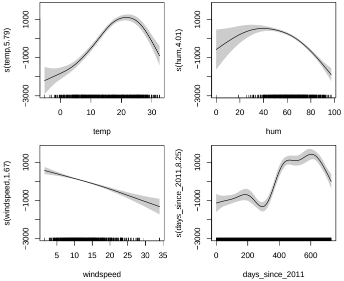
Interpretable Machine Learning

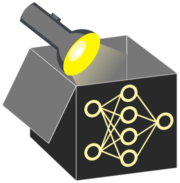
GAM & Boosting
Interpretable Models 1



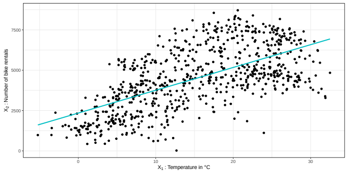
Learning goals

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

GENERALIZED ADDITIVE MODEL (GAM) ▸ TIBSHIRANI_1986



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



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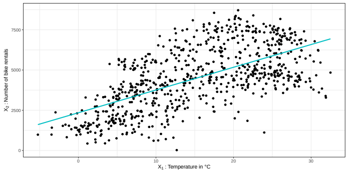
Workaround in LMs / GLMs:

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



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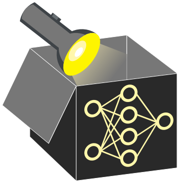

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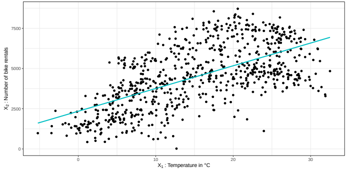


Idea of GAMs:

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

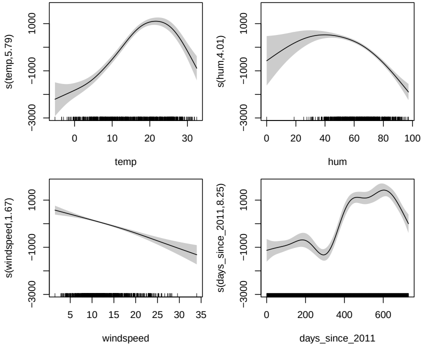
$$g(\mathbb{E}(y \mid \mathbf{x})) = \theta_0 + f_1(x_1) + f_2(x_2) + \ldots + f_p(x_p)$$

- Preserves additive structure and allows to model non-linear effects
- Splines have smoothness param. 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

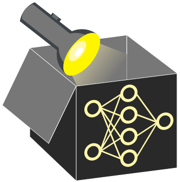
	edf	p-value
s(temp)	5.8	0.00
s(hum)	4.0	0.00
s(windspeed)	1.7	0.00
s(days_since_2011)	8.3	0.00



Interpretation

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

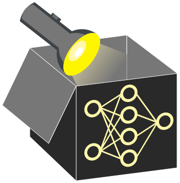
MODEL-BASED BOOSTING ▸ YU_2003 ▸ HOTHORN_2008



- Boosting iteratively combines weak base learners to create powerful ensemble
- Idea: Use simple BLs (e.g. univar., with splines) to ensure interpretability
- Possible to combine BL of same type (with distinct parameters $\boldsymbol{\theta}$ and $\boldsymbol{\theta}^{\star}$):

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

MODEL-BASED BOOSTING ▸ YU_2003 ▸ HOTHORN_2008



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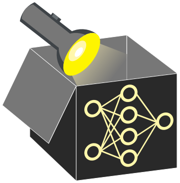
- In each iteration, fit a set of BLs, add best one to model (with step-size ν):

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

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

MODEL-BASED BOOSTING - LINEAR EXAMPLE



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

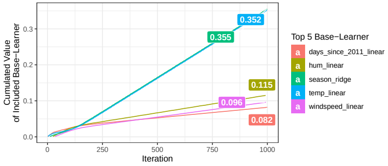
$$b^{[j]}(x_j, \theta) = x_j\theta + \theta_0 \quad \text{for } j = 1, \ldots p \quad \rightsquigarrow \text{ordinary linear regression}$$

- 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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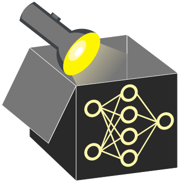

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$$b^{[j]}(x_j, \theta) = x_j\theta + \theta_0 \quad \text{for } j = 1, \dots p \quad \rightsquigarrow \text{ordinary linear regression}$$

- Here: Interpretation of weights as in LM
- After many iterations, it converges to same solution as LM
- Early stopping allows feature selection & may also prevent overfitting (regularization)

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
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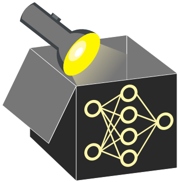
$\Rightarrow$ Converges to solution of LM

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)

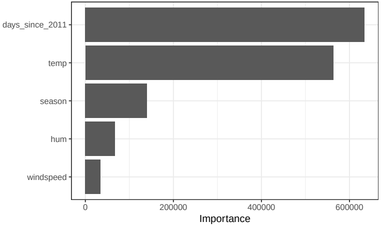
LINEAR EXAMPLE: INTERPRETATION



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

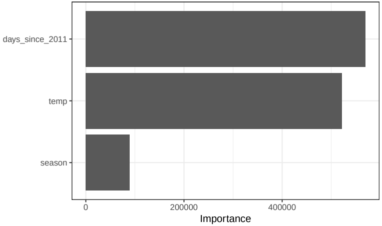
- E.g. iter. 1: `days_since_2011` with risk reduction (MSE) of 140,782.94
- For every iteration the change in risk can be attributed to a feature

1000 iterations



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

20 iterations



In-bag-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.) ▸ Schalk 2018
- BLs: linear and centered splines for numeric feat., categorical for season

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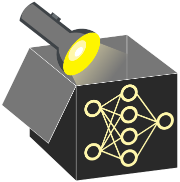

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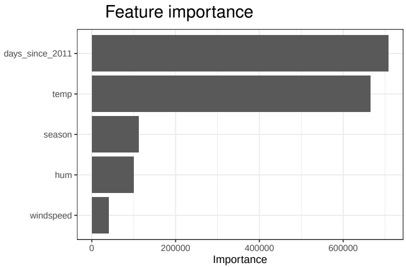

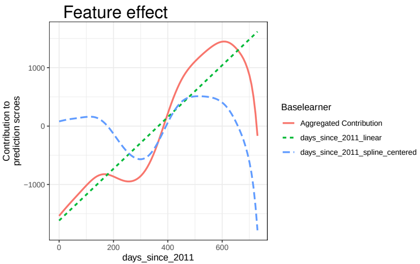

$\Rightarrow$ In-bag-risk: 250,202.0 ; OOB risk (10-fold CV): 267,497.0 (difference to lin. example: 178,953.0)
$\Rightarrow$ In-bag-risk: 434,686.0 ; OOB risk (10-fold CV): 446,450.0 (previous lin. example with 1000 iter.)

- 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