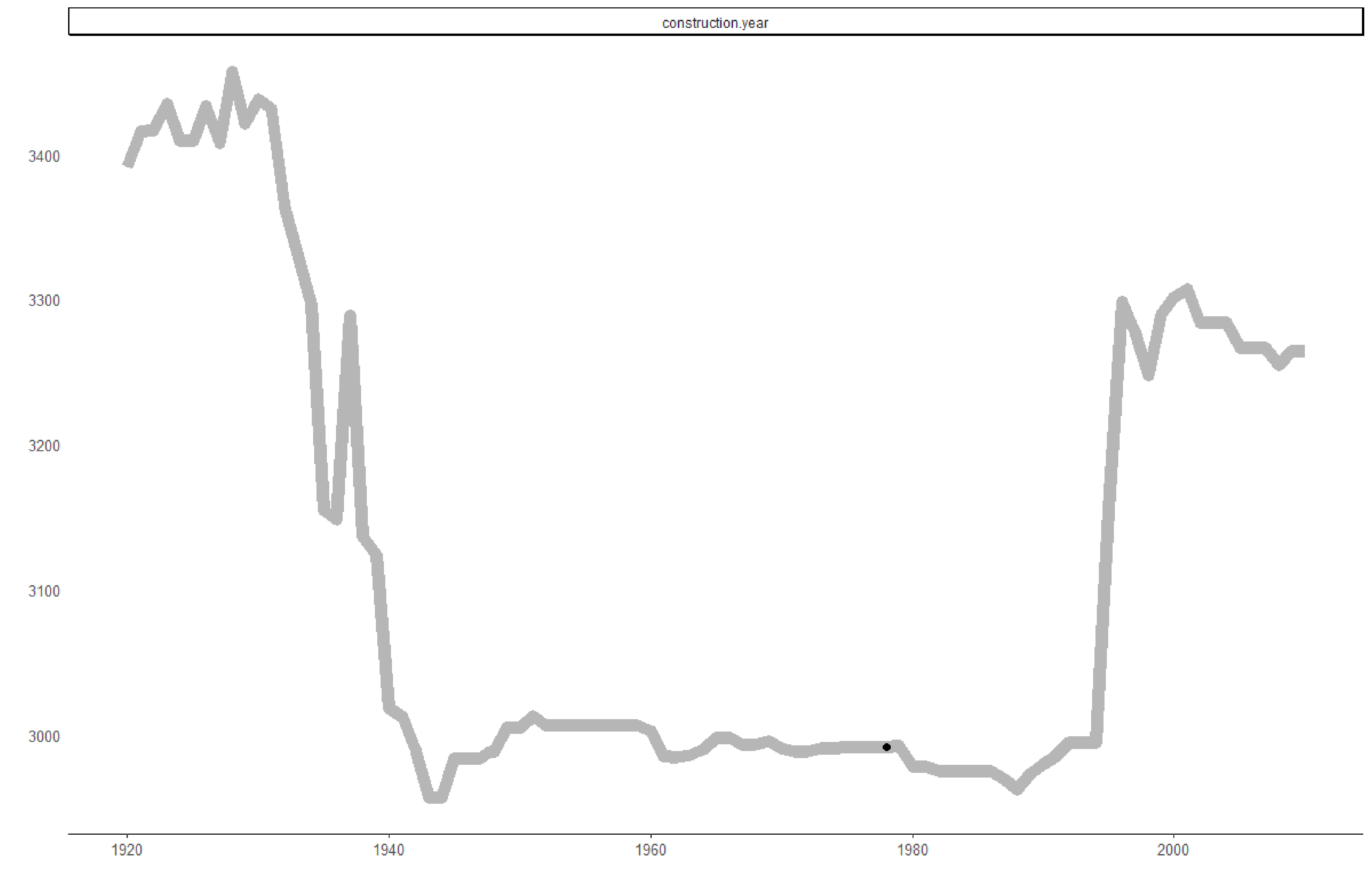
Use our knowledge about the model behaviour

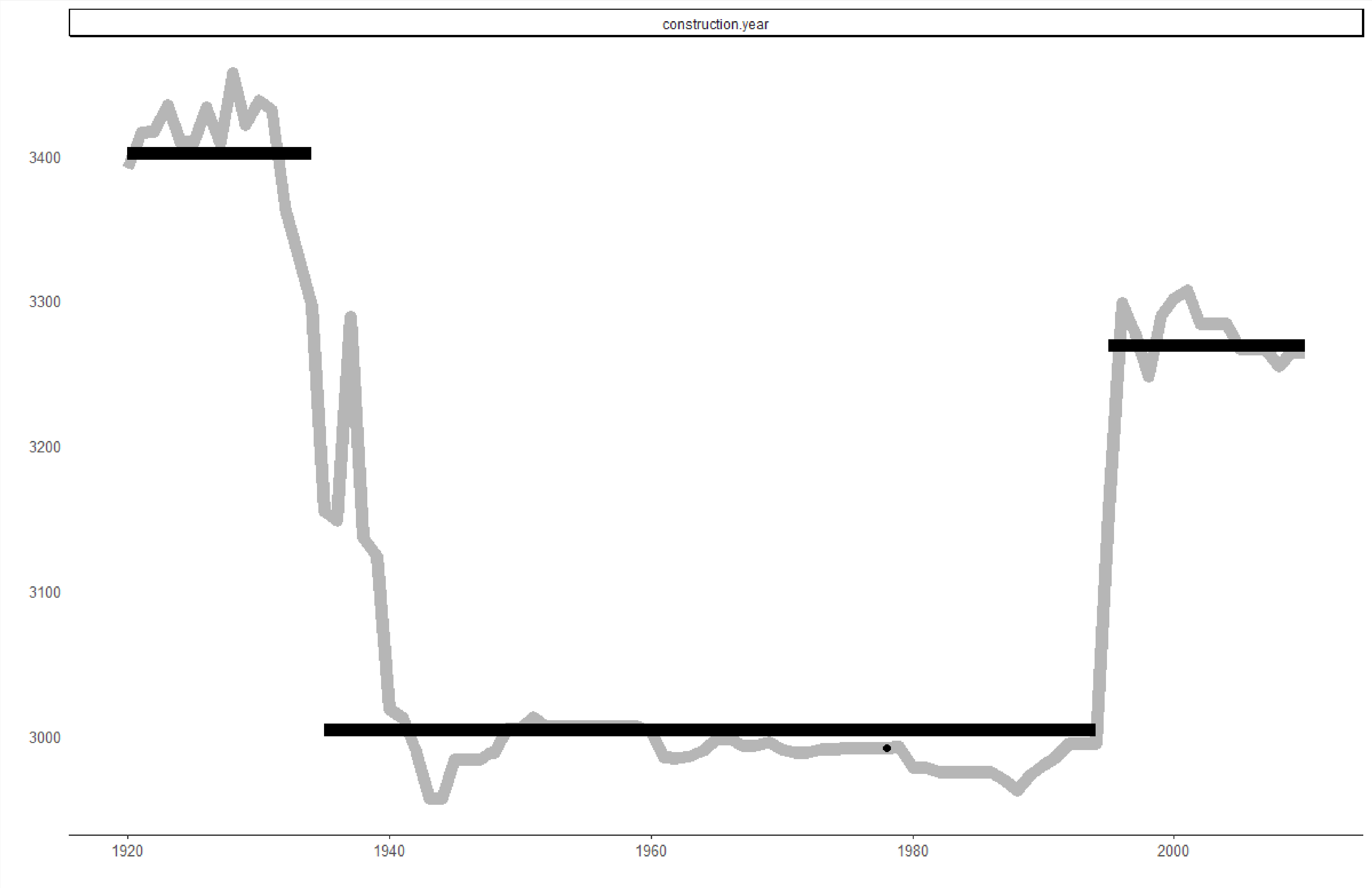
Partial Dependence Plots

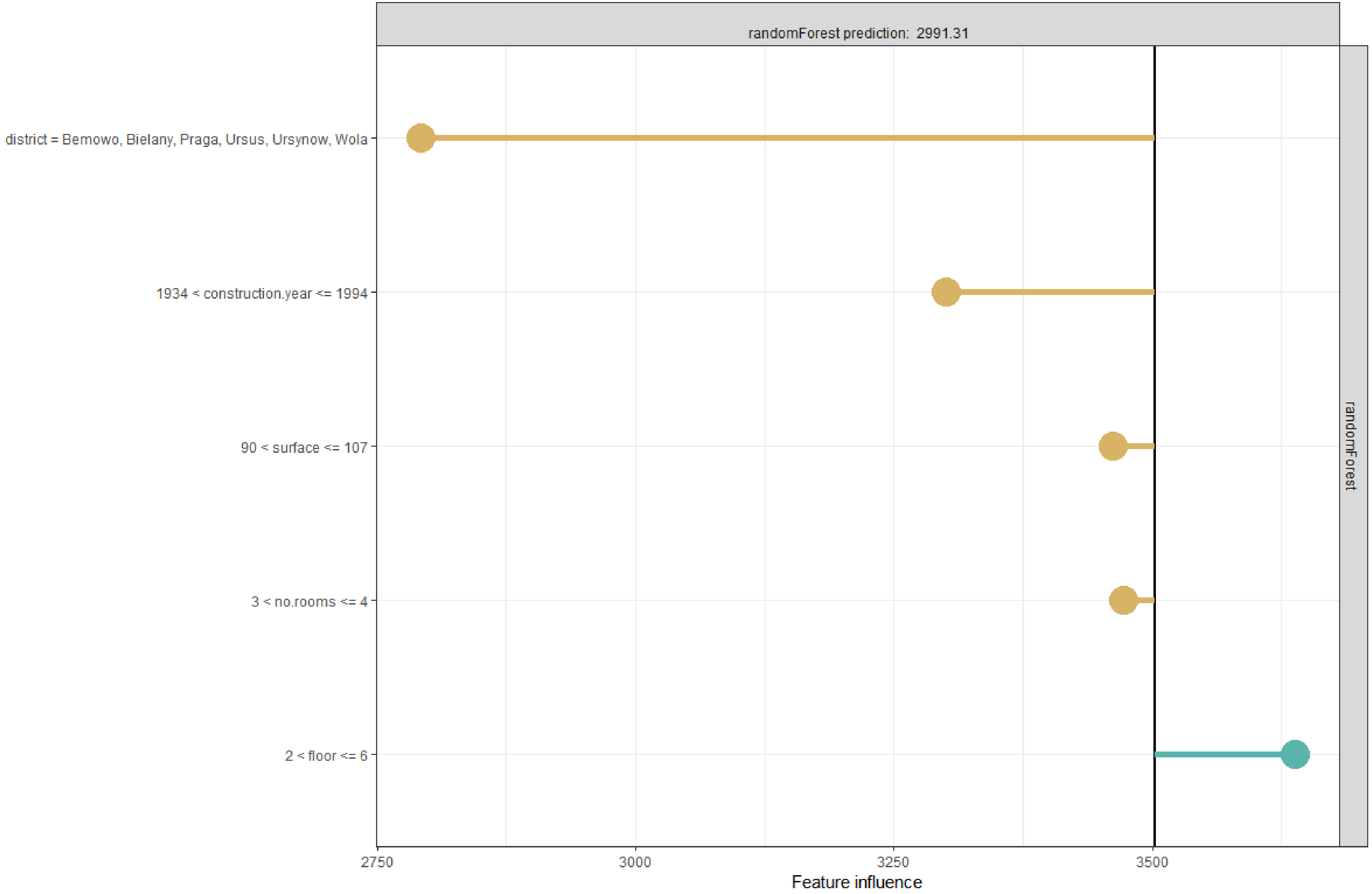


Ceteris Paribus Profiles




construction.year
3400
3300
3200
3100
3000
1920
1940
1960
1980
2000


construction.year
3400
3300
3200
3100
3000
1920
1940
1960
1980
2000


randomForest prediction: 2991.31
district = Bemowo, Bielany, Praga, Ursus, Ursynow, Wola
1934 < construction.year <= 1994
90 < surface <= 107
3 < no.rooms <= 4
2 < floor <= 6
randomForest
2750
3000
3250
3500
Feature influence

Summary

- Explanations of individual predictions rely on good interpretable features.
- For tabular data, the notion of an *interpretable feature* is not clear.
- We propose a method of creating interpretable features based on conditional behaviour of the model. It is implemented in R package **localModel**.

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