

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/vo_99/ciml-vo_99-cho1.pdf) and Chapter 2 (Limits of Learning; http://ciml.info/dl/vo_99/ciml-vo_99-cho2.pdf).

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 1

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

EN ↔ NL

Machine translation

Intent: **SHOWFLIGHT**

I want to fly to San Francisco on
Monday afternoon please

Intent classification

Image classification

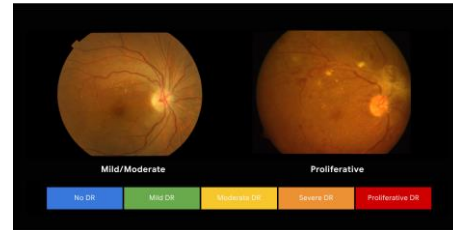


Digit recognition
MNIST dataset

IMAGENET

ImageNet has **21841** classes

<http://image-net.org/explore>



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



spam



not spam



not spam

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
```

Hand crafted rules: spam classification

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

Very precise. Sometimes easier to fix mistakes.



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

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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

Setting:

X : input space (set of possible instances)

Y : output space

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

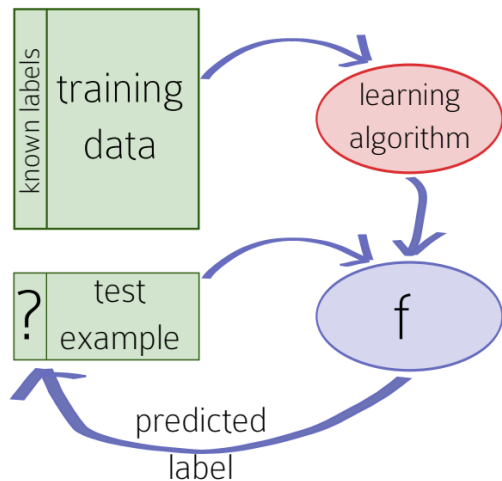
Learning:

Input: $\langle x^{(i)}, y^{(i)} \rangle$: training examples i : current training example

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

Output:

$f \in F$: hypothesis that approximates the target function



CIML, figure 1.1

Tasks & data

features target

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

Goal: Predict the target using the features

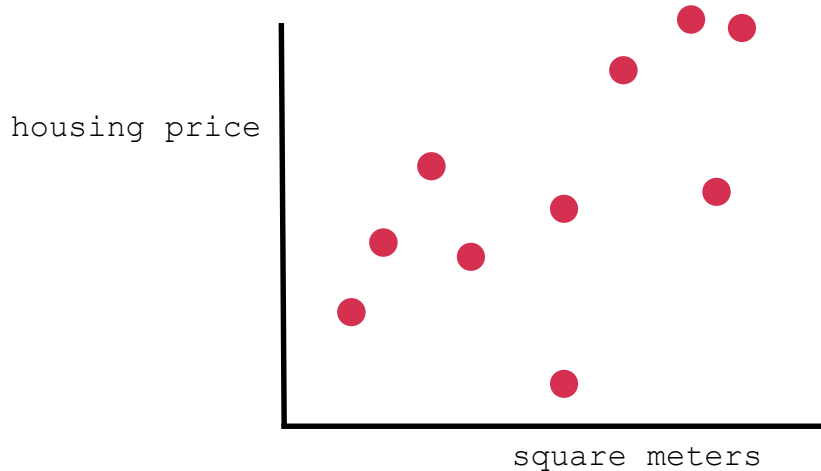
Housing price prediction:

This is a *regression* problem (target is a real number)

What are the dimensions of the features and the target?

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

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



Tasks & data

features target

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

Goal: Predict the target using the features

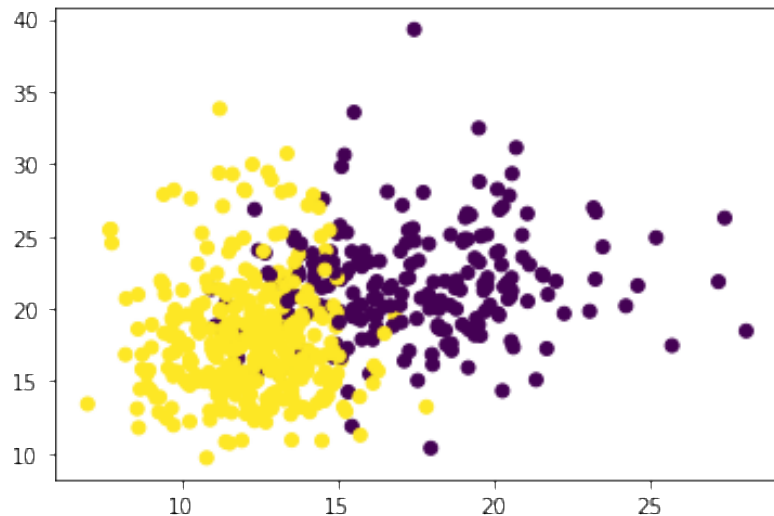
Breast cancer diagnosis (malignant or benign):

This is a *classification* problem (target is a category)

What are the dimensions of the features and the target?

$x^{(i)} \in \mathbb{R}^2$ (two)

$y^{(i)} \in \{0,1\}$ (one)



Tasks & data

features target

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

Goal: Predict the target using the features

Breast cancer diagnosis (malignant or benign):

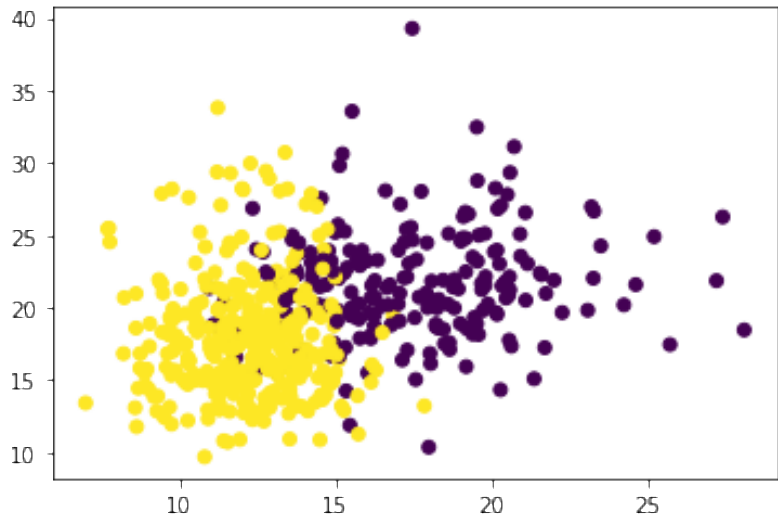
This is a *classification* problem (target is a category)

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!*

Training set

Test set

- **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)

Training data



class A

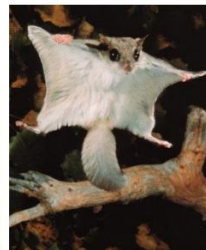


class B



Inductive bias

Test data



Question: How would you label the test data?

Underlying assumptions to generalize to new input!

Training data



class A

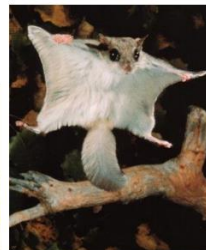


class B



Inductive bias

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)
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- **K-nearest neighbors**
- And many more...

Decision Trees

Asking the right questions

You: Is the course under consideration in Systems?

Me: Yes

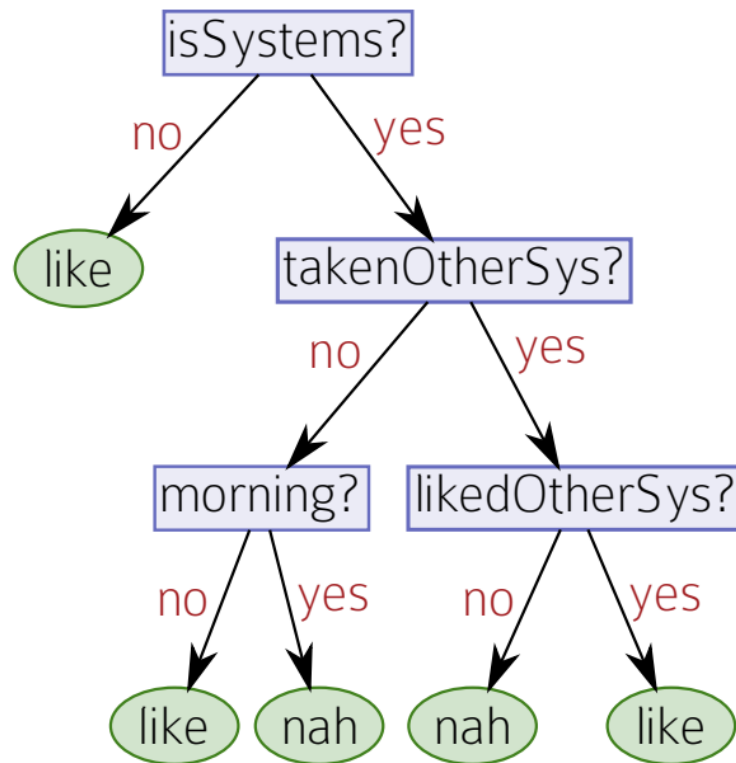
You: Has this student taken any other Systems courses?

Me: Yes

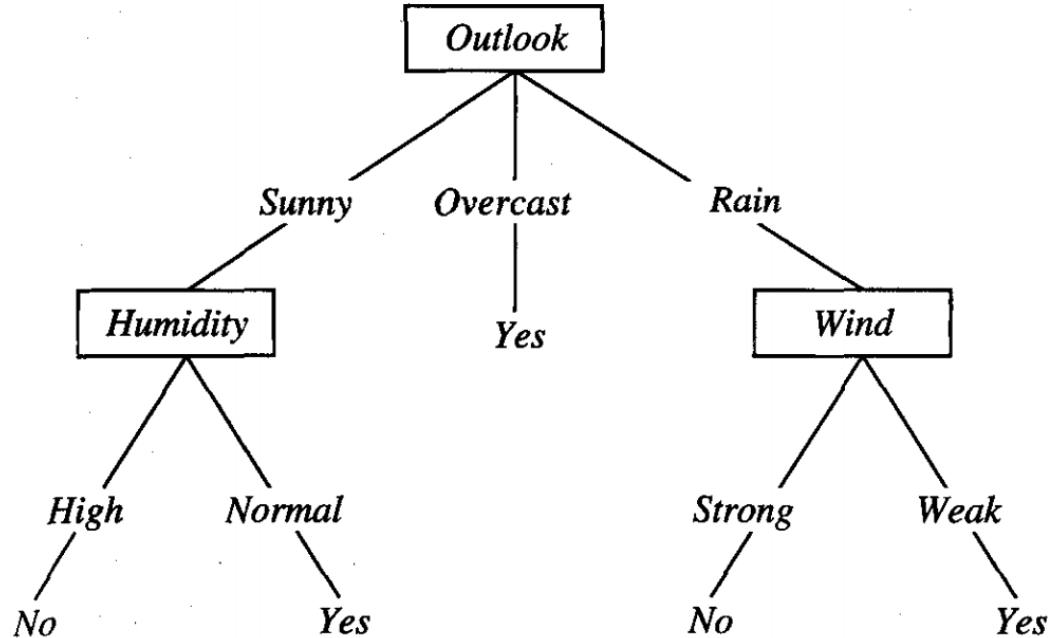
You: Has this student liked most previous Systems courses?

Me: No

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



Examples



Is it a good time to play tennis?

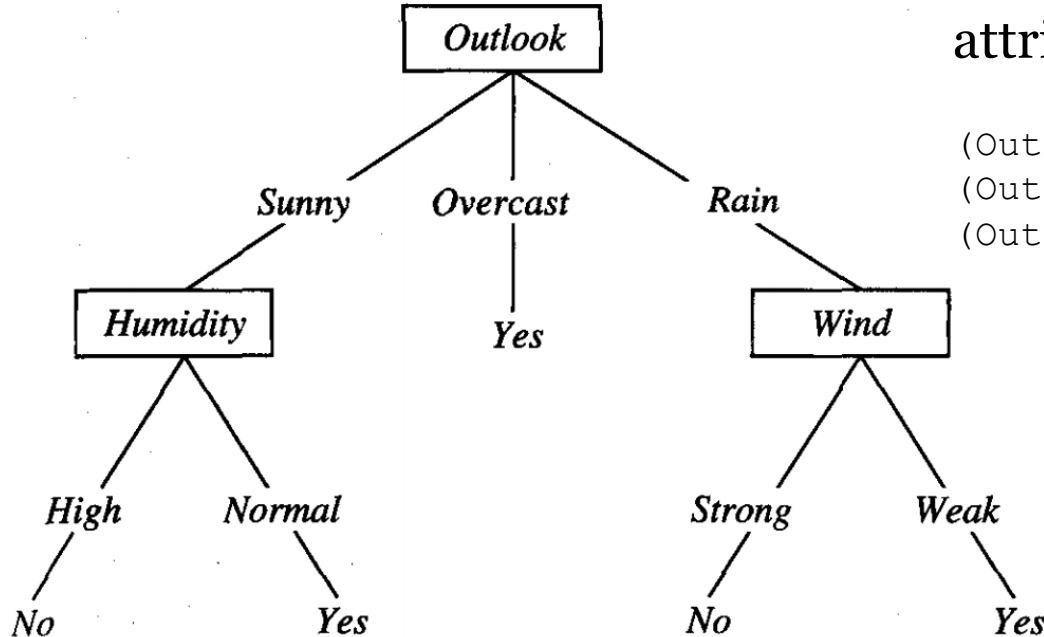
(Outlook = Sunny,
Temperature = Hot,
Humidity = High,
Wind = Strong)

Answer: No

Examples

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

$(\text{Outlook} = \text{Sunny} \wedge \text{Humidity} = \text{Normal}) \vee$
 $(\text{Outlook} = \text{Overcast}) \vee$
 $(\text{Outlook} = \text{Rain} \wedge \text{Wind} = \text{Weak})$



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

Supervised learning

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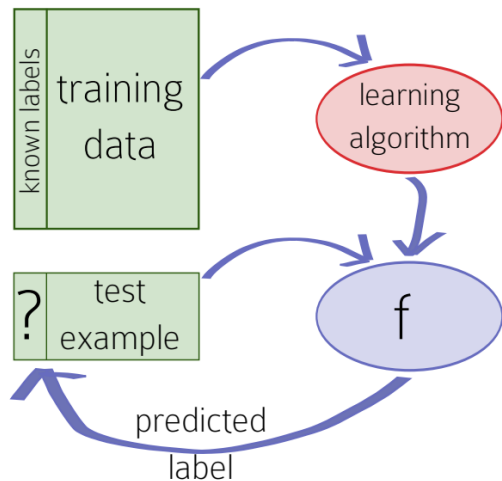
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CIML, figure 1.1

Supervised learning

Setting:

X : input space (set of possible instances)

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$y=1$: 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

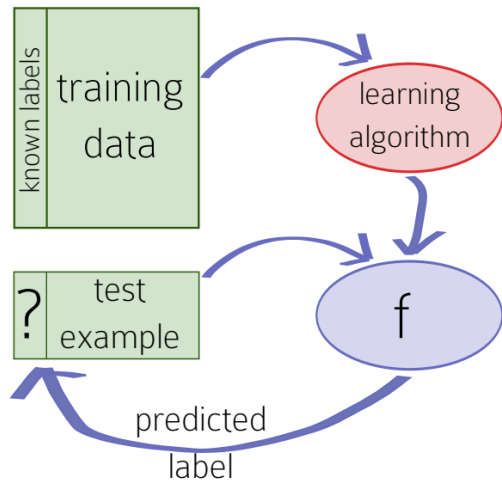
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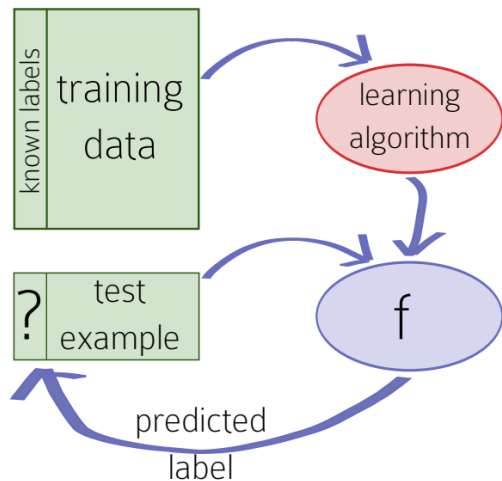
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CIML, figure 1.1

Learning decision trees

Find the ‘best’ tree $h \in H$, 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

Learning decision trees

Start with empty tree

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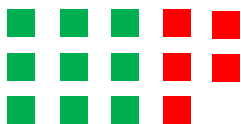
Select the best test to split the data on

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

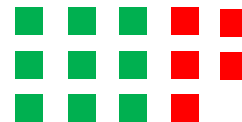
normal

[3+, 4-]

[6+, 1-]



Question:
which one would
you choose?



[9+, 5-]

Wind

weak

strong

[6+, 2-]

[3+, 3-]



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 😞

Selecting attributes to split

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

After split:

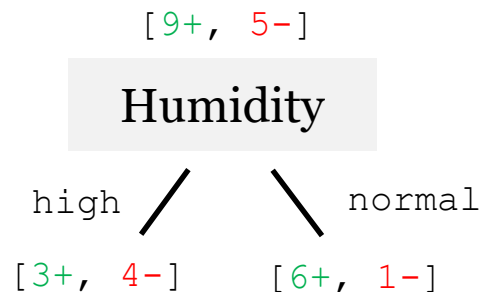
All instances have the same label 😄

Uniform distribution over labels 😞

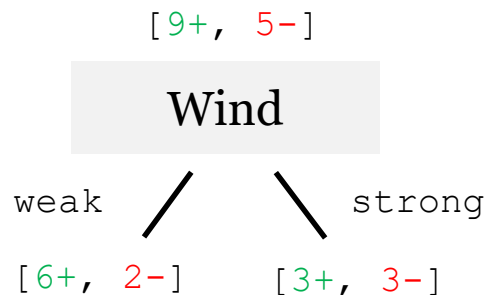
How can we quantify this intuition?

Selecting attributes to split: misclassification rate

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



$$(3 + 1) / 14 = 0.286$$



$$(2 + 3) / 14 = 0.357$$

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



Entropy = 0



Entropy = 1

[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:

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

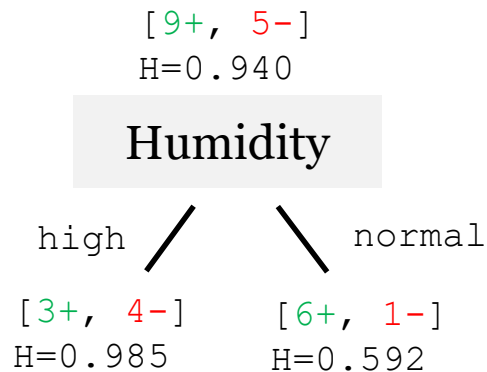
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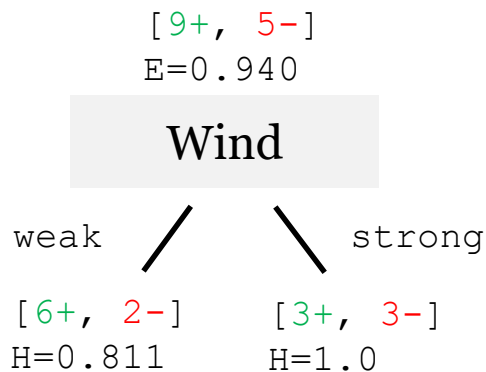
Information Gain:

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

Selecting attributes to split: Information Gain

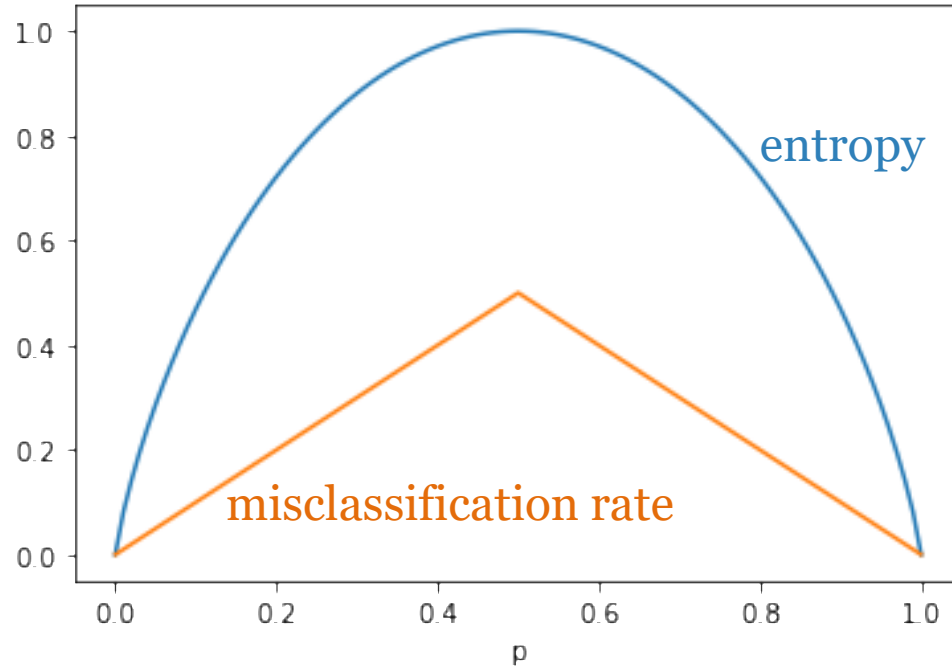


$$0.940 - (7/14) * 0.985 - (7/14) * 0.592 = 0.1515$$



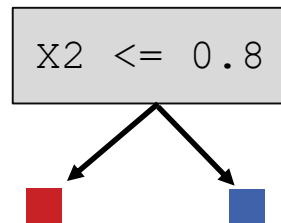
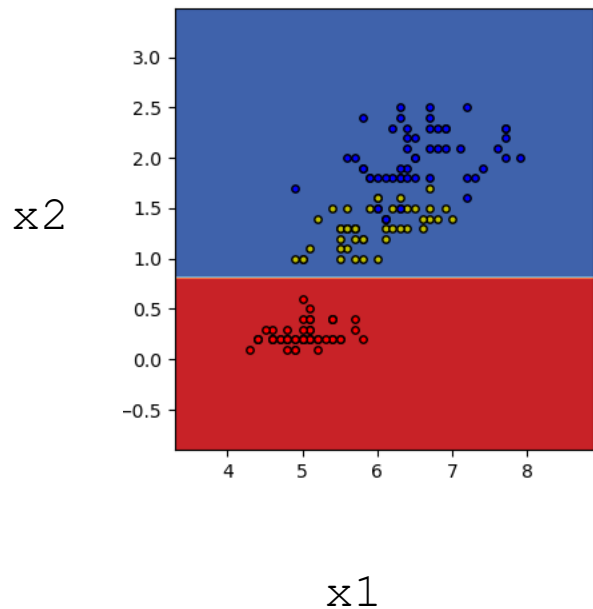
$$0.940 - (8/14) * 0.811 - (6/14) * 1 = 0.048$$

Selecting attributes to split

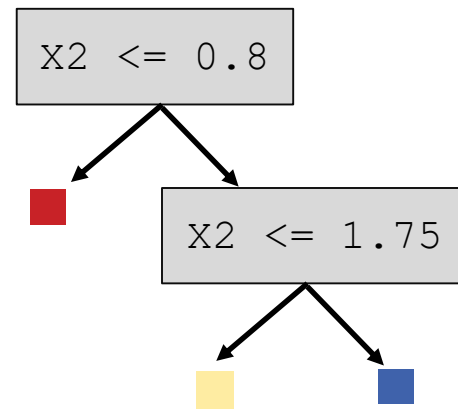
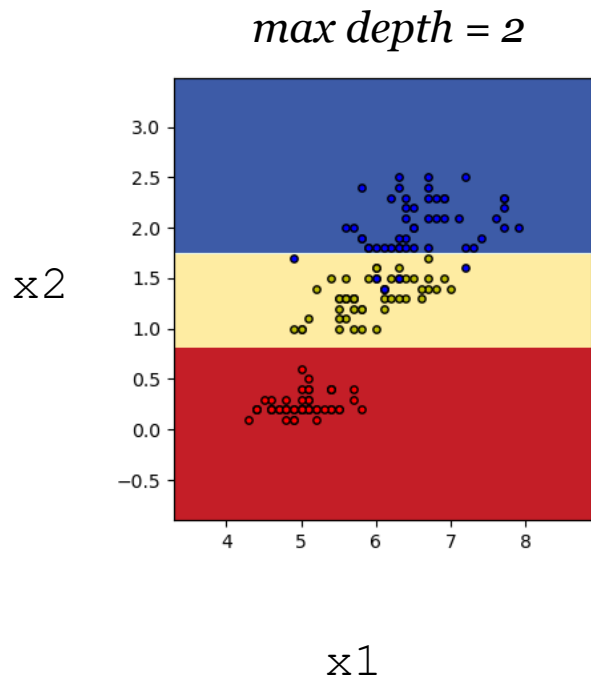


Decision boundary

max depth = 1

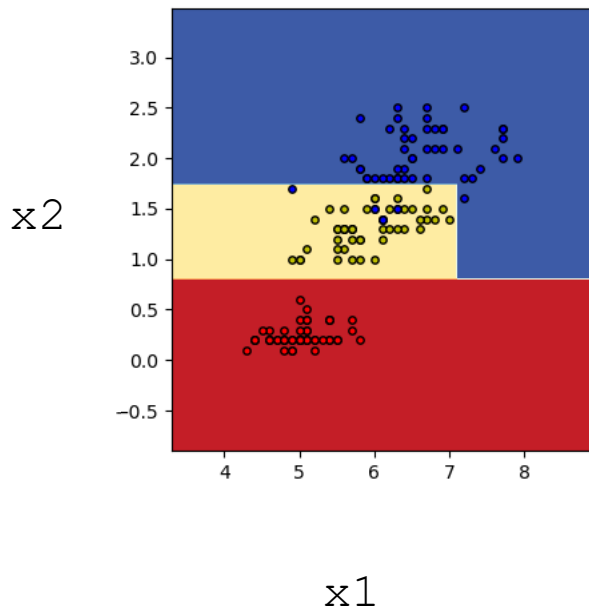


Decision boundary

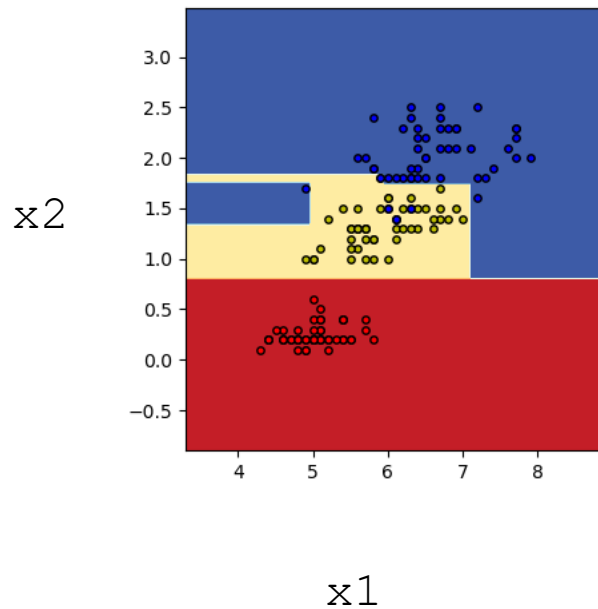


Decision boundary

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?

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

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

Confusion Matrix:

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

Classification: Accuracy

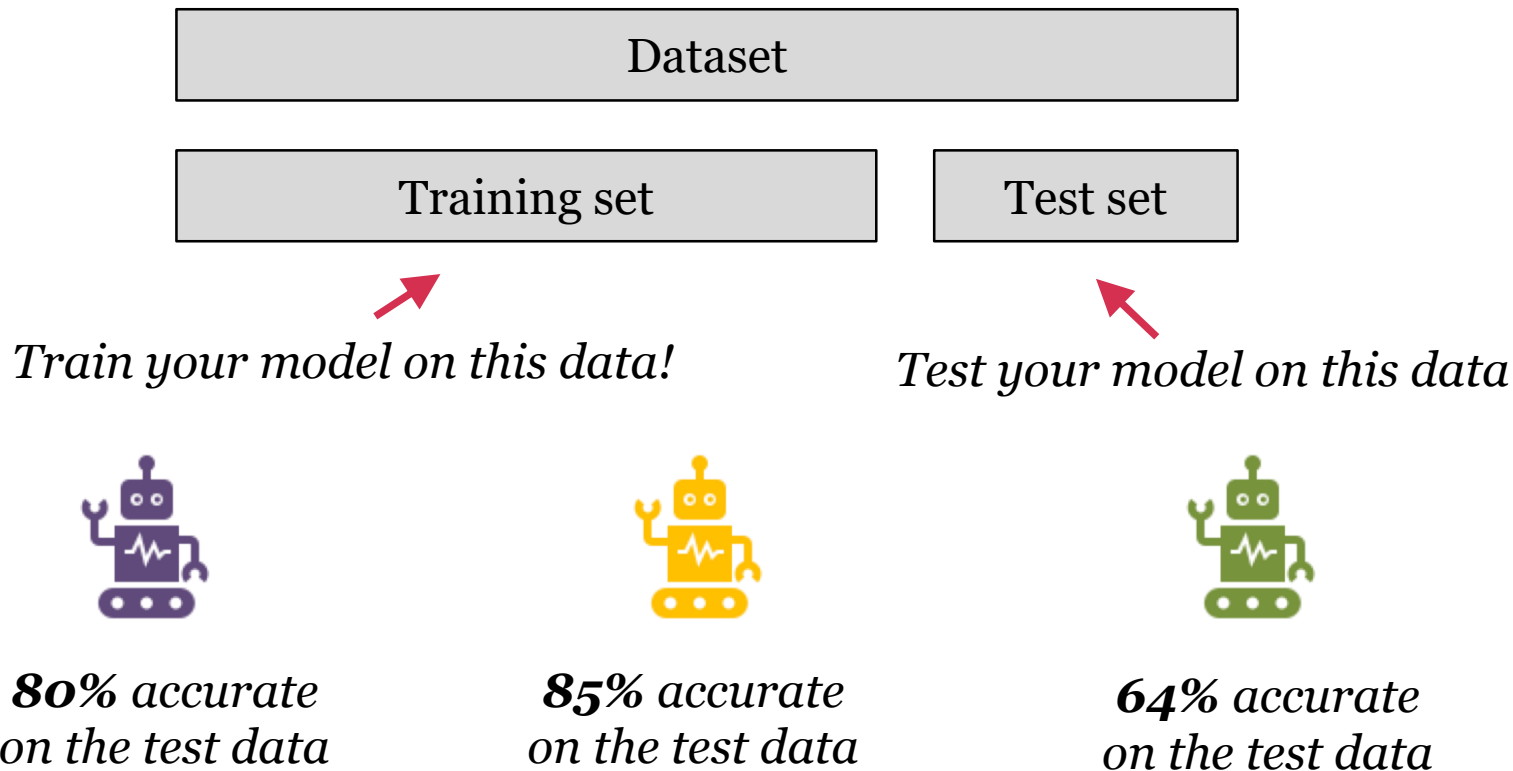
$$\frac{\text{\#correctly labeled instances}}{\text{\#total instances}}$$

Confusion Matrix:

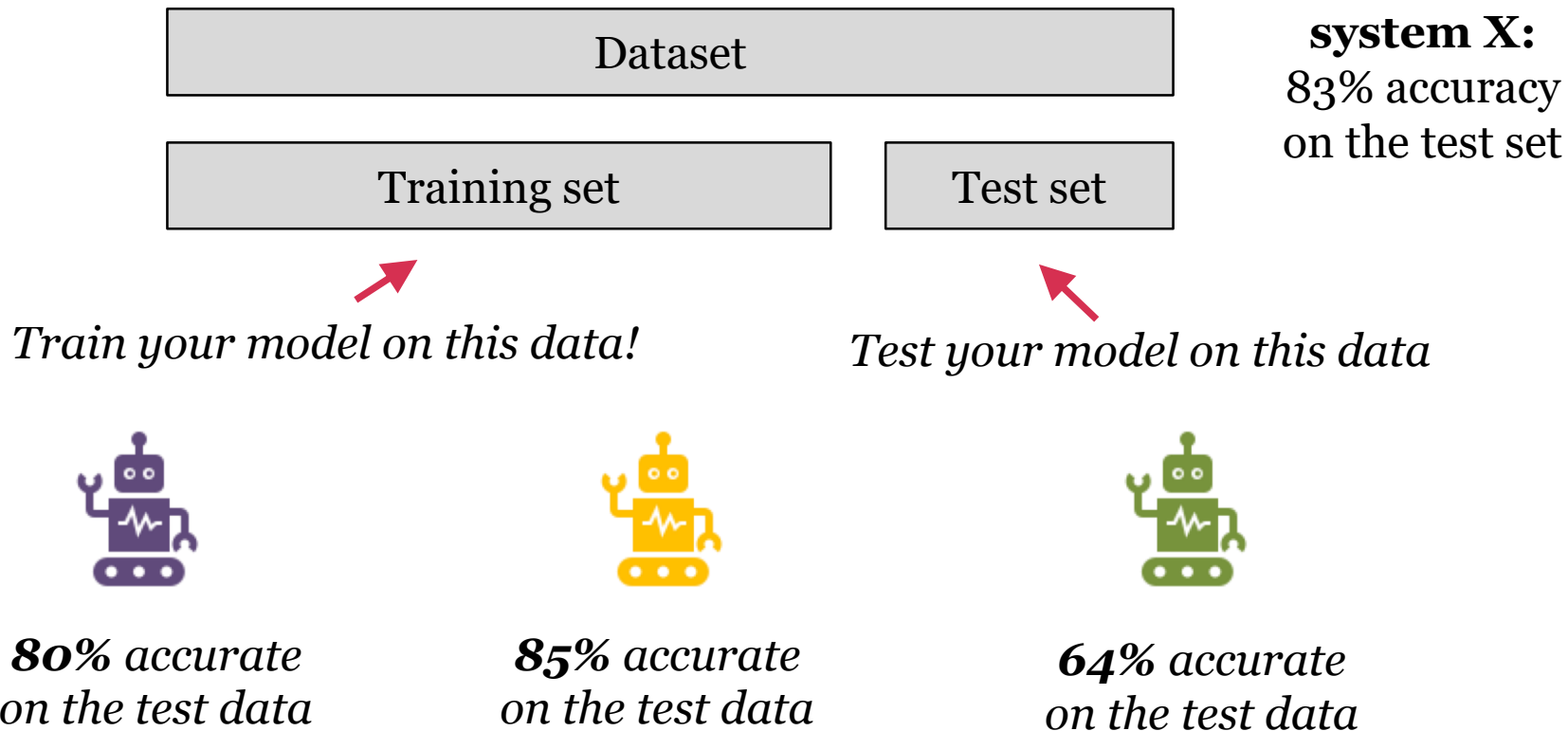
	Truth: A	Truth: B
Predicted: A	70	40
Predicted: B	30	60

$$\text{Accuracy: } 130/200 = 0.65$$

Train & test data



Train & test data



Train & test data

My model is better!! It is 85% accurate



Hold on...



Dataset

Training set

Test set

system X:
83% accuracy
on the 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!!

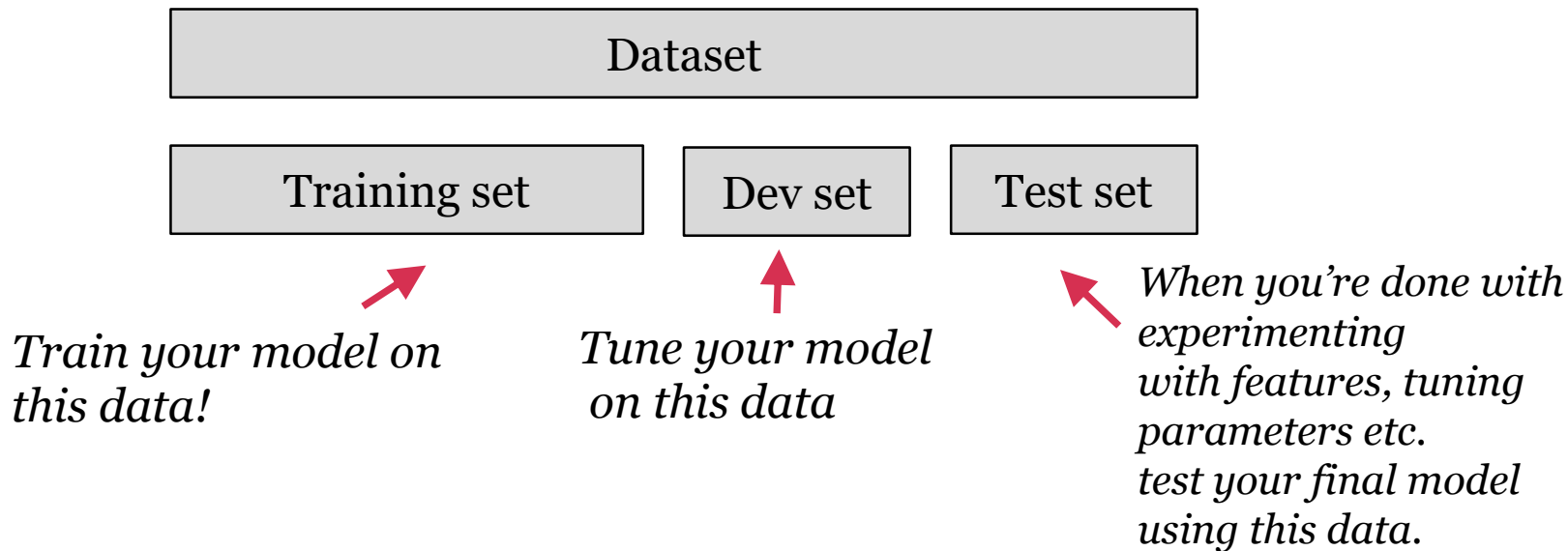
Training error is an optimistic estimate of your system's true error. So evaluate on a holdout test set. But...

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

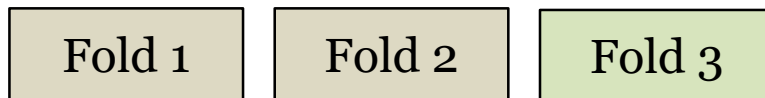
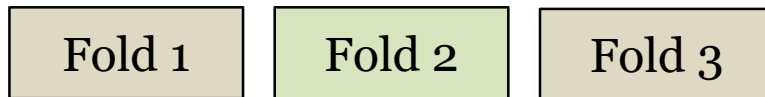
- Feature development
- Selecting the model
- ...



Train & dev & test data



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

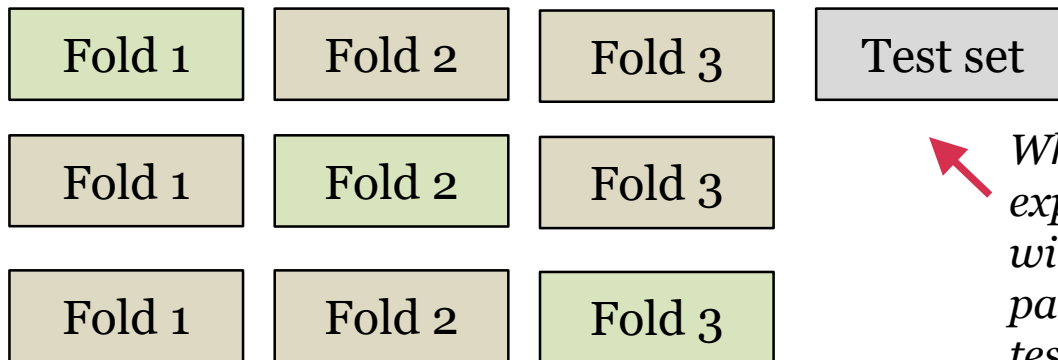
*E.g. train on folds 2 and 3, test on fold 1.
Usually 10 folds (i.e. 10-fold cross validation),
but depends on the data*



Cross validation

**leave-one-out
cross
validation:**

number of folds
= number of data
points



*When you're done with
experimenting
with features, tuning
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test your final model
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Train and tune your parameters on folds 1-3

*E.g. train on folds 2 and 3, test on fold 1.
Usually 10 folds (i.e. 10-fold cross validation),
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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.

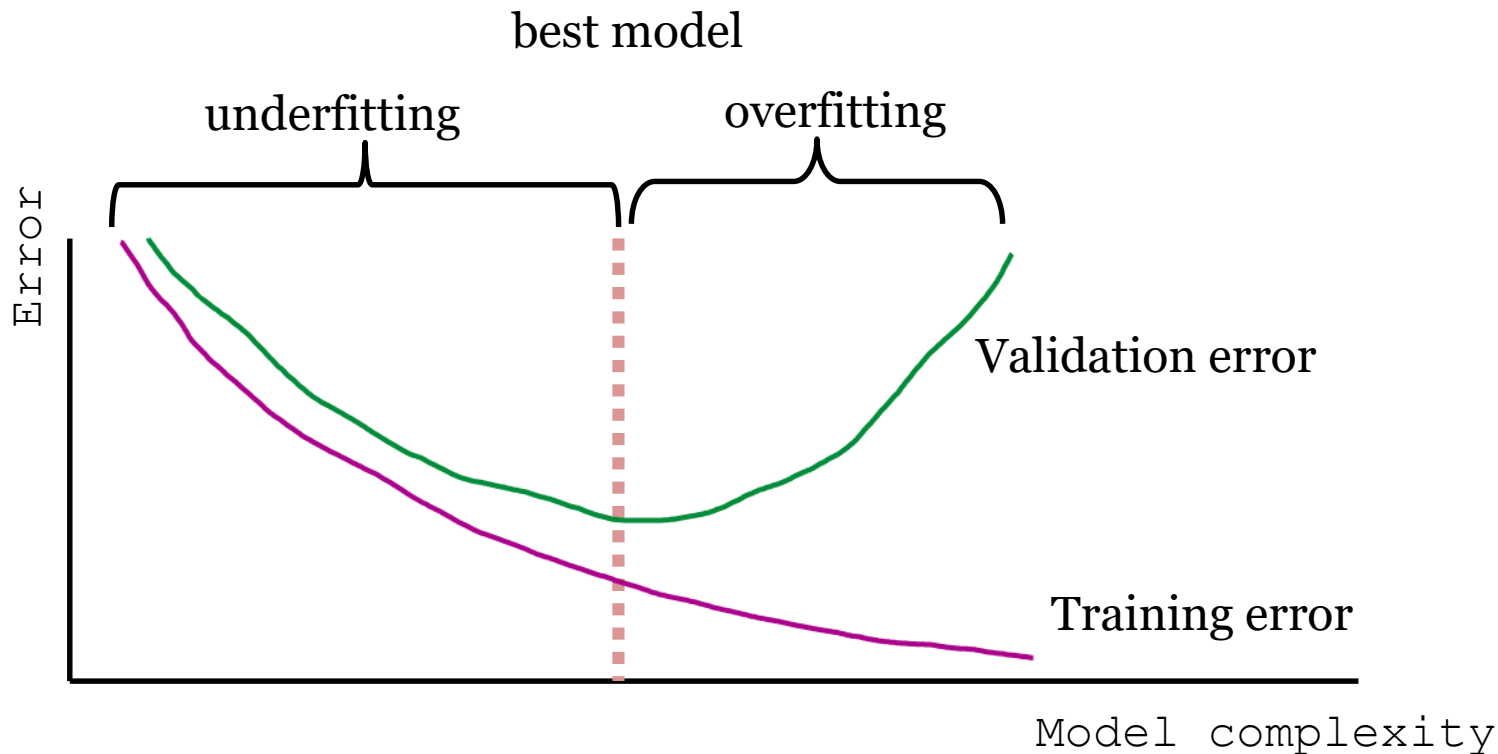
Example: a leaf for each instance in your training data (training error will be zero!) .

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
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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

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

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:

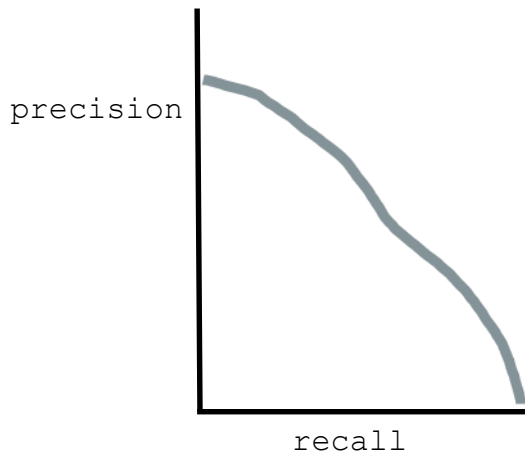
$$60/100 = 0.6$$

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

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

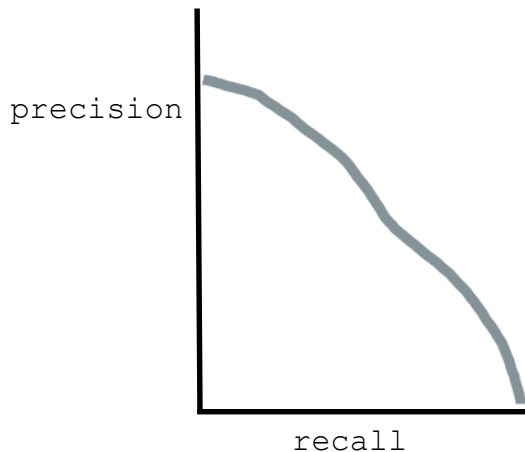
Only label messages as spam
if we're really *sure*.
Use the “confidence” of the
classifier

High confidence



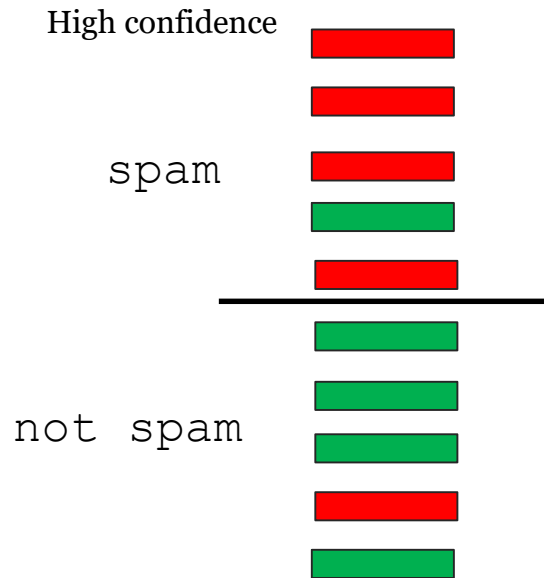
Low confidence

Precision recall curve



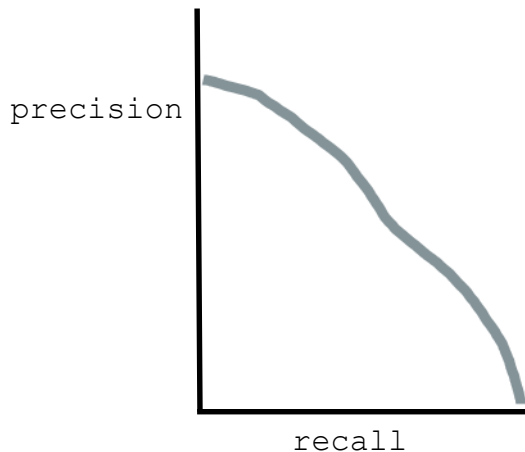
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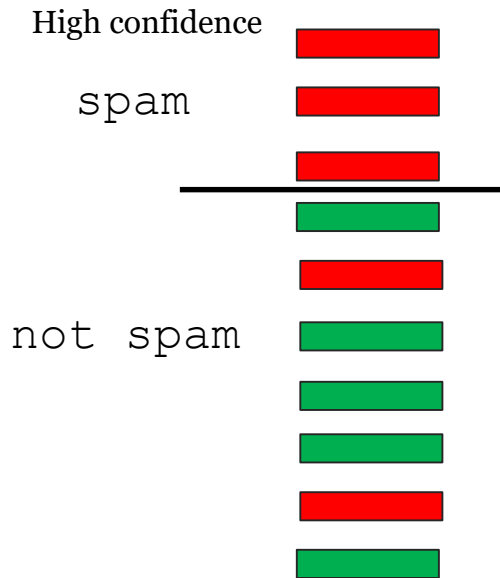
Precision = $4/5$
Recall = $4/5$

Precision recall curve



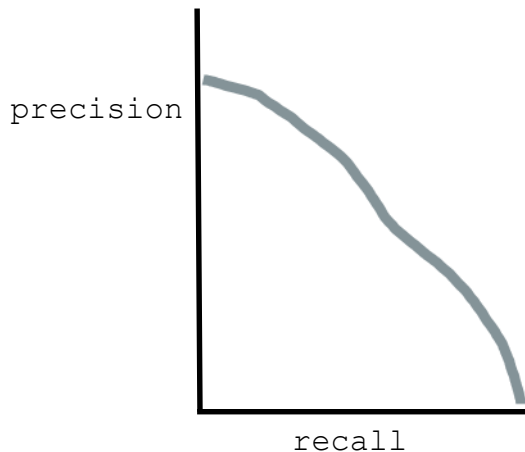
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Precision = $3/3 = 1$ ↑
Recall = $3/5$ ↓

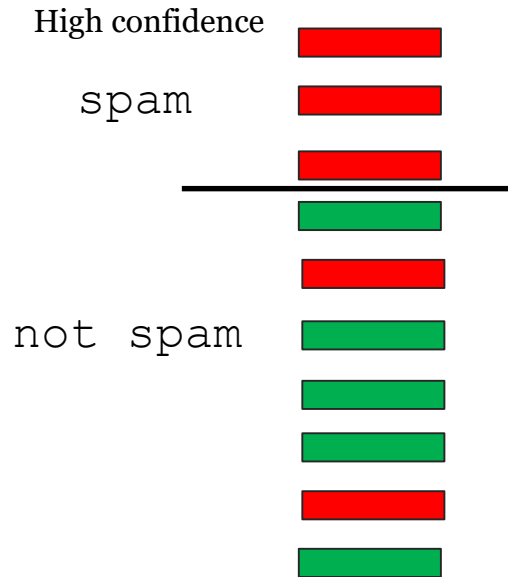
Precision recall curve



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

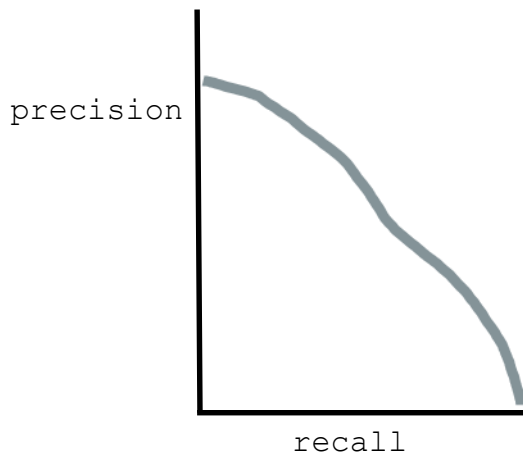
Only label messages as spam
if we're really *sure*.
Use the “confidence” of the
classifier

How can we compute the
confidence of a decision tree?

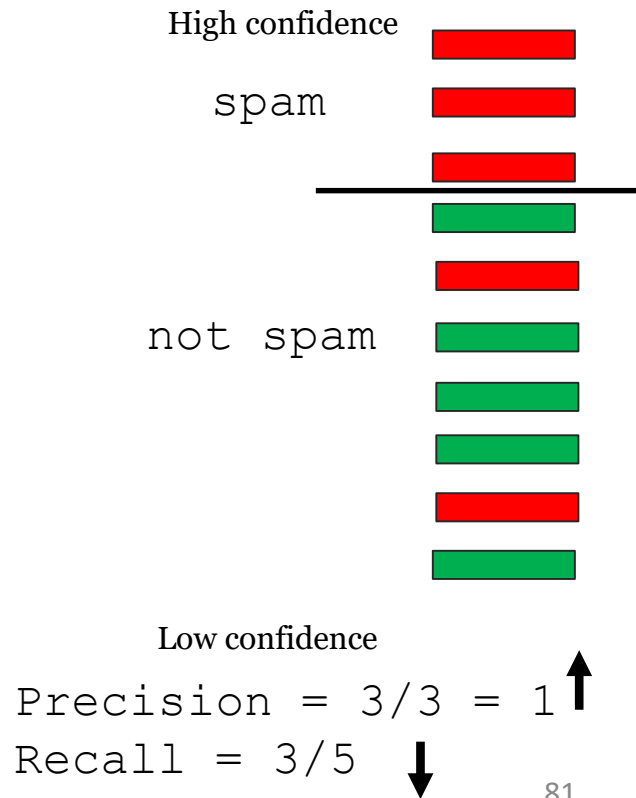


Precision = $3/3 = 1$ ↑
Recall = $3/5$ ↓

Precision recall curve



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



Evaluation

Combining recall and precision using F-measure

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

Often $\beta = 1$:

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

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.

IMGENET

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 +
wrap up**

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

1	real world goal	increase revenue
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ML process

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....

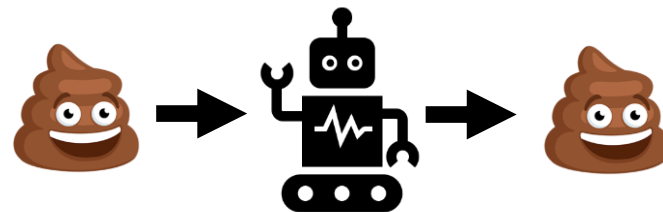
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ML process

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)



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.

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ML process

Usually a combination of multiple evaluation metrics.

Also take into account:

- Cost of errors (e.g. accidentally 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!

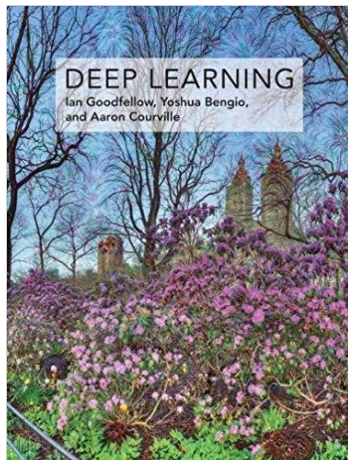
What do you need to know

- 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)

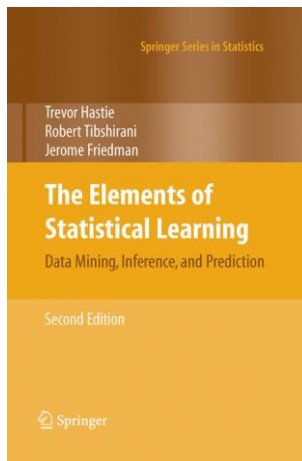
Resources

- `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.)

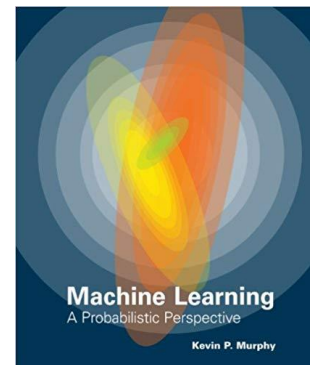
Books



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