Lecture 7a - Supervised Machine Learning I

Jesse Hoey
School of Computer Science
University of Waterloo

February 20, 2020

Readings: Poole & Mackworth (2nd ed.) Chapt. 7.1-7.3.1, 7.4
Learning is the ability to improve one’s behavior based on experience.

- The range of behaviors is expanded: the agent can do more.
- The accuracy on tasks is improved: the agent can do things better.
- The speed is improved: the agent can do things faster.
Components of a learning problem

The following components are part of any learning problem:

- **task** The behavior or task that’s being improved. For example: classification, acting in an environment
- **data** The experiences that are being used to improve performance in the task.
- **measure of improvement** How can the improvement be measured? For example: increasing accuracy in prediction, new skills that were not present initially, improved speed.
Types of learning

- Draw a conclusion from a knowledge base: **deduction** (top-down)
- Infer a representation from data: **induction** (bottom-up)
- The richer (more complex) the representation, the more useful it is for subsequent problem solving.
- The richer the representation, the more difficult it is to learn.
Common Learning Tasks

- **Supervised classification**: Given a set of pre-classified training examples, classify a new instance.
- **Unsupervised learning**: Find natural classes for examples.
- **Reinforcement learning**: Determine what to do based on rewards and punishments.
- **Transfer Learning**: Learning from an expert
- **Active Learning**: Learner actively seeks to learn
- **Inductive logic programming**: Build richer models in terms of logic programs.
Learning tasks can be characterized by the feedback given to the learner.

- **Supervised learning** What has to be learned is specified for each example.
- **Unsupervised learning** No classifications are given; the learner has to discover categories and regularities in the data.
- **Reinforcement learning** Feedback occurs after a sequence of actions. Credit assignment problem. Is a form of Supervised Learning.
Measuring Success

The measure of success is not how well the agent performs on the training examples, but how well the agent performs for new examples.

Consider two agents solving a binary classification task:

- $P$ claims the negative examples seen are the only negative examples. Every other instance is positive.
- $N$ claims the positive examples seen are the only positive examples. Every other instance is negative.

Both agents correctly classify every training example, but disagree on every other example.
The tendency to prefer one hypothesis over another is called a **bias**.

A bias is necessary to make predictions on unseen data.

Saying a hypothesis is better than $N$’s or $P$’s hypothesis isn’t something that’s obtained from the data.

To have any inductive process make predictions on unseen data, you need a bias.

What constitutes a good bias is an empirical question about which biases work best in practice.
Given a representation and a bias, the problem of learning can be reduced to one of search.

Learning is search through the space of possible representations looking for the representation or representations that best fits the data, given the bias.

These search spaces are typically prohibitively large for systematic search.

A learning algorithm is made of a search space, an evaluation function, and a search method.
Supervised Learning

Given:

- a set of input features $X_1, \ldots, X_n$
- a set of target features $Y_1, \ldots, Y_k$
- a set of training examples where the values for the input features and the target features are given for each example
- a set of test examples, where only the values for the input features are given

predict the values for the target features for the test examples.

- **classification** when the $Y_i$ are discrete
- **regression** when the $Y_i$ are continuous

**Very important**: keep training and test sets separate!
Data isn’t perfect:
  ▶ some of the features are assigned the wrong value
  ▶ the features given are inadequate to predict the classification
  ▶ there are examples with missing features

overfitting occurs when a distinction appears in the data, but doesn’t appear in the unseen examples. This occurs because of random correlations in the training set.
Evaluating Predictions

Suppose $Y$ is a feature and $e$ is an example:

- $Y(e)$ is the value of feature $Y$ for example $e$.
- $\hat{Y}(e)$ is the predicted value of feature $Y$ for example $e$.
- The **error** of the prediction is a measure of how close $\hat{Y}(e)$ is to $Y(e)$.
- There are many possible errors that could be measured.
Measures of error

$E$ is the set of examples. $T$ is the set of target features.

- **absolute error**

$$\sum_{e \in E} \sum_{Y \in T} |Y(e) - \hat{Y}(e)|$$
Measures of error

$E$ is the set of examples. $T$ is the set of target features.

- **absolute error**

$$\sum_{e \in E} \sum_{Y \in T} \left| Y(e) - \hat{Y}(e) \right|$$

- **sum of squares error**

$$\sum_{e \in E} \sum_{Y \in T} (Y(e) - \hat{Y}(e))^2$$
Measures of error

$E$ is the set of examples. $T$ is the set of target features.

- **absolute error**

$$\sum_{e \in E} \sum_{Y \in T} |Y(e) - \hat{Y}(e)|$$

- **sum of squares error**

$$\sum_{e \in E} \sum_{Y \in T} (Y(e) - \hat{Y}(e))^2$$

- **worst-case error**

$$\max_{e \in E} \max_{Y \in T} \left| Y(e) - \hat{Y}(e) \right|.$$
Measures of error

$E$ is the set of examples. $\mathbf{T}$ is the set of target features.

- **absolute error**
  \[ \sum_{e \in E} \sum_{Y \in \mathbf{T}} |Y(e) - \hat{Y}(e)| \]

- **sum of squares error**
  \[ \sum_{e \in E} \sum_{Y \in \mathbf{T}} (Y(e) - \hat{Y}(e))^2 \]

- **worst-case error**
  \[ \max_{e \in E} \max_{Y \in \mathbf{T}} |Y(e) - \hat{Y}(e)|. \]

- **cost-based error** takes into account costs of various errors.
When target features are $Y(e) \in \{0, 1\}$ and predicted features are $\hat{Y}(e) \in [0, 1]$ (predicted features: probability the target is 1):

- **likelihood of the data** (maximize this)

$$\prod_{e \in E} \prod_{Y \in T} P(\hat{Y}(e) | Y(e))$$

$$\prod_{e \in E} \prod_{Y \in T} \hat{Y}(e)^Y(e)(1 - \hat{Y}(e))^{(1 - Y(e))}$$
Measures of error (cont.)

When target features are \( Y(e) \in \{0, 1\} \) and predicted features are \( \hat{Y}(e) \in [0, 1] \) (predicted features: probability the target is 1):

- **likelihood of the data** (maximize this)

\[
\prod_{e \in E} \prod_{Y \in T} P(\hat{Y}(e) | Y(e))
\prod_{e \in E} \prod_{Y \in T} \hat{Y}(e)^{Y(e)} (1 - \hat{Y}(e))^{(1 - Y(e))}
\]

- **entropy** or **negative log likelihood** (minimize this: a cost)

\[
- \sum_{e \in E} \sum_{Y \in T} [Y(e) \log \hat{Y}(e) + (1 - Y(e)) \log(1 - \hat{Y}(e))]
\]
Not all errors are equal, e.g. predict:
- a patient has a disease when they do not
- a patient doesn’t have a disease when they do

need to map out both kinds of errors to find the best trade-off

<table>
<thead>
<tr>
<th></th>
<th>predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>T</td>
</tr>
<tr>
<td>actual</td>
<td>T</td>
</tr>
<tr>
<td></td>
<td>F</td>
</tr>
</tbody>
</table>

recall = sensitivity = \( \frac{TP}{TP+FN} \)

specificity = \( \frac{TN}{TN+FP} \)

precision = \( \frac{TP}{TP+FP} \)

F-measure = \( \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \)
Receiver Operating Curve

"perfect" agent
bias (model parameters)
agent "P" predicts T for all examples

"best you can do" agent

agent "N" predicts F for all examples
Many learning algorithms can be seen as deriving from:

- decision trees
- linear classifiers
- Bayesian classifiers
Example: user discussion board behaviors

<table>
<thead>
<tr>
<th>example</th>
<th>author</th>
<th>thread</th>
<th>length</th>
<th>where read</th>
<th>user’s action</th>
</tr>
</thead>
<tbody>
<tr>
<td>e1</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e2</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e3</td>
<td>unknown</td>
<td>follow up</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e4</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e5</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e6</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e7</td>
<td>unknown</td>
<td>follow up</td>
<td>short</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e8</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e9</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e10</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e11</td>
<td>unknown</td>
<td>follow up</td>
<td>short</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e12</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e13</td>
<td>known</td>
<td>follow up</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e14</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e15</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e16</td>
<td>known</td>
<td>follow up</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e17</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e18</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e19</td>
<td>unknown</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>?</td>
</tr>
</tbody>
</table>
### Example: user discussion board behaviors

<table>
<thead>
<tr>
<th>example</th>
<th>author</th>
<th>thread</th>
<th>length</th>
<th>where read</th>
<th>user’s action</th>
</tr>
</thead>
<tbody>
<tr>
<td>e1</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e2</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e3</td>
<td>unknown</td>
<td>follow up</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e4</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e5</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e6</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e7</td>
<td>unknown</td>
<td>follow up</td>
<td>short</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e8</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e9</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e10</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e11</td>
<td>unknown</td>
<td>follow up</td>
<td>short</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e12</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e13</td>
<td>known</td>
<td>follow up</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e14</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e15</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e16</td>
<td>known</td>
<td>follow up</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e17</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e18</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e19</td>
<td>unknown</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>?</td>
</tr>
</tbody>
</table>
Learning Decision Trees

- Representation is a decision tree.
- Bias is towards simple decision trees.
- Search through the space of decision trees, from simple decision trees to more complex ones.
Simple, successful technique for supervised learning from discrete data

Learn a *decision tree* from data:
- Nodes are input attributes/features
- Branches are labeled with input feature value(s)
- Leaves are predictions for target features (point estimates)
- Can have many branches per node
- Branches can be labeled with multiple feature values
Example Decision Trees

```
<table>
<thead>
<tr>
<th>Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>long</td>
</tr>
<tr>
<td>short</td>
</tr>
</tbody>
</table>

Thread

<table>
<thead>
<tr>
<th>new</th>
</tr>
</thead>
<tbody>
<tr>
<td>reads</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>follow_up</th>
</tr>
</thead>
<tbody>
<tr>
<td>reads</td>
</tr>
</tbody>
</table>

Author

<table>
<thead>
<tr>
<th>unknown</th>
</tr>
</thead>
<tbody>
<tr>
<td>skips</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>known</th>
</tr>
</thead>
<tbody>
<tr>
<td>reads</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>long</td>
</tr>
<tr>
<td>short</td>
</tr>
</tbody>
</table>

reads with probability 0.82

skips
Learning a decision tree

- Incrementally split the training data
- Recursively solve sub-problems
- Hard part: how to split the data?
- Criteria for a good decision tree (bias):
  - small decision tree,
  - good classification (low error on training data),
  - good generalisation (low error on test data)
//X is input features, Y is output features,  
//E is training examples  
//output is a decision tree, which is either  
// - a point estimate of Y, or  
// - of the form <X_i, T_1, ..., T_N> where  
//  X_i is an input feature and T_1, ..., T_N are decision trees

procedure DecisionTreeLearner(X,Y,E) 
if stopping criteria is met then  
    return pointEstimate(Y,E)
else 
    select feature X_i ∈ X  
    for each value x_i of X_i do  
        E_i = all examples in E where X_i = x_i  
        T_i = DecisionTreeLearner(X \{X_i}, Y, E_i)  
    end for  
    return <X_i, T_1, ..., T_N>
end procedure
procedure ClassifyExample(e,X,Y,DT)
    S ← DT
    while S is internal node of the form < X_i, T_1, \ldots, T_N > do
        j ← X_i(e)
        S ← T_j
    end while
    return S
end procedure
Remaining issues

- Stopping criteria
- Selection of features
- Point estimate (final return value at leaf)
- Reducing number of branches (partition of domain)
Stopping Criteria

- How do we decide to stop splitting?
- The stopping criteria is related to the final return value
- Depends on what we will need to do
- Possible stopping criteria:
  - No more features
  - Performance on training data is good enough
Feature Selection

• Ideal: choose sequence of features that result in smallest tree
• Actual: myopically split - as if only allowed one split, which feature would give best performance?
• heuristics for best performing feature:
  ▶ Most even split
  ▶ Maximum information gain
  ▶ GINI index
  ▶ ... others domain dependent ...
Good Feature Selection
Bad Feature Selection

Where read

- work
  - thread
    - length
      - short
      - long
      - reads
      - skips
    - reads
  - thread
    - length
      - short
      - long
      - reads
      - skips

- home
  - thread
    - length
      - short
      - long
      - reads
      - skips
  - thread
    - length
      - short
      - long
      - reads
      - skips

Author

- known
  - thread
    - follow up
      - length
        - short
        - long
        - reads
        - skips
    - reads
  - thread
    - follow up
      - length
        - short
        - long
        - reads
        - skips

- unknown
  - thread
    - follow up
      - length
        - short
        - long
        - reads
        - skips
    - reads
  - thread
    - follow up
      - length
        - short
        - long
        - reads
        - skips

Information Theory

- A **bit** is a binary digit: 0 or 1
- n bits can distinguish $2^n$ items
- Can do better by taking probabilities into account

Example:
Distinguish $\{a, b, c, d\}$ with $P(a) = 0.5$, $P(b) = 0.25$, $P(c) = P(d) = 0.125$
If we encode
  - $a:00$  
  - $b:01$  
  - $c:10$  
  - $d:11$
uses on average 2 bits

But if we encode
  - $a:0$  
  - $b:10$  
  - $c:110$  
  - $d:111$
uses on average

$$P(a) \times 1 + P(b) \times 2 + P(c) \times 3 + P(d) \times 3 = 1.75 \text{ bits}$$
- In general, need $-\log_2 P(x)$ bits to encode $x$

- Each symbol requires on average

$$-P(x) \log_2 P(x) \text{ bits}$$

- To transmit an entire sequence distributed according to $P(x)$, we need on average

$$\sum_x -P(x) \log_2 P(x) \text{ bits}$$

of information per symbol we wish to transmit

- **information content** or *entropy* of the sequence
Information gain

Given a set $E$ of $N$ training examples, if the number of examples with output feature $Y = y_i$ is $N_i$, then

$$P(Y = y_i) = P(y_i) = \frac{N_i}{N}$$

(the point estimate)

Total information content for the set $E$ is:

$$I(E) = -\sum_{y_i \in Y} P(y_i) \log P(y_i)$$

So, after splitting $E$ up into $E_1$ and $E_2$ (size $N_1$, $N_2$) based on input attribute $X_i$, the information content

$$I(E_{split}) = \frac{N_1}{N} I(E_1) + \frac{N_2}{N} I(E_2)$$

and we want the $X_i$ that maximises the information gain:

$$I(E) - I(E_{split})$$
Example: user discussion board behaviors

<table>
<thead>
<tr>
<th>example</th>
<th>author</th>
<th>thread</th>
<th>length</th>
<th>where read</th>
<th>user’s action</th>
</tr>
</thead>
<tbody>
<tr>
<td>e1</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e2</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e3</td>
<td>unknown</td>
<td>follow up</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e4</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e5</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e6</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e7</td>
<td>unknown</td>
<td>follow up</td>
<td>short</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e8</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e9</td>
<td>known</td>
<td>follow up</td>
<td>long</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e10</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e11</td>
<td>unknown</td>
<td>follow up</td>
<td>short</td>
<td>home</td>
<td>skips</td>
</tr>
<tr>
<td>e12</td>
<td>known</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>skips</td>
</tr>
<tr>
<td>e13</td>
<td>known</td>
<td>follow up</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e14</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e15</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e16</td>
<td>known</td>
<td>follow up</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e17</td>
<td>known</td>
<td>new</td>
<td>short</td>
<td>home</td>
<td>reads</td>
</tr>
<tr>
<td>e18</td>
<td>unknown</td>
<td>new</td>
<td>short</td>
<td>work</td>
<td>reads</td>
</tr>
<tr>
<td>e19</td>
<td>unknown</td>
<td>new</td>
<td>long</td>
<td>work</td>
<td>?</td>
</tr>
</tbody>
</table>
Final return value

- Point estimate of $Y$ (output features) over all examples
- Point estimate is just a prediction of target features
  - mean value,
  - median value,
  - most likely classification,
  - etc.

E.g.

$$P(Y = y_i) = \frac{N_i}{N}$$

Where
  - $N_i$ is the number of training samples at the leaf with $Y = Y_i$
  - $N$ is the total number of training samples at the leaf.
Using a Priority Queue to Learn the DT

- The “vanilla” version we saw grows all branches for a node.
- But there might be some branches that are more worthwhile to expand.
- Idea: sort the leaves using a priority queue ranked by how much information can be gained with the best feature at that leaf.
- Always expand the leaf at the top of the queue.
procedure DecisionTreeLearner(X,Y,E)
Start with a single node (index 0) with
- whole data set $E_0 \equiv E$,
- the point estimate for $E_0$, $y_0$,
- the best next feature to split $E_0$ on, $X_0$ and
- the amount of information gain $\Delta I_0$ if $E_0$ split on $X_0$.
Repeat until a stopping criteria is reached
- find the tree leaf (index $i$) with the highest information-Gain $\Delta I_i$:
  → leaf $i$ is the next split to do.
- Split the data at that leaf ($E_i$) according to the Best-Feature $X_i$
  → two datasets $E_i+$ and $E_i-$
- Add 2 children to node $i$, one with $E_i+$ and one with $E_i-$
- for each new child: compute and store in the child nodes:
  - point estimate,
  - best next feature to split on (of all the remaining features), and
  - information gain for that split
procedure DecisionTreeLearner(X,Y,E)

\[ DT = \text{pointEstimate}(Y, E) = \text{initial decision tree} \]
\[ \{X', \Delta I\} \leftarrow \text{best feature and Information Gain value for } E \]
\[ PQ \leftarrow \{DT, E, X', \Delta I\} = \text{priority queue of leaves ranked by } \Delta I \]

while stopping criteria is not met do:

\[ \{S_l, E_l, X_l, \Delta I_l\} \leftarrow \text{leaf at the head of } PQ \]

for each value \( x_i \) of \( X_l \) do

\[ E_i = \text{all examples in } E_l \text{ where } X_l = x_i \]
\[ \{X_j, \Delta I_j\} = \text{best feature and value for } E_i \]
\[ T_i \leftarrow \text{pointEstimate}(Y, E_i) \]

insert \( \{T_i, E_i, X_j, \Delta I_j\} \) into \( PQ \) according to \( \Delta I_j \)

end for

\[ S_l \leftarrow \langle X_l, T_1, \ldots, T_N \rangle \]

end while

return \( DT \)

end procedure
Overfitting

Sometimes the decision tree is “too good” at classifying the training data, and will not generalise very well. This often occurs when there is not much data.

3 attributes: bad weather, burnt toast, train late

training data:
A: true, true, true;
A: false, false, false;
A: false, false, false;
A: true, false, false;
A: false, true, false;
A: true, false, true;
A: false, false, false;
Overfitting

Sometimes the decision tree is “too good” at classifying the training data, and will not generalise very well. This often occurs when there is not much data. 

3 attributes: bad weather, burnt toast, train late

training data:
A: true, true, true;
A: false, false, false;
A: false, false, false;
A: true, false, false;
A: false, true, false;
A: true, false, true;
A: false, false, false;
A: true, true, true;
A: true, false, true;
A: false, true, false;
A: true, false, true;
A: false, true, false;
A: false, true, false;
...

Split: badweather

<table>
<thead>
<tr>
<th>Value</th>
<th>Count</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>true</td>
<td>9</td>
<td>0.53</td>
</tr>
<tr>
<td>false</td>
<td>8</td>
<td>0.47</td>
</tr>
</tbody>
</table>

Leaf

<table>
<thead>
<tr>
<th>Value</th>
<th>Count</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>true</td>
<td>9</td>
<td>0.90</td>
</tr>
<tr>
<td>false</td>
<td>1</td>
<td>0.10</td>
</tr>
</tbody>
</table>

Leaf

<table>
<thead>
<tr>
<th>Value</th>
<th>Count</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>true</td>
<td>0</td>
<td>0.00</td>
</tr>
<tr>
<td>false</td>
<td>7</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Overfitting

Some methods to avoid overfitting

- Regularization: e.g. Prefer small decision trees over big ones, so add a 'complexity' penalty to the stopping criteria - stop early
- Pseudocounts: add some data based on prior knowledge
- Cross validation
Overfitting

Test set errors caused by:

- **bias**: the error due to the algorithm finding an imperfect model.
  - **representation bias**: model is too simple
  - **search bias**: not enough search

- **variance**: the error due to lack of data.

- **noise**: the error due to the data depending on features not modeled or because the process generating the data is inherently stochastic.

- **bias-variance trade-off**:
  - Complicated model, not enough data (low bias, high variance)
  - Simple model, lots of data (high bias, low variance)
Overfitting

- capacity of a model is its ability to fit a wide variety of functions.
- capacity is like the inverse of bias - a high capacity model has low bias and vice-versa.

![Graph showing underfitting, appropriate capacity, and overfitting](image-url)
Cross Validation

Split training data into a training and a validation set.

Use the validation set as a "pretend" test set.

Optimise the decision maker to perform well on the validation set, not the training set.

Can do this multiple times with different validation sets.
Uncertainty (Poole & Mackworth (2nd ed.) Chapter 8)