Lecture 6 – Tree-based methods, Bagging and Boosting

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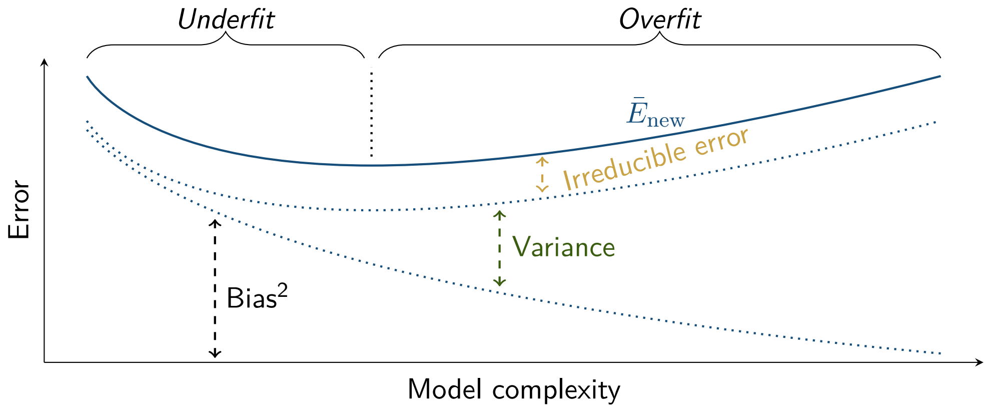
Summary of Lecture 5



Finding a balanced fit (neither over- nor underfit) is called the
the bias-variance tradeoff.

Contents – Lecture 6

1. Classification and regression trees (CART)
2. Bagging – *a general variance reduction technique*
3. Random forests
4. Boosting

The idea behind tree-based methods

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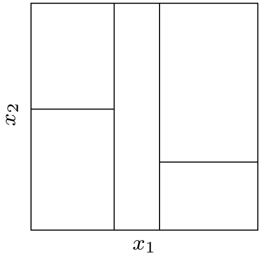
One **flexible** way of designing this function is to partition the input space into disjoint regions and fit a simple model in each region.



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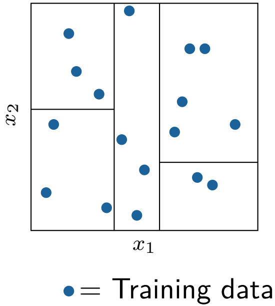

- **Classification:** Majority vote within the region.
- **Regression:** Mean of training data within the region.

Finding the partition

The key challenge in using this strategy is to find a good partition.

Even if we restrict our attention to seemingly simple regions (e.g. “boxes”), finding an ***optimal*** partition w.r.t. minimizing the training error is ***computationally infeasible!***

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Instead, we use a "greedy" approach: **recursive binary splitting**.

1. Select one input variable x_j and a cut-point s. Partition the input space into two half-spaces,

$$\{\mathbf{x} : x_j < s\} \qquad \{\mathbf{x} : x_j \geq s\}.$$

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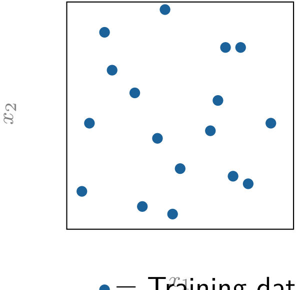
$$\{\mathbf{x} : x_j < s\} \qquad \{\mathbf{x} : x_j \geq s\}.$$

2. Repeat this splitting for each region until some stopping criterion is met (e.g., no region contains more than 5 training data points).

Recursive binary splitting

Partitioning of input space



● = Training data

Tree representation

Recursive binary splitting

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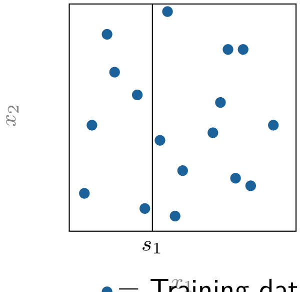

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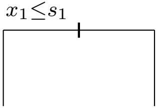

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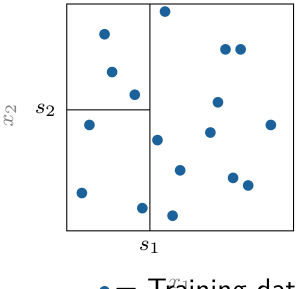

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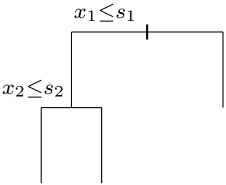

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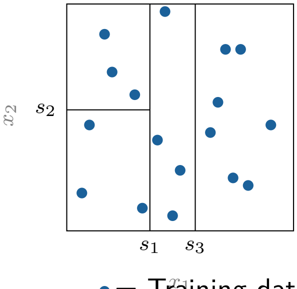

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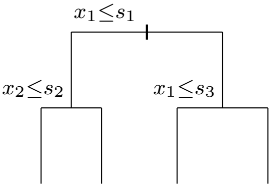

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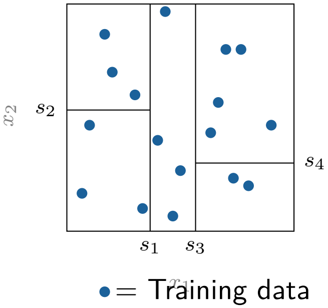

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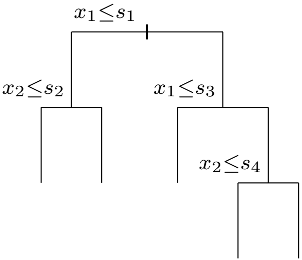

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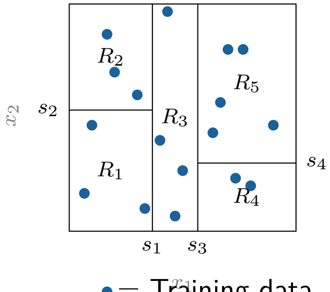

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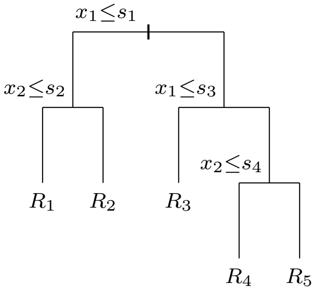

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Regression trees (I/II)

Once the input space is partitioned into L regions, $R_1, R_2, \dots, R_L$ the prediction model is

$$\widehat{y}_\star = \sum_{\ell=1}^{L} \widehat{y}_\ell \mathbb{I}\{\mathbf{x}_\star \in R_\ell\},$$

where $\mathbb{I}\{\mathbf{x}_\star \in R_\ell\}$ is the indicator function

$$\mathbb{I}\{\mathbf{x}_\star \in R_\ell\} = \begin{cases} 1 & \text{if } \mathbf{x}_\star \in R_\ell \\ 0 & \text{if } \mathbf{x}_\star \notin R_\ell \end{cases}$$

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For regression trees we use

$$\widehat{y}_\ell = \text{avarage}\{y_i : \mathbf{x}_i \in R_\ell\}$$

Regression trees (II/II) - How do we find the partition?

Recursive binary splitting is **greedy** - each split is made in order to minimize the loss **without looking ahead** at future splits.

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We then seek (j,s) that minimize

$$\sum_{i:\mathbf{x}_i \in R_1(j,s)} (y_i - \widehat{y}_1(j,s))^2 + \sum_{i:\mathbf{x}_i \in R_2(j,s)} (y_i - \widehat{y}_2(j,s))^2$$

where

$$\widehat{y}_1 = \text{avarage}\{y_i : \mathbf{x}_i \in R_1(j,s)\}$$
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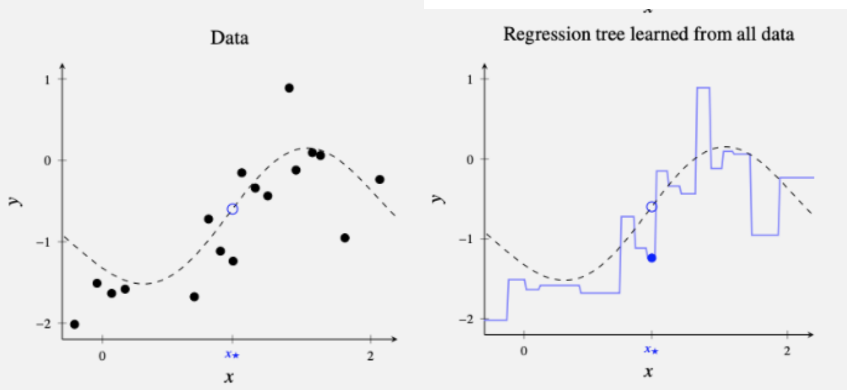
This optimization problem is easily solved by "brute force" by evaluating all possible splits.

Example: Regression trees



Classification trees

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$$\widehat{\pi}_{\ell m} = \frac{1}{n_\ell} \sum_{i:\mathbf{x}_i \in R_\ell} \mathbb{I}\{y_i = m\}$$

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be the proportion of training data points in the lth region that belong to the mth class. Then we approximate

$$p(y = m \,|\, \mathbf{x}_\star) \approx \sum_{\ell=1}^{L} \widehat{\pi}_{\ell m} \mathbb{I}\{\mathbf{x}_\star \in R_\ell\}$$

Classification trees

Secondly, the squared loss used to construct the tree needs to be replaced by a measure suitable to categorical outputs.

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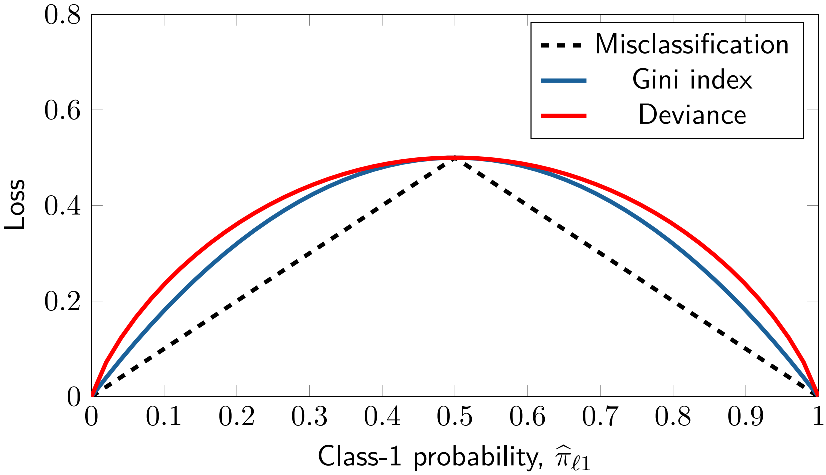
Three common error measures are,

$$
\begin{aligned}
\text{Misclassification error:} \quad & 1 - \max_m \widehat{\pi}_{\ell m} \\
\text{Entropy/deviance:} \quad & -\textstyle\sum_{m=1}^{M} \widehat{\pi}_{\ell m} \log \widehat{\pi}_{\ell m} \\
\text{Gini index:} \quad & \textstyle\sum_{m=1}^{M} \widehat{\pi}_{\ell m}(1 - \widehat{\pi}_{\ell m})
\end{aligned}
$$

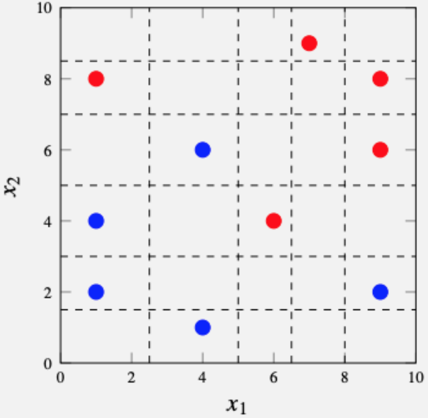
Classification error measures

For a binary classification problem ($M = 2$)



Example using entropy

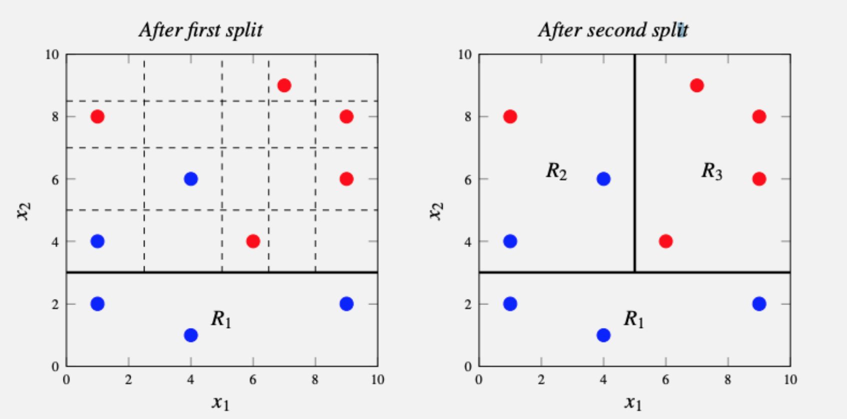
x_1	x_2	y
9.0	2.0	Blue
1.0	4.0	Blue
4.0	6.0	Blue
4.0	1.0	Blue
1.0	2.0	Blue
1.0	8.0	Red
6.0	4.0	Red
7.0	9.0	Red
9.0	8.0	Red
9.0	6.0	Red



Example using entropy

Split (R_1)	n_1	$\widehat{\pi}_{1B}$	$\widehat{\pi}_{1R}$	Q_1	n_2	$\widehat{\pi}_{2B}$	$\widehat{\pi}_{2R}$	Q_2	$n_1Q_1 + n_2Q_2$
$x_1 < 2.5$	3	2/3	1/3	0.64	7	3/7	4/7	0.68	6.69
$x_1 < 5.0$	5	4/5	1/5	0.50	5	1/5	4/5	0.50	5.00
$x_1 < 6.5$	6	4/6	2/6	0.64	4	1/4	3/4	0.56	6.07
$x_1 < 8.0$	7	4/7	3/7	0.68	3	1/3	2/3	0.64	6.69
$x_2 < 1.5$	1	1/1	0/1	0.00	9	4/9	5/9	0.69	6.18
$x_2 < 3.0$	3	3/3	0/3	0.00	7	2/7	5/7	0.60	**4.18**
$x_2 < 5.0$	5	4/5	1/5	0.50	5	1/5	4/5	0.06	5.00
$x_2 < 7.0$	7	5/7	2/7	0.60	3	0/3	3/3	0.00	**4.18**
$x_2 < 8.5$	9	5/9	4/9	0.69	1	0/1	1/1	0.00	6.18

Example using entropy



Improving CART

The flexibility/complexity of classification and regression trees (CART) is decided by the tree depth.

- ! To obtain a **small bias** the tree need to be grown deep,
- ! but this results in a **high variance!**

The performance of (simple) CARTs is often unsatisfactory!

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To improve the practical performance:

- Bagging and Random Forests
- Boosted trees

Bagging (I/II)

For now, assume that we have access to B **independent** datasets $\mathcal{T}^1, \dots, \mathcal{T}^B$. We can then train a separate deep tree $\widehat{y}^b(\mathbf{x})$ for each dataset, $1, \dots, B$.

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- Each $\widehat{y}^b(\mathbf{x})$ has a **low bias** but **high variance**
- By averaging

$$\widehat{y}_{\text{bag}}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^{B} \widehat{y}^b(\mathbf{x})$$

the bias is kept small, but variance is reduced by a factor B!

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Bagging (II/II)

Obvious problem We only have access to one training dataset.

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For each bootstrapped dataset $\widetilde{\mathcal{T}}^b$ we train a tree $\widetilde{y}^b(\mathbf{x})$. Averaging these,

$$\widetilde{y}^b_{\text{bag}}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^{B} \widetilde{y}^b(\mathbf{x})$$

is called "bootstrap aggregation", or bagging.

Bagging - Toy example

ex) Assume that we have a training set

$$\mathcal{T} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), (\mathbf{x}_3, y_3), (\mathbf{x}_4, y_4)\}.$$

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We generate, say, $B = 3$ datasets by bootstrapping:

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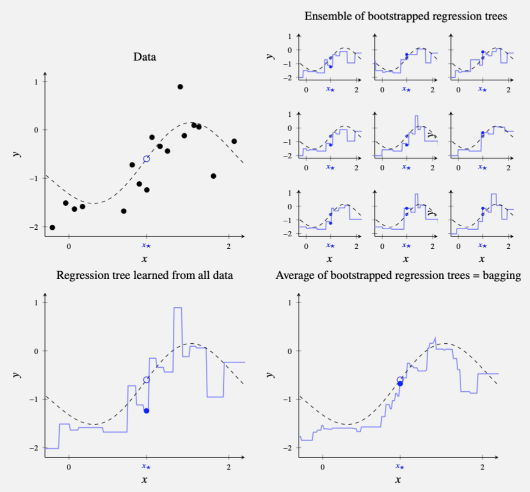
Compute $B = 3$ (deep) regression trees $\tilde{y}^1(\mathbf{x})$, $\tilde{y}^2(\mathbf{x})$ and $\tilde{y}^3(\mathbf{x})$, one for each dataset $\widetilde{\mathcal{T}}^1$, $\widetilde{\mathcal{T}}^2$, and $\widetilde{\mathcal{T}}^3$, and average

$$\tilde{y}_{\text{bag}}(\mathbf{x}) = \frac{1}{3}\sum_{b=1}^{3} \tilde{y}^b(\mathbf{x})$$

Example: Regression trees



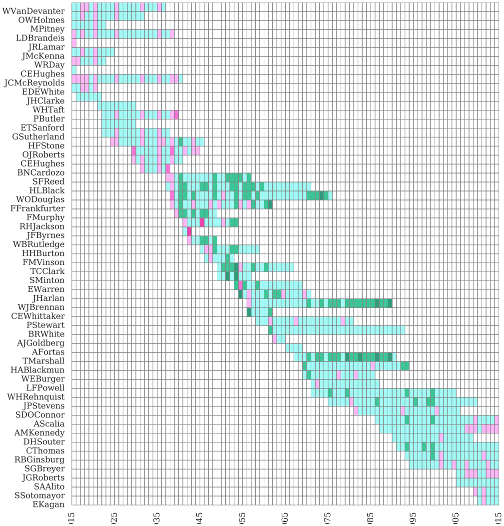
Application) Predicting US Supreme Court behavior

Random forest classifier built on SCDB data[1] to predict the votes of Supreme Court justices:

$$Y \in \{\texttt{affirm}, \texttt{reverse}, \texttt{other}\}$$

Result: 70% correct classifications

D. M. Katz, M. J. Bommarito II and J. Blackman. **A General Approach for Predicting the Behavior of the Supreme Court of the United States**. *arXiv.org*, arXiv:1612.03473v2, January 2017.



[1] `http://supremecourtdatabase.org`

Application) Predicting US Supreme Court behavior

Not only have random forests proven to be "unreasonably effective" in a wide array of supervised learning contexts, but in our testing, random forests outperformed other common approaches including support vector machines [. . .] and feedforward artificial neural network models such as multi-layer perceptron

— Katz, Bommarito II and Blackman (arXiv:1612.03473v2)

Random forests

Bagging can drastically improve the performance of CART!

However, the B bootstrapped dataset are ***correlated***
$\Rightarrow$ the variance reduction due to averaging is diminished.

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A **random forest** is constructed by bagging, but for each split in each tree only a ***random subset*** of $q \leq p$ inputs are considered as splitting variables.

Rule of thumb: $q = \sqrt{p}$ for classification trees and $q = p/3$ for regression trees.[2]

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Random forest pseudo-code

Algorithm Random forest for regression

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      i. Select q out of the p input variables uniformly at random.

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      iii. Split the node into two children with $\{x_j \leq s\}$ and $\{x_j > s\}$.
2. Final model is the average the B ensemble members,

$$\widehat{y}_\star^{\text{rf}} = \frac{1}{B} \sum_{b=1}^{B} \widetilde{y}_\star^b.$$

Random forests

The random input selection used in random forests:

- ▼ increases the bias, but often very slowly
- ▼ adds to the variance (σ^2) of each tree
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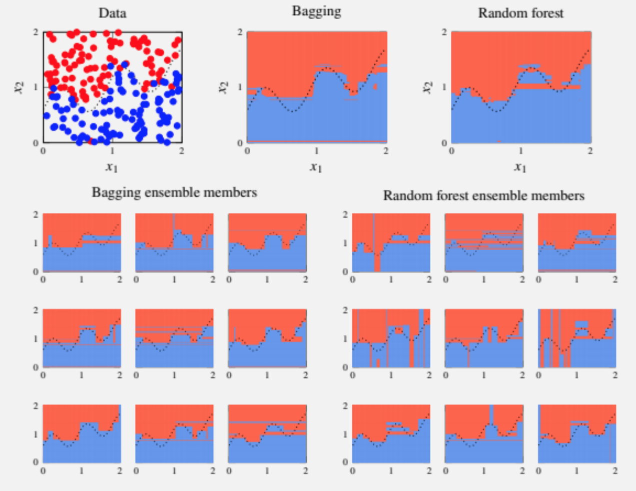
The reduction in correlation is typically the dominant effect $\Rightarrow$ there is an overall reduction in MSE!

ex)Random forest on regression data



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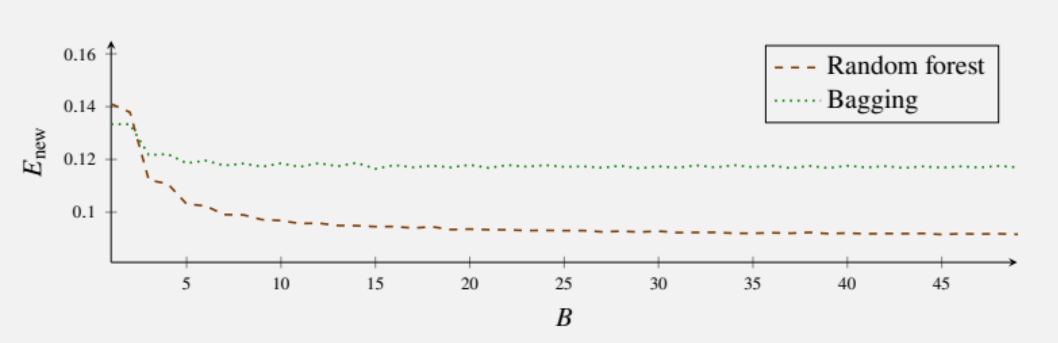

Advantages of random forests

Random forests have several **computational advantages**:

- Easy to do in parallel!
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. . . and they also come with some other benefits:

- Often works well off-the-shelf – few tuning parameters
- Requires little or no input preparation
- Implicit input selection

ex) Automatic music generation

ALYSIA: automated music generation using random forests.

- User specifies the lyrics
- ALYSIA generates accompanying music via
  - *rythm model*
  - *melody model*
- Trained on a corpus of pop songs.

https://www.youtube.com/watch?v=whgudcj82_I
https://www.withalysia.com/

M. Ackerman and D. Loker. **Algorithmic Songwriting with ALYSIA**. *In: Correia J., Ciesielski V., Liapis A. (eds) Computational Intelligence in Music, Sound, Art and Design. EvoMUSART*, 2017.

Boosting

Even a simple (classification or regression) model can typically capture some aspects of the input-output relationship.

Can we then learn an ***ensemble*** of "weak models", each describing some part of this relationship, and combine these into one "strong model"?

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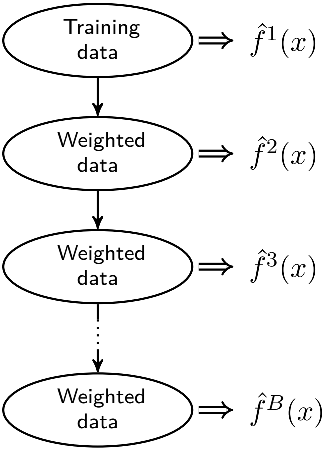
- One of the most successful machine learning ideas!

Boosting


Training data
$\Longrightarrow \hat{f}^1(x)$
Weighted data
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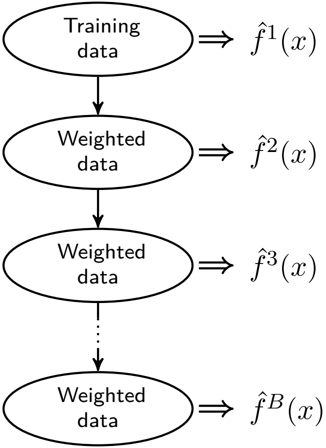
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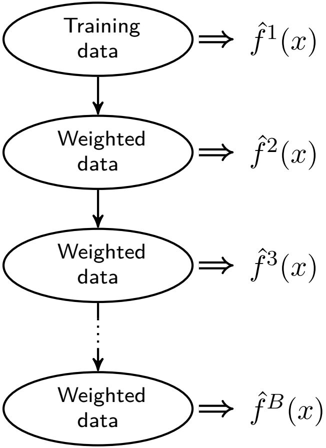

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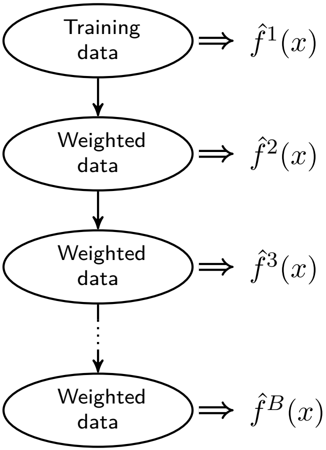
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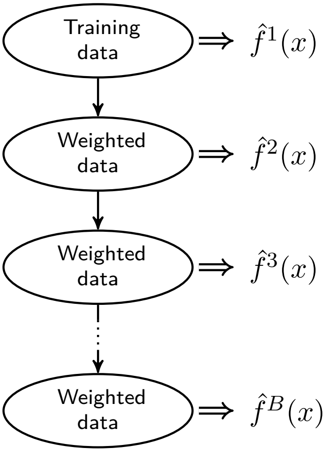
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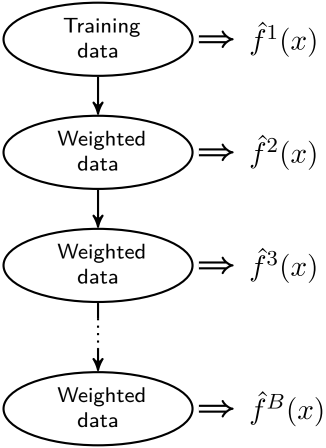
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Binary classification

We will restrict our attention to binary classification.

- Class labels are -1 and 1, i.e. $y \in \{-1, 1\}$.
- We have access to some (weak) base classifier, e.g. a classification tree.

Note. Using labels -1 and 1 is mathematically convenient as it allows us to express a majority vote between B classifiers $\widehat{G}^1(\mathbf{x}), \ldots, \widehat{G}^B(\mathbf{x})$ as

$$\text{sign}\left(\sum_{b=1}^{B} \widehat{G}^b(\mathbf{x})\right) = \begin{cases} +1 & \text{if more plus-votes than minus-votes,} \\ -1 & \text{if more minus-votes than plus-votes.} \end{cases}$$

Boosting procedure (for classification)

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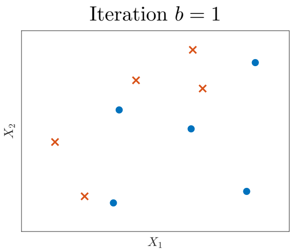
The predictions of the B classifiers, $\widehat{G}^{(1)}(\mathbf{x}), \ldots, \widehat{G}^{(B)}(\mathbf{x})$, are combined using a **weighted** majority vote:

$$\widehat{G}^B_{\text{boost}}(\mathbf{x}) = \text{sign}\left(\sum_{b=1}^{B} \alpha^{(b)} \widehat{G}^{(b)}(\mathbf{x})\right).$$

ex) Boosting illustration



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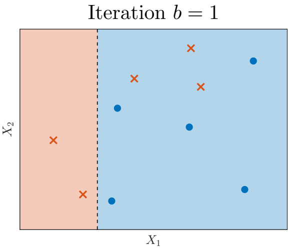

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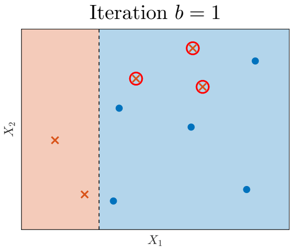

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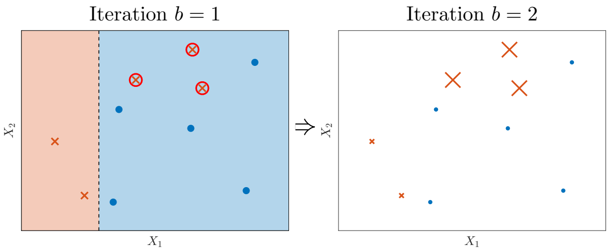

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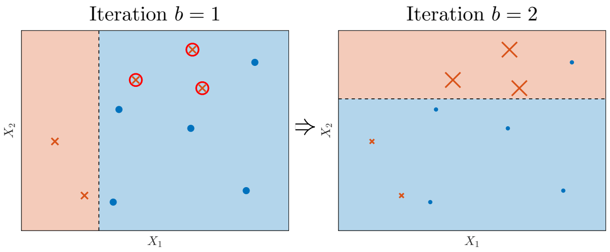

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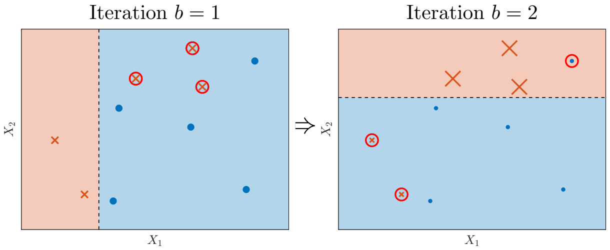

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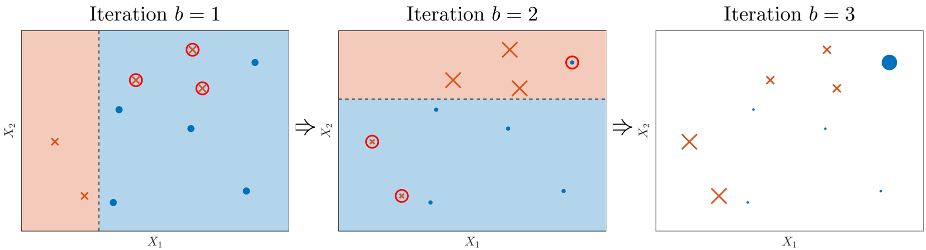

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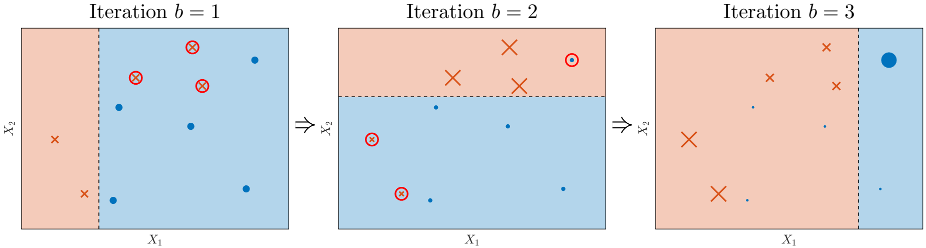

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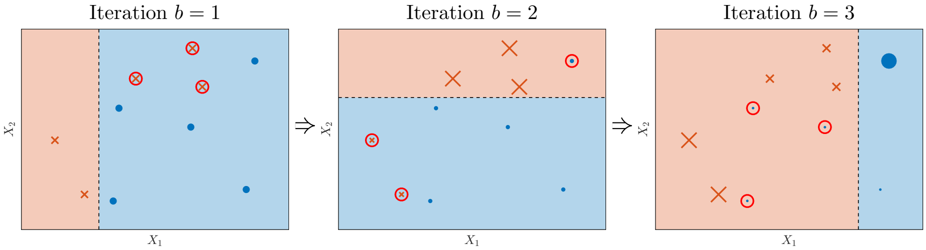

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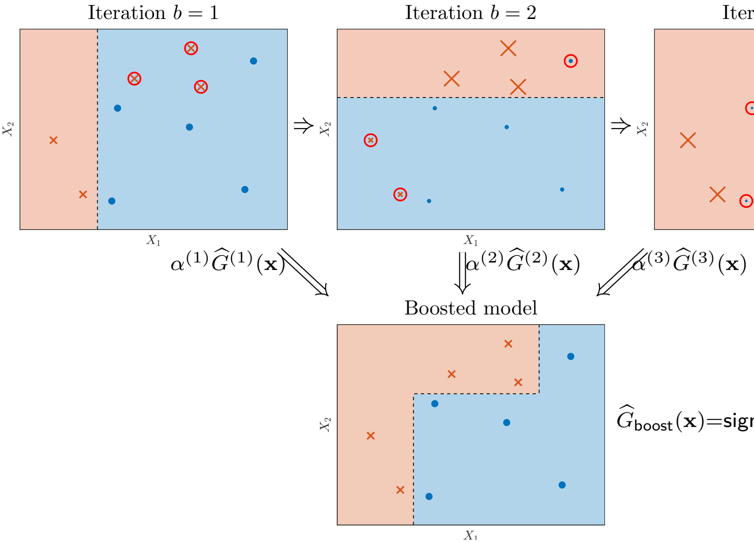


$$\widehat{G}_{\text{boost}}(\mathbf{x}) = \text{sign}\left(\sum_{b=1}^{3} \alpha^{(b)}\widehat{G}^{(b)}(\mathbf{x})\right)$$

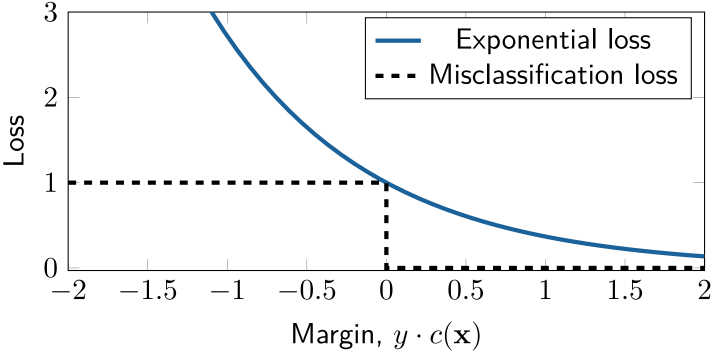
The technical details. . .

Q1: How do we reweight the data?

Q2: How are the coefficients $\alpha^{(1)}, \dots, \alpha^{(B)}$ computed?

Exponential loss

Loss functions for binary classifier $\widehat{G}(\mathbf{x}) = \text{sign}(c(\mathbf{x}))$.



Exponential loss function $L(y, c(\mathbf{x})) = \exp(-y \cdot c(\mathbf{x}))$ plotted vs. **margin** $y \cdot c(\mathbf{x})$. The misclassification loss $\mathbb{I}\{y \neq \widehat{G}(\mathbf{x})\} = \mathbb{I}\{y \cdot c(\mathbf{x}) < 0\}$ is plotted as comparison.

AdaBoost pseudo-code

1. Assign weights $w_i^1 = 1/n$ to all data points.
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      iii. Compute new weights

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      iv. *Normalize.* Set $w_i^{b+1} \leftarrow w_i^{b+1} / \sum_{j=1}^n w_j^{b+1}$, for $i = 1, \ldots, n$.

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Y. Freund and R. E. Schapire. **Experiments with a New Boosting Algorithm**. *Proceedings of the 13th International Conference on Machine Learning (ICML)*. Bari, Italy, 1996.

2003 Gödel Prize

Boosting vs. bagging

Bagging	**Boosting**
Learns base models in parallel	Learns base models sequentially
Uses bootstrapped datasets	Uses reweighted datasets
Does not overfit as B becomes large	Can overfit as B becomes large
Reduces variance but not bias (requires deep trees as base models)	Also reduces bias! (works well with shallow trees)

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Reduces variance but not bias (requires deep trees as base models)	Also reduces bias! (works well with shallow trees)

N.B. Boosting does ***not*** require each base model to have low bias. Thus, a shallow classification tree (say, 4-8 terminal nodes) or even a tree with a single split (2 terminal nodes, a “stump”) is often sufficient.

A few concepts to summarize lecture 6

CART: Classification and regression trees. A class of nonparametric methods based on partitioning the input space into regions and fitting a simple model for each region.

Recursive binary splitting: A greedy method for partitioning the input space into “boxes” aligned with the coordinate axes.

Gini index and deviance: Commonly used error measures for constructing classification trees.

Ensemble methods: Umbrella term for methods that average or combine multiple models.

Bagging: Bootstrap aggregating. An ensemble method based on the statistical bootstrap.

Random forests: Bagging of trees, combined with random feature selection for further variance reduction (and computational gains).