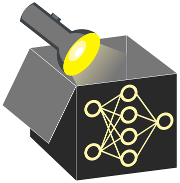
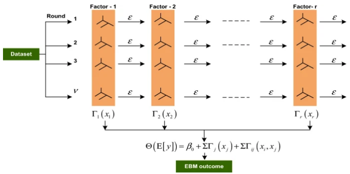
Interpretable Machine Learning



Explainable Boosting Machines (EBM)

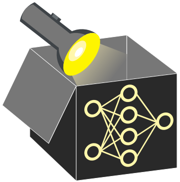
Interpretable Models 1



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

RECAP: SPLIT SELECTION DECISION TREE



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

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

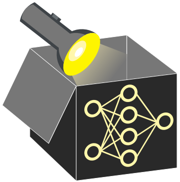
- **Sum of squared errors (SSE) = residual sum of squares (RSS)**:

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

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

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

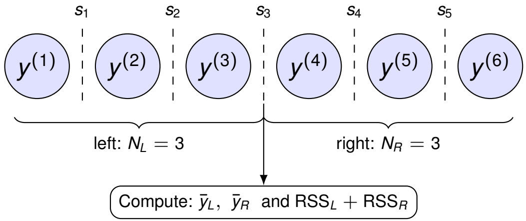
NAIVE SPLIT SELECTION: EXPLICIT COMPUT.



- 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:

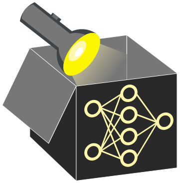
    $\bar{y}_L = \frac{1}{N_L} \sum_{i \in \mathcal{I}_L} y^{(i)}, \quad \bar{y}_R = \frac{1}{N_R} \sum_{i \in \mathcal{I}_R} y^{(i)}$, with $N_L = |\mathcal{I}_L|, \quad N_R = |\mathcal{I}_R|$
  - Compute RSS after splitting at s_k:

    $\text{RSS}_{\text{split}}(s_k) = \text{RSS}_L(s_k) + \text{RSS}_R(s_k) = \sum_{i \in \mathcal{I}_L} (y^{(i)} - \bar{y}_L)^2 + \sum_{i \in \mathcal{I}_R} (y^{(i)} - \bar{y}_R)^2$
- Select split point s_k that minimizes $\text{RSS}_{\text{split}}(s_k)$
- **Compute cost:** $O(n^2)$ per feat. (recompute mean & RSS at each split)



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

EFFICIENT SPLIT SELECTION



- **Setup:** For feature X_j, sort the data $(x_j^{(i)}, y^{(i)})_{i=1}^n$ by increasing $x_j^{(i)}$
- **Define group statistics (cumulative sums) after split at s_k:**

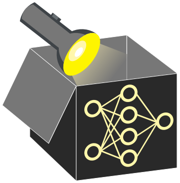
$$S_L = \sum_{i \in \mathcal{I}_L} y^{(i)}, \qquad SS_L = \sum_{i \in \mathcal{I}_L} (y^{(i)})^2, \qquad N_L = |\mathcal{I}_L|$$
$$S_R = S_n - S_L, \qquad SS_R = SS_n - SS_L, \qquad N_R = n - N_L$$

- **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

EFFICIENT SPLIT SELECTION



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

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

- **Reduction in RSS:**

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

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

- **Search:** Choose best split $s_k^\star = \arg\max_{s_k} \Delta\text{RSS}(s_k)$
- **Complexity per feature:**
  $O(n \log n)$ (sorting) + $O(n)$ (cumulative sums and scan)

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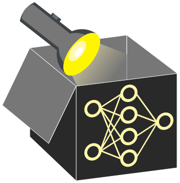
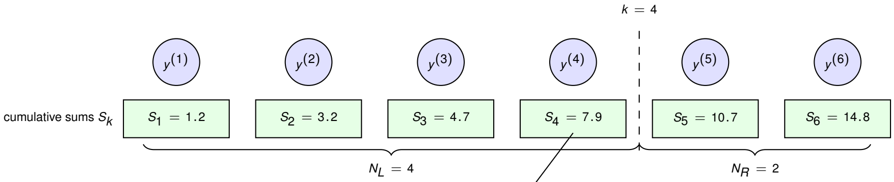
EFFICIENT SPLIT SELECTION - EXAMPLE



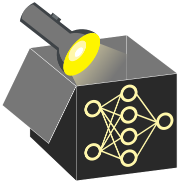
$$\boxed{y^{(1)}=1.2,\ y^{(2)}=2.0,\ y^{(3)}=1.5,\ y^{(4)}=3.2,\ y^{(5)}=2.8,\ y^{(6)}=4.1} \quad (\,x_j^{(1)} \leq \cdots \leq x_j^{(6)}\,)$$



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

- $G(k)$ omits $-S_n^2/n$ (identical for all splits $\Rightarrow$ does not affect $\arg\max$).
- Only cumulative sums S_k are required, no SS_k is stored or updated.
- $\mathcal{O}(1)$ per split $\Rightarrow \mathcal{O}(n)$ per feature.

EXPLAINABLE BOOSTING MACHINES (EBM)



Recall GAM:

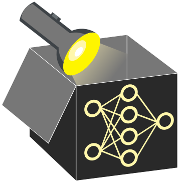
$$g\big(\mathbb{E}[y \mid \mathbf{x}]\big) = \theta_0 + f_1(x_1) + f_2(x_2) + \ldots + f_p(x_p),$$

- 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**

EBM idea: GAMs train with **gradient boosting** over **shallow bagged trees**

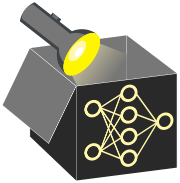
- **GAMs** - feature-wise interpretability via separate shape functions $f_j(x_j)$
  $\rightsquigarrow$ Potentially include pairwise interactions manually
- **Gradient Boosting** - incrementally fits residuals to improve predictive performance while retaining additivity
- **Shallow Bagged Trees** - low-depth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

EBM - TWO-STAGE MODEL CONSTRUCTION



1. **Stage 1: Fit Main Effects (Univariate Terms)** ▸ Lou 2012
   - Train EBM using only feature-wise shape functions $f_j(x_j)$
   - Freeze the univariate model after convergence
2. **Stage 2: Add Selected Pairwise Interactions** ▸ Lou 2013
   - Apply **FAST** to rank all $O(p^2)$ feat 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: $\hat{f}() = \sum_{j=1}^{p} f_j(x_j) + \sum_{(i,j)\in\mathcal{K}} f_{ij}(x_i, x_j)$

UNIVARIATE EBM - INITIALIZATION



- Set all shape functions to zero:

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

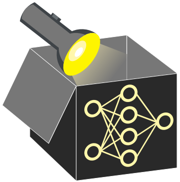
- Compute initial model prediction:

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

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

$$\tilde{r}^{[0]} = -\frac{\partial L}{\partial \hat{y}} = y - \hat{y}^{[0]} = y$$

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:

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

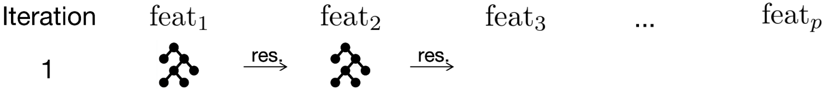
- Update prediction:

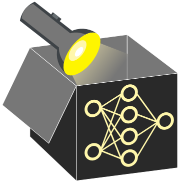
$$\hat{y}^{[1]} = \sum_{j=1}^{p} f_j^{[1]}(x_j)$$

- Recompute pseudo-residuals:

$$\tilde{r}^{[1]} = -\frac{\partial L}{\partial \hat{y}} = y - \hat{y}^{[1]}$$

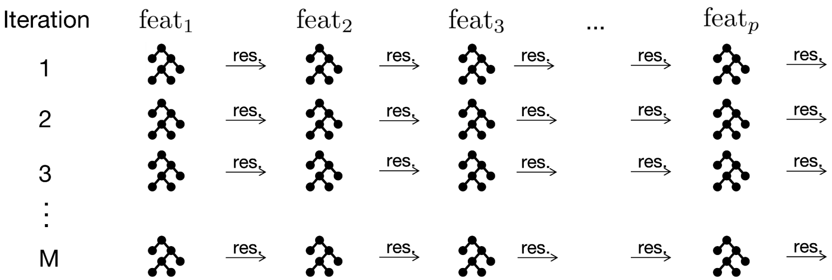
UNIVARIATE EBM CYCLE THROUGH FEATURES

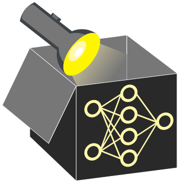




- 1st boosting iteration:
  Cycle through each feature $j = 2, \ldots, p$:
  - Fit shallow bagged tree $T_j^{[1]}$ using feature x_j and previous residual $\tilde{r}^{[j-1]}$
  - Update f_j: $f_j^{[1]}(x_j) = f_j^{[0]}(x_j) + \eta \cdot T_j^{[1]}(x_j)$
  - Recompute $\hat{y}$ and residuals: $\tilde{r}^{[j]}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

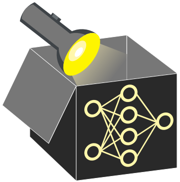
UNIVARIATE EBM ITERATE BOOSTING PROCESS





- Repeat feature-wise updates for M boosting iterations (e.g., $M = 10000$)
- In each boosting iteration:
  - Cycle over all features $j = 1, \ldots, p$ 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



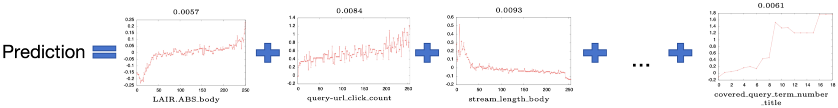
- Final model consists of M shallow trees per feature:

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

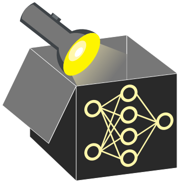
- For each feature x_j, combine its M trees into a shape function:

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

- 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



EBM WITH PAIRWISE INTERACTIONS



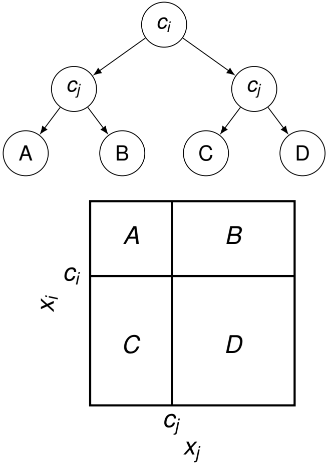
Generalized Additive Models plus Interactions (GA2M):

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

- **Motivation**: Univariate EBM does not model interactions
- **Challenge**: $O(p^2)$ potential pairwise interactions $\rightsquigarrow$ often infeasible
- **Solution - FAST algorithm** ▸ Lou 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 asecond-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

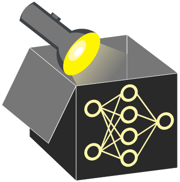
FAST: PAIR-WISE INTERACTION STRENGTH

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

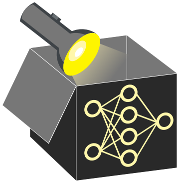


tree T_{ij} with 4 leaves

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



FAST: PAIR-WISE INTERACTION STRENGTH



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

$$\begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline\end{array} \Rightarrow \begin{array}{|c|c|}\hline \hat{y}_A & \hat{y}_B \\ \hline \hat{y}_C & \hat{y}_D \\ \hline\end{array} \Rightarrow RSS_1$$

$$\begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline\end{array} \Rightarrow \begin{array}{|c|c|}\hline \hat{y}_A & \hat{y}_B \\ \hline \hat{y}_C & \hat{y}_D \\ \hline\end{array} \Rightarrow RSS_2$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$\begin{array}{|c|c|}\hline A & B \\ \hline C & D \\ \hline\end{array} \Rightarrow \begin{array}{|c|c|}\hline \hat{y}_A & \hat{y}_B \\ \hline \hat{y}_C & \hat{y}_D \\ \hline\end{array} \Rightarrow RSS_{b^2}$$

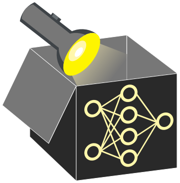
1. **Discretize** : Map each axis to $b \leq 256$ ordered bins (quantile or equal-width).
2. **Iterate** over b^2 candidate cuts (c_i, c_j).
3. **Fit** : For each cut, assign a constant $\hat{y}_r = \text{mean}(y \in r)$ to $r \in \{A, B, C, D\}$.
4. **Compute RSS summed over all regions**:

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

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

5. **Select** : Keep the split with minimal RSS.
$\rightsquigarrow$ largest RSS drop = strongest interaction.

FAST: USE RSS DROP



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:

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

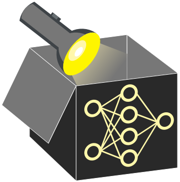
- Plug into RSS summed over all regions:

$$\text{RSS}(c_i, c_j) = \sum_r \left(\sum_{(x,y)\in r} y^2 - \frac{1}{n_r} \left(\sum_{(x,y)\in r} y \right)^2 \right) = \sum_r \sum_{(x,y)\in r} y^2 + \sum_r \frac{S_r^2}{n_r}$$

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

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

FAST: USE RSS DROP



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

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

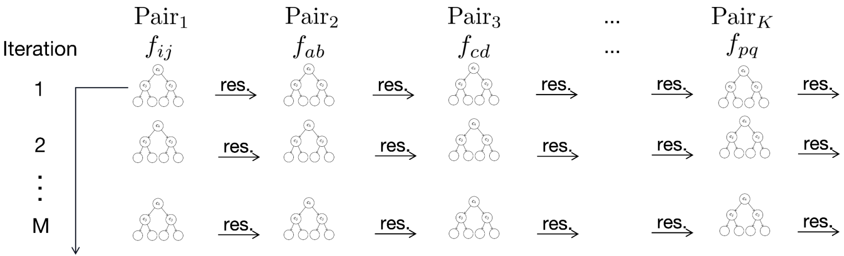
The parent term S_n^2/n is constant across all cuts. Hence

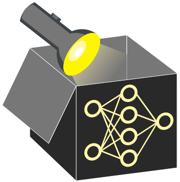
$$\textbf{maximize } \Delta\text{RSS}(c_i, c_j) = \sum_r \frac{S_r^2}{n_r} \quad \Longleftrightarrow \quad \textbf{minimize } \text{RSS}(c_i, c_j).$$

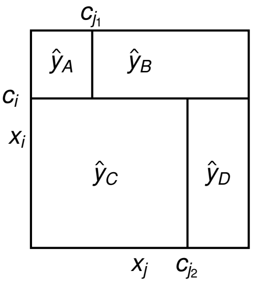
Why is this efficient?

- 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
- For the best cut: Compare and select the largest $\Delta\text{RSS}(c_i, c_j)$.

EBM - BOOSTING PAIRWISE INTERACTIONS

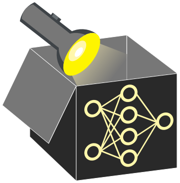




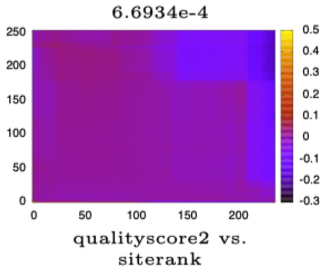


- **Goal:** Fit each selected interaction $f_{ij}(x_i, x_j)$ on residuals from main effects
- Use tree-like predictor, inspired by FAST
  - Use two axis-aligned cuts (c_i, c_j)
  - Plus one refinement cut to increase flexibility while keeping interpretability
- Reuse region-wise sums from FAST lookup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

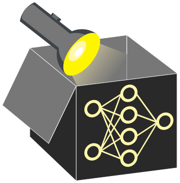
EBM - PREDICTION WITH PAIRWISE INTERACTIONS



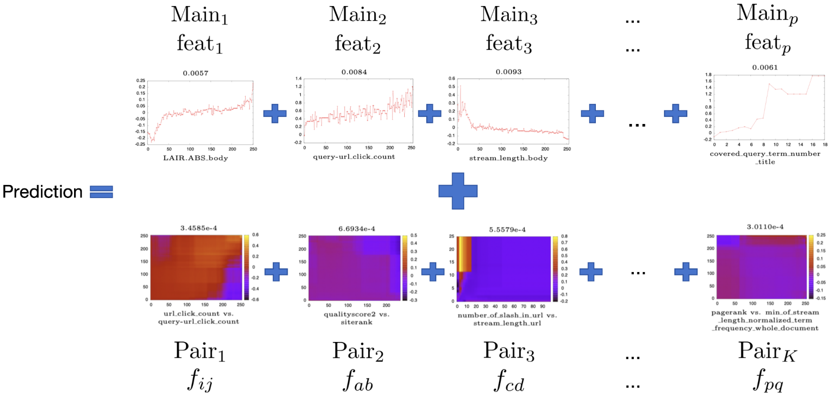
- Each selected pair (x_i, x_j) is modeled by M boosted predictors trained on their residual interaction
- These are aggregated into a single bivariate function $f_{ij}(x_i, x_j)$
- The function is visualized as a 2D heatmap:
  - Axes: feature values of x_i and x_j
  - Color: contribution to the final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



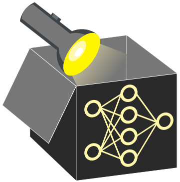
EBM - FINAL MODEL STRUCTURE



- **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



EBM *VS.* MODEL-BASED BOOSTING



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

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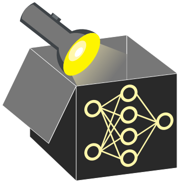

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- **Iteration policy**
  - **EBM**: round-robin ($\forall j$) each boosting pass; tiny learning rate $\eta \approx 0.01$.
  - **MB-boost**: greedy; update the *single* component that yields the largest loss reduction.

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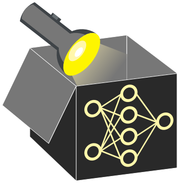

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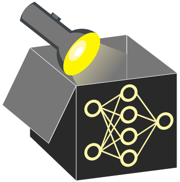
- **Regularisation**
  - **EBM**: many iterations M (5–10k); early stopping via *internal* CV on out-of-bag samples; bagging further lowers variance.
  - **MB-boost**: shrinkage $\nu \in (0, 1]$; early stop by CV/AIC; component selection acts like an L_0/L_1 penalty $\rightarrow$ sparsity.

EBM *VS.* MODEL-BASED BOOSTING



- **Interactions**
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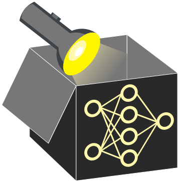

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    - one 1-D step plot for each f_j
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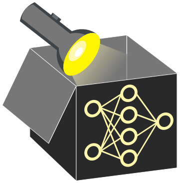

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- **Take-away**
  - *EBM* provides fast, interpretable, and interaction-sparse models
  - *MB-boost* offers flexible stat modeling with built-in variable selection