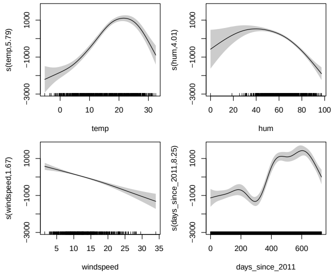
Interpretable Machine Learning

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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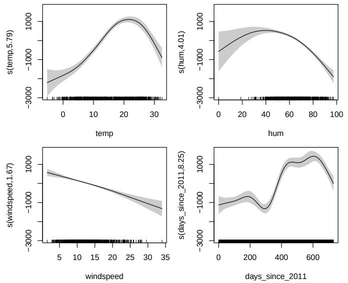
Interpretable Models 1



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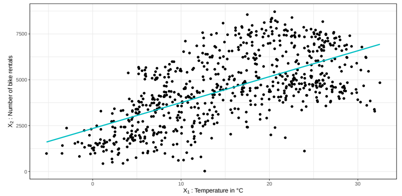
GENERALIZED ADDITIVE MODEL (GAM)

Hastie and Tibshirani (1986)

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



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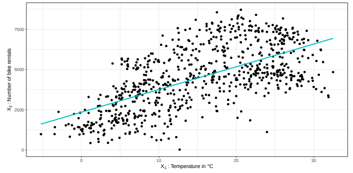

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- Including high-order effects
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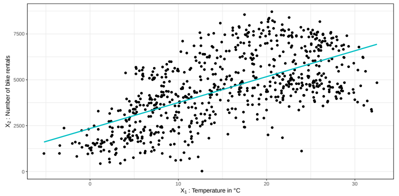

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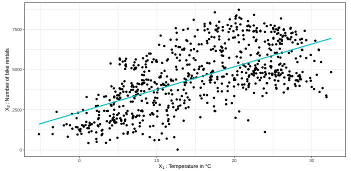

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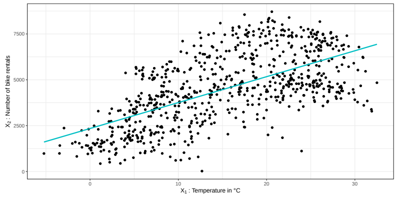

Idea of GAMs:

- 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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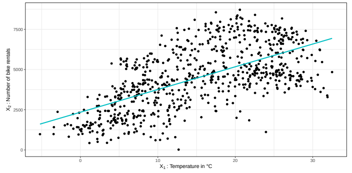

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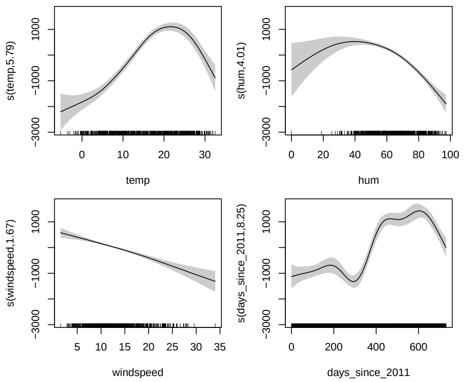
GENERALIZED ADDITIVE MODEL (GAM) - EXAMPLE

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



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- Interpretation is performed visually and relative to average prediction
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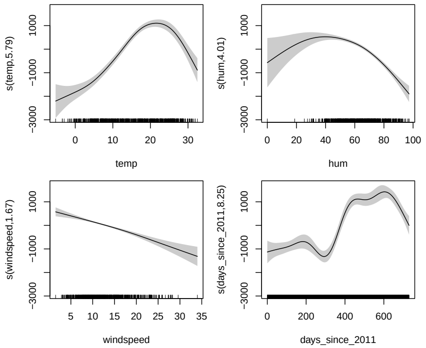

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MODEL-BASED BOOSTING

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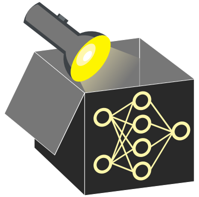

- Boosting iteratively combines weak base learners to create powerful ensemble
- Idea: Use simple BLs (e.g univariate, with splines) to ensure interpretability
- Possible to combine BL of same type (with distinct parameters $\boldsymbol{\theta}$ and $\boldsymbol{\theta}^{\star}$):

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

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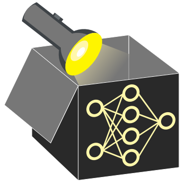

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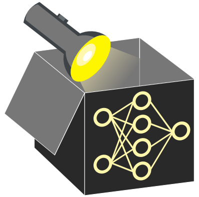

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- In each iteration, fit a set of BLs, add best one to model (with step-size ν):

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

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

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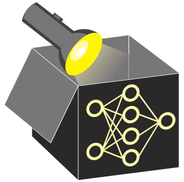

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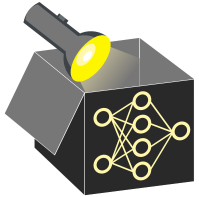

Simple case: Use linear model with single feature (including intercept) as BL

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

- 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
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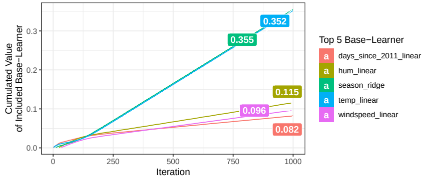
$\Rightarrow$ Converges to solution of LM

Relative frequency of selected BLs across iterations



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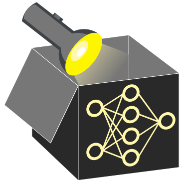

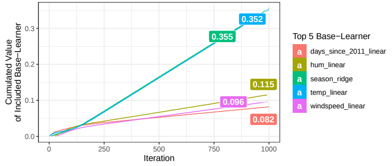

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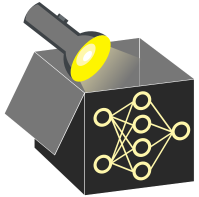

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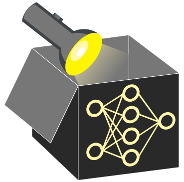
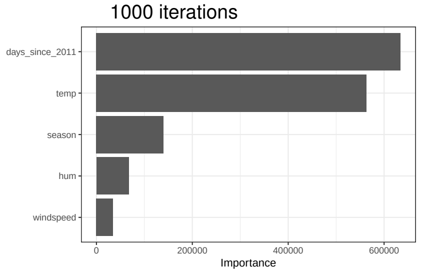


LINEAR EXAMPLE: INTERPRETATION

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



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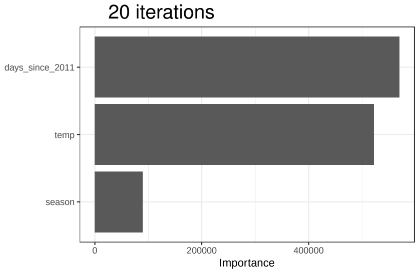

In-bag-risk: 693,505.0
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⇒ Difference in risk: 258,819.0
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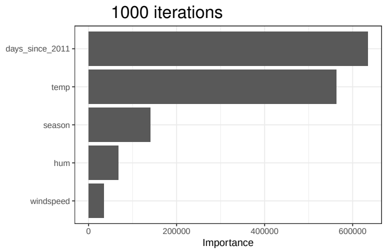

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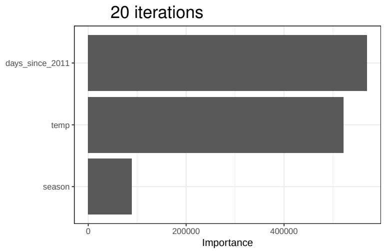

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- BLs: linear and centered splines for numeric features, categorical for season

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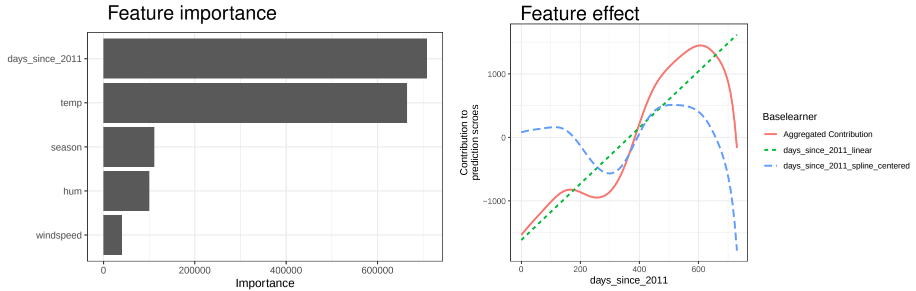

⇒ In-bag-risk: 250,202.0 ; OOB risk (10-fold CV): 267,497.0 (difference to lin. example: 178,953.0)
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- Total effect for `days_since_2011`
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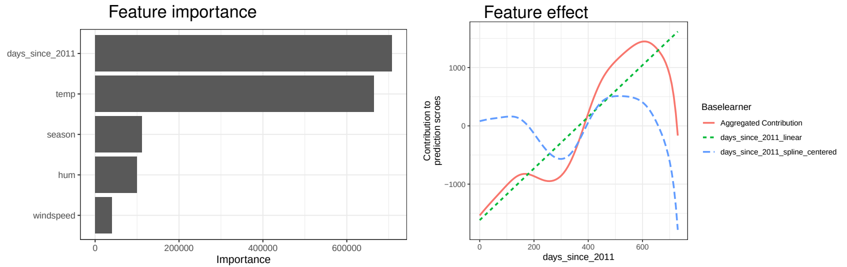

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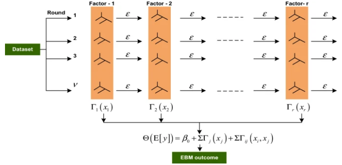
Explainable Boosting Machines (EBM)



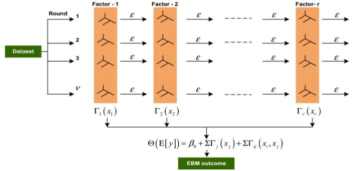
Learning goals

- Understand link between GAM and EBM
- Learn univariate EBMs
  ≙ GAM + boosting + shallow bagged trees
- Extend to GA2M: GAMs with selected pairwise interactions
- Detect interactions efficiently using FAST algorithm

Interpretable Machine Learning

Explainable Boosting Machines (EBM)

Interpretable Models 1



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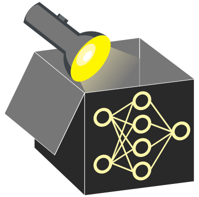
RECAP: SPLIT SELECTION DECISION TREE



- **Impurity (Regression):** Variance of target Y in a node:

$$\text{Var}(Y) = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \bar{y})^2 = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)})^2 - \bar{y}^2$$

- **Sum of squared errors (SSE) = residual sum of squares (RSS):**

$$\text{RSS} = n \cdot \text{Var}(Y) = \sum_{i=1}^{n}(y^{(i)} - \bar{y})^2 = \cdots = \sum_{i=1}^{n}(y^{(i)})^2 - \frac{1}{n}\left(\sum_{i=1}^{n} y^{(i)}\right)^2$$

$$\text{Hence: } \boxed{\text{RSS} = SS_n - \frac{S_n^2}{n} \quad \text{with} \quad S_n = \sum_{i=1}^{n} y^{(i)},\; SS_n = \sum_{i=1}^{n}(y^{(i)})^2}$$

- **Split criterion:**
  - **Minimize post-split RSS:** $\text{RSS}_{\text{split}} = \text{RSS}_L + \text{RSS}_R$
  - **Maximize reduction in RSS:** $\Delta\text{RSS} = \text{RSS}_{\text{parent}} - (\text{RSS}_L + \text{RSS}_R)$

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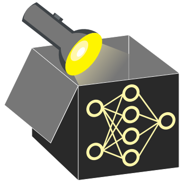

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$$\text{Var}(Y) = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \bar{y})^2 = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)})^2 - \bar{y}^2$$

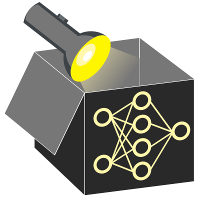
- **Sum of squared errors (SSE) = residual sum of squares (RSS):**

$$\text{RSS} = n \cdot \text{Var}(Y) = \sum_{i=1}^{n}(y^{(i)} - \bar{y})^2 = \cdots = \sum_{i=1}^{n}(y^{(i)})^2 - \frac{1}{n}\left(\sum_{i=1}^{n} y^{(i)}\right)^2$$

$$\text{Hence: } \boxed{\text{RSS} = SS_n - \frac{S_n^2}{n} \quad \text{with} \quad S_n = \sum_{i=1}^{n} y^{(i)},\; SS_n = \sum_{i=1}^{n}(y^{(i)})^2}$$

- **Split criterion:**
  - **Minimize post-split RSS:** $\text{RSS}_{\text{split}} = \text{RSS}_L + \text{RSS}_R$
  - **Maximize reduction in RSS:** $\Delta\text{RSS} = \text{RSS}_{\text{parent}} - (\text{RSS}_L + \text{RSS}_R)$

NAIVE SPLIT SELECTION: EXPLICIT COMPUTATION



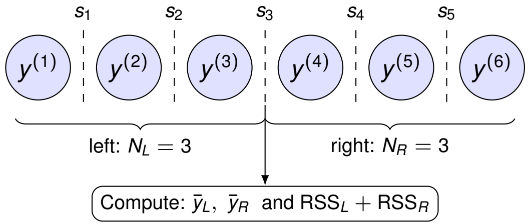
- For a given feature X_j, sort the pairs $(x_j^{(i)}, y^{(i)})$ by increasing $x_j^{(i)}$.
- For each of the $n-1$ potential split points at $s_k = \frac{1}{2}(x_j^{(k)} + x_j^{(k+1)})$:
  - Define partitions: $\mathcal{I}_L = \{i : x^{(i)} \leq s_k\}, \quad \mathcal{I}_R = \{i : x^{(i)} > s_k\}$
  - Compute group means and counts after splitting at s_k:

    $$\bar{y}_L = \frac{1}{N_L} \sum_{i \in \mathcal{I}_L} y^{(i)}, \quad \bar{y}_R = \frac{1}{N_R} \sum_{i \in \mathcal{I}_R} y^{(i)}, \text{ with } N_L = |\mathcal{I}_L|, \quad N_R = |\mathcal{I}_R|$$

  - Compute RSS after splitting at s_k:

    $$\text{RSS}_{\text{split}}(s_k) = \text{RSS}_L(s_k) + \text{RSS}_R(s_k) = \sum_{i \in \mathcal{I}_L} (y^{(i)} - \bar{y}_L)^2 + \sum_{i \in \mathcal{I}_R} (y^{(i)} - \bar{y}_R)^2$$

- Select split point s_k that minimizes $\text{RSS}_{\text{split}}(s_k)$
- **Computational cost:** $O(n^2)$ per feature (recompute mean & RSS at each split)



$\mathcal{O}(n^2)$ operations (recompute for each split s_j per feature)

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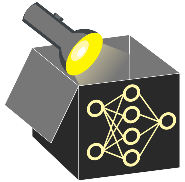

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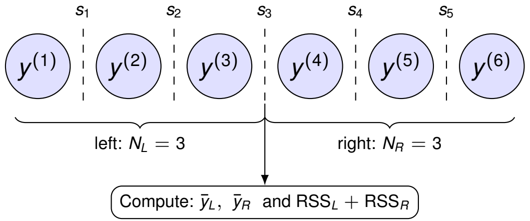

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EFFICIENT SPLIT SELECTION

- **Setup:** For feature X_j, sort the data $(x_j^{(i)}, y^{(i)})_{i=1}^n$ by increasing $x_j^{(i)}$
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$$S_R = S_n - S_L, \qquad SS_R = SS_n - SS_L, \qquad N_R = n - N_L$$

- **RSS for child nodes and parent node:**

$$\text{RSS}_L(s_k) = SS_L - \frac{S_L^2}{N_L}, \text{RSS}_R(s_k) = SS_R - \frac{S_R^2}{N_R}, \text{RSS}_{\text{parent}} = SS_L + SS_R - \frac{S_n^2}{n}$$

HB

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All squared-target terms SS_L, SS_R cancel. Only first-order sums are needed.

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- **Complexity per feature:** $O(n \log n)$ (sorting) + $O(n)$ (cumulative sums & scan)

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EFFICIENT SPLIT SELECTION - EXAMPLE

$\boxed{y^{(1)}=1.2,\ y^{(2)}=2.0,\ y^{(3)}=1.5,\ y^{(4)}=3.2,\ y^{(5)}=2.8,\ y^{(6)}=4.1}$ $(x_j^{(1)} \leq \cdots \leq x_j^{(6)})$

$k = 4$

	$y^{(1)}$	$y^{(2)}$	$y^{(3)}$	$y^{(4)}$	$y^{(5)}$	$y^{(6)}$
cumulative sums S_k	$S_1 = 1.2$	$S_2 = 3.2$	$S_3 = 4.7$	$S_4 = 7.9$	$S_5 = 10.7$	$S_6 = 14.8$

$N_L = 4$ $N_R = 2$

$$\boxed{\begin{aligned} G(k{=}4) &= \frac{S_4^2}{4} + \frac{(S_6 - S_4)^2}{2} \\ &= \frac{7.9^2}{4} + \frac{(14.8 - 7.9)^2}{2} \approx 39.41 \end{aligned}}$$

- $G(k)$ omits $-S_n^2/n$ (identical for all splits $\Rightarrow$ does not affect arg max).
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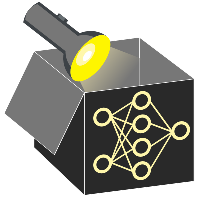
Interpretable Machine Learning – 4 / 20

EXPLAINABLE BOOSTING MACHINES (EBM)



Recall GAM:

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

- One shape function f_j per feature x_j
  $\rightsquigarrow$ **Feature-level interpretability**
- Captures non-linear univariate effects
  $\rightsquigarrow$ **Better performance / more flexible than GLMs**

Idea of EBM: GAMs trained with **gradient boosting** over **shallow bagged trees**

- **GAMs** - provide feature-wise interpretability via separate shape functions $f_j(x_j)$
  $\rightsquigarrow$ Potentially include pairwise interactions manually
- **Gradient Boosting** - incrementally fits residuals to improve predictive performance while retaining additivity
- **Shallow Bagged Trees** - low-depth trees (2–4 leaves) reduce variance and create interpretable shape functions

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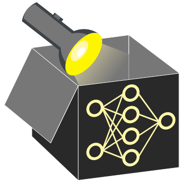

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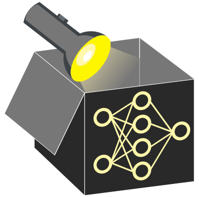
EBM - TWO-STAGE MODEL CONSTRUCTION



1. **Stage 1: Fit Main Effects (Univariate Terms)** ▸ Lou et al. 2012
   - Train EBM using only feature-wise shape functions $f_j(x_j)$
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   - Apply **FAST** to rank all $O(p^2)$ feature pairs by potential reduction in RSS
   - Select top K pairwise interactions and store them in $\mathcal{K}$
   - Use boosting to fit pairwise interaction terms $f_{ij}(x_i, x_j)$ on residuals
   - Final model: $\hat{f}(\mathbf{x}) = \sum_{j=1}^{p} f_j(x_j) + \sum_{(i,j)\in\mathcal{K}} f_{ij}(x_i, x_j)$

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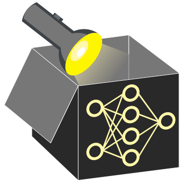

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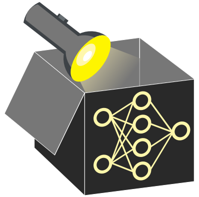
UNIVARIATE EBM - INITIALIZATION



- Set all shape functions to zero:

$$f_j^{[0]}(x_j) = 0 \quad \text{for all } j = 1, \ldots, p$$

- Compute initial model prediction:

$$\hat{y}^{[0]} = \sum_{j=1}^{p} f_j^{[0]}(x_j) = 0$$

- Compute initial pseudo-residuals (e.g., for squared loss):

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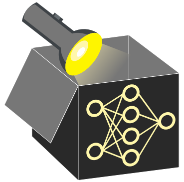
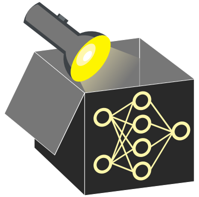
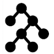


UNIVARIATE EBM – FIRST FEATURE UPDATE



Iteration	feat_1		feat_2	feat_3	...	feat_p
1		$\xrightarrow{\text{res.}}$				

- Fit shallow bagged tree $T_1^{[1]}$ (2–4 leaves) to training data $\left\{\left(x_1, \tilde{r}^{[0]}\right)^{(i)}\right\}_{i=1}^n$

  $\rightsquigarrow$ Use only feature x_1 as input and $\tilde{r}^{[0]}$ as target
- Update first shape function with learning rate η:

$$f_1^{[1]}(x_1) = f_1^{[0]}(x_1) + \eta \cdot T_1^{[1]}(x_1)$$

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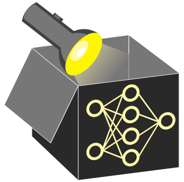

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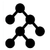
1		$\xrightarrow{\text{res.}}$				

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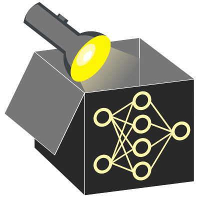
UNIVARIATE EBM – CYCLE THROUGH FEATURES



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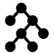
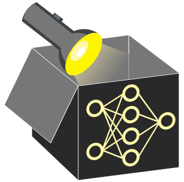
1		$\xrightarrow{\text{res.}}$		$\xrightarrow{\text{res.}}$			

- 1st boosting iteration:
  Cycle through each feature $j = 2, \ldots, p$:
  - Fit shallow bagged tree $T_j^{[1]}$ using feature x_j and previous residual $\tilde{r}^{[j-1]}$
  - Update f_j: $f_j^{[1]}(x_j) = f_j^{[0]}(x_j) + \eta \cdot T_j^{[1]}(x_j)$
  - Recompute $\hat{y}$ and residuals: $\tilde{r}^{[j]} = y - \hat{y}^{[j]}$
- After one full pass over features, we complete one boosting iteration

UNIVARIATE EBM CYCLE THROUGH FEATURES



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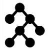
1		$\xrightarrow{\text{res.}}$		$\xrightarrow{\text{res.}}$			

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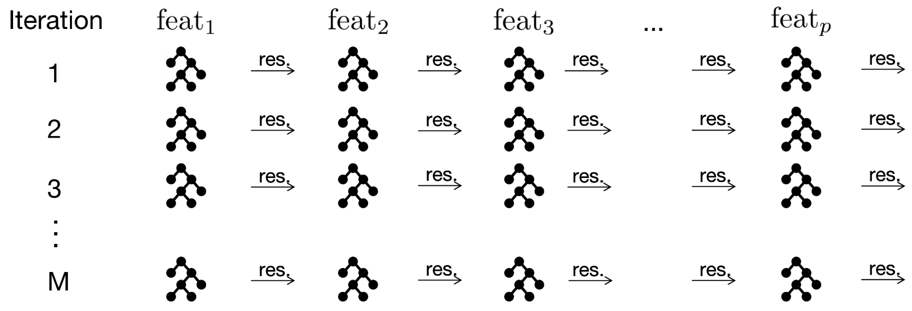
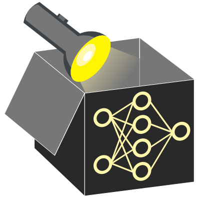
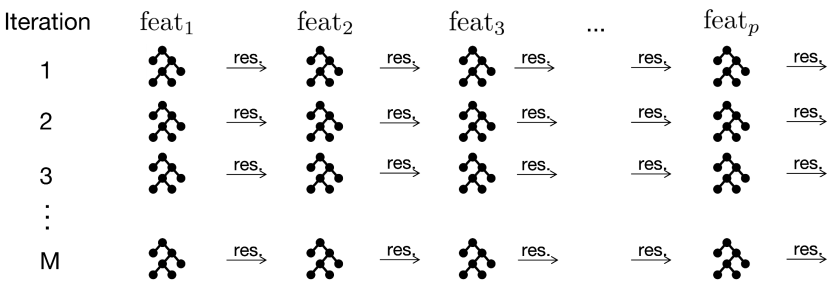
UNIVARIATE EBM – ITERATE BOOSTING PROCESS

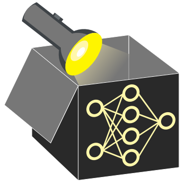




- Repeat feature-wise updates for M boosting iterations (e.g., $M = 10000$)
- In each boosting iteration:
  - Cycle over all features $j = 1, \dots, p$ individually
  - Update only one f_j at a time using residuals from previous state
- Use small learning rate η to ensure smooth updates and order-invariance

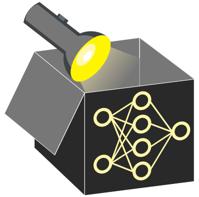
UNIVARIATE EBM ITERATE BOOSTING PROCESS





- Repeat feature-wise updates for M boosting iterations (e.g., $M = 10000$)
- In each boosting iteration:
  - Cycle over all features $j = 1, \dots, p$ individually
  - Update only one f_j at a time using residuals from previous state
- Use small learning rate η to ensure smooth updates and order-invariance

UNIVARIATE EBM - PREDICTION & INTERPRETABILITY



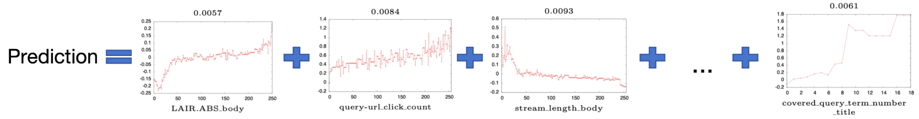
- Final model consists of M shallow trees per feature:

$$\text{EBM Model} = \sum_{j=1}^{p} \sum_{m=1}^{M} \eta \cdot T_j^{[m]}(x_j)$$

- For each feature x_j, combine its M trees into a shape function:

$$\hat{f}_j(x_j) = \sum_{m=1}^{M} \eta \cdot T_j^{[m]}(x_j)$$

- Plot $\hat{f}_j(x_j)$ vs. x_j $\rightsquigarrow$ Shows univariate marginal effect of feature j
- One plot per feature $\rightsquigarrow$ Model is fully explainable via p additive plots



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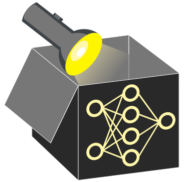
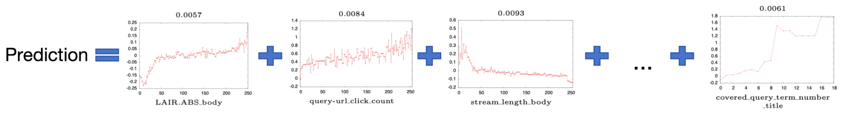
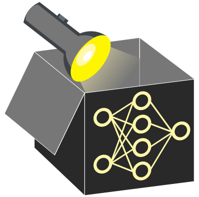




EBM WITH PAIRWISE INTERACTIONS



Generalized Additive Models plus Interactions (GA2M):

$$g\big(\mathbb{E}[y \mid \mathbf{x}]\big) = \theta_0 + \sum_{j=1}^{p} f_j(x_j) + \sum_{i<j} f_{ij}(x_i, x_j)$$

- **Motivation**: Univariate EBM does not model interactions
- **Challenge**: $O(p^2)$ potential pairwise interactions $\rightsquigarrow$ often infeasible
- **Solution - FAST algorithm** ▸ Lou et al. 2013:
  - Efficiently estimates importance of all feature pairs
  - Ranks pairs by reduction in residual sum of squares (RSS)
  - Avoids fitting EBM with each pairwise interaction
- **Result**: Add only top-ranked interactions f_{ij} via a second-stage boosting step
  $\rightsquigarrow$ Performed after the univariate EBM has been trained
- **Interpretability preserved**: Each $f_{ij}(x_i, x_j)$ visualized as a 2D heatmap

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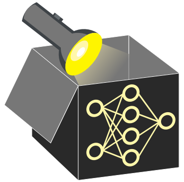

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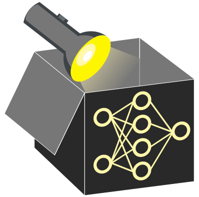
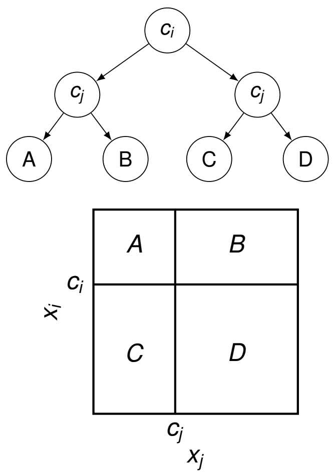
Interpretable Machine Learning – 12 / 20

FAST: PAIR-WISE INTERACTION STRENGTH

We evaluate a 4-leaf, axis-aligned tree T_{ij} over the 2D feature projection (x_i, x_j).





tree T_{ij} with 4 leaves

1. **Discretize** : Map each axis to $b \leq 256$ ordered bins (quantile or equal-width).

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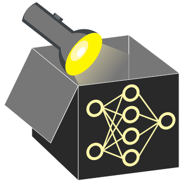

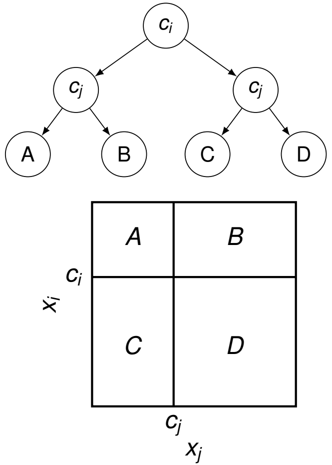

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Interpretable Machine Learning – 13 / 20

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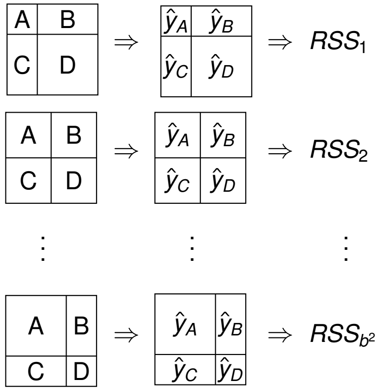

❶ **Discretize** : Map each axis to $b \leq 256$ ordered bins (quantile or equal-width).

❷ **Iterate** over b^2 candidate cuts (c_i, c_j).

❸ **Fit** : For each cut, assign a constant $\hat{y}_r = \text{mean}(y \in r)$ to $r \in \{A, B, C, D\}$.

❹ **Compute RSS summed over all regions**:

$$\text{RSS}(c_i, c_j) = \sum_r \sum_{(x,y)\in r} (y - \hat{y}_r)^2$$

$$= \sum_r \left(\sum_{(x,y)\in r} y^2 - \frac{1}{n_r} \left(\sum_{(x,y)\in r} y \right)^2 \right)$$

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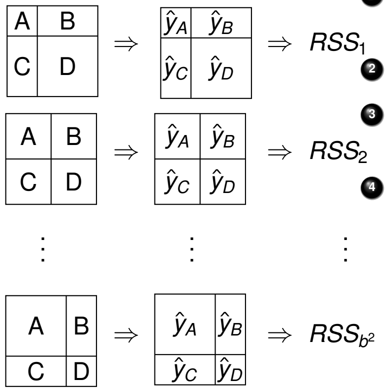

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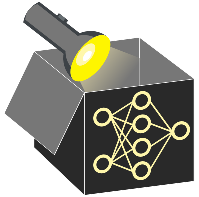

To evaluate a cut pair (c_i, c_j), we use precomputed per-region statistics:

- For each region $r \in \{A, B, C, D\}$, compute:

$$S_r = \sum_{(x,y)\in r} y, \quad n_r = |\{(x,y) \in r\}|, \quad \hat{y}_r = S_r / n_r$$

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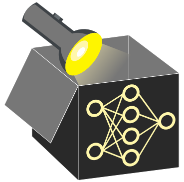
- For a candidate cut, compute **RSS drop**:

$$\begin{aligned} \Delta\text{RSS}(c_i, c_j) &= \text{RSS}_{\text{parent}} - \text{RSS}(c_i, c_j) \\ &= \left(\sum_{i=1}^{n} \left(y^{(i)} \right)^2 - \frac{S_n^2}{n} \right) - \sum_r \sum_{(x,y)\in r} y^2 + \sum_r \frac{S_r^2}{n_r} \end{aligned}$$



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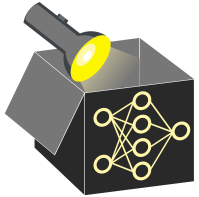

Because $\sum_{i=1}^{n} \left(y^{(i)}\right)^2 = \sum_r \sum_{(x,y)\in r} y^2$, *all squared target terms cancel*:

$$\boxed{\Delta\mathrm{RSS}(c_i, c_j) = \sum_r \frac{S_r^2}{n_r} - \frac{S_n^2}{n}}$$

The parent term S_n^2/n is constant across all cuts. Hence

$$\textbf{maximize } \Delta\mathrm{RSS}(c_i, c_j) = \sum_r \frac{S_r^2}{n_r} \iff \textbf{minimize } \mathrm{RSS}(c_i, c_j).$$

Why is this efficient?

- Precompute cummulative sums of y and counts across the binned grid
- Enables fast lookup of region statistics S_r, n_r for any cut
- No additional data scan or recomputation needed across the b^2 candidate cuts
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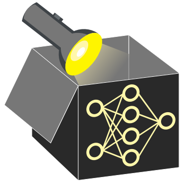
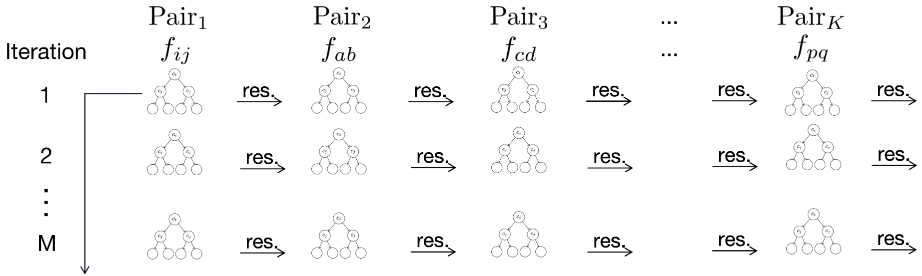
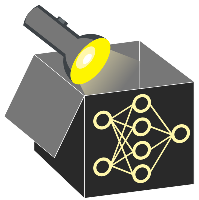
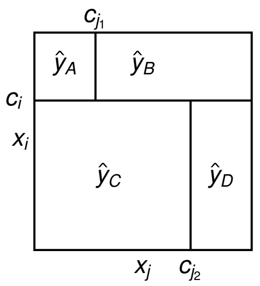


EBM - BOOSTING PAIRWISE INTERACTIONS







- **Goal:** Fit each selected interaction $f_{ij}(x_i, x_j)$ on residuals from main effects
- Use tree-like predictor, inspired by FAST
  - Use two axis-aligned cuts (c_i, c_j)
  - Plus one refinement cut to increase flexibility while keeping interpretability
- Reuse region-wise sums from FAST lookup tables
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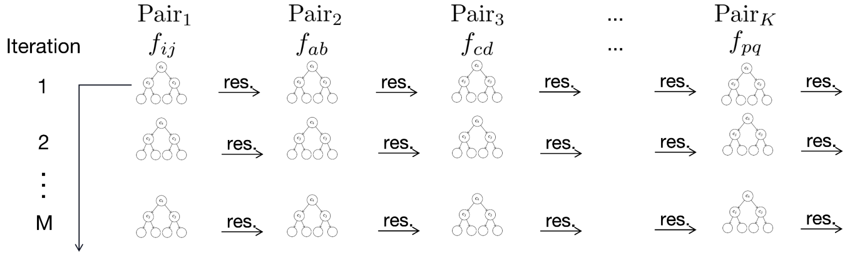

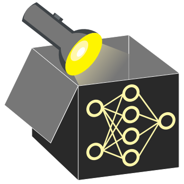

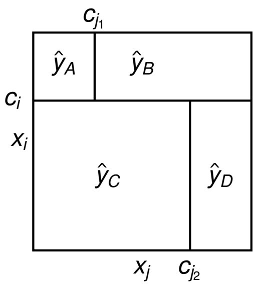

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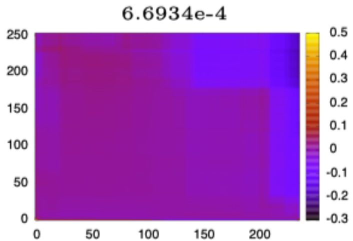
EBM - PREDICTION WITH PAIRWISE INTERACTIONS

- Each selected pair (x_i, x_j) is modeled by M boosted predictors trained on their residual interaction
- These are aggregated into a single bivariate function $f_{ij}(x_i, x_j)$
- The function is visualized as a 2D heatmap:
  - Axes: feature values of x_i and x_j
  - Color: contribution to the final prediction
  - Preserves human interpretability
- One heatmap is generated per selected pairwise interaction



qualityscore2 vs. siterank

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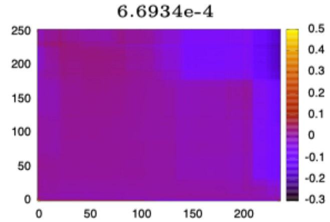

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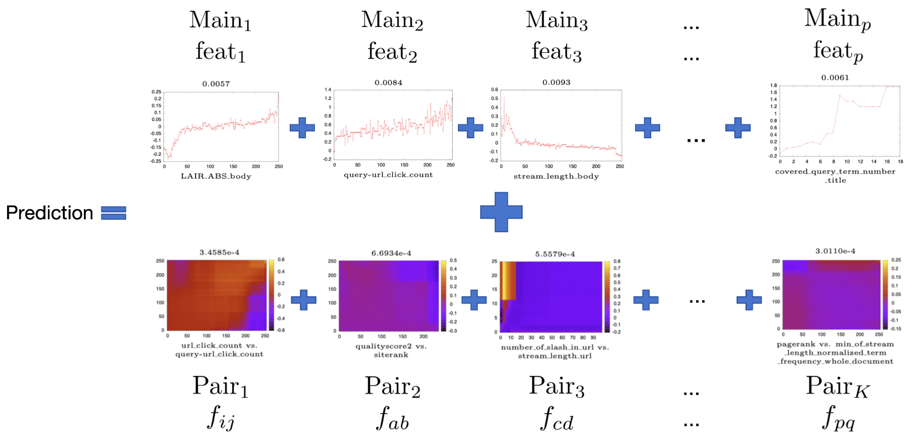
EBM - FINAL MODEL STRUCTURE

- **Main effects:** One shape function $f_j(x_j)$ per feature (visualized as 1D plots)
- **Pairwise interactions:** Selected functions $f_{ij}(x_i, x_j)$ added for top K pairs (visualized as 2D heatmaps)
- **Prediction:** Additive sum of all univariate and selected bivariate contributions



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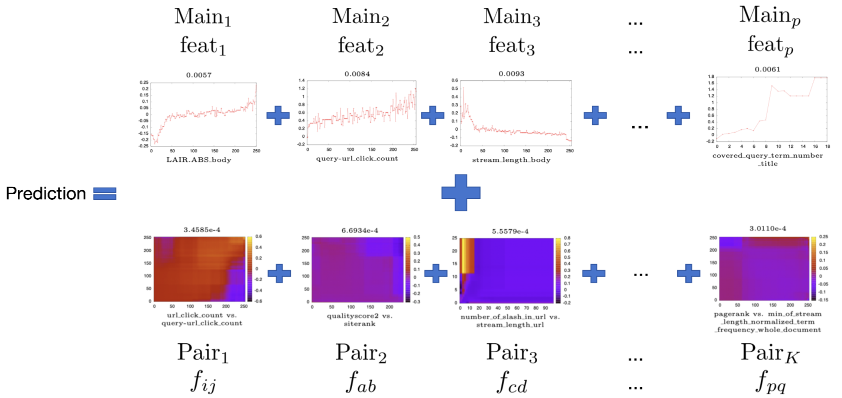

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EBM *VS.* MODEL-BASED BOOSTING

- **Base learner**
  - **EBM**: bagged 2–4-leaf trees, *one feature* per tree ⇒ step-function shape f_j ▸ Lou et al. 2012
  - **MB-boost**: user chooses component-wise learner (linear term, P-spline, tree, random effect, . . .) ▸ Bühlmann & Hothorn 2007

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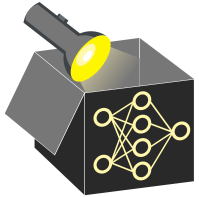

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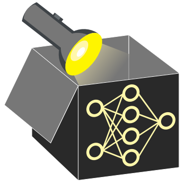

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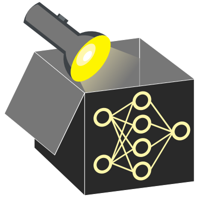

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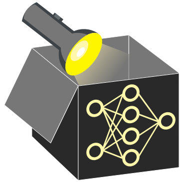
- **Regularisation**
  - **EBM**: many iterations M (5–10k); early stopping via *internal* CV on out-of-bag samples; bagging further lowers variance.
  - **MB-boost**: shrinkage $\nu \in (0, 1]$; early stop by CV/AIC; component selection acts like an L_0/L_1 penalty $\rightarrow$ sparsity.

EBM *VS.* MODEL-BASED BOOSTING



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  - **MB-boost**: shrinkage $\nu \in (0, 1]$; early stop by CV/AIC; component selection acts like an L_0/L_1 penalty $\rightarrow$ sparsity.

EBM *VS.* MODEL-BASED BOOSTING

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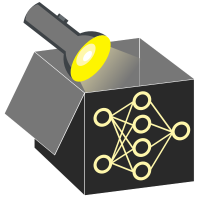

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  - **EBM**:
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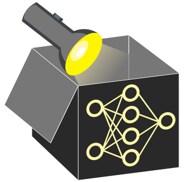

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