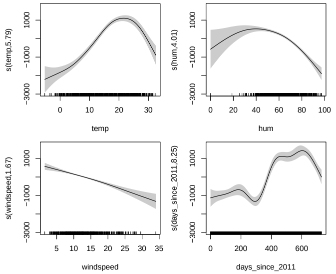
Interpretable Machine Learning

GAM & Boosting



Learning goals

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

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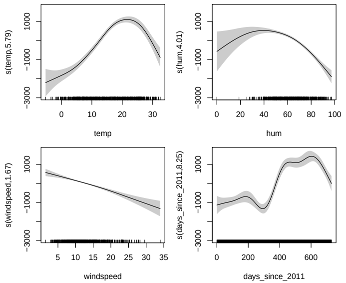
Interpretable Models 1



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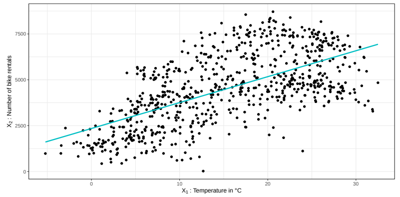
GENERALIZED ADDITIVE MODEL (GAM)

▸ Hastie and Tibshirani (1986)

Problem: LM not great if features act on outcome non-linearly



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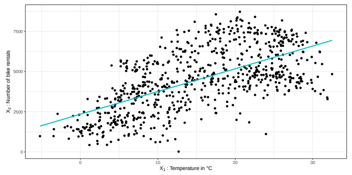

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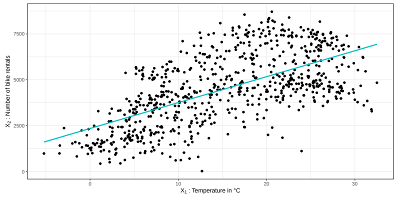
- Categorization of features (i.e., intervals/ buckets of feature values)



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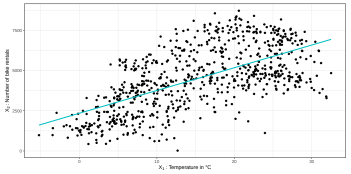

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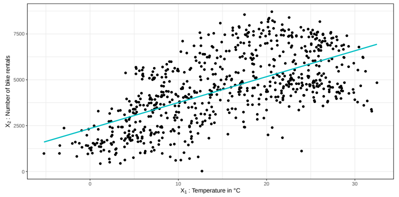

Idea of GAMs:

- 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

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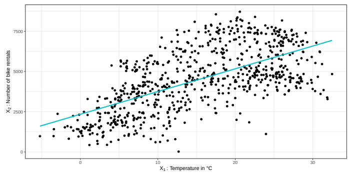

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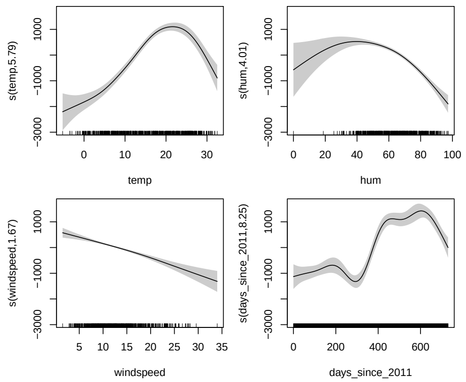
GENERALIZED ADDITIVE MODEL (GAM) - EXAMPLE

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 is performed visually and relative to average prediction
- Edf: effective degrees of freedom ⇝ represents degree of smoothness/complexity

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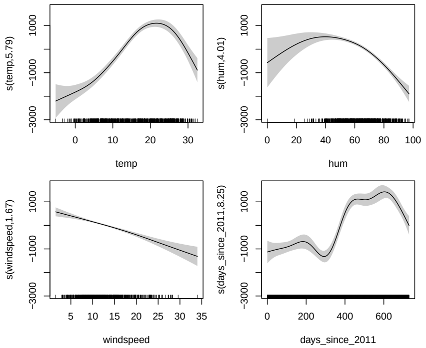

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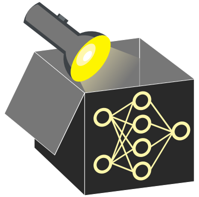
MODEL-BASED BOOSTING ▸ Bühlmann, Yu 2003 ▸ Bühlmann, Hothorn 2008



- Boosting iteratively combines weak base learners to create powerful ensemble
- Idea: Use simple BLs (e.g univariate, with splines) to ensure interpretability
- Possible to combine 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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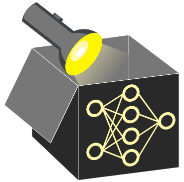

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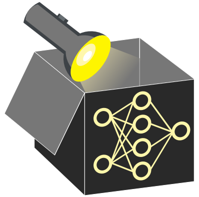

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- In each iteration, fit a set of BLs, add best one to model (with step-size ν):

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

- Final model is additive GAM, we can read off effect curves

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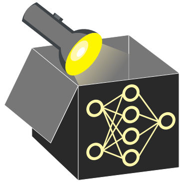

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MODEL-BASED BOOSTING - LINEAR EXAMPLE

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

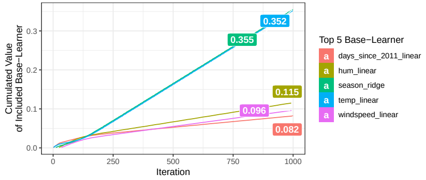
$$b^{[j]}(x_j, \theta) = x_j\theta + \theta_0 \quad \text{for } j = 1, \dots p \quad \rightsquigarrow \text{ordinary linear regression}$$

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

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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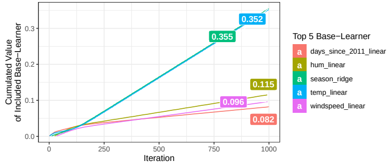

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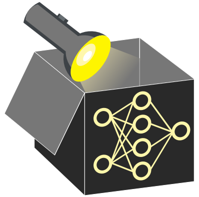

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$\Rightarrow$ 3 BLs selected after 20 iter. (feature selection)

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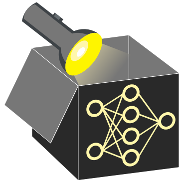
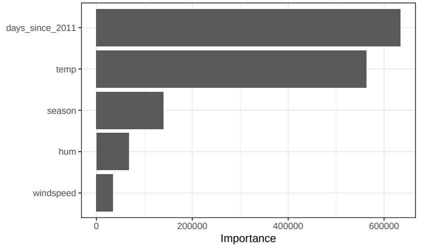


LINEAR EXAMPLE: INTERPRETATION

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

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

1000 iterations



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

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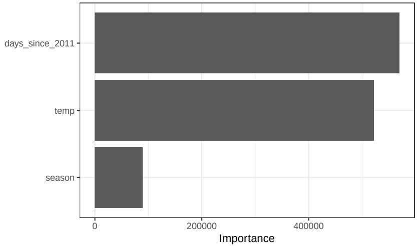

In-bag-risk: 693,505.0
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⇒ Difference in risk: 258,819.0
Difference in OOB risk: 259,326.0

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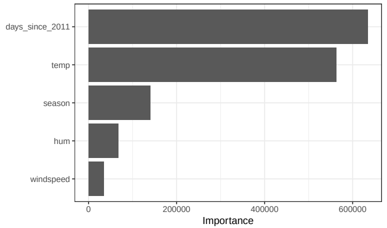

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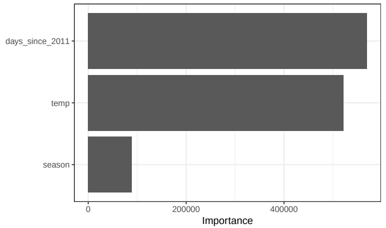

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- Fit model on bike data with different BL types (1000 iter.) ▸ Daniel Schalk et al. 2018
- BLs: linear and centered splines for numeric features, categorical for season

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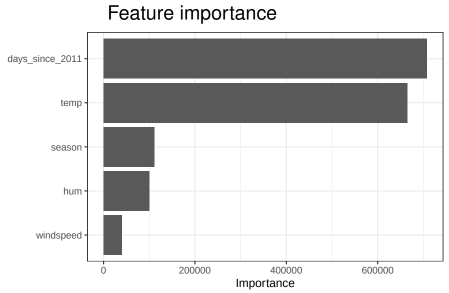

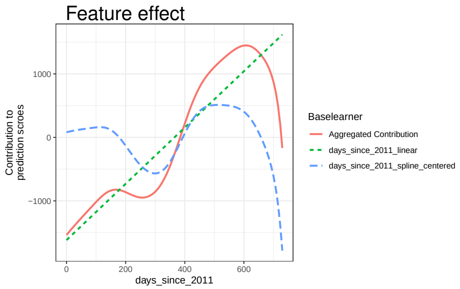

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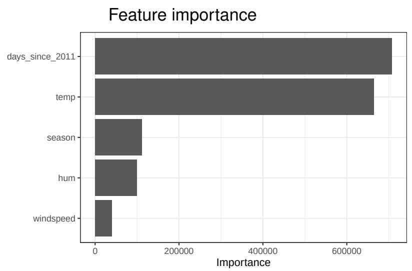

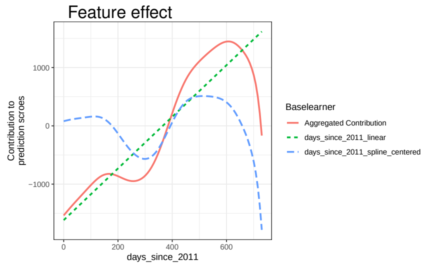

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