Machine Learning

Ensemble methods

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2nd semester a.y. 2024/2025 · May 12, 2025

Main idea: Combine many weak learners into a stronger ensemble model.

Objective: To improve performance and robustness.

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Reduce the high bias by aggregation!

Random forest: Intuition

Figures by Richard Kershner

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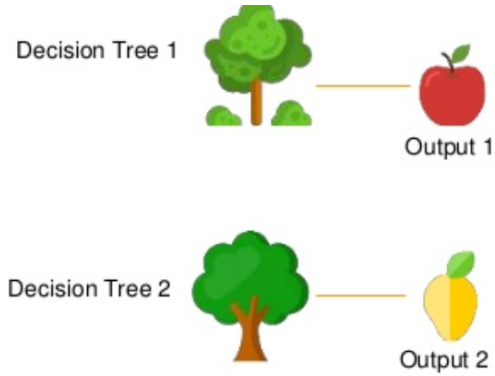

Construct multiple decision trees.

Each decision tree outputs a prediction for a given input.

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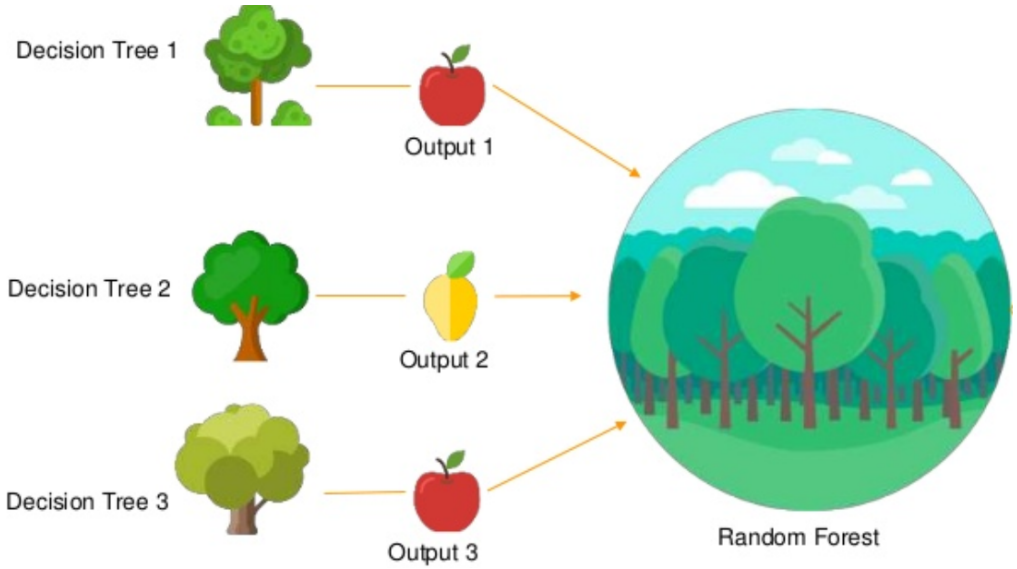

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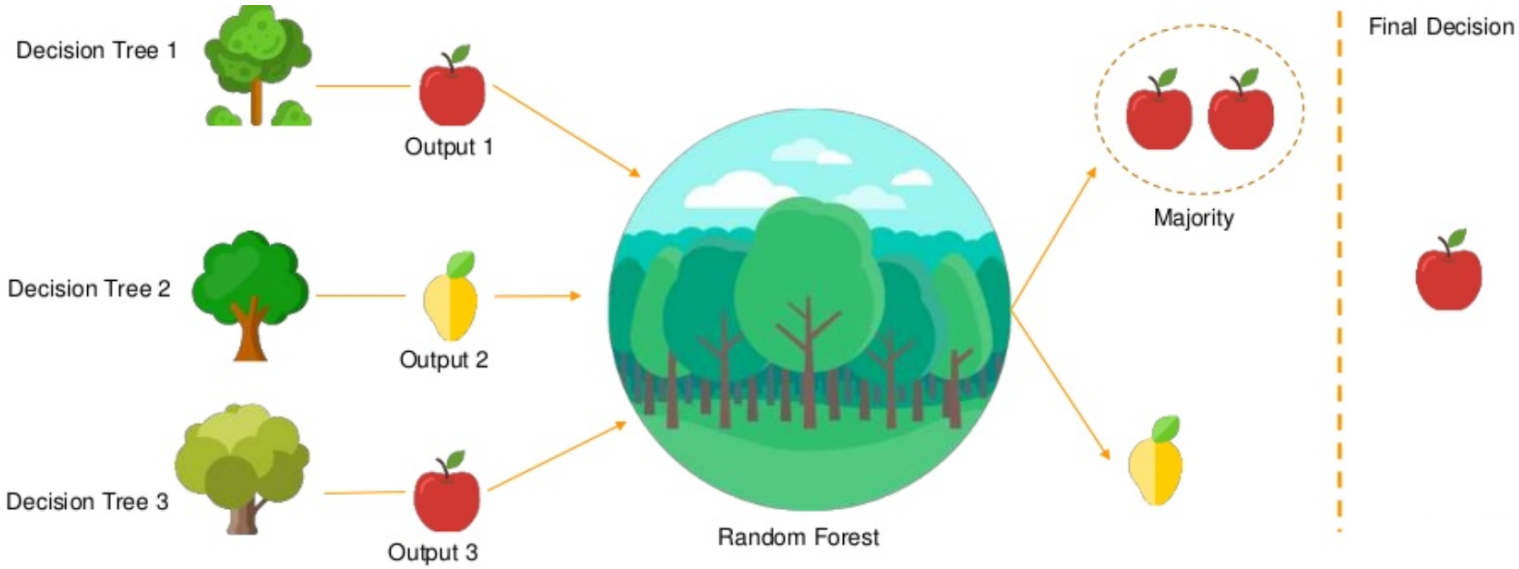


Construct multiple decision trees.

Each decision tree outputs a prediction for a given input.

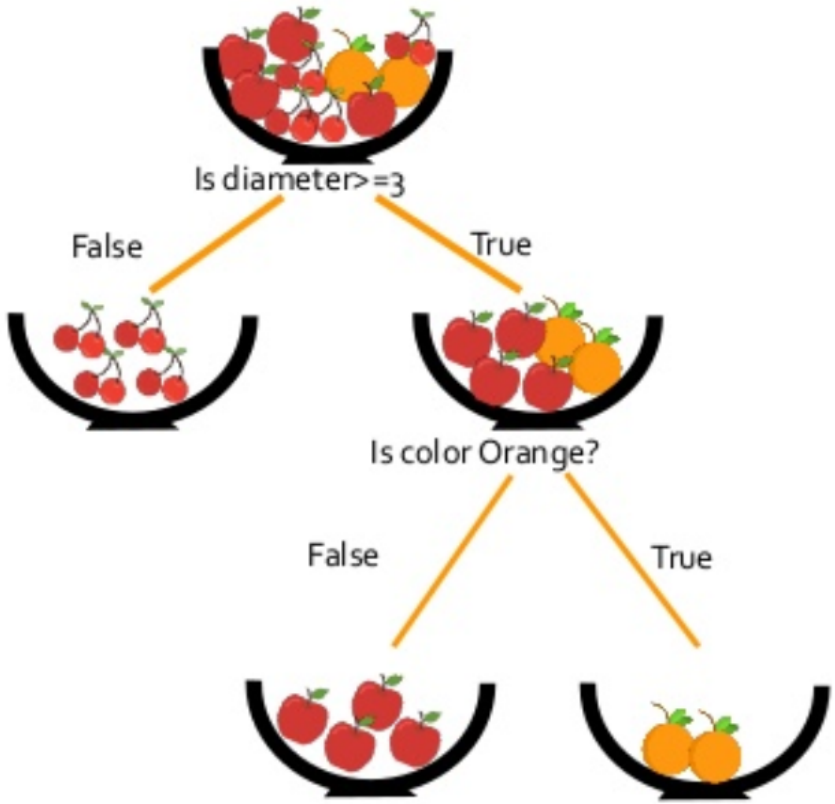
The predictions from each tree are combined into one final prediction.

In the example, the final decision is "apple with probability 66%".

Figures by Richard Kershner

Decision tree

A decision tree is a binary tree in which each branch represents a possible decision. A path through the tree is therefore a course of action.

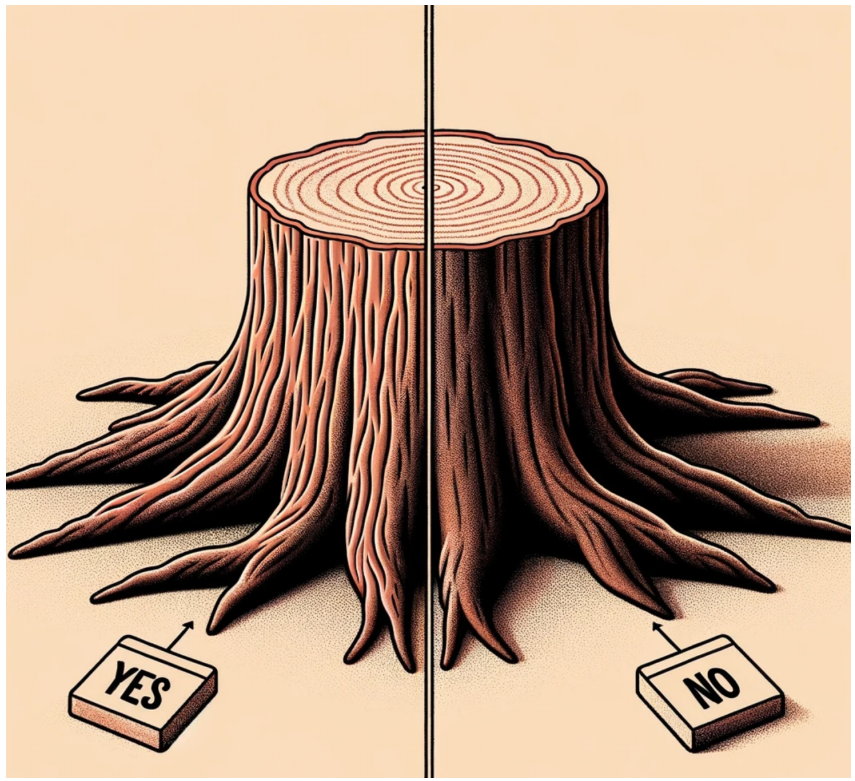


The data is iteratively partitioned into subsets from the root to the leaves.

Decision stump

An even weaker model is a decision stump.

A one-level decision tree, splitting data based on a single feature.



Information gain

Intermediate nodes are decision nodes.

Leaf nodes store the final decision (i.e. the classification result).

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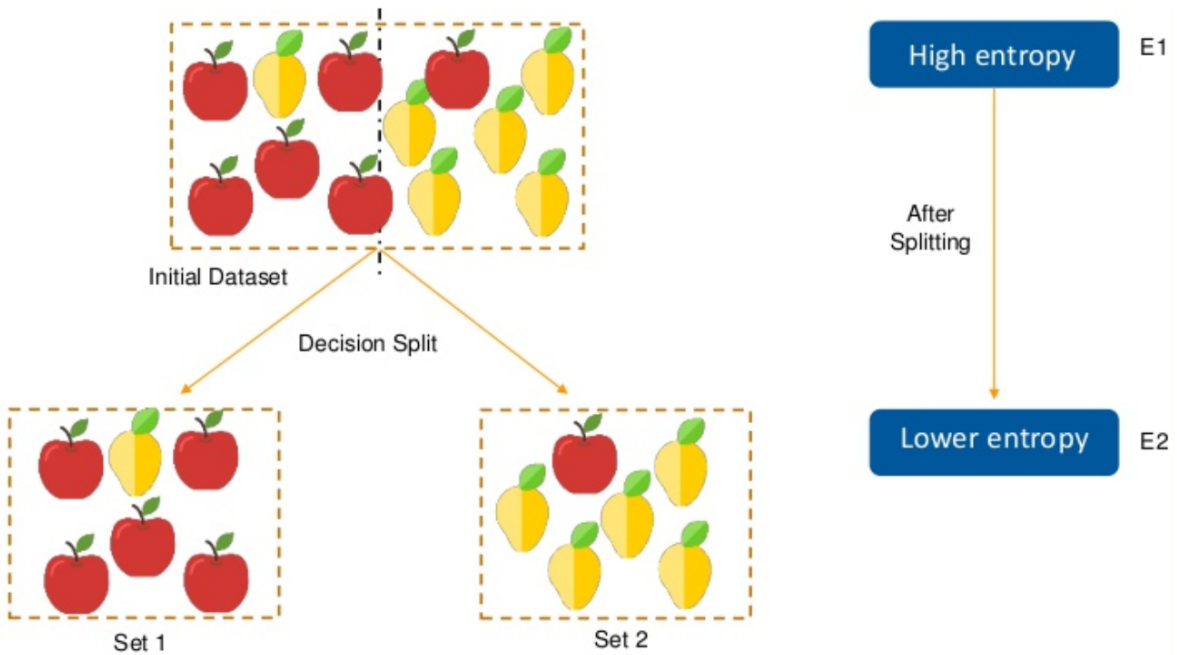

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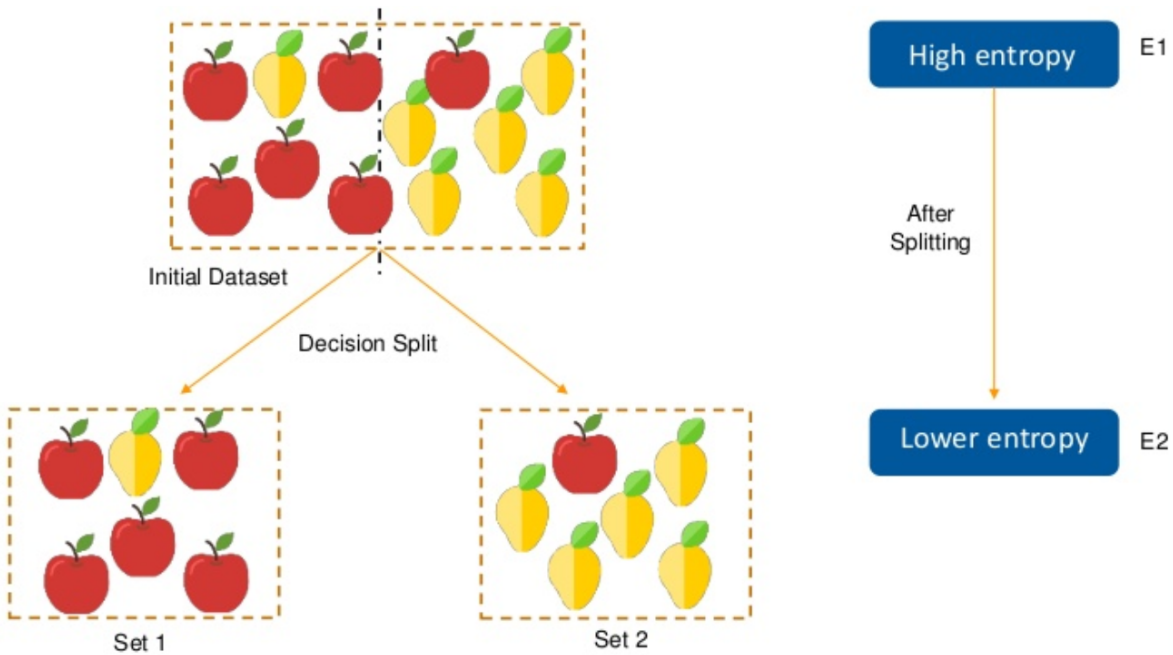

The split should be as discriminative as possible: maximize the information gain $E2 - E1$.

Training

Problem: Classify the types of fruit based on their features.

We start from a set of data points that have high entropy.

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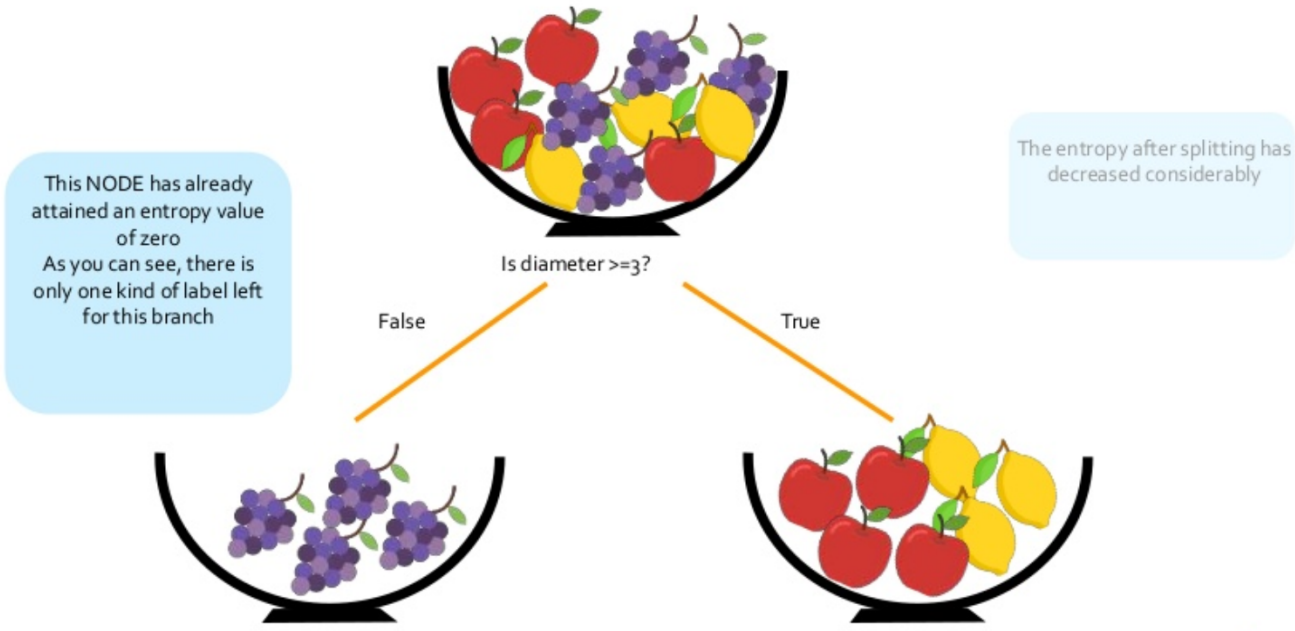
Keep splitting until the dataset is empty or accuracy is high enough.

Accuracy



A leaf is where no more splitting is required or possible (zero entropy).

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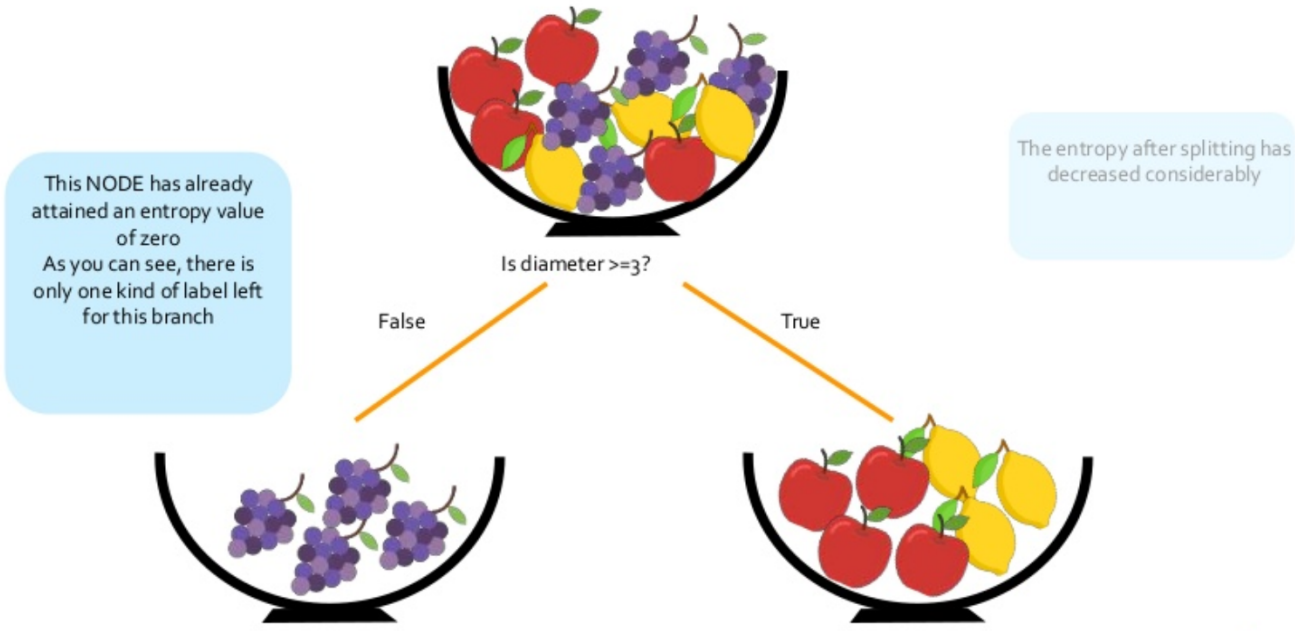

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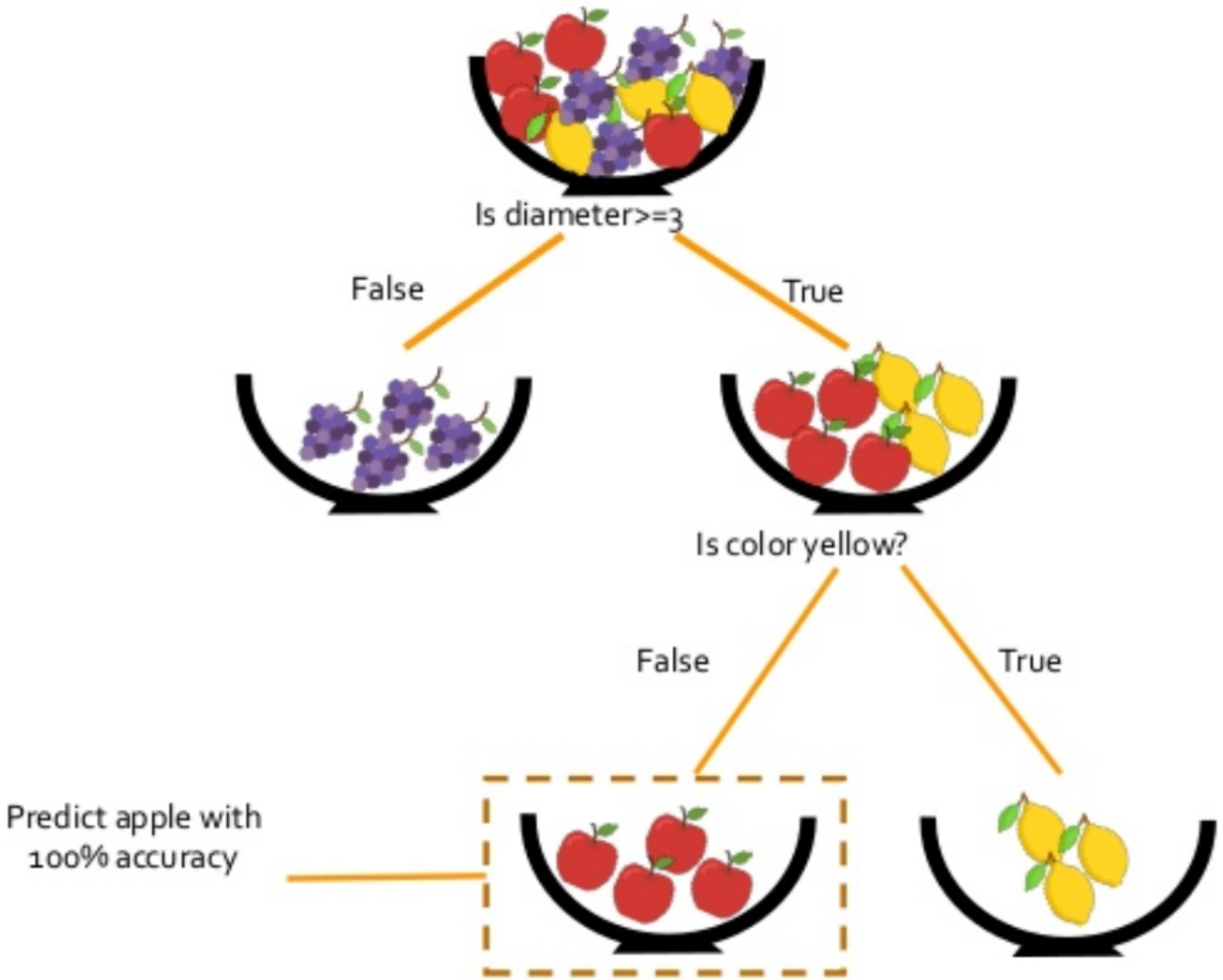
At each leaf, accuracy with respect to label ℓ is measured as:

$$\frac{\#\text{ data points with label } \ell}{\#\text{ data points}}$$

Accuracy


Is diameter>=3
False
True
Is color yellow?
False
True
Predict apple with
100% accuracy

Feature interaction

Each tree splits features to make predictions.

Thus, deeper nodes represent interactions between features.

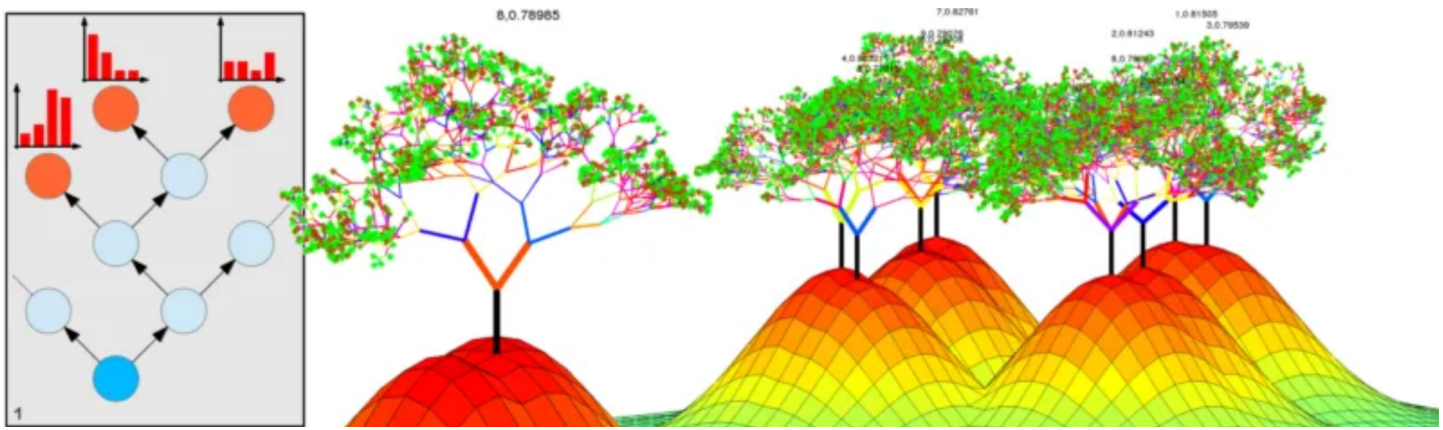


Figure: Sonali Dasgupta

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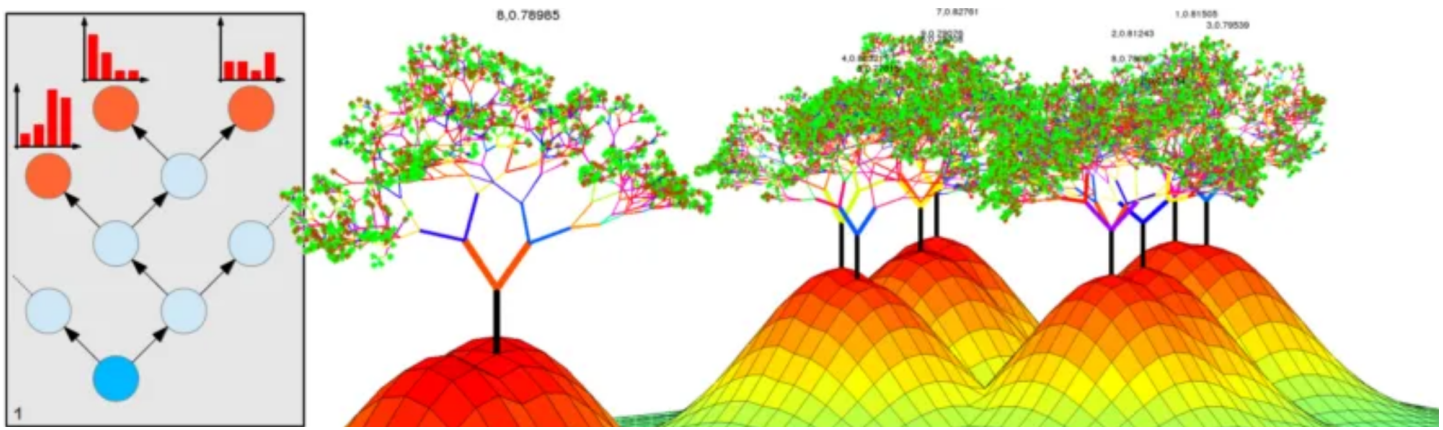

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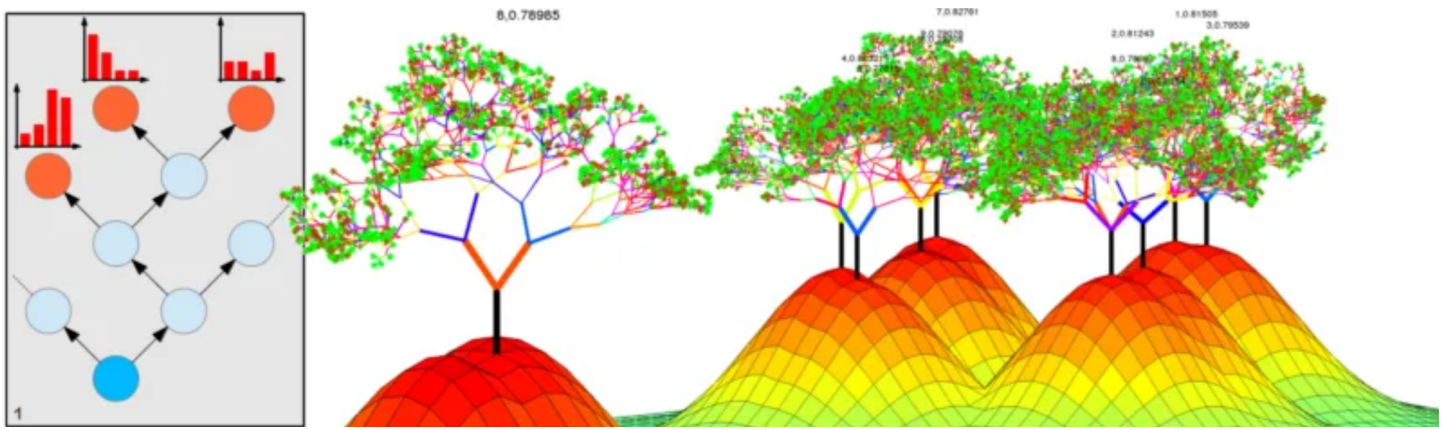

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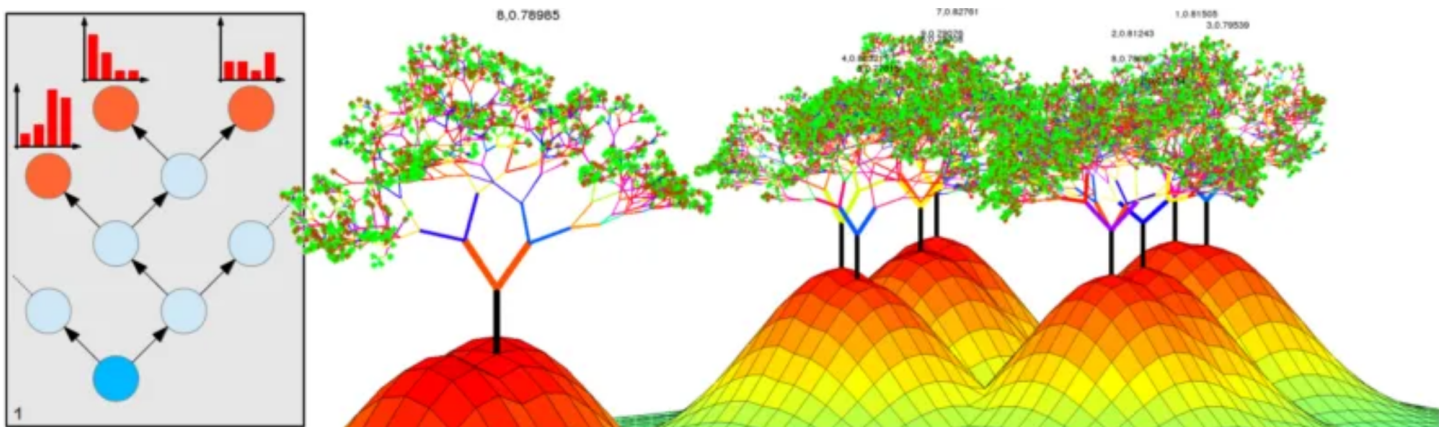

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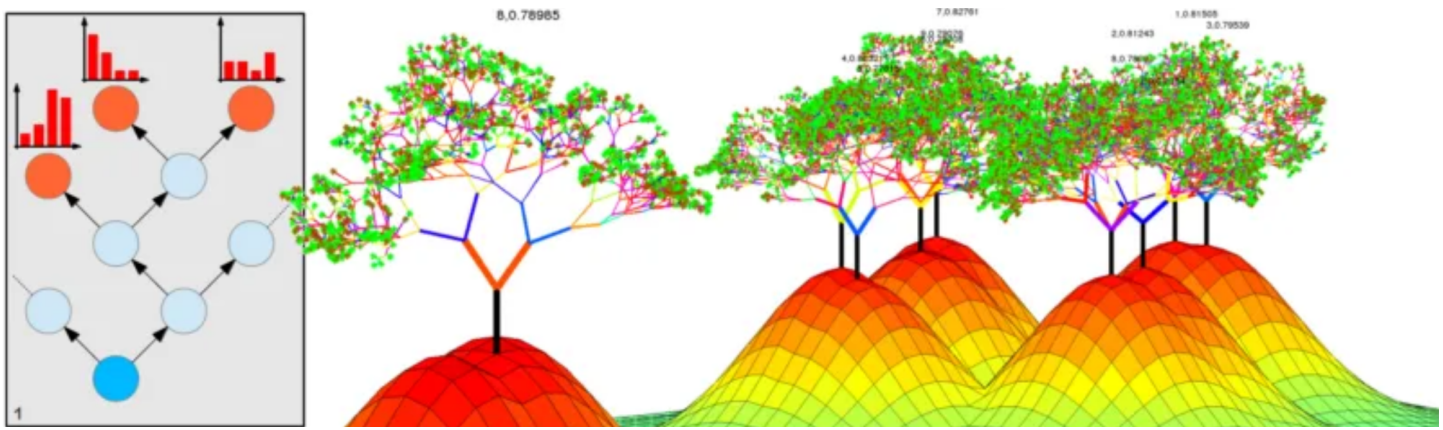
- Deep trees capture complex interactions but risk overfitting.



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Regression forests

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- Each tree outputs a probability distribution over all the classes.
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For regression problems:

- Each tree outputs a continuous value.
- Internal splits minimize the MSE.
- Leaf nodes contain the average value.

Regression forests: Example

- **Training data:** mobile phones
- **Features:** screen brightness, battery level, number of apps
- **Target value** to predict: temperature

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- Keep the split that results in the lowest weighted average MSE.

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4. Average the tree predictions to get the forest prediction.

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Bagging vs. Boosting

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- **Bagging:** Reduces variance by training on different subsets of data.

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- **Boosting:** Reduces bias by focusing on errors of previous models.

  Example: AdaBoost, XGBoost, LightGBM.

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Boosting

Main idea: Sequentially train weak learners, focusing each time on the incorrectly predicted data; then, combine these models.

- AdaBoost: At each iteration, re-weight the training data to focus on the difficult samples.
- Gradient Boosting: At each iteration, focus on the residual errors of the previous model.

AdaBoost

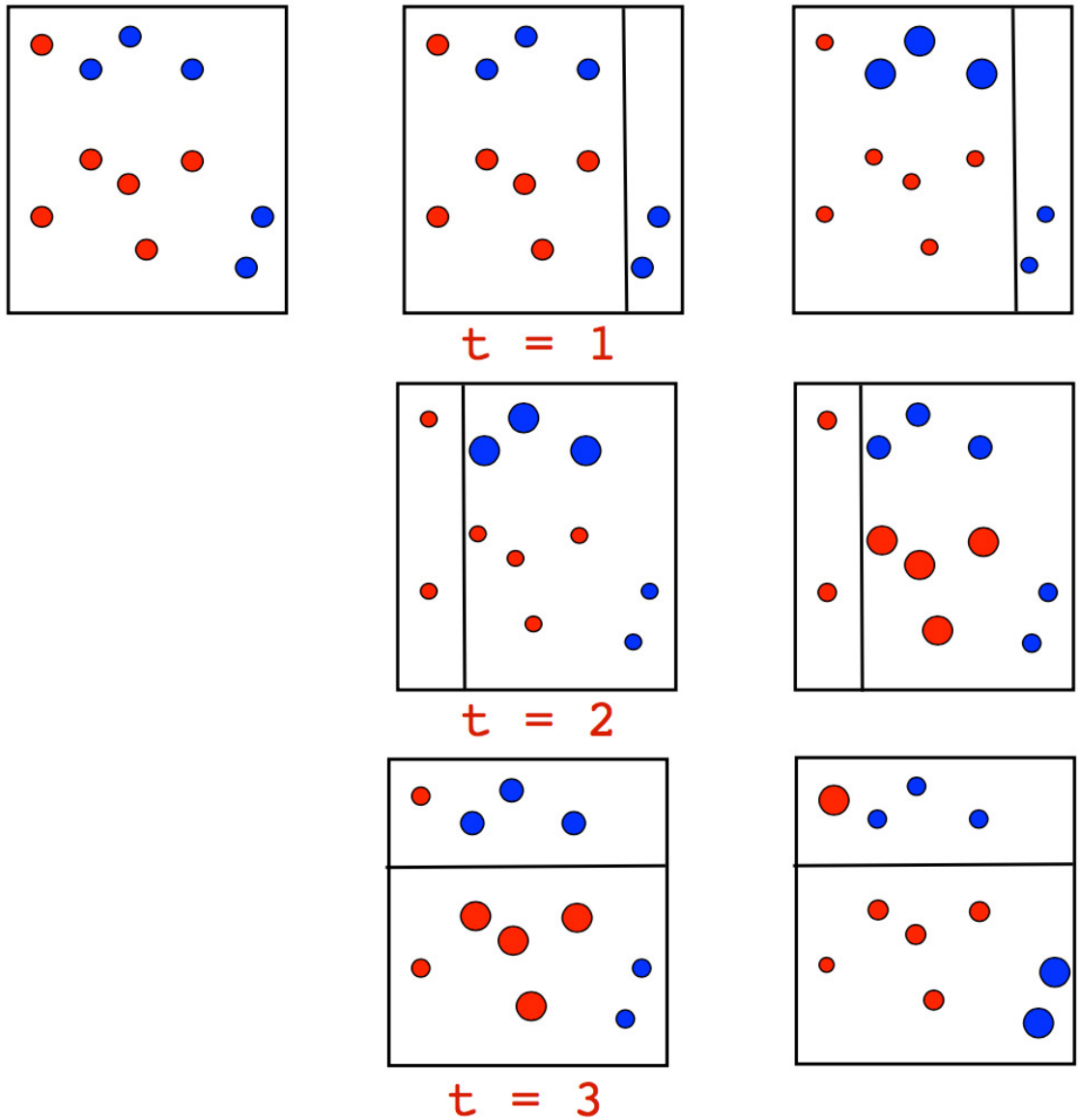
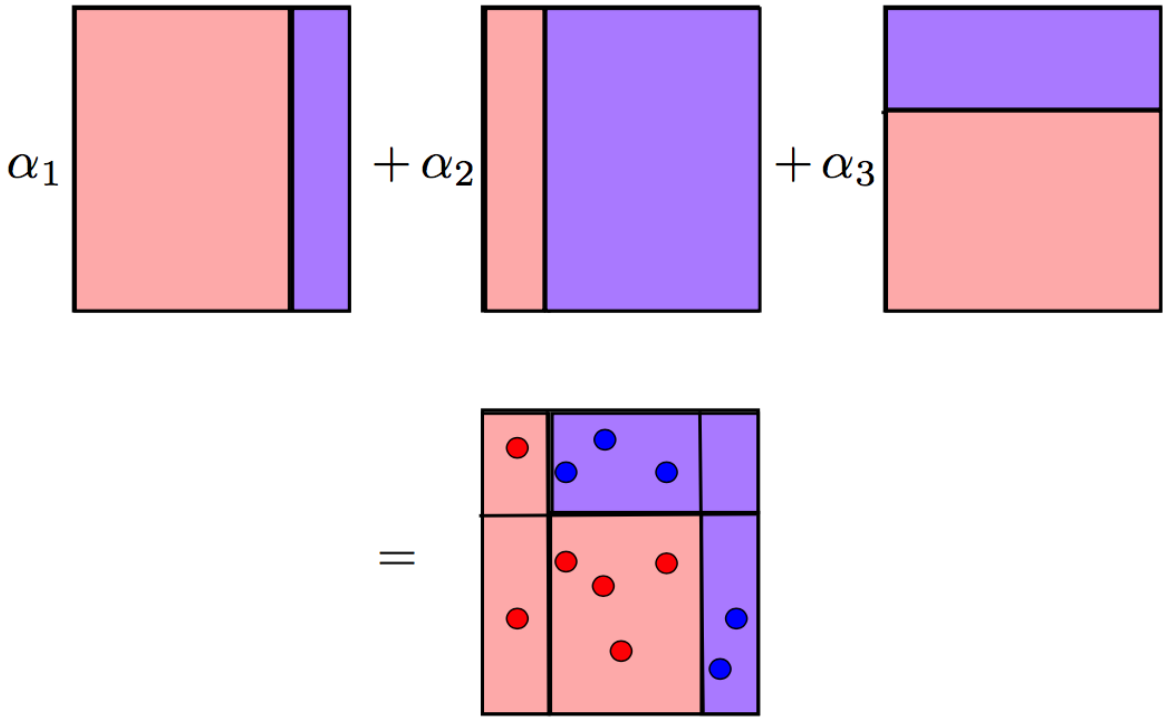


Figure: Yury Kashnitsky

AdaBoost



The α_i are proportional to the accuracy of each weak learner.

AdaBoost tends to overfit.

Figure: Yury Kashnitsky

AdaBoost

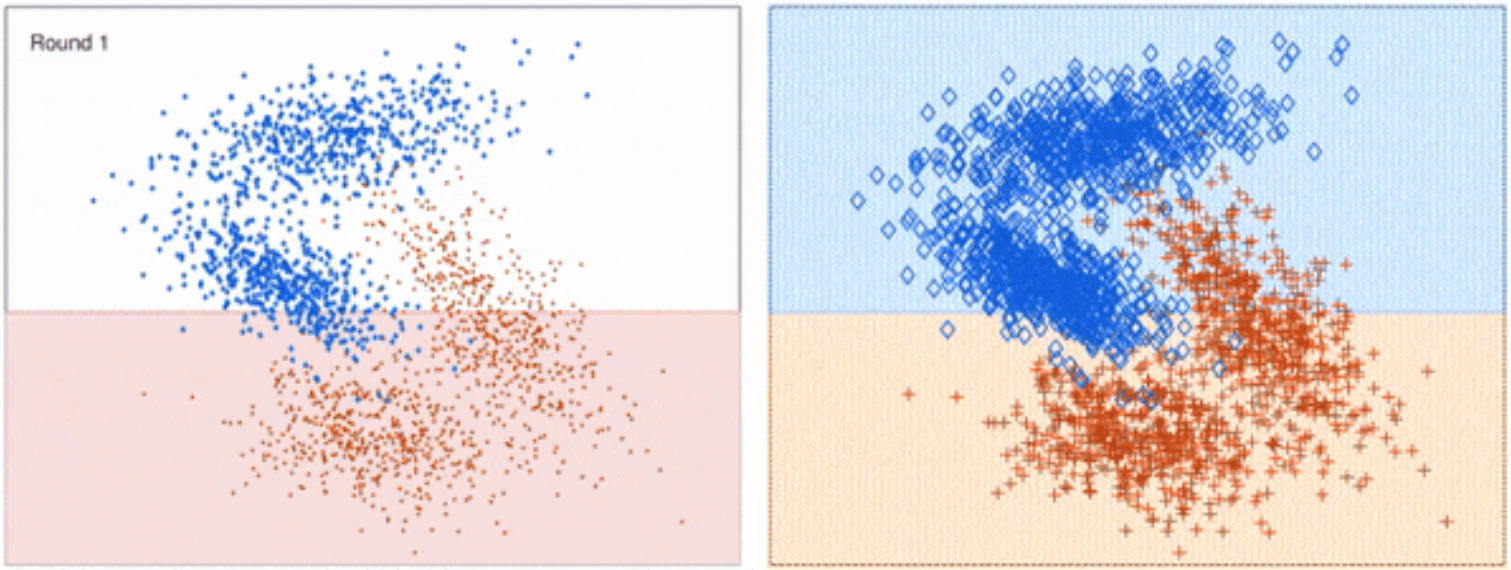


Figure: Kai O. Arras

Example: Toxic content

Gradient boosting

Let's illustrate this with least-squares regression for $F : X \to \mathbb{R}$:

$$L(y, F(x)) = \sum_i (F(x_i) - y_i)^2$$

Now iterate for $m = 0, \ldots$:

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The final solution is the combination $F_0(x) + \sum_m h_m(x)$.

Gradient boosting

Why is it called "gradient" boosting?

Given the MSE loss:

$$L(y, F(x)) = \sum_i (F(x_i) - y_i)^2$$

Its (negative) derivative w.r.t. the predictions $F(x)$ is:

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For this reason, the derivatives $-\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}$ are also called pseudo-residuals r_i.

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Since $h_{m+1} \propto -\frac{\partial L}{\partial F}$, this really looks like standard gradient descent!

$$F_{m+1}(x) = F_m(x) + \gamma h_{m+1}(x)$$

where γ is the learning rate.

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Note: The weak model $h_{m+1}(x)$ is trained using the pseudo-residuals for the training set $\{(x_i, r_i)\}$, **not** using the labels $\{(x_i, y_i)\}$!

Gradient boosting in practice

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- Remember: you compute the pseudo-residuals as the derivatives:

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This ensures that each subsequent model in the boosting process focuses on correcting the errors of the previous models.

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Deep learning:

- Works very well with very large datasets.
- Learns features by itself, e.g. as local spatial patterns.
- Allows transfer learning, e.g. via fine-tuning.
- Flexible for many tasks (e.g., generation, sequence prediction, etc.).

Suggested reading

"Understanding random forests: from theory to practice"

`https://arxiv.org/pdf/1407.7502`

"Ensembles: Gradient boosting, random forests, bagging, voting, stacking"

`https://scikit-learn.org/stable/modules/ensemble.html`