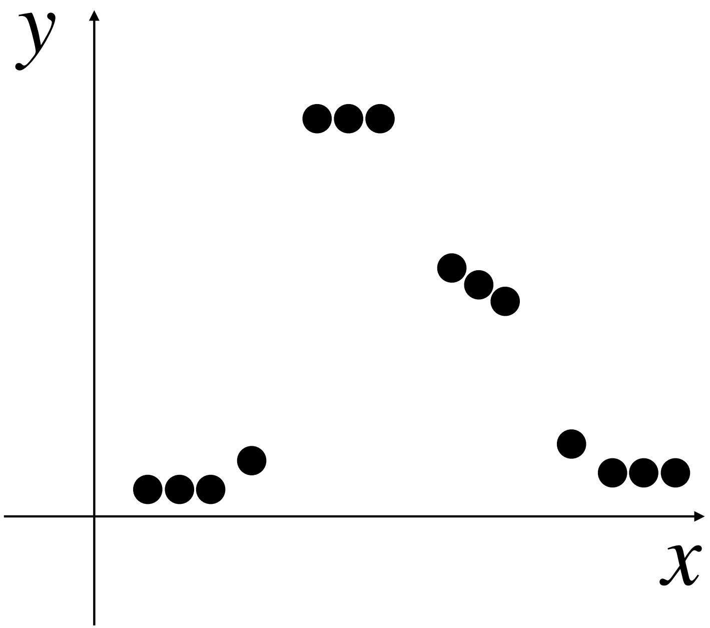
Ensemble Methods:
Bagging & Random Forest

Recap on Decision (Regression) Tree

Regression dataset $\mathscr{D} = \{x_i, y_i\}_{i=1}^{n}, \quad (x_i, y_i) \sim P$



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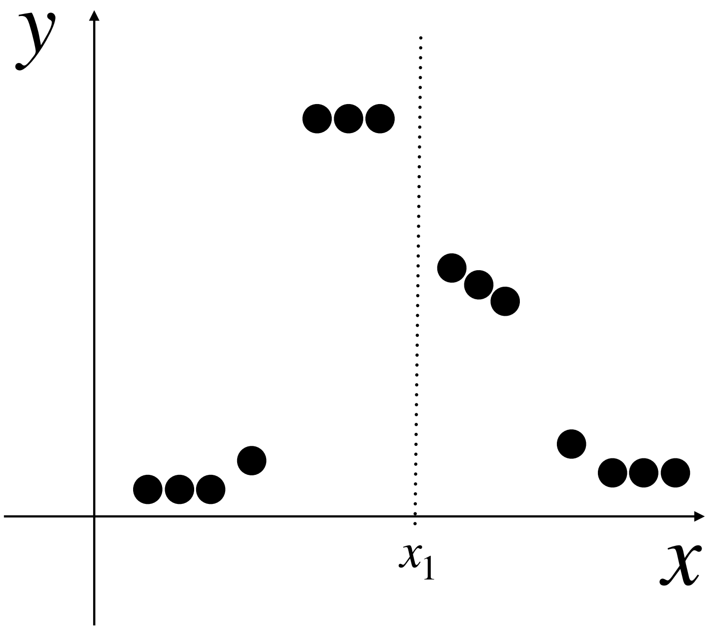

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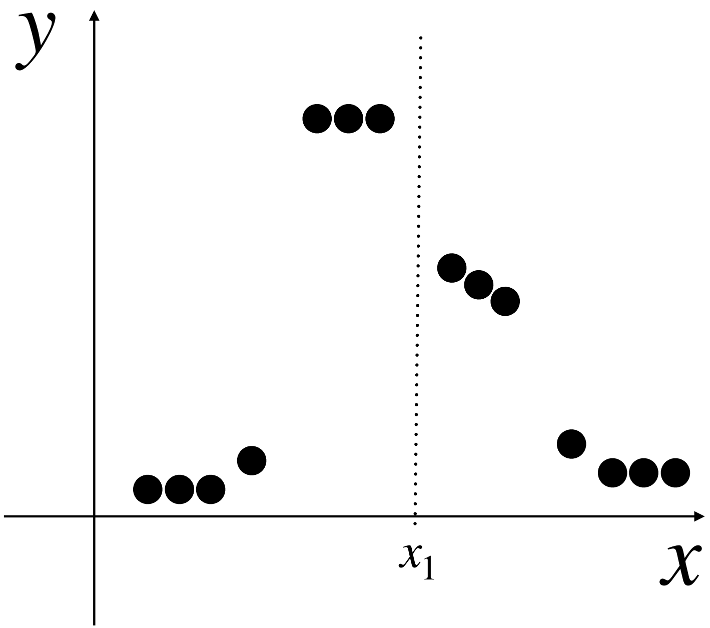

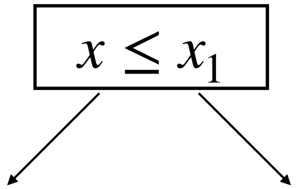

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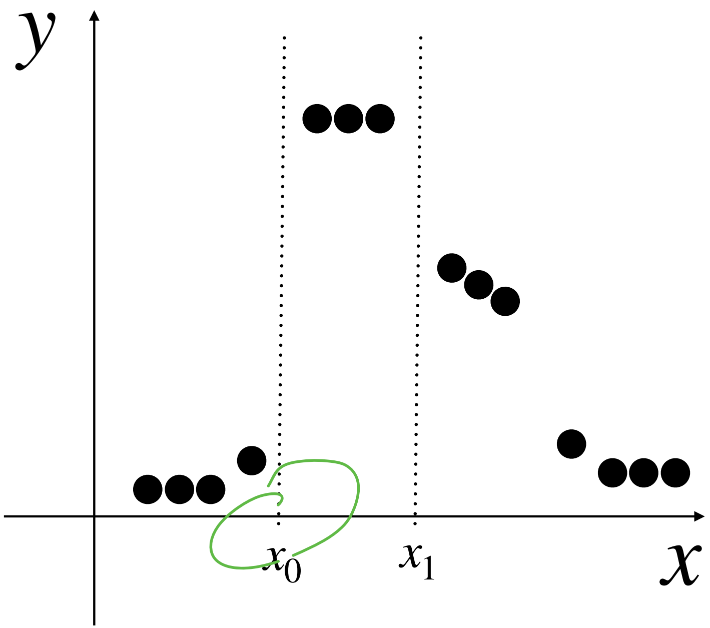

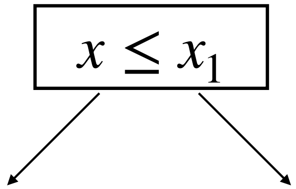

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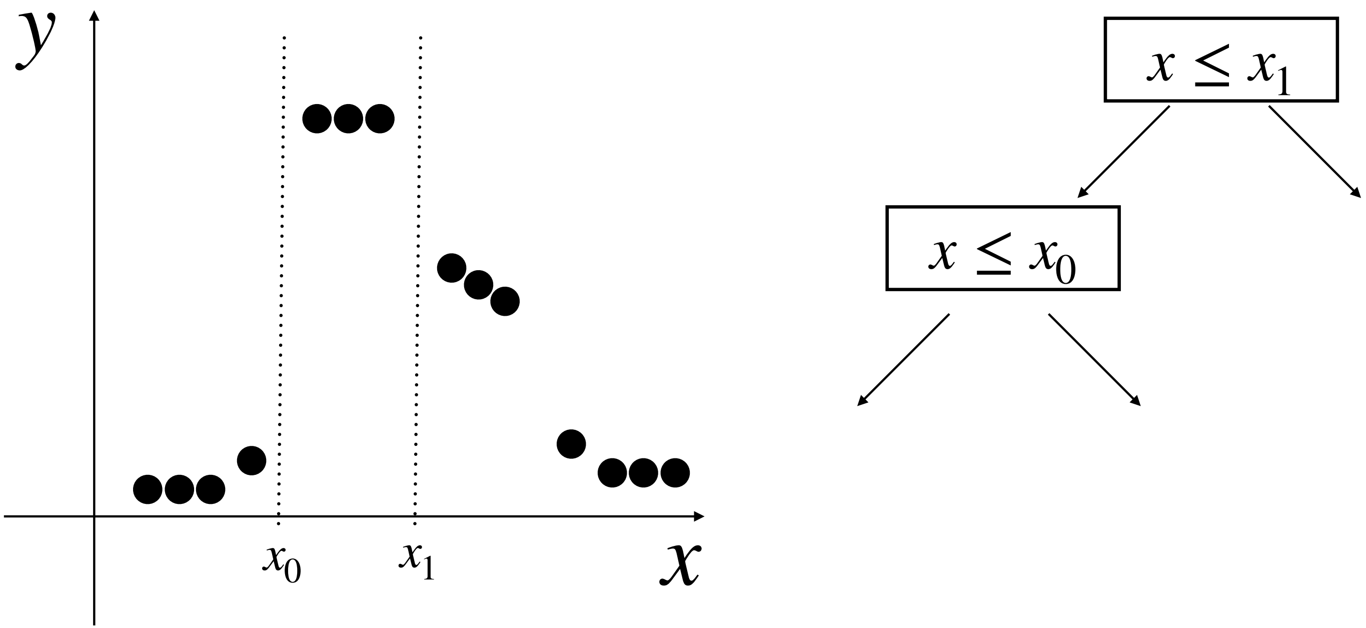

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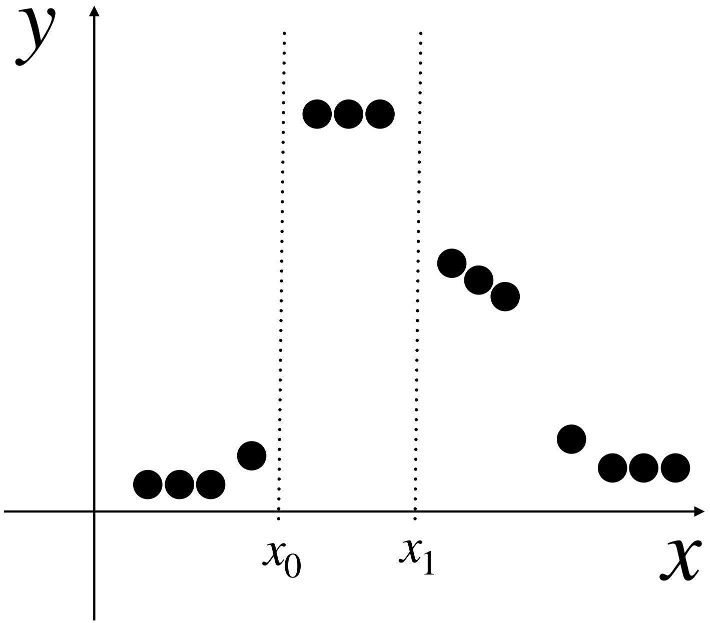

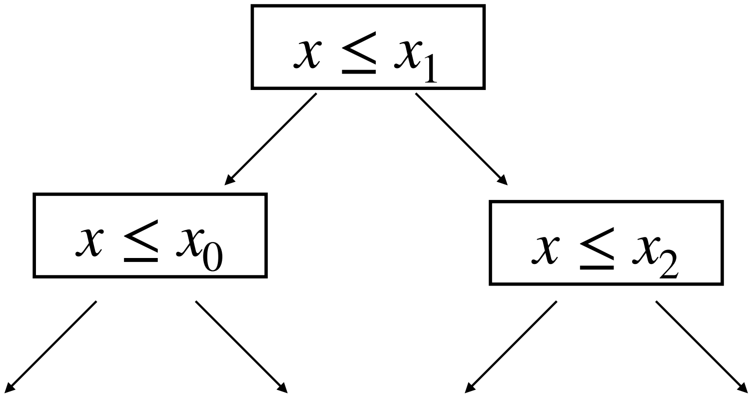

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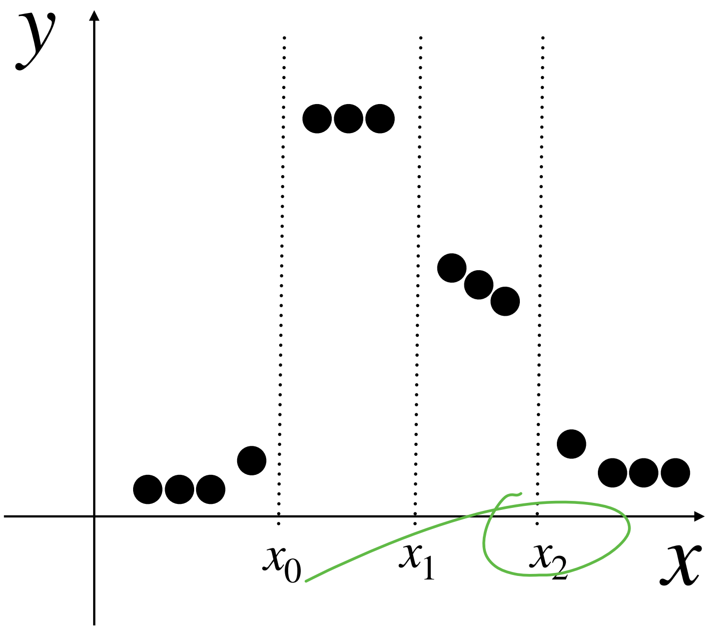

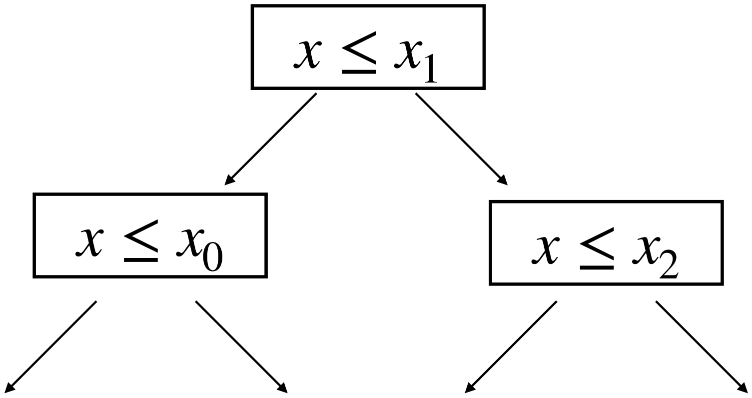

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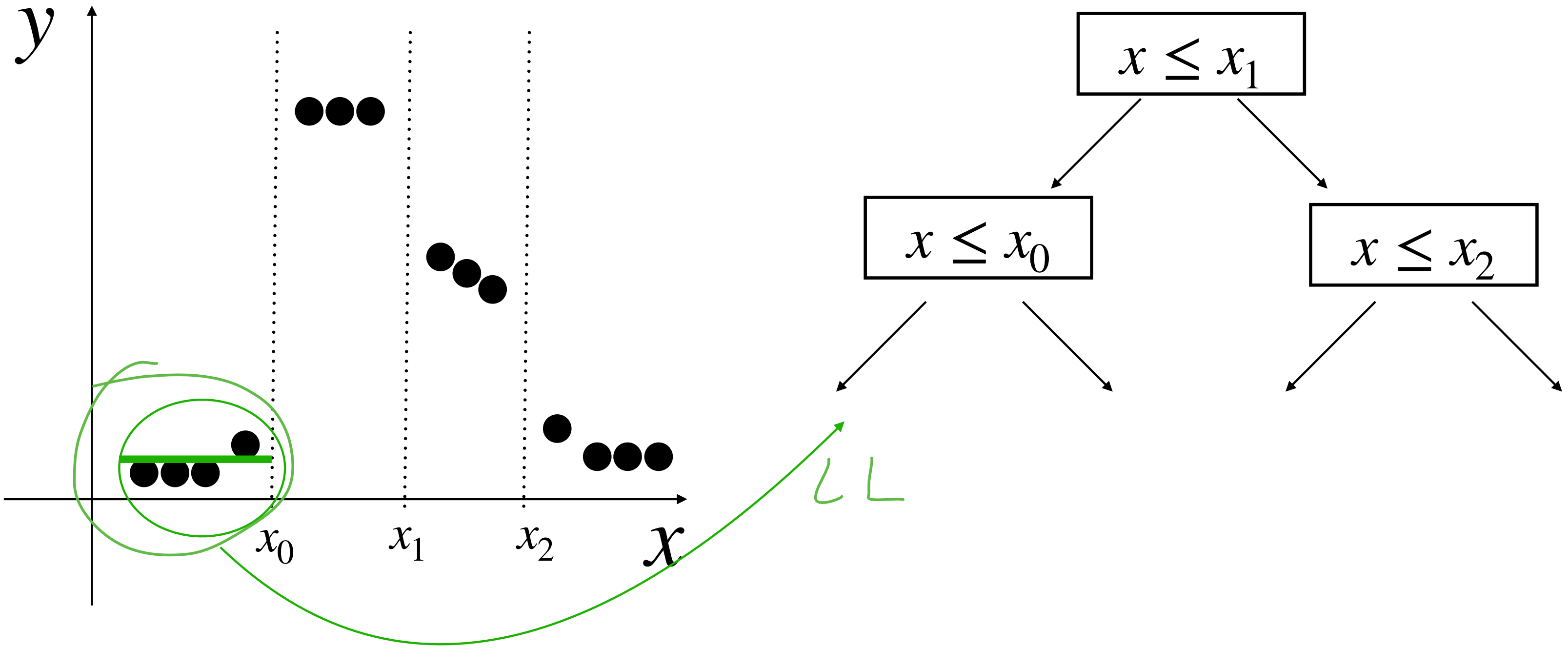

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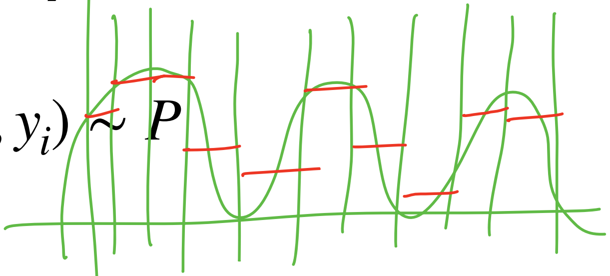

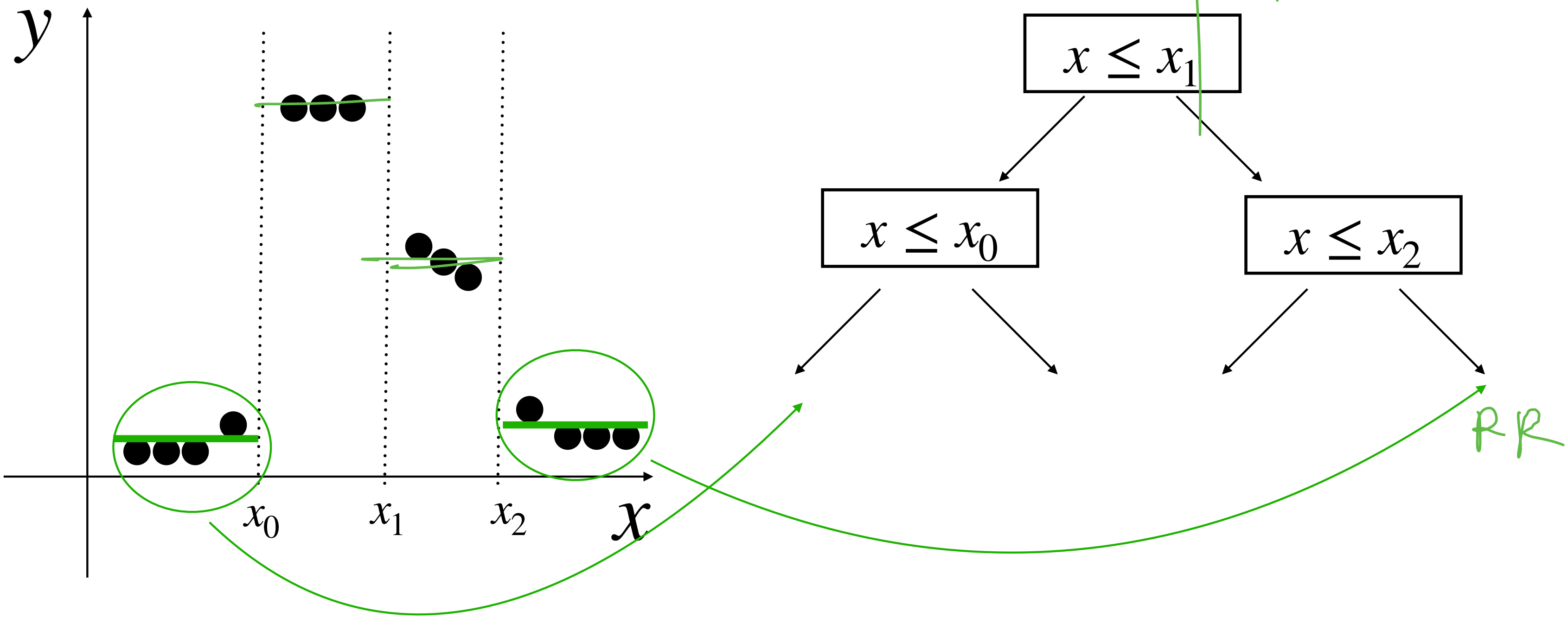

Issues of Decision Trees

Decision Tree can have high variance, i.e., overfilling!

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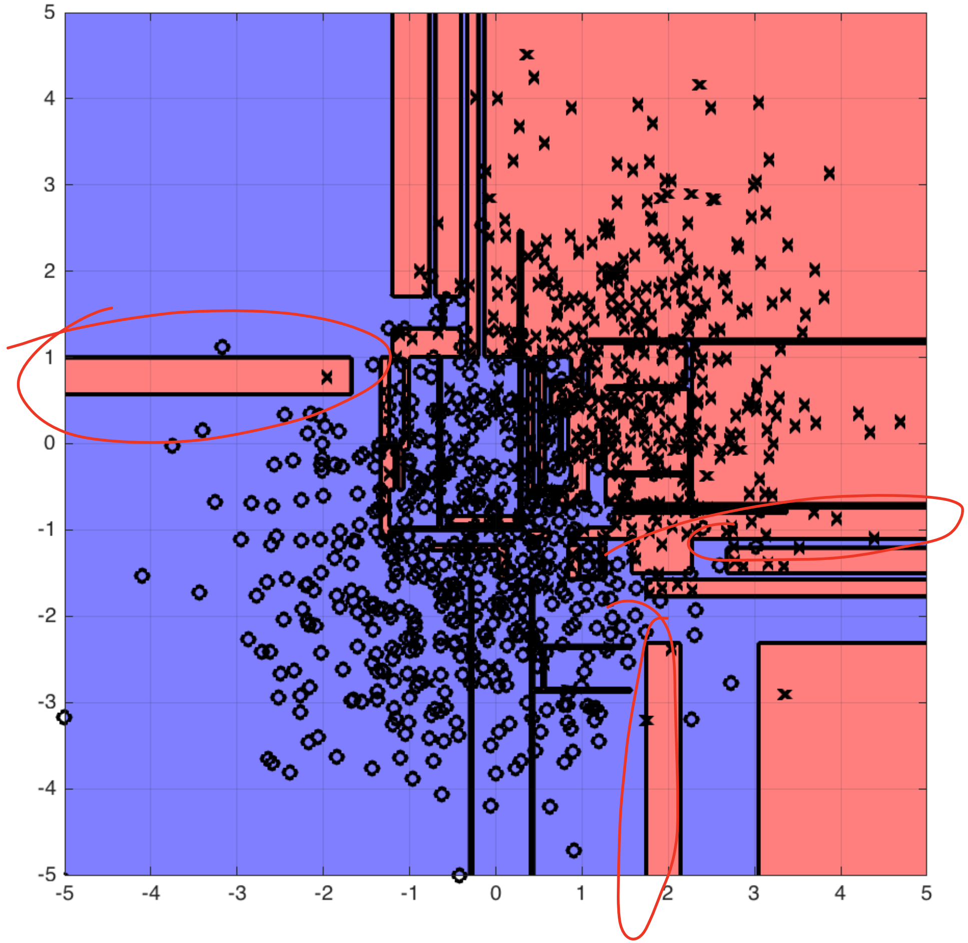

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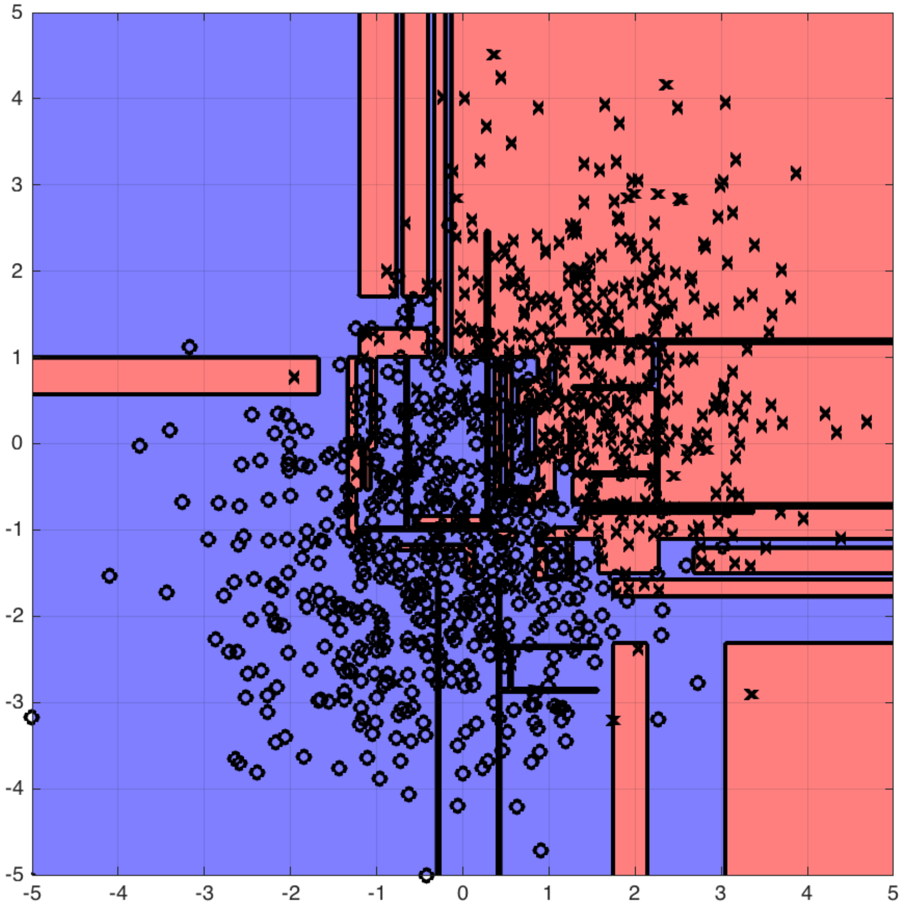

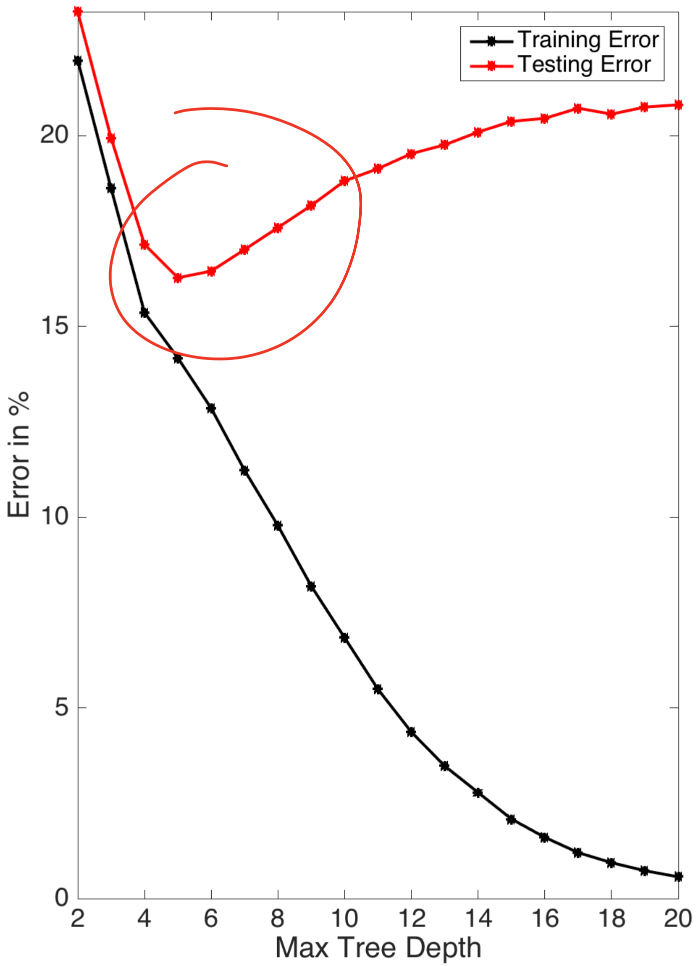

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Common regularizations in Decision Trees

1. Minimum number of examples per leaf

No split if # of examples < threshold

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1. Minimum number of examples per leaf

No split if # of examples < threshold

2. Maximum Depth

No split if it hits depth limit

3. Maximum number of nodes

Stop the tree if it hits max # of nodes

Outline of Today

1. Variance Reduction using averaging

2. Bagging: Bootstrap Aggregation

3. Random Forest

Variance Reduction via Averaging

Consider i.i.d random variables $\{x_i\}_{i=1}^{n}, \quad x_i \sim \mathcal{N}(0, \sigma^2)$

$$\text{Var}(x_i) = \sigma^2$$

Variance Reduction via Averaging

Consider i.i.d random variables $\{x_i\}_{i=1}^n, \quad x_i \sim \mathcal{N}(0,\sigma^2)$

$$\text{Var}(x_i) = \sigma^2$$

$n = 2$

Q: what is the variance of $\bar{x} = \sum_{i=1}^{n} x_i / n$

$n \to \infty$

$\bar{x} \mapsto E[x] = 0$

$$\text{Var}(\bar{x}) = \frac{\sigma^2}{n}$$

$n \to \infty \quad \text{Var}(\bar{x}) \to 0$

Variance Reduction via Averaging

Consider i.i.d random variables $\{x_i\}_{i=1}^n, \quad x_i \sim \mathcal{N}(0, \sigma^2)$

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Q: what is the variance of $\bar{x} = \sum_{i=1}^{n} x_i / n$

Avg significantly reduced variance!

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$n=3 \qquad x_i \sim N(0, \sigma^2)$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \sigma^2 & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{2,1} & \sigma^2 & \sigma_{2,3} \\ \sigma_{3,1} & \sigma_{3,2} & \sigma^2 \end{bmatrix}\right)$$

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$$\sigma_{i,j} = \mathbb{E}[x_i x_j] \qquad \sigma_{ij} > 0$$

Variance Reduction via Averaging

Consider (possibly correlated) random variables $\{x_i\}_{i=1}^n, \quad x_i \sim \mathcal{N}(0,\sigma^2)$

Q: what is the variance of $\bar{x} = \sum_{i=1}^{3} x_i/3$

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Consider (possibly correlated) random variables $\{x_i\}_{i=1}^{n}, \quad x_i \sim \mathcal{N}(0,\sigma^2)$

$$\mathrm{Var}\left(\frac{x_1+x_2+x_3}{3}\right) = \mathbb{E}\left[\left(\frac{x_1+x_2+x_3}{3}\right)^2\right]$$

Q: what is the variance of $\bar{x} = \sum_{i=1}^{3} x_i/3$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \sigma^2 & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{2,1} & \sigma^2 & \sigma_{2,3} \\ \sigma_{3,1} & \sigma_{3,2} & \sigma^2 \end{bmatrix}\right)$$

A: $\mathrm{Var}(\bar{x}) = \sigma^2/3 + \sum_{i \neq j} \sigma_{i,j}/9$ $= 1$

$\sigma = 1$

$\sigma_{i,j} = 1$

$$\sigma_{i,j} = \mathbb{E}[x_i x_j]$$

Variance Reduction via Averaging

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Worst case: when these RVs are positively correlated, averaging may not reduce variance

Outline of Today

1. Variance Reduction using averaging

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Why Bagging

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$\hat{h}$ is a random quantity + it has high variance

Q: can we learn multiple $\hat{h}$ and perform averaging to reduce variance?

Yes, we do this via Bootstrap

Detour: Bootstrapping

$z_i = (x_i, y_i)$

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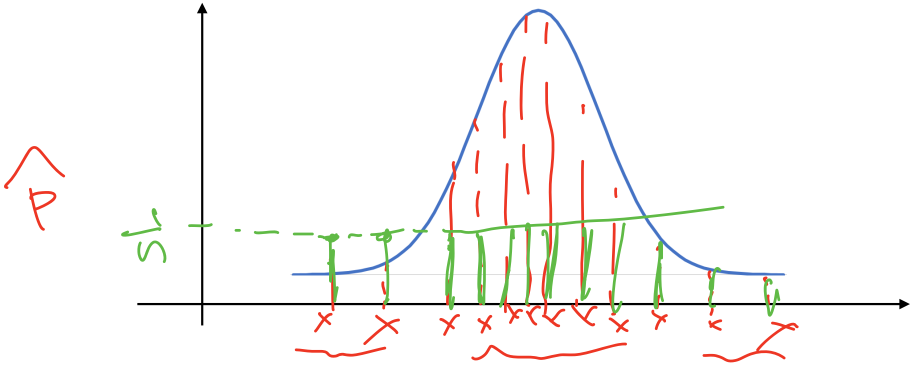

Bootstrapping

$$\widehat{P}(z_i) = 1/n, \forall i \in [n]$$

Why $\hat{P}$ can be regarded as an approximation of P?

$$E_{z \sim p}[z]$$

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$$\mathbb{E}_{z \sim \hat{P}}[z] = \sum_{i=1}^{n} \frac{z_i}{n}$$

$\hat{P}$ $\varphi(z_i)$

$= \frac{1}{n}$

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LLN

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$$\mathbb{E}_{z\sim\hat{P}}[z^3] \longmapsto \mathbb{E}_{z\sim P}[z^3]$$

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2. In fact for any $f : Z \rightarrow \mathbb{R}$

f(z) ex, z³

$$\mathbb{E}_{z\sim\hat{P}}[f(z)] = \sum_{i=1}^{n} \frac{f(z_i)}{n} \rightarrow \mathbb{E}_{z\sim P}[f(z)]$$

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A: $(1 - 1/n)^n \rightarrow 1/e, n \rightarrow \infty$

0.36

Bagging: Bootstrap Aggregation

Consider dataset $\mathscr{D} = \{x_i, y_i\}_{i=1}^n$, $(x_i, y_i) \sim P, x_i \in \mathbb{R}^d, y_i \in \{-1,1\}$

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2. Treat $\hat{P}$ as the ground truth, draw k datasets $\mathcal{D}_1, \mathcal{D}_2, \ldots, \mathcal{D}_k$ from $\hat{P}$

$D_1 \sim \hat{P}$

$D_2 \sim \hat{P}$

$D_3 \sim \hat{P}$

$\vdots$

$D_k \sim \hat{P}$

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3. For each $i \in [k]$, train classifier, e.g., $\hat{h}_i = \text{ID3}(\mathcal{D}_i)$

$\rightarrow \{\hat{h}_1, \ldots, \hat{h}_k\}$

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$|D_i|$

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$\hat{h}_i(x) \to y_i \in R$

4. Averaging / Aggregation, i.e., $\bar{h} = \sum_{i=1}^k \hat{h}_i / k$

$\bar{h}(x) = \sum_{i=1}^{k} y_i / k$

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The step that reduces Var!

Bagging in Test Time

Given a test example x_{test} (binary classification)

We can use $\{\hat{h}_i\}_{i=1}^{k}$ to form a distribution over labels:

$$\hat{y} = \begin{bmatrix} p \\ 1 - p \end{bmatrix}$$

prob of +1

prob of −1

Bagging in Test Time

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We can use $\{\hat{h}_i\}_{i=1}^{k}$ to form a distribution over labels:

$$\hat{y} = \begin{bmatrix} p \\ 1 - p \end{bmatrix}$$

where:

$$p = \frac{\text{\# of trees predicting } +1}{k}$$

Bagging reduces variance

$$\bar{h} = \sum_{i=1}^{k} \hat{h}_i / k$$

What happens when $k \to \infty$?

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What happens when $k \to \infty$?

$\hat{h}_i = ID3(D_i) \quad D_i \sim \hat{P}$

$$\bar{h} \to \mathbb{E}_{\mathcal{D} \sim \hat{P}} \left[\mathrm{ID3}(\mathcal{D}) \right]$$

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↓ $\hat{P} \to P$, when $n \to \infty$

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The expected decision tree (under true P)

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The expected decision tree (under true P)

Deterministic, i.e., zero variance

Outline of Today

1. Variance Reduction using averaging

2. Bagging: Bootstrap Aggregation

3. Random Forest

Motivation of Random Forest

Consider any two hypothesis $\hat{h}_i, \hat{h}_j, i \neq j$ in Bagging

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$$\hat{h}_j \leftarrow D_j \sim \hat{P}$$

$$D_i \cap D_j \neq \emptyset$$

Motivation of Random Forest

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Recall that: $\text{Var}(\bar{x}) = \sigma^2/3 + \sum_{i \neq j} \sigma_{i,j}/9$

σ_{ij} as the correlation between $\hat{h}_i$ $\hat{h}_j$

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Recall that: $\text{Var}(\bar{x}) = \sigma^2/3 + \sum_{i \neq j} \sigma_{i,j}/9$

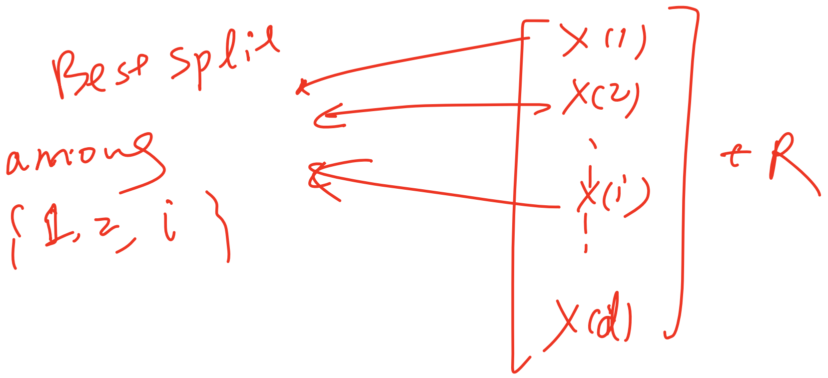
To avoid positive correlation, we want to make $\hat{h}_i, \hat{h}_j$ as independent as possible

Random Forest

Key idea:

In ID3, for every split, **randomly select** k $(k < d)$ many features, find the split **only using these k features**

k=3



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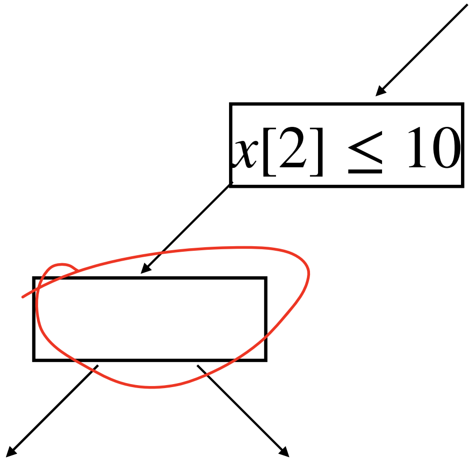

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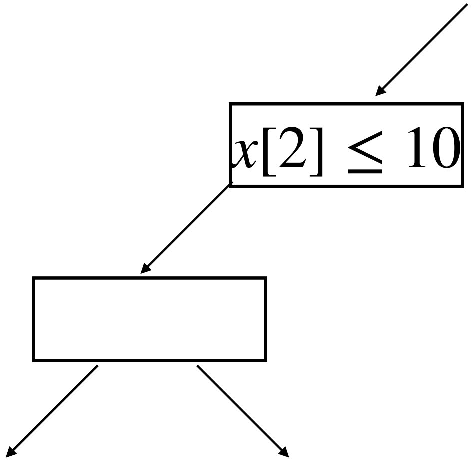

Regular ID3: looking for split in all d dimensions

Random Forest

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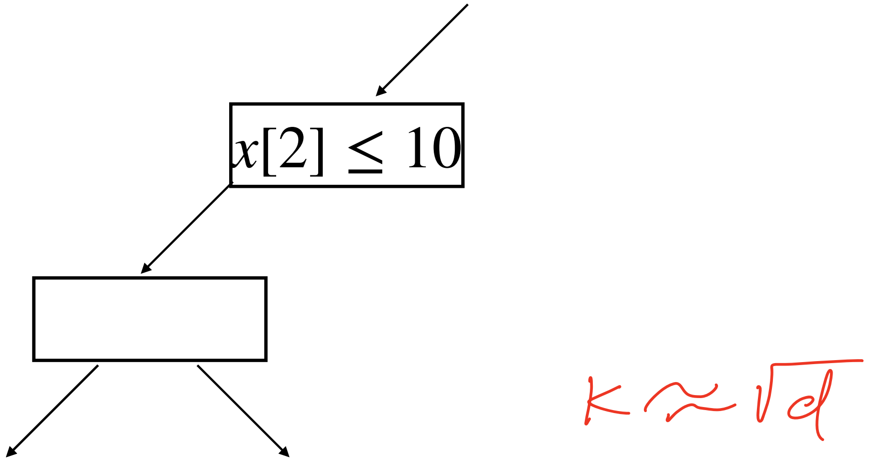


Regular ID3: looking for split in all d dimensions

ID3 in RF: looking for split in k randomly picked dimensions

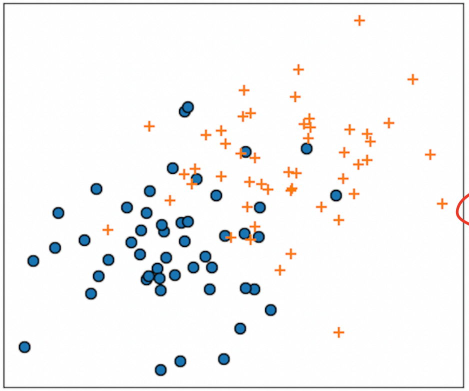
Benefit of Random Forest

By always randomly selecting subset of features for **every tree, and every split**:

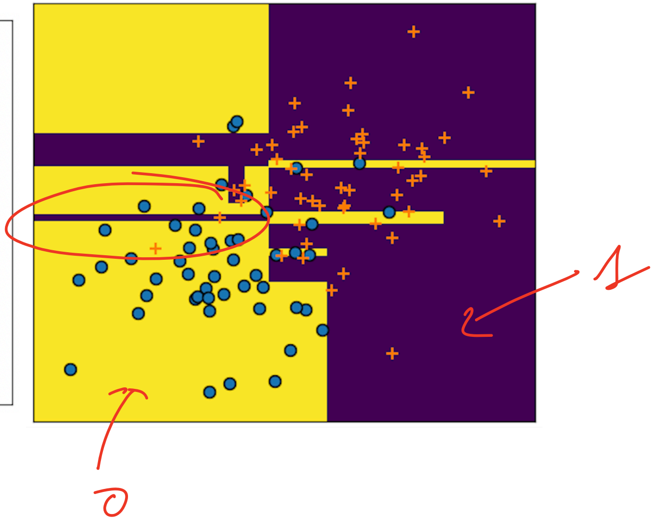
We further reduce the correlation between $\hat{h}_i$ & $\hat{h}_j$

D_i D_j

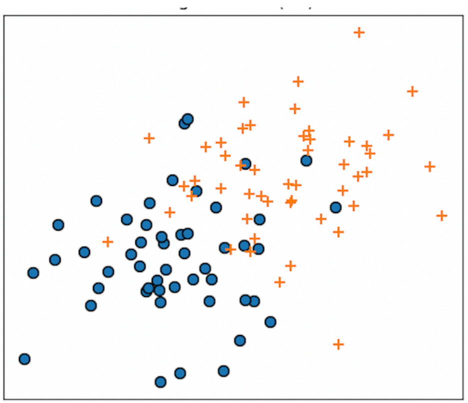
Demo of Random Forest



DT w/ Depth 10



Demo of Random Forest



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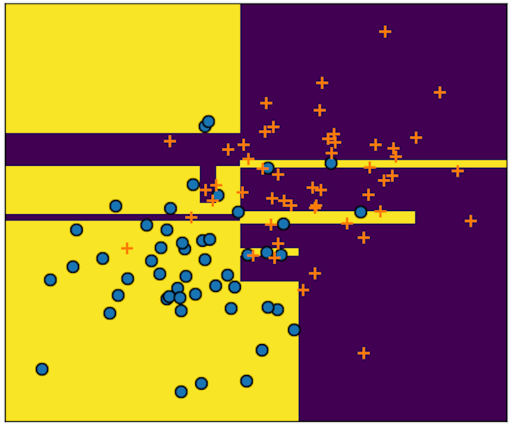
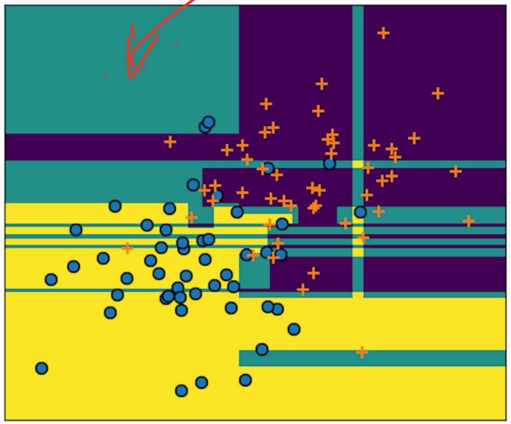
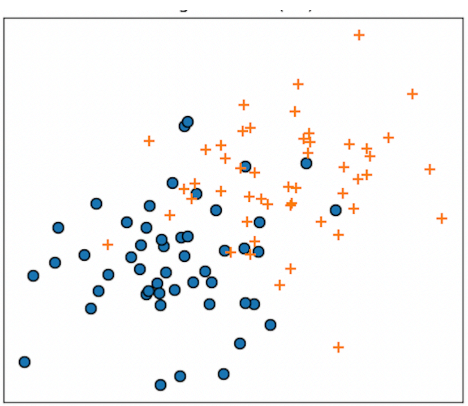


RF w/ 2 trees



Demo of Random Forest



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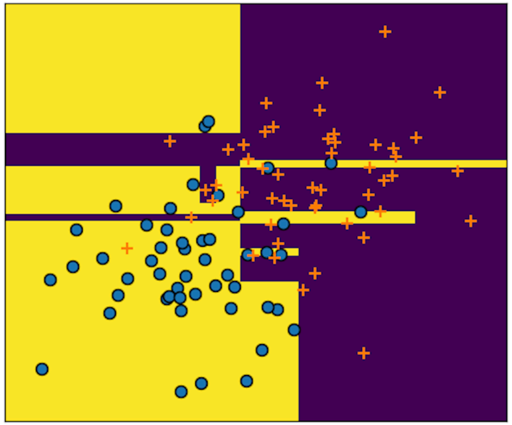

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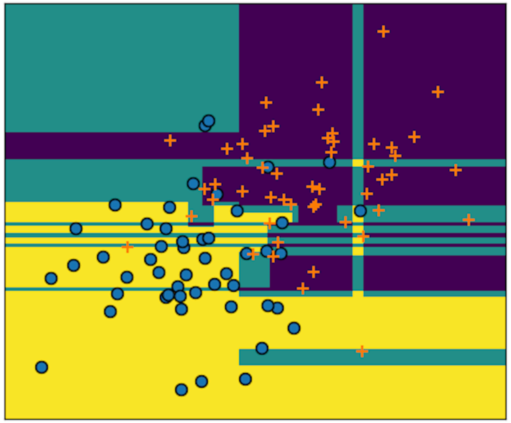
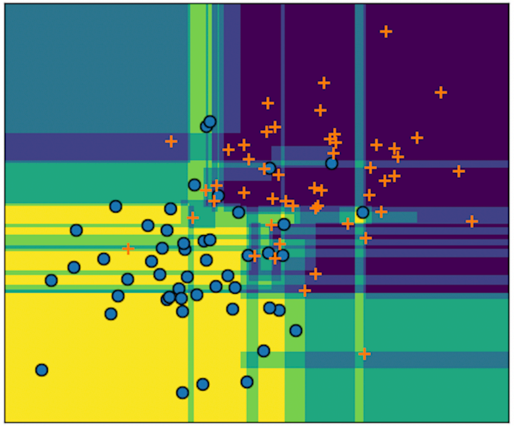
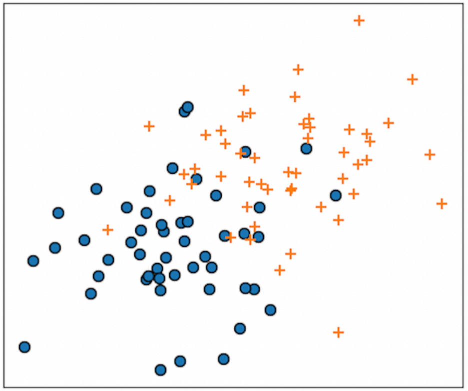


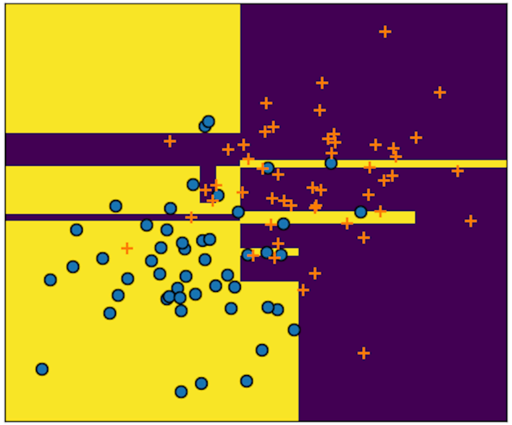
RF w/ 5 trees



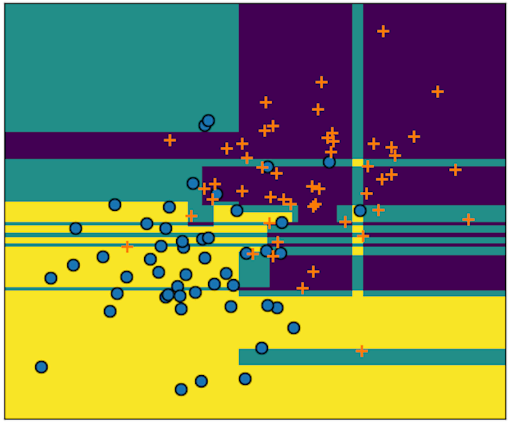
Demo of Random Forest



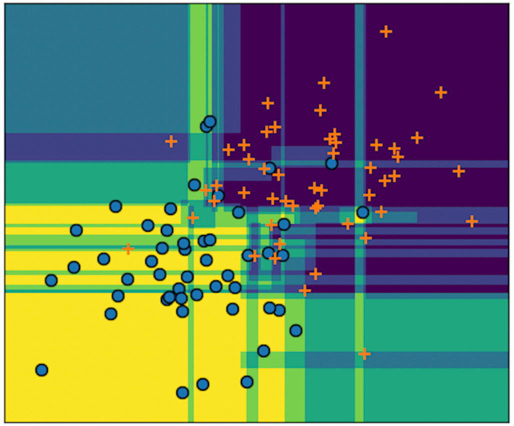
DT w/ Depth 10



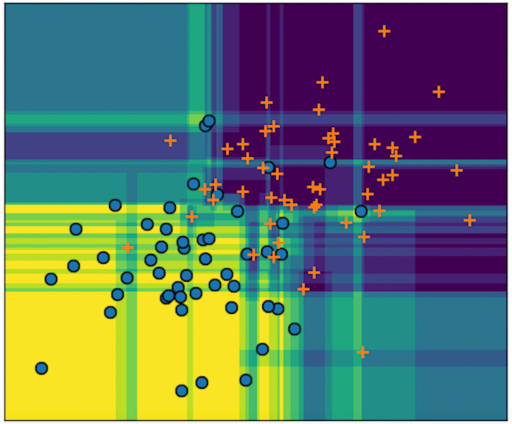
RF w/ 2 trees



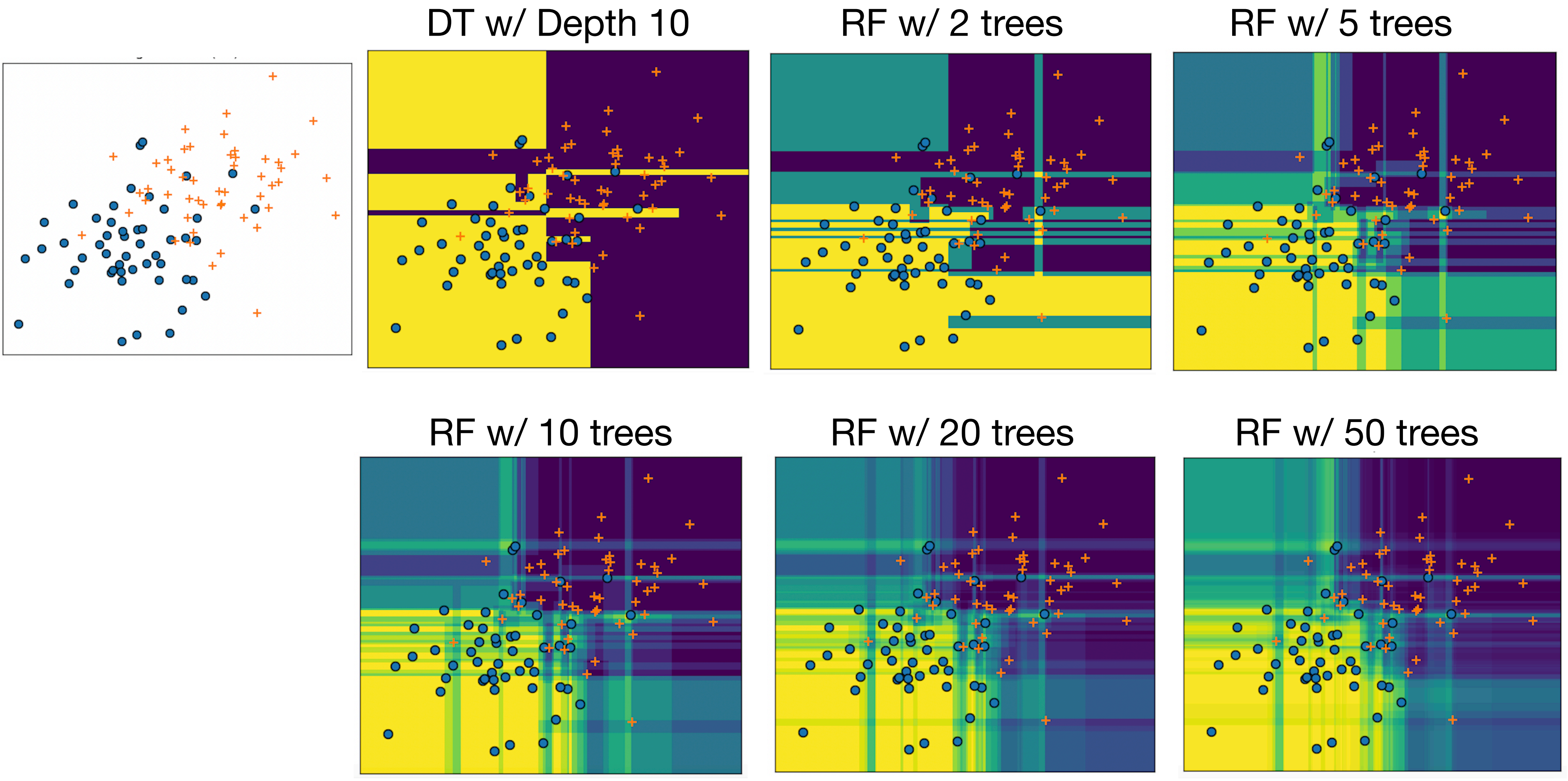
RF w/ 5 trees



RF w/ 10 trees



Demo of Random Forest



Summary for today

An approach to reduce the variance of our classifier:

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1. Create datasets via bootstrapping + train classifiers on them + averaging

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1. Create datasets via bootstrapping + train classifiers on them + averaging

2. To further reduce correlation between classifiers, RF randomly selects subset of dimensions for every split.