Announcements

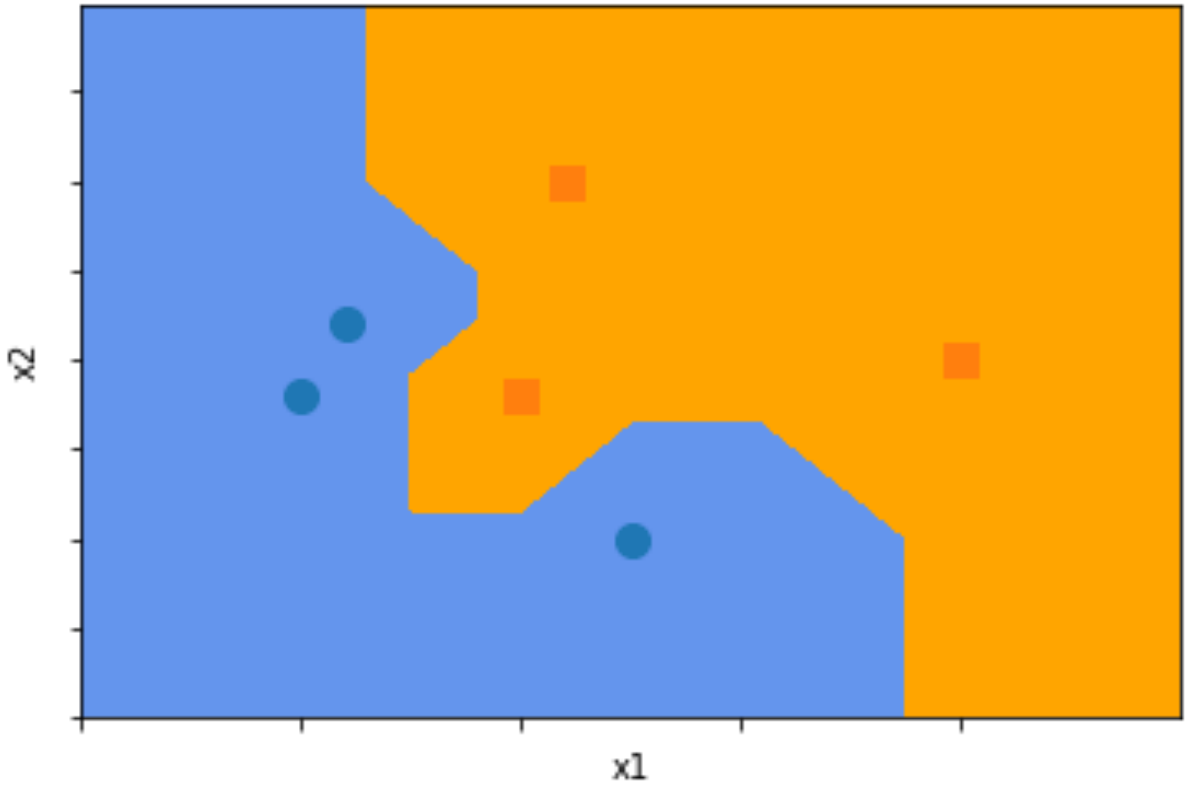
- Homework 3 is due **tonight (Monday, October 3) at 8pm**
  - Homework 4 posted, due **Wednesday, October 19 at 8pm**
- Project group form due **tomorrow (Tuesday, October 4) at 8pm)**
- Quiz 4 is due **Thursday, October 6 at 8pm**

Recap: KNN & Decision Trees

- **Loss minimization**
  - What is the model family?
  - What is the loss function?

- Not all algorithms fit cleanly into “loss minimization” framework
  - Algorithm does not minimize loss, but goal is still to minimize a loss such as accuracy of MSE or error rate

Recap: KNN



Recap: KNN

- **No learning algorithm!**

- **Prediction algorithm:**
  - **Input:** Feature vector x
  - **Step 1:** Find k neighbors closest to x (e.g., in L_2 distance)
  - **Step 2:** Combine predictions from these neighbors (e.g., majority, average)
  - **Output:** Combined prediction

- **Loss minimization**
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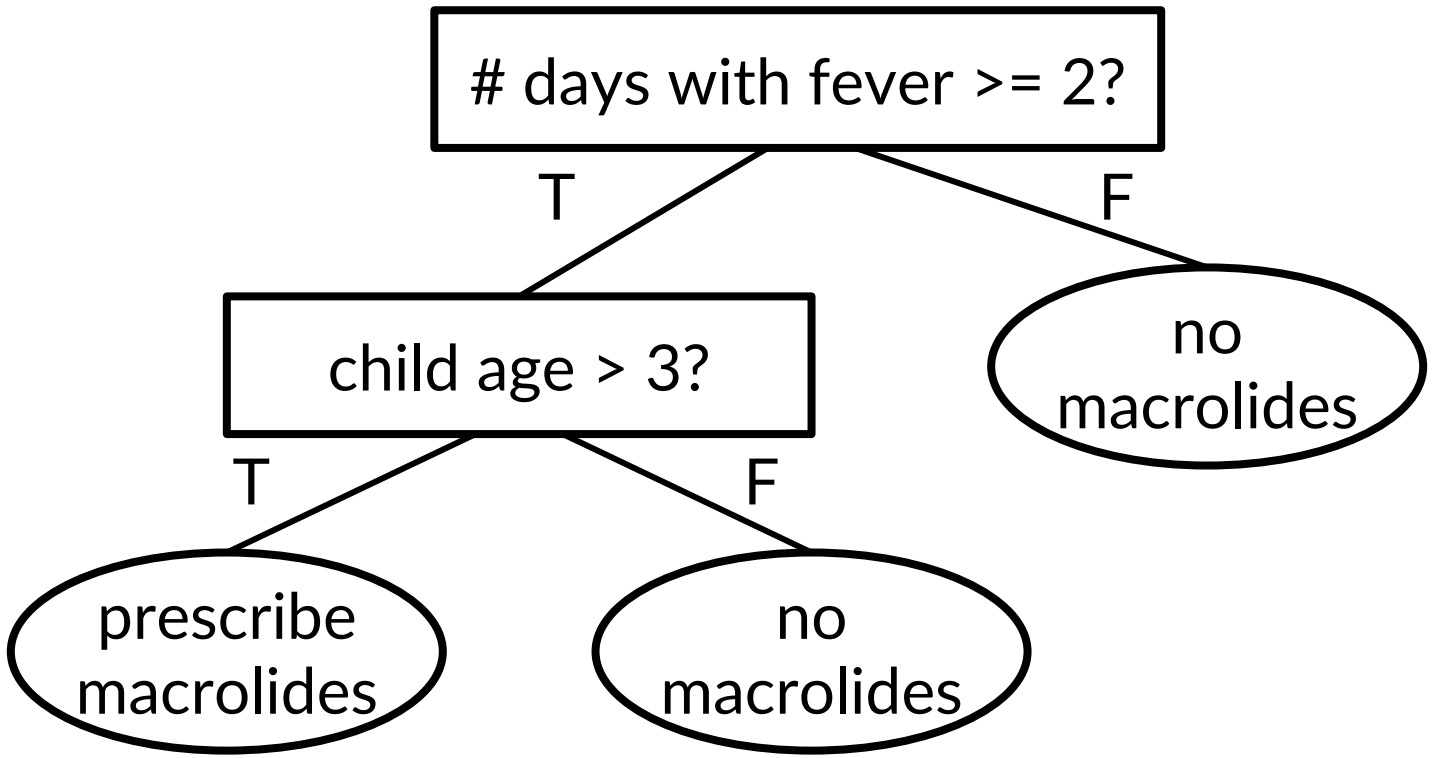
- **Loss minimization**
  - What is the model family? $f_\beta(x) = \mathrm{KNN}(x; \beta)$, where $\beta = Z$ is training data
  - What is the loss function? Classification accuracy, MSE, etc.

Recap: Decision Trees



Decision tree example from: Martignon and Monti. (2010). Conditions for risk assessment as a topic for probabilistic education. *Proceedings of the Eighth International Conference on Teaching Statistics* (ICOTS8).

Recap: Decision Trees

- **Learning algorithm:**
  - **Input:** Training dataset Z
  - **Step 1:** Construct decision tree by iteratively splitting Z using some criterion
  - **Step 2:** Prune tree to avoid overfitting
  - **Output:** Pruned tree
- **Prediction algorithm:** Label at a leaf node of the tree
- **Loss minimization**
  - What is the model family?
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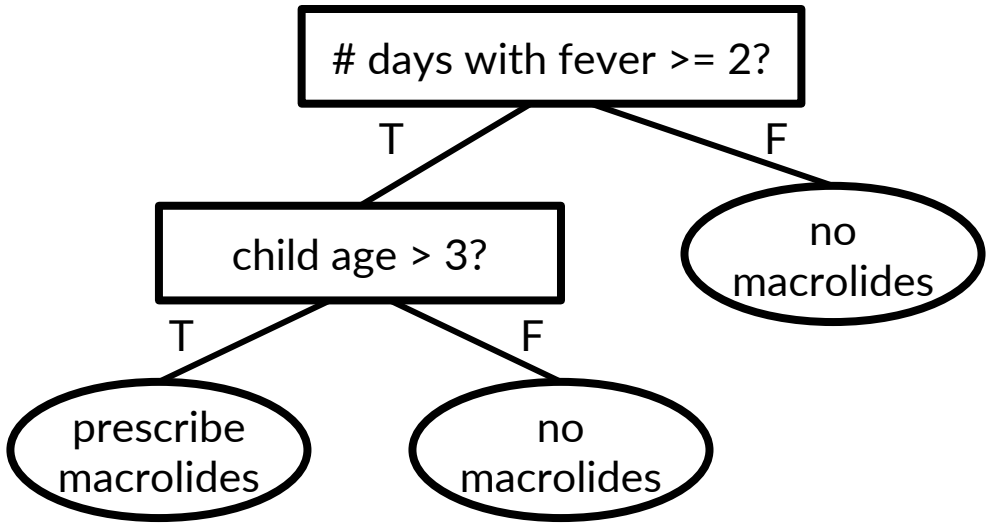
  - **Step 2:** Prune tree to avoid overfitting
  - **Output:** Pruned tree
- **Prediction algorithm:** Label at a leaf node of the tree
- **Loss minimization**
  - What is the model family? $f_\beta(x) = \mathrm{DecisionTree}(x; \beta)$
  - What is the loss function? Classification accuracy, MSE, etc.

Recap: Random Forests

- Train many decision trees and average them!
  - Increases model capacity, thereby reducing bias
- Very powerful model family in practice

Recap: Random Forests

- Decision trees can be very high-capacity model families!
  - If we grow them very large (but we worked very hard to avoid overfitting)
  - Naturally capture feature interactions



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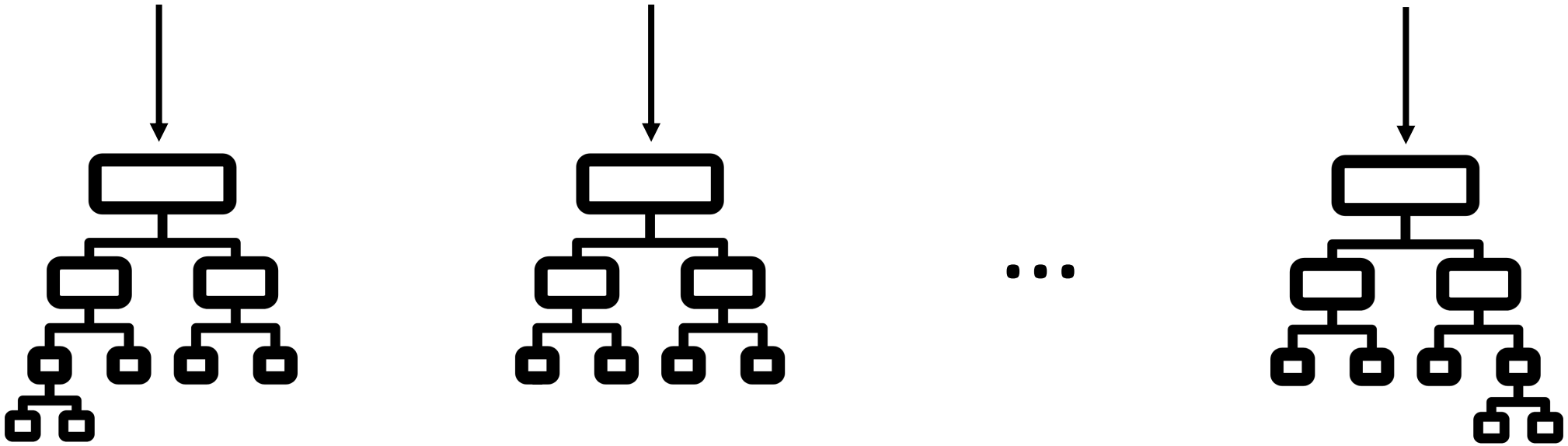
Recap: Random Forests



Recap: Random Forests

- Train many decision trees and average them!
  - Increases model capacity, thereby reducing bias
- Very powerful model family in practice
- **Today:** How to learn ensembles such as random forests

Lecture 9: Learning Ensembles

CIS 4190/5190

Fall 2022

Strategies for Increasing Model Capacity

- **Approaches so far:**
  - Richer model family
  - Feature engineering

- **Today:** Ensembles
  - Increase capacity of existing, low capacity models (e.g., decision trees)
  - Helps avoid overfitting

Ensemble Learning

- **Step 1:** Learn a set of "base" models $f_1, \ldots, f_k$
- **Step 2:** Construct model $F(x)$ that combines predictions of $f_1, \ldots, f_k$

Example: Netflix Movie Recommendations

- **Goal:** Predict how a user will rate a movie based on:
  - The user's ratings for other movies
  - Other users' ratings for this movie (and others)
  - **No features!**

- **Netflix Prize (2007-2009):** $1 million for the first team to do 10% better than the existing Netflix recommendation system

- **Winner:** BellKor's Pragmatic Chaos
  - An ensemble of 800+ rating systems

Ensembles of Decision Trees

- **Strategy 1:** Random forests
- **Strategy 2:** Gradient boosted decision trees
- Among the most powerful and widely-used models for “tabular” data (i.e., not images, text, graphs, or other highly structured data)

Ensemble Design Decisions

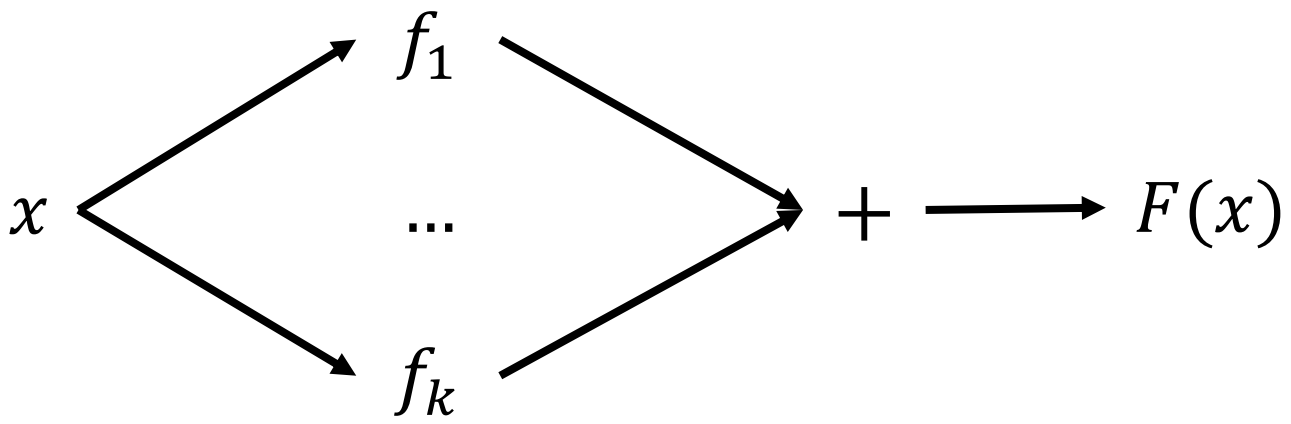
- How to learn the base models?
- How to combine the learned base models?

Ensemble Design Decisions

- How to learn the base models?
- **How to combine the learned base models?**

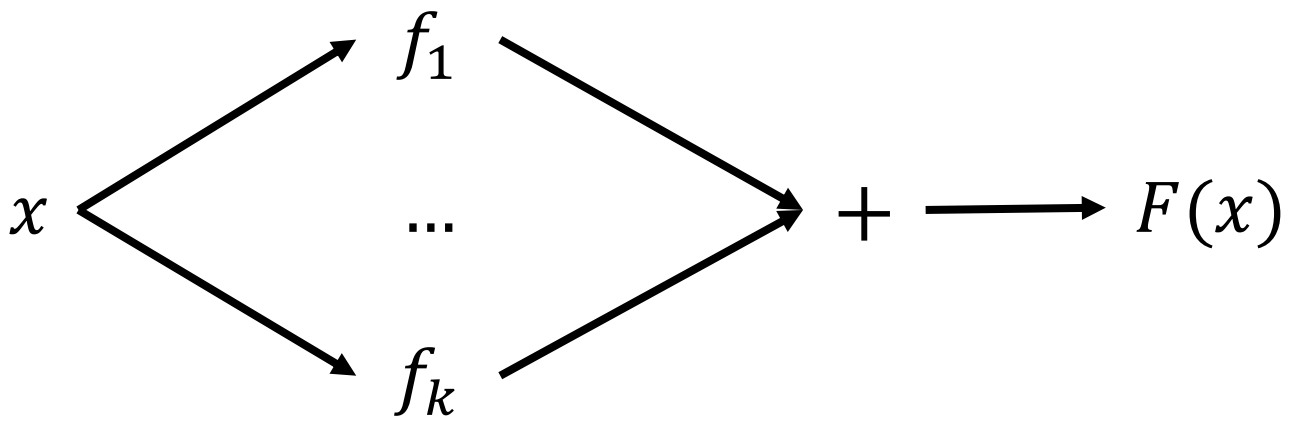
Combining Learned Base Models

- **Regression:** Average predictions $F(x) = \frac{1}{k}\sum_{i=1}^{k} f_i(x)$
  - Works well if the base models have similar performance



Combining Learned Base Models

- **Classification:** Majority vote $F(x) = 1\left(\sum_{i=1}^{k} f_i(x) \geq \frac{k}{2}\right)$ (for binary)
  - Can also average probabilities for classification



Combining Learned Base Models

- Can use weighted average:

$$F(x) = \sum_{i=1}^{k} \beta_i \cdot f_i(x)$$

- Can fit weights using linear regression on second training set

- More generally, can fit a second layer model

$$F(x) = g_\beta\big(f_1(x), \ldots, f_k(x)\big)$$

Combining Learned Base Models

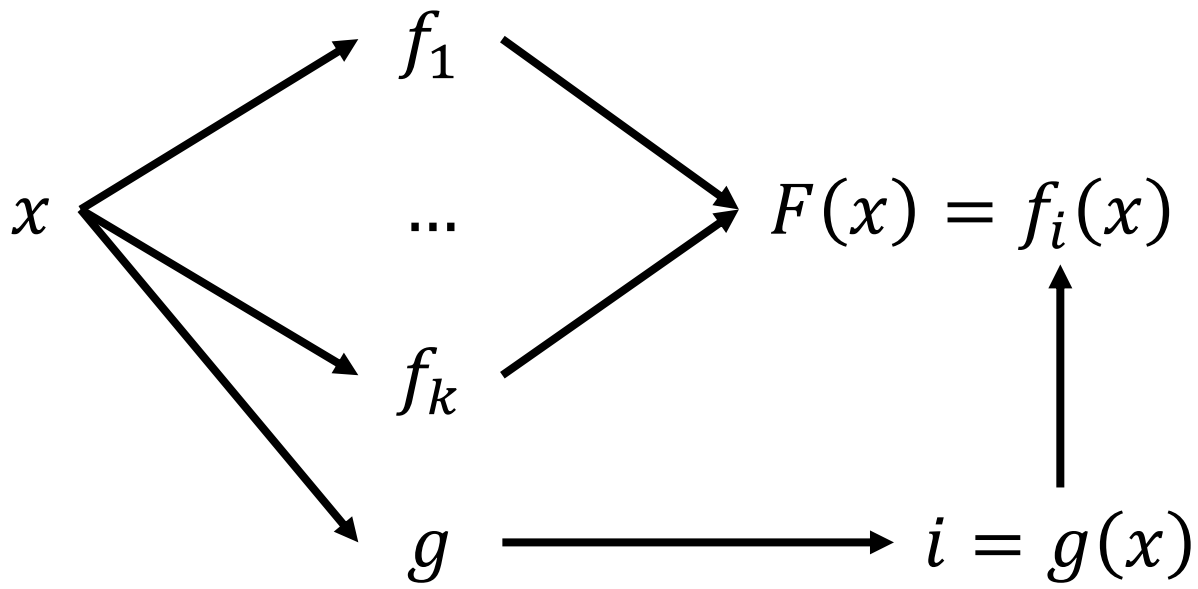
- Second model as “mixture of experts”:

$$F(x) = \sum_{i=1}^{k} g(x)_i \cdot f_i(x)$$

- Second stage model predicts weights over “experts” $f_i(x)$

Combining Learned Base Models

- Second model as “mixture of experts”:
  - **Special case:** $g(x)$ is one-hot
  - **Advantage:** Only need to run $g(x)$ and $f_{g(x)}(x)$



Ensemble Design Decisions

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Ensemble Design Decisions

- **How to learn the base models?**

- How to combine the learned base models?

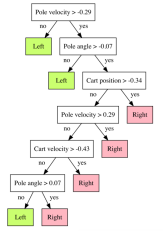
Learning Base Models

- Successful ensembles require **diversity**
  - Different model families
  - Different training data
  - Different features
  - Different hyperparameters

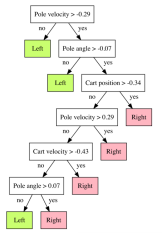
- **Intuition:** Models should make **independent** mistakes

Learning Base Models

- **Intuition:** Models should make **independent** mistakes



$\text{acc} = \frac{3}{4}$



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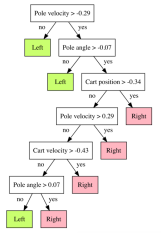


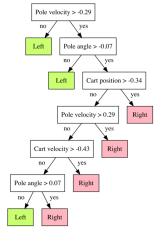
$\text{acc} = \frac{3}{4}$

F $\quad \text{acc} = 1 - \left(1 - \frac{3}{4}\right)^3 - 3 \cdot \frac{3}{4} \cdot \left(1 - \frac{3}{4}\right)^2 \approx 0.84$

x_1	x_2	x_3	x_4
✓	✓	✗	✓
✗	✓	✓	✓
✓	✗	✓	✓
✓		✓	✓

Learning Base Models

- **Intuition:** Models should make **independent** mistakes



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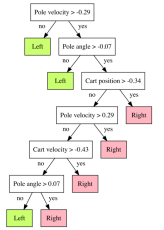

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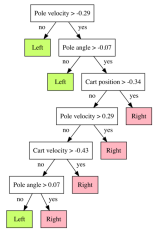
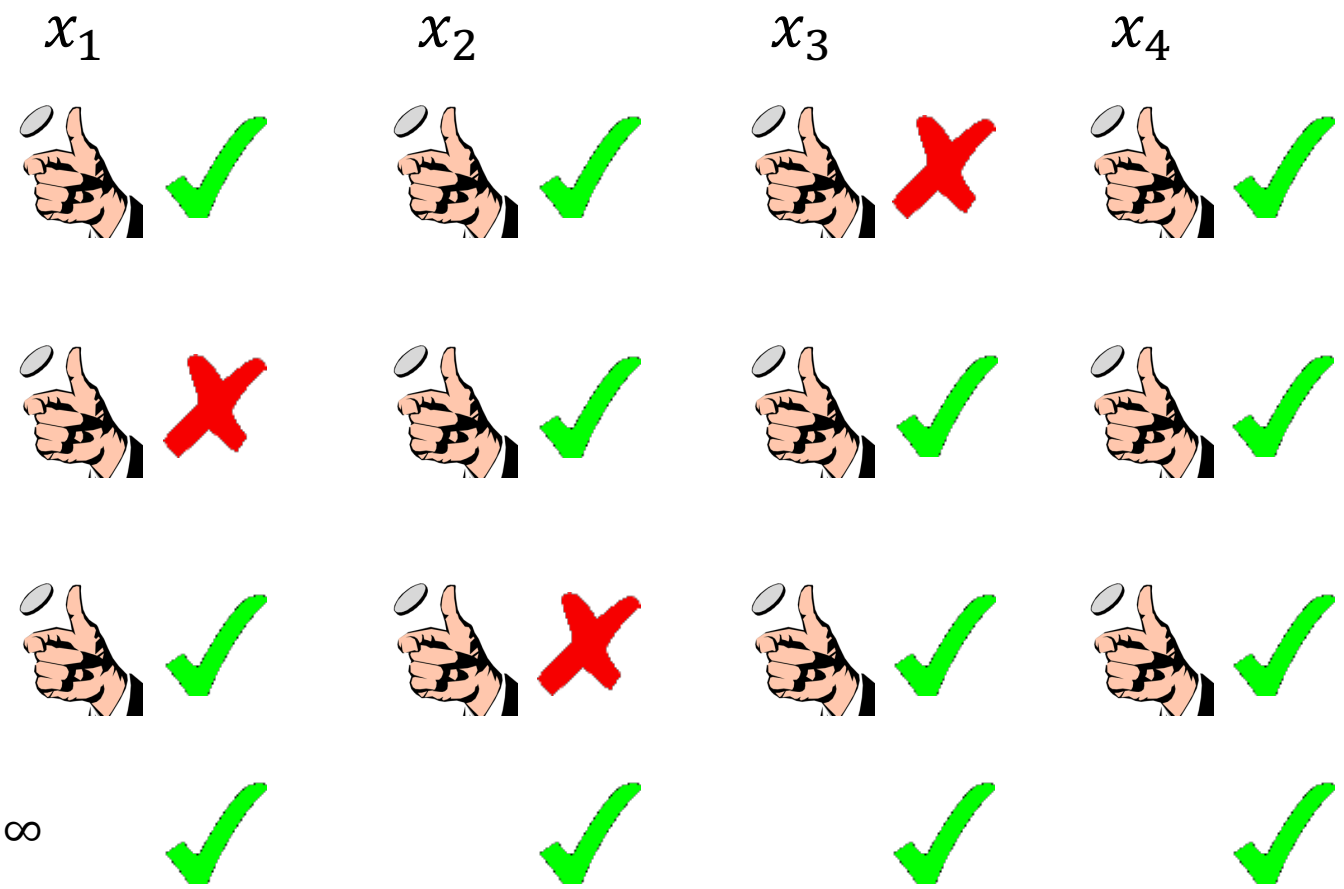


$\text{acc} = \frac{3}{4}$

F $\quad \text{acc} \to 1 \text{ as } k \to \infty$



Learning Base Models

- Ensemble can be built from different learning algorithms
  - **Example:** Decision tree, logistic regression, kNN, …
- What if we want an ensemble of decision trees?
  - **Issue:** Decision tree learning algorithm is deterministic
  - **Solution:** Randomize the learning algorithm (may sacrifice performance)!
- Randomize decisions inside learning algorithm
  - **Example:** Randomize splits weighted (somehow) by information gain
  - **Issue:** Very specific to the algorithm
  - **Solution:** Randomize input to learning algorithm (i.e., training data)!

Randomizing Learning Algorithms

- **Bagging:** Randomize training data ("Boostrap Aggregating")
  - **Random examples:** Subsample examples $\{(x, y)\}$ (obtain $X \in \mathbb{R}^{n' \times d}$)
    Random features: Subsample features x_j (obtain $X \in \mathbb{R}^{n \times d'}$)

- Meta-strategy that can build ensembles from arbitrary base learners

- Can be thought of as a form of regularization

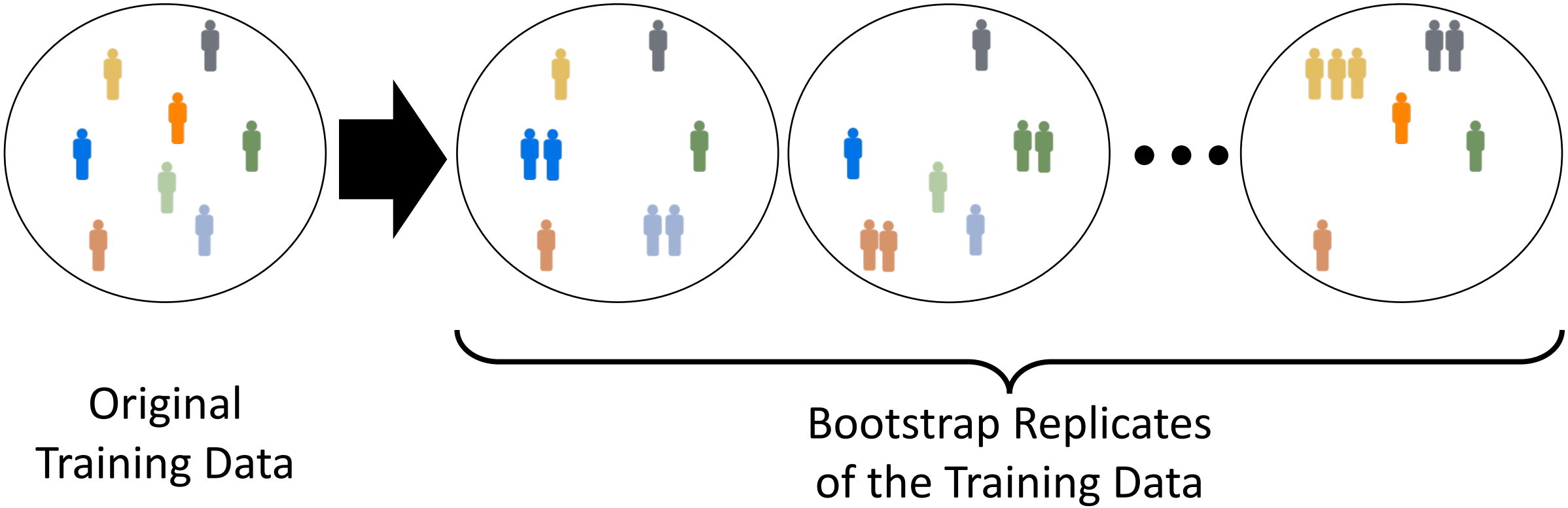
Aside: Bootstrap

- Subsample examples $\{(x, y)\}$ **with replacement** (obtain $X \in \mathbb{R}^{n \times d}$)

- Excludes $\left(1 - \frac{1}{n}\right)^n$ of the training examples
  - Separately in each of the replicates
  - As $n \to \infty$, excludes $\to \frac{1}{e} \approx 36.8\%$ examples

- Has good statistical properties

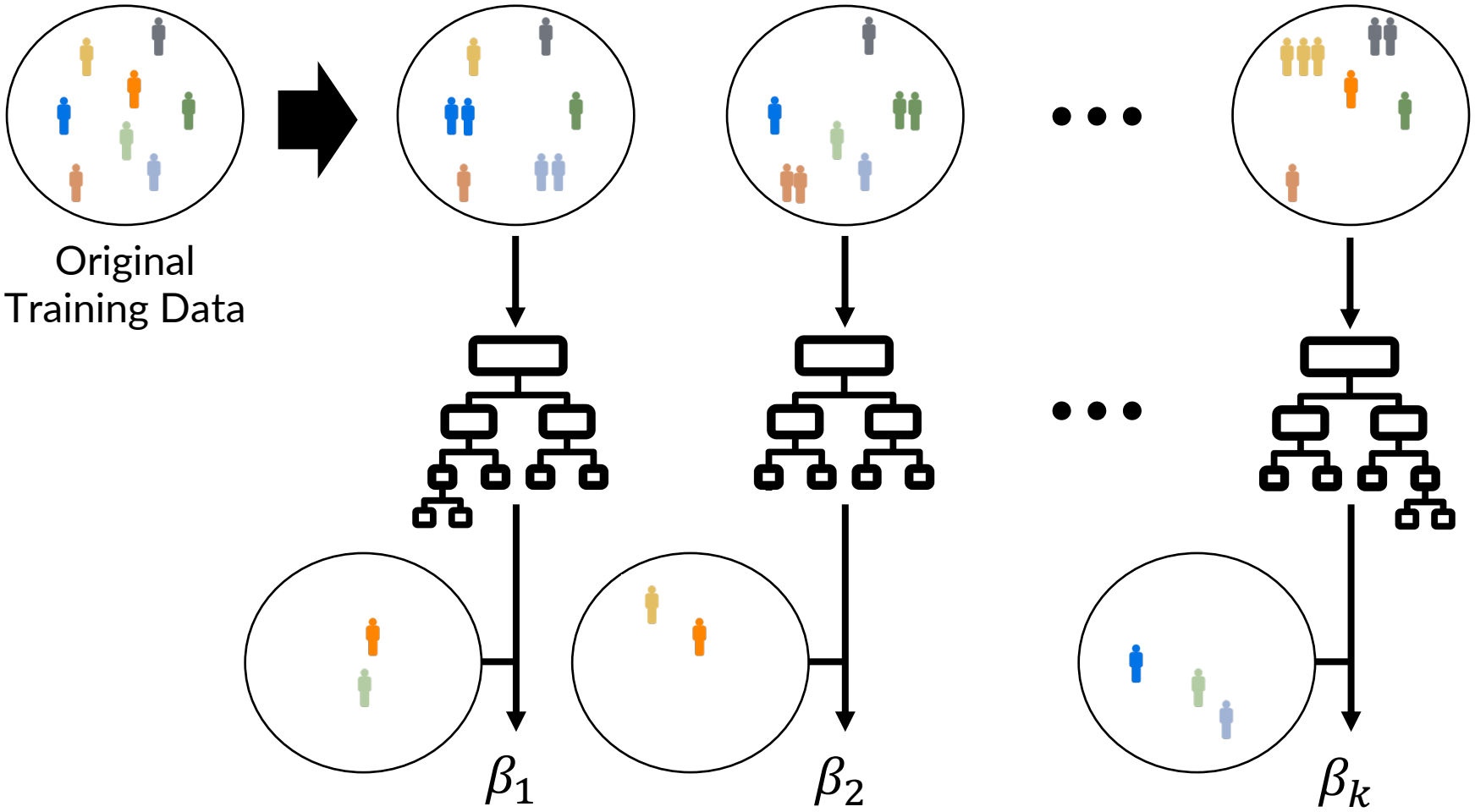
Randomizing Learning Algorithms



Ensemble Learning

- **Step 1:** Create bootstrap replicates of the original training dataset
- **Step 2:** Train a classifier for each replicate
- **Step 3 (Optional):** Use held-out validation set to weight models
  - Can just use average predictions

Ensemble Learning



Random Forests

- Ensemble of decision trees using bagging
  - Typically use simple average (over probabilities for classification)
- Often among the best performing models
- **Intuition:**
  - Large decision trees are good nonlinear models, but high variance
  - Random forests average over many decision trees to reduce variance without increasing bias

Random Forests

- **Tweak 1:** Randomize features in learning algorithm instead of bagging
  - At DT node splitting step, subsample $\approx \sqrt{d}$ features
  - Allows each tree to use all features, but not at every node
  - **Aside:** If a few features are highly predictive, then they will be selected in many trees, causing the base models to be highly correlated

- **Tweak 2:** Train **unpruned** decision trees
  - Ensures base models have higher capacity
  - **Intuition:** Skipping pruning increases variance (randomness increases bias)

Bias Variance Tradeoff for Random Forests

- Naïvely, skipping pruning yields high variance
- Introduce randomness to increase bias
  - Without randomness, all models in the random forest would be the same (large) decision tree, so the random forest would still have very large variance
- Carefully select randomness to tune bias variance tradeoff

AdaBoost (Freund & Schapire 1997)

- Like bagging, meta-algorithm that turns base models into ensemble
  - **Provably learns** for base models achieving any error rate > 0.5
- Uses **different training example weights** (instead of different subsamples or different features) to introduce diversity
  - In particular, **upweights** currently incorrectly predicted examples
- Base models should satisfy the following:
  - High-bias/low-capacity (e.g., depth-limited decision trees, linear classifiers)
  - Able to incorporate sample weights during learning
  - **Specific to classification (discuss general losses later)**

Aside: Learning with Weighted Examples

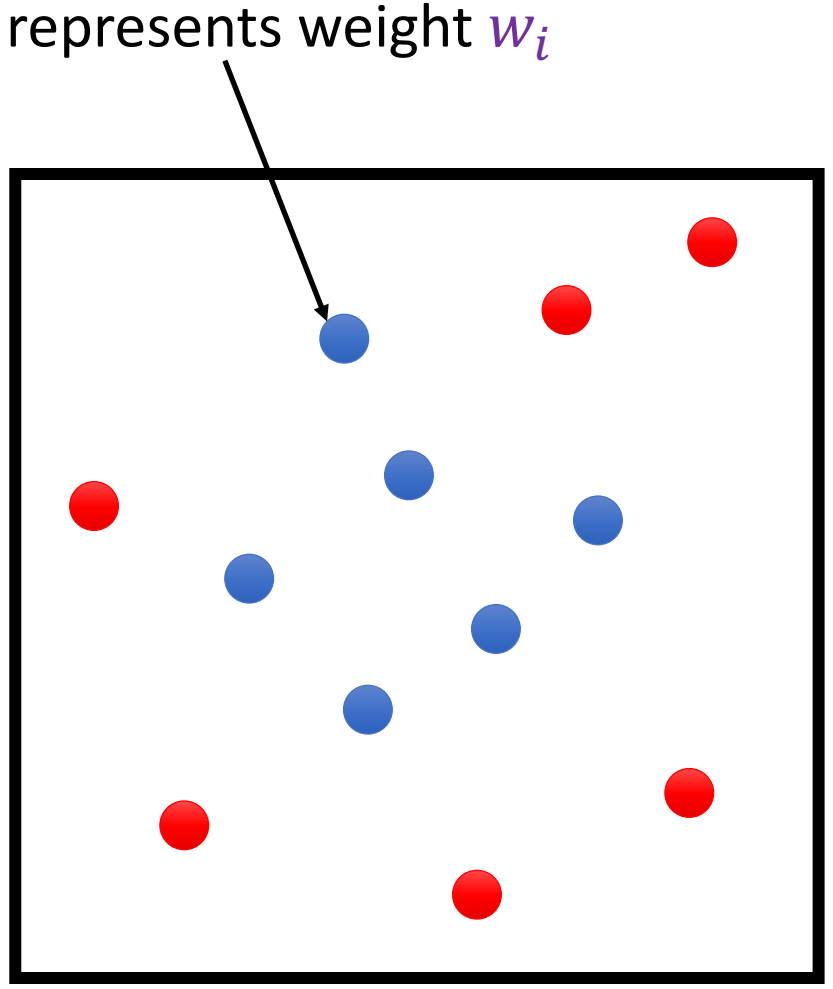
- Many algorithms can directly incorporate weights into the loss
- For maximum likelihood estimation:

$$\ell(\beta; Z, w) = \sum_{i=1}^{n} w_i \cdot \log p_\beta(y_i \mid x_i)$$

- Alternatively, can subsample the data proportional to weights w_i

AdaBoost

1. $w_1 \leftarrow \left(\frac{1}{n}, \ldots, \frac{1}{n}\right)$ ($w_{1,i}$ weight for (x_i, y_i))
2. **for** $t \in \{1, \ldots, T\}$
3. $\quad f_t \leftarrow \text{Train}(Z, w_t)$
4. $\quad \epsilon_t \leftarrow \text{Error}(f_t, Z, w_t)$
5. $\quad \beta_t \leftarrow \frac{1}{2} \ln \frac{1-\epsilon_t}{\epsilon_t}$
6. $\quad w_{t+1,i} \propto w_{t,i} \cdot e^{-\beta_t \cdot y_i \cdot f_t(x_i)}$ (for all i)
7. **return** $F(x) = \text{sign}(\sum_{t=1}^{T} \beta_t \cdot f_t(x))$



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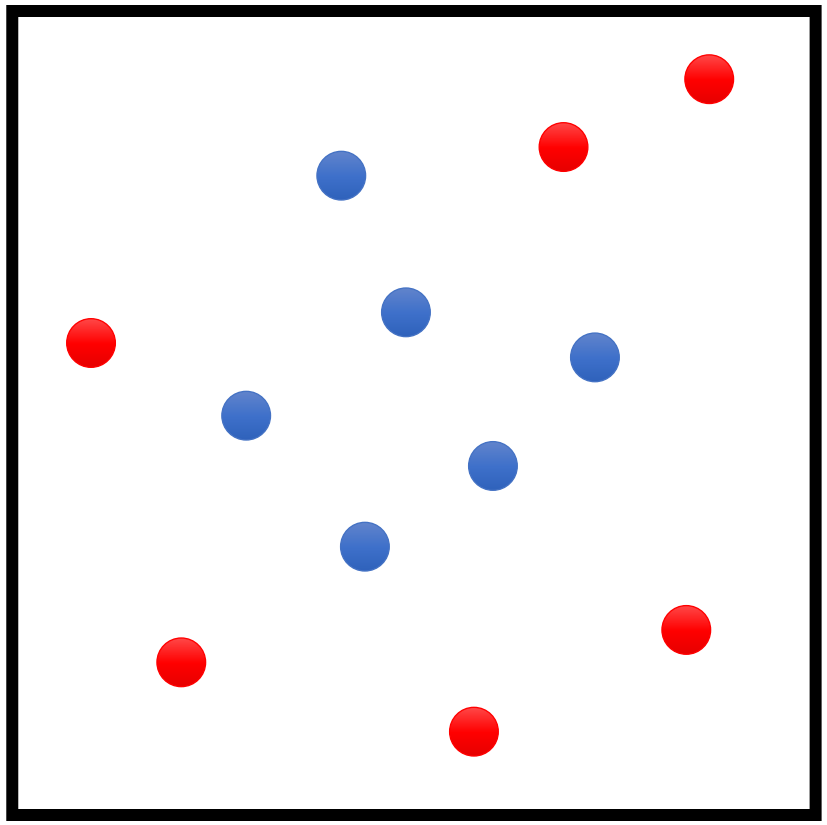

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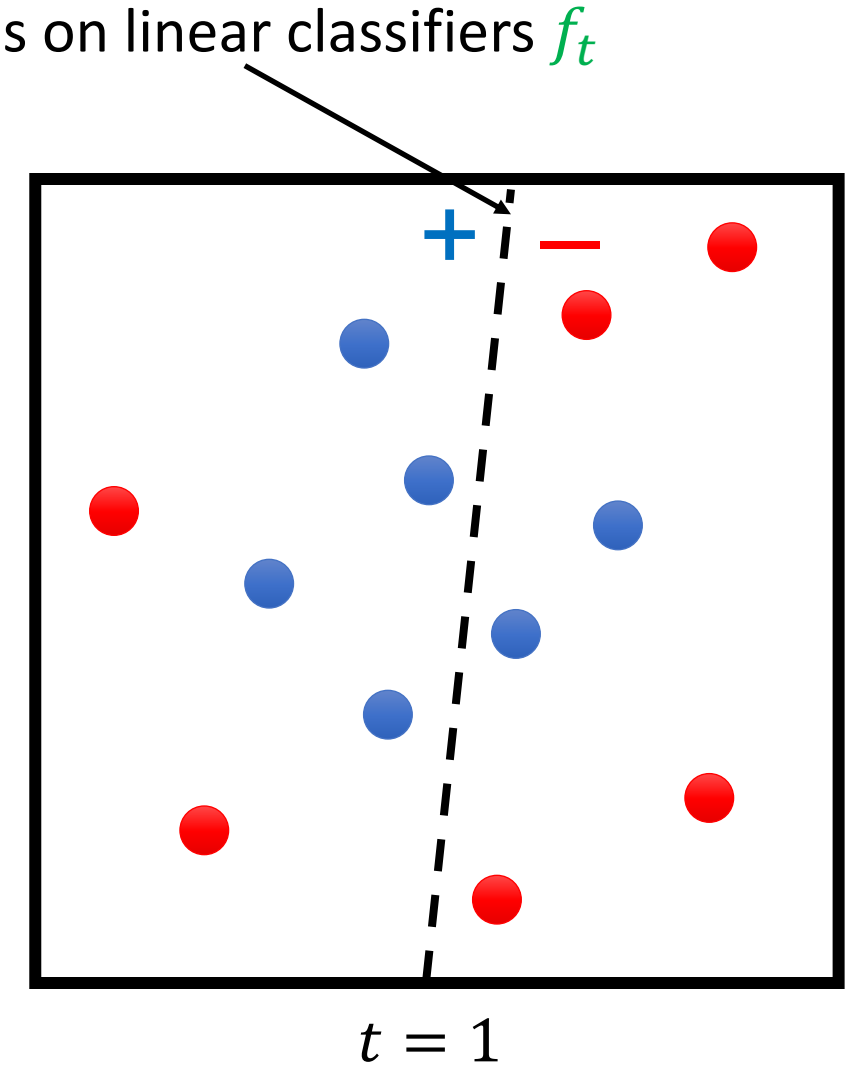

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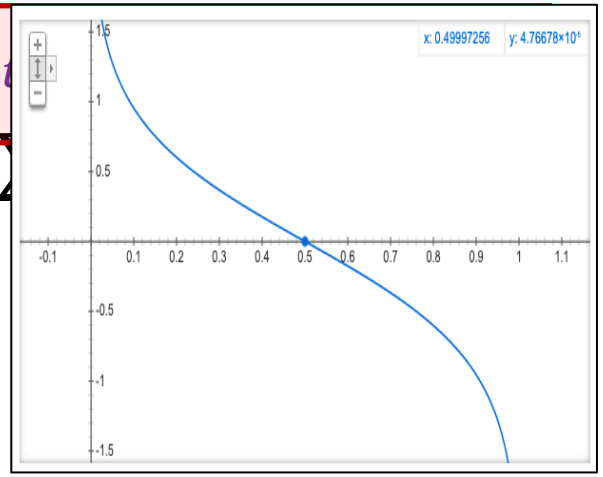
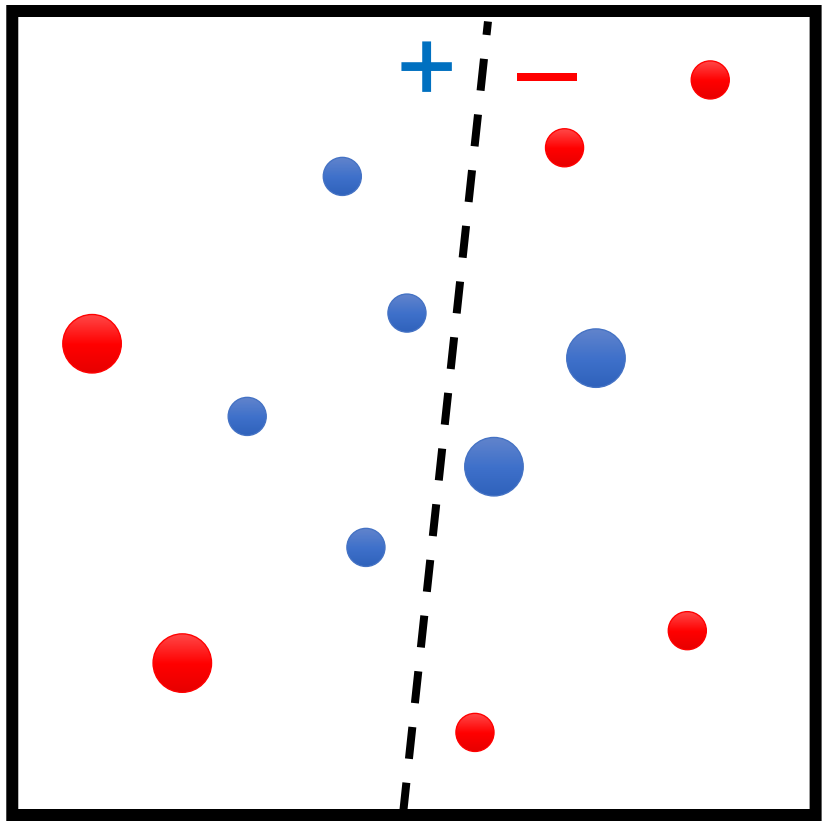
6. $w_{t+1,i} \propto w_{t,i} \cdot e^{-\beta_t}$
7. **return** $F(x) = \text{sign}(\ldots)$

β_t becomes larger as ϵ_t becomes smaller





$t = 1$

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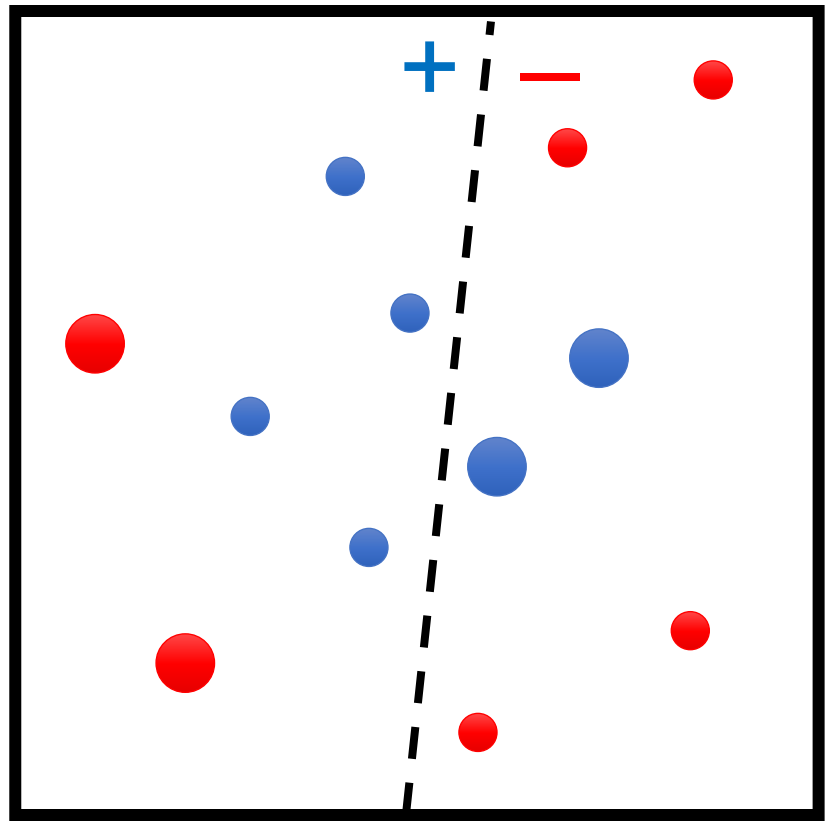
6. $\quad w_{t+1,i} \propto w_{t,i} \cdot e^{-\beta_t \cdot y_i \cdot f_t(x_i)}$ (for all i)
7. **return** $F(x) = \text{sign}(\sum_{t=1}^{T} \beta_t \cdot f_t(x))$

Use convention $y_i \in \{-1, +1\}$

If correct ($y_i = f_t(x_i)$) then multiply by $e^{-\beta_t}$

If incorrect ($y_i \neq f_t(x_i)$) then multiply by e^{β_t}



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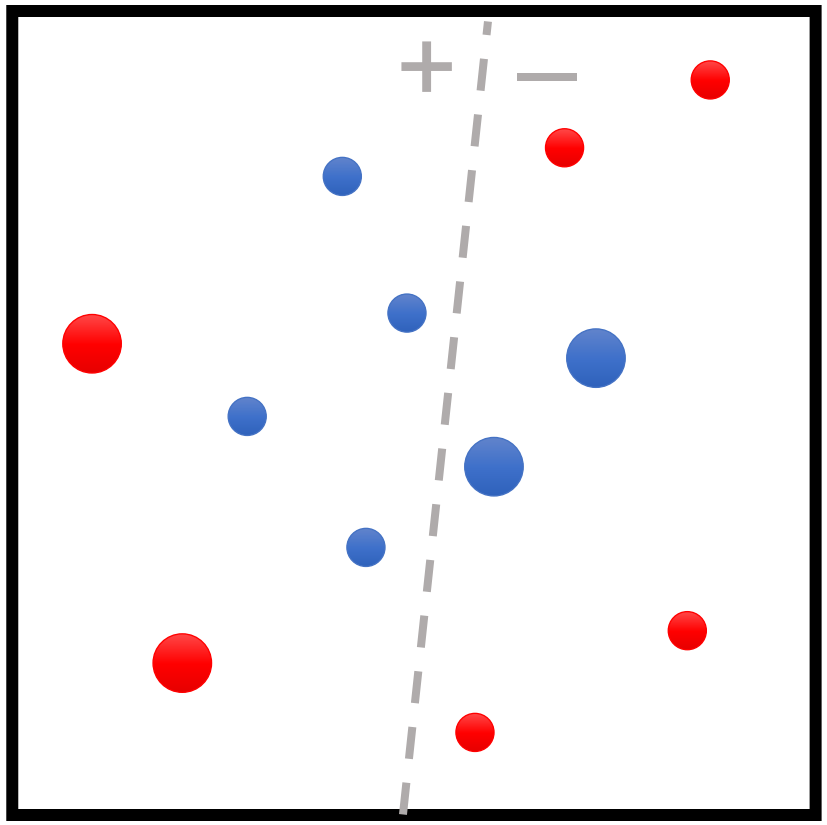

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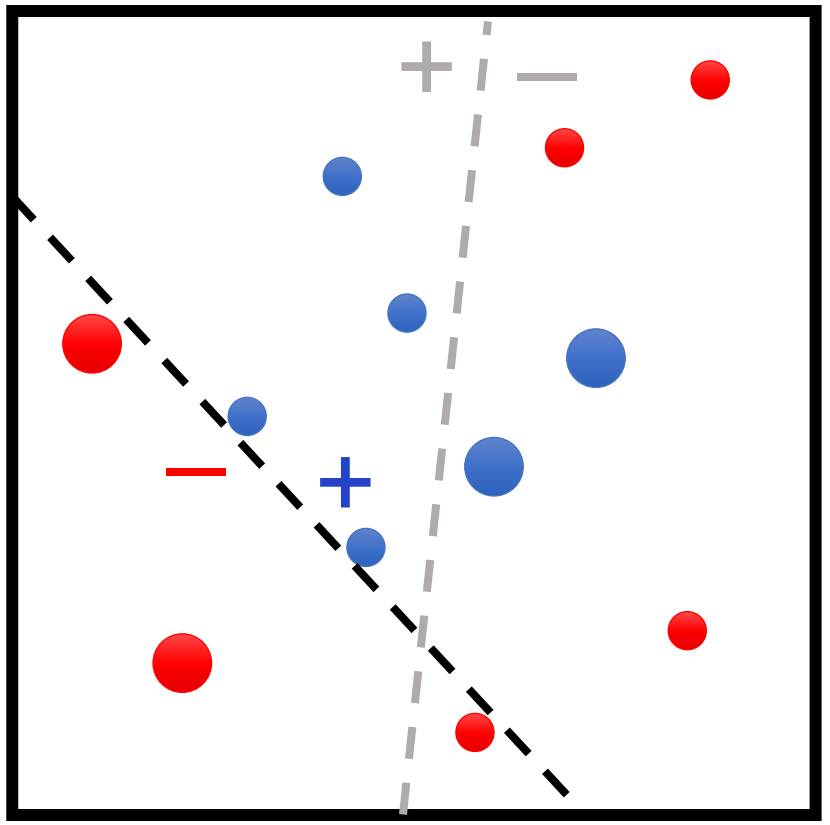

$t = 2$

AdaBoost

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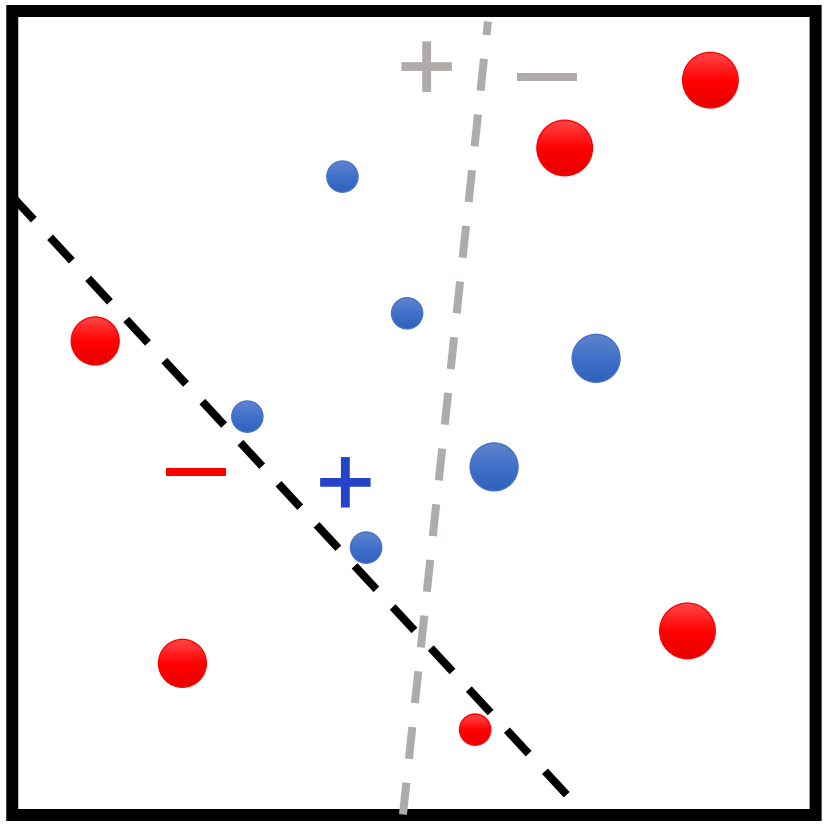
7. **return** $F(x) = \text{sign}(\sum_{t=1}^{T} \beta_t \cdot f_t(x))$



$t = 2$

AdaBoost

1. $w_1 \leftarrow \left(\frac{1}{n}, \ldots, \frac{1}{n}\right)$ ($w_{1,i}$ weight for (x_i, y_i))
2. **for** $t \in \{1, \ldots, T\}$
3. $\quad f_t \leftarrow \text{Train}(Z, w_t)$
4. $\quad \epsilon_t \leftarrow \text{Error}(f_t, Z, w_t)$
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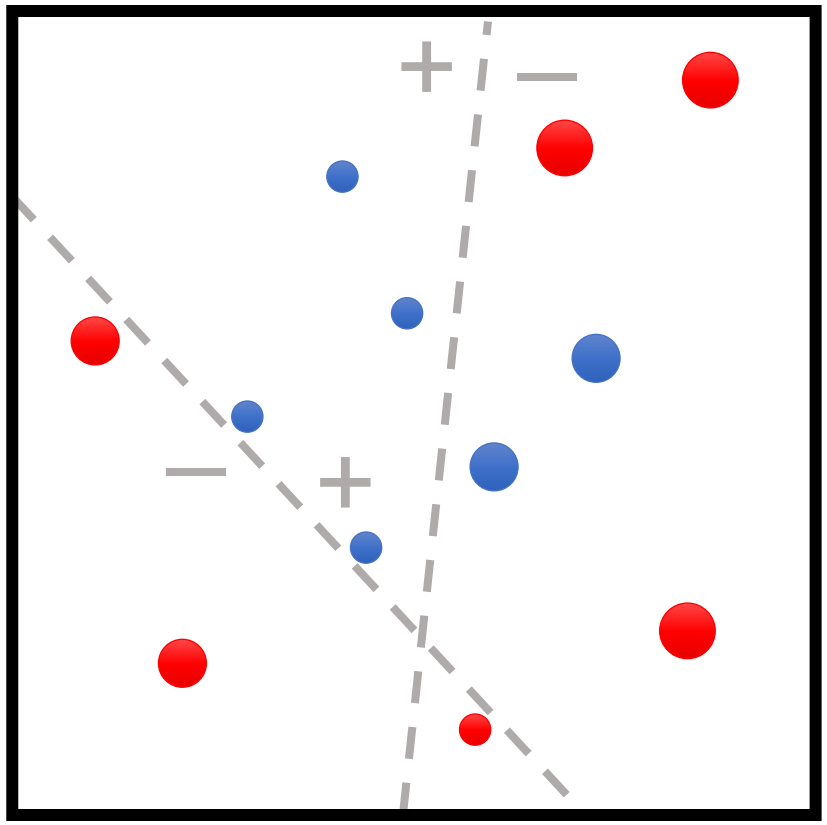

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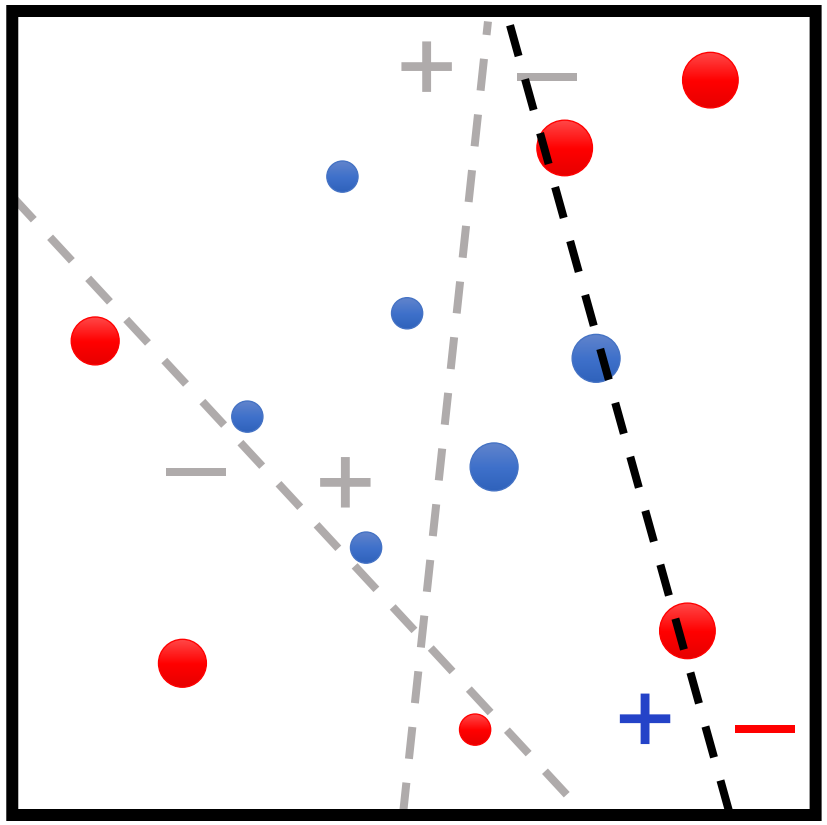

$t = 3$

AdaBoost

1. $w_1 \leftarrow \left(\frac{1}{n}, \ldots, \frac{1}{n}\right)$ ($w_{1,i}$ weight for (x_i, y_i))
2. **for** $t \in \{1, \ldots, T\}$
3. $\quad f_t \leftarrow \text{Train}(Z, w_t)$
4. $\quad \epsilon_t \leftarrow \text{Error}(f_t, Z, w_t)$
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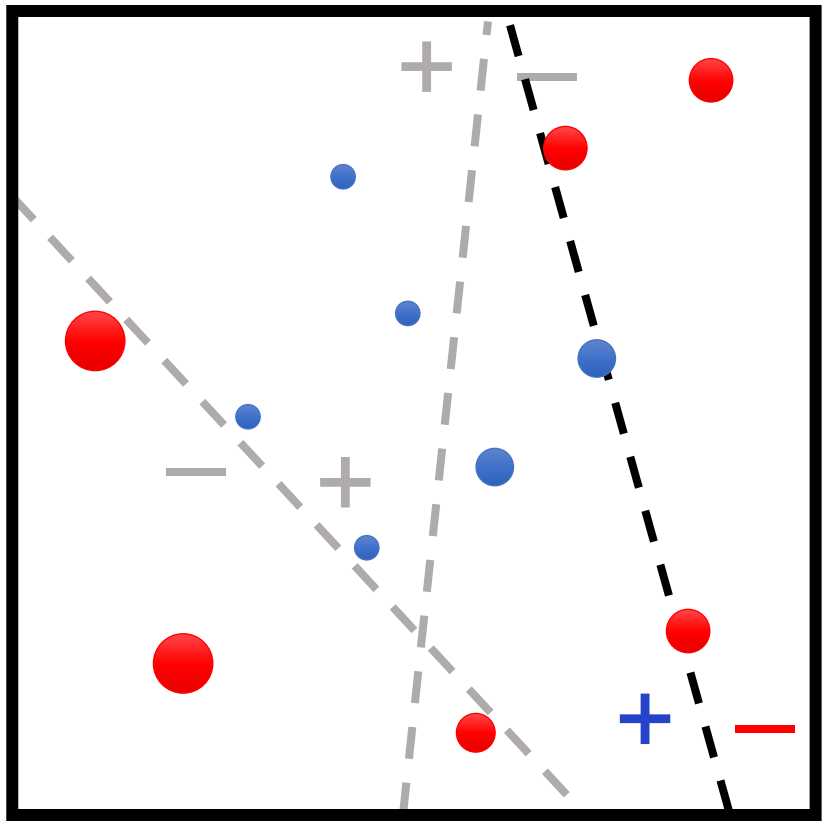

$t = 3$

AdaBoost

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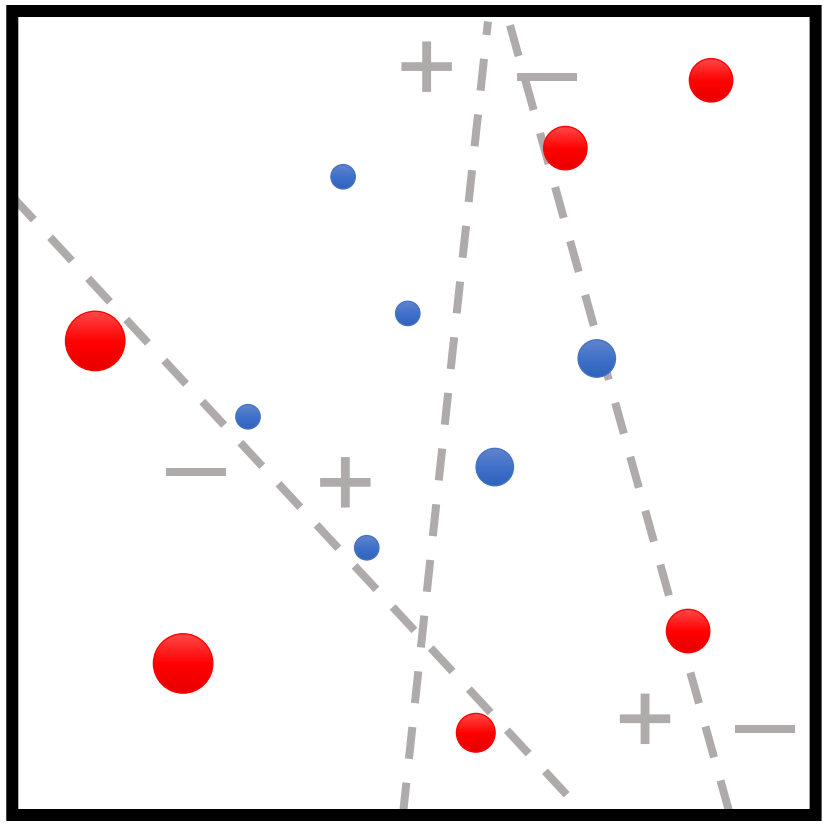

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AdaBoost

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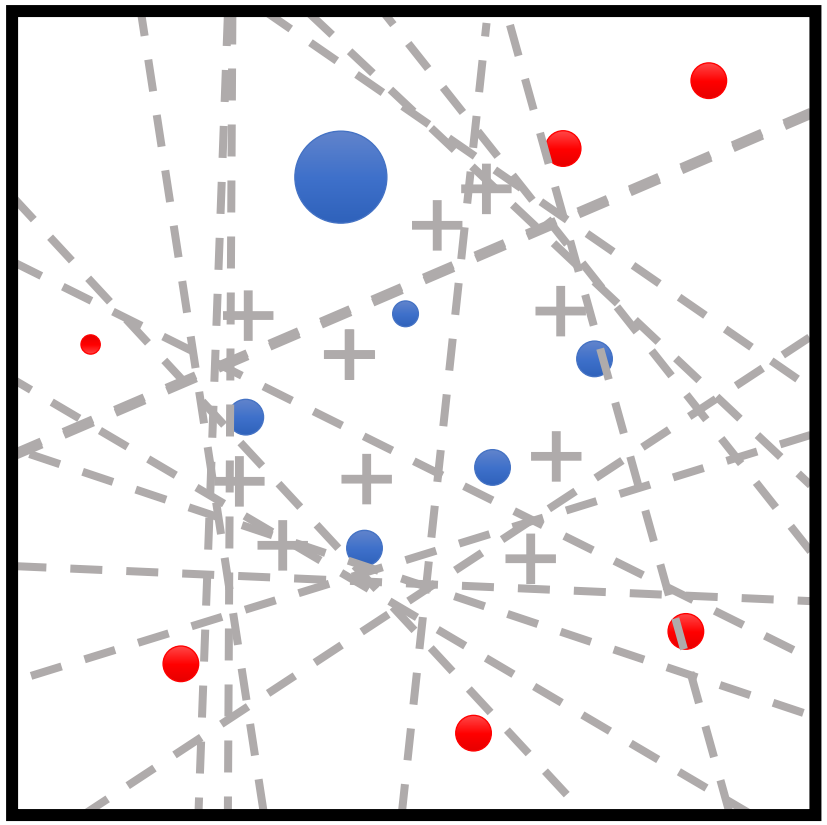

Under certain assumptions, training error goes to zero in $O(\log n)$ iterations

$t = T$

AdaBoost

1. $w_1 \leftarrow \left(\frac{1}{n}, \ldots, \frac{1}{n}\right)$ ($w_{1,i}$ weight for (x_i, y_i))
2. **for** $t \in \{1, \ldots, T\}$
3. $\quad f_t \leftarrow \text{Train}(Z, w_t)$
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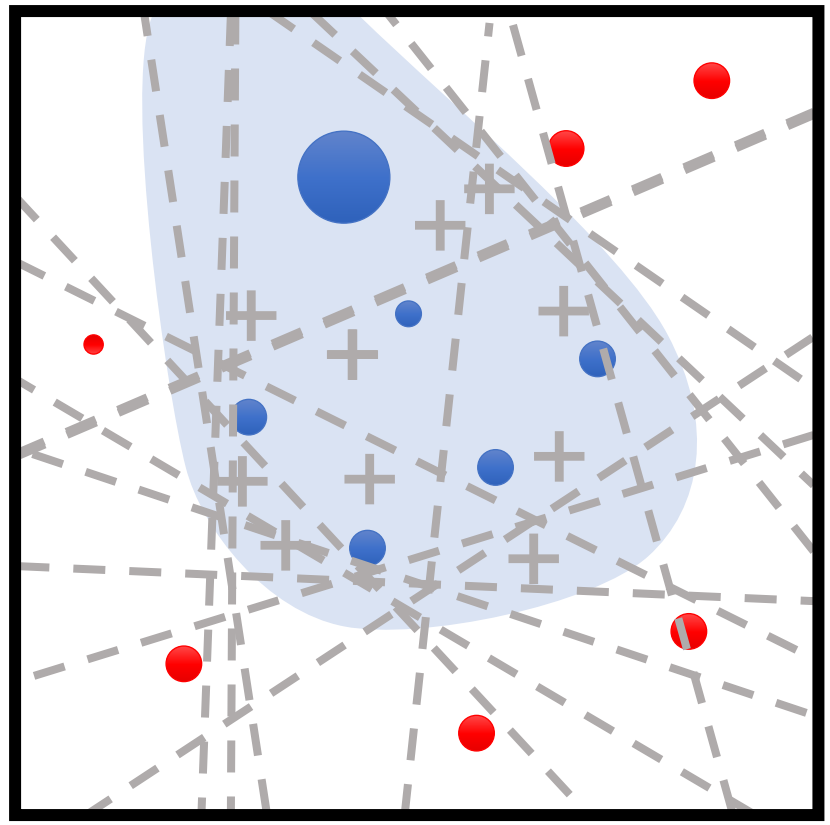
6. $\quad w_{t+1,i} \propto w_{t,i} \cdot e^{-\beta_t \cdot y_i \cdot f_t(x_i)}$ (for all i)
7. **return** $F(x) = \text{sign}(\sum_{t=1}^{T} \beta_t \cdot f_t(x))$

final model is average of base models weighted by their performance

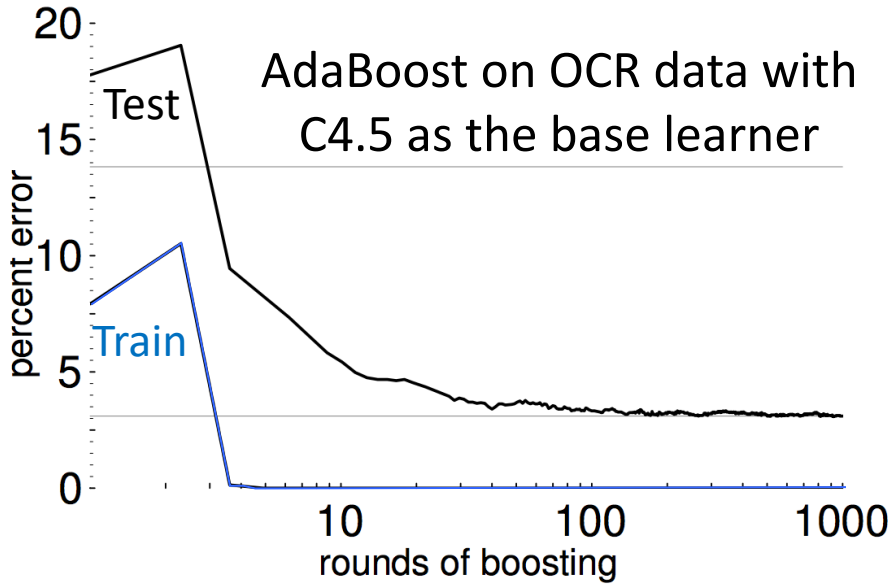


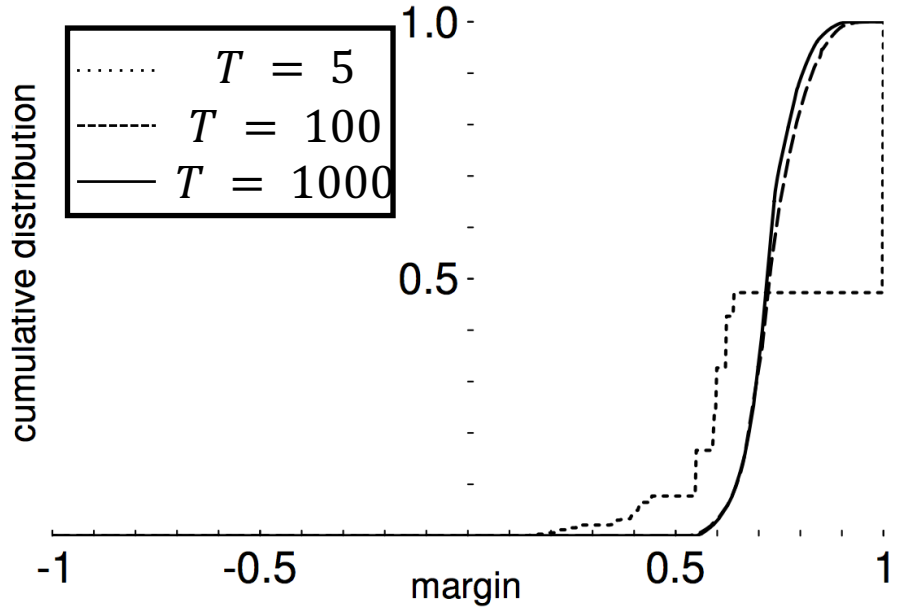
AdaBoost Weighting Strategy

- On each iteration:
  - Misclassified examples are upweighted
  - Correctly classified are downweighted
- If an example is repeatedly misclassified, it will eventually be upweighted so much that it is correctly classified
- Emphasizes “hardest” parts of the input space
  - Instances with highest weight are often outliers

AdaBoost and Overfitting

- Basic ML theory predicts AdaBoost always overfits as $T \to \infty$
  - Hypothesis keeps growing more complex!
  - In practice, AdaBoost often does not overfit





AdaBoost Summary

- **Strengths:**
  - Fast and simple to implement
  - No hyperparameters (except for T)
  - Very few assumptions on base models

- **Weaknesses:**
  - Can be susceptible to noise/outliers when there is insufficient data
  - No way to parallelize
  - Small gains over complex base models
  - **Specific to classification!**

Boosting as Gradient Descent

- Both algorithms: $\text{new model} = \text{old model} + \text{update}$
- **Gradient Descent:**

$$\theta_{t+1} = \theta_t - \alpha \cdot \nabla_\theta L(\theta_t; Z)$$

- **Boosting:**

$$F_{t+1}(x) = F_t(x) + \beta_{t+1} \cdot f_{t+1}(x)$$

- Here, $F_t(x) = \sum_{i=1}^{n} \beta_t \cdot f_t(x)$

Boosting as Gradient Descent

- **Suppose that:**
  - $\beta_t = 1$ for all t
  - $F_{t+1}(x_i) = y_i$ is a perfect predictor on the training data

- Then, boosting has the form

$$f_{t+1}(x_i) = \underbrace{y_i - F_t(x_i)}$$

"residuals", i.e., error of the current model

- **Idea:** Train f_{t+1} to predict residuals $y_i - F_t(x_i)$

Boosting as Gradient Descent

- **Algorithm:** For each $t \in \{1, \dots, T\}$:
  - **Step 1:** Train f_{t+1} using dataset

$$Z_{t+1} = \{(x_i, y_i - F_t(x_i))\}_{i=1}^{n}$$

  - **Step 2:** Take

$$F_{t+1}(x) = F_t(x) + f_{t+1}(x)$$

- Return the final model F_T

Boosting as Gradient Descent

- Residuals are the gradient of the squared error $L(y, \hat{y}) = \frac{1}{2}(y - \hat{y})^2$:

$$\text{residual}_i = y_i - F_t(x) = \left[-\frac{\partial L}{\partial \hat{y}}\right]_{F_t(x)}$$

- For general losses, we can train f_{t+1} using

$$Z_{t+1} = \left\{\left(x_i, \left[-\frac{\partial L}{\partial \hat{y}}\right]_{F_t(x)}\right)\right\}_{i=1}^{n}$$

Gradient Boosting in Practice

- Gradient boosting with depth-limited decision trees (e.g., depth 3) is one of the most powerful off-the-shelf classifiers available
  - **Caveat:** Inherits decision tree hyperparameters

- XGBoost is a very efficient implementation suitable for production use
  - A popular library for gradient boosted decision trees
  - Optimized for computational efficiency of training and testing
  - Used in many competition winning entries, across many domains
  - https://xgboost.readthedocs.io