Machine Learning (CSE 446): Decision Trees (continued)

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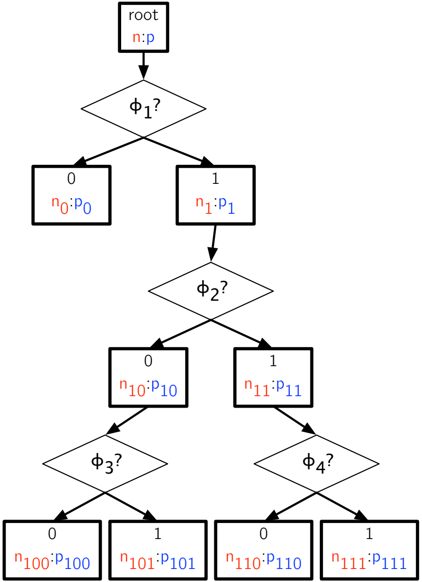
Decision Tree: Making a Prediction



Data: decision tree t, input example x
Result: predicted class
if t *has the form* $\text{Leaf}(y)$ **then**
    return y;
else
    # $t.\phi$ is the feature associated with t;
    # t.child(v) is the subtree for value v;
    return $\text{DTreeTest}(t.\text{child}(t.\phi(x)), x)$;
end

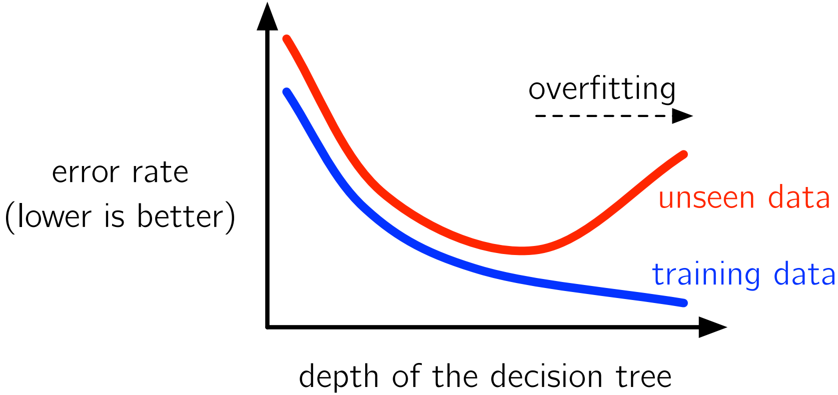
Algorithm 1: DTreeTest

Greedily Building a Decision Tree (Binary Features)

Data: data D, feature set Φ
Result: decision tree
if *all examples in* D *have the same label* y*, or* Φ *is empty and* y *is the best guess* **then**
  return $\textsc{Leaf}(y)$;
else
  for *each feature* ϕ *in* Φ **do**
    partition D into D_0 and D_1 based on ϕ-values;
    let mistakes(ϕ) $=$ (non-majority answers in D_0) $+$ (non-majority answers in D_1);
  end
  let ϕ^* be the feature with the smallest number of mistakes;
  return $\textsc{Node}(\phi^*, \{0 \rightarrow \textsc{DTreeTrain}(D_0, \Phi \setminus \{\phi^*\}), 1 \rightarrow \textsc{DTreeTrain}(D_1, \Phi \setminus \{\phi^*\})\})$;
end

Algorithm 2: $\textsc{DTreeTrain}$

Danger: Overfitting



Some Notation

- Let ℓ be a loss function; $\ell(y, \hat{y})$ is what we lose by outputting $\hat{y}$ when y is the correct output. For classification:

$$\ell(y, \hat{y}) = [\![y \neq \hat{y}]\!]$$

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- The training data $D = \langle (x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N) \rangle$ are assumed to be i.i.d. samples from $\mathcal{D}$.
- The space of classifiers we're considering is $\mathcal{F}$; f is a classifier from $\mathcal{F}$, chosen by our learning algorithm.

Overfitting, More Formally

- Classifier f's average loss on **training data**:

$$\hat{\epsilon}(f) = \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, f(x_n))$$

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- f has overfit D when:

$$\exists f' \in \mathcal{F} \text{ s.t. } \hat{\epsilon}(f) < \hat{\epsilon}(f') \wedge \epsilon(f') < \epsilon(f)$$

This is the fundamental problem of ML.

Inductive, Supervised Machine Learning

- Input: loss function ℓ and training data D drawn i.i.d. from $\mathcal{D}$
- Output: f such that $\epsilon(f)$ is low over $\mathcal{D}$, with respect to ℓ

Never forget that $\epsilon(f) \neq \hat{\epsilon}(f)$.

Is your training data D really drawn from $\mathcal{D}$?

Back to decision trees . . .

Avoiding Overfitting by Stopping Early

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In each case, we have a **hyperparameter** $(d_{max}, \Delta, N_{min})$, which you should **tune** on **development data**.

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- Choose the t_i that performs best on development data.

More Things to Know

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- For continuous-valued features, we use threshholds, e.g., $\phi(x) \le \tau$.
  In this case, you must choose τ.
  If the sorted values of ϕ are $\langle v_1, v_2, \ldots, v_N \rangle$, you only need to consider $\tau \in \left\{ \frac{v_n + v_{n+1}}{2} \right\}_{n=1}^{N-1}$ (midpoints between consecutive feature values).

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- For continuous-valued **outputs**, what value makes sense as the prediction at a leaf? What loss should we use instead of $[\![y \neq \hat{y}]\!]$?

Machine Learning (CSE 446): Limits of Learning

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The Bayes Optimal Classifier

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Theorem: The Bayes optimal classifier achieves minimal zero/one error ($\ell(y, \hat{y}) = [\![y \neq \hat{y}]\!]$) of any deterministic classifier.

Proof

Consider (deterministic) f' that claims to be better than $f^{(\mathsf{BO})}$ and x such that $f^{(\mathsf{BO})}(x) \neq f'(x)$.

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By definition,

$$\mathcal{D}(x, f^{(\mathsf{BO})}(x)) = \max_y \mathcal{D}(x,y) \geq \mathcal{D}(x, f'(x))$$

$$\Rightarrow \left(\sum_y \mathcal{D}(x,y)\right) - \mathcal{D}(x, f^{(\mathsf{BO})}(x)) \leq \left(\sum_y \mathcal{D}(x,y)\right) - \mathcal{D}(x, f'(x))$$

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This must hold for all x. Hence f' is no better than $f^{(\mathsf{BO})}$.

One Limit of Learning

You cannot do better than $\epsilon(f^{\mathsf{BO}})$.