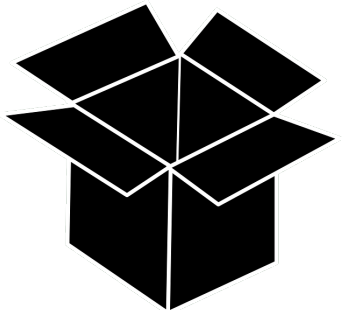


Interpretable Machine Learning

Interpretable Models



Learning goals

- Examples for interpretable models: linear and polynomial regression models, generalized linear models, generalized additive models, model-based boosting, rule-based learning
- Methodological summary, motivation behind the model, model interpretations

LINEAR AND POLYNOMIAL REGRESSION

- For linear regression models, we only estimate the model parameters. The model equation is manually specified and known in advance:

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + \cdots + \epsilon$$

$$Y = X^T \beta + \mathcal{E}$$

- The model equation is identical across the entire feature space.
- The predictive power of LMs is determined by specifying the correct model structure. A polynomial regression model is an extension of the LM that includes higher order terms or interactions. This way we can additively model non-linear data and make use of the entire LM toolbox.

LINEAR AND POLYNOMIAL REGRESSION

- By knowing the model equation, we can exactly determine feature effects (e.g., beta coefficients, effect plots) and importance scores (e.g., p-values, t-statistics). For higher order effects or interactions, beta coefficients cannot be interpreted in isolation, i.e., we need to use marginal effects or effect plots with simultaneous changes in feature values.
- Note that for inference-based metrics (p-values, t-statistics, confidence intervals) to be valid, the error term needs to be normally distributed with zero mean, i.e., $\epsilon \sim N(0, \sigma^2)$. It follows that $(y|x) \sim N(x^T \beta, \sigma^2)$. This restricts the usage of LMs in practice, as the distribution of the error term is a prior assumption about the data.

LINEAR AND POLYNOMIAL REGRESSION MODELS

Call:

```
lm(formula = cnt ~ (hum + temp)^2, data = data_bike)
```

Residuals:

Min	1Q	Median	3Q	Max
-4635.2	-1122.0	-82.6	1017.2	3528.9

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	2112.4	695.5	3.037	0.00247 **
hum	-1568.5	1150.5	-1.363	0.17320
temp	8085.1	1437.0	5.627	2.63e-08 ***
hum:temp	-1998.9	2344.8	-0.852	0.39423

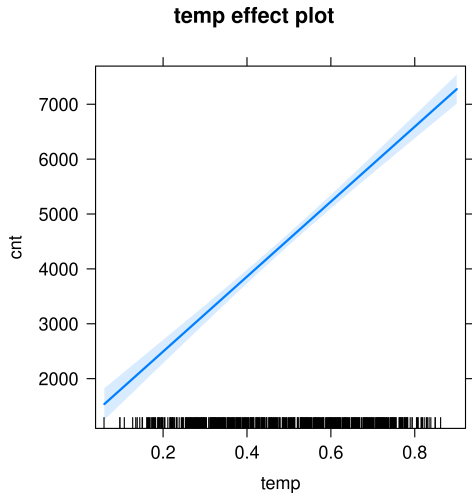
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1469 on 727 degrees of freedom

Multiple R-squared: 0.4274, Adjusted R-squared: 0.425

F-statistic: 180.9 on 3 and 727 DF, p-value: < 2.2e-16

LINEAR AND POLYNOMIAL REGRESSION MODELS



GENERALIZED LINEAR REGRESSION MODELS

- Generalized linear models (GLMs) are more flexible regarding the target distribution. They keep the linear predictor $X^T\beta$ which now explains the transformed, expected conditional target through a link function g :

$$\begin{aligned}g(\mathbb{E}_Y(Y|X)) &= X^T\beta \\ \mathbb{E}_Y(Y|X) &= g^{-1}(X^T\beta)\end{aligned}$$

- GLMs are a framework for target distributions of the exponential family, e.g., Gaussian, Binomial, Poisson, Exponential, Gamma. A Gaussian target distribution with identity link corresponds to a linear / polynomial regression model.

GENERALIZED LINEAR REGRESSION MODELS

- The link function describes how the linear predictor $X^T \beta$ relates to the expected, conditional target $\mathbb{E}_Y(Y|X)$, e.g., if the target is distributed binomially, a natural link function is the logit link $\log \left(\frac{\mathbb{E}_Y(Y|X)}{1 - \mathbb{E}_Y(Y|X)} \right)$.
- We need to specify the correct model equation, target distribution, and link function in order to receive a good model fit.
- As the model equation is still known, interpretations are possible the same way as for polynomial regression models. However, even linear terms become non-linear through the link function (if the identity link is not used)!

GENERALIZED LINEAR REGRESSION MODELS

Call:

```
glm(formula = cnt ~ (hum + temp)^2, family = Gamma(link = "inverse"),
     data = data_bike)
```

Deviance Residuals:

Min	1Q	Median	3Q	Max
-2.84829	-0.31351	-0.01372	0.22187	0.75445

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	2.618e-04	4.648e-05	5.633	2.54e-08 ***
hum	2.404e-04	7.902e-05	3.042	0.00243 **
temp	-1.846e-04	8.243e-05	-2.239	0.02545 *
hum:temp	-2.603e-04	1.400e-04	-1.859	0.06342 .

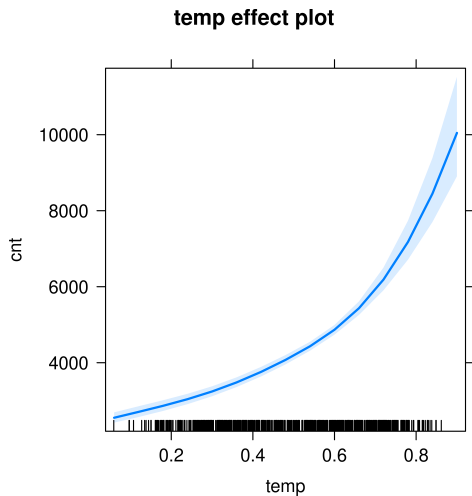
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for Gamma family taken to be 0.1454719)

Null deviance: 189.26 on 730 degrees of freedom
Residual deviance: 132.01 on 727 degrees of freedom
AIC: 12966

Number of Fisher Scoring iterations: 5

GENERALIZED LINEAR REGRESSION MODELS



GENERALIZED ADDITIVE MODELS

- A generalized additive model (GAM) adds flexibility and predictive power to the GLM framework by replacing pre-specified terms with smoothing functions:

$$g(\mathbb{E}_Y(y|x)) = \beta_0 + \beta_1 h_1(x_1) + \dots + \beta_p h_p(x_p) + \dots$$

- For the component functions, we may either specify a parametric form (e.g., a regression splines), or a non-parametric one, e.g., locally estimated scatterplot smoothing (LOESS).
- This makes GAMs much more adaptive. The estimated model is largely determined by the structure of the data instead of premade assumptions as in LMs and GLMs. However, we still need to specify the order and type of the component functions to be estimated, e.g., which interactions to include.

GENERALIZED ADDITIVE MODELS

- Furthermore, the smoothing degree of each component function can be tuned to avoid overfitting. Regularization increases interpretability, as the interpretations drawn from the model can be transferred more easily to new data.
- A GAM retains interpretability by keeping the additive model equation (as long as the component functions are interpretable). As the model equation is known, we can use similar interpretation methods as for LMs and GLMs, e.g., evaluating the estimated components that depend on the features of interest.

GENERALIZED ADDITIVE MODELS

Family: gaussian
Link function: identity

Formula:
cnt ~ s(hum, temp)

Parametric coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	4504.35	46.83	96.18	<2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

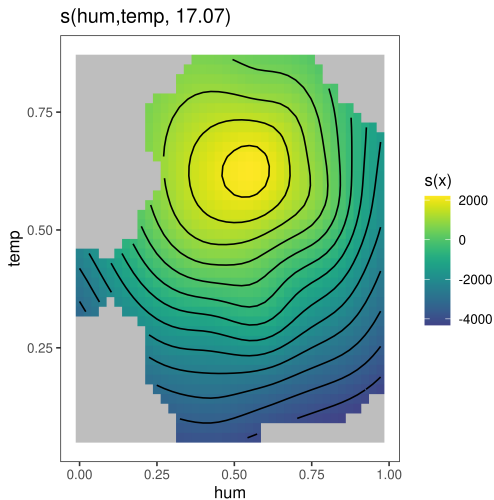
Approximate significance of smooth terms:

	edf	Ref.df	F	p-value
s(hum,temp)	17.07	22.1	44.09	<2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) = 0.573 Deviance explained = 58.3%
GCV = 1.6439e+06 Scale est. = 1.6033e+06 n = 731

GENERALIZED ADDITIVE MODELS



MODEL-BASED BOOSTING

- Boosting iteratively joins weak base learners to create a powerful ensemble model.
- Idea: Combine boosting with interpretable base learners (e.g., single feature LM). The resulting ensemble is also interpretable.
- Consider two linear base learners $b_j(x, \Theta)$ and $b_j(x, \Theta^*)$ with the same type, but distinct parameter vectors Θ and Θ^* . They can be combined in a base learner of the same type:

$$b_j(x, \Theta) + b_j(x, \Theta^*) = b_j(x, \Theta + \Theta^*)$$

MODEL-BASED BOOSTING

- We create a selection of interpretable base learners. In each iteration, all base learners are trained on the so-called pseudo residuals, and the one with the best fit is added to the previously computed model:

$$\hat{f}^{[1]}(x) = f_0 + \beta b_3(x_3, \theta^{[1]})$$

$$\hat{f}^{[2]}(x) = f_0 + \beta b_3(x_3, \theta^{[1]}) + \beta b_3(x_3, \theta^{[2]})$$

$$\hat{f}^{[3]}(x) = f_0 + \beta b_3(x_3, \theta^{[1]}) + \beta b_3(x_3, \theta^{[2]}) + \beta b_1(x_1, \theta^{[3]})$$

$$\hat{f}^{[3]}(x) = f_0 + \beta \left(b_3(x_3, \theta^{[1]} + \theta^{[2]}) + b_1(x_1, \theta^{[3]}) \right)$$

- The final model has an additive structure (equivalent to a GAM), where each component function is interpretable itself.

MODEL-BASED BOOSTING

Model-based Boosting

Call:

```
mboost(formula = cnt ~ bols(hum) + bols(temp) + bspatial(hum, temp), data = data_bike)
```

Squared Error (Regression)

Loss function: $(y - f)^2$

Number of boosting iterations: mstop = 100

Step size: 0.1

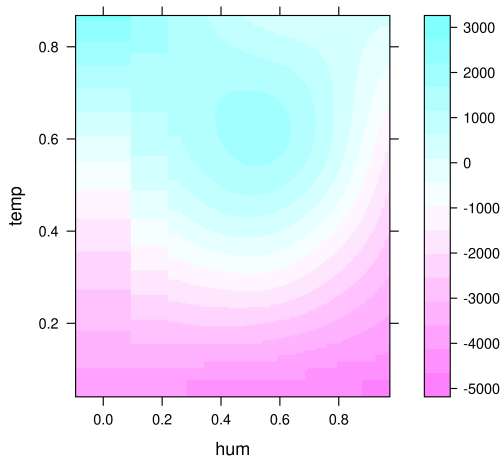
Offset: 4504.349

Number of baselearners: 3

Selection frequencies:

```
bspatial(hum, temp)
1
```


MODEL-BASED BOOSTING



RULE-BASED LEARNING

- Decision rules follow a general structure: IF the conditions are met, THEN make a certain prediction. Rule-based learning aims to capture a set of decision rules that accurately describe the data.
- Although a single decision rule is very intelligibile, a large collection of decision rules might not be. An interpretable rule-based model should therefore be based on as few rules as possible.
- Descripte Rule Discovery (DRD) is based on mining databases for frequent item sets, and converting these into a set of decision rules, e.g., a rule {mobile phone} \Rightarrow {mobile phone case} might stem from mobile phones and phone cases being bought together frequently. DRD is not suited to create a model that makes predictions on unseen data.

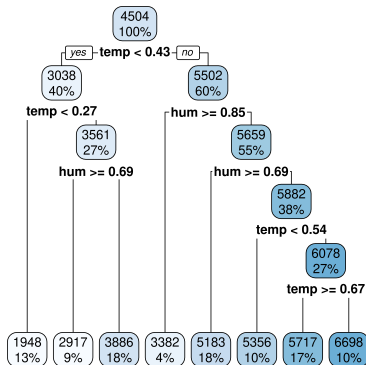
RULE-BASED LEARNING

- Instead, we are interested in Predictive Rule Learning (PRL), which aims to discover a set of rules that cover the entire feature space, thereby being able to predict for any data instance. There are innumerable rule-based learning algorithms, e.g., decision tree learning, OneR, Sequential Covering, or Bayesian Rule Lists.
- Decision tree learning, e.g, classification and regression trees (CART), is the most popular group of rule-based models, as every tree can be represented by a collection of decision rules. A decision tree recursively partitions the data by optimizing an objective function, e.g., minimizing the data impurity. A succession of tree splits corresponds to a decision rule with the succeeding split conditions as a conjunction.

RULE-BASED LEARNING

- The RuleFit algorithm combines polynomial regression with rule ensembles for automatic interaction detection. In the first stage, a tree ensemble is trained to produce decision rules (where the predictions are discarded and only the splits are utilized), e.g., $x_1 < 0 \wedge x_2 > 1$. In the second stage, a linear model with main effects is augmented with each decision rule being represented by a single dummy feature.

RULE-BASED LEARNING



cnt
1948 when temp < 0.27
2917 when temp is 0.27 to 0.43 & hum >= 0.69
3382 when temp >= 0.43 & hum >= 0.85
3886 when temp is 0.27 to 0.43 & hum < 0.69
5183 when temp >= 0.43 & hum is 0.69 to 0.85
5356 when temp is 0.43 to 0.54 & hum < 0.69
5717 when temp >= 0.67 & hum < 0.69
6698 when temp is 0.54 to 0.67 & hum < 0.69