COMS 4771 Lecture 4

1. K-D trees for nearest neighbor search.
2. Decision trees.

K-D trees for nearest neighbor search

Tree structures for one-dimensional data

A data structure for fast NN search in $\mathbb{R}^1$

Sort training data so that $x_1 \leq x_2 \leq \cdots \leq x_n$, then construct binary tree.

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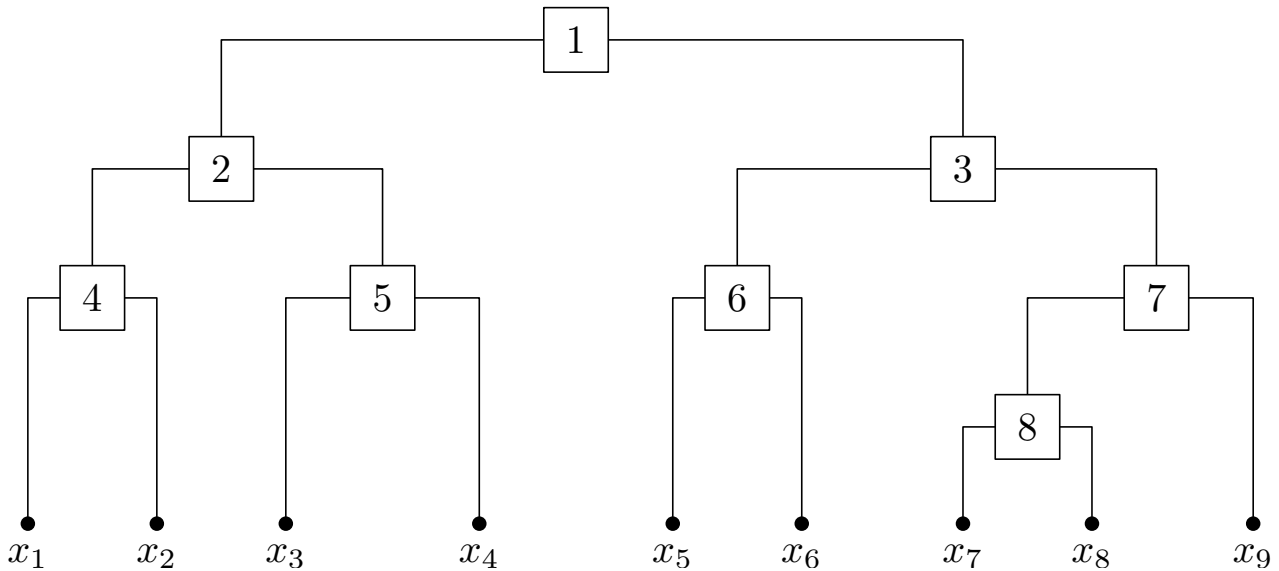

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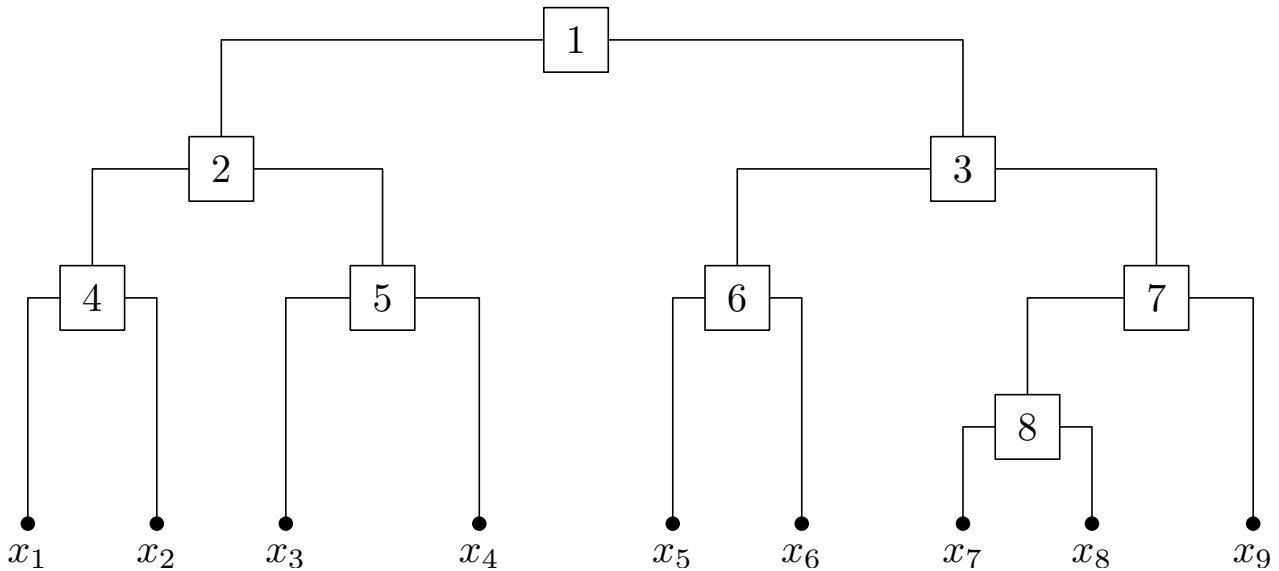

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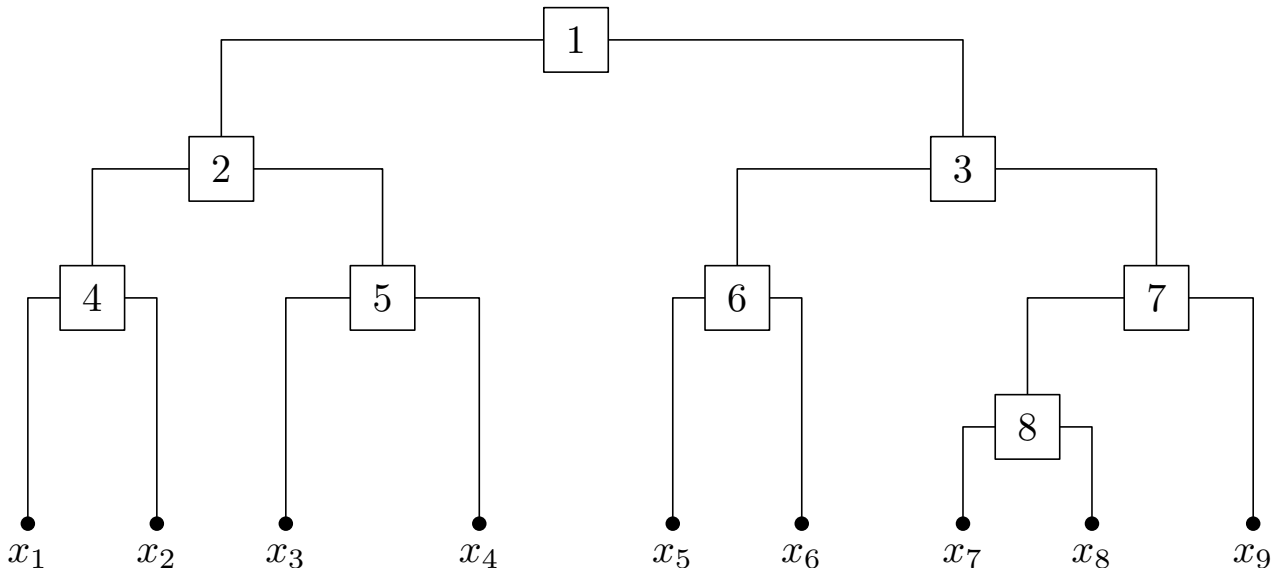

With each tree node, remember **midpoint** between rightmost point in left child, and leftmost point in right child. **This permits very efficient NN search.**

If tree is (approximately) balanced, then $O(\log(n))$ time to find NN!

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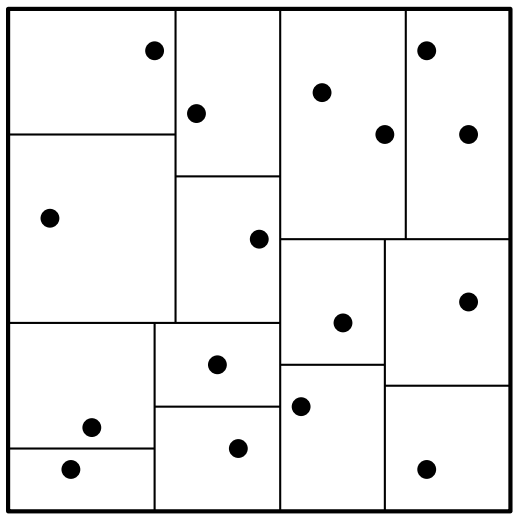
Given points $S \subset \mathbb{R}^d$:

1. Pick a coordinate $j \in \{1, 2, \ldots, d\}$.
2. Let m be the median of $\{x_j : \boldsymbol{x} \in S\}$.
3. Split points into halves:

$$L := \{\boldsymbol{x} \in S : x_j < m\},$$
$$R := \{\boldsymbol{x} \in S : x_j \geq m\}.$$

4. Recurse on L and R.



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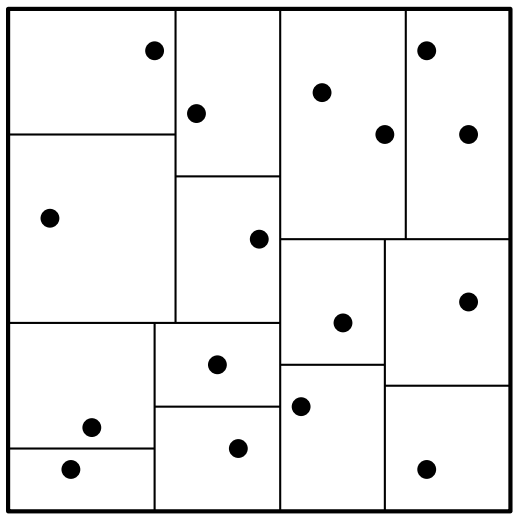

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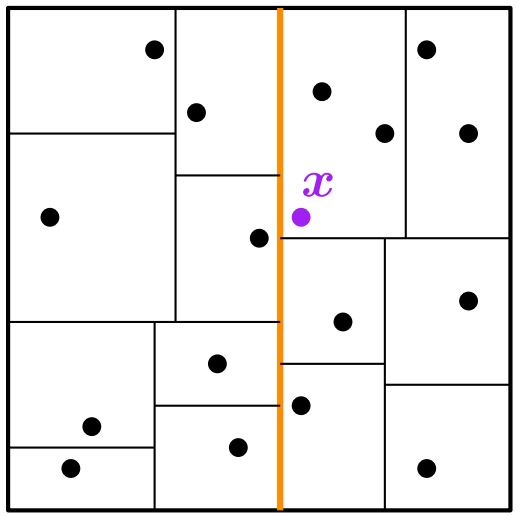

Easy to lookup points in S (in $O(\log(n))$ time), but how about NN search?

Same $O(\log(n))$-time routing of a test point $\boldsymbol{x} \in \mathbb{R}^d$ is **overly optimistic**:
might not yield the NN!

Searching K-D trees using geometry

For K-D trees:
L and R are separated by a hyperplane $H = \left\{ \boldsymbol{z} \in \mathbb{R}^d : z_j = m \right\}$.

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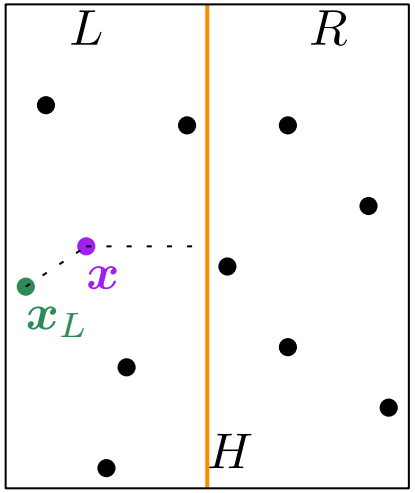

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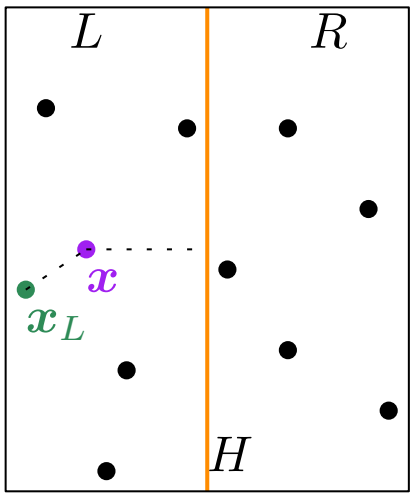
By geometry,

$$\min_{\boldsymbol{x}' \in R} \|\boldsymbol{x} - \boldsymbol{x}'\|_2 \geq \text{distance from } \boldsymbol{x} \text{ to } H$$
$$= |x_j - m|.$$



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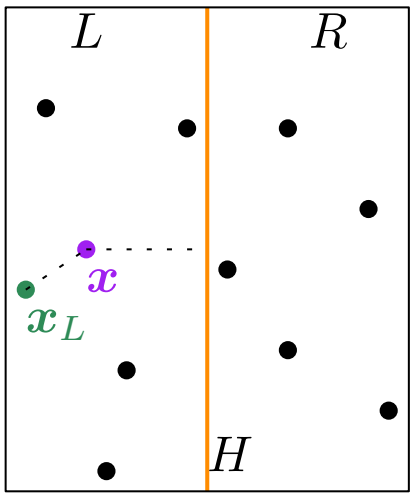

A valid check: if $\|\boldsymbol{x} - \boldsymbol{x}_L\|_2 < |x_j - m|$, then

$$\|\boldsymbol{x} - \boldsymbol{x}_L\|_2 < \min_{\boldsymbol{x}' \in R} \|\boldsymbol{x} - \boldsymbol{x}'\|_2.$$

In this case, we can skip searching R and immediately return $\boldsymbol{x}_L$.

Efficient NN search?

For certain kinds of binary space partition trees (similar to K-D trees), NN search typically completes in $O(2^d \log(n))$ time.

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Question: Can we use trees to directly build good classifiers?

Decision trees

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Directly optimize tree structure for good classification.

A **decision tree** is a function $f : \mathcal{X} \to \mathcal{Y}$, represented by a binary tree in which:

- Each **tree node** is associated with a splitting rule $h : \mathcal{X} \to \{0, 1\}$.
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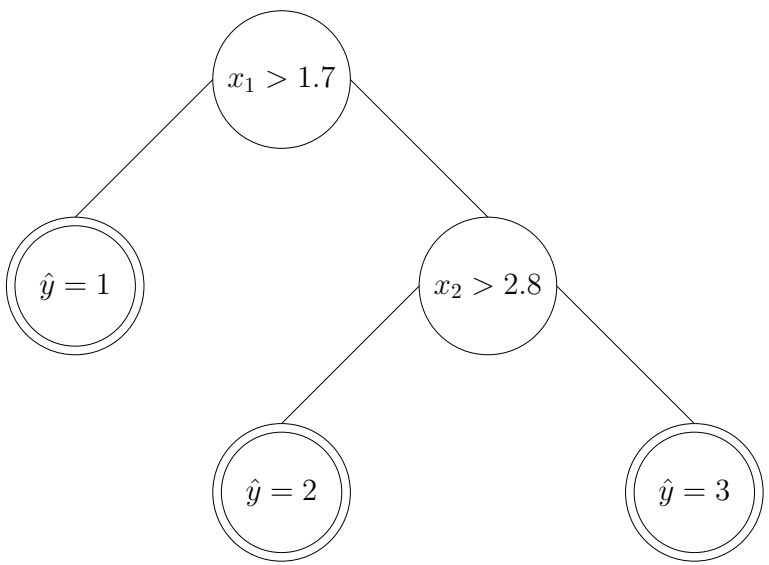
When $\mathcal{X} = \mathbb{R}^d$, typically only consider splitting rules of the form

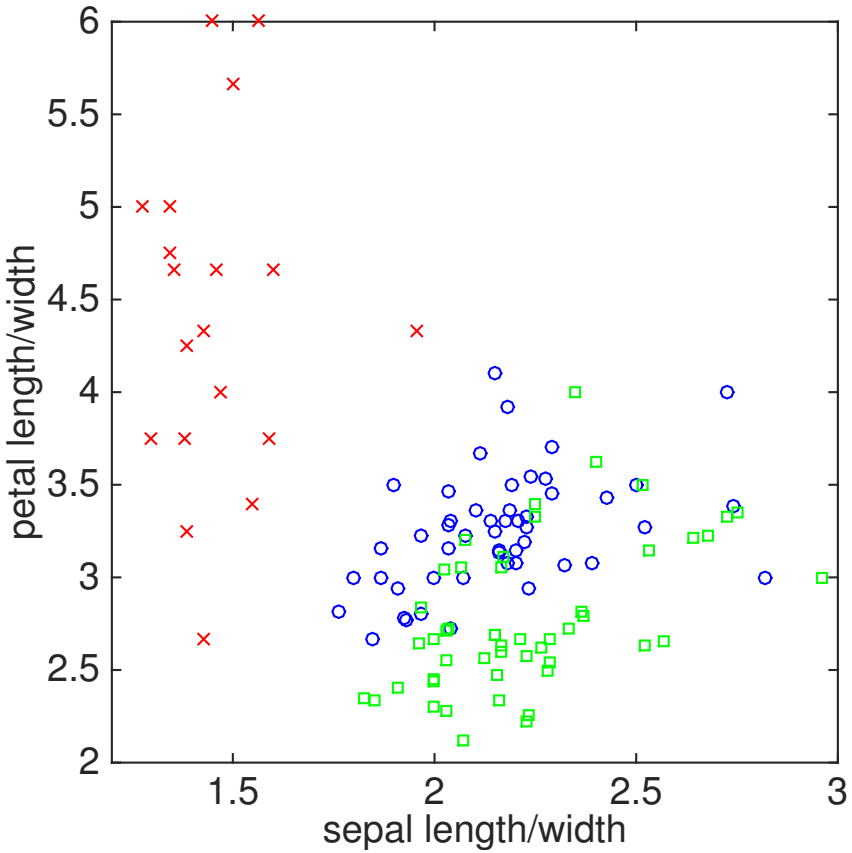
$$h(\boldsymbol{x}) = \mathbb{1}\{x_i > t\}$$

for some $i \in [d]$ and $t \in \mathbb{R}$.
Called *axis-aligned*, *coordinate*, or *Stoller* splits.

(Notation: $[d] := \{1, 2, \ldots, d\}$)



Decision tree example



Classifying irises by sepal and petal measurements

- $\mathcal{X} = \mathbb{R}^2$, $\mathcal{Y} = \{1, 2, 3\}$
- $x_1 =$ ratio of sepal length to width
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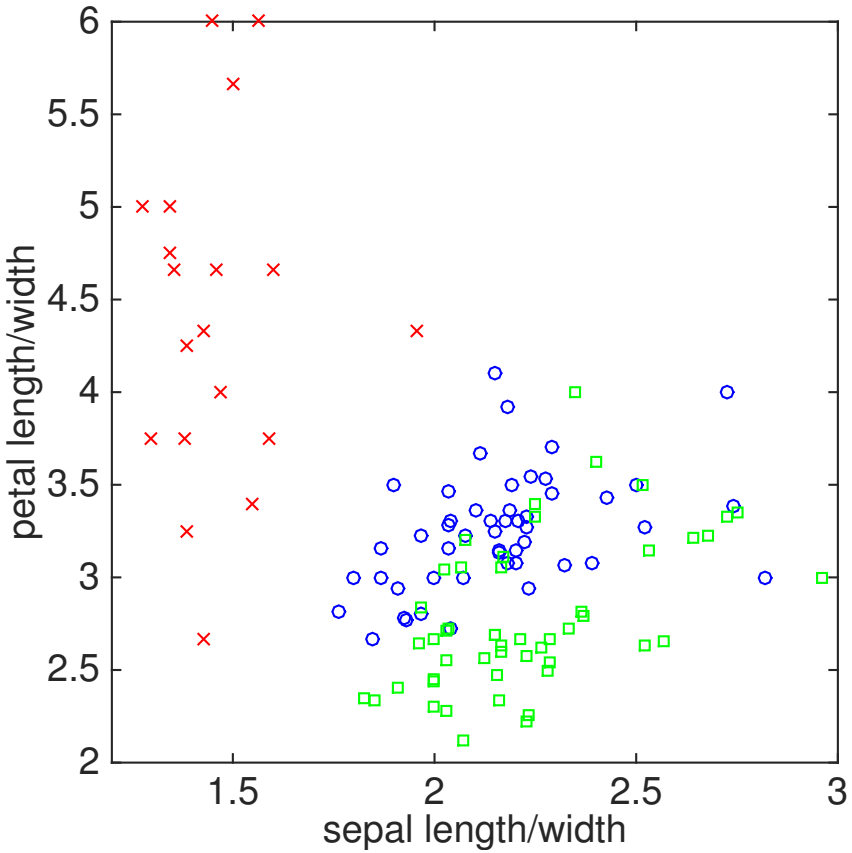

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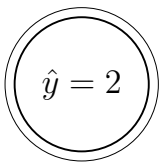

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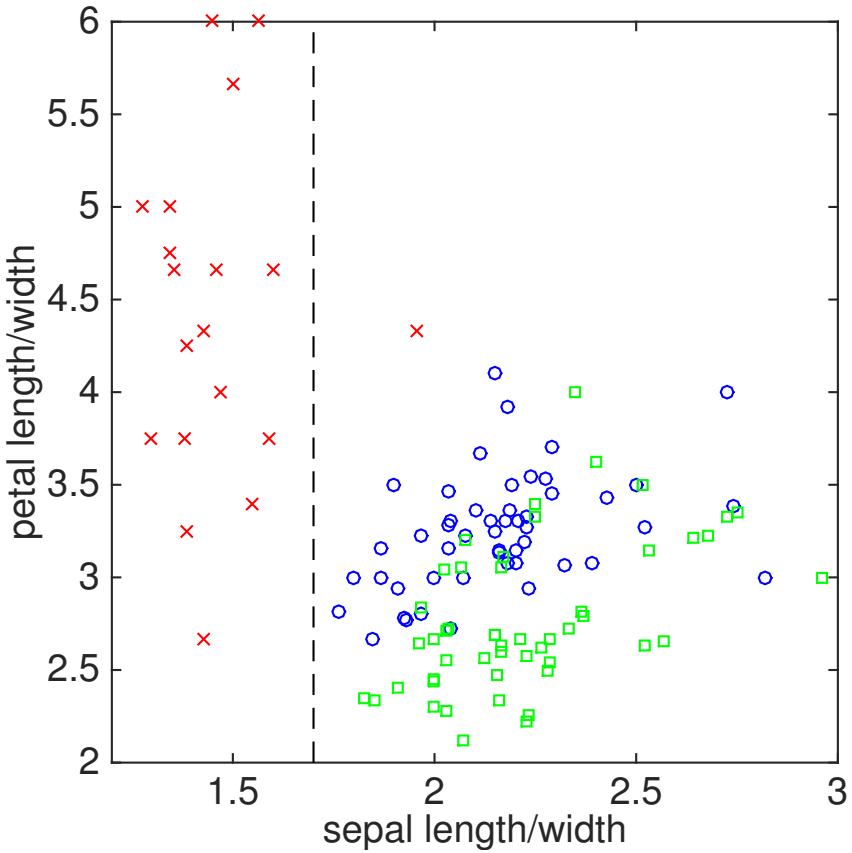

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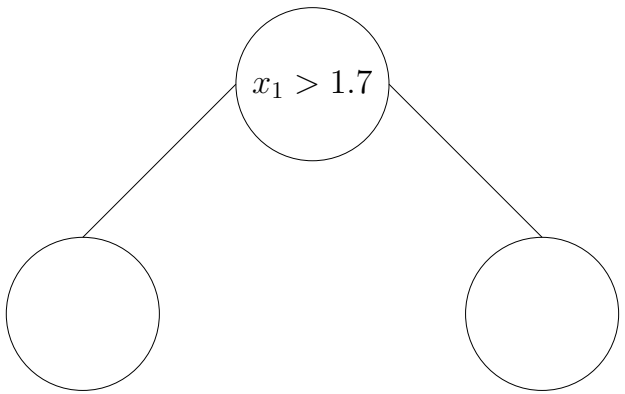

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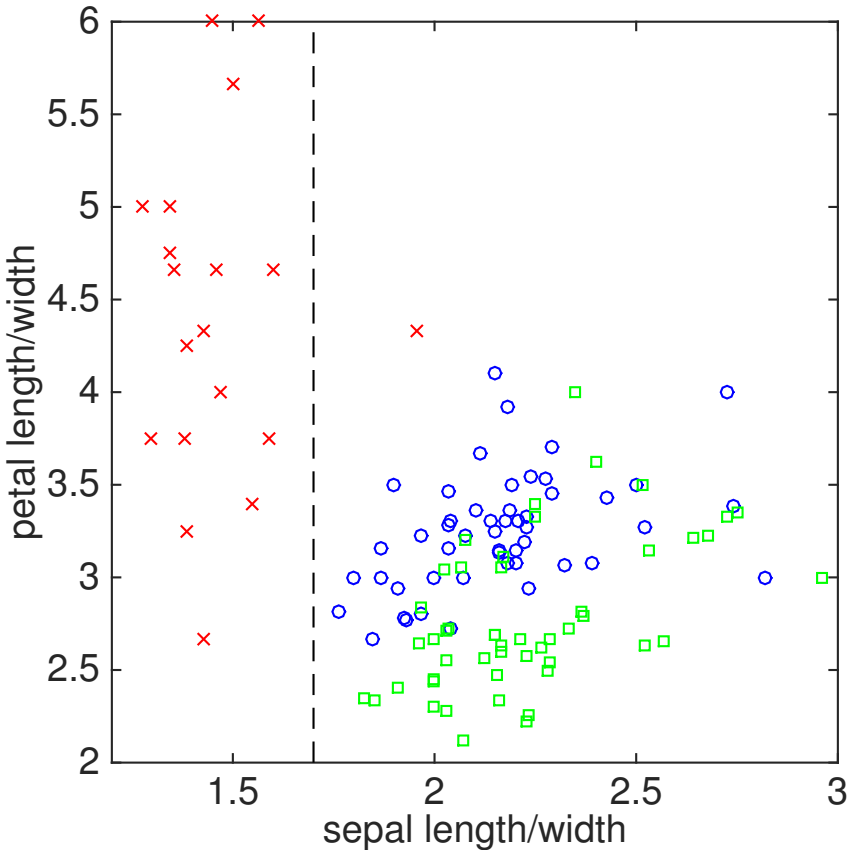

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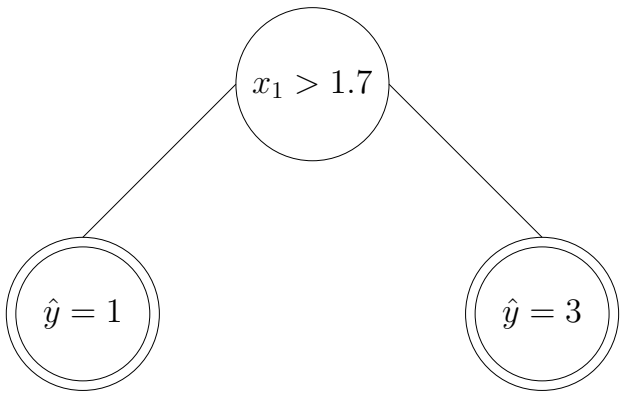

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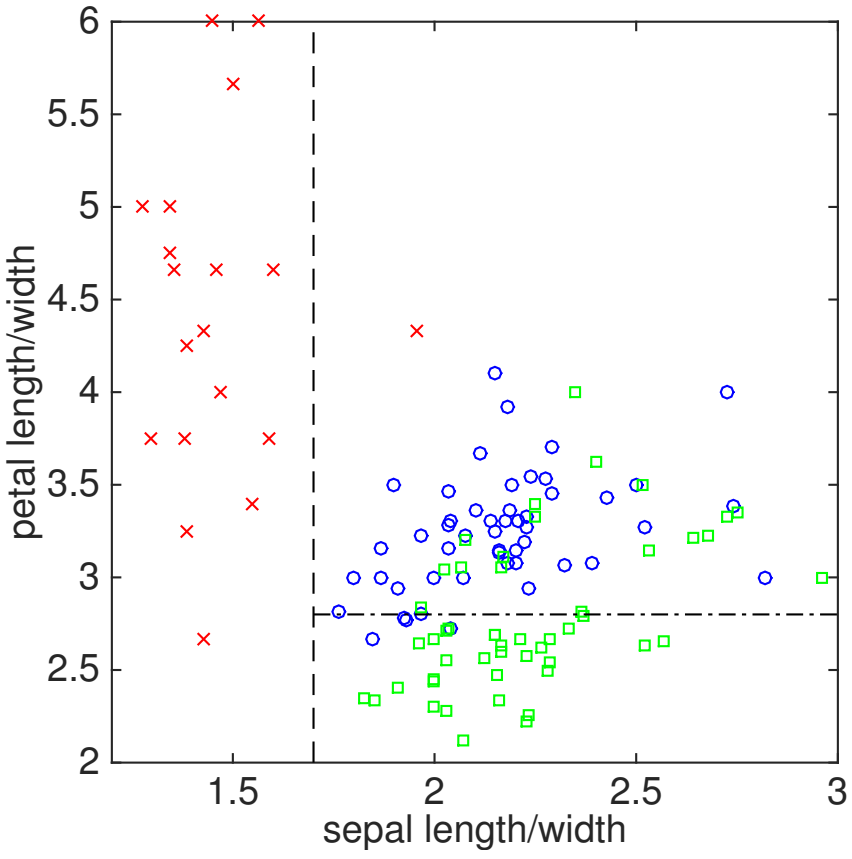

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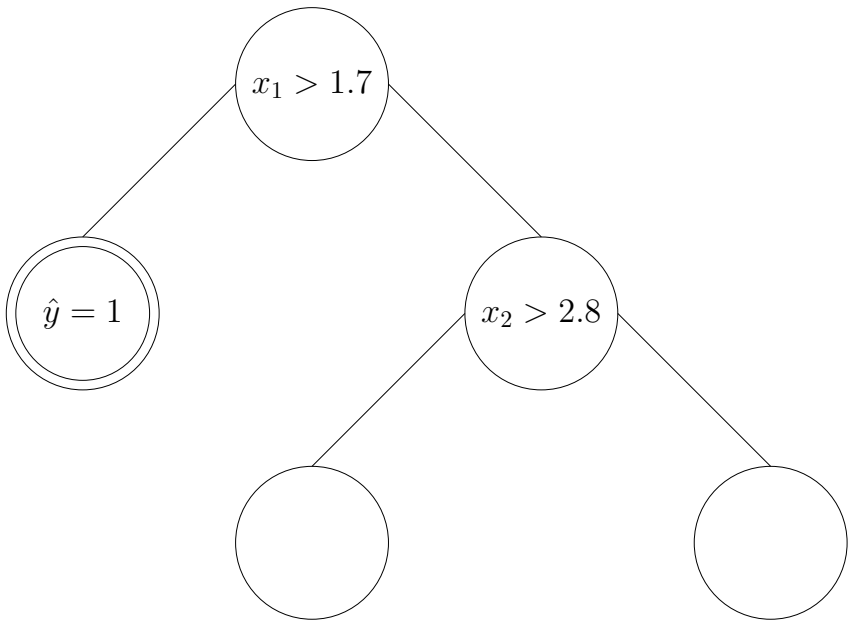

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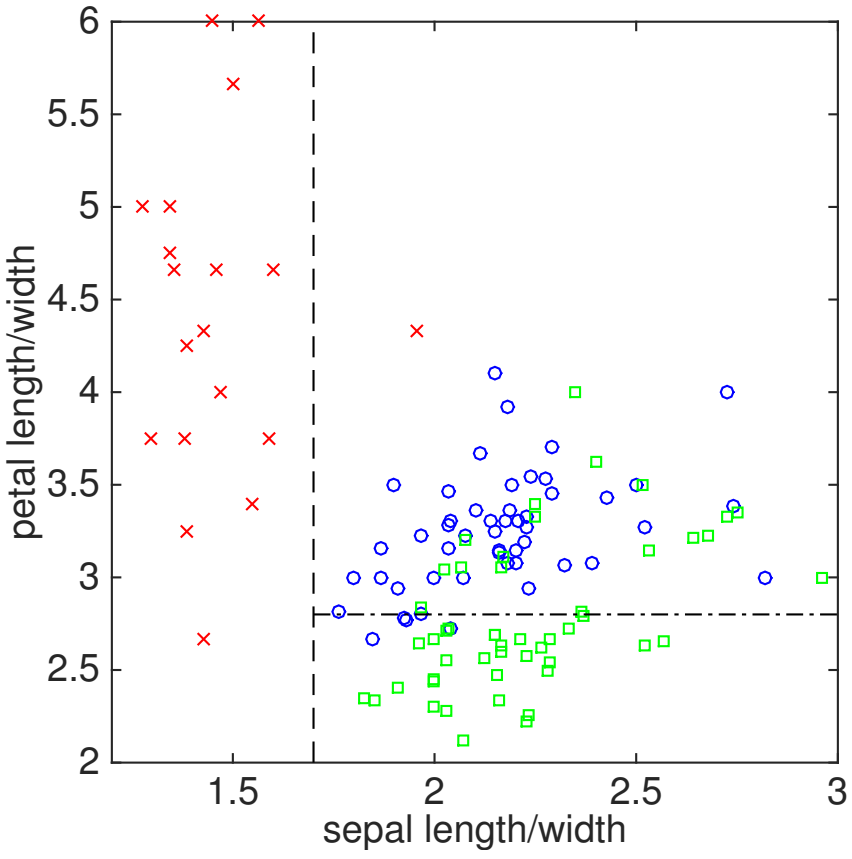

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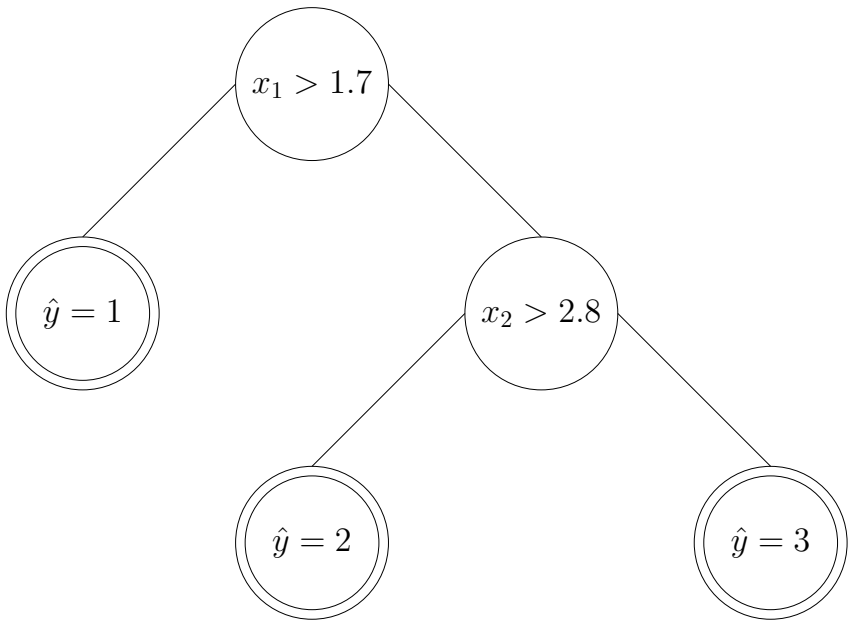
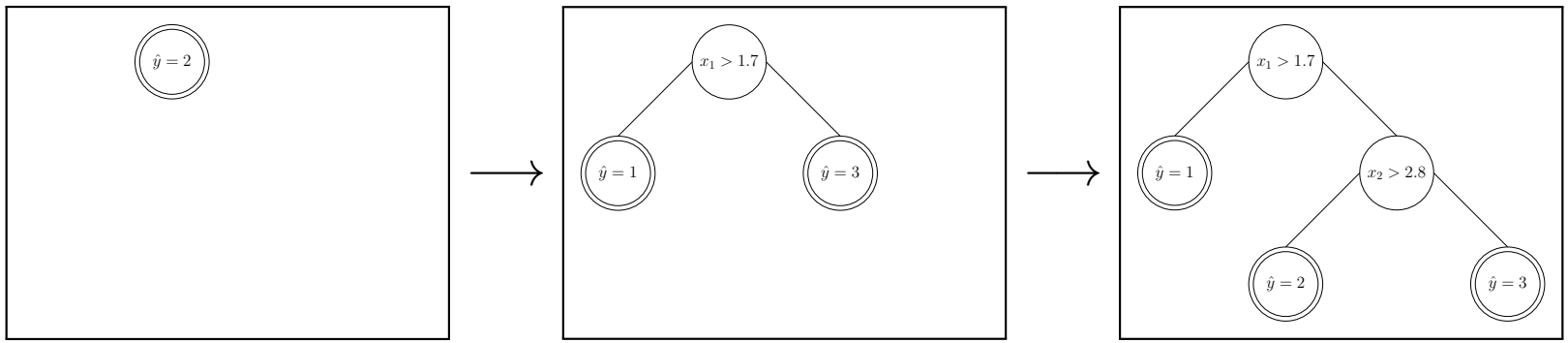


Basic decision tree learning algorithm



Basic "top-down" greedy algorithm

- Initially, tree is a single leaf node containing all (training) data.
- Loop:
  - Pick the leaf ℓ and rule h that maximally reduces uncertainty.
  - Split data in ℓ using h, and grow tree accordingly.

  ...until some stopping criterion is satisfied.

[**Label of a leaf** is the **plurality label** among the data contained in the leaf.]

Notions of uncertainty: binary case ($\mathcal{Y} = \{0, 1\}$)

Suppose in a set of examples $S \subseteq \mathcal{X} \times \{0, 1\}$, a p fraction are labeled as 1.

1. **Classification error**:

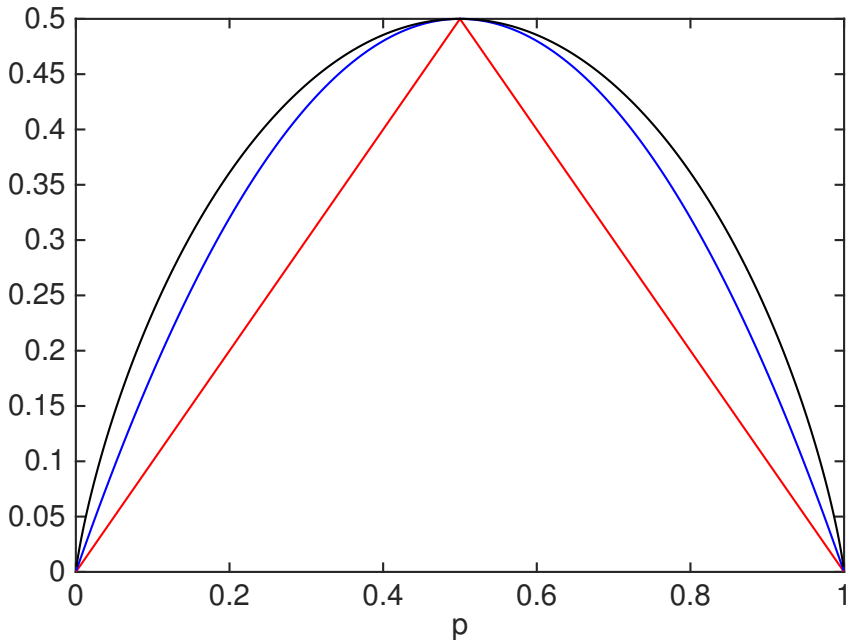
$$u(S) := \min\{p,\, 1 - p\}$$

2. **Gini index**:

$$u(S) := 2p(1 - p)$$

3. **Entropy**:

$$u(S) := p \log \frac{1}{p} + (1-p) \log \frac{1}{1-p}$$



Gini index and entropy (after some rescaling) are concave upper-bounds on classification error.

Notions of uncertainty: general case

Suppose in $S \subseteq \mathcal{X} \times \mathcal{Y}$, a p_k fraction are labeled as k (for each $k \in \mathcal{Y}$).

1. **Classification error**:
$$u(S) := 1 - \max_{k \in \mathcal{Y}} p_k$$
2. **Gini index**:
$$u(S) := 1 - \sum_{k \in \mathcal{Y}} p_k^2$$
3. **Entropy**:
$$u(S) := \sum_{k \in \mathcal{Y}} p_k \log \frac{1}{p_k}$$

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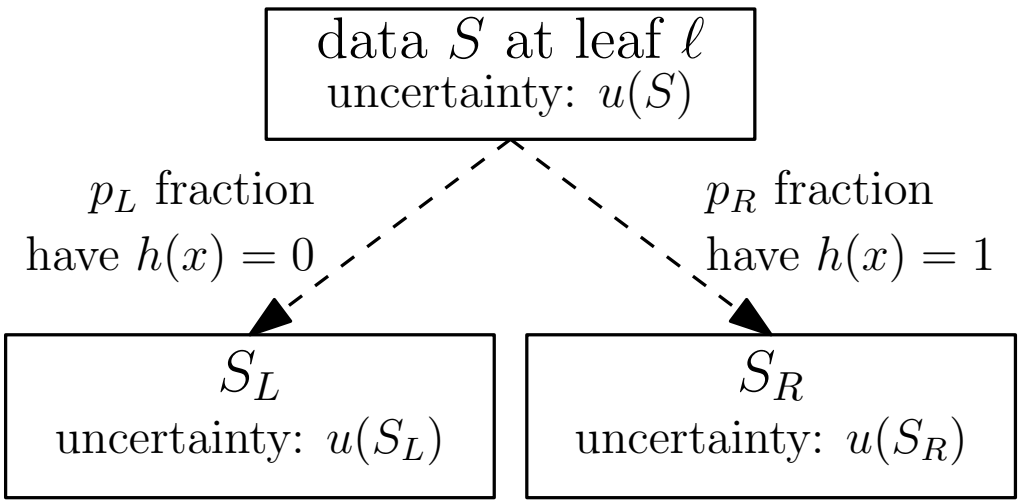
Each is *maximized* when $p_k = 1/|\mathcal{Y}|$ for all $k \in \mathcal{Y}$ (i.e., equal numbers of each label in S).

Each is *minimized* when $p_k = 1$ for a single label $k \in \mathcal{Y}$ (so S is **pure** in label).

Uncertainty reduction

Suppose the data S at a leaf ℓ is split by a rule h into S_L and S_R, where $p_L := |S_L|/|S|$ and $p_R := |S_R|/|S|$.



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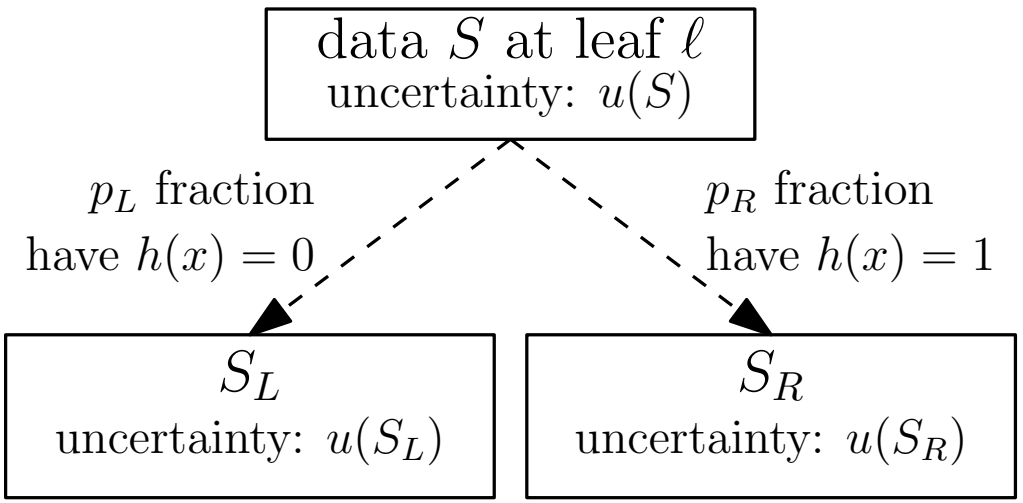

The **reduction in uncertainty** from using rule h at leaf ℓ is

$$u(S) - \Big(p_L \cdot u(S_L) + p_R \cdot u(S_R)\Big).$$

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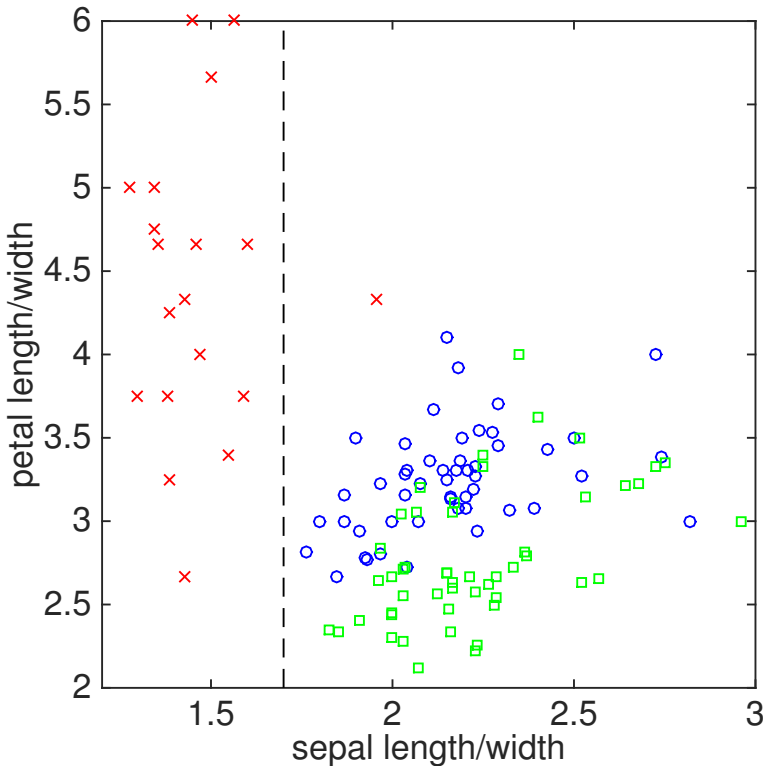

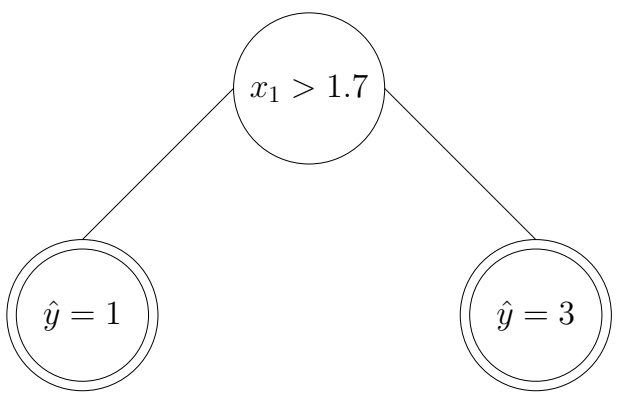

One leaf (with $\hat{y} = 1$) already has zero uncertainty (a pure leaf).

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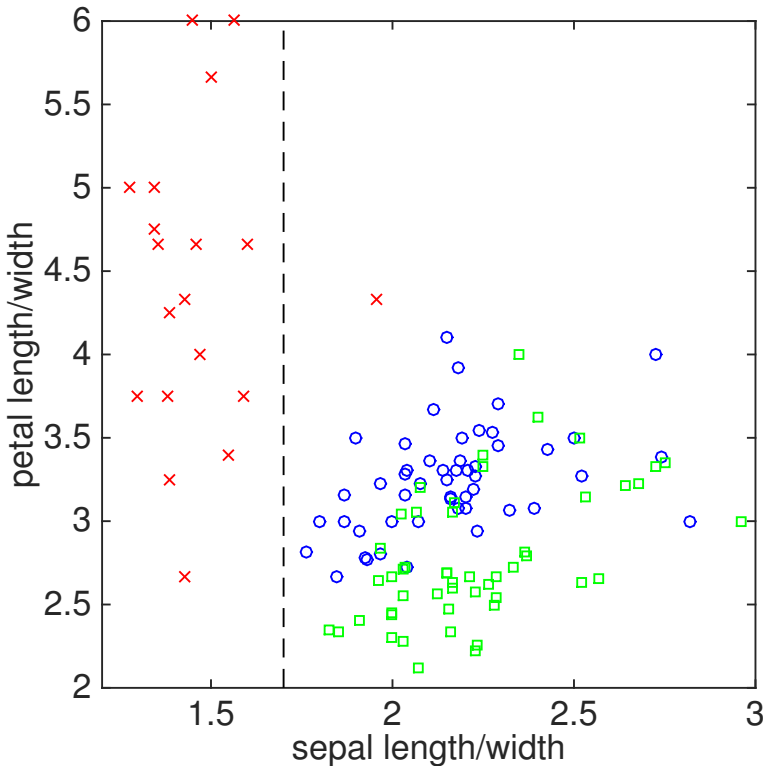

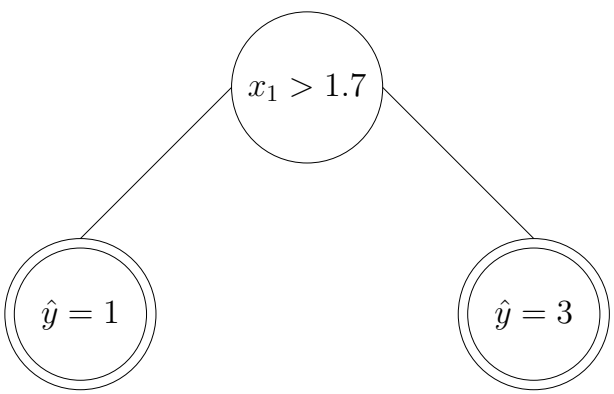

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Other leaf (with $\hat{y} = 3$) has Gini index

$$u(S) = 1 - \left(\frac{1}{101}\right)^2 - \left(\frac{50}{101}\right)^2 - \left(\frac{50}{101}\right)^2$$
$$= 0.5098.$$

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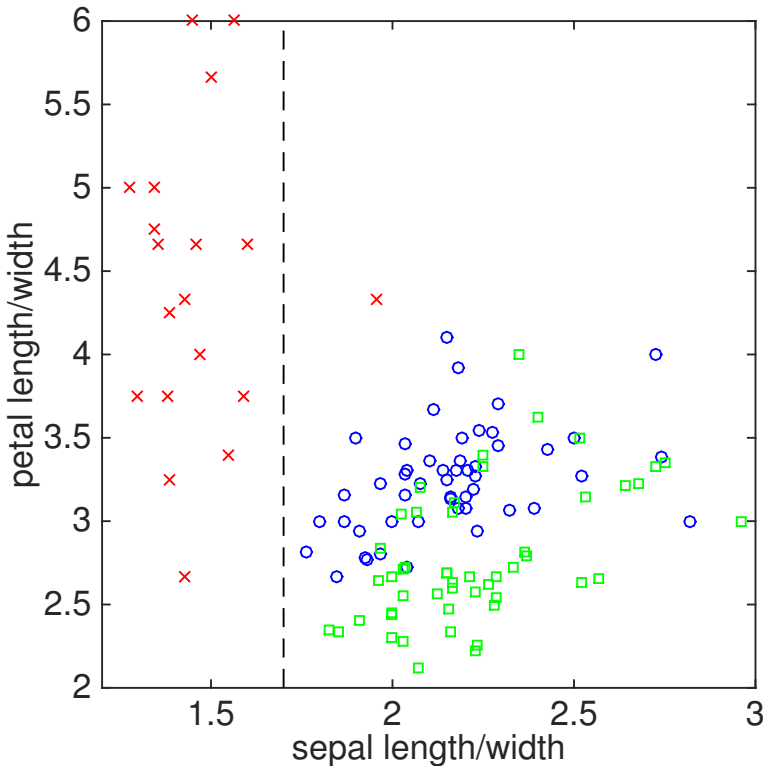

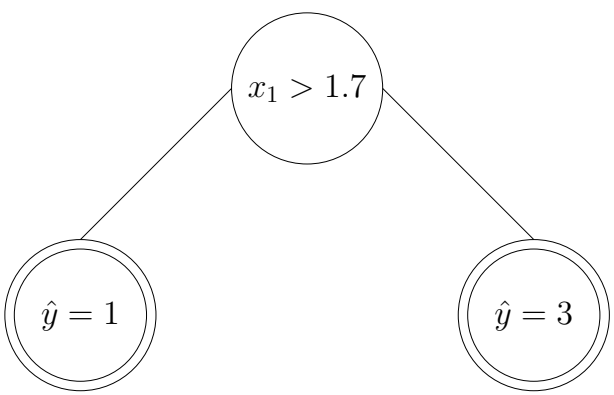

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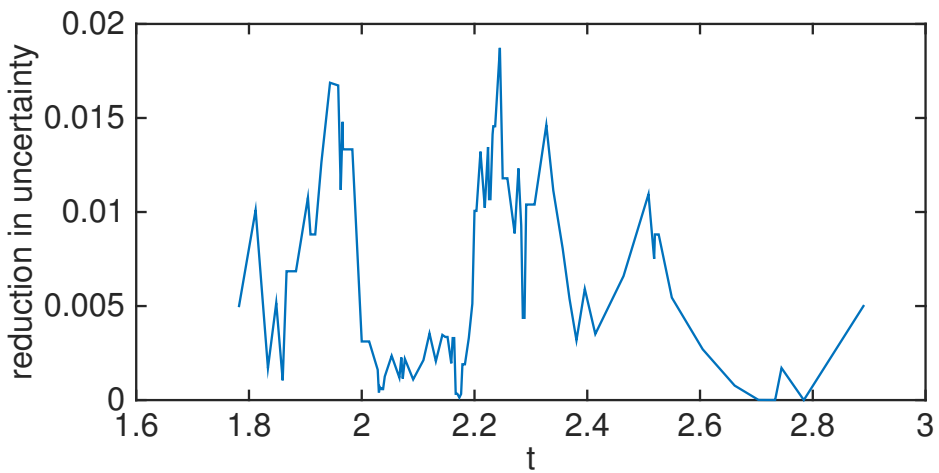

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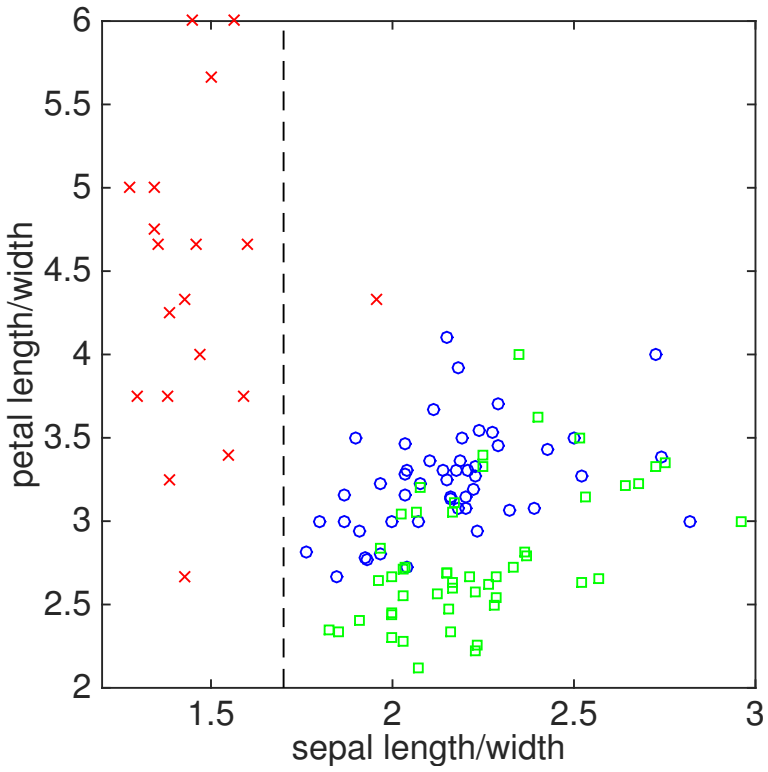
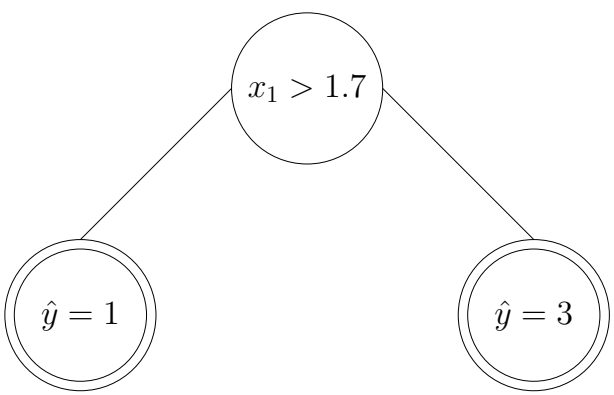


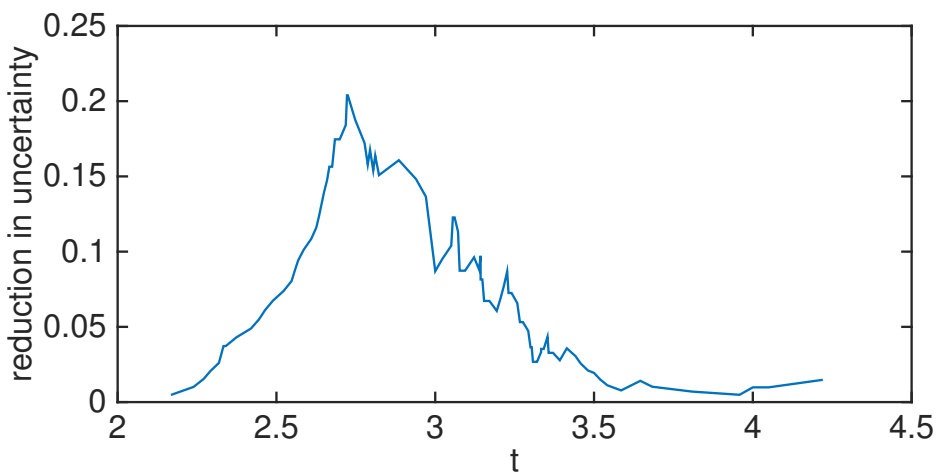


One leaf (with $\hat{y} = 1$) already has zero uncertainty (a pure leaf).

Other leaf (with $\hat{y} = 3$) has Gini index

$$u(S) = 1 - \left(\frac{1}{101}\right)^2 - \left(\frac{50}{101}\right)^2 - \left(\frac{50}{101}\right)^2$$
$$= 0.5098.$$

Split S with $\mathbb{1}\{x_2 > t\}$ to S_L, S_R:



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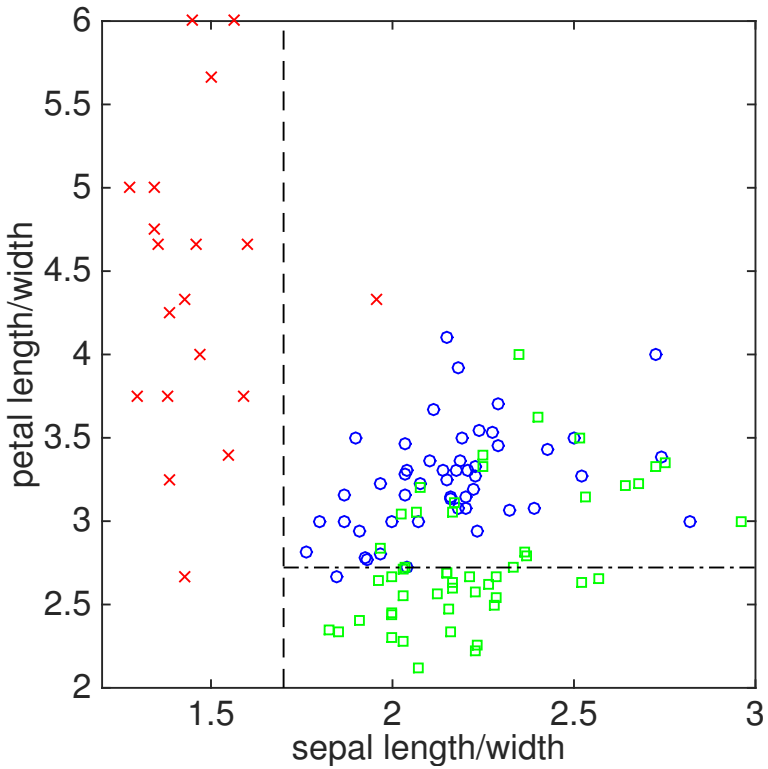

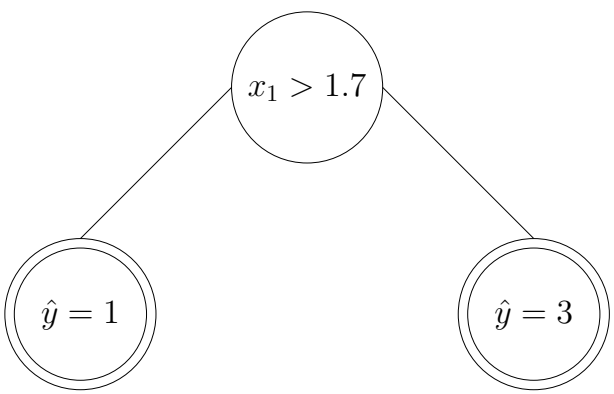

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Split S with $\mathbb{1}\{x_2 > 2.7222\}$ to S_L, S_R:

$u(S_L) = 1 - \left(\frac{0}{30}\right)^2 - \left(\frac{1}{30}\right)^2 - \left(\frac{29}{30}\right)^2 = 0.0605,$

$u(S_R) = 1 - \left(\frac{1}{71}\right)^2 - \left(\frac{49}{71}\right)^2 - \left(\frac{21}{71}\right)^2 = 0.4197.$

Reduction in uncertainty:

$$0.5098 - \left(\frac{30}{101} \cdot 0.0605 + \frac{71}{101} \cdot 0.4197\right) = 0.2039.$$

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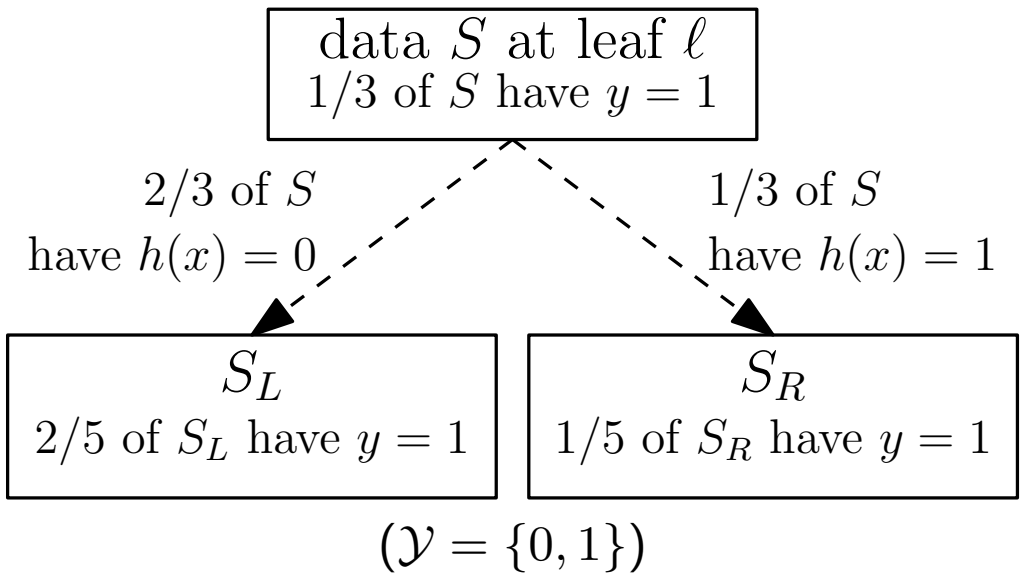

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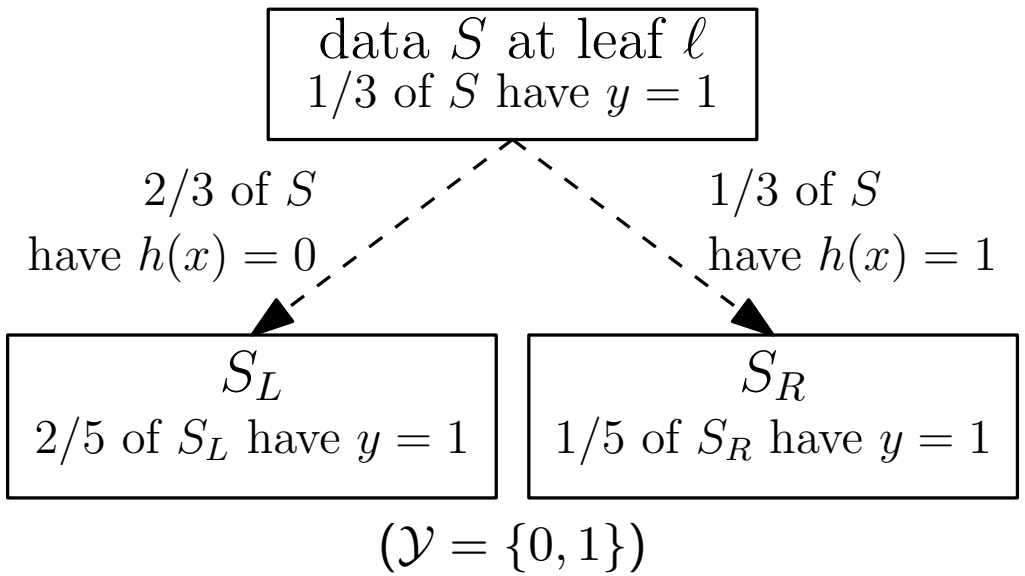
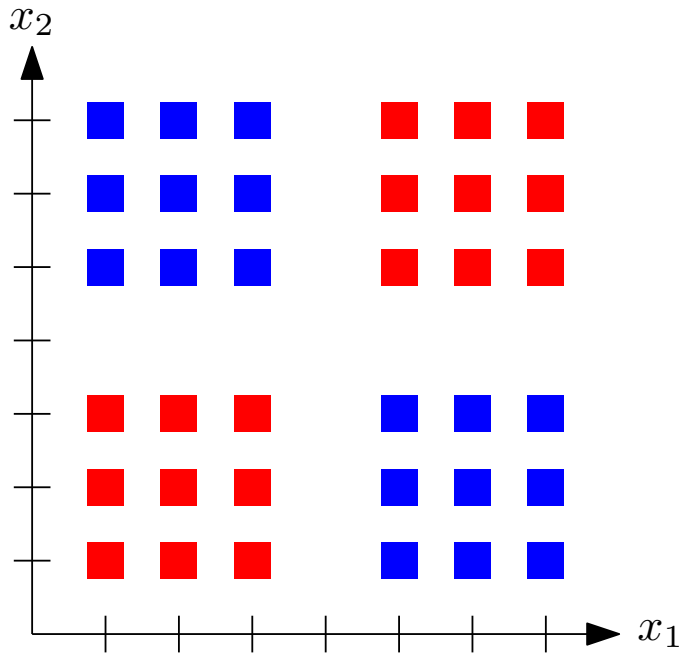


Reduction in classification error: $\frac{1}{3} - \left(\frac{2}{3} \cdot \frac{2}{5} + \frac{1}{3} \cdot \frac{1}{5}\right) = 0$

Reduction in Gini index: $\frac{4}{9} - \left(\frac{2}{3} \cdot \frac{12}{25} + \frac{1}{3} \cdot \frac{8}{25}\right) = \frac{4}{225}$

Limitations of uncertainty notions

Suppose $\mathcal{X} = \mathbb{R}^2$ and $\mathcal{Y} = \{\text{red}, \text{blue}\}$, and the data is as follows:



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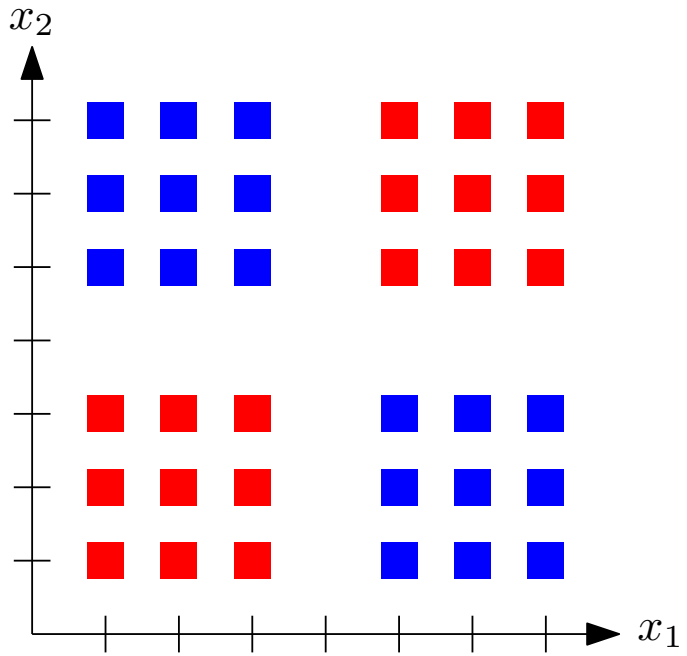

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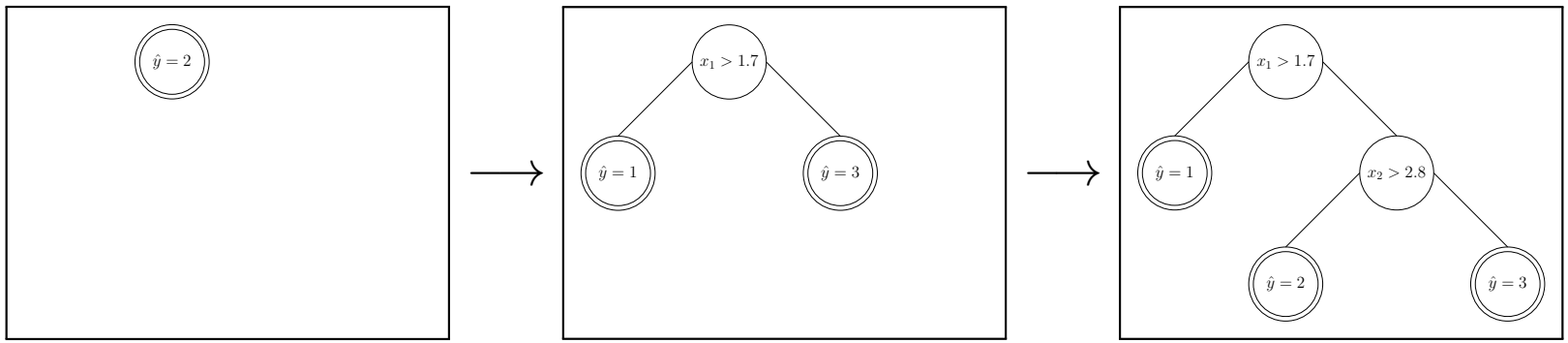
Upshot:
Zero reduction in uncertainty is not necessarily a desirable stopping condition.

Basic decision tree learning algorithm



Basic "top-down" greedy algorithm

- Initially, tree is a single leaf node containing all (training) data.
- Loop:
  - Pick the leaf ℓ and rule h that maximally reduces uncertainty.
  - Split data in ℓ using h, and grow tree accordingly.

  ...until some stopping criterion is satisfied.

[**Label of a leaf** is the **plurality label** among the data contained in the leaf.]

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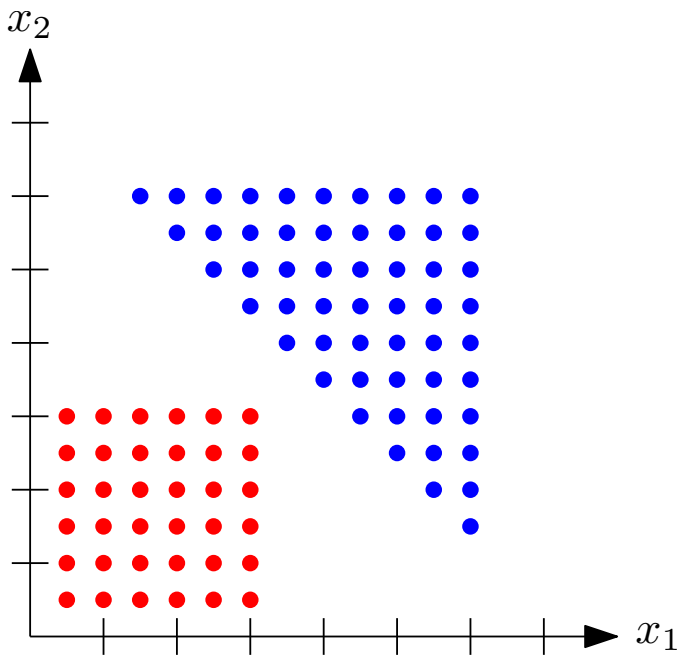

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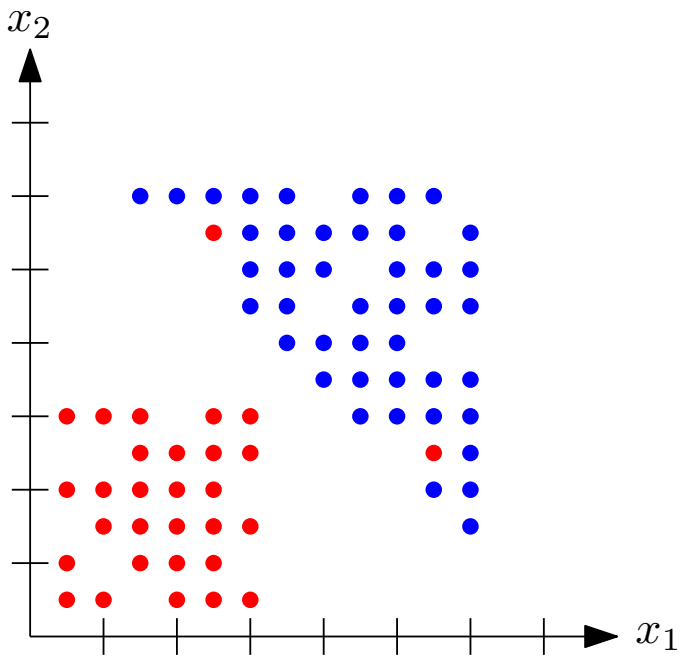

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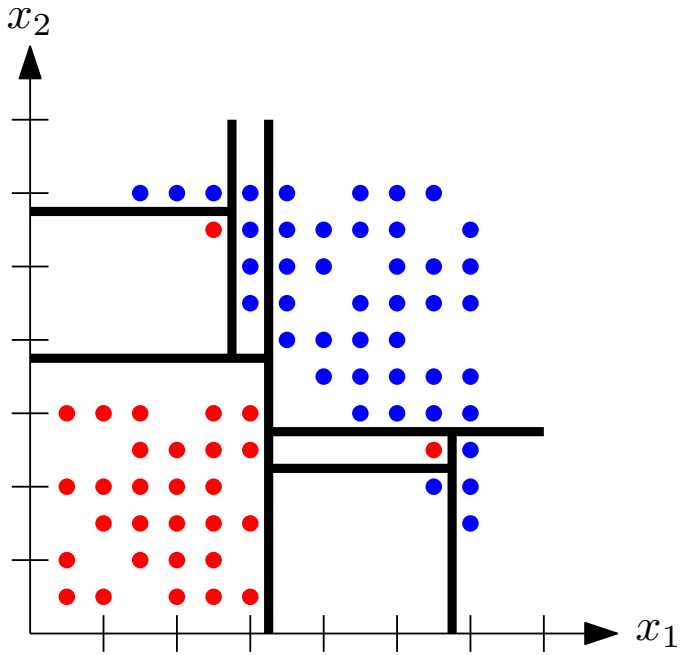
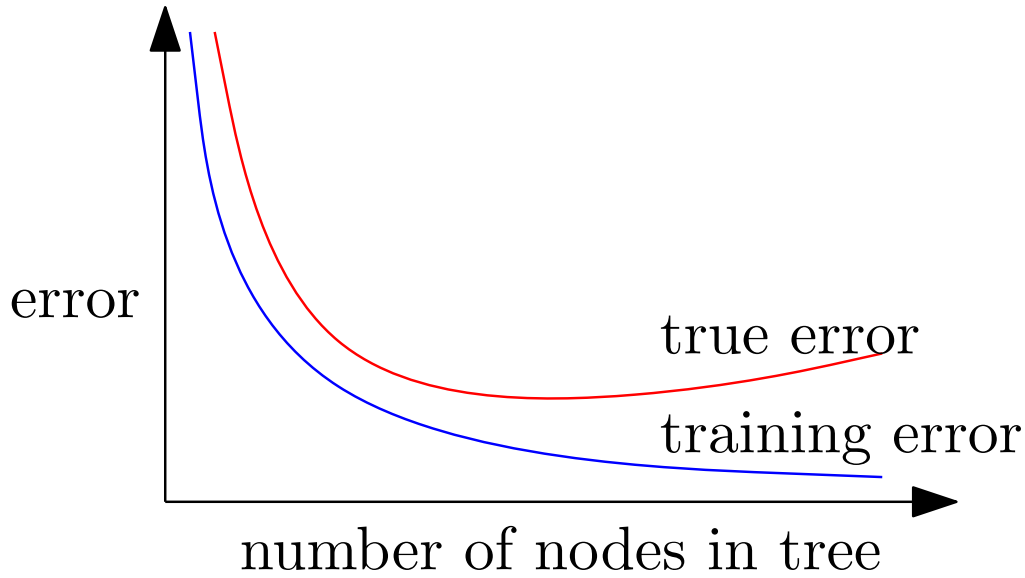


Overfitting



- Training error **goes to zero** as the number of nodes in the tree increases.
- True error decreases initially, but eventually **increases due to overfitting**.

Preventing overfitting

Split training data S into two parts, S' and S'':

- Use first part S' to **grow the tree until all leaves are pure**.
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Independence of S' and S'' make it unlikely for spurious structures in each to perfectly align.

Example: Spam filtering

Data

- 4601 e-mail messages, 39.4% are spam.
- $\mathcal{Y} = \{\text{spam}, \text{not spam}\}$
- E-mails represented by 57 features:
  - 48: percentange of e-mail words that is specific word (e.g., "free", "business")
  - 6: percentage of e-mail characters that is specific character (e.g., "!").
  - 3: other features (e.g., average length of ALL-CAPS words).

Results

Using variant of greedy algorithm to grow tree; prune tree using validation set.

Chosen tree has just **17 leaves**. Test error is 9.3%.

	$\hat{y} = \text{not spam}$	$\hat{y} = \text{spam}$
$y = \text{not spam}$	57.3%	4.0%
$y = \text{spam}$	5.3%	33.4%

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