Machine Learning (ML) 101

Methods in AI research

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Practicalities

- **Literature for today:** Hal Daumé III, A Course in Machine Learning, Chapter 1 (Decision Trees; http://ciml.info/dl/v0_99/ciml-v0_99-ch01.pdf) and Chapter 2 (Limits of Learning; http://ciml.info/dl/v0_99/ciml-v0_99-ch02.pdf).

- **Speech & Language processing** Section 25.2 (Dialog State: Interpreting Dialog Acts)

RECAP !

Last time

- **Dialog systems**
  - Chatbots vs. goal-based dialogue systems
  - We came across approaches for which we needed to:
    - Select a response from the dataset ('information retrieval' approach)
    - Classify domain, intent, slot for frame-based approaches
    - Classify dialog acts
  - Rule-based vs. **machine learning** approaches

Natural Language

Egesiel Magalhães S.	**Loan Offer** - Do you need a Loan @ 2% PA? Mail us your: Names,Home Add,Mob No,Email id,Amount Needed,Lo...
Mr. Karim Zongo	**PLEASE THIS IS VERY URGENT.** - Compliment of the day, I am Mr. Karim Zongo Have a Business Proposal of $5...
CITIBANK OF NEW YORK	**NEW MESSAGE FROM CITIBANK NEW YORK** - CITIBANK INTERNATIONAL NEW YORK DIRECTOR, FOREIGN OPE...
MRS. CHRISTY MCCOOL	**MY DONATION OF 4 MILLION DOLLARS ARE YOU INTERESTED ?** - I am writing to seek your consent to conduct...

Spam classification

Intent: **SHOWFLIGHT**

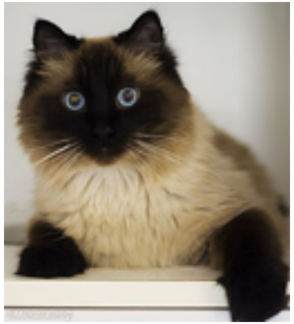
```
I want to fly to San Francisco on
Monday afternoon please
```

Intent classification

EN ←→ NL

Machine translation

Image classification

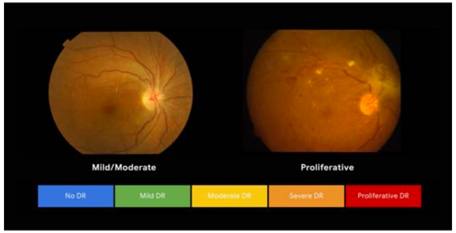


IMAGENET

ImageNet has **21841** classes

http://image-net.org/explore

Digit recognition
MNIST dataset



Diagnosing Diabetic Eye Disease
https://ai.google/healthcare/

What is Machine Learning?

There are many definitions, here is a useful one:

A computer program is said to ***learn*** *from experience* ***E*** *with respect to some class of tasks* ***T*** *and performance measure* ***P****, if its performance at tasks in* ***T****, as measured by* ***P****, improved with experience* ***E****.*

Tom Mitchell, Machine Learning 1997

What is Machine Learning?

Three components:

- Task T
- Experience E
- Performance measure P

Detect the dialog act of an utterance

T: Classify the dialog act of an utterance

P: The fraction of utterances correctly classified

E: A set of utterances labeled with their dialog acts

What is Machine Learning?

Three components:

- Task T
- Experience E
- Performance measure P

Self-driving cars

T: Drive on public highways using vision sensors

P: Average distance traveled before an error

E: Sequence of images and steering commands from human drivers

Experience

1. Supervised learning
2. Unsupervised learning
3. Reinforcement learning

Experience

The focus of our lectures!

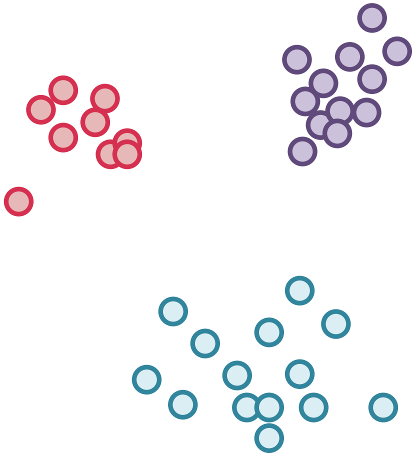
1. Supervised learning
2. Unsupervised learning
3. Reinforcement learning

Learn a model using **labelled** instances

Example: image classification, dialog act classification.

Experience

1. Supervised learning
2. Unsupervised learning
3. Reinforcement learning



Learn a model using **unlabelled** data

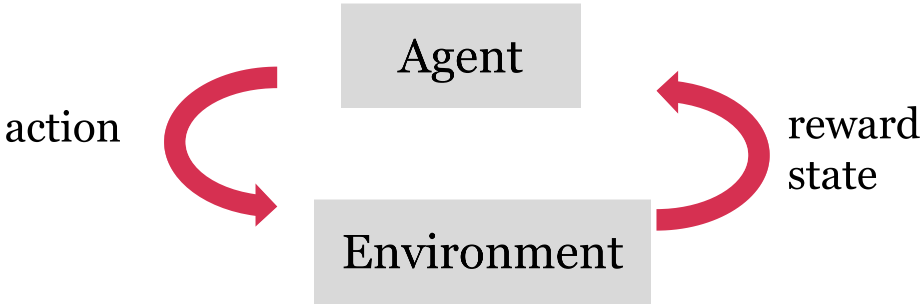
Example: community detection

Experience

1. Supervised learning

2. Unsupervised learning

3. Reinforcement learning



Agent: conversational agent
Environment: user
Reward: 1..5 poor-excellent dialog
Action: utterance by agent

Supervised learning

RECAP!

Hand crafted rules: dialog systems

To recognize SET-ALARM intent:

```
wake me (up) | set (the|an) alarm | get me up
```

Hand crafted rules: spam classification

```
Spam list => spam
'Buy' AND ('cheap' OR 'free') => spam
```

Very precise. Sometimes easier to fix mistakes.

Manually crafting rules takes a **lot** of time and is **difficult** to do.

High maintenance cost (e.g. need to adapt to changing language use)

Hand crafted rules: time-consuming!

- 232 industry categories and 504 occupation categories

- Manual rules
  - Development time = **192** person-months

- Machine learning
  - Development time = **4** person-months
  - More accurate!

COMMERCIAL APPLICATIONS OF MASSIVELY PARALLEL SUPERCOMPUTERS FOR THE 90’S

Waltz 1991.

Hand crafting rules for some tasks would be *really* difficult!

For example: author identification of texts

- It's (usually) not about the use of *specific* words, but about small differences between (relative) frequencies of words and grammatical constructions.

But collecting labels is easy…

Supervised learning

- Learn a machine learning model using **labeled example instances**

- Need to define **features**, characteristics of the instances that the model uses for predictions (words in a document, movie ratings, etc..)

Supervised learning

- Learn a machine learning model using **labeled example instances**

- Need to define **features**, characteristics of the instances that the model uses for predictions (words in a document, movie ratings, etc..)

Domain classification for dialog systems

```
I want to fly to San
Francisco on Monday
afternoon please
```

```
Domain: AIRLINE
```

Features: words

Supervised learning

- Learn a machine learning model using **labeled example instances**

- Need to define **features**, characteristics of the instances that the model uses for predictions (words in a document, movie ratings, etc..)

Features for house price prediction:

- Overall condition of the house
- Neighborhood
- Condition of the basement
- Number of bedrooms
- Construction date
- First floor square meters
- Number of schools in within 2 km
- Condition of the kitchen
- ..

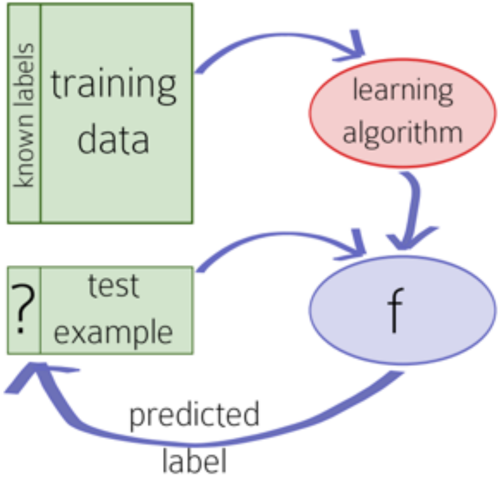
Supervised learning

- Learn a machine learning model using **labeled example instances**

- Need to define **features**, characteristics of the instances that the model uses for predictions (words in a document, movie ratings, etc..)

Question: What features could we use to predict whether a credit card transaction is fraudulent or genuine?

Supervised learning



CIML, figure 1.1

Setting:

X: input space (set of possible instances)
Y: output space

H = {f|f : X → Y}: set of hypotheses (the set of all possible classifiers we consider)

Learning:

i: current training example

Input: $<x^{(i)}, y^{(i)}>$: training examples
Learning algorithm: Defines a data-driven search over the hypothesis space

Output:

f ∈ F: hypothesis that approximates the target function

Tasks & data

features output

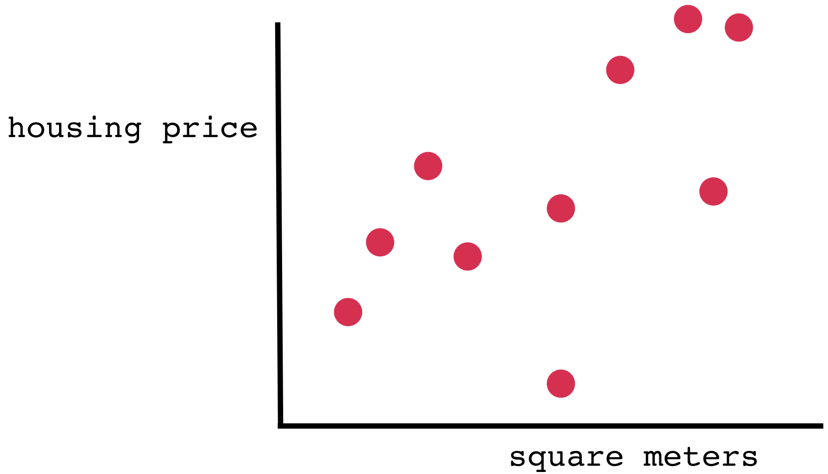
Input: $\{<x^{(1)}, y^{(1)}>, \ldots, <x^{(N)}, y^{(N)}>\}$

Goal: Predict the target using the features

Housing price prediction:
This is a *regression* problem (target is a real number)

What are the dimensions of the features and the target?

$x^{(i)} \in \mathbb{R}$ (one)
$y^{(i)} \in \mathbb{R}$ (one)



Tasks & data

features output

Input: $\{<x^{(1)}, y^{(1)}>, \ldots, <x^{(N)}, y^{(N)}>\}$

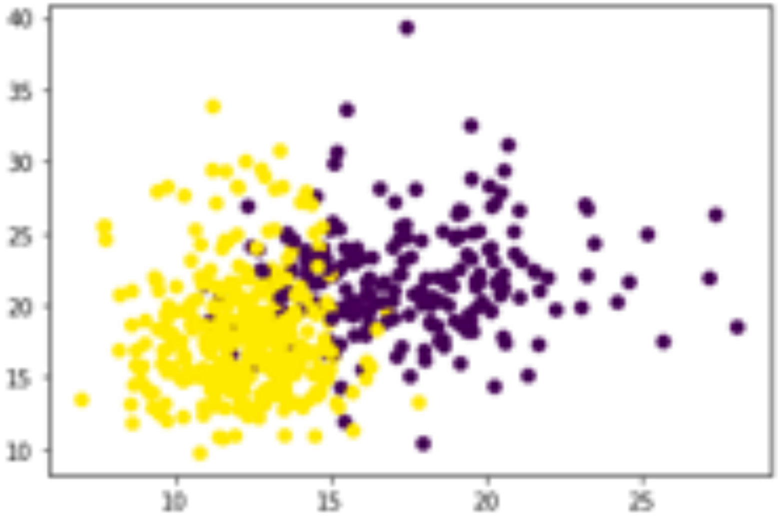
Goal: Predict the target using the features

Breast cancer diagnosis (malignant or benign):
This is a *classification* problem (target is a category)

The focus of our lectures!

What are the dimensions of the features and the target?

$x^{(i)} \in \mathbb{R}^2$ (two)
$y^{(i)} \in \{0,1\}$ (one)



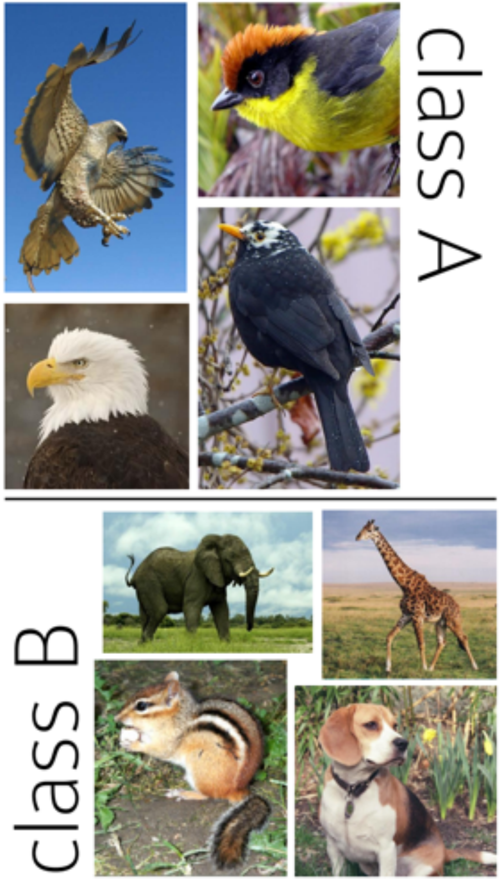
Learning

- **Generalization**
  - Training versus test examples
  - *Memorization is not enough!*

- **Inductive bias**
  - Allows a learning algorithm to prioritize one solution (or interpretation) over another, independent of the observed data (Battaglia et al. 2018, Mitchell 1980)

Inductive bias

Training data



[CIML 2.1 and 2.2]

Test data

ABBA:
bird vs. non-bird

AABB:
Fly vs. no-fly

Underlying assumptions to generalize to new input!

Supervised machine learning for classification

- Naive Bayes
- Logistic Regression
- Support Vector Machines (SVM)
- Neural networks
- Decision trees
- K-nearest neighbors
- And many more…

Supervised machine learning for classification

- Naive Bayes
- **Logistic Regression**
- Support Vector Machines (SVM)
- **Neural networks**
- **Decision trees**
- **K-nearest neighbors**
- And many more…

Decision Trees

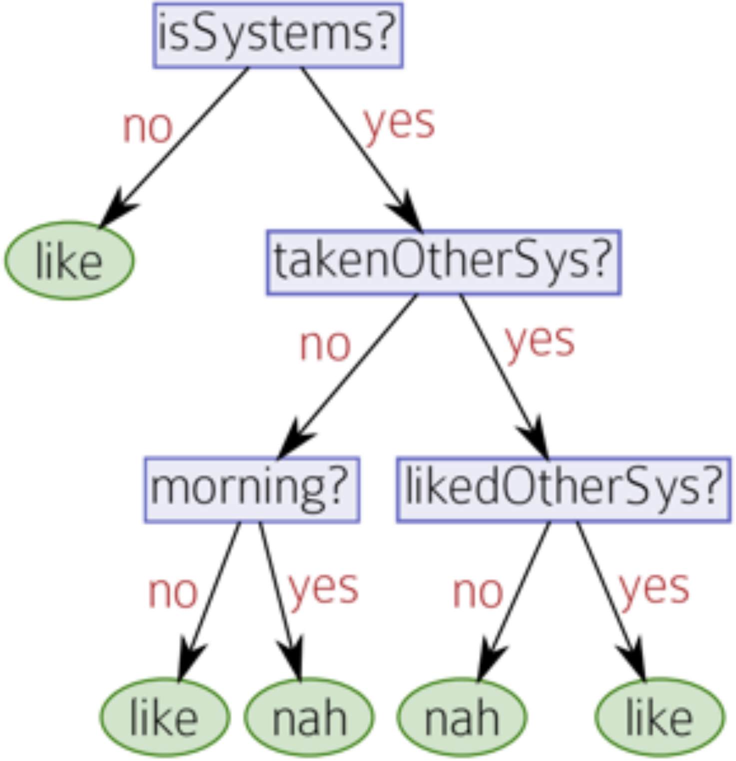
Asking the right questions

You: Is the course under consideration in Systems?
Me: Yes

You: Has this student taken any other Systems courses?
Me: Yes

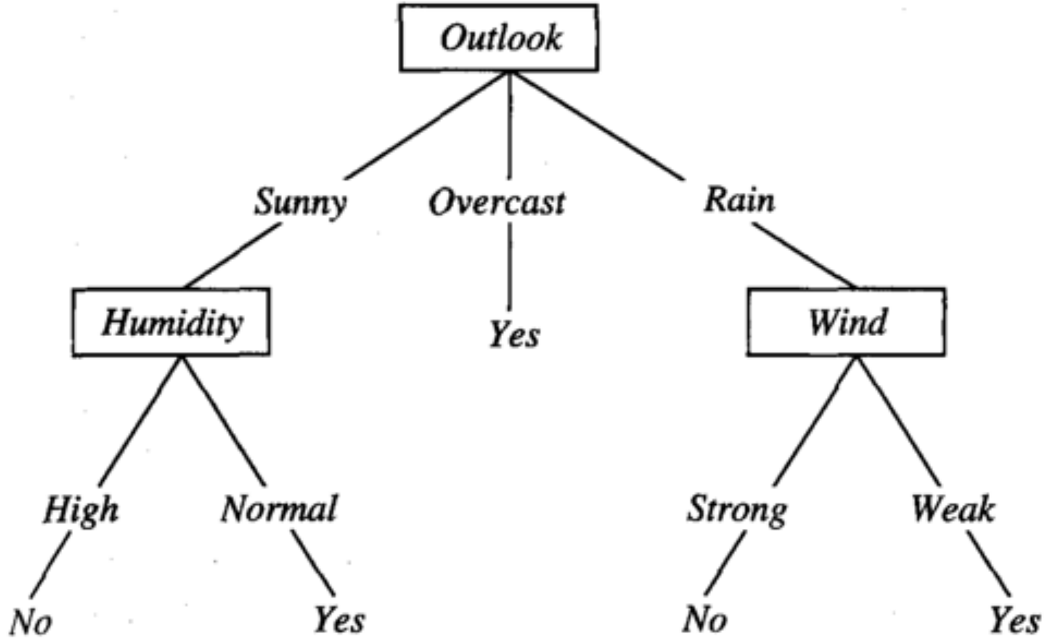
You: Has this student liked most previous Systems courses?
Me: No

You: **I predict this student will not like this course.**



CML book

Examples



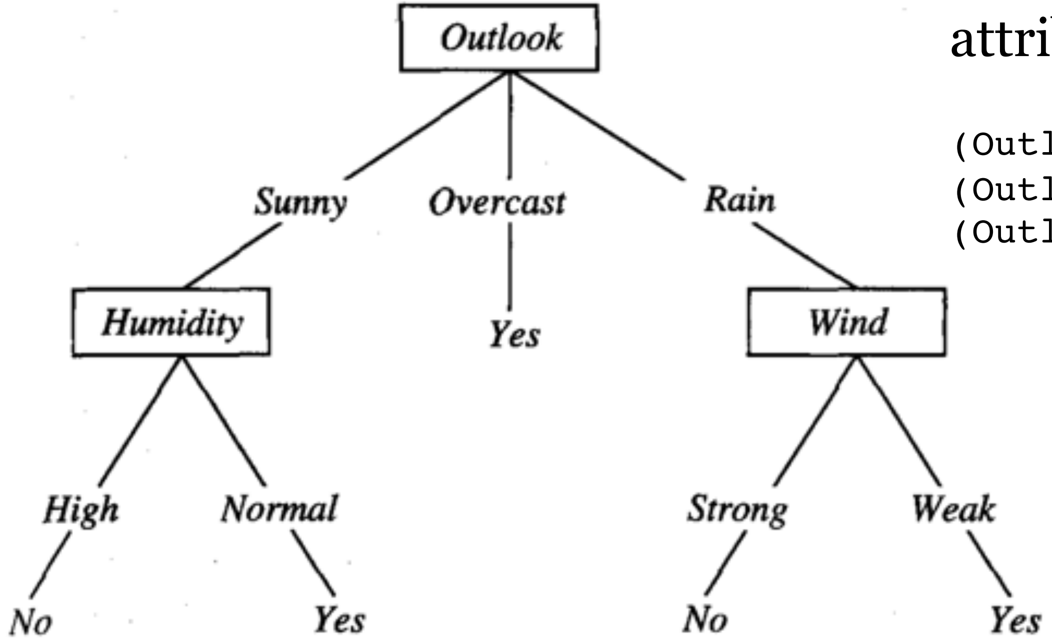
Is it a good time to play tennis?

`(Outlook = Sunny, Temperature = Hot, Humidity = High, Wind = Strong)`

Answer: **No**

Machine Learning, Tom Mitchell (p. 53)

Examples



Decision trees represent disjunction of conjunctions of constraints on the attribute values

```
(Outlook = Sunny ∧ Humidity = Normal) V
(Outlook = Overcast) V
(Outlook = Rain ∧ Wind = Weak)
```

Decision trees can be represented as if-then rules (helps interpretability ☺)

Machine Learning, Tom Mitchell (p. 53)

Examples

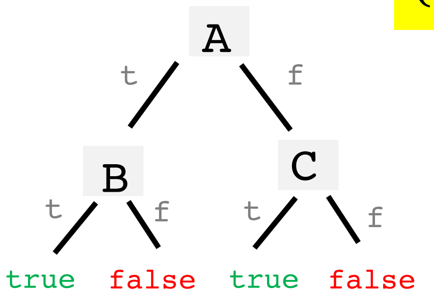
Question: create a decision tree for

```
A∧B ∨ ¬A ∧ C  ((A and B) or (not A and C))
```

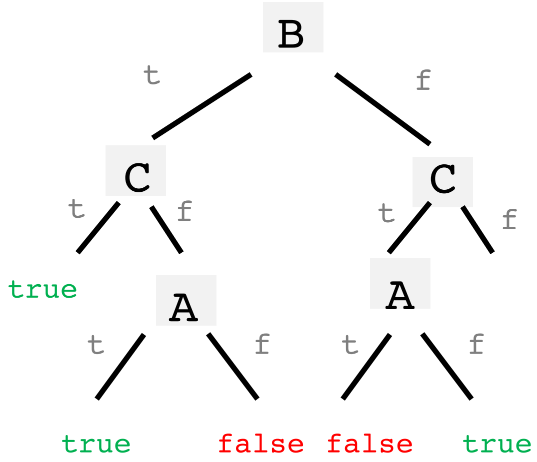
Examples

Question: create a decision tree for

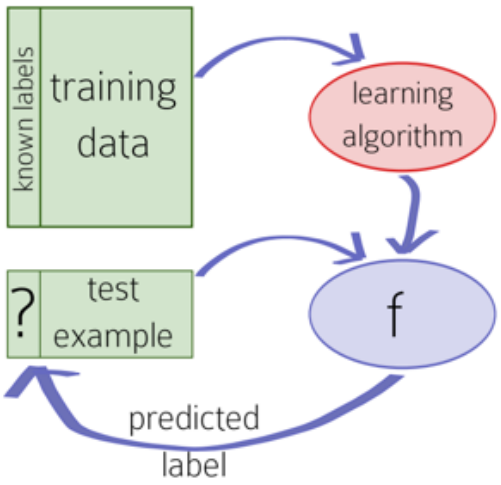
```
A∧B ∨ ¬A ∧ C   ((A and B) or (not A and C))
```



Different trees
(different sizes)



Supervised learning



CIML, figure 1.1

Setting:

X: input space (set of possible instances)

Y: output space

y=1: likes the course 0: doesn't like course

H = {f|f : $X \rightarrow$ Y}: set of hypotheses (the set of all possible classifiers we consider) Set of all possible decision trees

Learning:

i: current training example

Input: <$x^{(i)}$, $y^{(i)}$>: training examples

Learning algorithm: Defines a data-driven search over the hypothesis space

Output:

f ∈ F: hypothesis that approximates the target function

Learning decision trees

Find the 'best' tree h ∈ H, i.e. the tree that minimizes training error, or maximizes training accuracy

What about doing an exhaustive search? 😔
Computationally infeasible

Instead: We use a greedy search

Learning decision trees

```
Start with empty tree

Base cases:
If all instances have the same label →
   create a leaf with that label and exit
If no features left to split →
    create a leaf with the majority label

Else:
Select the best test to split the data on
Split the data according to the test
Recurse on each subset of the data
```

Selecting attributes to split

Is it a good time to play tennis?

[9+, 5-]
Humidity
high: [3+, 4-]
normal: [6+, 1-]

[9+, 5-]
Wind
weak: [6+, 2-]
strong: [3+, 3-]

Machine Learning, Tom Mitchell

Question:
which one would you choose?

Selecting attributes to split

We want to be more certain about the label after splitting:

After split:

All instances have the same label 😃

Uniform distribution over labels 😔

How can we quantify this intuition?

Selecting attributes to split: misclassification rate

What is the error when choosing the majority label after a split?

[9+, 5-]

Humidity

high / \ normal

[3+, 4-] [6+, 1-]

(3 + 1) / 14 = 0.286

[9+, 5-]

Wind

weak / \ strong

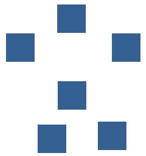
[6+, 2-] [3+, 3-]

(2 + 3) / 14 = 0.357

Selecting attributes to split: Information Gain

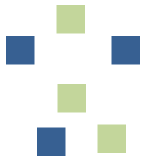
Entropy:

$$H(S) = -\sum_i p_i \log_2 p_i$$



Entropy = 0

p_i: the probability of class i (i.e. the fraction of instances of class i in S)



Entropy = 1

Entropy comes from information theory

[9+, 5-] $-(9/14)\log_2(9/14) - (5/14)\log_2(5/14) = 0.940$

[7+, 7-] $-(7/14)\log_2(7/14) - (7/14)\log_2(7/14) = 1$

[14+, 0-] $-(14/14)\log_2(14/14) - (0/14)\log_2(0/14) = 0$

Selecting attributes to split: Information Gain

Entropy:

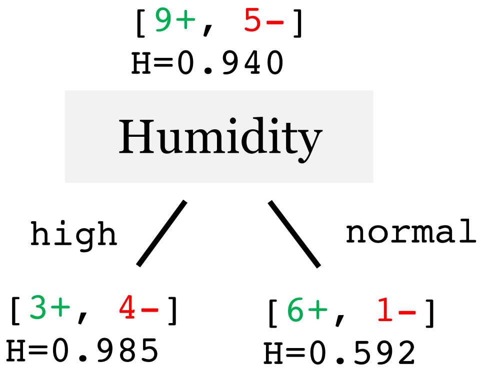
$$H(S) = -\sum_i p_i \log_2 p_i$$

p_i: the probability of class i (i.e. the fraction of instances of class i in S)

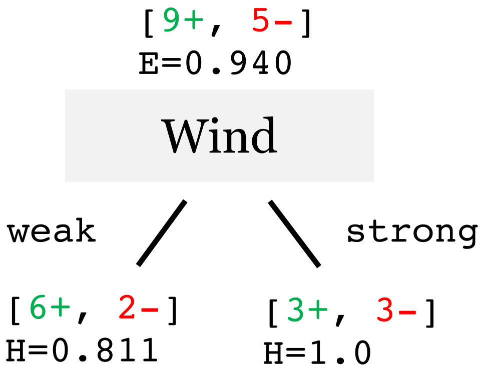
Entropy comes from information theory

Information Gain:
Entropy before you split – entropy after split (weighted by probability of following each branch)

Selecting attributes to split: Information Gain

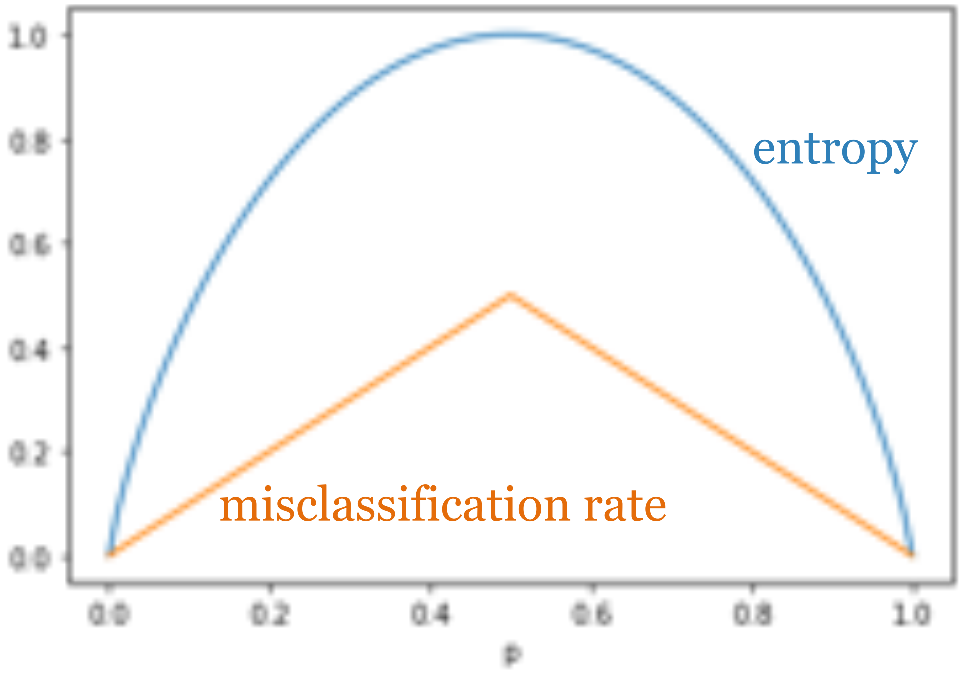


0.940 – (7/14) * 0.985 – (7/14) * 0.592 = 0.1515



0.940 – (8/14) * 0.811 – (6/14) * 1 = 0.048

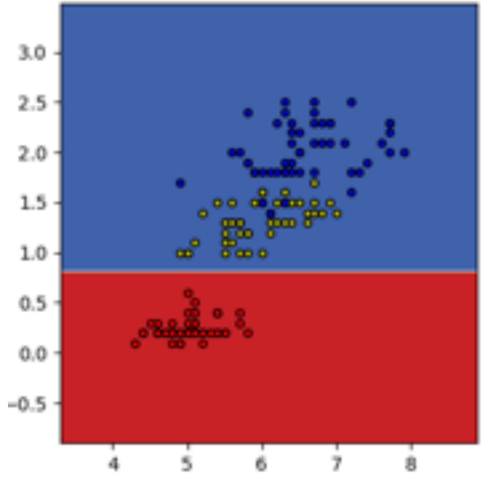
Selecting attributes to split



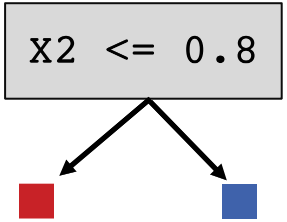
Decision boundary

max depth = 1

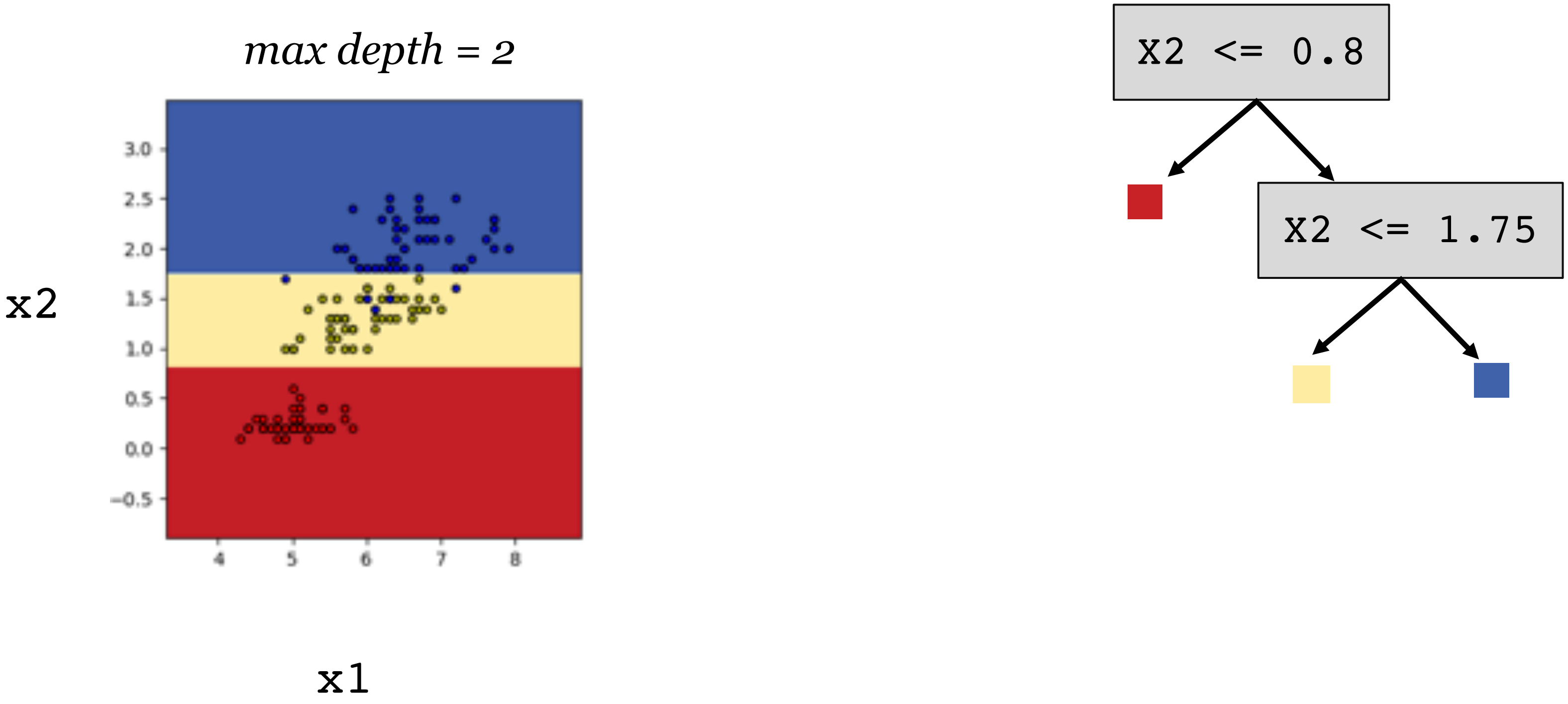
x2



x1

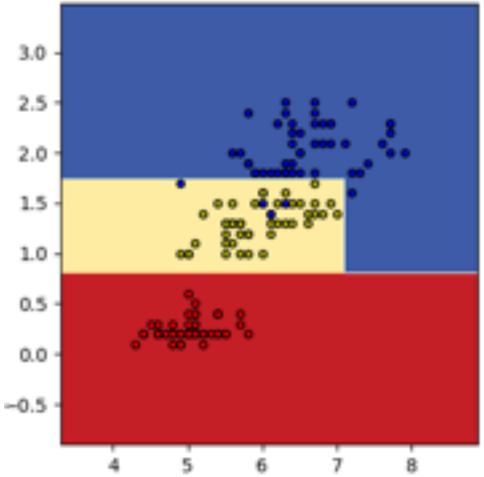


Decision boundary

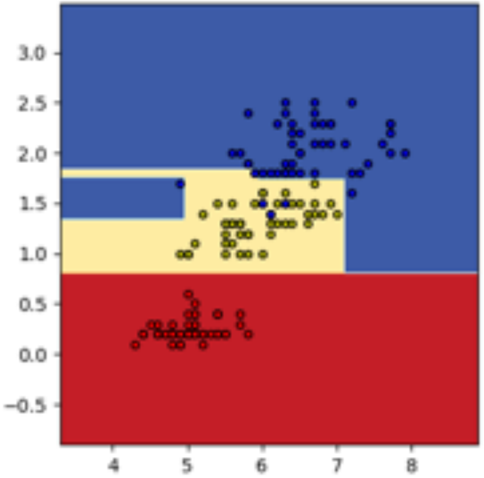


Decision boundary

max depth = 3



max depth = 25



Inductive bias

Underlying assumptions to generalize to new input!
What type of solutions are we more likely to prefer?

E.g., prefer smaller models with similar training accuracy (e.g. shallow decision trees), i.e. decisions can be made by only looking at a small number of features.

Model selection

Model selection

- **Features:** Words, user profile, etc.
- **Model:** Decision trees, or maybe something different?

We are interested in how well the model **generalizes**!

i.e. how does it perform on data it hasn't seen before?

Classification: Accuracy

$$\frac{\texttt{\#correctly labeled instances}}{\texttt{\#total instances}}$$

	Truth: A	Truth: B
Predicted: A	70	40
Predicted: B	30	60

Accuracy: 130/200 = 0.65

Train & test data

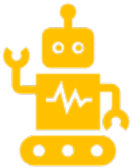
Dataset

Training set | Test set

Train your model on this data!

Test your model on this data

80% *accurate*
on the test data



85% *accurate*
on the test data

64% *accurate*
on the test data

Train & test data

Ok let's use the yellow model!! It is 85% accurate

Hold on...

Dataset

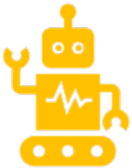
Training set

Test set

Train your model on this data!

Test your model on this data

***80%** accurate*
on the test data



***85%** accurate*
on the test data

***64%** accurate*
on the test data

Warning!!

Training error is an optimistic estimate of your system's true error. So evaluate on a holdout test set. But…

Test set is only unbiased if you **NEVER** do **ANY** learning on the test set.

- Feature development
- Selecting the model
- …

Train & dev & test data

Dataset

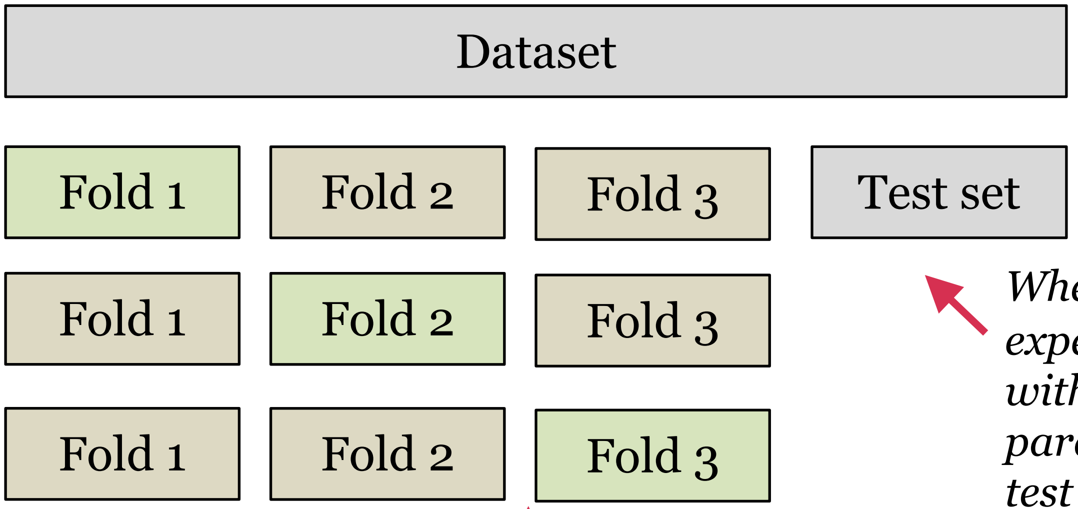
Training set | Dev set | Test set

Train your model on this data!

Tune your model on this data

When you're done with experimenting with features, tuning parameters etc. test your final model using this data.

Cross validation



When you're done with experimenting with features, tuning parameters etc. test your final model using this data.

Train and tune your parameters on folds 1-3

E.g. train on folds 2 and 3, test on fold 1.
Usually 10 folds, but depends on the data

Overfitting and underfitting

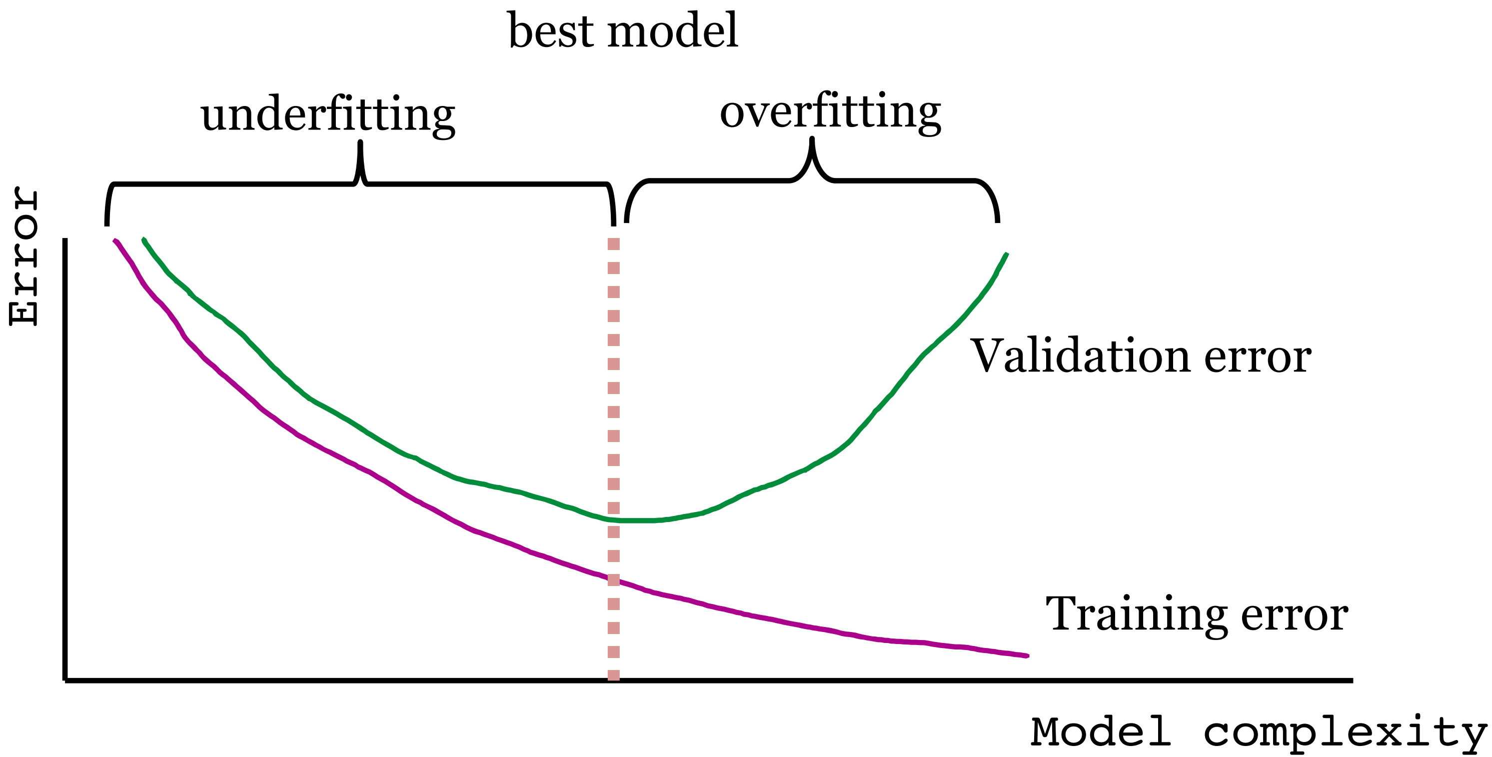
Underfitting: The model is too simple. It could have learned something but didn't.
Example: A decision tree which always predicts the same label (majority class)

Overfitting: The model pays too much attention to idiosyncrasies of the training data.
Example: a leaf for each instance in your training data (training error will be zero!) .

Constrain to simpler trees

- Max. depth
- Max. number of leaves
- Minimum number of instances per leaf

Overfitting and underfitting



Parameters vs. hyper parameters

- **Parameters:** The weights or structure selected by the learning algorithm

- **Hyperparameters:** 'Parameters that control the other parameters'. 'Things' we can tune but are not selected by the learning algorithm.

Parameters vs. hyper parameters

- **Parameters:** The weights or structure selected by the learning algorithm
- **Hyperparameters:** 'Parameters that control the other parameters'. 'Things' we can tune but are not selected by the learning algorithm.

Decision trees

Parameters:
structure of a specific decision tree

Hyperparameters:
Maximum depth, minimum number of instances per leaf, ..

Cannot be naively adjusted using the training data, because increasing max depth will always reduce the training error!

Evaluation metrics

Y	X1	X2
0	0	1
0	0	0
0	0	1
1	0	1
1	0	1
1	1	1
1	1	0
1	1	0
1	1	0
1	1	0

Accuracy

$$\frac{\texttt{\#correctly labeled instances}}{\texttt{\#total instances}}$$

Question: What is the accuracy of a classifier that would predict the majority label?

Accuracy is not suitable when the label distributions are (heavily) skewed!

Evaluation metrics

	Truth: A	Truth: B
Predicted: A	True Positive (TP)	False Positive (FP)
Predicted: B	False Negative (FN)	True Negative (TN)

$$accuracy = \frac{\#TP + \#TN}{\#TP + \#FP + \#FN + \#TN}$$

Evaluation metrics

	Truth: A	Truth: B
Predicted: A	70 (TP)	40 (FP)
Predicted: B	30 (FN)	60 (TN)

Precision for class A:
70/110 = 0.64

$$precision = \frac{\#TP}{\#TP + \#FP}$$

What fraction of the ones that you have identified belong to that class?

Of all messages labeled as spam, what fraction is actually spam?

Evaluation metrics

	Truth: A	Truth: B
Predicted: A	70 (TP)	40 (FP)
Predicted: B	30 (FN)	60 (TN)

Precision for class A:
70/110 = 0.64

Precision for class B:
60/90= 0.67

$$precision = \frac{\#TP}{\#TP + \#FP}$$

What fraction of the ones that you have identified belong to that class?

Of all messages labeled as spam, what fraction is actually spam?

Evaluation metrics

	Truth: A	Truth: B
Predicted: A	70 (TP)	40 (FP)
Predicted: B	30 (FN)	60 (TN)

Recall A:
70/100 = 0.7

$$recall = \frac{\#TP}{\#TP + \#FN}$$

What fraction of the ones that belong to the class have you identified?

Of all the messages that are actually spam, what fraction has the system labeled as spam?

Evaluation metrics

	Truth: A	Truth: B
Predicted: A	70 (TP)	40 (FP)
Predicted: B	30 (FN)	60 (TN)

Recall A:
70/100 = 0.7

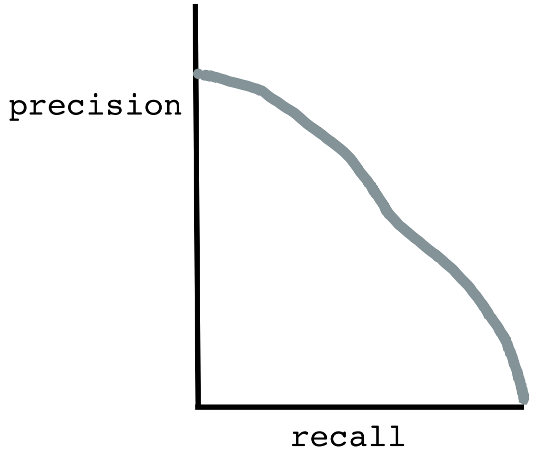
Recall B:
60/100 = 0.6

$$recall = \frac{\#TP}{\#TP + \#FN}$$

What fraction of the ones that belong to the class have you identified?

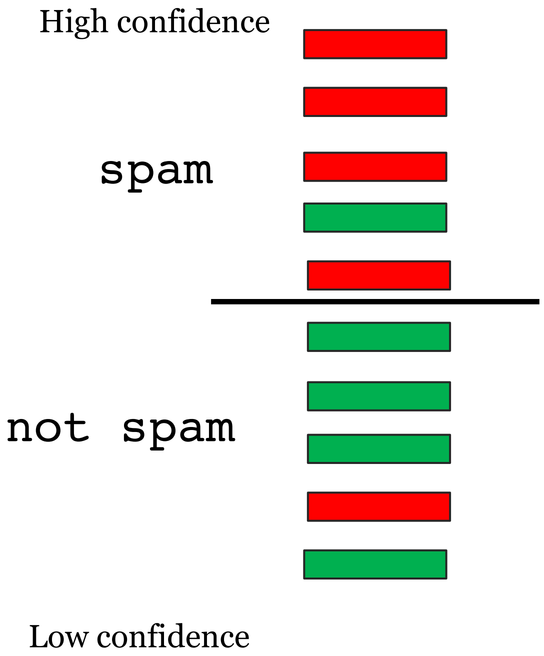
Of all the messages that are actually spam, what fraction has the system labeled as spam?

Precision recall curve



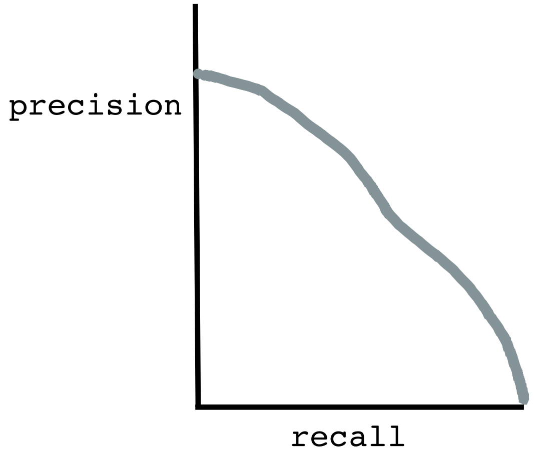
Spam classification
Accidentally labeling a message as spam: BAD
Accidentally labeling a spam message as ok: ANNOYING

Only label messages as spam if we're really *sure*.
Use the "confidence" of the classifier




```
Precision = 4/5
Recall = 4/5
```

Precision recall curve



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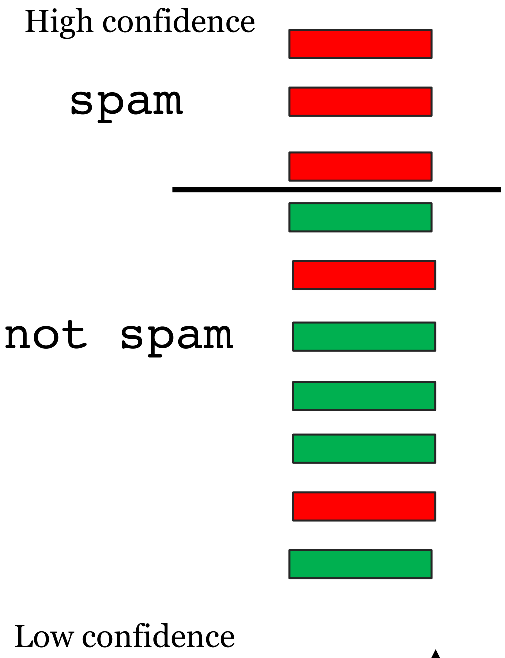
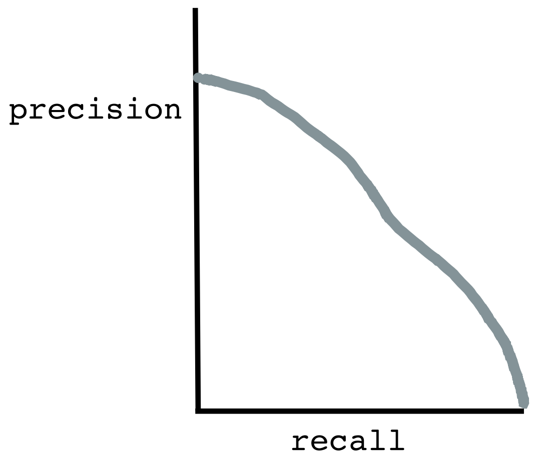


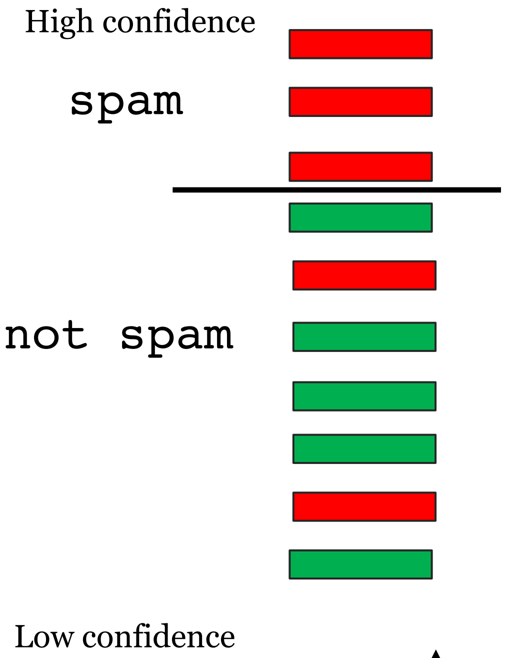
Precision = 3/3 = 1
Recall = 3/5

How can we compute the confidence of a decision tree?

Precision recall curve



Question: Come up with a task for which *precision* is more important, and a task for which *recall* is more important



Precision = 3/3 = 1 ↑

Recall = 3/5 ↓

Evaluation

Combining recall and precision using F-measure

$$F_\beta = (1+\beta^2)\frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

Often **β** = 1:

$$F_1 = \frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

Multiclass classification

- Many classification tasks are *binary* (e.g. spam or not spam).
- But… often there are more than 2 classes. This is called **multiclass** classification.

IMAGENET

ImageNet has **21841** classes

Speech act classification
15 speech acts in the project dataset

F1 for multiclass problems

- F1 scores for individual classes
- In addition:
  - Micro F1 average: Calculate F1 by counting total nr of true positives, false negatives and false positives
  - Macro F1 average: Calculate metrics for each class, and aggregate by taking an (unweighted) average

ML process

1	real world goal	increase revenue
2	real world mechanism	better ad display
3	learning problem	classify click-through
4	data collection	interaction w/ current system
5	collected data	query, ad, click
6	data representation	bow^2, $\pm$ click
7	select model family	decision trees, depth 20
8	select training data	subset from april'16
9	train model & hyperparams	final decision tree
10	predict on test data	subset from may'16
11	evaluate error	zero/one loss for $\pm$ click
12	deploy!	(hope we achieve our goal)

CIML, figure 2.4

ML process

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CIML, figure 2.4

Decide *what and how* to collect data!

Often (in ML): Use datasets others created

- Many publicly available labelled datasets (https://archive.ics.uci.edu/ml/index.php, Kaggle (https://www.kaggle.com/), etc
- Shared tasks (competitions.. leader boards)

But… often these datasets are not sufficient
(specific domains, new tasks, industry, etc…) → You need to collect your own data

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ML process

Decide *what and how* to collect data!

Some labels can be collected 'automatically'

- E.g. whether user clicked on an ad

When annotating your own data:

- Develop annotation guidelines (sometimes called code book, especially in the social sciences)
- Compute inter-annotator agreement and within-annotator agreement.
- If humans can't agree about the right label....

CIML, figure 2.4

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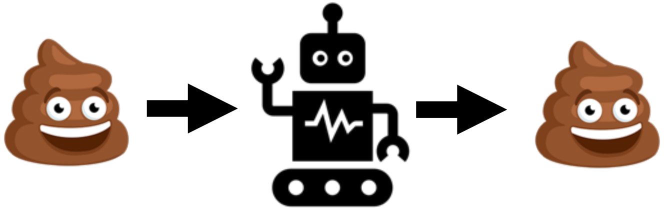
ML process

Decide *what and how* to collect data!

Be suspicious of 'ground truth' or 'gold labels'!

- Annotator noise
- Inherent ambiguity
- Some concepts are very hard to formalize! (hate speech detection)

CIML, figure 2.4



garbage in, garbage out

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ML process

Decision trees, or something else?

In addition:

- **Baseline model:** Compare your model against very stupid baselines (e.g. majority baseline) and simple machine learning methods
- **Oracle model:** If your system depends on various components (e.g. a dialog system), test overall performance with 'oracle' components.

CIML, figure 2.4

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CIML, figure 2.4

ML process

Usually a combination of multiple evaluation metrics.

Also take into account:

- Cost of errors (e.g. accidently labeling a spam e-mail as 'ok' vs. a self-driving car not detecting a pedestrian crossing a street)
- Brittleness
- Biases
- Etc..

Before deciding to deploy it!

Question!

You are a reviewer for the *best AI conference* and asked to review a submitted article. (Or, you're a journalist wanting to write a piece about a newly released system. Or, you're a software developer deciding whether to implement a new AI system.)

```
"Our system is the best. Its
training errors are so low!"
```

Nope, training errors are optimistic estimates.

Question!

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```
"Our system is the best. Its
test error is only 0.10 with
d=3"
```

This is suspicious. Looks like the best result was reported by choosing a d based on the test data.

Question!

You are a reviewer for the *best AI conference* and asked to review a submitted article. (Or, you're a journalist wanting to write a piece about a newly released system. Or, you're a software developer deciding whether to implement a new AI system.)

```
“Our system is the best. Its test
error is only 0.10. We chose d=3
based on cross-validation”
```

Yup, the hyper parameters are selected based on cross validation on the training data.

What do you need to know

- Pros and cons of rule-based vs. supervised learning
- Differences between supervised, unsupervised, reinforcement learning
- Decision Trees (algorithm, entropy, error rate)
- Concepts such as decision boundary, overfitting, underfitting, inductive bias, hyperparameters
- How to set up machine learning experiments (cross validation, evaluation metrics, precision recall tradeoff)

Example questions

- Draw a decision tree for simple problems.
    - Be able to compute the best split according to information gain and misclassification rate

- Frame a problem as a machine learning problem.

- Compute evaluation metrics (precision, recall, accuracy, F1).

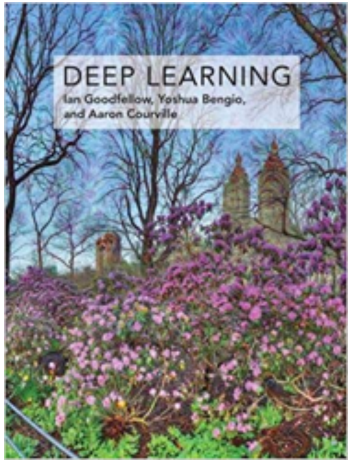
Resources

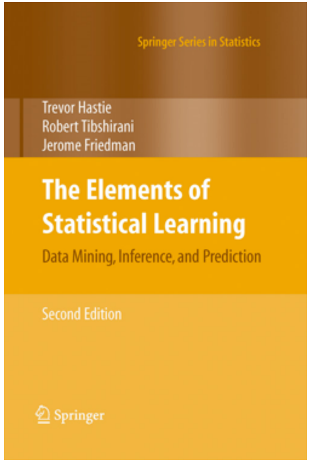
- `scikit-learn` https://scikit-learn.org. Python library with many implementations for ML models (incl. decision trees), as well as pre processing and evaluation

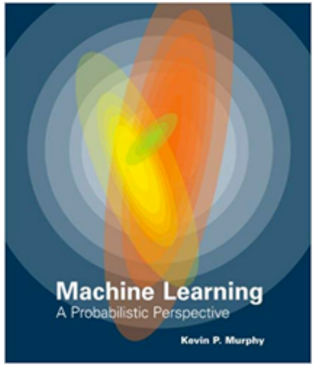
- kaggle https://www.kaggle.com/. Improve your ML skills by participating in competitions with shared datasets.

- There are many online tutorials and online courses (e.g. ML courses by Andrew Ng, Fast AI, etc.)

Books







Freely available online!:
http://www.deeplearningbook.org/

Freely available online!:
https://web.stanford.edu/~hastie/ElemStatLearn/

Thanks

Some slides based on (or inspired by) slides by Matt Gormley and Carlos Guestrin, Soheil Feizi