Lecture 7a - Supervised Machine Learning I

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Readings: Poole & Mackworth (2nd ed.)Chapt. 7.1-7.3.1,7.4

Learning

Learning is the ability to improve 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

- Make a prediction from a knowledge base (causes and laws): deduction (top-down)
- Infer laws from data (causes and effects): induction (bottom-up)
- Infer causes from experience and knowledge: abduction (we will not cover this)
- 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.

Feedback

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 (unseen) 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.

Bias

- 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.

Learning as search

- 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! (see "N and P" agents slide)

Noise

- 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

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

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

- sum of squares error

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

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- worst-case error:

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

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- worst-case error:

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

- A cost-based error takes into account costs of various errors.

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)

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

$$\prod_{e \in E} \prod_{Y \in T} \hat{Y}(e)^{Y(e)} (1 - \hat{Y}(e))^{(1-Y(e))}$$

Measures of error (cont.)

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$$\prod_{e \in E} \prod_{Y \in T} \hat{Y}(e)^{Y(e)} (1 - \hat{Y}(e))^{(1-Y(e))}$$

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

$$-\sum_{e \in E} \sum_{Y \in T} [Y(e) \log \hat{Y}(e) + (1 - Y(e)) \log(1 - \hat{Y}(e))]$$

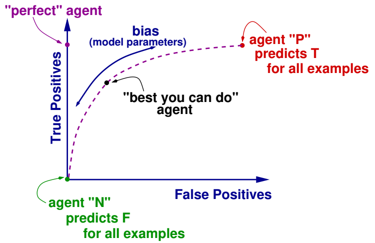
Precision and Recall

- 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

		predicted T	predicted F
actual	T	true positive (TP)	false negative (FN)
	F	false positive (FP)	true negative (TN)

- recall = sensitivity = TP/(TP+FN)
- specificity = TN/(TN+FP)
- precision = TP/(TP+FP)
- F1-measure = 2*Precision*Recall/(Precision+Recall) gives even weight to precision and recall

Receiver Operating Curve (ROC)



The ROC gives
full range of performance of an algorithm across different biases

Basic Models for Supervised Learning

Many learning algorithms can be seen as deriving from:

- decision trees
- linear classifiers (incl. neural networks)
- Bayesian classifiers

Example: user discussion board

- Consider an application that predicts if a user will read or skip a discussion board article
- User action depends on the following attributes or features of articles:
  - the author of the article is known or unknown to the user,
  - the thread is new or a follow up,
  - the article's length is long or short,
  - the user reads the article at home or at work.
- Try to predict, based only on your prior knowledge of threaded discussion boards, what the user's action will be (read or skip) for the following examples:

example	author	thread	length	where read	user's action
t1	unknown	new	long	work	
t2	known	new	short	home	
t3	unknown	follow up	short	work	
t4	unknown	follow up	long	home	
t5	known	follow up	short	home	

Dataset: discussion board behaviors

After seeing this dataset, Now what is your prediction?

example	author	thread	length	where read	user's action
e1	known	new	long	home	skips
e2	unknown	new	short	work	reads
e3	unknown	follow up	long	work	skips
e4	known	follow up	long	home	skips
e5	known	new	short	home	reads
e6	known	follow up	long	work	skips
e7	unknown	follow up	short	work	skips
e8	unknown	new	short	work	reads
e9	known	follow up	long	home	skips
e10	known	new	long	work	skips
e11	unknown	follow up	short	home	skips
e12	known	new	long	work	skips
e13	known	follow up	short	home	reads
e14	known	new	short	work	reads
e15	known	new	short	home	reads
e16	known	follow up	short	work	reads
e17	known	new	short	home	reads
e18	unknown	new	short	work	reads
e19	unknown	new	long	work	?
e20	unknown	follow up	long	home	?

Example: user discussion board behaviors

It appears the user mostly skips long articles (yellow lines) with two exceptions (green lines)

example	author	thread	length	where read	user's action
e1	known	new	long	home	skips
e2	unknown	new	short	work	reads
e3	unknown	follow up	long	work	skips
e4	known	follow up	long	home	skips
e5	known	new	short	home	reads
e6	known	follow up	long	work	skips
e7	unknown	follow up	short	work	skips
e8	unknown	new	short	work	reads
e9	known	follow up	long	home	skips
e10	known	new	long	work	skips
e11	unknown	follow up	short	home	skips
e12	known	new	long	work	skips
e13	known	follow up	short	home	reads
e14	known	new	short	work	reads
e15	known	new	short	home	reads
e16	known	follow up	short	work	reads
e17	known	new	short	home	reads
e18	unknown	new	short	work	reads
e19	unknown	new	long	work	?
e20	known	follow up	short	home	?

Learning Decision Trees

Simple, successful technique for supervised learning from discrete data

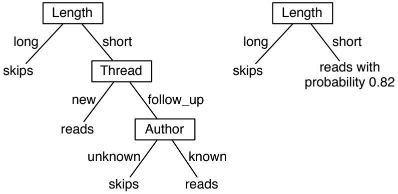
- Representation is a decision tree.
- Bias is towards simple decision trees.
- Search through the space of decision trees, from simple decision trees to more complex ones.

Decision Trees

- 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

Which decision tree is better for the discussion board example?



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)

Decision tree learning: pseudocode

//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 $< X_i, T_1, \ldots, T_N >$ where
// X_i is an input feature and $T_1, \ldots, T_N$ are decision trees

procedure DecisionTreeLearner(X,Y,E)
if stopping criteria is met **then**
  return pointEstimate(Y,E)
else
  select feature $X_i \in X$
  for each value x_i of X_i **do**
    E_i = all examples in E where $X_i = x_i$
    T_i = DecisionTreeLearner($X \setminus \{X_i\}, Y, E_i$)
  end for
  return $< X_i, T_1, \ldots, T_N >$
end procedure

Decision tree classification: pseudocode

//X is is input features, Y is output features,
//e is test example
//DT is a decision tree
//output is a prediction of Y for e

procedure ClassifyExample(e,X,Y,DT)
$S \leftarrow DT$
while S is internal node of the form $< X_i, T_1, \ldots, T_N >$ **do**
  $j \leftarrow X_i(e)$
  $S \leftarrow T_j$
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 for N-ary features)

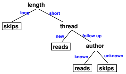
Stopping Criteria

- 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

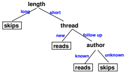
Feature Selection

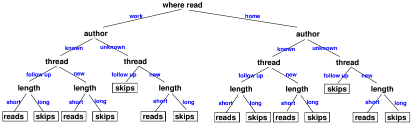
- Ideal: choose sequence of features that result in smallest tree
- Actual: myopically split - as if only allowed one split, which feature would give best performance?
- heuristics for best performing feature:
  - Most even split
  - Maximum information gain
  - GINI index
  - ... others domain dependent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

Good Feature Selection



Bad Feature Selection





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 bits

Information Theory

- In general, need $-\log_2 P(x)$ bits to encode x
- Each symbol requires on average

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

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

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

  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 (assume $\log \equiv \log_2$):

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

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

Build a decision tree for this dataset, using information gain to split,
then make predictions for two unlabeled test examples

example	**author**	**thread**	**length**	**where read**	**user's action**
e1	known	new	long	home	skips
e2	unknown	new	short	work	reads
e3	unknown	follow up	long	work	skips
e4	known	follow up	long	home	skips
e5	known	new	short	home	reads
e6	known	follow up	long	work	skips
e7	unknown	follow up	short	work	skips
e8	unknown	new	short	work	reads
e9	known	follow up	long	home	skips
e10	known	new	long	work	skips
e11	unknown	follow up	short	home	skips
e12	known	new	long	work	skips
e13	known	follow up	short	home	reads
e14	known	new	short	work	reads
e15	known	new	short	home	reads
e16	known	follow up	short	work	reads
e17	known	new	short	home	reads
e18	unknown	new	short	work	reads
e19	unknown	new	long	work	?
e20	unknown	follow up	long	home	?

(see dtexample.pdf handout)

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

Priority Queue (PQ) Decision Tree: Pseudocode V1

procedure DecisionTreeLearner(X,Y,E)
Start PQ 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 ΔI_0 if E_0 split on X_0.
- add node 0 to PQ

Repeat until a stopping criteria is reached:
- find leaf (index i) with highest information gain (head of PQ)
  $\rightarrow$ leaf i is the next split to do.
- Split the data at that leaf (E_i) according to the Best-Feature X_i
  $\rightarrow$ 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
- add child nodes to PQ by information gain

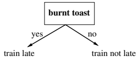
Decision tree learning: pseudocode V2

procedure DecisionTreeLearner(X,Y,E)
$DT = pointEstimate(Y,E)$ = initial decision tree
$\{X', \Delta I\} \leftarrow$ best feature and Information Gain value for E
$PQ \leftarrow \{DT, E, X', \Delta I\}$ = priority queue of leaves ranked by ΔI
while stopping criteria is not met **do:**
    $\{S_l, E_l, X_l, \Delta I_l\} \leftarrow$ leaf at the head of PQ
    for each value x_i of X_l **do**
        E_i = all examples in E_l where $X_l = x_i$
        $\{X_j, \Delta I_j\}$ = best feature and value for E_i
        $T_i \leftarrow pointEstimate(Y, E_i)$
        insert $\{T_i, E_i, X_j, \Delta I_j\}$ into PQ according to ΔI_j
    end for
    $S_l \leftarrow < X_l, T_1, \ldots, T_N >$
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
Attributes:
bad weather (W), I burnt my toast (T), my train is late (L)
training data:
W , T , L ;
true, true, true;
false, false, false;
false, false, false;
true, false, false;

best decision tree (info gain):



Decision tree predicts the train based on burnt toast

Overfitting

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Attributes:

bad weather (W), I burnt my toast (T), my train is late (L)

training data:

W , T , L ;

true, true, true;

false, false, false;

false, false, false;

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false, true, false;

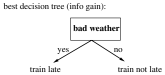
true, false, true;

false,false, false;

true, true, true;

true, false, true;

false, true, false;

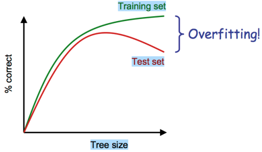


Decision tree predicts the train based on the weather

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



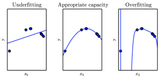
Overfitting

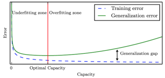
Test set errors caused by:

- 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)
- see handout `biasvariance.pdf`

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





→ slight wrinkle in this story (see `https://www.bradyneal.com/bias-variance-tradeoff-textbooks-update` and `https://arxiv.org/abs/1810.08591`.

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)