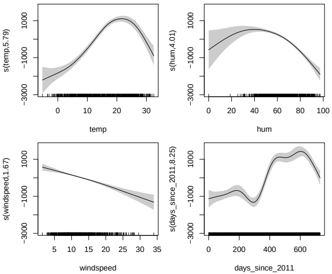
Interpretable Machine Learning

GAM & Boosting



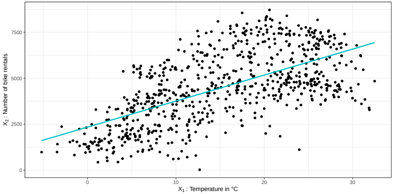
Learning goals

- Generalized additive model
- Model-based boosting with simple base learners
- Feature effect and importance in model-based boosting

GENERALIZED ADDITIVE MODEL (GAM)

▸ Hastie and Tibshirani (1986)

Problem: LM not suitable if relationship between features and target variable is not linear



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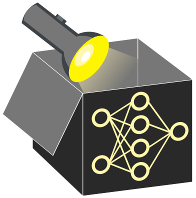
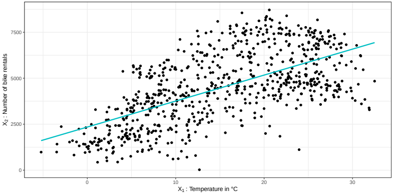


Problem: LM not suitable if relationship between features and target variable is not linear

Workaround in LMs / GLMs:

- Feature transformations (e.g., exp or log)
- Including high-order effects
- Categorization of features (i.e., intervals/ buckets of feature values)



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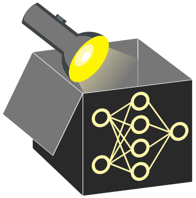

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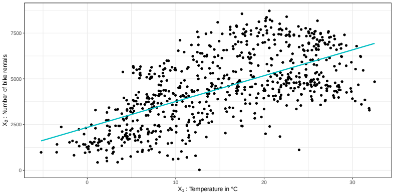


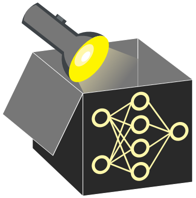
Idea of GAMs:

- Instead of linear terms $\theta_j x_j$, use flexible functions $f_j(x_j) \rightsquigarrow$ splines

$$g(\mathbb{E}(y \mid \mathbf{x})) = \theta_0 + f_1(x_1) + f_2(x_2) + \ldots + f_p(x_p)$$

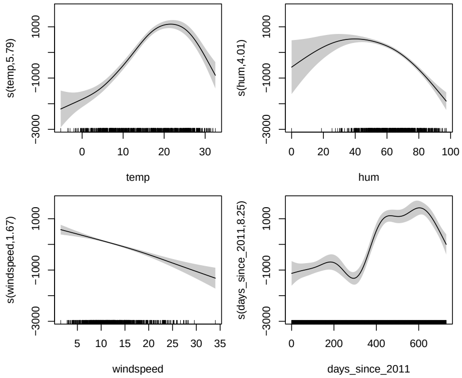
- Preserves additive structure and allows to model non-linear effects
- Splines have a smoothness parameter to control flexibility (prevent overfitting)
  $\rightsquigarrow$ Needs to be chosen, e.g., via cross-validation

GENERALIZED ADDITIVE MODEL (GAM) - EXAMPLE



Fit a GAM with smooth splines for four numeric features of bike rental data
⇝ more flexible and better model fit but less interpretable than LM

	edf	p-value
s(temp)	5.8	0.00
s(hum)	4.0	0.00
s(windspeed)	1.7	0.00
s(days_since_2011)	8.3	0.00

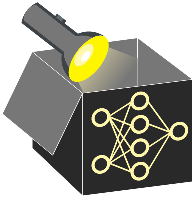


Interpretation

- Interpretation needs to be done visually and relative to average prediction
- Edf (effective degrees of freedom) represents complexity of smoothness

MODEL-BASED BOOSTING

▸ Bühlmann and Yu 2003



- Recall: Boosting iteratively combines weak base learners (BL)
- Idea: Use simple linear BL to ensure interpretability (in general also spline BL possible)

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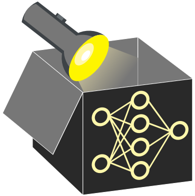

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- Possible to combine linear BL of same type (with distinct parameters $\boldsymbol{\theta}$ and $\boldsymbol{\theta}^{\star}$):

$$b^{[j]}(\mathbf{x}, \boldsymbol{\theta}) + b^{[j]}(\mathbf{x}, \boldsymbol{\theta}^{\star}) = b^{[j]}(\mathbf{x}, \boldsymbol{\theta} + \boldsymbol{\theta}^{\star})$$

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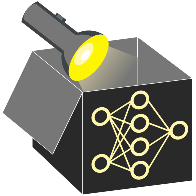

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- In each iteration, fit a set of BLs and add the best BL to previous model (using step-size ν):

$$\hat{f}^{[1]} = \hat{f}_0 + \nu b^{[3]}(\mathbf{x}_3, \boldsymbol{\theta}^{[1]})$$

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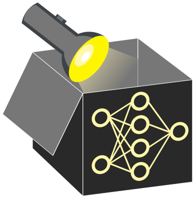

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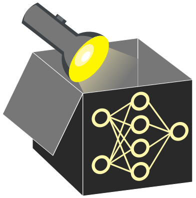

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&= \hat{f}_0 + \nu \left(b^{[3]}(\mathbf{x}_3, \boldsymbol{\theta}^{[1]} + \boldsymbol{\theta}^{[2]}) + b^{[1]}(\mathbf{x}_1, \boldsymbol{\theta}^{[3]}) \right) \\
&= \hat{f}_0 + \hat{f}_3(\mathbf{x}_3) + \hat{f}_1(\mathbf{x}_1)
\end{aligned}$$

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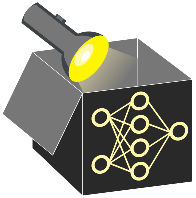

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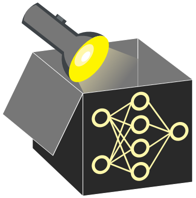
&= \hat{f}_0 + \hat{f}_3(\mathbf{x}_3) + \hat{f}_1(\mathbf{x}_1)
\end{aligned}$$

- Final model is additive (as GAMs), where each component function is interpretable

MODEL-BASED BOOSTING - LINEAR EXAMPLE

Simple case: Use linear model with single feature (including intercept) as BL



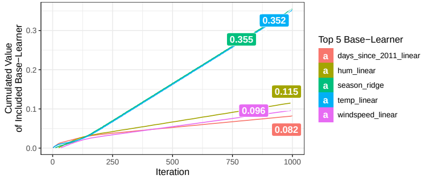
$$b^{[j]}(x_j, \theta) = x_j\theta + \theta_0 \quad \text{for } j = 1, \dots p \qquad \rightsquigarrow \text{ordinary linear regression}$$

- Here: Interpretation of weights as in LM
- After many iterations, it converges to same solution as least square estimate of LMs

1000 iter. with $\nu = 0.1$	Intercept	Weights
days_since_2011	-1791.06	4.9
hum	1953.05	-31.1
season	0	WINTER: -323.4 SPRING: 539.5 SUMMER: -280.2 FALL: 67.2
temp	-1839.85	120.4
windspeed	725.70	-56.9
offset	4504.35	

$\Rightarrow$ Converges to solution of LM

Relative frequency of selected BLs across iterations



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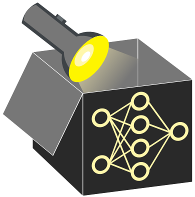

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- After many iterations, it converges to same solution as least square estimate of LMs
- Early stopping allows feature selection and might prevent overfitting (regularization)

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$\Rightarrow$ Converges to solution of LM

20 iter. with $\nu = 0.1$	Intercept	Weights
days_since_2011	-1210.27	3.3
season	0	WINTER: -276.9 SPRING: 137.6 SUMMER: 112.8 FALL: 20.3
temp	-1118.94	73.2
offset	4504.35	

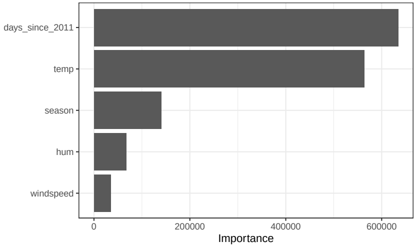
$\Rightarrow$ 3 BLs selected after 20 iter. (feature selection)

LINEAR EXAMPLE: INTERPRETATION

Feature importance: aggregated change in risk in each iteration per feature.

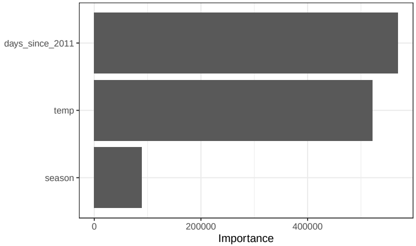
- E.g. iteration 1: `days_since_2011` causes a risk reduction (MSE) of 140,782.94
- For every iteration the change in risk can be attributed to a feature

1000 iterations



Overall risk: 434,686.0
OOB risk (10-fold CV): 446,450.0

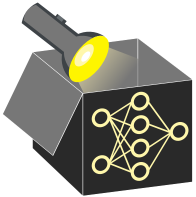
20 iterations



Overall risk: 693,505.0
OOB risk (10-fold CV): 705,776.0

$\Rightarrow$ Difference in risk: 258,819.0
Difference in OOB risk: 259,326.0

NON-LINEAR EXAMPLE: INTERPRETATION



- Fit model on bike data with different BL types (1000 iter.) ▸ Daniel Schalk et al. 2018
- BLs: linear and centered splines for numeric features, categorical for season

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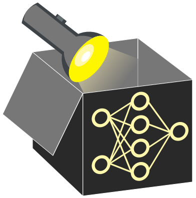

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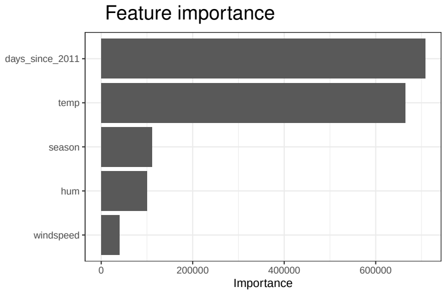

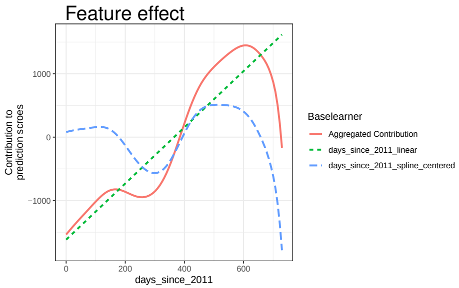

$\Rightarrow$ In-bag-Risk: 250,202.0 ; OOB risk (10-fold CV): 267,497.0 (Difference: 178,953.0)

- Feature importance (risk reduction over iter.) $\rightsquigarrow$ `days_since_2011` most important
- Total effect for `days_since_2011`
  $\rightsquigarrow$ Combination of partial effects of linear BL and centered spline BL