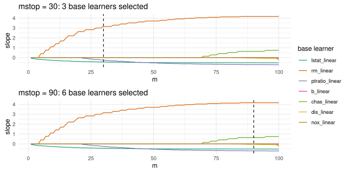
Introduction to Machine Learning

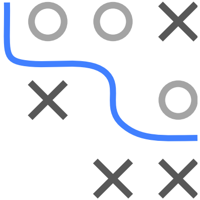
Boosting
Gradient Boosting: CWB Basics 1



Learning goals

- Concept of CWB
- Which base learners do we use
- Built-in feature selection

COMPONENTWISE GRADIENT BOOSTING



GB (with trees), has strong predictive performance but is difficult to interpret unless the base learners are stumps.

The aim of CWB is to find a model that exhibits:

- strong predictive performance,
- interpretable components,
- automatic selection of components,
- is sparser than a model fitted with maximum-likelihood estimation.

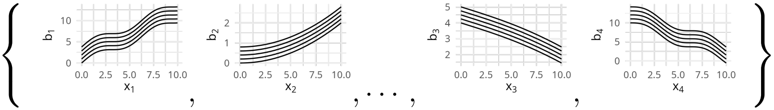
This is achieved by using “nice” base learners which yield familiar statistical models in the end.

Because of this, CWB is also often referred to as **model-based boosting**.

BASE LEARNERS

In GB only one kind of base learner $\mathcal{B}$ is used, e.g., regression trees.

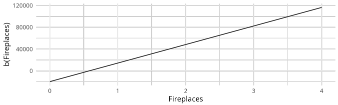
For CWB we generalize this to multiple base learner sets $\{\mathcal{B}_1, ...\mathcal{B}_J\}$ with associated parameter spaces $\{\mathbf{\Theta}_1, ...\mathbf{\Theta}_J\}$, where $j \in \{1, 2, \dots, J\}$ indexes the type of base learner.



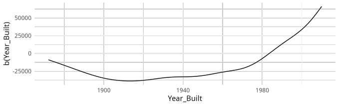
In each iteration, base learners are fitted to the **pseudo residuals** $\tilde{r}^{[m]}$.

BASE LEARNERS / 2

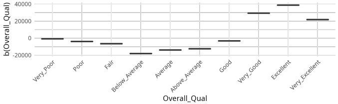
We restrict the base learners to additive model components, i.e.,



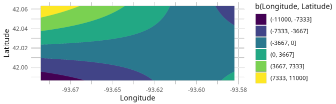
linear effect



non-linear (spline) effect



dummy encoded linear model of a cat. feature



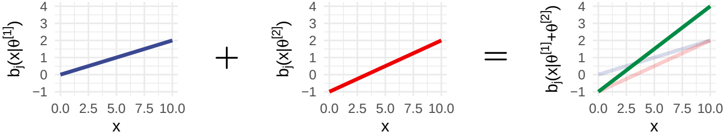
tensor product spline for interaction modelling (e.g. spatial effects)

More advanced base learners could also be Markov random fields, random effects, or trees.

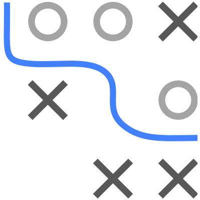
BASE LEARNERS / 3

Two BLs of the same type can simply be added by adding up their parameter vectors:

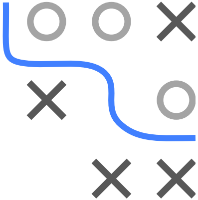
$$b_j(\mathbf{x}, \boldsymbol{\theta}^{[1]}) + b_j(\mathbf{x}, \boldsymbol{\theta}^{[2]}) = b_j(\mathbf{x}, \boldsymbol{\theta}^{[1]} + \boldsymbol{\theta}^{[2]}).$$



Thus, if $\{b_j(\mathbf{x}, \boldsymbol{\theta}^{[1]}), b_j(\mathbf{x}, \boldsymbol{\theta}^{[2]})\} \in \mathcal{B}_j$, then $b_j(\mathbf{x}, \boldsymbol{\theta}^{[1]} + \boldsymbol{\theta}^{[2]}) \in \mathcal{B}_j$.



COMPONENTWISE BOOSTING ALGORITHM



Different from GB, multiple base learners $b_j \in \mathcal{B}_j$, $j = 1, \dots, J$, are fitted and only best-fitting one is selected and updated.

Algorithm Componentwise Gradient Boosting.

Initialize $f^{[0]}(\mathbf{x}) = \arg\min_{\theta_0 \in \mathbb{R}} \sum_{i=1}^{n} L(y^{(i)}, \theta_0)$
for $m = 1 \to M$ **do**
    For all i: $\tilde{r}^{[m](i)} = -\left[\frac{\partial L(y,f)}{\partial f}\right]_{f=f^{[m-1]}(\mathbf{x}^{(i)}),y=y^{(i)}}$
    for $j = 1 \to J$ **do**
        Fit regression base learner $b_j \in \mathcal{B}_j$ to the vector of pseudo-residuals $\tilde{r}^{[m]}$:
        $\hat{\boldsymbol{\theta}}_j^{[m]} = \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}_j} \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - b_j(\mathbf{x}^{(i)}, \boldsymbol{\theta}))^2$
    end for
    $j^{[m]} = \arg\min_j \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_j(\mathbf{x}^{(i)}, \hat{\boldsymbol{\theta}}_j^{[m]}))^2$
    Update $f^{[m]}(\mathbf{x}) = f^{[m-1]}(\mathbf{x}) + \alpha \hat{b}_j(\mathbf{x}, \hat{\boldsymbol{\theta}}_{j^{[m]}}^{[m]})$
end for
Output $\hat{f}(\mathbf{x}) = f^{[M]}(\mathbf{x})$

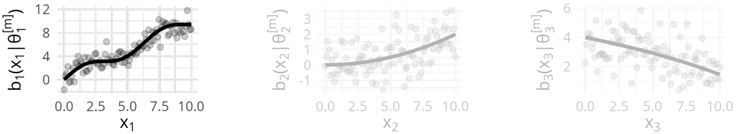
(Same as for GB, New inner loop for CWB)

COMPONENTWISE BOOSTING ALGORITHM

Algorithm Componentwise Gradient Boosting (inner loop).

for $j = 1 \to J$ **do**
  Fit regression base learner $b_j \in \mathcal{B}_j$ to the vector of pseudo-residuals $\tilde{r}^{[m]}$:
  $\hat{\boldsymbol{\theta}}_j^{[m]} = \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}_j} \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - b_j(\mathbf{x}^{(i)}, \boldsymbol{\theta}))^2$
end for
$j^{[m]} = \arg\min_j \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_j(\mathbf{x}^{(i)}, \hat{\boldsymbol{\theta}}_j^{[m]}))^2$

Iteration m, $j = 1$, $\sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_1(x_1^{(i)}, \hat{\boldsymbol{\theta}}_1^{[m]}))^2 = 24.4$:



COMPONENTWISE BOOSTING ALGORITHM

Algorithm Componentwise Gradient Boosting (inner loop).

for $j = 1 \to J$ **do**

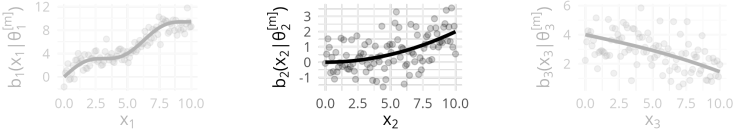
Fit regression base learner $b_j \in \mathcal{B}_j$ to the vector of pseudo-residuals $\tilde{r}^{[m]}$:

$$\hat{\boldsymbol{\theta}}_j^{[m]} = \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}_j} \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - b_j(\mathbf{x}^{(i)}, \boldsymbol{\theta}))^2$$

end for

$$j^{[m]} = \arg\min_j \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_j(\mathbf{x}^{(i)}, \hat{\boldsymbol{\theta}}_j^{[m]}))^2$$

Iteration m, $j = 2$, $\sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_2(x_2^{(i)}, \hat{\boldsymbol{\theta}}_2^{[m]}))^2 = 43.2$:



COMPONENTWISE BOOSTING ALGORITHM

Algorithm Componentwise Gradient Boosting (inner loop).

for $j = 1 \rightarrow J$ **do**

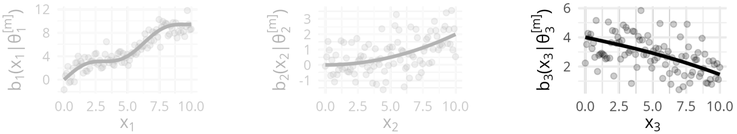
  Fit regression base learner $b_j \in \mathcal{B}_j$ to the vector of pseudo-residuals $\tilde{r}^{[m]}$:

  $\hat{\theta}_j^{[m]} = \arg\min_{\theta \in \Theta_j} \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - b_j(\mathbf{x}^{(i)}, \theta))^2$

end for

$j^{[m]} = \arg\min_j \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_j(\mathbf{x}^{(i)}, \hat{\theta}_j^{[m]}))^2$

Iteration m, $j = 3$, $\sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_3(x_3^{(i)}, \hat{\theta}_3^{[m]}))^2 = 35.2$:



COMPONENTWISE BOOSTING ALGORITHM

Algorithm Componentwise Gradient Boosting (inner loop).

for $j = 1 \to J$ **do**

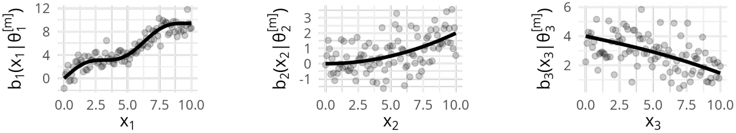
Fit regression base learner $b_j \in \mathcal{B}_j$ to the vector of pseudo-residuals $\tilde{r}^{[m]}$:

$$\hat{\theta}_j^{[m]} = \arg\min_{\theta \in \Theta_j} \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - b_j(\mathbf{x}^{(i)}, \theta))^2$$

end for

$$j^{[m]} = \arg\min_j \sum_{i=1}^{n} (\tilde{r}^{[m](i)} - \hat{b}_j(\mathbf{x}^{(i)}, \hat{\theta}_j^{[m]}))^2$$

Iteration m: $\Rightarrow j^{[m]} = 1$



FEATURE SELECTION IN CWB

In CWB, we often define BLs on a single feature

$$b_j(x_j, \theta) \quad \text{for } j = 1, 2, \ldots, p.$$

Allows natural form of feature selection:

- When we select the best BL in one iter of CWB, we thereby also only select one (associated) feature
- Note that a feature (or rather a BL associated with it) can be selected in multiple iters, so $\leq M$ features are selected