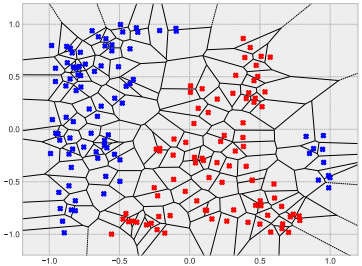
k-nn and decision trees

CS 446 / ECE 449

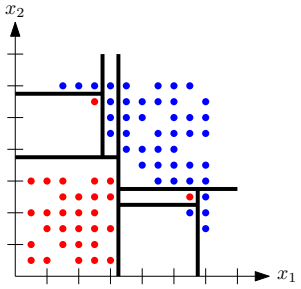
2022-02-16 19:35:44 -0600 (0670b06)

Plan for today

Today we'll cover two standard machine learning methods.



Nearest neighbors ("k-nn").



Decision trees.

`pytorch` **meta-algorithm.**

1. Clean/augment data (lecture 10).
2. Pick model/architecture (anything from lectures 2-13).
3. Pick a loss function measuring model fit to data.
4. Run a gradient descent variant to fit model to data.
5. Tweak 1-4 until training error is small.
6. Tweak 1-5, possibly reducing model complexity, until testing error is small.

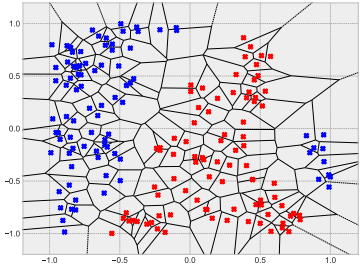
k-nn and decision trees will **not** use GD!

1-nearest-neighbor (1-nn)

1. Pick a distance function $\rho(\cdot, \cdot)$.
2. Memorize training set $((\boldsymbol{x}_i, y_i))_{i=1}^n$.
3. Given $\boldsymbol{x}$, output label y_i of closest $\boldsymbol{x}_i$, meaning

$$\rho(\boldsymbol{x}, \boldsymbol{x}_i) = \min_j \rho(\boldsymbol{x}, \boldsymbol{x}_j).$$

(Break ties arbitrarily but consistently.)



In this way, 1-nn uses the training set to form a Voronoi partition of the input space.

k-nearest-neighbor (k-nn)

1. Pick a distance function $\rho(\cdot, \cdot)$ and integer $k \geq 1$.
2. Memorize training set $((\boldsymbol{x}_i, y_i))_{i=1}^n$.
3. Given $\boldsymbol{x}$,
   - (Classification case) output plurality (most frequent) label y amongst k closest training examples ("k" nearest neighbors).
   - (Regression case) output average label y amongst k closest training examples ("k" nearest neighbors).

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Remarks.

- If $(\boldsymbol{x}_i)_{i=1}^n$ are distinct, 1-nn gets 0 training error.
- k-nn may fail to get 0 training error. (What is an example?)
- Why use k-nn?

`pytorch` **meta-algorithm.**

⋮

6. Tweak 1-5, possibly reducing model complexity, until testing error is small.

- Here, k and the distance function are the model hyper-parameters.
- 1-nn can have bad testing error.
- For carefully chosen k, e.g., $\mathcal{O}(\ln n)$, k-nn is guaranteed to achieve optimal test error.
  ("Optimal" means "bayes error rate", the best population risk over all possible predictors.)
- Higher k smooths the predictor, and gives a "less complex" model in an interesting way.

Example: OCR ("optical character recognition") for digits

Task: classify handwritten digits into $\{0, \ldots, 9\}$.

Digits from standard MNIST dataset
(Lecun, Cortes, Burges).

- Test error of k-nn with ℓ_2 distance:

OCR digits classification

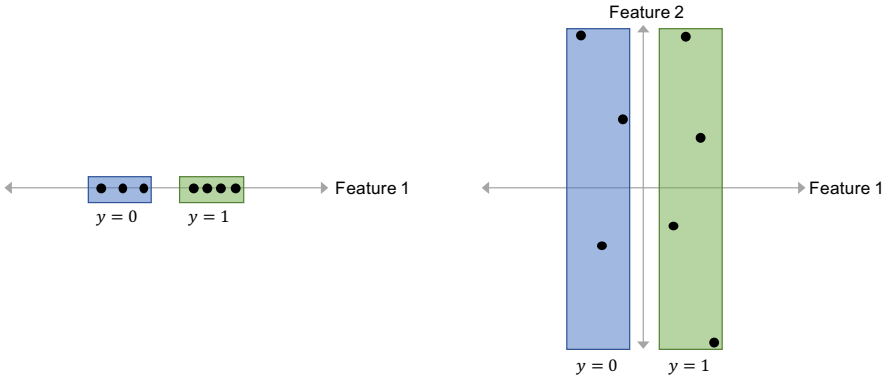
k	1	3	5	7	9
Test error rate	0.0309	0.0295	0.0312	0.0306	0.0341

- Test error of 1-nn with different distances:

Distance	ℓ_2	ℓ_3	Tangent	Shape
Test error rate	3.09%	2.83%	1.10%	0.63%

k-nn and features

Caution: nearest neighbor classifier can be broken by bad/noisy features!



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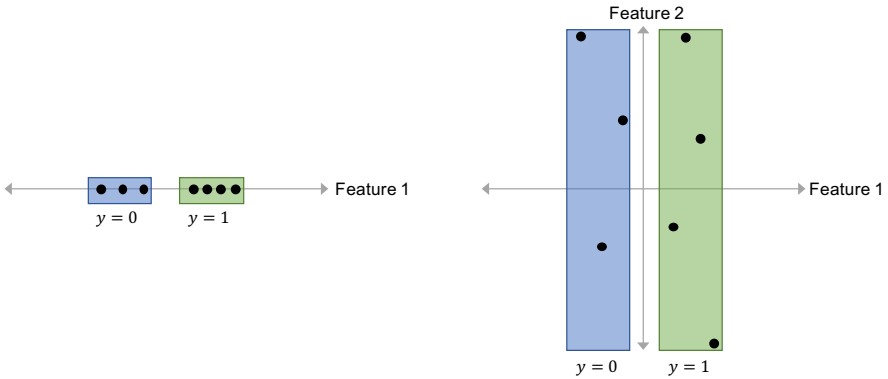

Curse of dimension. Given poly(d) random unit norm points in $\mathbb{R}^d$, with probability $> 99\%$, each is squared distance $2 \pm O\left(1/\sqrt{d}\right)$ from all others.

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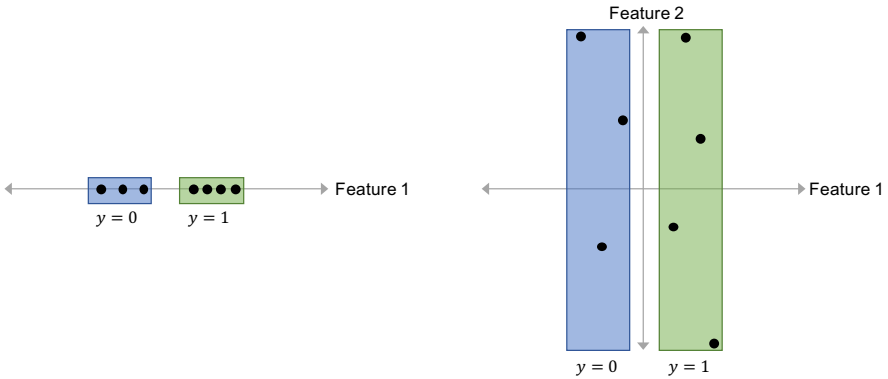

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Popular approach: train a deep network $f : \mathbb{R}^d \to \mathbb{R}^p$, and run k-nn on its outputs!

Computation

Naive k-nn takes $\mathcal{O}(n)$ time for each prediction
(and needs $\mathcal{O}(n)$ storage at all times).

There are many ways to speed this up;
see for instance `algorithm` parameter of
`sklearn.neighbors.KNeighborsClassifier`.
There is also locality sensitive hashing (LSH).
(These are all beyond the scope of this course.)

Decision trees

Decision trees

A **decision tree** is a binary tree which recursively partitions/refines the input space:

- Each **tree node** is associated with a splitting rule $g\colon \mathcal{X} \to \{0, 1\}$ (interpreted as "recurse left" and "recurse right").
- Each **leaf node** is associated with a label $\hat{y}$.

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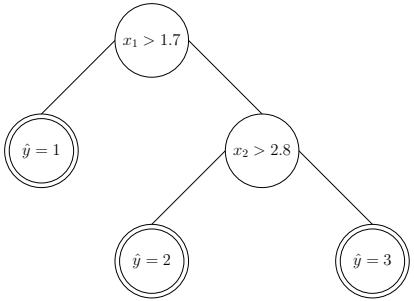
When $\mathcal{X} = \mathbb{R}^d$, typically only consider splitting rules of the form

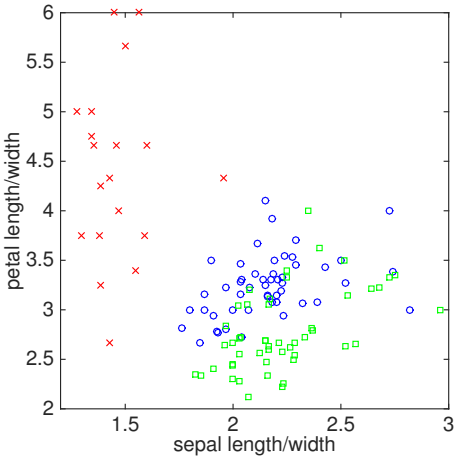
$$g(\boldsymbol{x}) \;=\; \mathbb{1}\{x_i > t\}$$

for some $i \in [d]$ and $t \in \mathbb{R}$.
Called axis-aligned or coordinate 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
- x_2 = ratio of petal length to width

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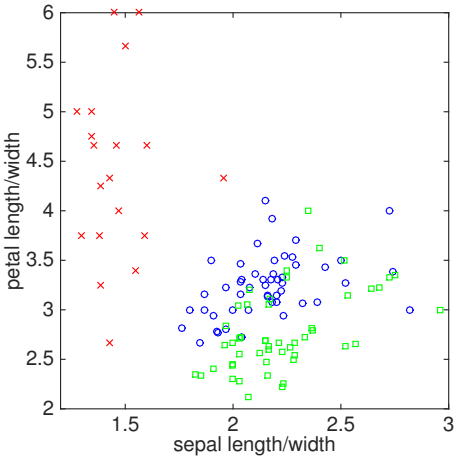

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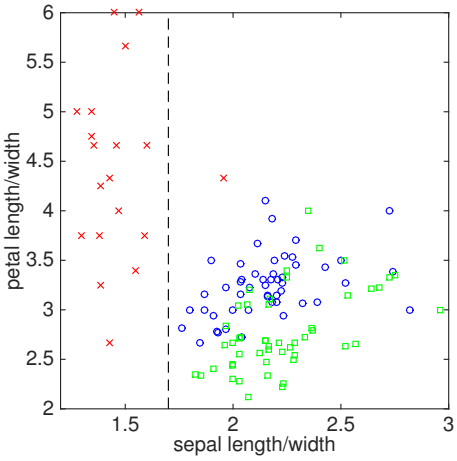

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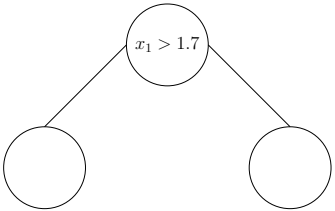

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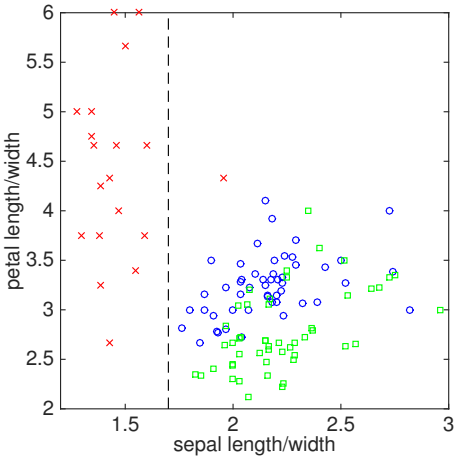

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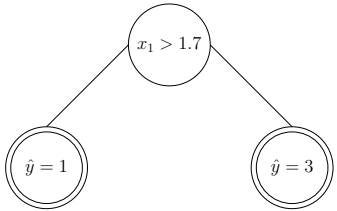

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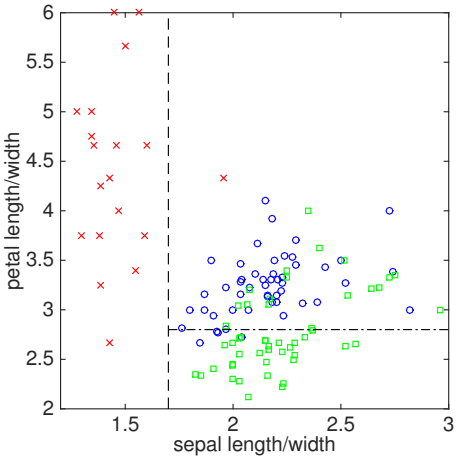

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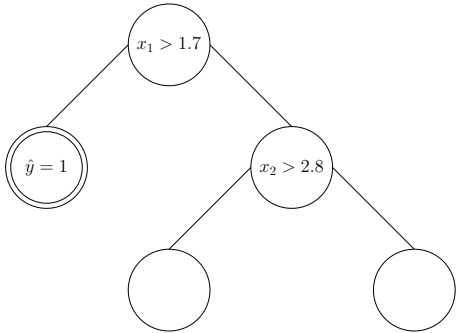

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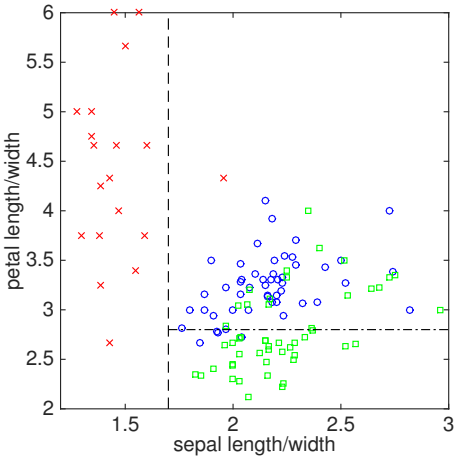

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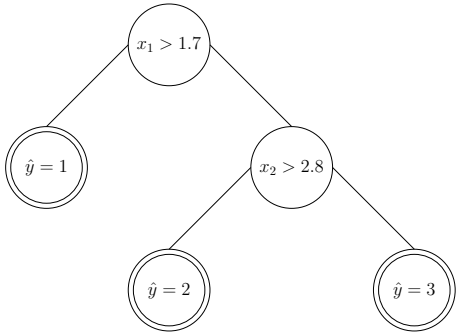

Notions of uncertainty for binary classification

Basic decision tree algorithm (further details soon):
recursively partition data, minimizing **uncertainty**.

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Example **uncertainty** measures for binary classification,
given example set S, suppose $p|S|$ are labeled $+1$.

1. **Classification error**:

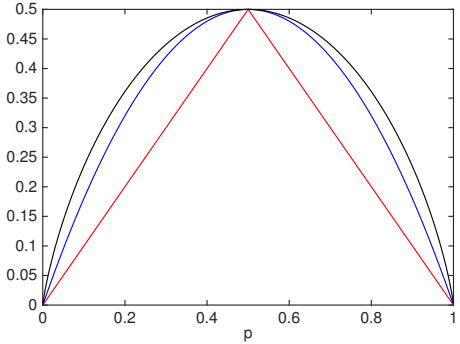
$$u(S) \;:=\; \min\{p,\, 1-p\}$$

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 for multiclass classification

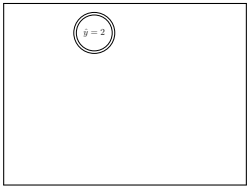
Consider examples set S, of which $p_y|S|$ have label y.

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

Each is maximized when $p_y = 1/K$ for all $y \in \mathcal{Y}$
(i.e., all labels appear equally).

Each is minimized when $p_y = 1$ for a single label $y \in \mathcal{Y}$
(i.e., S is **pure**).

Basic decision tree learning algorithm



Basic "top-down" greedy (training) algorithm.

- Pick an per-node uncertainty measure u; the uncertainty of a tree $\mathcal{T}$ is

$$u(\mathcal{T}) := \frac{1}{n} \sum_{\text{leaf } S \in \mathcal{T}} |S| \cdot u(S).$$

- Place all data in single root tree node.

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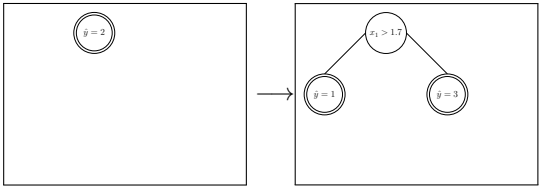

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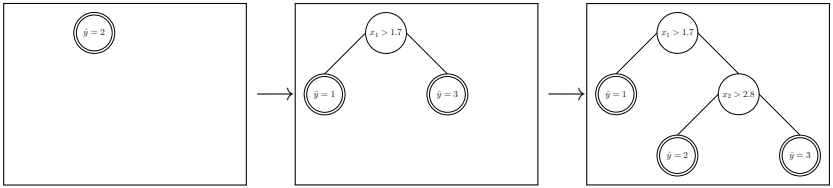

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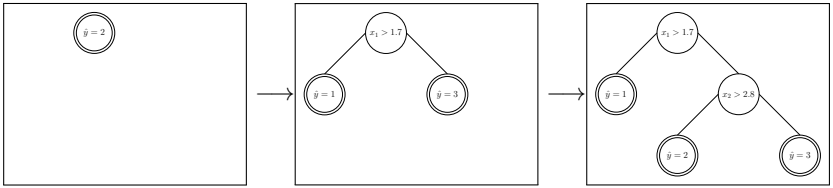

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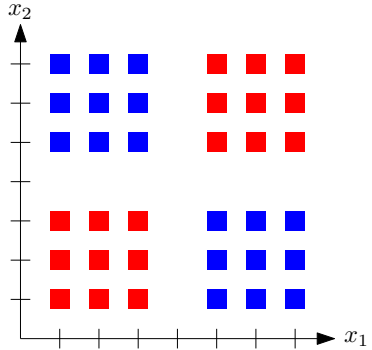
To predict on new data (as before): traverse tree to corresponding leaf, output the plurality (or average) label of its training data.

Failure of greedy uncertainty reduction

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



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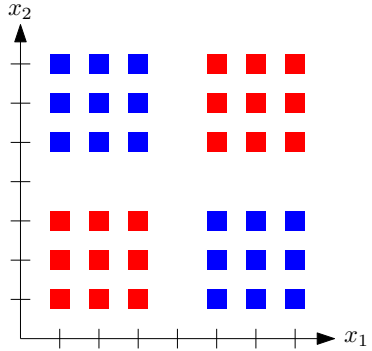

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Remark: if we do a random nonempty split, the subsequent step can make progress.

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   Serious danger of **overfitting**.

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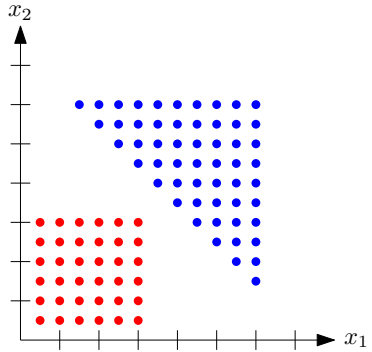

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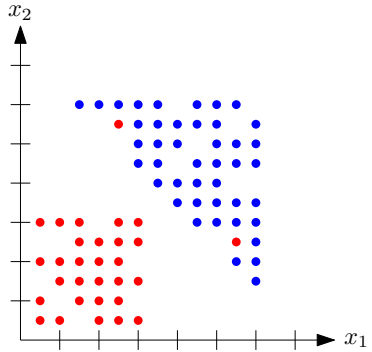

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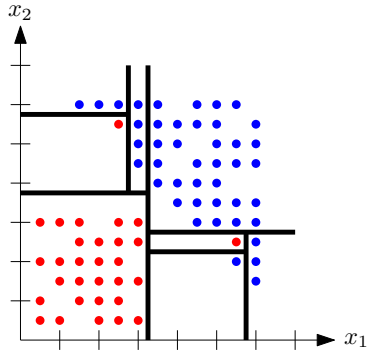
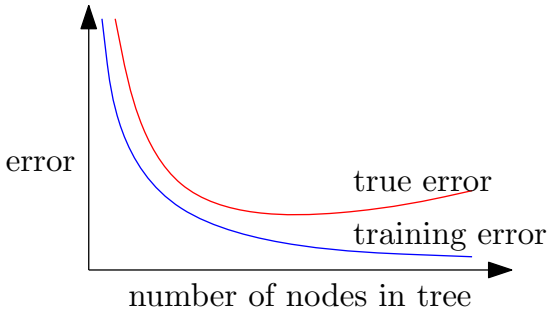


Overfitting



- Training error **goes to zero** as the number of nodes in the tree increases.
- True error decreases initially, but eventually **increases due to overfitting**.
  (Fix this by stopping early, or by pruning tree afterwards.)
- The stopping rule is related to **reducing model complexity** (step 6 in the pytorch meta-algorithm).

Example: Spam filtering

Data

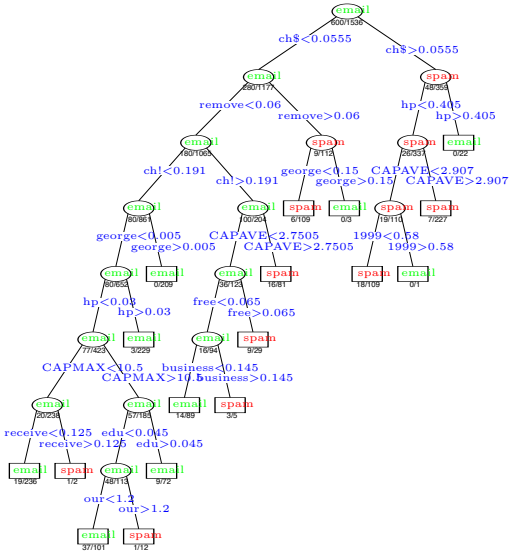
- 4601 e-mail messages, 39.4% are spam.
- $\mathcal{Y} = \{\text{spam}, \text{not spam}\}$
- E-mails represented by 57 features:
  - 48: percentange of e-mail words that is specific word (e.g., "free", "business")
  - 6: percentage of e-mail characters that is specific character (e.g., "!").
  - 3: other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

Results

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

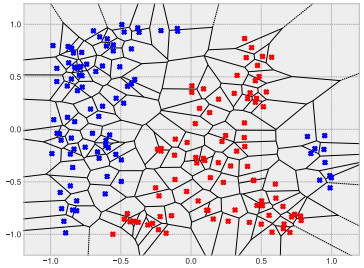
Chosen tree has just **17 leaves**. Test error is 9.3%.

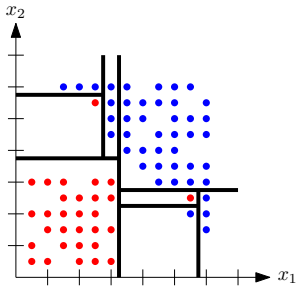
	$\hat{y} = \text{not spam}$	$\hat{y} = \text{spam}$
$y = \text{not spam}$	57.3%	4.0%
$y = \text{spam}$	5.3%	33.4%



Note this is **somewhat interpretable**. Interpretability is a popular and active subject these days, partially since deep networks are used extensively but hard to interpret.

Summary for today





Nearest neighbors.
Training/fitting: memorize data.
Testing/predicting: find k closest memorized points, return plurality/average label.
Overfitting? Vary k.

Decision trees.
Training/fitting: greedily partition space, reducing "uncertainty".
Testing/predicting: traverse tree, output leaf label.
Overfitting? Limit or prune tree.

Note: both methods naturally handle binary classification, multi-class classification, and regression.