CMSC 471:
Machine Learning

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Some slides courtesy Tim Finin

Why study learning?

- **Discover** new things or structure previously unknown
  - Examples: data mining, scientific discovery
- Fill in skeletal or **incomplete specifications** in a domain
  - Large, complex systems can't be completely built by hand & require dynamic updating to incorporate new info.
  - Learning new characteristics expands the domain or expertise and lessens the "brittleness" of the system
- Acquire models automatically directly from data rather than by manual programming
- Build agents that can **adapt** to users, other agents, and their environment
- Understand and improve efficiency of **human learning**

What does it mean to learn?

Wesley has been taking an AI course

Geordi, the instructor, needs to determine if Wesley has "learned" the topics covered, at the end of the course

What is a "reasonable" exam?

- (Bad) Choice 1: History of pottery
  - Wesley's performance is not indicative of what was learned in AI
- (Bad) Choice 2: Questions answered during lectures
  - Open book?

A good test should test ability to answer "related" but "new" questions on the exam

Generalization

Model, parameters and hyperparameters

Model: mathematical formulation of system (e.g., classifier)

Parameters: primary "knobs" of the model that are set by a learning algorithm

Hyperparameter: secondary "knobs"

http://www.uiparade.com/wp-content/uploads/2012/01/ui-design-pure-css.jpg


Instance of data
(“datum”)

score(Instance of data (“datum”))

scoring model

$$\text{score}_{\theta}(\;\;)$$

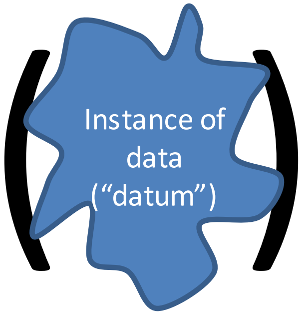
Instance of dat
("datum")

$$\Downarrow$$

objective

$$F(\theta)$$

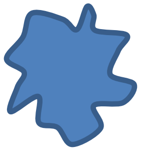
scoring model

$\mathrm{score}_\theta($  $)$

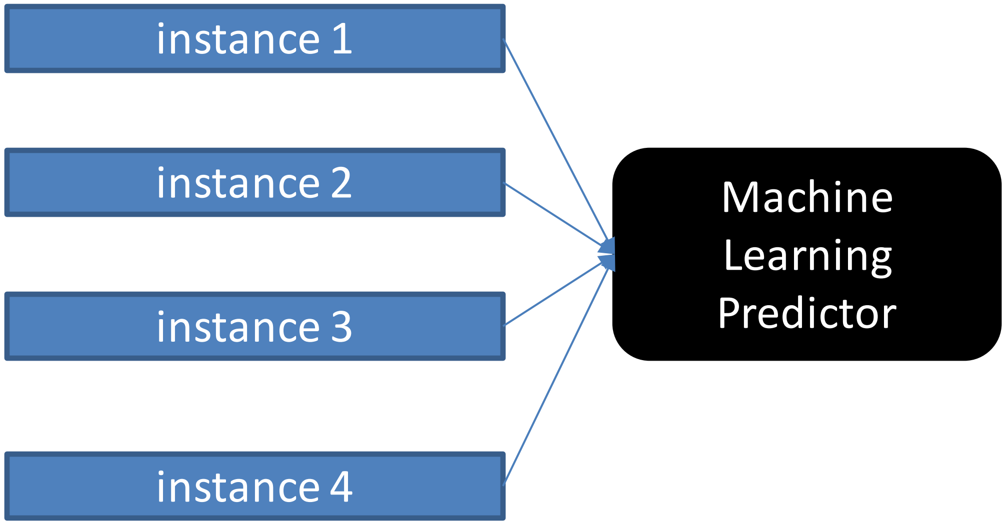
$\Downarrow$

objective

$F(\theta)$

(implicitly) dependent on the observed data X= 

Machine Learning Framework: Learning



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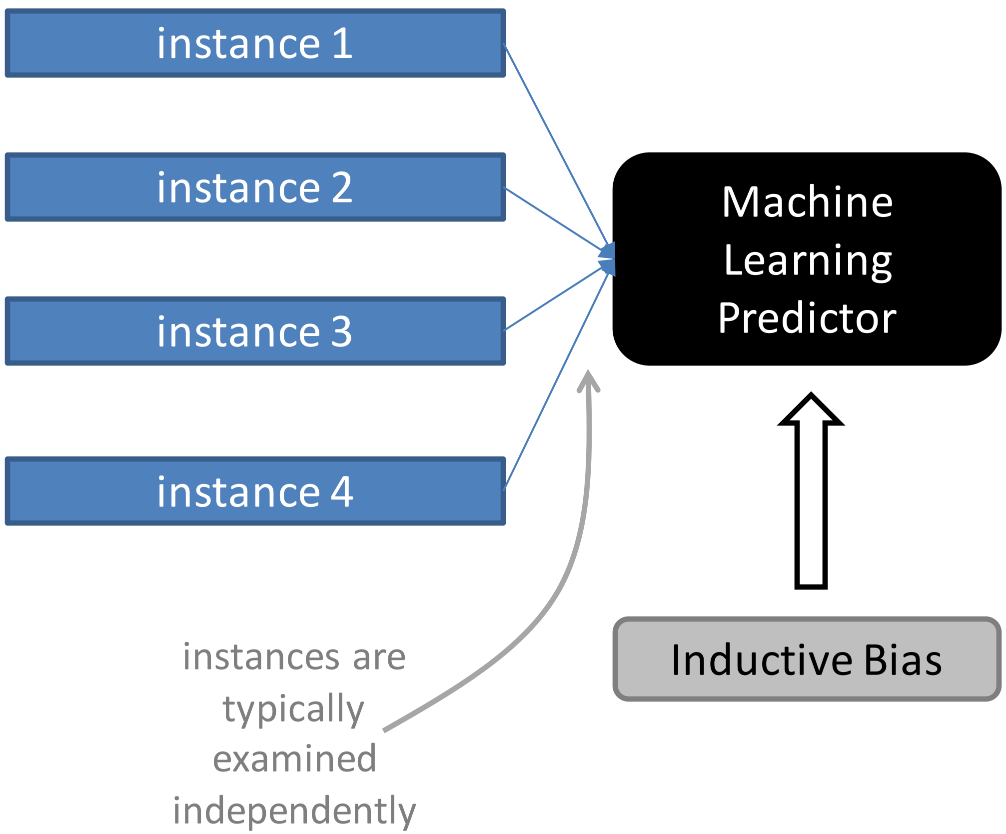

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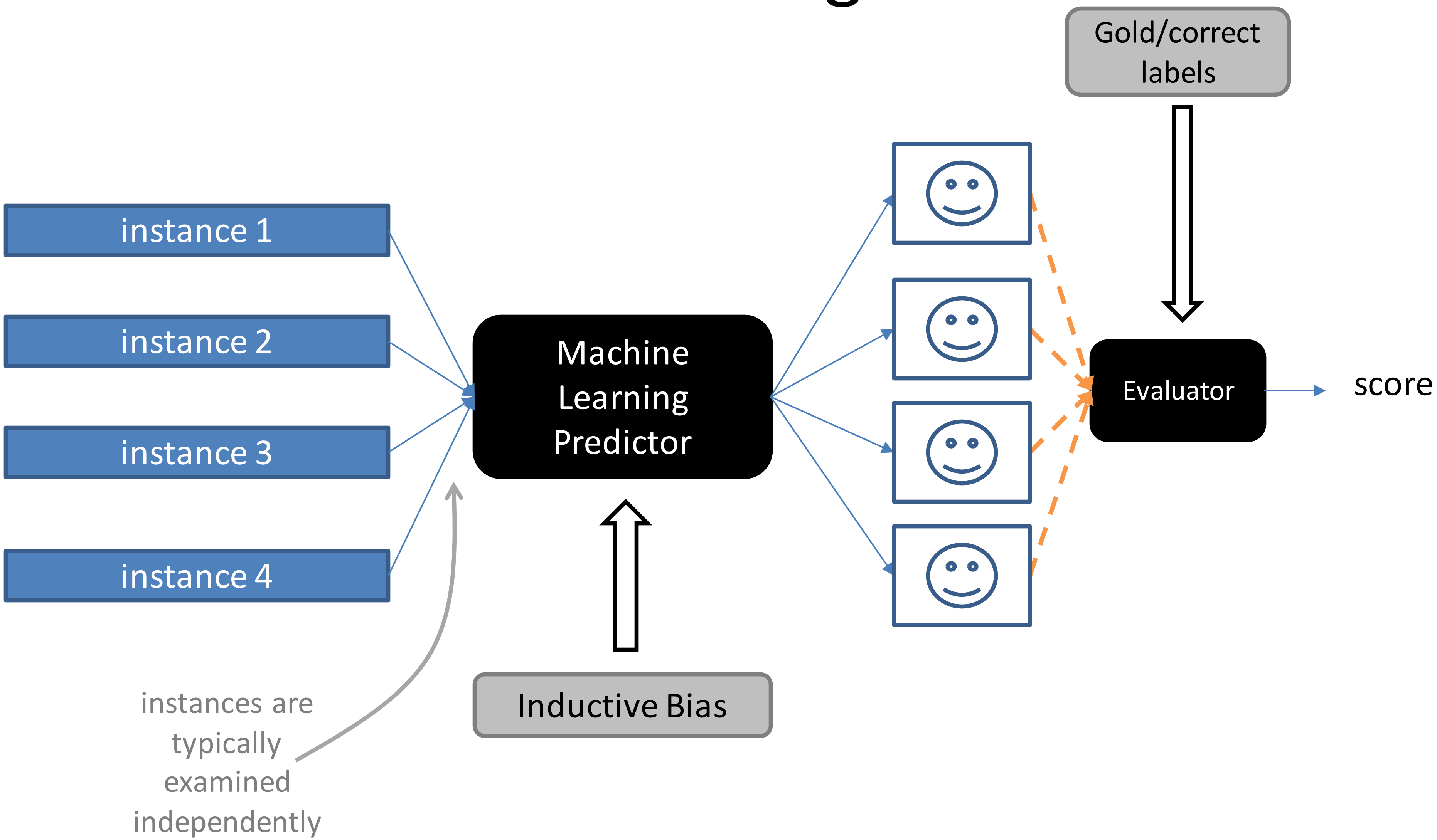

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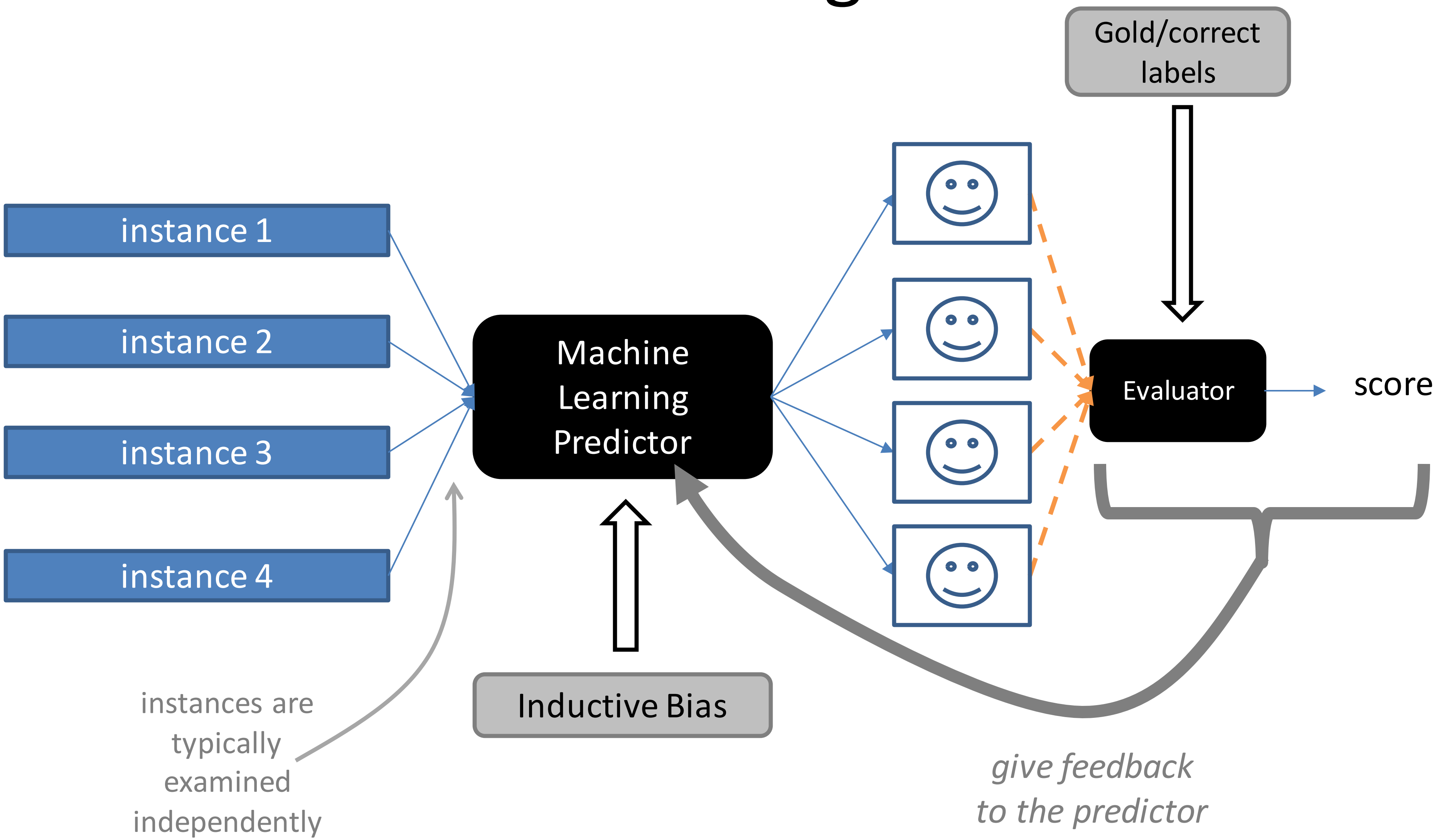


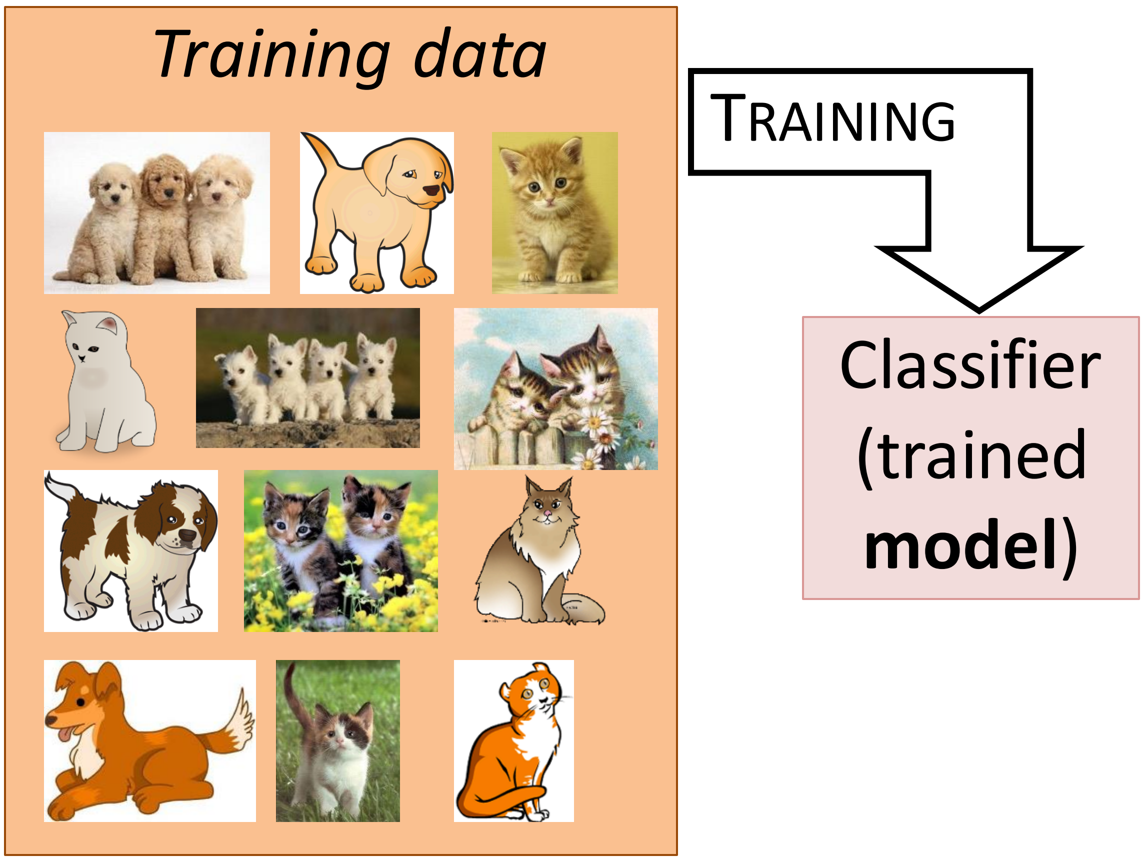
Classify with Goodness

$$\text{predicted label}$$

$$= \underset{\text{label}}{\arg\max}\ \text{score}(\text{example}, \text{label})$$

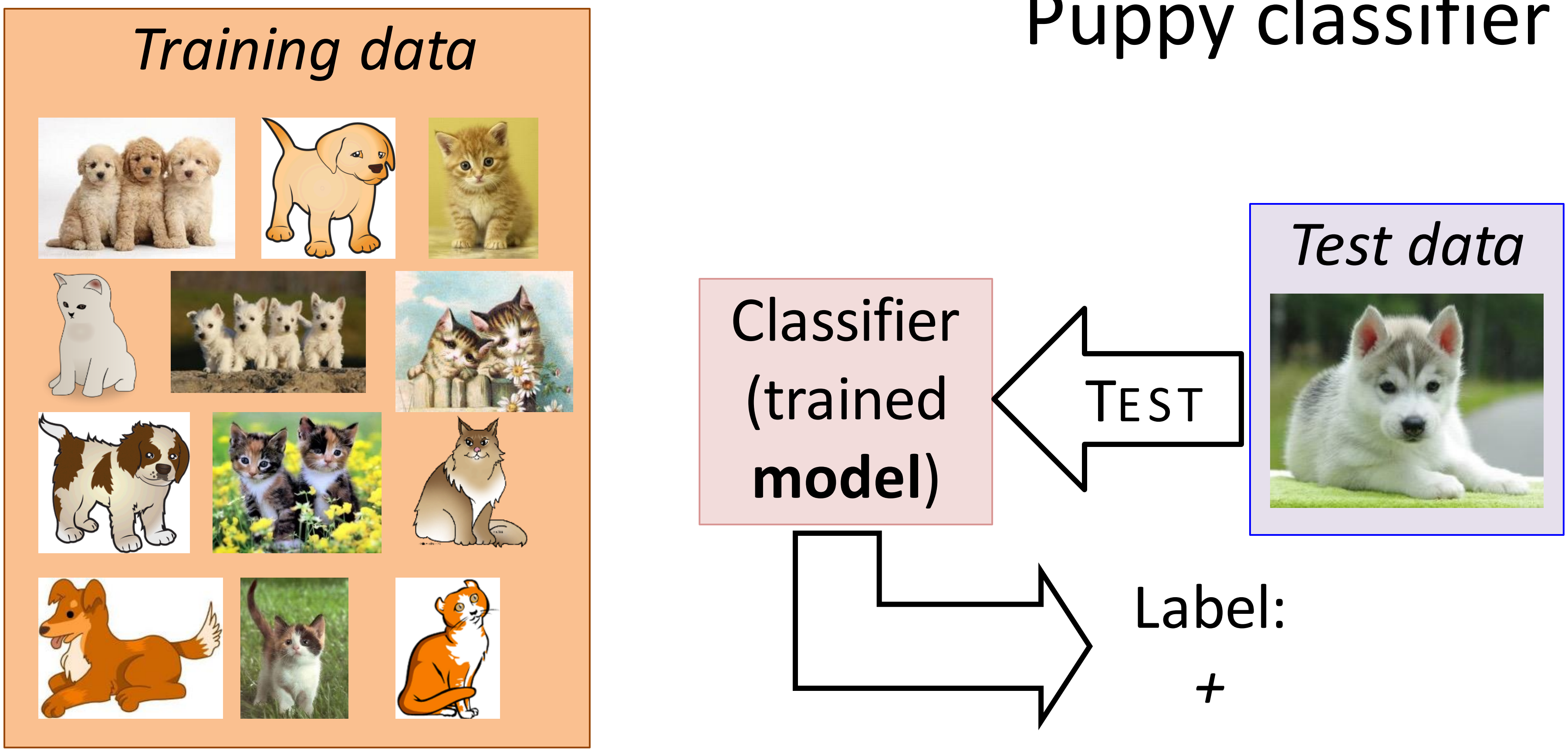
ML Framework Example

Puppy classifier



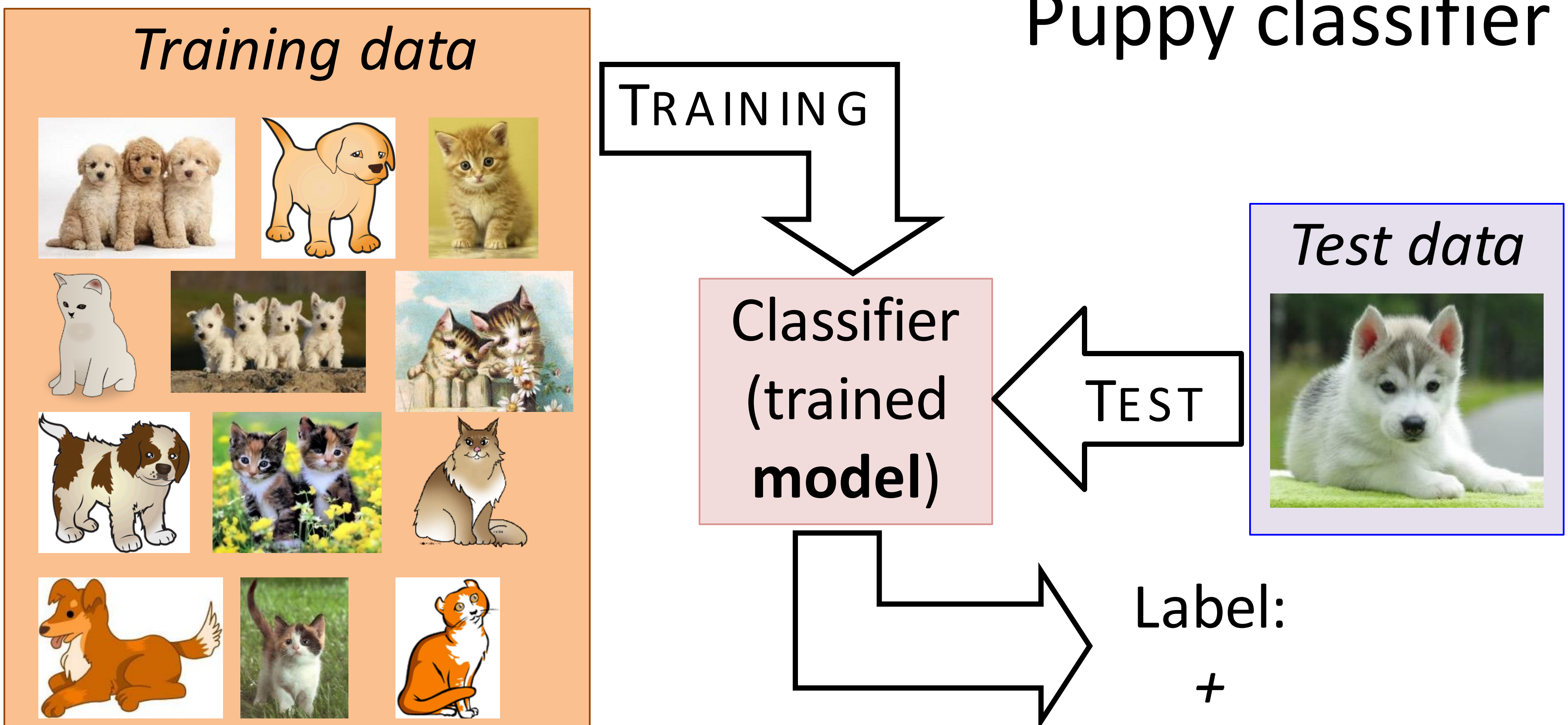
ML Framework Example

Puppy classifier



ML Framework Example

Puppy classifier



ML Framework Example

Puppy classifier

Training data, X

Text-ure	*Ears*	*Legs*	*Class*
Fuzzy	Round	4	+
Slimy	Missing	8	-
Fuzzy	Pointy	4	-
Fuzzy	Round	4	+
Fuzzy	Pointy	4	+
…			

TRAINING

Classifier (trained **model**)

TEST

Test data

x_1 = <Fuzzy, Pointy, 4>

Label: +

General ML Consideration: Inductive Bias

What do we know *before* we see the data, and how does that influence our modeling decisions?

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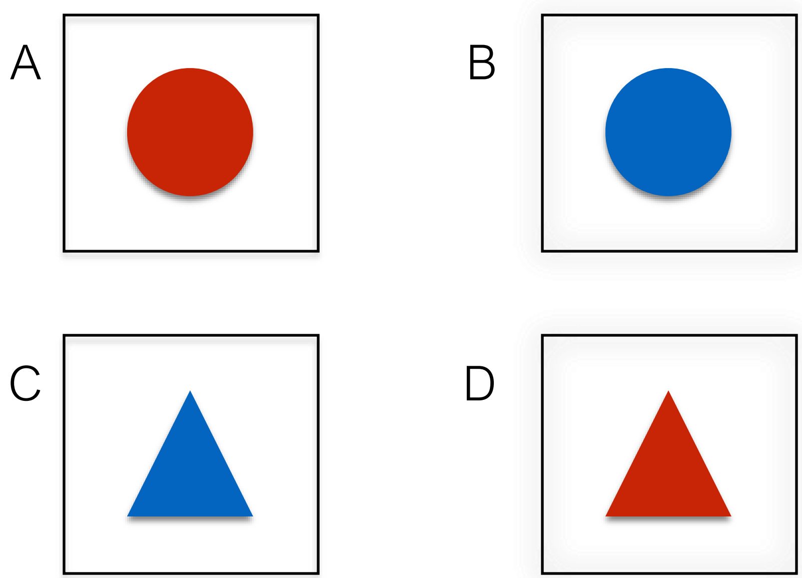

Partition these into two groups…

Courtesy Hamed Pirsiavash

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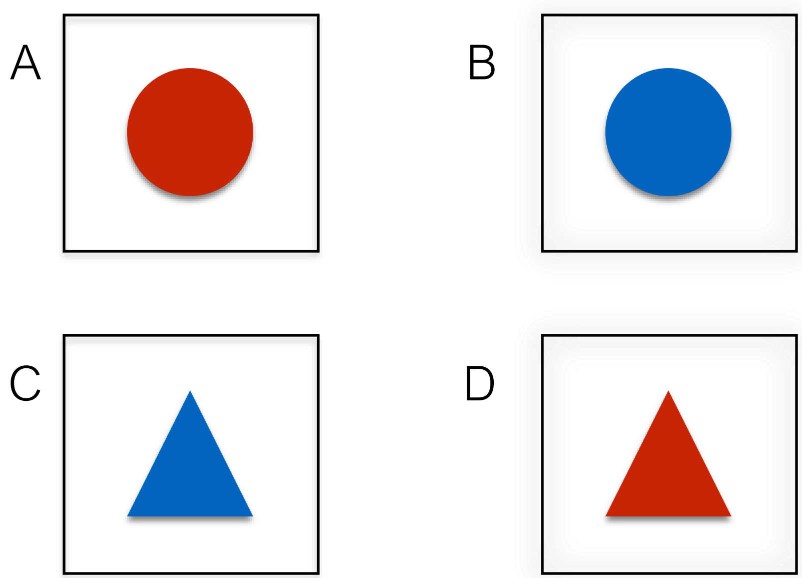

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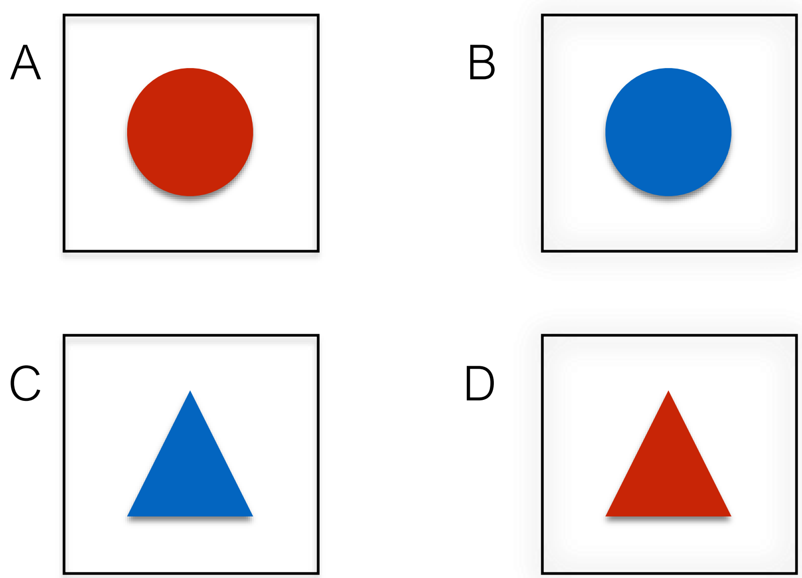

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Who selected ● vs. ▲ ?

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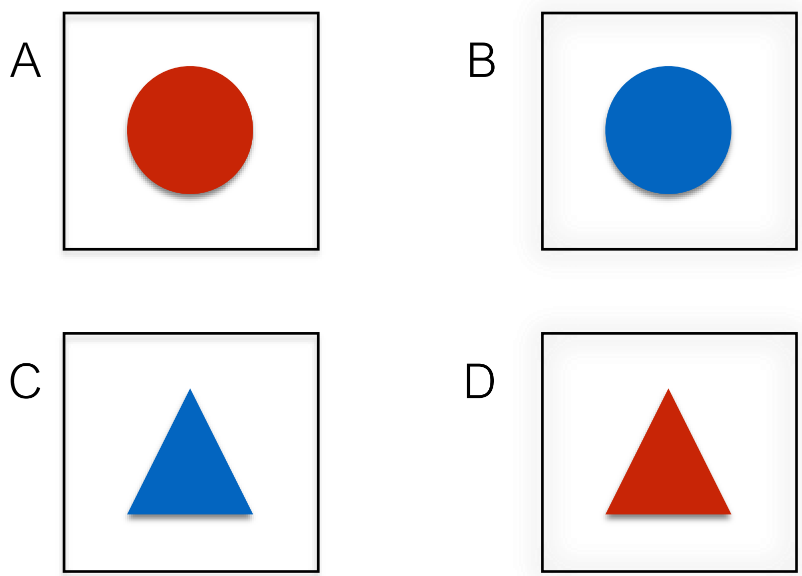

Partition these into two groups

Who selected red vs. blue?

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Tip: Remember how your own biases/interpretation are influencing your approach

Courtesy Hamed Pirsiavash

AI & ML

AI and Learning Today

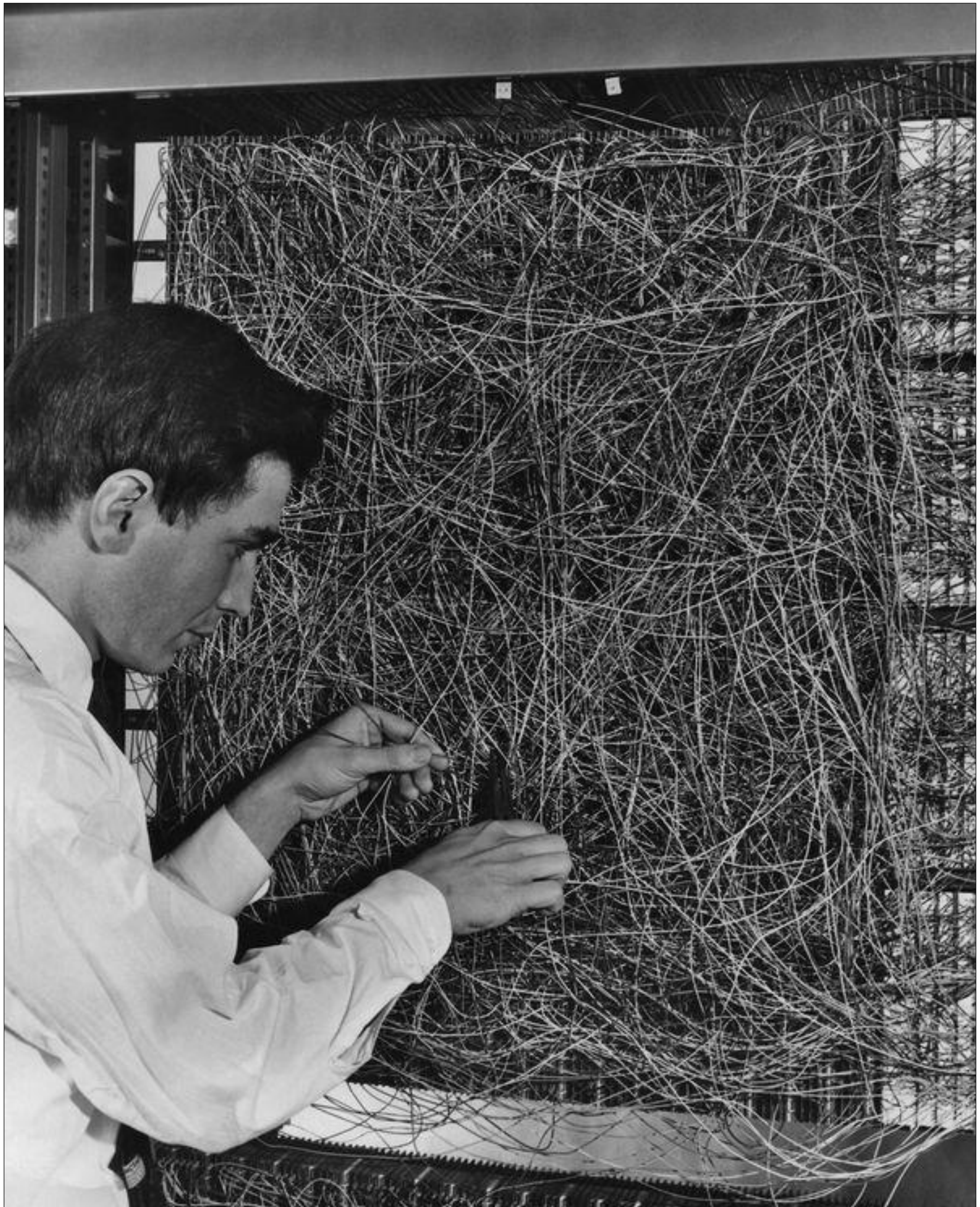
- 50s&60s: neural network learning popular

  Marvin Minsky did neural networks for his dissertation
- Mid 60s: replaced by paradigm of manually encoding & using symbolic knowledge

  Cf. Perceptrons, Minsky & Papert book showed limitations of perceptron model of neural networks
- 90s: more data & Web drove interest in statistical machine learning techniques & data mining
- Now: machine learning techniques & big data play biggest driver in almost all successful AI systems

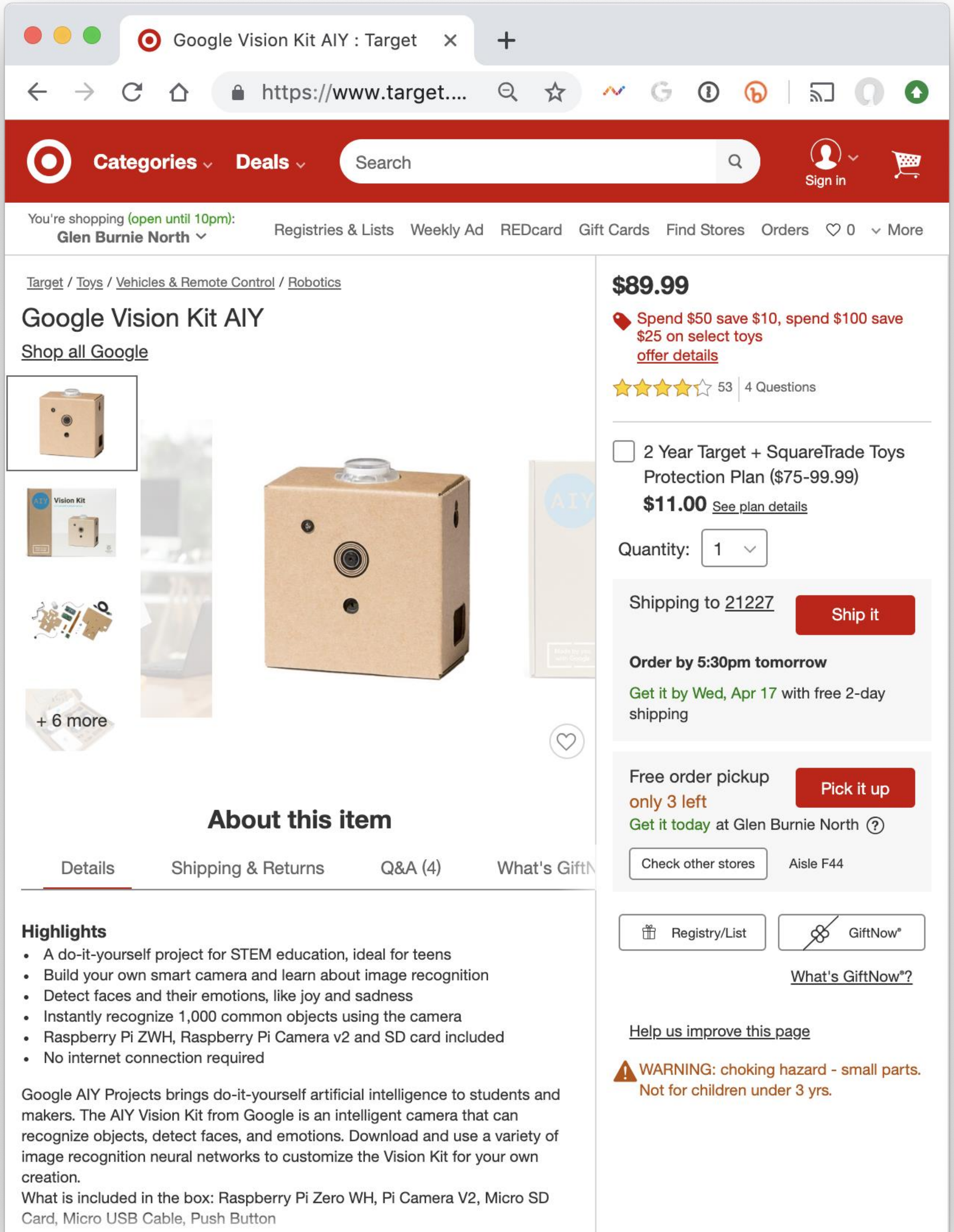
  … and neural networks are the current favorite approach

seeAlso: Timeline of machine learning



Neural Networks 1960

A man adjusting the random wiring network between the light sensors and association unit of scientist Frank Rosen-blatt's Perceptron, or MARK 1 computer, at the Cornell Aeronautical Laboratory, Buffalo, New York, circa 1960. The machine is designed to use a type of artificial neural network, known as a perceptron.



Neural Networks 2020

Google's AIY Vision Kit ($89.99 at Target) is an intelligent camera that can recognize objects, detect faces and emotions. Download and use a variety of image recognition neural networks to customize the Vision Kit for your own creation. Included in the box: Raspberry Pi Zero WH, Pi Camera V2, Micro SD Card, Micro USB Cable, Push Button.

Currently $58.85 on Amazon

Machine Learning Successes

- Games: chess, go, poker
- Text sentiment analysis
- Email spam detection
- Recommender systems (e.g., Netflix, Amazon)
- Machine translation
- Speech understanding
- SIRI, Alexa, Google Assistant, …
- Autonomous vehicles
- Individual face recognition
- Understanding digital images
- Credit card fraud detection
- Showing annoying ads

The Big Idea and Terminology

Given some data, learn a model of how the world works that lets you predict new data

- **Training Set:** Data from which you learn initially
- **Model:** What you learn; a "model" of how inputs are associated with outputs
- **Test set:** New data you test your model against
- **Corpus:** A body of text data (pl.: corpora)
- **Representation:** The computational expression of data

Major Machine learning paradigms (1)

- **Rote**: 1-1 mapping from inputs to stored representation, learning by memorization, association-based storage & retrieval
- **Induction:** Use specific examples to reach general conclusions
- **Clustering**: Unsupervised discovery of natural groups in data

Major Machine learning paradigms (2)

- **Analogy:** Find correspondence between different representations
- **Discovery**: Unsupervised, specific goal not given
- **Genetic algorithms:** *Evolutionary* search techniques, based on *survival of the fittest*
- **Reinforcement:** Feedback (positive or negative reward) given at the end of a sequence of steps
- **Deep learning:** *artificial neural networks* with *representation learning* for ML tasks

CORE TERMINOLOGY

Three Axes for Thinking About Your ML Problem

Classification Regression Clustering	Fully-supervised Semi-supervised Un-supervised	Probabilistic Generative Conditional Spectral Neural Memory-based Exemplar …
*the **task**: what* kind *of problem are you solving?*	*the **data**: amount of human input/number of labeled examples*	*the **approach**: how any data are being used*

Types of learning problems

- **Supervised**: learn from training examples
  - Regression:
  - Classification: Decision Trees, SVM
- **Unsupervised**: learn w/o training examples
  - Clustering
  - Dimensionality reduction
  - Word embeddings
- **Reinforcement learning:** improve performance using feedback from actions taken
- Lots more we won't cover
  - Hidden Markov models, Learning to rank, Semi-supervised learning, Active learning …

Machine Learning Problems

	Supervised Learning	***Unsupervised Learning***
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Supervised learning

- Given training examples of inputs & corres-ponding outputs, produce “correct” outputs for new inputs
- Two important scenarios:
  - **Classification:** outputs typically labels (goodRisk, badRisk); learn decision boundary to separate classes
  - **Regression:** aka *curve fitting* or *function approxima-tion*; Learn a *continuous* input-output mapping from examples, e.g., for a zip code, predict house sale price given its square footage

Unsupervised Learning

Given only *unlabeled* data as input, learn some sort of structure, e.g.:

- **Clustering**: group Facebook friends based on similarity of post texts and friends
- **Embeddings**: Find sets of words whose meanings are related (e.g., doctor, hospital)
- **Topic modelling**: Induce N topics and words most common in documents about each

Inductive Learning Framework

- Raw input data from sensors or a database preprocessed to obtain **feature vector**, **X**, of **relevant** features for classifying examples
- Each **X** is a list of (attribute, value) pairs
- ***n*** attributes (a.k.a. features): fixed, positive, and finite
- Features have fixed, finite number # of possible values
  - Or continuous within some well-defined space, e.g., “age”
- Each example is a point in an *n*-dimensional feature space
  - X = [Person:Sue, EyeColor:Brown, Age:Young, Sex:Female]
  - X = [Cheese:*f*, Sauce:*t*, Bread:*t*]
  - X = [Texture:Fuzzy, Ears:Pointy, Purrs:Yes, Legs:4]

Inductive Learning Framework Example

Puppy classifier

Training data, X

Text-ure	*Ears*	*Legs*	*Class*
Fuzzy	Round	4	+
Slimy	Missing	8	-
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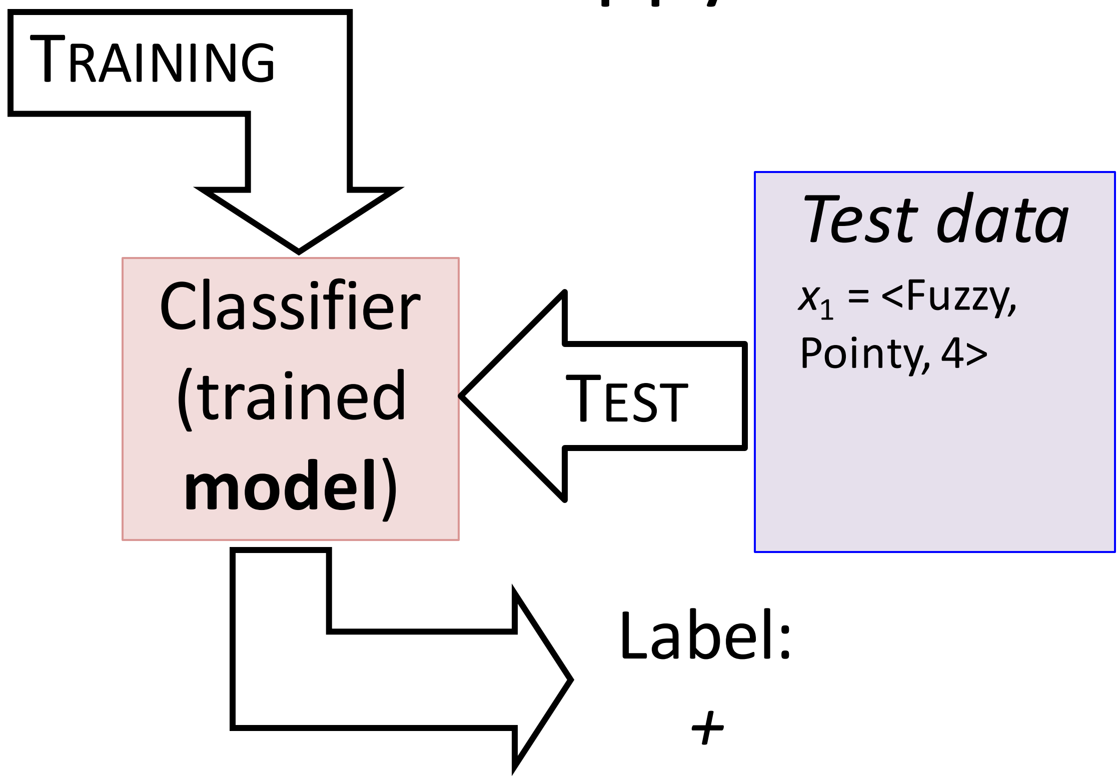

Classification Examples

Assigning subject categories, topics, or genres

Spam detection

Authorship identification

Age/gender identification

Language Identification

Sentiment analysis

…

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Input:

an instance

a fixed set of classes $C = \{c_1, c_2, \ldots, c_J\}$

Output: a predicted class c from C

Classification: Hand-coded Rules?

Assigning subject categories, topics, or genres

Spam detection

Authorship identification

Age/gender identification

Language Identification

Sentiment analysis

…

Rules based on combinations of words or other features

spam: black-list-address OR ("dollars" AND "have been selected")

Accuracy can be high

If rules carefully refined by expert

Building and maintaining these rules is expensive

Can humans faithfully assign uncertainty?

Classification: Supervised Machine Learning

Assigning subject categories, topics, or genres

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…

Input:

an instance d

a fixed set of classes $C = \{c_1, c_2, \ldots, c_J\}$

A training set of m hand-labeled instances $(d_1,c_1),\ldots,(d_m,c_m)$

Output:

a learned classifier γ that maps instances to classes

Classification: Supervised Machine Learning

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γ learns to associate certain ***features*** of instances with their labels

Classification: Supervised Machine Learning

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Naïve Bayes

Logistic regression

Support-vector machines

k-Nearest Neighbors

…

Classification Example: Face Recognition

Class	Image
Avrim	
Avrim	
Avrim	
Avrim	

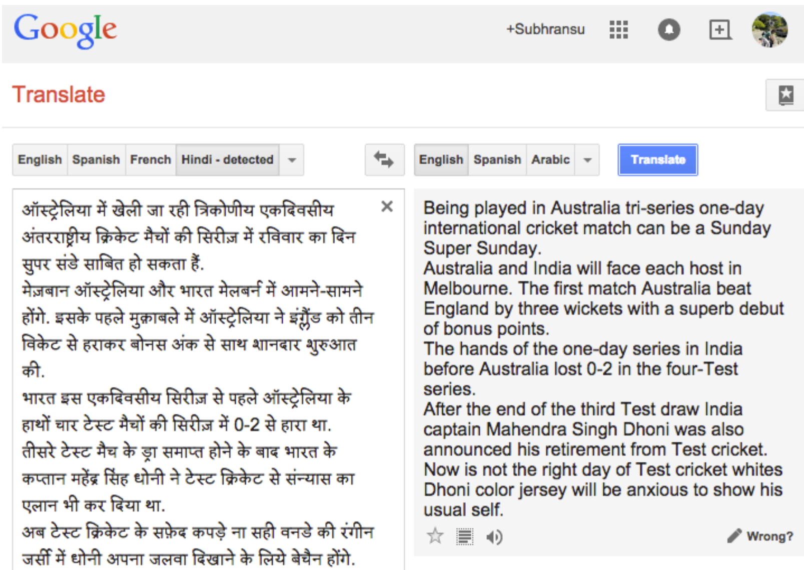
Class	Image
Tom	
Tom	
Tom	
Tom	

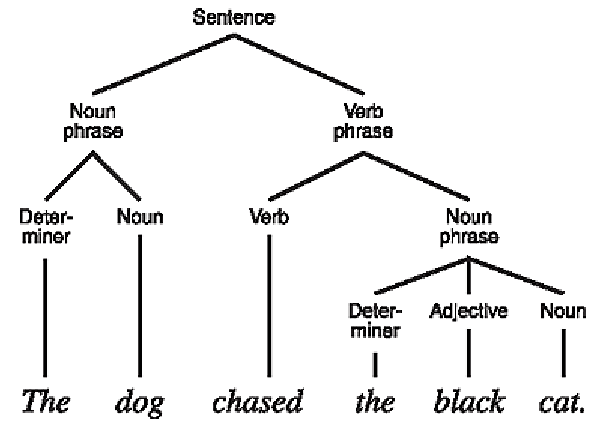
What is a good *representation* for images?

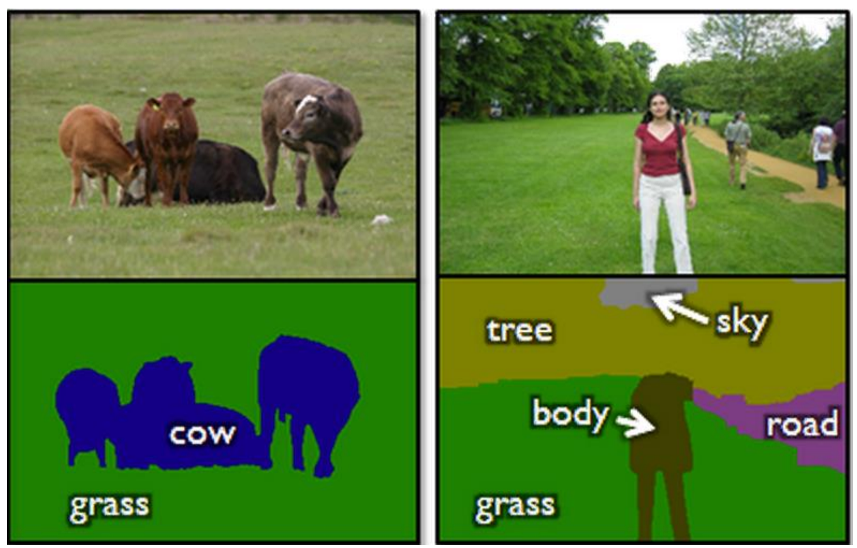
Pixel values? Edges?

Courtesy from Hamed Pirsiavash

Classification Example:
Sequence & Structured Prediction







Courtesy Hamed Pirsiavash

Ingredients for classification

Inject *your* knowledge into a learning system

Feature representation

Training data:
labeled examples

Model

Courtesy Hamed Pirsiavash

Ingredients for classification

Inject *your* knowledge into a learning system

Problem specific

Difficult to learn from bad ones

Feature representation

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Courtesy Hamed Pirsiavash

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Inject *your* knowledge into a learning system

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Difficult to learn from bad ones

Labeling data == $$$

Sometimes data is available for “free”

Feature representation

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Ingredients for classification

Inject *your* knowledge into a learning system

Problem specific

Difficult to learn from bad ones

Feature representation

Labeling data == $$$

Sometimes data is available for "free"

Training data:

labeled examples

No single learning algorithm is always good ("no free lunch")

Different learning algorithms work differently

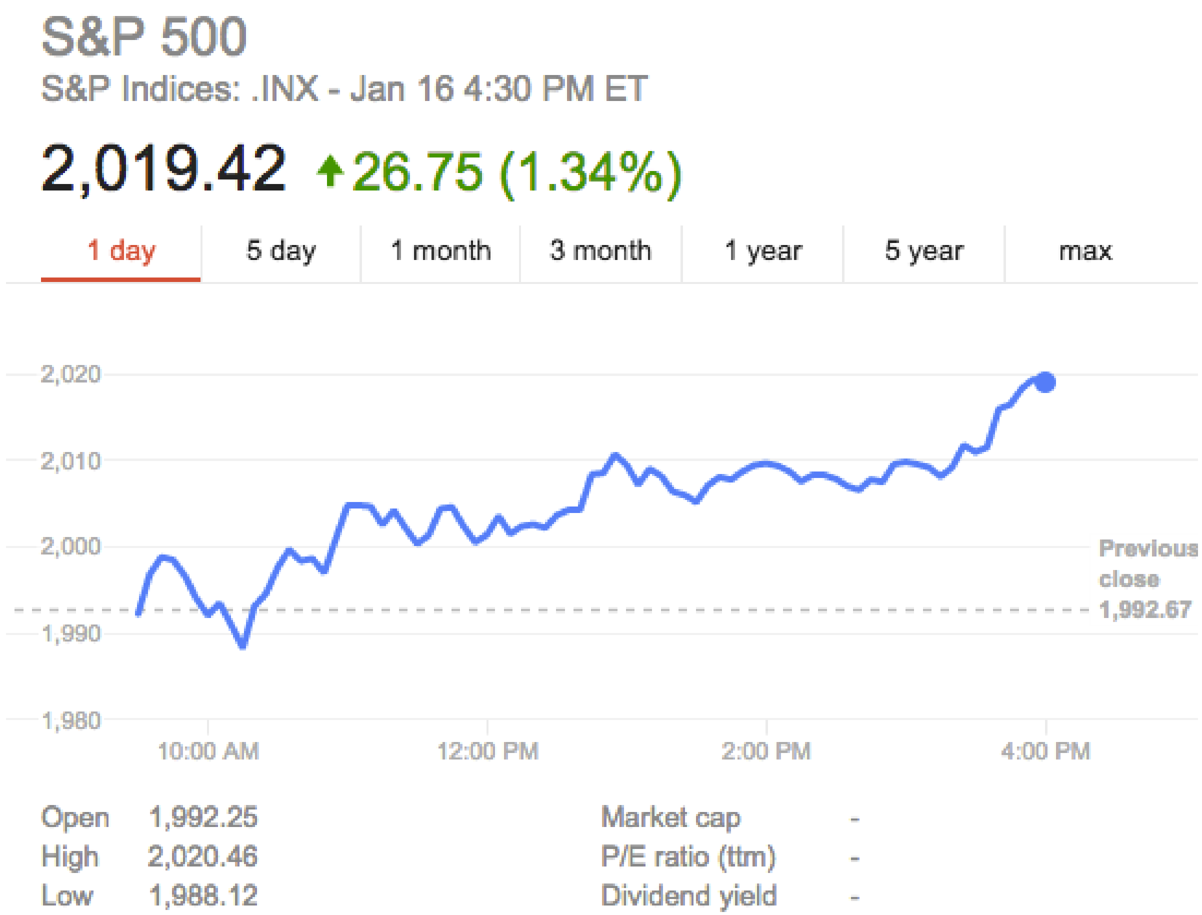
Model

Courtesy Hamed Pirsiavash

Regression

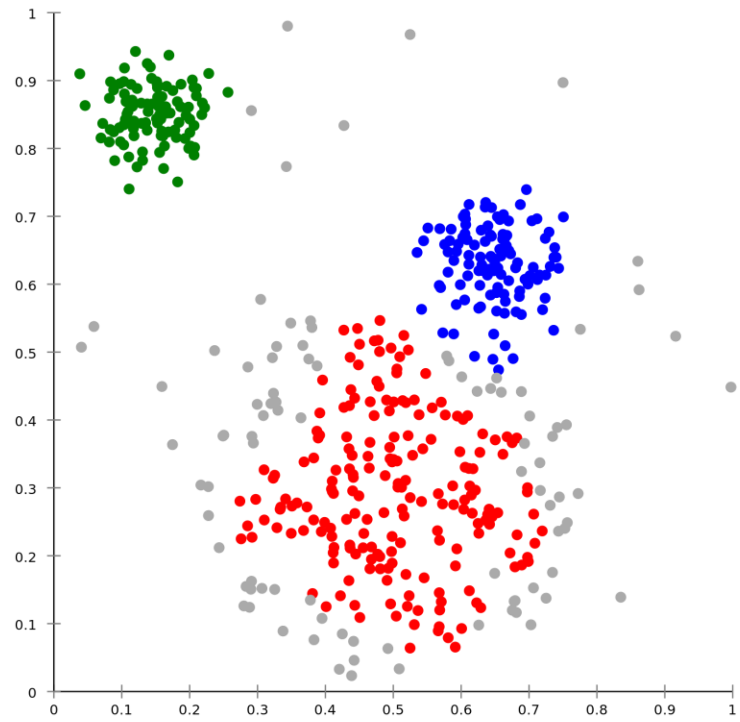
Like classification, but real-valued

Regression Example: Stock Market Prediction



Courtesy Hamed Pirsiavash

Unsupervised learning: Clustering

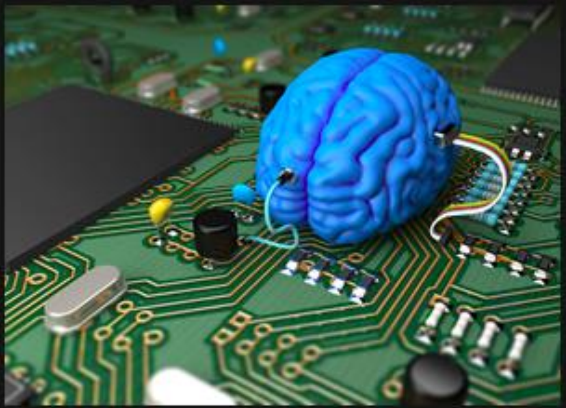


Courtesy Hamed Pirsiavash

ML FOR USERS

Deep Learning

What society thinks I do



What my friends think I do

What other computer scientists think I do

What mathematicians think I do

What I think I do

```
from [redacted] import *
```

keras
torch

What I actually do

Our Jobs

Help you learn the ropes...

https://raftinginthesmokies.com/wp-content/uploads/2019/02/ropes-challenge-course.jpeg

Our Jobs

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Our Jobs

Help you learn the ropes...

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… and apply your knowledge using whatever tools your org. uses!

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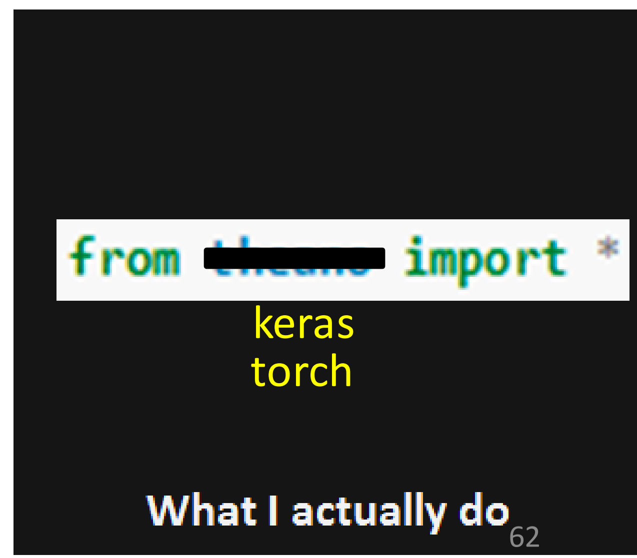

Toolkit Basics

- Machine learning involves working with data
  - analyzing, manipulating, transforming, …
- More often than not, it's numeric or has a natural numeric representation
- Natural language text is an exception, but this too can have a numeric representation
- A common data model is as a N-dimensional matrix or tensor
- These are supported in Python via libraries

Typical Python Libraries

numpy, scipy

- Basic mathematical libraries for dealing with matrices and scientific/mathematical functions

pandas, matplotlib

- Libraries for data science & plotting

sklearn (scikit-learn)

- A whole bunch of implemented classifiers

torch (pytorch) and tensorflow

- Frameworks for building neural networks

Lots of documentation available for all of these online!

What is Numpy?

- NumPy supports features needed for ML
  - Typed N-dimensional arrays (matrices/tensors)
  - Fast numerical computations (matrix math)
  - High-level math functions
- Python does numerical computations slowly and lacks an efficient matrix representation
- 1000 x 1000 matrix multiply
  - Python triple loop takes > 10 minutes!
  - Numpy takes ~0.03 seconds

NumPy Arrays Can Represent ..

Structured lists of numbers

- **Vectors**
- **Matrices**
- Images
- Tensors
- Convolutional Neural Networks

$$\begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix}$$

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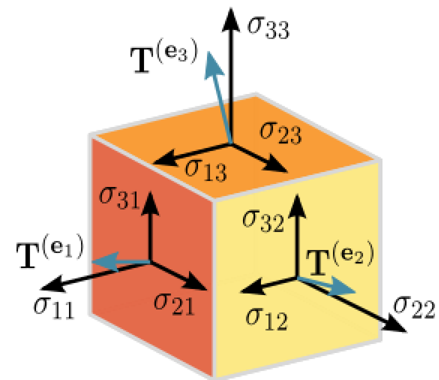
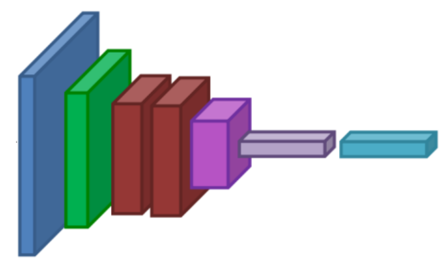




NumPy Arrays, Basic Properties

```
>>> import numpy as np
>>> a= np.array([[1,2,3],[4,5,6]],dtype=np.float32)
>>> print(a.ndim, a.shape, a.dtype)
2  (2, 3)  float32
>> print(a)
[[1. 2. 3.]
 [4. 5. 6.]]
```

Arrays:

1. Can have any number of dimensions, including zero (a scalar)
2. Are **typed**: np.uint8, np.int64, np.float32, np.float64
3. Are **dense:** each element of array exists and has the same type

NumPy Array Indexing, Slicing

```
a[0,0]  # top-left element
a[0,-1] # first row, last column
a[0,:]  # first row, all columns
a[:,0]  # first column, all rows
a[0:2,0:2]  # 1st 2 rows, 1st 2 columns
```

Notes:

- Zero-indexing
- Multi-dimensional indices are comma-separated)
- Python notation for slicing

SciPy

- SciPy builds on the NumPy array object
- Adds additional mathematical functions and *sparse arrays*
- **Sparse array:** one where most elements = 0
- An efficient representation only implicitly encodes the non-zero values
- Access to a missing element returns 0

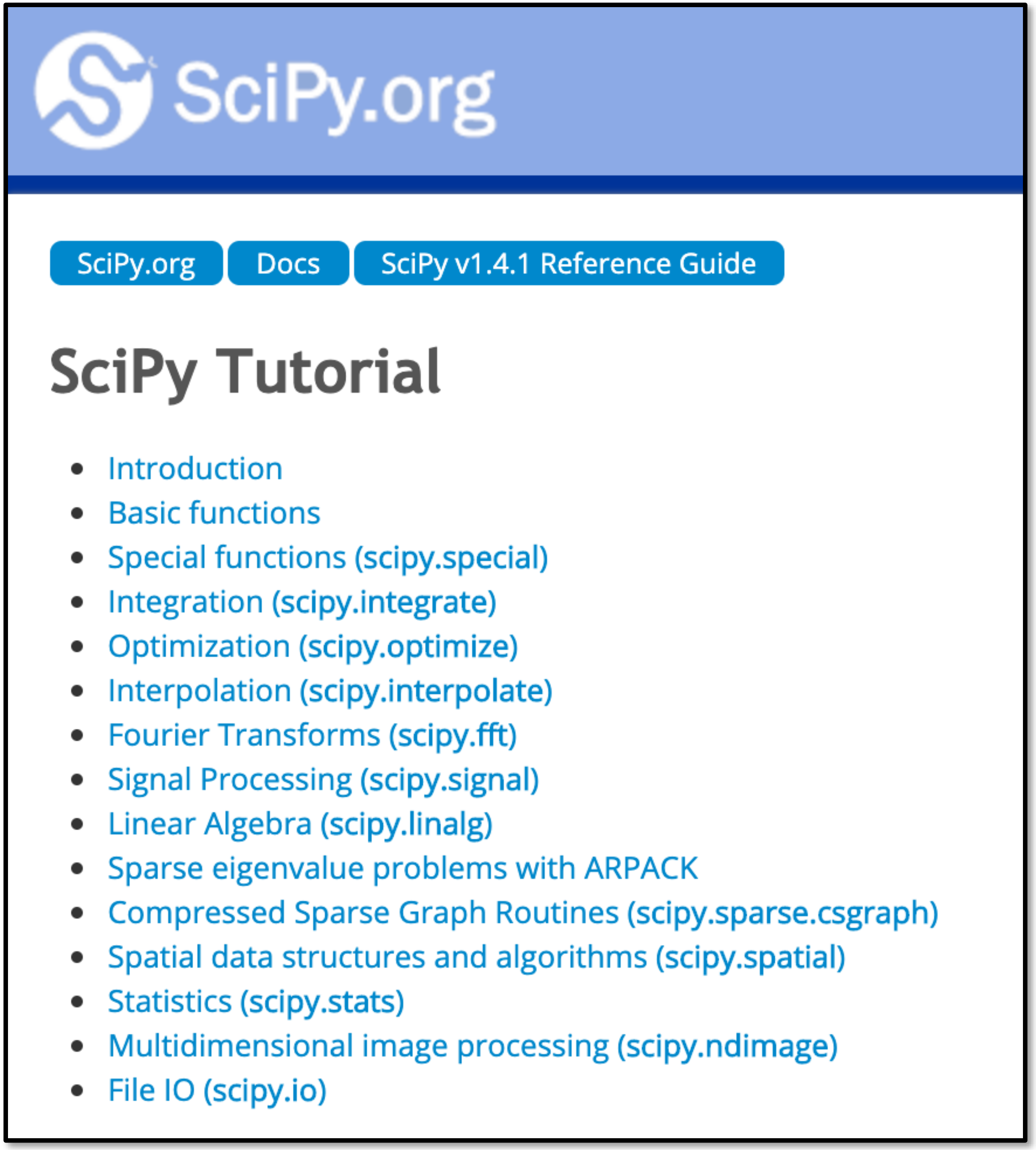
SciPy sparse array use case

- NumPy and SciPy arrays are numeric
- We can represent a document's content by a vector of features
- Each feature is a possible word
- A feature's value might be any of:
  - TF: number of times it occurs in the document;
  - TF-IDF: … normalized by how common the word is
  - and maybe normalized by document length …

SciPy sparse array use case

- Maybe only model 50k most frequent words found in a document collection, ignoring others
- Assign each unique word an index (e.g., dog:137)
  - Build python dict **w** from vocabulary, so w['dog']=137
- The sentence "the dog chased the cat"
  - Would be a *numPy vector* of length 50,000
  - Or a *sciPy sparse vector* of length 4
- An 800-word news article may only have 100 unique words; The Hobbit has about 8,000

More on SciPy



SciPy.org

SciPy.org | Docs | SciPy v1.4.1 Reference Guide

SciPy Tutorial

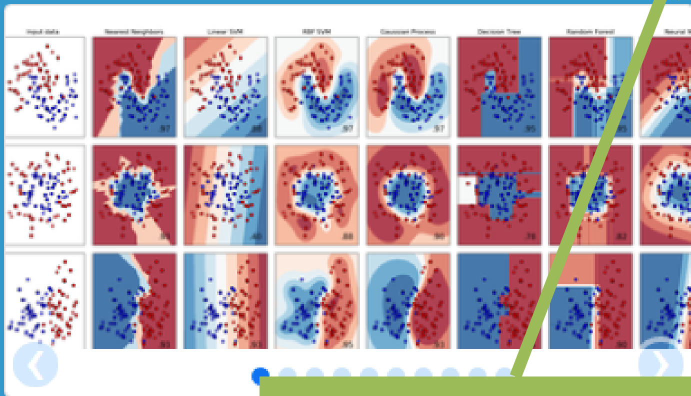
- Introduction
- Basic functions
- Special functions (scipy.special)
- Integration (scipy.integrate)
- Optimization (scipy.optimize)
- Interpolation (scipy.interpolate)
- Fourier Transforms (scipy.fft)
- Signal Processing (scipy.signal)
- Linear Algebra (scipy.linalg)
- Sparse eigenvalue problems with ARPACK
- Compressed Sparse Graph Routines (scipy.sparse.csgraph)
- Spatial data structures and algorithms (scipy.spatial)
- Statistics (scipy.stats)
- Multidimensional image processing (scipy.ndimage)
- File IO (scipy.io)

See the [SciPy tutorial] Web pages

scikit learn

Home Installation Documentation Examples

https://sklearn.org/



scikit-learn

Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Documentation online

Many tutorials

Classification

Identifying to which category an object belongs to.

Applications: Spam detection, Image recognition.
Algorithms: SVM, nearest neighbors, random forest, ... — Examples

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.
Algorithms: SVR, ridge regression, Lasso, ... — Examples

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: k-Means, spectral clustering, mean-shift, ... — Examples

Dimensionality reduction

Reducing the number of random variables to consider.

Applications: Visualization, Increased efficiency
Algorithms: PCA, feature selection, non-negative matrix factorization. — Examples

Model selection

Comparing, validating and choosing parameters and models.

Goal: Improved accuracy via parameter tuning
Modules: grid search, cross validation, metrics. — Examples

Preprocessing

Feature extraction and normalization.

Application: Transforming input data such as text for use with machine learning algorithms.
Modules: preprocessing, feature extraction. — Examples

How easy is this?

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.linear_model import LogisticRegression
>>> X, y = load_iris(return_X_y=True)
```

features on data

labels

```
>>> clf = LogisticRegression(random_state=0).fit(X, y)
```

DATA & EVALUATION

http://archive.ics.uci.edu/ml

UCI Machine Learning Repos

archive.ics.uci.edu/ml/

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UCI

Machine Learning Repository

Center for Machine Learning and Intelligent Systems

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View ALL Data Sets

Welcome to the UC Irvine Machine Learning Repository!

We currently maintain 233 data sets as a service to the machine learning community. You may **view all data sets** through our searchable interface. Our old web site is still available, for those who prefer the old format. For a general overview of the Repository, please visit our About page. For information about citing data sets in publications, please read our citation policy. If you wish to donate a data set, please consult our donation policy. For any other questions, feel free to contact the Repository librarians. We have also set up a mirror site for the Repository.

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233 data sets

Latest News:

2010-03-01: Note from donor regarding Netflix data
2009-10-16: Two new data sets have been added.
2009-09-14: Several data sets have been added.
2008-07-23: Repository mirror has been set up.
2008-03-24: New data sets have been added!
2007-06-25: Two new data sets have been added: UJI Pen Characters, MAGIC Gamma Telescope
2007-04-13: Research papers that cite the repository have been associated to specific data sets.

Featured Data Set: Yeast

Task: Classification
Data Type: Multivariate
 # Attributes: 8
 # Instances: 1484

Predicting the Cellular Localization Sites of Proteins

Newest Data Sets:

2012-10-21: QtyT40I10D100K
2012-10-19: Legal Case Reports
2012-09-29: seeds
2012-08-30: Individual household electric power consumption
2012-08-15: Northix
2012-08-06: PAMAP2 Physical Activity Monitoring
2012-08-04: Restaurant & consumer data
2012-08-03: CNAE-9

Most Popular Data Sets (hits since 2007):

386214: Iris
272233: Adult
237503: Wine
195947: Breast Cancer Wisconsin (Diagnostic)
182423: Car Evaluation
151635: Abalone
135419: Poker Hand
113024: Forest Fires

UCI Machine Learning Repository: Zoo Data Set

http://archive.ics.uci.edu/ml/datasets/Zoo

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View ALL Data Sets

Zoo Data Set

Download: Data Folder, Data Set Description

Abstract: Artificial, 7 classes of animals

http://archive.ics.uci.edu/ml/datasets/Zoo

Data Set Characteristics:	Multivariate	**Number of Instances:**	101	**Area:**	Life
Attribute Characteristics:	Categorical, Integer	**Number of Attributes:**	17	**Date Donated**	1990-05-15
Associated Tasks:	Classification	**Missing Values?**	No	**Number of Web Hits:**	18038

Zoo data

animal name: string
hair: Boolean
feathers: Boolean
eggs: Boolean
milk: Boolean
airborne: Boolean
aquatic: Boolean
predator: Boolean
toothed: Boolean
backbone: Boolean
breathes: Boolean
venomous: Boolean
fins: Boolean
legs: {0,2,4,5,6,8}
tail: Boolean
domestic: Boolean
catsize: Boolean
type: {mammal, fish, bird, shellfish, insect, reptile, amphibian}

101 examples

aardvark,1,0,0,1,0,0,1,1,1,1,0,0,4,0,0,1,mammal
antelope,1,0,0,1,0,0,0,1,1,1,0,0,4,1,0,1,mammal
bass,0,0,1,0,0,1,1,1,1,0,0,1,0,1,0,0,fish
bear,1,0,0,1,0,0,1,1,1,1,0,0,4,0,0,1,mammal
boar,1,0,0,1,0,0,1,1,1,1,0,0,4,1,0,1,mammal
buffalo,1,0,0,1,0,0,0,1,1,1,0,0,4,1,0,1,mammal
calf,1,0,0,1,0,0,0,1,1,1,0,0,4,1,1,1,mammal
carp,0,0,1,0,0,1,0,1,1,0,0,1,0,1,1,0,fish
catfish,0,0,1,0,0,1,1,1,1,0,0,1,0,1,0,0,fish
cavy,1,0,0,1,0,0,0,1,1,1,0,0,4,0,1,0,mammal
cheetah,1,0,0,1,0,0,1,1,1,1,0,0,4,1,0,1,mammal
chicken,0,1,1,0,1,0,0,0,1,1,0,0,2,1,1,0,bird
chub,0,0,1,0,0,1,1,1,1,0,0,1,0,1,0,0,fish
clam,0,0,1,0,0,0,1,0,0,0,0,0,0,0,0,0,shellfish
crab,0,0,1,0,0,1,1,0,0,0,0,0,4,0,0,0,shellfish
…

Defining Appropriate Features

Feature functions help extract useful features (characteristics) of the data

They turn *data* into *numbers*

Features that are not 0 are said to have **fired**

Defining Appropriate Features

Feature functions help extract useful features (characteristics) of the data

They turn *data* into *numbers*

Features that are not 0 are said to have fired

Often binary-valued (0 or 1), but can be real-valued

Features

Define a feature f_{clue}(, label) for each type of clue you want to consider

The feature f_{clue} fires if the clue applies to/can be found in the (, label) pair

sklearn example
(in-class, live coding)

Zoo example

AIMA Code Example

```
aima-python> python
>>> from learning import *
>>> zoo
<DataSet(zoo): 101 examples, 18 attributes>
>>> dt = DecisionTreeLearner()
>>> dt.train(zoo)
>>> dt.predict(['shark',0,0,1,0,0,1,1,1,1,0,0,1,0,1,0,0])
'fish'
>>> dt.predict(['shark',0,0,0,0,0,1,1,1,1,0,0,1,0,1,0,0])
'mammal’
```

Central Question: How Well Are We Doing?

Classification

- Precision, Recall, F1
- Accuracy
- Log-loss
- ROC-AUC
- …

Regression

- (Root) Mean Square Error
- Mean Absolute Error
- …

Clustering

- Mutual Information
- V-score
- …

the ***task****: what* kind *of problem are you solving?*

Central Question: How Well Are We Doing?

Classification

Regression

Clustering

the ***task****: what* kind *of problem are you solving?*

- Precision, Recall, F1
- Accuracy
- Log-loss
- ROC-AUC
- …

- (Root) Mean Square Error
- Mean Absolute Error
- …

- Mutual Information
- V-score
- …

This does not have to be the same thing as the loss function you optimize

Evaluation methodology (1)

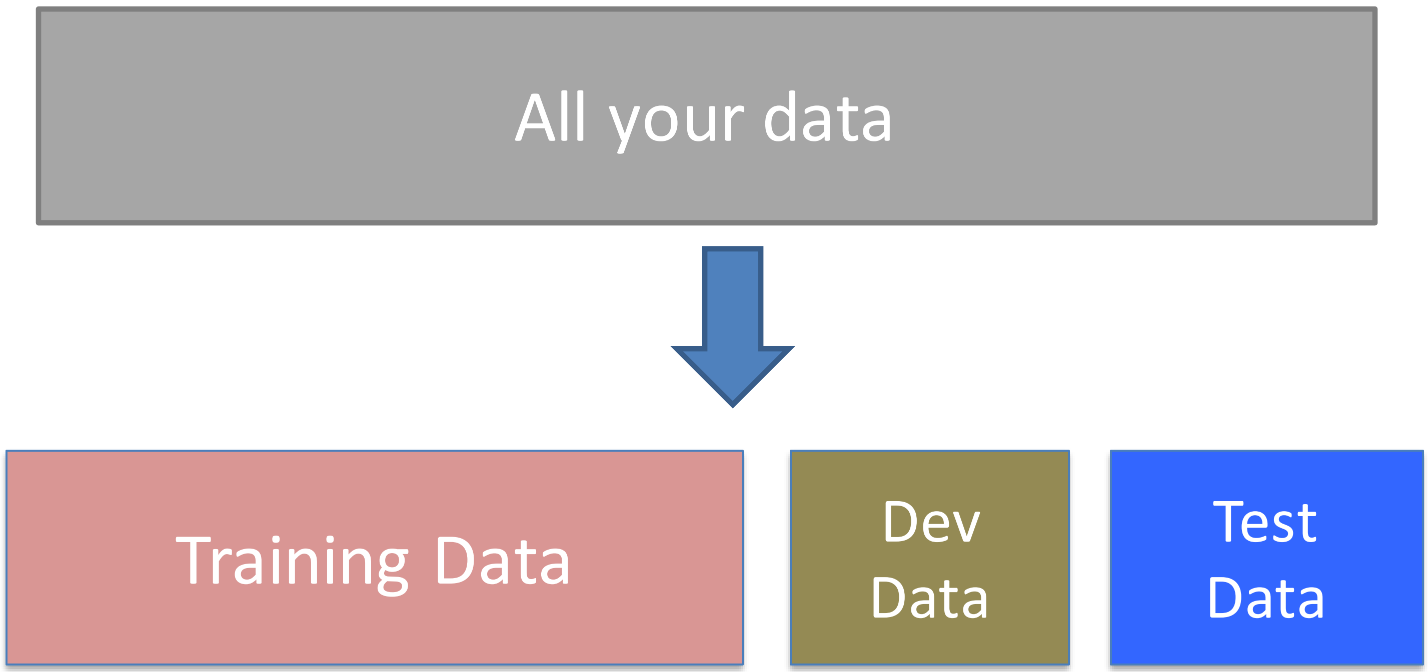
Standard methodology:

1. Collect large set of examples with correct classifications (aka ground truth data)
2. Randomly divide collection into two disjoint sets: ***training*** and ***test*** *(e.g., via a 90-10% split)*
3. Apply learning algorithm to **training** set giving hypothesis H
4. Measure performance of H on the held-out **test** set

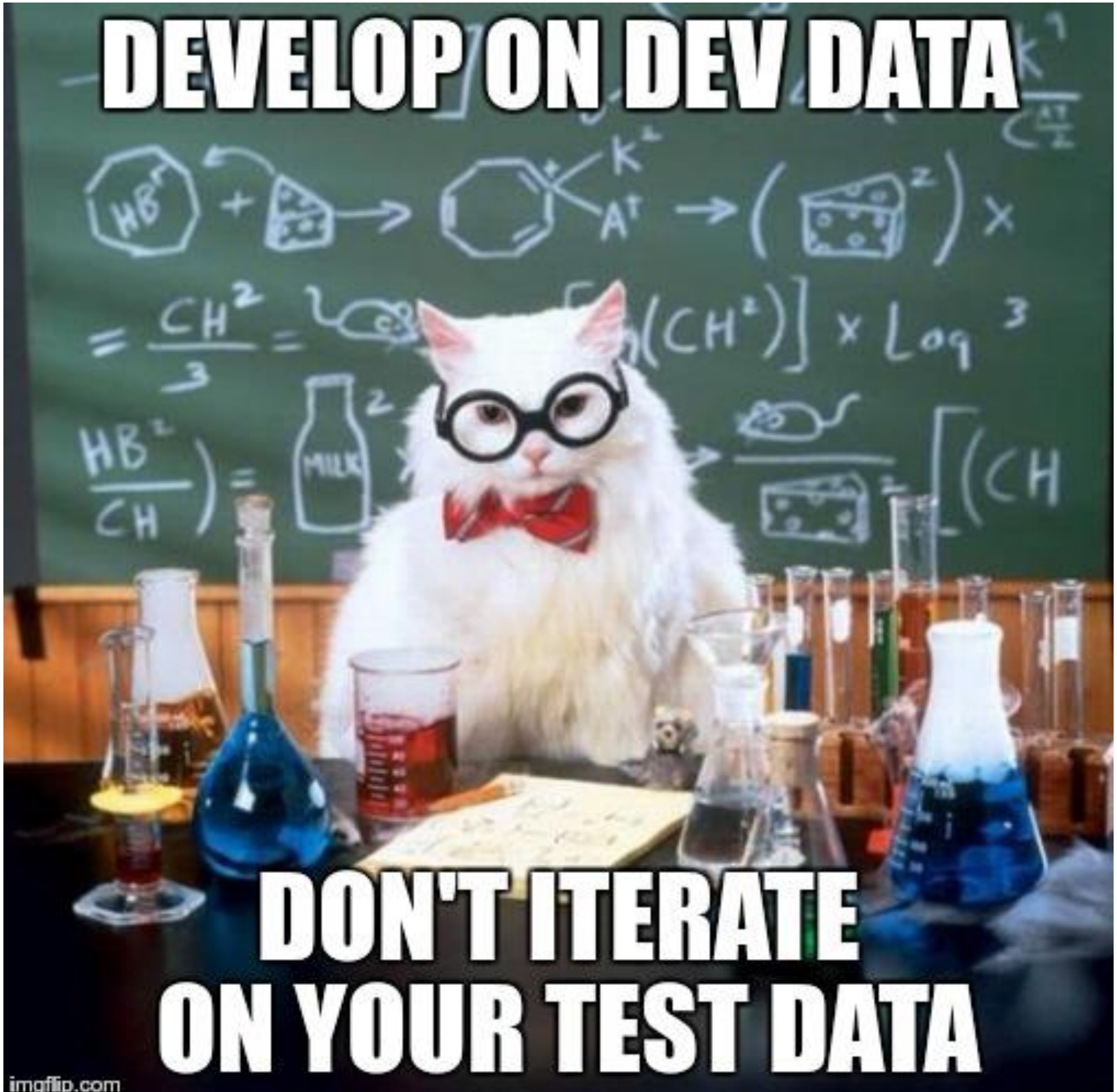
Evaluation methodology (2)

- Important: keep the training and test sets disjoint!
- Study efficiency & robustness of algorithm: repeat steps 2-4 for different training sets & training set sizes
- On modifying algorithm, restart with step 1 to avoid evolving algorithm to work well on just this collection

Experimenting with Machine Learning Models



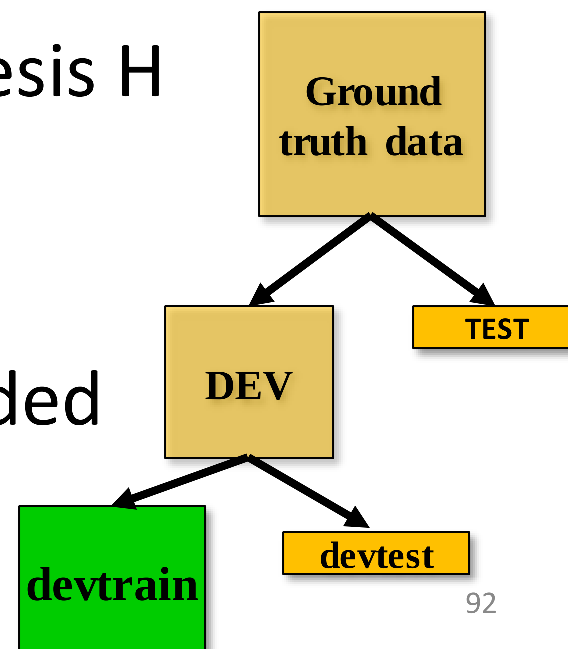
Rule #1


DEVELOP ON DEV DATA
DON'T ITERATE ON YOUR TEST DATA
imgflip.com

Evaluation methodology (3)

Common variation on methodology:

1. Collect set of examples with correct classifications
2. Randomly divide it into two disjoint sets: ***development*** & ***test****;* further divide development into ***devtrain*** & ***devtest***
3. Apply ML to *devtrain,* giving hypothesis H
4. Measure performance of H w.r.t. *devtest* data
5. Modify approach, repeat 3-4 as needed
6. Final test on *test* data



Evaluation methodology (4)

- Only **devtest** data used for evaluation during system **development**
- When all development has ended, **test** data used for **final evaluation**
- Ensures final system not influenced by test data
- If more development needed, get new dataset!

Co

1. classifications

2. sets:

development

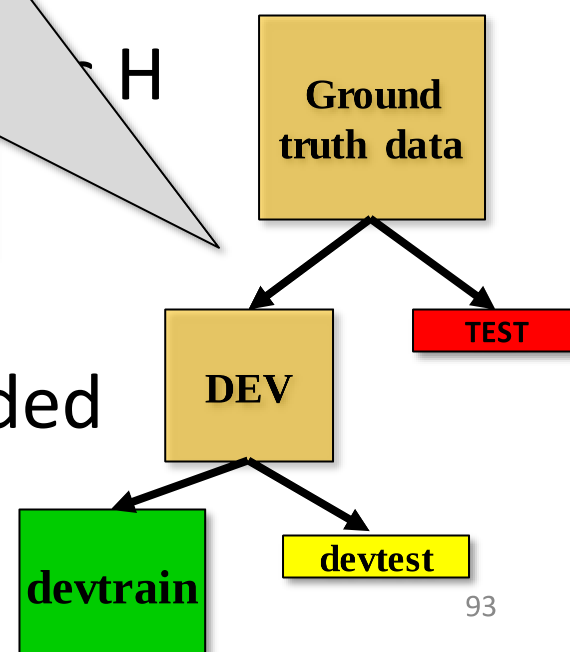
3. H

4.

devtest data

5. Modify approach, repeat 3-4 as needed

6. Final test on *test* data



Zoo evaluation

train_and_test(learner, data, start, end) uses data[start:end] for test and rest for train

```
>>> dtl = DecisionTreeLearner
>>> train_and_test(dtl(), zoo, 0, 10)
1.0
>>> train_and_test(dtl(), zoo, 90, 100)
0.80000000000000004
>>> train_and_test(dtl(), zoo, 90, 101)
0.81818181818181823
>>> train_and_test(dtl(), zoo, 80, 90)
0.90000000000000002
```

Zoo evaluation

train_and_test(learner, data, start, end) uses data[start:end] for test and rest for train

- We hold out 10 data items for test; train on the other 91; show the accuracy on the test data
- Doing this four times for different test subsets shows accuracy from 80% to 100%
- What’s the true accuracy of our approach?

K-fold Cross Validation

- **Problem:** getting *ground truth* data expensive
- **Problem: n**eed different test data for each test
- **Problem:** experiments needed to find right *feature space* & parameters for ML algorithms
- **Goal:** minimize training+test data needed
- **Idea:** split training data into K subsets; use K-1 for *training* and one for *development testing*
- Repeat K times and average performance
- Common K values are 5 and 10

Zoo evaluation

- AIMA code has a cross_validation function that runs K-fold cross validation
- cross_validation(learner, data, K, N) does N iterations, each time randomly selecting 1/K data points for test, leaving rest for train

```
>>> cross_validation(dtl(), zoo, 10, 20)
0.9550000000000007
```

- This is a very common approach to evaluating the accuracy of a model during development
- Best practice is still to hold out a <u>final</u> test data set

Leave one out

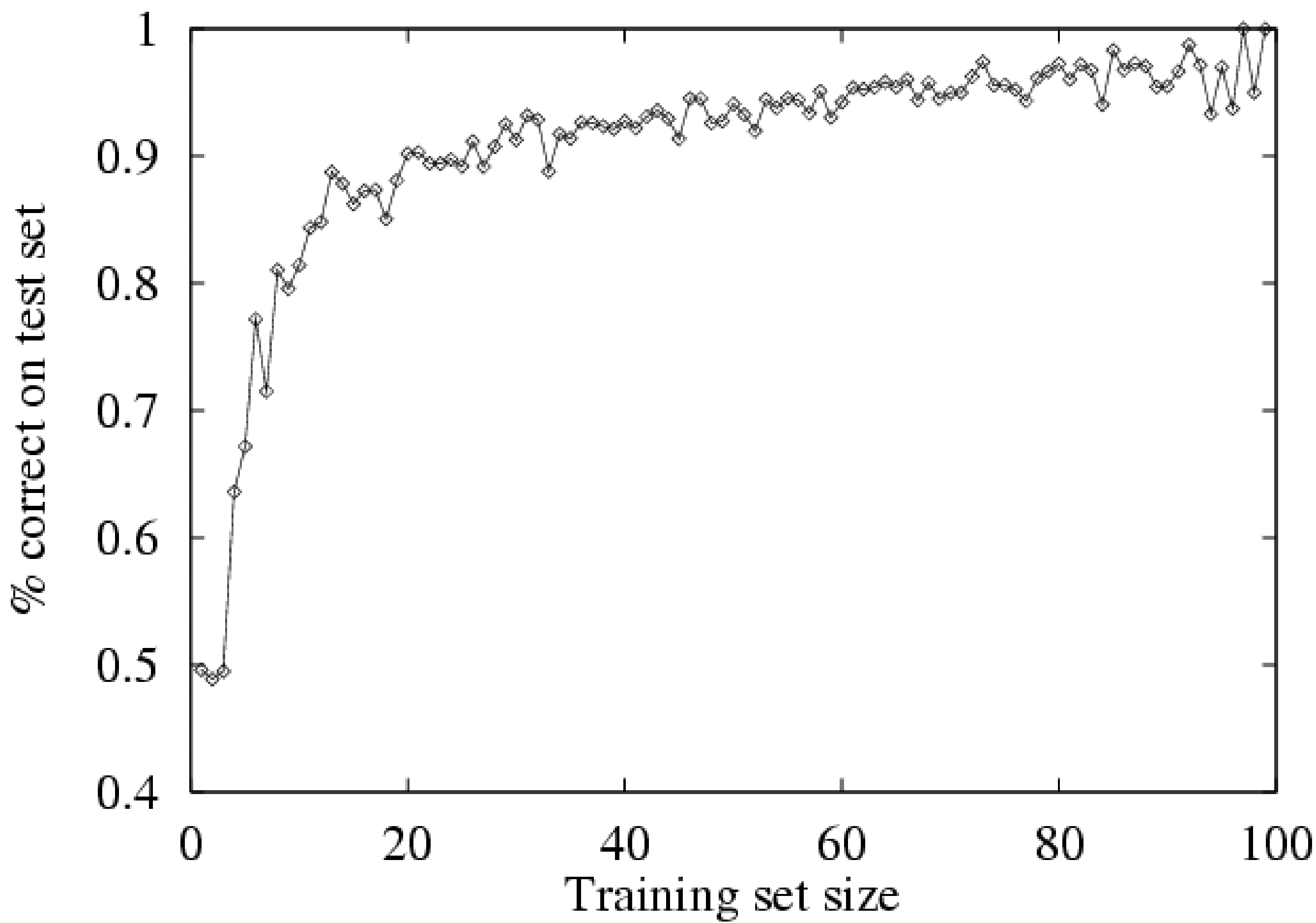
- AIMA code also has a leave1out function that runs a different set of experiments to estimate accuracy of the model
- leave1out(learner, data) does len(data) trials, each using one element for test, rest for train

```
>>> leave1out(dtl(), zoo)
0.970297029702970297027
```

- K-fold cross validation can be too pessimistic, since it only trains with 80% or 90% of the data
- The leave one out evaluation is an alternative

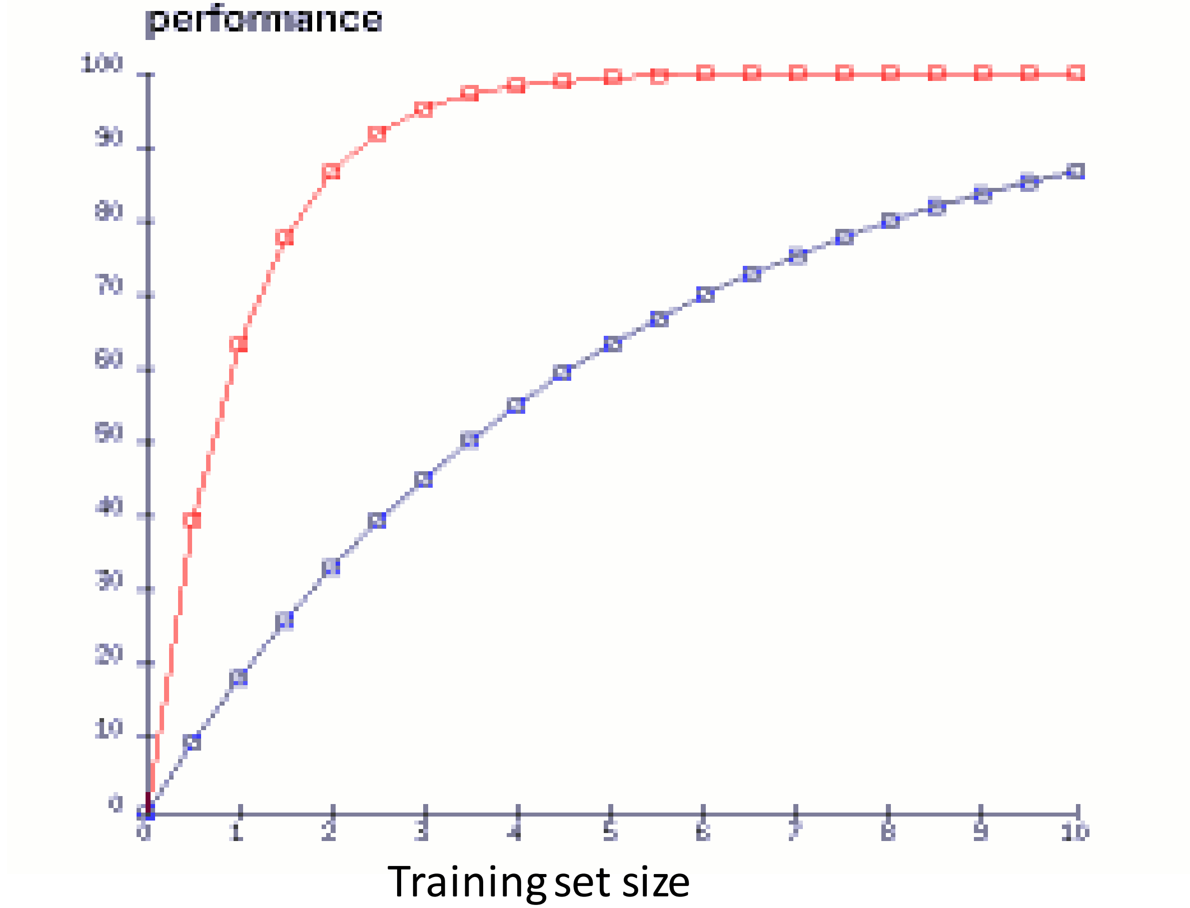
Learning curve (1)

A learning curve shows accuracy on test set as a function of training set size or (for neural networks) running time



Learning curve

- When evaluating ML algorithms, steeper learning curves are better
- They represents faster learning with less data



Here the system with the red curve is better since it requires less data to achieve given accuracy

Classification Evaluation: the 2-by-2 contingency table

Let’s assume there are two classes/labels

● ○

Assume ● is the “positive” label

Given X, our classifier predicts either label

p(● |X) vs. p(○ |X)

Classification Evaluation: the 2-by-2 contingency table

	What is the actual label?	
What label does our system predict? (↓)	Actually Correct	Actually Incorrect
Selected/ Guessed		
Not selected/ not guessed		

Classes/Choices

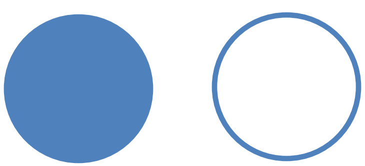
Classification Evaluation: the 2-by-2 contingency table

	What is the actual label?	
What label does our system predict? (↓)	**Actually Correct**	**Actually Incorrect**
Selected/ Guessed	True Positive (TP) *Actual* *Guessed*	
Not selected/ not guessed		

Classes/Choices

Classification Evaluation: the 2-by-2 contingency table

	What is the actual label?	
What label does our system predict? (↓)	**Actually Correct**	**Actually Incorrect**
Selected/ Guessed	True Positive (TP) *Actual* *Guessed*	False Positive (FP) *Actual* *Guessed*
Not selected/ not guessed		



Classes/Choices

Classification Evaluation: the 2-by-2 contingency table

	What is the actual label?	
What label does our system predict? (↓)	Actually Correct	Actually Incorrect
Selected/ Guessed	True Positive (TP) *Actual* *Guessed*	False Positive (FP) *Actual* *Guessed*
Not selected/ not guessed	False Negative (FN) *Actual* *Guessed*	

Classes/Choices

Classification Evaluation: the 2-by-2 contingency table

	What is the actual label?	
What label does our system predict? (↓)	Actually Correct	Actually Incorrect
Selected/ Guessed	True Positive *Actual* (TP) *Guessed*	False Positive *Actual* (FP) *Guessed*
Not selected/ not guessed	False Negative *Actual* (FN) *Guessed*	True Negative *Actual* (TN) *Guessed*

Classes/Choices

Classification Evaluation: the 2-by-2 contingency table

What label does our system predict? (↓)	*What is the actual label?* Actually Correct	Actually Incorrect
Selected/ Guessed	True Positive (TP) Actual · Guessed	False Positive (FP) Actual · Guessed
Not selected/ not guessed	False Negative (FN) Actual · Guessed	True Negative (TN) Actual · Guessed

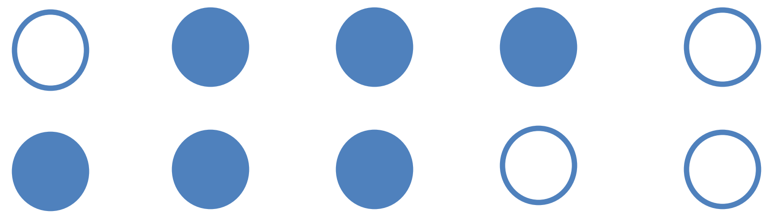
Classes/Choices

Construct this table by *counting* the number of TPs, FPs, FNs, TNs

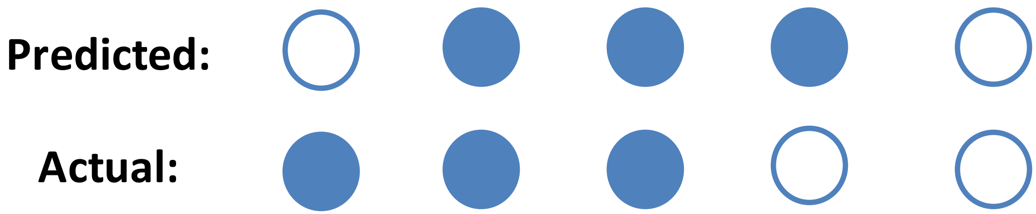
Contingency Table Example

Predicted:

Actual:



Contingency Table Example



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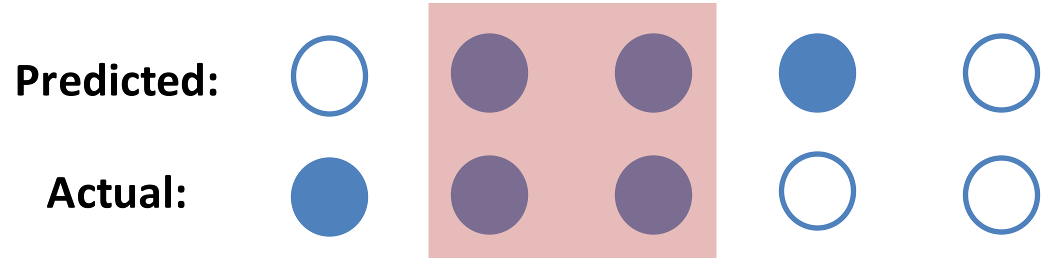
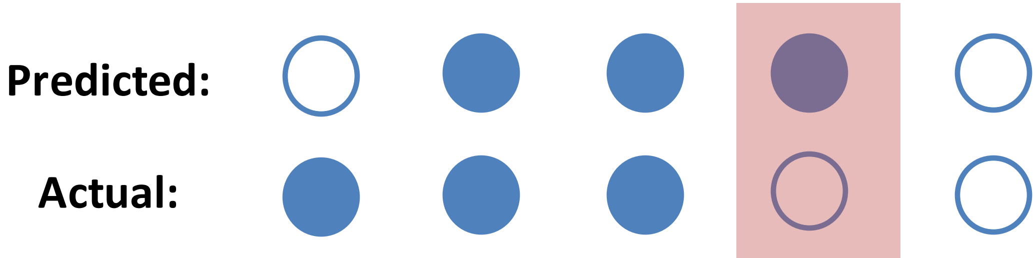
Contingency Table Example



	What is the actual label?	
What label does our system predict? (↓)	**Actually Correct**	**Actually Incorrect**
Selected/ Guessed	True Positive (TP) = 2	False Positive (FP)
Not selected/ not guessed	False Negative (FN)	True Negative (TN)

Contingency Table Example

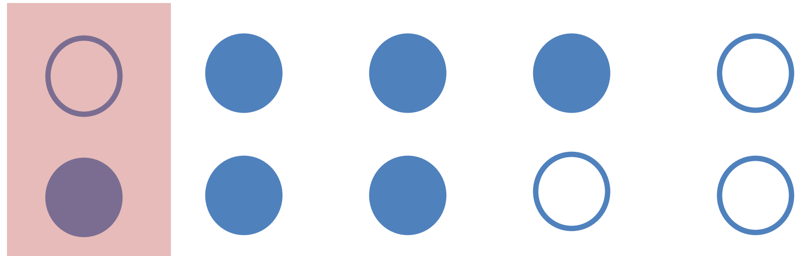


	What is the actual label?	
What label does our system predict? (↓)	**Actually Correct**	**Actually Incorrect**
Selected/ Guessed	True Positive (TP) = 2	False Positive (FP) = 1
Not selected/ not guessed	False Negative (FN)	True Negative (TN)

Contingency Table Example

Predicted:

Actual:



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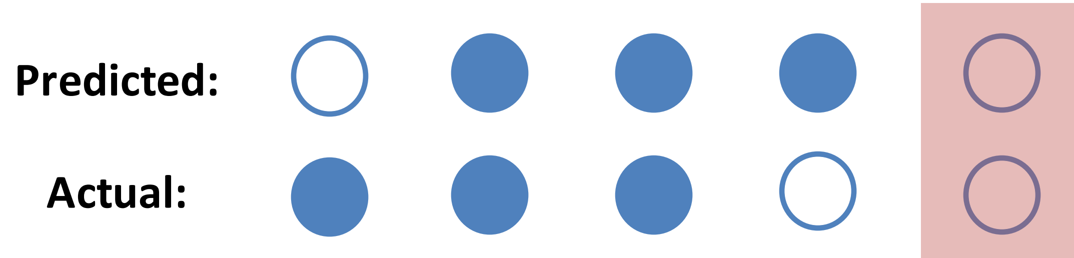
Contingency Table Example



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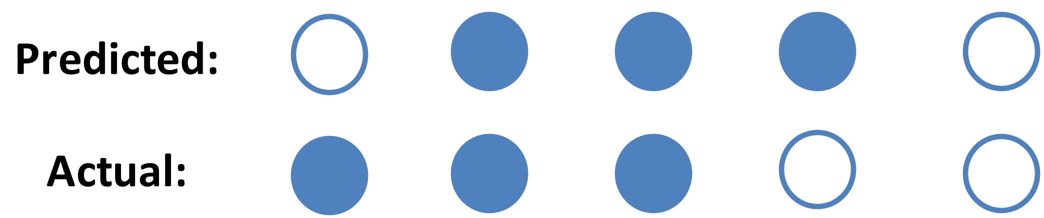
Contingency Table Example



	What is the actual label?	
What label does our system predict? (↓)	**Actually Correct**	**Actually Incorrect**
Selected/ Guessed	True Positive (TP) = 2	False Positive (FP) = 1
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Classification Evaluation: Accuracy, Precision, and Recall

Accuracy: % of items correct

$$\frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

	Actually Correct	Actually Incorrect
Selected/Guessed	True Positive (TP)	False Positive (FP)
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Classification Evaluation: Accuracy, Precision, and Recall

Accuracy: % of items correct

$$\frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

Precision: % of selected items that are correct

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

	Actually Correct	Actually Incorrect
Selected/Guessed	True Positive (TP)	False Positive (FP)
Not select/not guessed	False Negative (FN)	True Negative (TN)

Classification Evaluation: Accuracy, Precision, and Recall

Accuracy: % of items correct

$$\frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

Precision: % of selected items that are correct

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

Recall: % of correct items that are selected

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

	Actually Correct	Actually Incorrect
Selected/Guessed	True Positive (TP)	False Positive (FP)
Not select/not guessed	False Negative (FN)	True Negative (TN)

Classification Evaluation: Accuracy, Precision, and Recall

Accuracy: % of items correct

$$\frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

Precision: % of selected items that are correct

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

Min: 0 ☹
Max: 1 😁

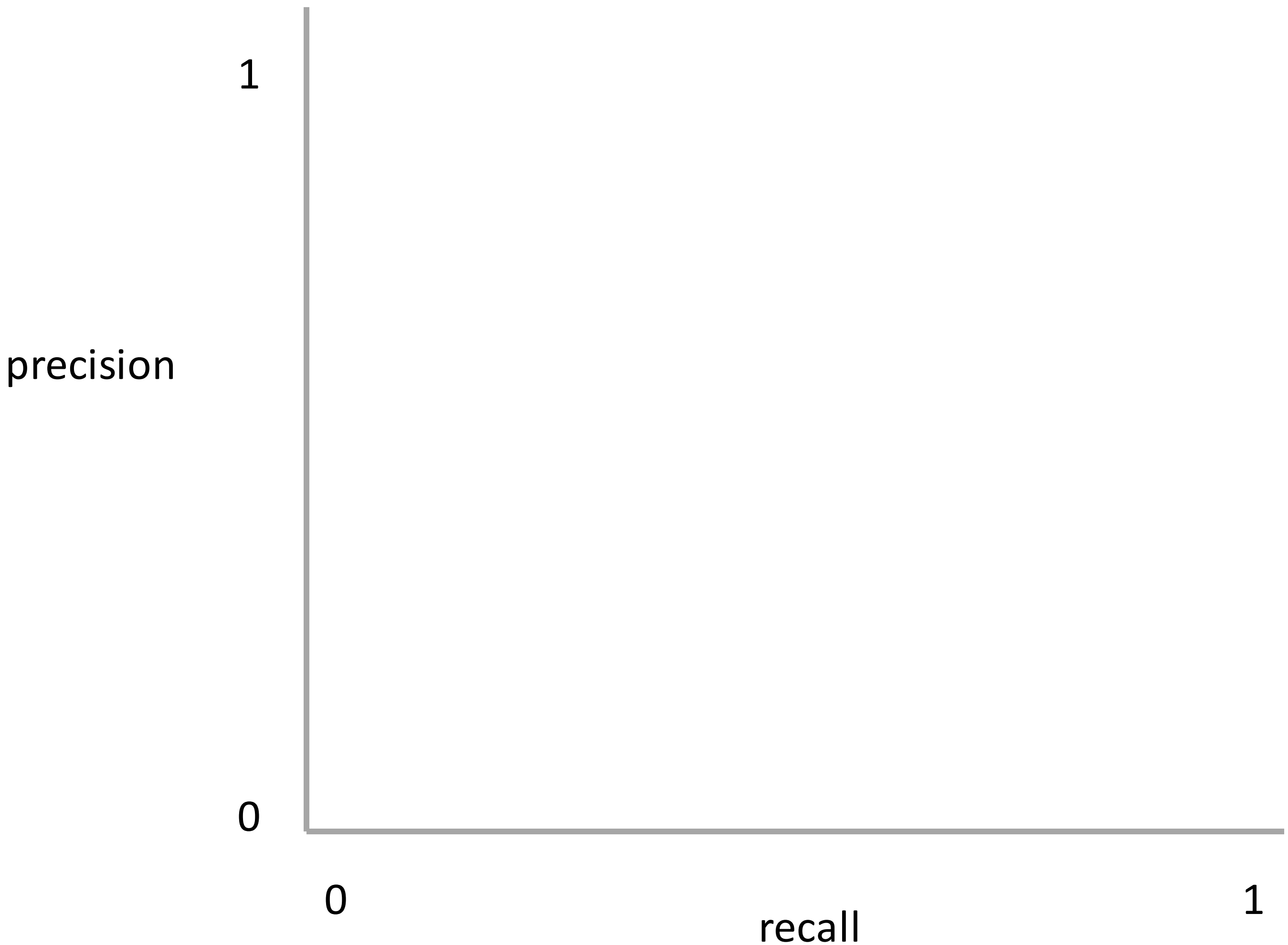
Recall: % of correct items that are selected

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

	Actually Correct	**Actually Incorrect**
Selected/Guessed	True Positive (TP)	False Positive (FP)
Not select/not guessed	False Negative (FN)	True Negative (TN)

Precision and Recall Present a Tradeoff

Q: Where do you want your ideal model ?



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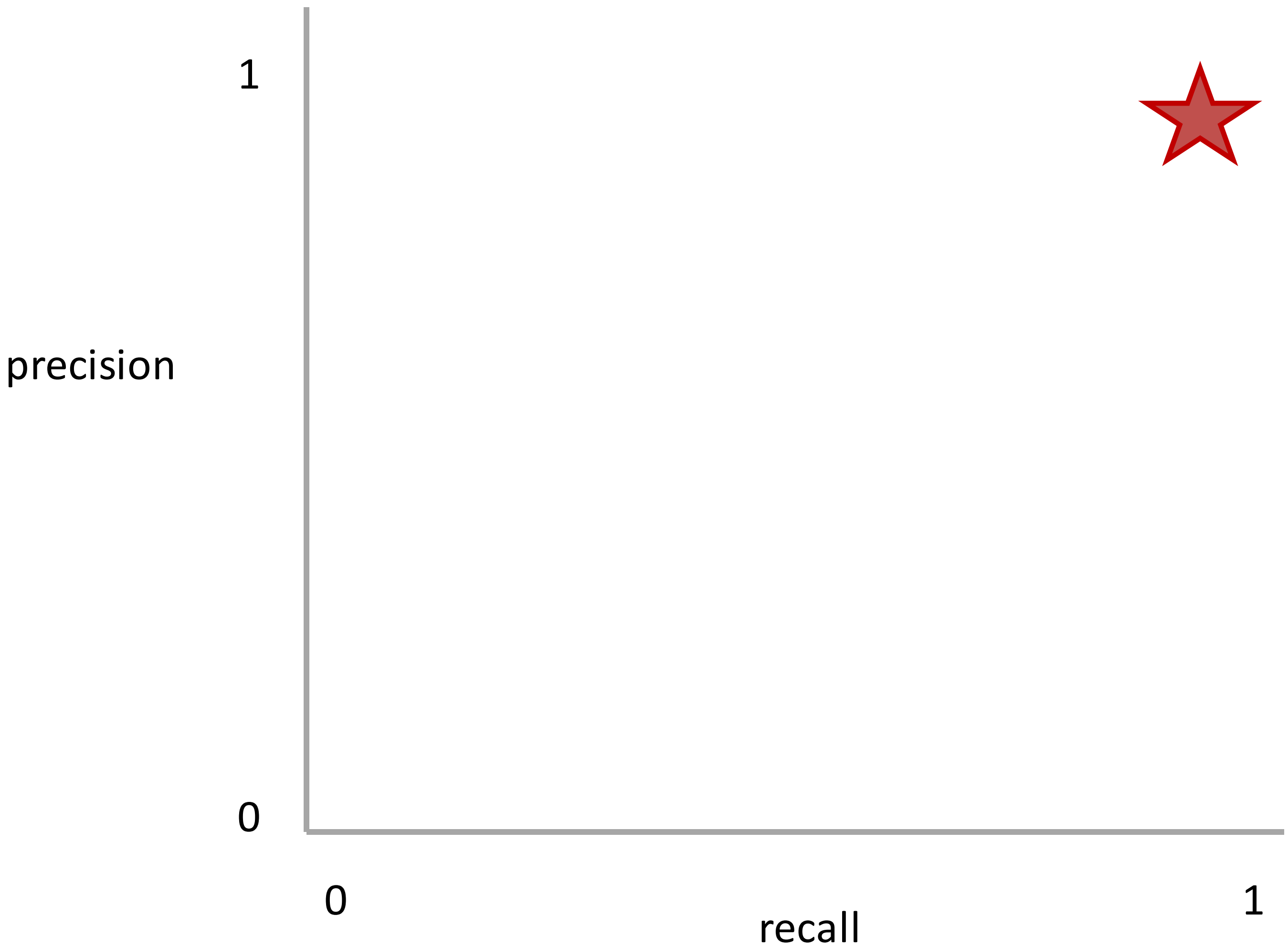
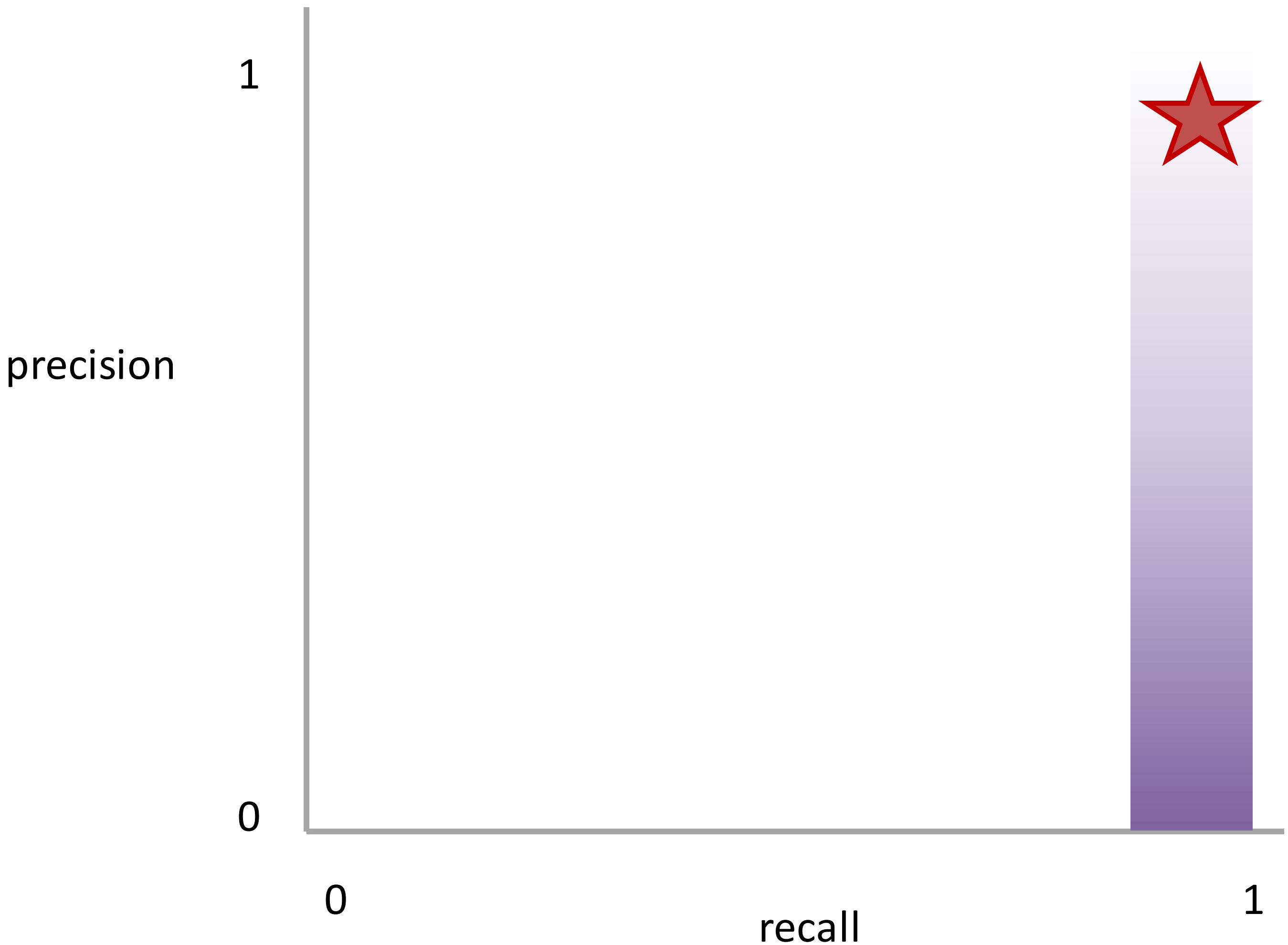


Q: Where do you want your ideal model ?

Q: You have a model that always identifies correct instances. Where on this graph is it?

Precision and Recall Present a Tradeoff

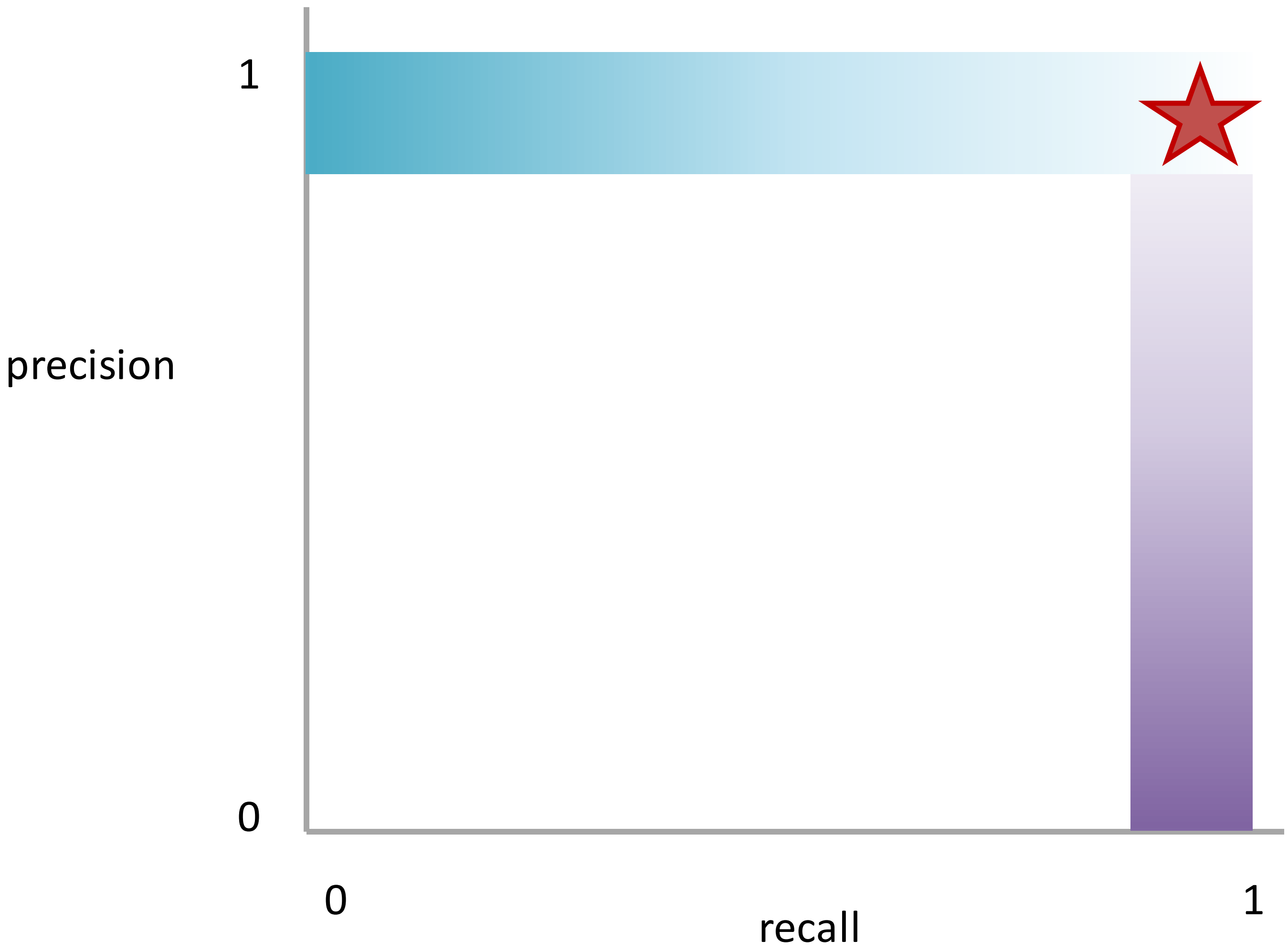


Q: Where do you want your ideal model?

Q: You have a model that always identifies correct instances. Where on this graph is it?

Q: You have a model that only make correct predictions. Where on this graph is it?

Precision and Recall Present a Tradeoff



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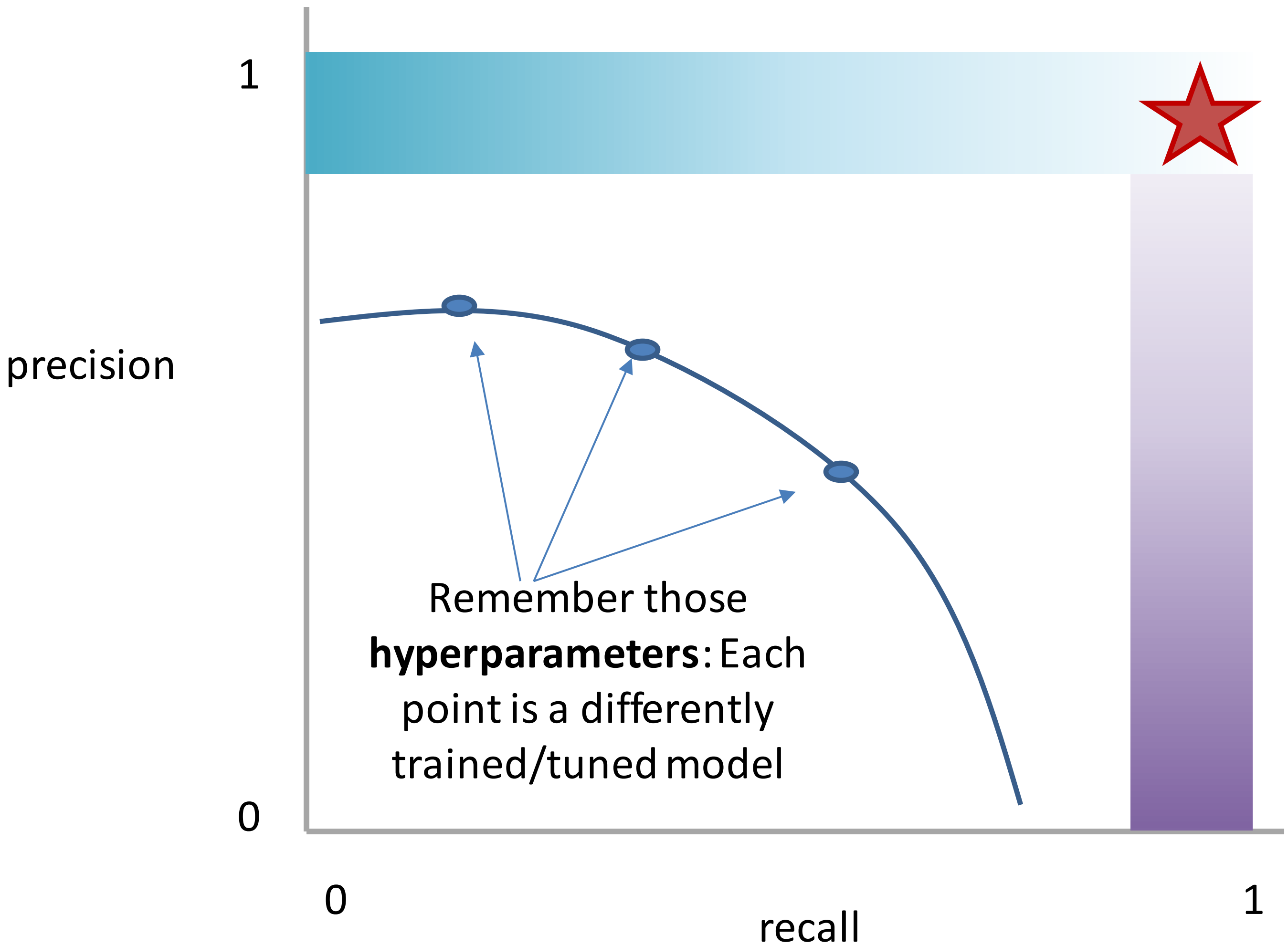


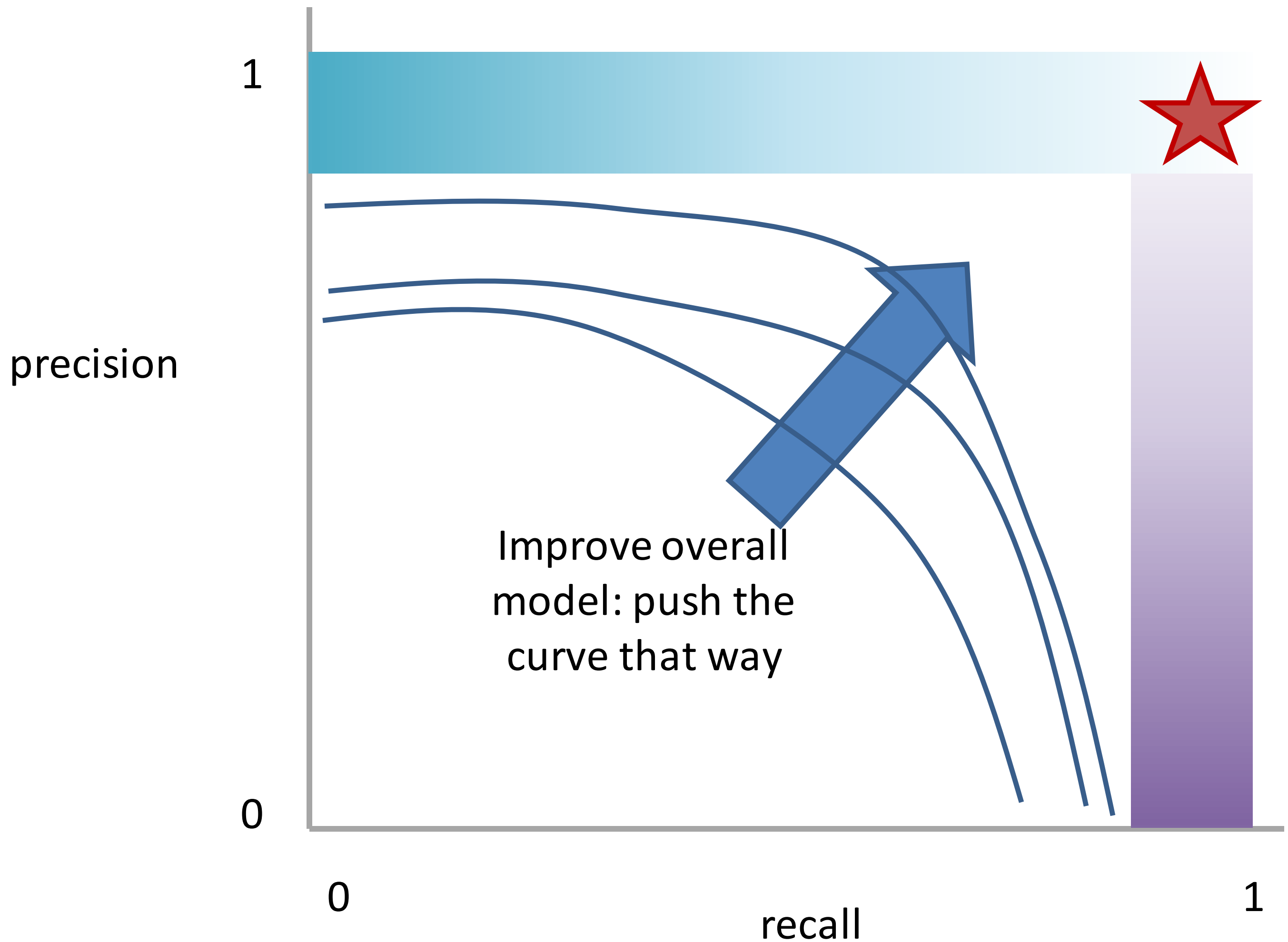
Q: Where do you want your ideal model ?

Q: You have a model that always identifies correct instances. Where on this graph is it?

Q: You have a model that only make correct predictions. Where on this graph is it?

Idea: measure the tradeoff between precision and recall

Precision and Recall Present a Tradeoff



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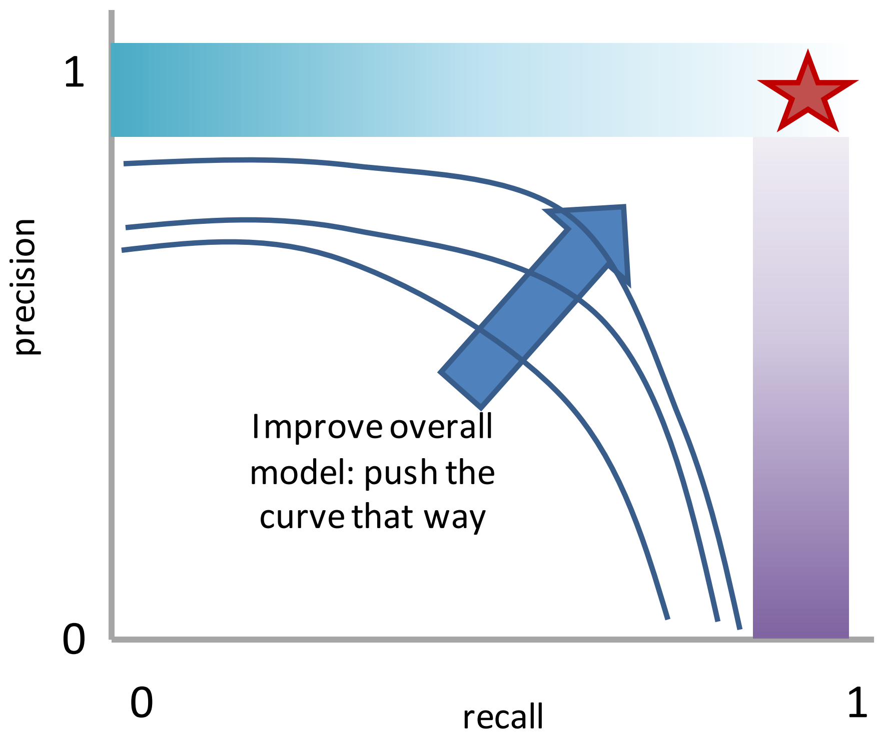
Q: You have a model that always identifies correct instances. Where on this graph is it?

Q: You have a model that only make correct predictions. Where on this graph is it?

Idea: measure the tradeoff between precision and recall

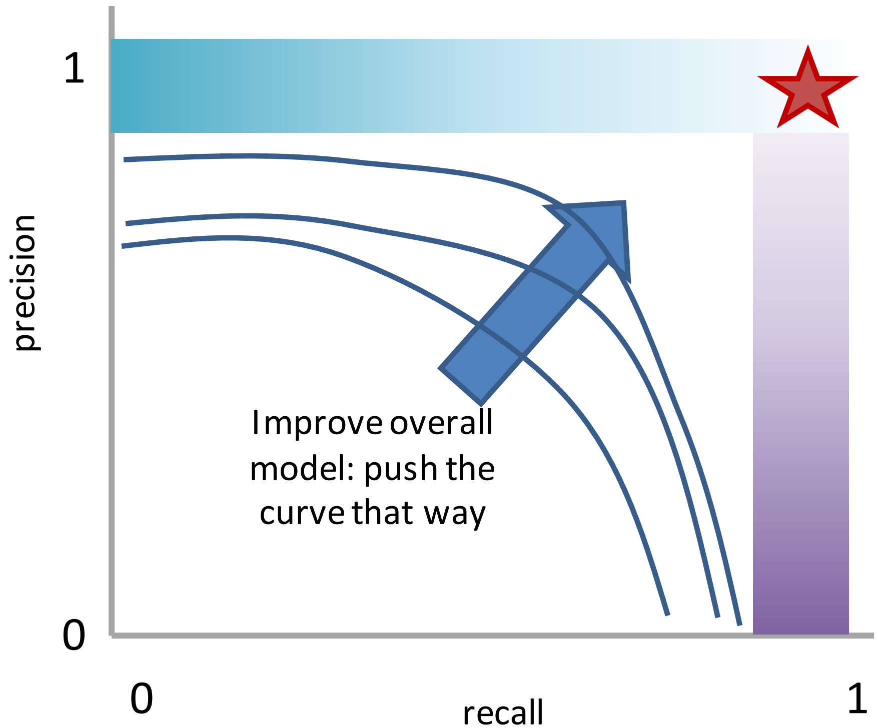
Measure this Tradeoff: Area Under the Curve (AUC)

AUC measures the area under this tradeoff curve



Min AUC: 0 ☹
Max AUC: 1 😁

Measure this Tradeoff: Area Under the Curve (AUC)



Min AUC: 0 ☹
Max AUC: 1 😁

AUC measures the area under this tradeoff curve

1. Computing the curve

   You need true labels & predicted labels with some score/confidence estimate

   Threshold the scores and for each threshold compute precision and recall

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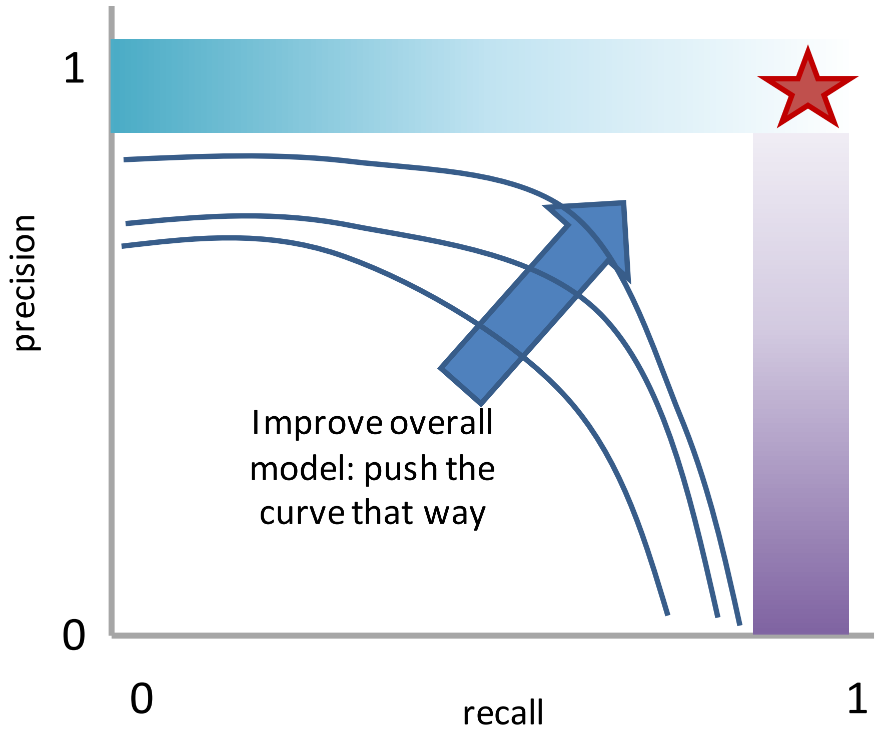

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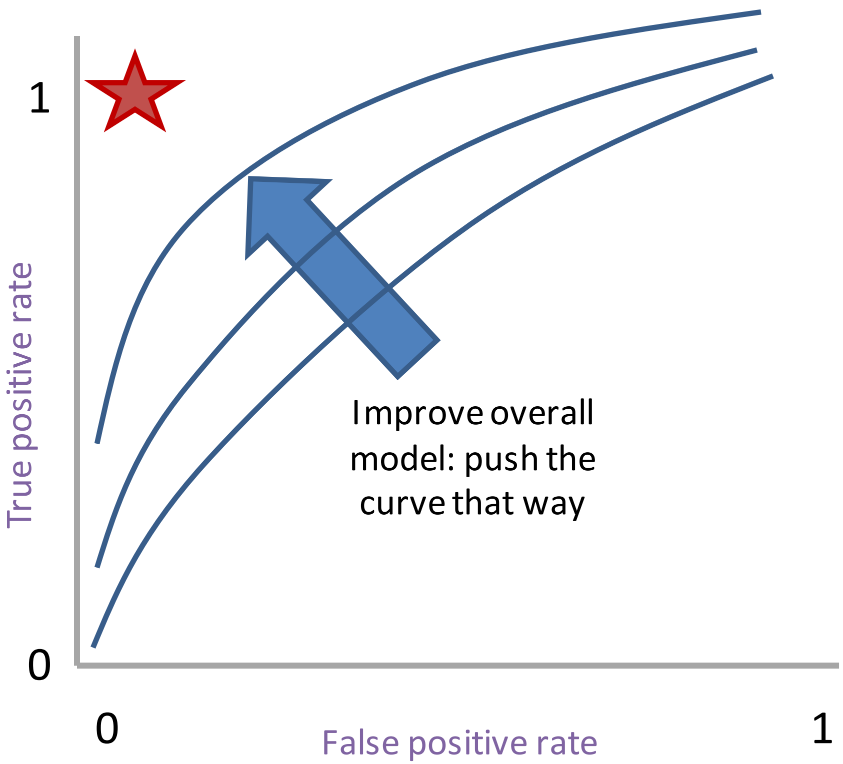
   Threshold the scores and for each threshold compute precision and recall

2. Finding the area

   How to implement: trapezoidal rule (& others)

In practice: external library like the sklearn.metrics module

Measure A Slightly Different Tradeoff: ROC-AUC



Min ROC-AUC: 0.5 ☹
Max ROC-AUC: 1 😁

AUC measures the area under this tradeoff curve

1. Computing the curve

   You need true labels & predicted labels with some score/confidence estimate

   Threshold the scores and for each threshold compute metrics

2. Finding the area

   How to implement: trapezoidal rule (& others)

In practice: external library like the sklearn.metrics module

Main variant: ROC-AUC

Same idea as before but with some flipped metrics

A combined measure: F

Weighted (harmonic) average of **P**recision & **R**ecall

$$F = \frac{1}{\alpha \frac{1}{P} + (1 - \alpha) \frac{1}{R}}$$

A combined measure: F

Weighted (harmonic) average of **P**recision & **R**ecall

$$F = \frac{1}{\alpha\frac{1}{P} + (1-\alpha)\frac{1}{R}} = \frac{(1+\beta^2) \ * P \ * R}{(\beta^2 * P) + R}$$

algebra
(not important)

A combined measure: F

Weighted (harmonic) average of **P**recision & **R**ecall

$$F = \frac{(1+\beta^2) \; * P \; * R}{(\beta^2 * P) + R}$$

Balanced F1 measure: β=1

$$F_1 = \frac{2 \; * P \; * R}{P + R}$$

P/R/F in a Multi-class Setting: Micro- vs. Macro-Averaging

If we have more than one class, how do we combine multiple performance measures into one quantity?

Macroaveraging: Compute performance for each class, then average.

Microaveraging: Collect decisions for all classes, compute contingency table, evaluate.

P/R/F in a Multi-class Setting: Micro- vs. Macro-Averaging

Macroaveraging: Compute performance for each class, then average.

$$\text{macroprecision} = \sum_c \frac{\mathrm{TP_c}}{\mathrm{TP_c} + \mathrm{FP_c}} = \sum_c \text{precision}_c$$

(missing 1/C)

Microaveraging: Collect decisions for all classes, compute contingency table, evaluate.

$$\text{microprecision} = \frac{\sum_{\mathrm{c}} \mathrm{TP_c}}{\sum_{\mathrm{c}} \mathrm{TP_c} + \sum_{\mathrm{c}} \mathrm{FP_c}}$$

P/R/F in a Multi-class Setting: Micro- vs. Macro-Averaging

Macroaveraging: Compute performance for each class, then average.

when to prefer the macroaverage?

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when to prefer the microaverage?

$$\text{microprecision} = \frac{\sum_{\mathrm{c}} \mathrm{TP_c}}{\sum_{\mathrm{c}} \mathrm{TP_c} + \sum_{\mathrm{c}} \mathrm{FP_c}}$$

Micro- vs. Macro-Averaging: Example

Class 1

	Truth : yes	Truth : no
Classifier: yes	10	10
Classifier: no	10	970

Class 2

	Truth : yes	Truth : no
Classifier: yes	90	10
Classifier: no	10	890

Micro Ave. Table

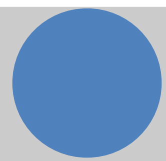
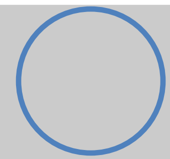
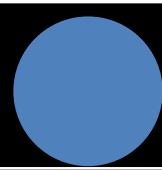
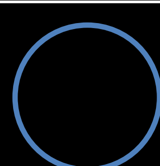
	Truth : yes	Truth : no
Classifier: yes	100	20
Classifier: no	20	1860

Macroaveraged precision: $(0.5 + 0.9)/2 = 0.7$

Microaveraged precision: $100/120 = .83$

Microaveraged score is dominated by score on frequent classes

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
				
Guessed Value		#	#	#
		#	#	#
		#	#	#

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
		●	○	▭
Guessed Value	●	80	9	11
	○	7	86	7
	▭	2	8	9

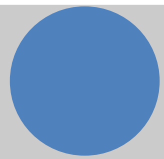
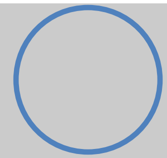
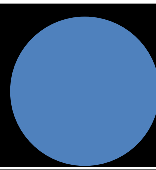
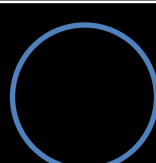
Q: Is this a good result?

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
		●	○	▭
Guessed Value	●	30	40	30
	○	25	30	50
	▭	30	35	35

Q: Is this a good result?

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
				
Guessed Value		7	3	90
		4	8	88
		3	7	90

Q: Is this a good result?

DECISION TREES & RANDOM FORESTS

Decision Trees

"20 Questions": http://20q.net/

Goals: 1. Figure out what questions to ask

2. In what order

3. Determine how many questions are enough

4. What to predict at the end

Adapted from Hamed Pirsiavash

Example: Learning a decision tree

Course ratings dataset

Rating	Easy?	AI?	Sys?	Thy?	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
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0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Adapted from Hamed Pirsiavash

Example: Learning a decision tree

Course ratings dataset

Rating is the label

Rating	Easy?	AI?	Sys?	Thy?	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Adapted from Hamed Pirsiavash

Example: Learning a decision tree

Course ratings dataset

Questions are features

Rating is the label

Rating	Easy?	AI?	Sys?	Thy?	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
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0	y	n	n	y	y
0	n	y	n	y	n
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-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Adapted from Hamed Pirsiavash

Example: Learning a decision tree

Course ratings dataset

Questions are features

Responses are feature values

Rating is the label

Idea: Predict the label by forming a tree where each node branches on values of particular features

Rating	Easy?	AI?	Sys?	Thy?	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
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0	y	n	n	y	y
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-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Adapted from Hamed Pirsiavash

Example: Learning a decision tree

Course ratings dataset

Questions are features

Responses are feature values

Rating is the label

Easy?

Rating	Easy?	AI?	Sys?	Thy?	Morning?
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+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
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-1	n	n	y	y	n
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-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
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Adapted from Hamed Pirsiavash

Example: Learning a decision tree

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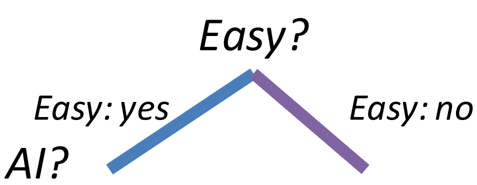
Rating is the label



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+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
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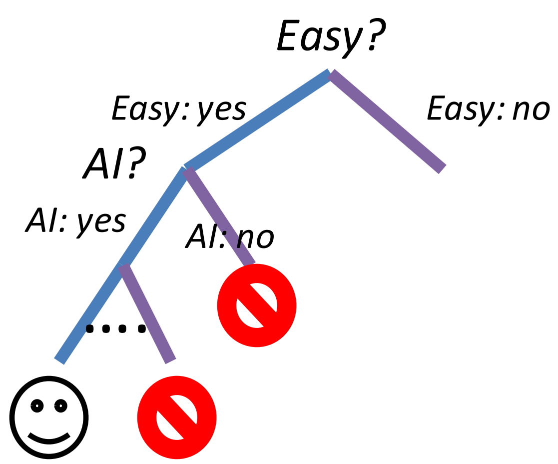

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+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
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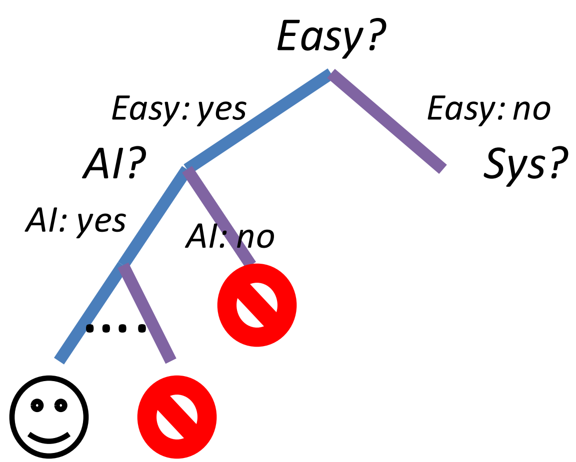

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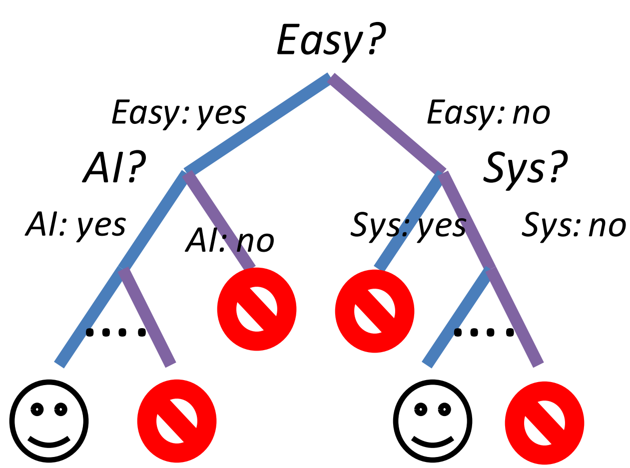

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+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Adapted from Hamed Pirsiavash

Ensembles

Key Idea: “Wisdom of the crowd“

groups of people can often make better decisions than individuals

Apply this to ML

Learn multiple classifiers and combine their predictions

Combining Multiple Classifiers by Voting

Train several classifiers and take majority of predictions

For regression use mean or median of the predictions

For ranking and collective classification use some form of averaging

A common family of approaches is called **bagging**

Bagging: Split the Data

Q: What can go wrong with option 1?

Option 1: Split the data into K pieces and train a classifier on each

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A: Small sample → poor performance

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Option 2: Bootstrap aggregation (bagging) resampling

Bagging: Split the Data

Q: What can go wrong with option 1?

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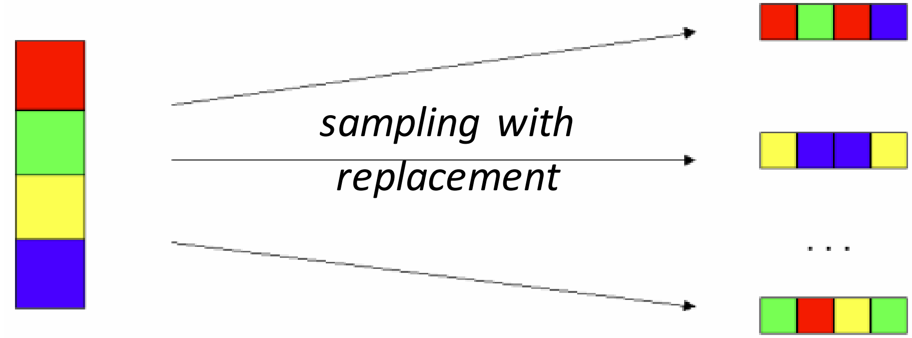
Option 1: Split the data into K pieces and train a classifier on each

Option 2: Bootstrap aggregation (bagging) resampling

- Obtain datasets $D_1, D_2, \ldots, D_N$ using bootstrap resampling from D

Given a dataset D…



get new datasets D̂ by random sampling with replacement from D

Courtesy Hamed Pirsiavash

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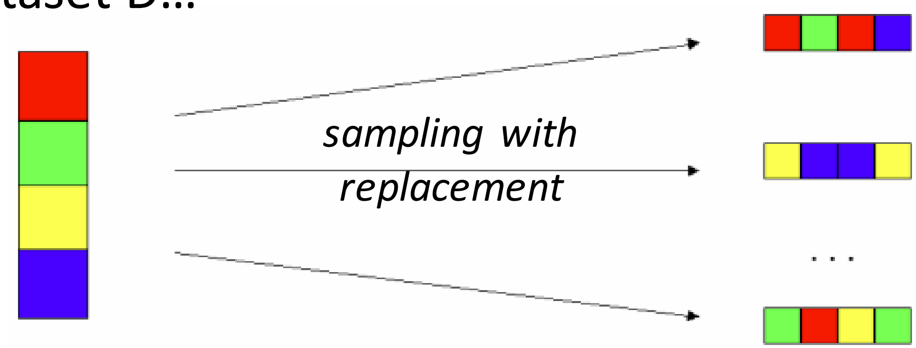


get new datasets $\hat{D}$ by random sampling with replacement from D

Courtesy Hamed Pirsiavash

Bagging Decision Trees

How would it work?

Bagging Decision Trees

How would it work?

Bootstrap sample S samples $\{(X_1, Y_1), \ldots, (X_S, Y_S)\}$

Train a tree t_s on (X_s, Y_s)

At test time: $\hat{y} = \text{avg}(t_1(x), \ldots t_S(x))$

Random Forests

Bagging trees with one modification

At each split point, choose a random subset of features of size **k** and pick the best among these

Train decision trees of depth **d**

Average results from multiple randomly trained trees

Q: What's the difference between bagging decision trees and random forests?

Random Forests

Bagging trees with one modification

At each split point, choose a random subset of features of size **k** and pick the best among these

Train decision trees of depth **d**

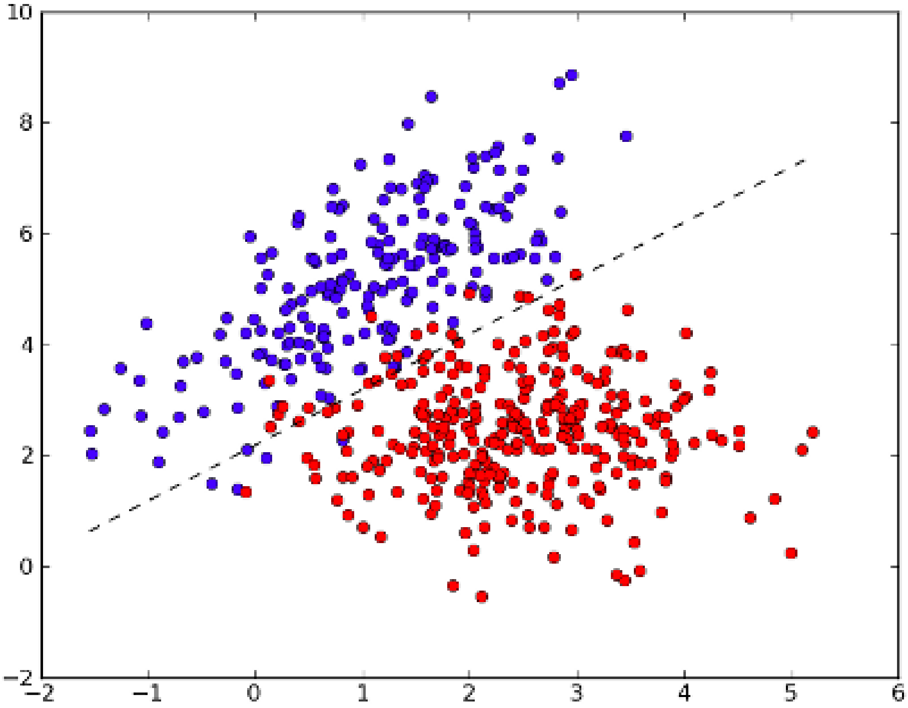
Average results from multiple randomly trained trees

Q: What's the difference between bagging decision trees and random forests?

A: Bagging → highly correlated trees (reuse good features)

LINEAR MODELS

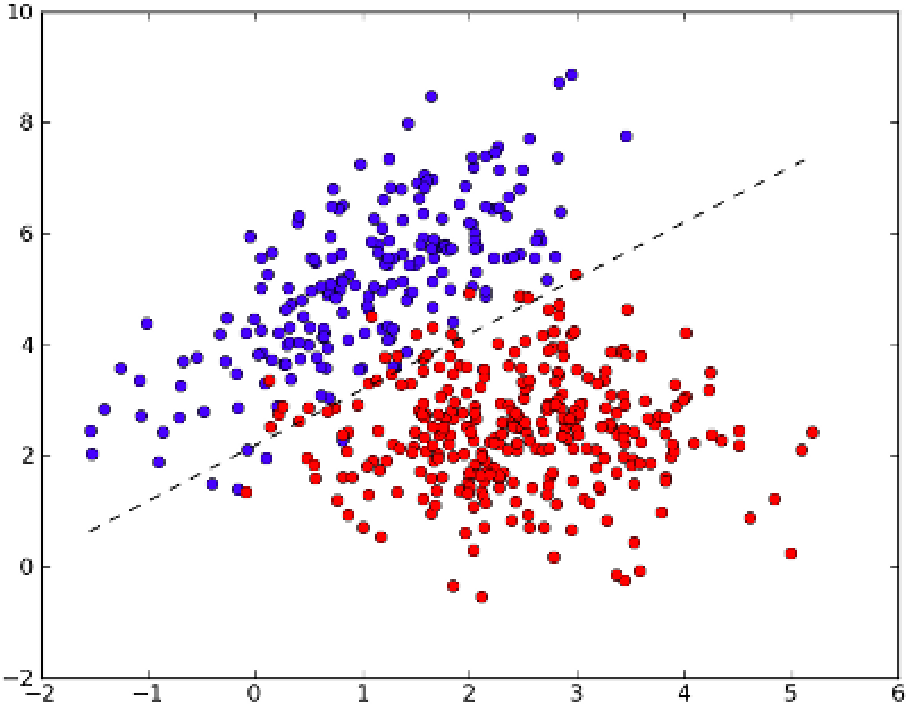
Linear Models



- Can be used for either regression or classification
- A number of instances for classification. Common ones are:
  - Perceptron
  - Linear SVM
  - Logistic regression
    - (yes, even though "regression" is in the name ☺)

Image courtesy Hamed Pirsiavash

Linear Models: Core Idea



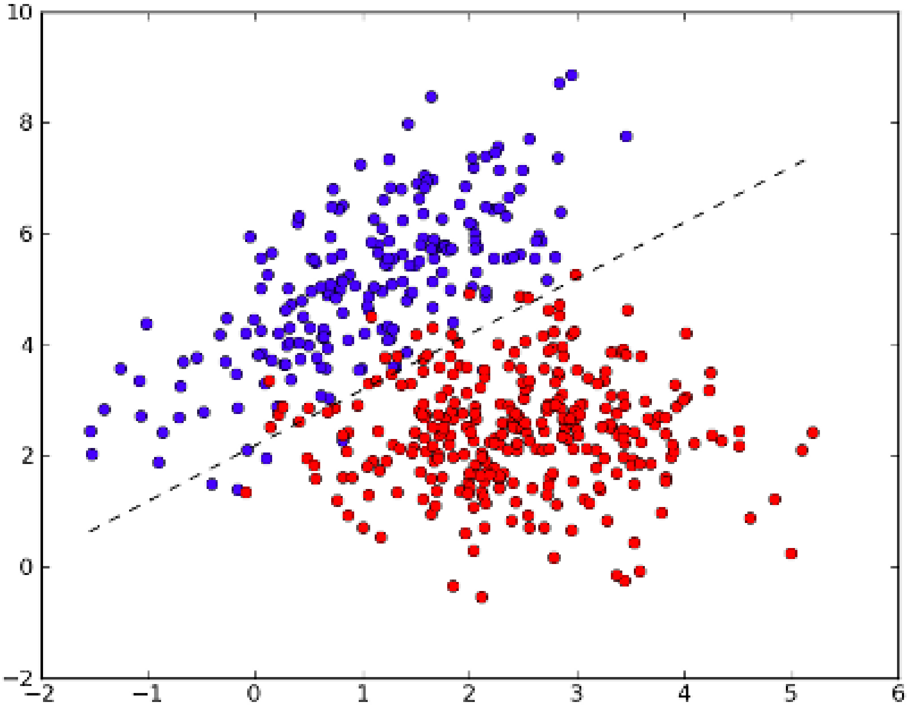
Model the relationship between the input data X and corresponding labels Y via a linear relationship (non-zero intercepts b are okay)

$$Y = W^T X + b$$

Items to learn: W, b

Image courtesy Hamed Pirsiavash

Linear Models: Core Idea



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For regression: the output of this equation *is* the predicted value

Image courtesy Hamed Pirsiavash

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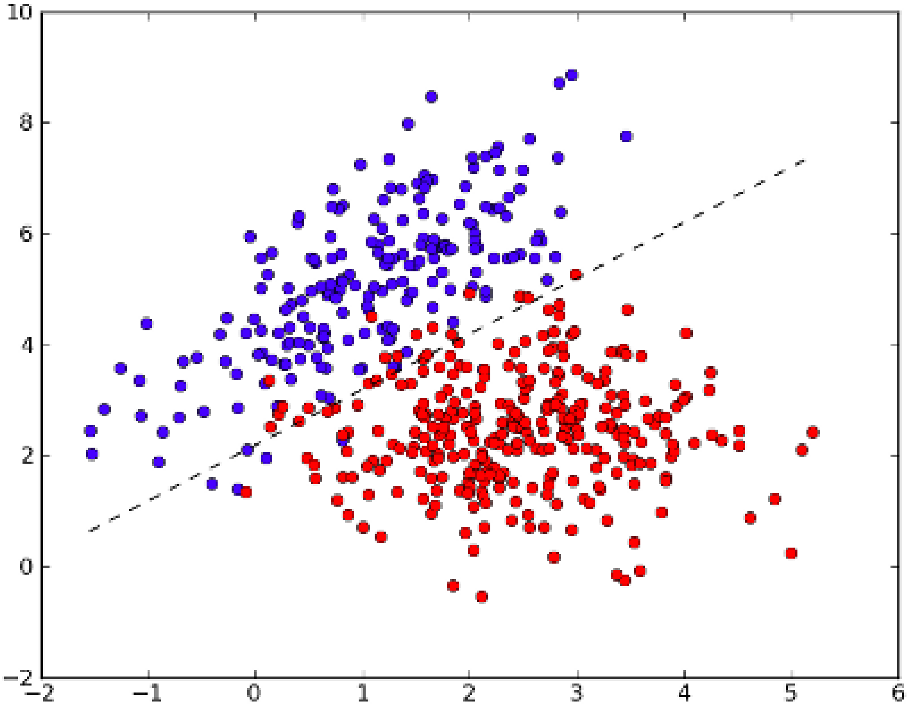

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$$Y = W^T X + b$$

Items to learn: W, b

For regression: the output of this equation *is* the predicted value

For classification: one class is on one side of this line, the other class is on the other

Image courtesy Hamed Pirsiavash

Linear Models in sklearn

1.1. Linear Models
1.1.1. Ordinary Least Squares
1.1.2. Ridge regression and classification
1.1.3. Lasso
1.1.4. Multi-task Lasso
1.1.5. Elastic-Net
1.1.6. Multi-task Elastic-Net
1.1.7. Least Angle Regression
1.1.8. LARS Lasso
1.1.9. Orthogonal Matching Pursuit (OMP)
1.1.10. Bayesian Regression
1.1.11. Logistic regression
1.1.12. Generalized Linear Regression
1.1.13. Stochastic Gradient Descent - SGD
1.1.14. Perceptron
1.1.15. Passive Aggressive Algorithms
1.1.16. Robustness regression: outliers and modeling errors
1.1.17. Polynomial regression: extending linear models with basis functions

These all have easy-to-use interfaces, with the same core interface:

- Training: model.fit(X=training_features, y=training_labels)

- Prediction: model.predict(X=eval_features)

https://scikit-learn.org/stable/modules/linear_model.html

Linear Models in sklearn

1.1. Linear Models

1.1.1. Ordinary Least Squares
1.1.2. Ridge regression and classification
1.1.3. Lasso
1.1.4. Multi-task Lasso
1.1.5. Elastic-Net
1.1.6. Multi-task Elastic-Net
1.1.7. Least Angle Regression
1.1.8. LARS Lasso
1.1.9. Orthogonal Matching Pursuit (OMP)
1.1.10. Bayesian Regression
1.1.11. Logistic regression
1.1.12. Generalized Linear Regression
1.1.13. Stochastic Gradient Descent - SGD
1.1.14. Perceptron
1.1.15. Passive Aggressive Algorithms
1.1.16. Robustness regression: outliers and modeling errors
1.1.17. Polynomial regression: extending linear models with basis functions

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Linear Models in pytorch

Docs > torch.nn > Linear

LINEAR

CLASS `torch.nn.Linear(in_features, out_features, bias=True)`

Applies a linear transformation to the incoming data: $y = xA^T + b$

This module supports TensorFloat32.

Variables

- **~Linear.weight** – the learnable weights of the module of shape $(\text{out\_features}, \text{in\_features})$. The values are initialized from $\mathcal{U}(-\sqrt{k}, \sqrt{k})$, where $k = \frac{1}{\text{in\_features}}$
- **~Linear.bias** – the learnable bias of the module of shape (out_features). If `bias` is `True`, the values are initialized from $\mathcal{U}(-\sqrt{k}, \sqrt{k})$ where $k = \frac{1}{\text{in\_features}}$

Examples:

```
>>> m = nn.Linear(20, 30)
>>> input = torch.randn(128, 20)
>>> output = m(input)
>>> print(output.size())
torch.Size([128, 30])
```

These are “building blocks” not full models.

Take CMSC 478 (or 678), or independent study to learn about this in more detail!

https://pytorch.org/docs/stable/generated/torch.nn.Linear.html

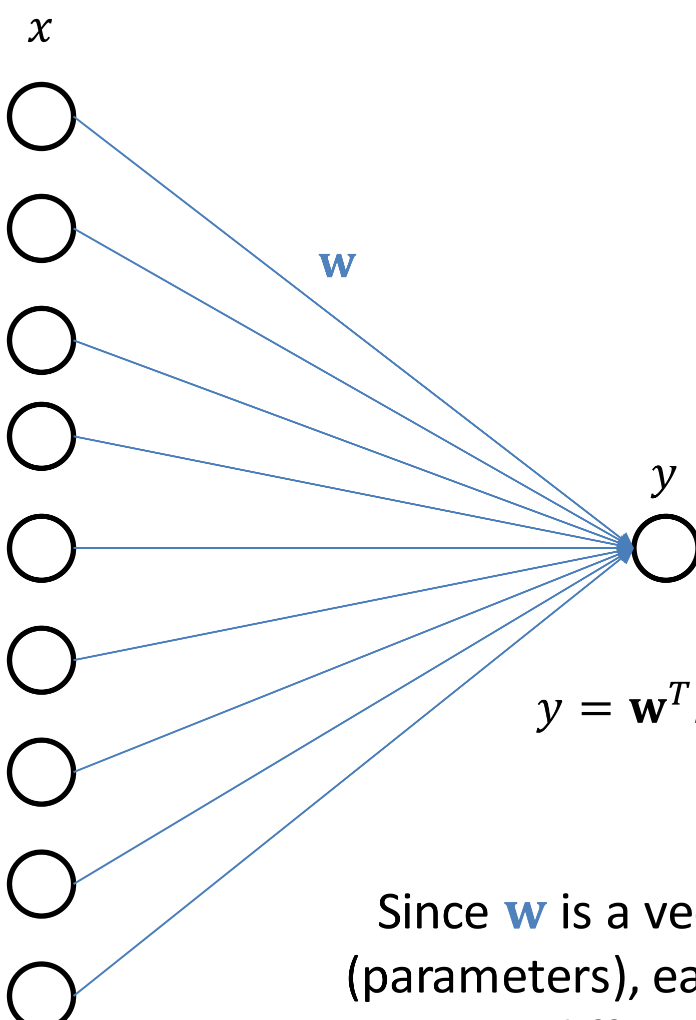
A Simple Linear Model

$$\text{predict } y_i \text{ from } \mathbf{x_i}$$

value y_i

data point x_i, as a vector of features

A Graphical View of Linear Models



$$y = \mathbf{w}^T x + b$$

Since $\mathbf{w}$ is a vector of weights (parameters), each arc from x to y is a different parameter

A Simple Linear Model for Regression

vector w of weights

$$y_i = \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}}$$

value y_i

data point x_i, as a vector of features

A Simple Linear Model for Regression

vector w of weights

bias b (WLOG, 0)

$$y_i = \mathbf{w}^{\mathbf{T}}\mathbf{x_i} + b$$

value y_i

data point x_i, as a vector of features

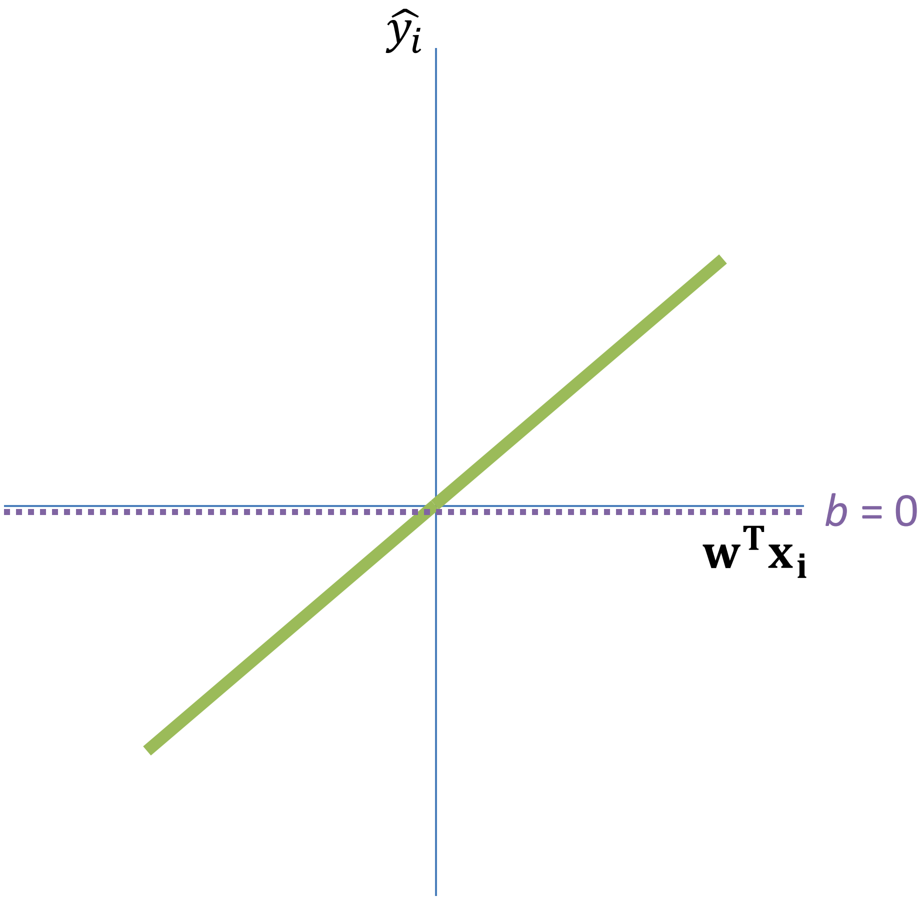
A Simple Linear Model for Regression

vector w of weights

$$y_i = \mathbf{w}^\mathbf{T}\mathbf{x}_\mathbf{i} + 0$$

value y_i

data point x_i, as a vector of features



A Simple Linear Model for Classification

vector w of weights

bias b (WLOG, 0)

$$y_i = \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}} + b$$

label y_i, (WLOG, binary {0, 1} value)

data point x_i, as a vector of features

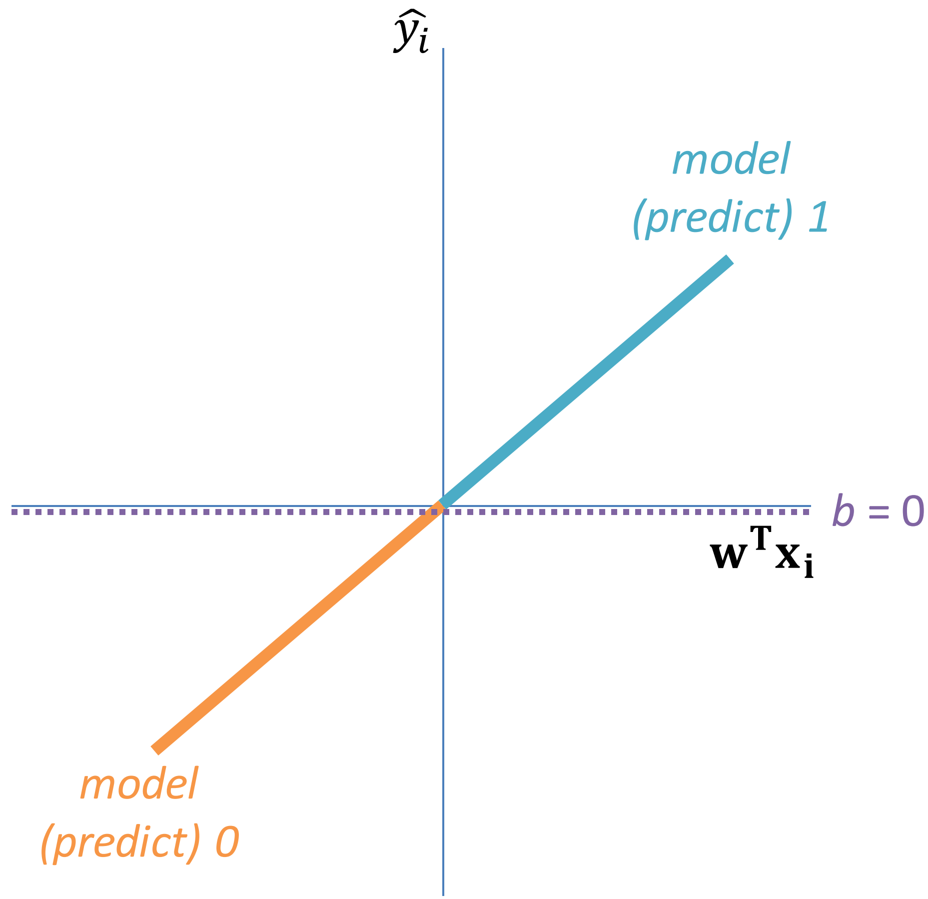
A Simple Linear Model for Classification

vector w of weights

$$y_i = \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}}$$

label y_i, (WLOG, binary {0, 1} value)

data point x_i, as a vector of features



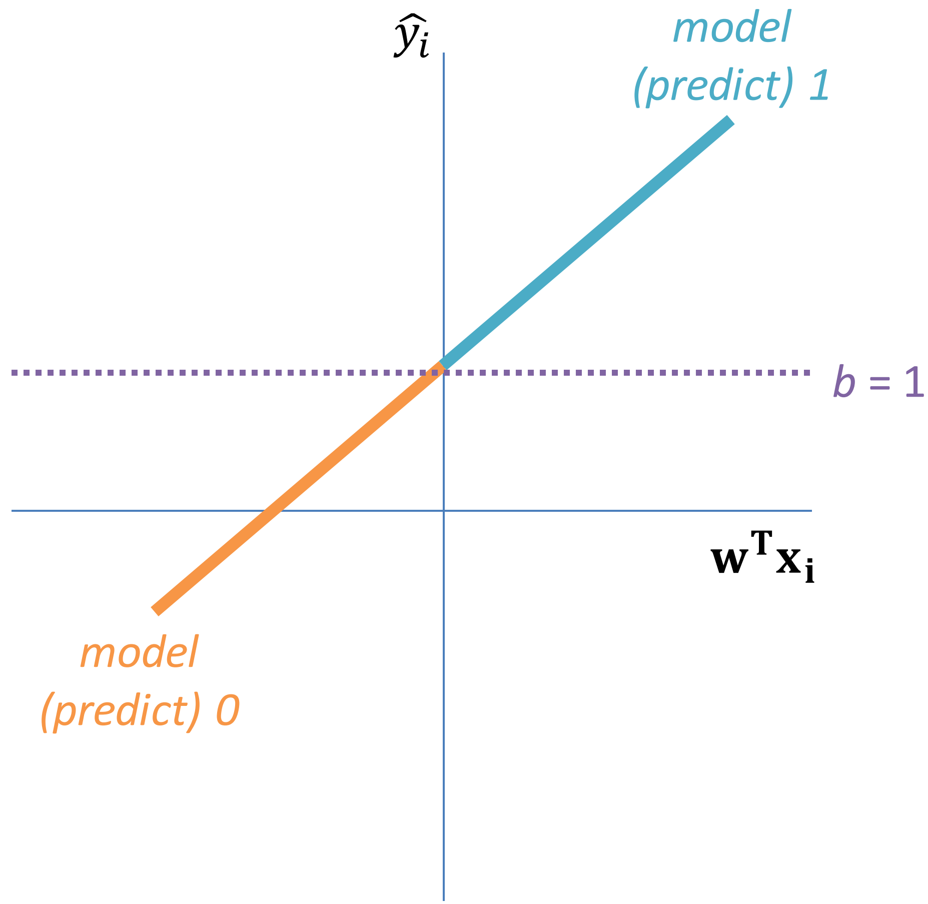
A Simple Linear Model for Classification

vector w of weights

$$y_i = \mathbf{w}^{\mathbf{T}}\mathbf{x_i} + 1$$

label y_i, (WLOG, binary {0, 1} value)

data point x_i, as a vector of features



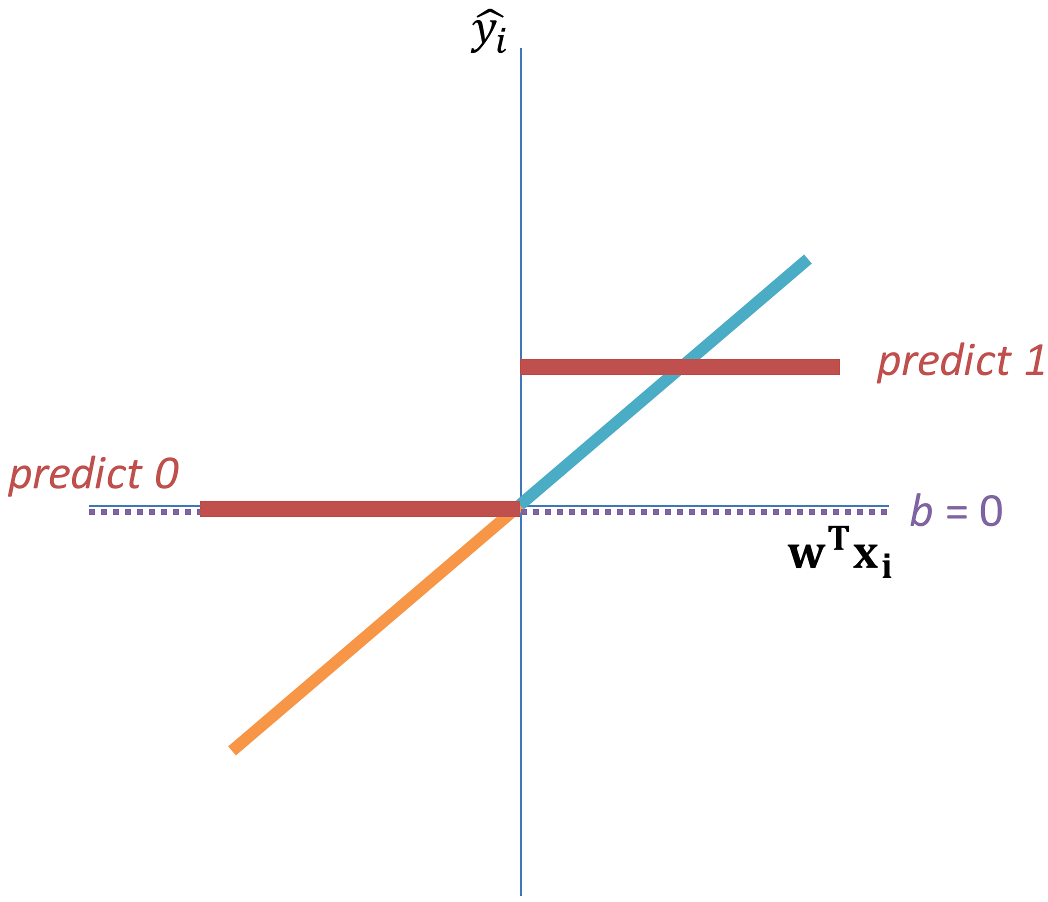
A Simple Linear Model for Classification

vector w of weights

$$y_i = \mathbf{w}^\mathbf{T}\mathbf{x_i}$$

label y_i, (WLOG, binary {0, 1} value)

data point x_i, as a vector of features



A Simple Linear Model for Classification

vector w of weights

$$y_i = \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}}$$

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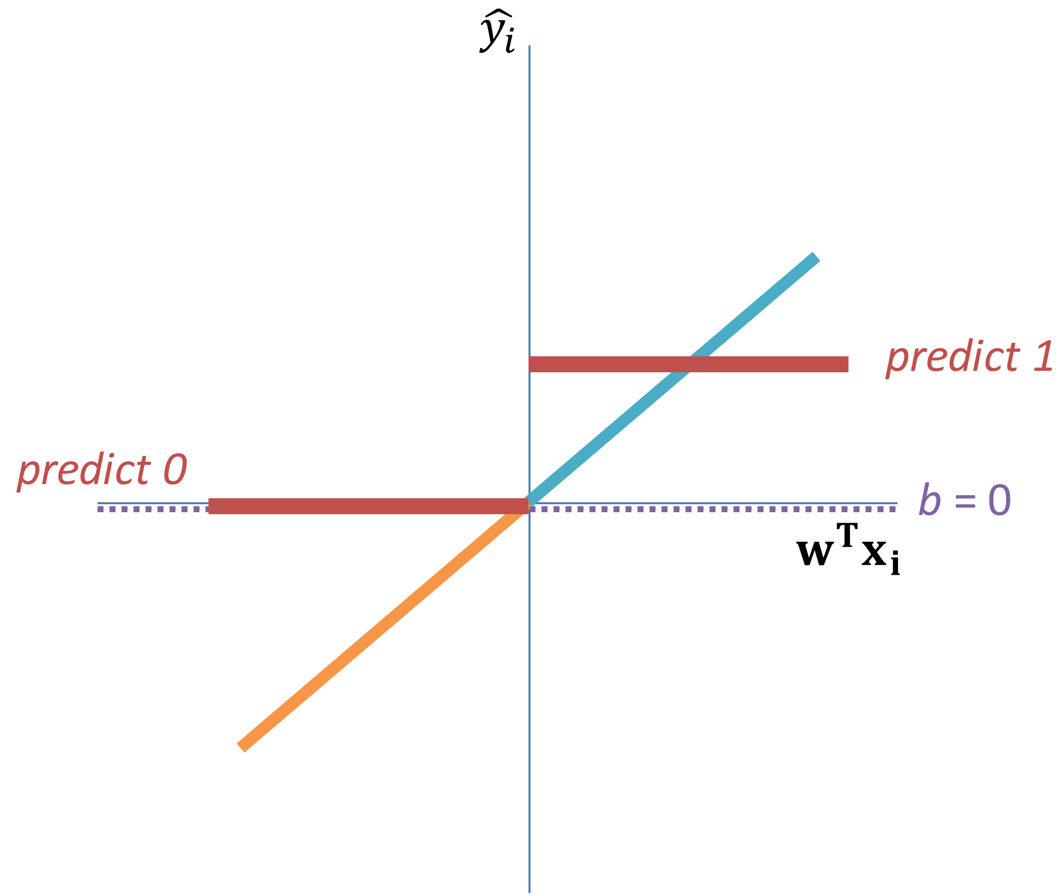


decision rule: $\hat{y}_i = \begin{cases} 0, & \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}} < 0 \\ 1, & \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}} \geq 0 \end{cases}$

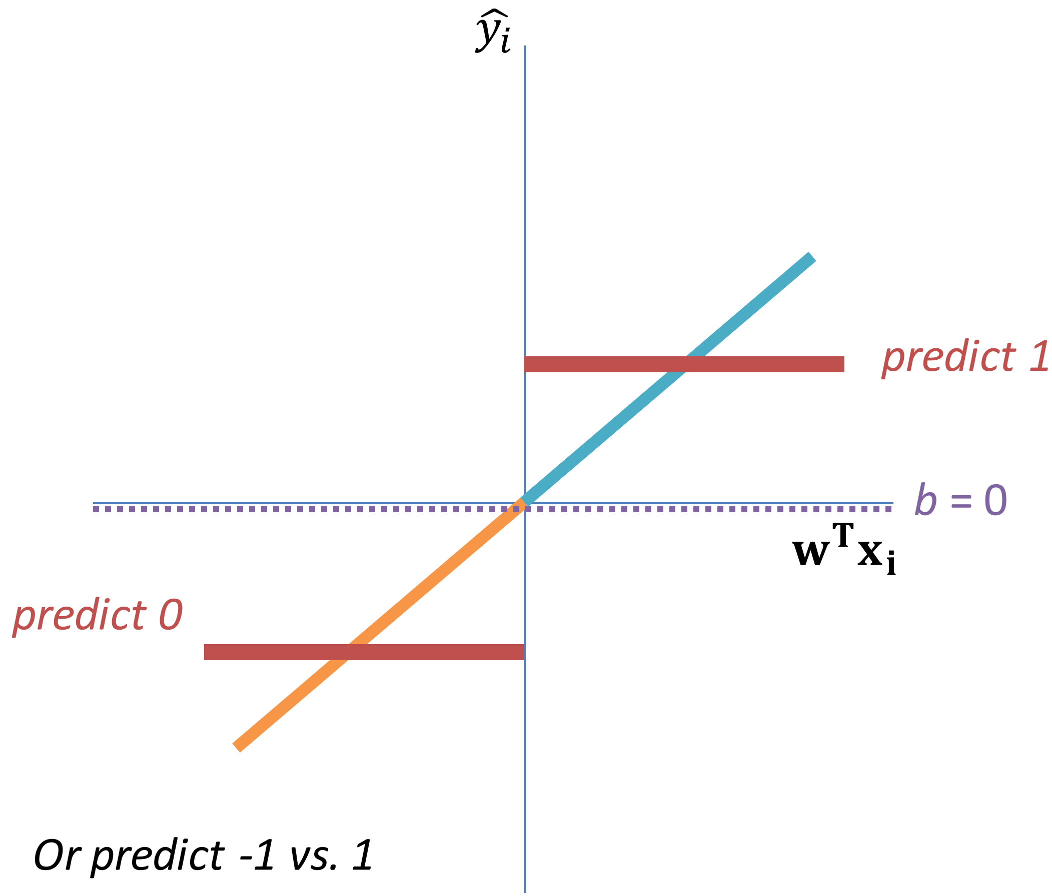
A Simple Linear Model for Classification

vector w of weights

$$y_i = \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}}$$

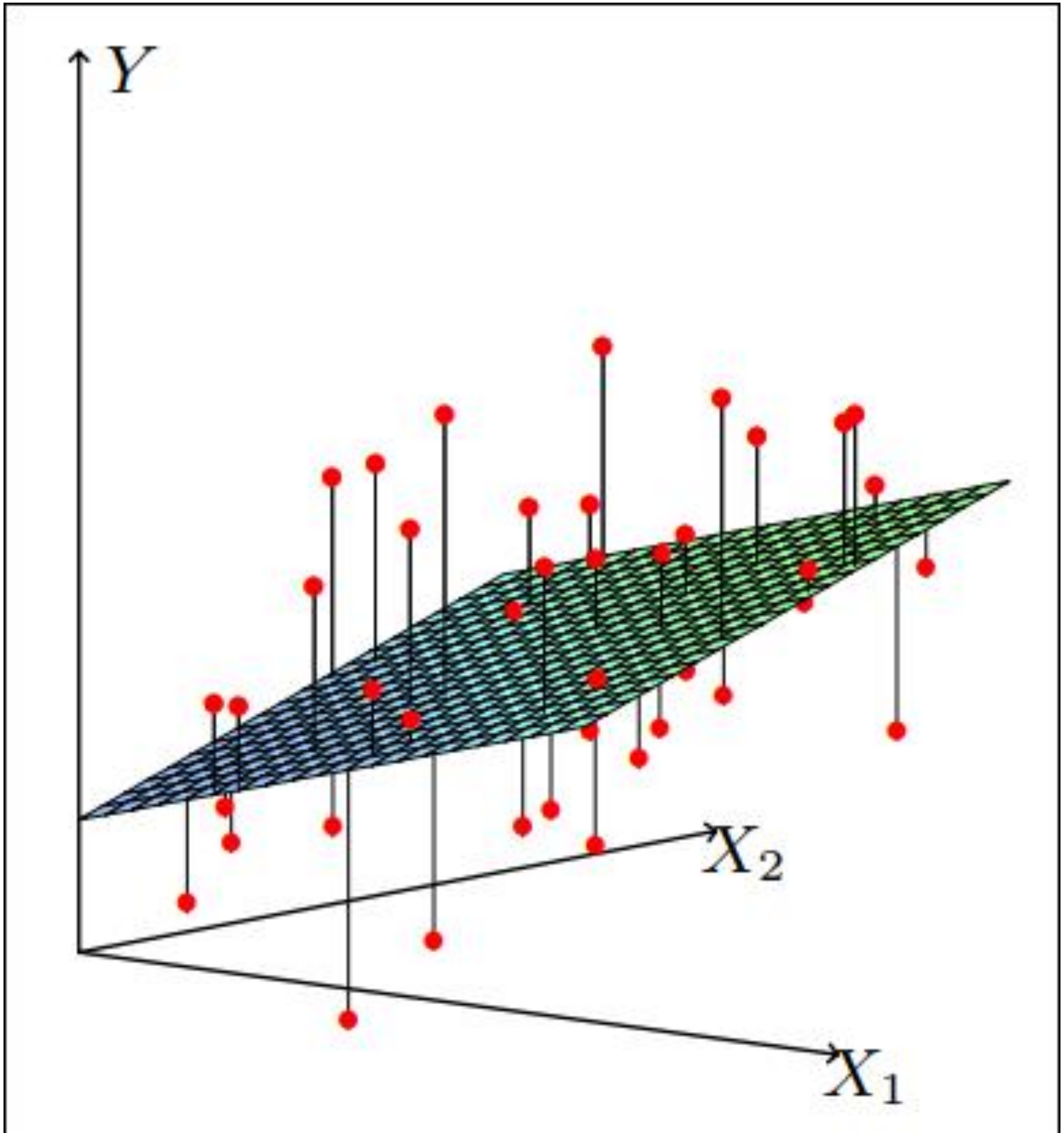
label y_i, (WLOG, binary {0, 1} value)

data point x_i, as a vector of features



Or predict -1 vs. 1

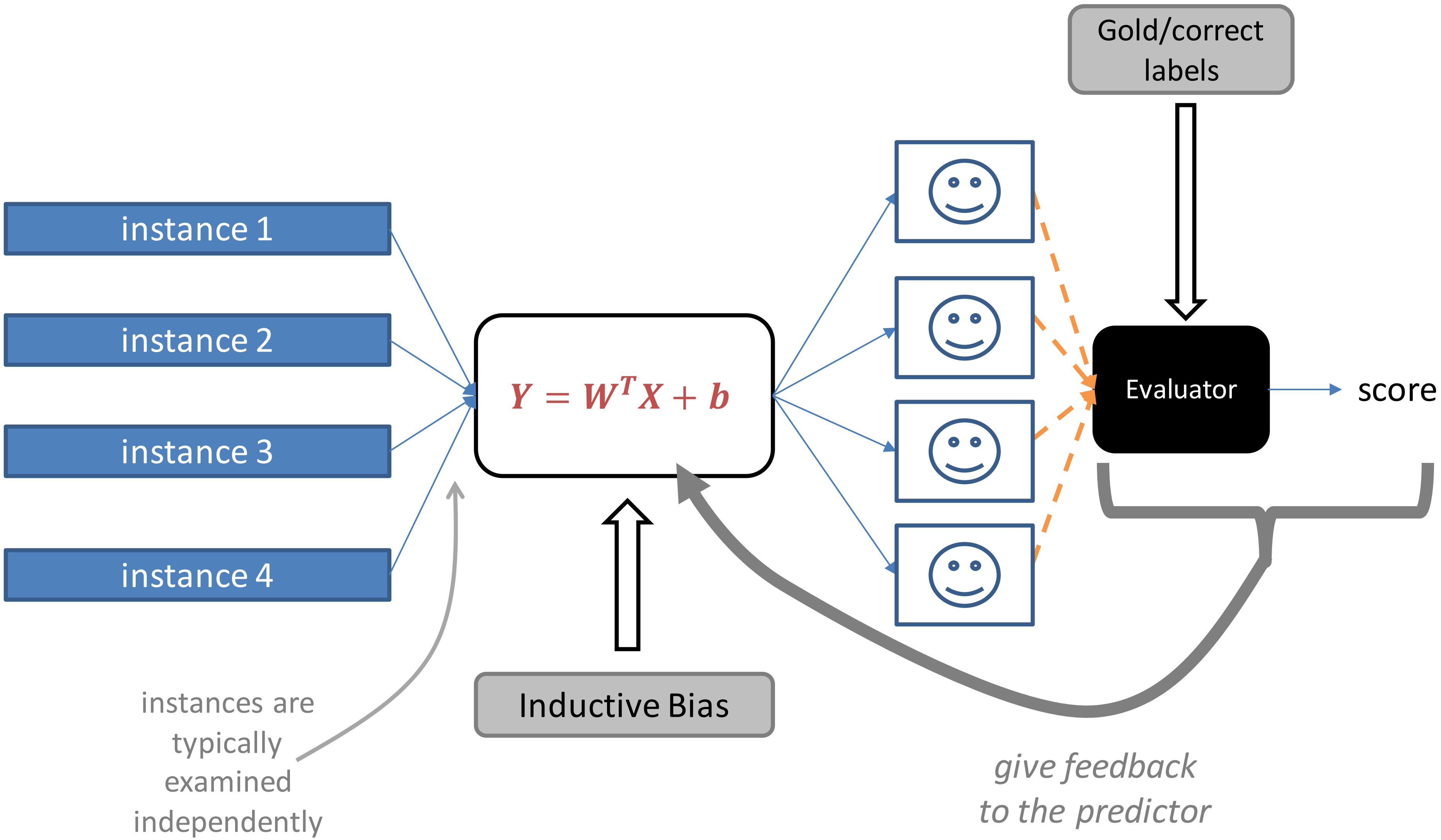
decision rule: $\widehat{y_i} = \begin{cases} -1, & \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}} < 0 \\ 1, & \mathbf{w}^{\mathbf{T}}\mathbf{x}_{\mathbf{i}} \geq 0 \end{cases}$



Linear Models in Multiple Dimensions

ESL, Fig 3.1

Linear Models in the Basic Framework



Central Question: How Well Are

Reminder!

The performance score does not have to be the same thing as the loss function you optimize

Classification

- Precision, Recall, F1
- Accuracy
- Log-loss
- ROC-AUC
- …

Regression

- (Root) Mean Square Error
- Mean Absolute Error
- …

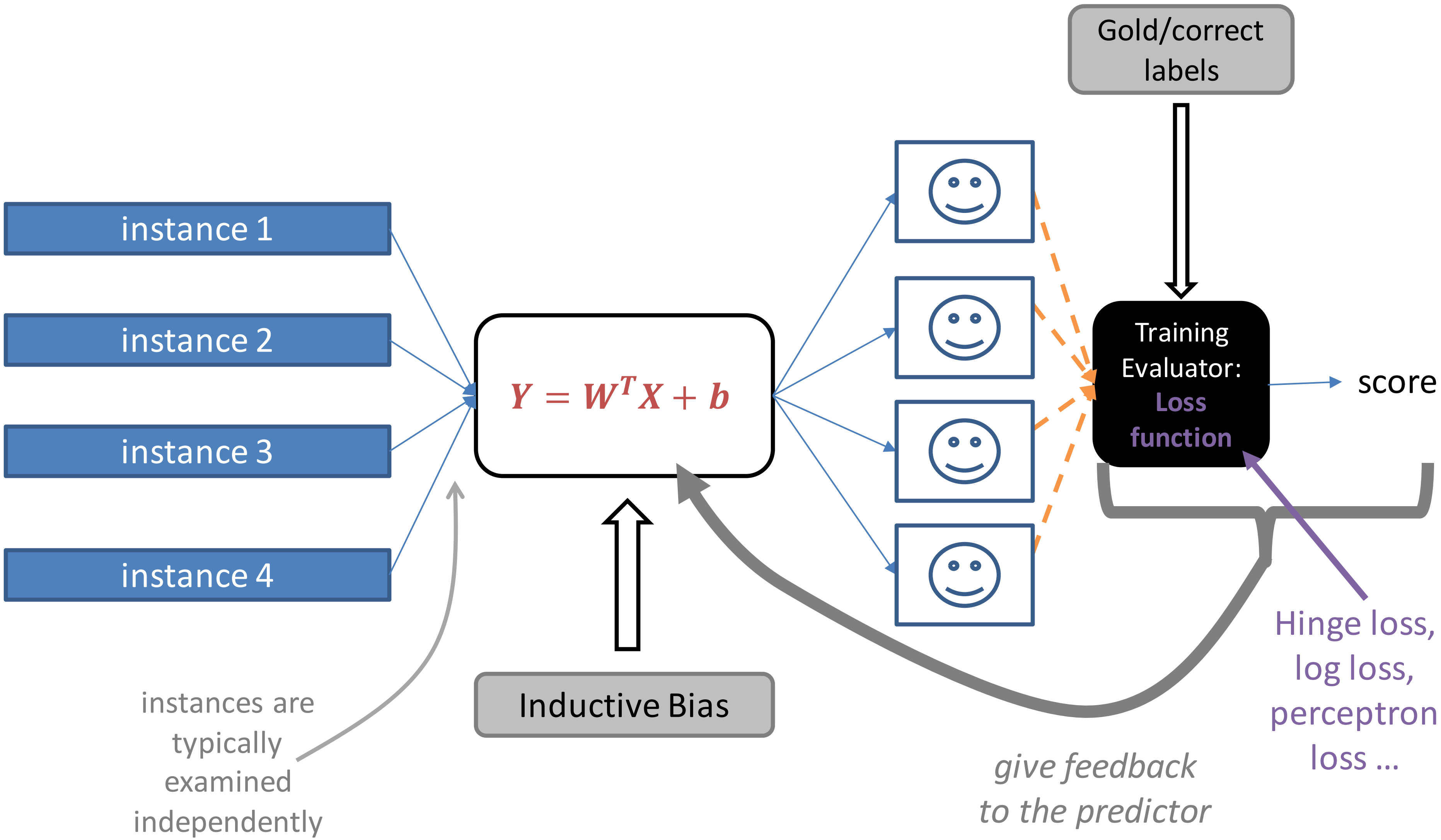
Clustering

- Mutual Information
- V-score
- …

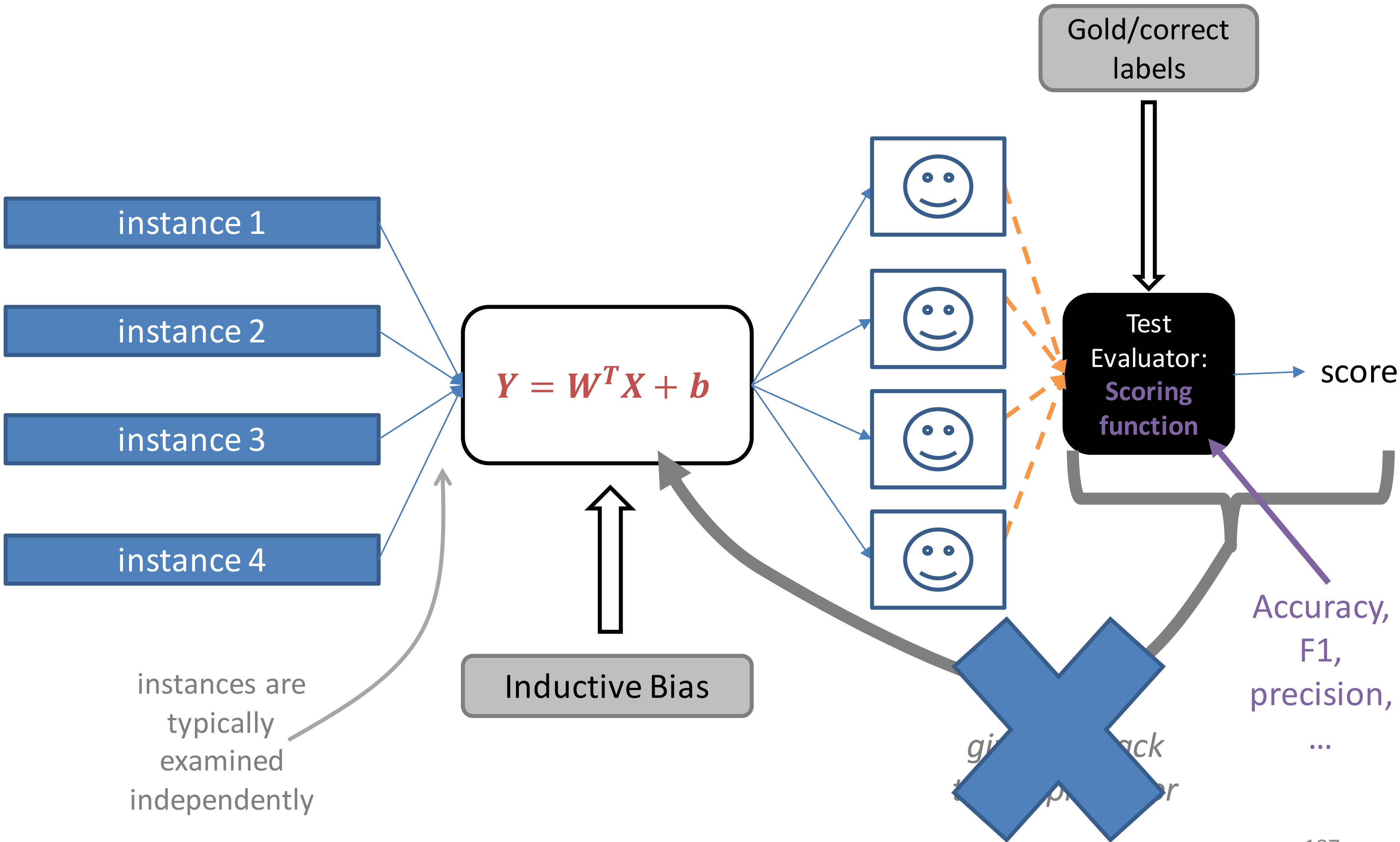
the ***task****: what* kind *of problem are you solving?*

How do we learn these linear classification methods?

Change the loss function. (478/678 topics)



How do we evaluate these linear classification methods? Change the eval function.



What if

- We want a unified way to predict more than two classes?

- We want a probabilistic (bounded, interpretable) score?

- We want to use *transformations* of our data x to help make decisions?

What if

- We want a unified way to predict more than two classes?
- We want a probabilistic (bounded, interpretable) score?
- We want to use *transformations* of our data x to help make decisions?

Terminology

common ML term	Log-Linear Models
as statistical regression	(Multinomial) logistic regression
	Softmax regression
based in information theory	Maximum Entropy models (MaxEnt)
a form of	Generalized Linear Models
viewed as	Discriminative Naïve Bayes
to be cool today :)	Very shallow (sigmoidal) neural nets

Turning Scores into Probabilities

score(s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships. h: The Bulls basketball team is based in Chicago. , ENTAILED) > score(s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships. h: The Bulls basketball team is based in Chicago. , NOT ENTAILED)

p(ENTAILED | s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships. h: The Bulls basketball team is based in Chicago.) > p(NOT ENTAILED | s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships. h: The Bulls basketball team is based in Chicago.)

KEY IDEA

Core Aspects to Maxent Classifier p(y|x)

- **features** $f(x, y)$ between x and y that are meaningful;
- **weights** θ (one per feature) to say how important each feature is; and
- a way to **form probabilities** from f and θ

$$p(y \mid x) = \frac{\exp(\theta^T f(x, y))}{\sum_{y'} \exp(\theta^T f(x, y'))}$$

Discriminative Document Classification

s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.

h: The Bulls basketball team is based in Chicago.

ENTAILED

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These extractions are all **features** that have **fired** (likely have some significance)

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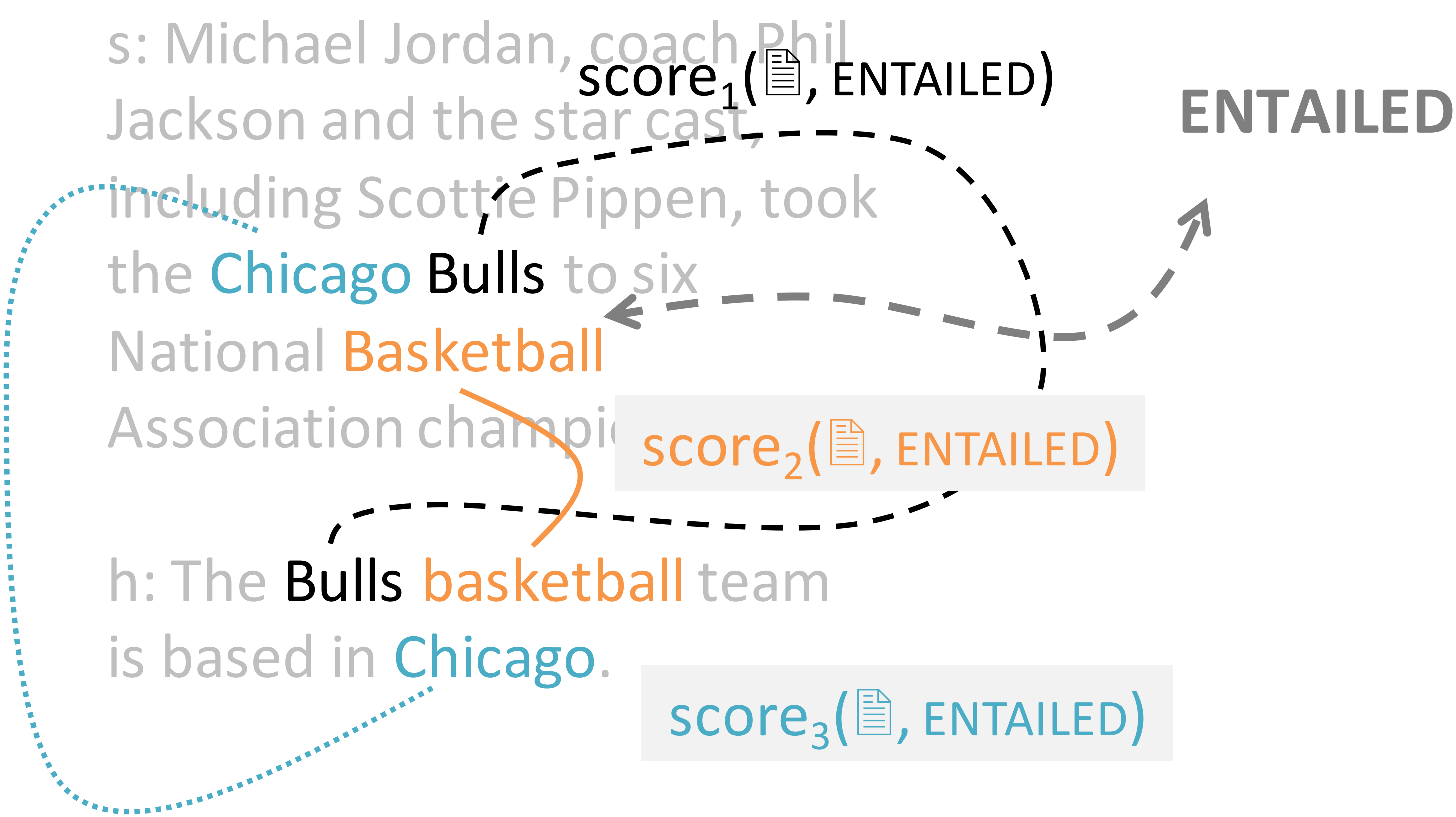
These extractions are all **features** that have **fired** (likely have some significance)

We need to *score* the different extracted clues.



Score and Combine Our Clues

score$_1$(🗎, ENTAILED)

score$_2$(🗎, ENTAILED)

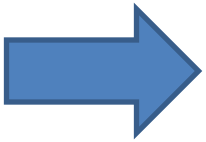
score$_3$(🗎, ENTAILED)

…

score$_k$(🗎, ENTAILED)

…

COMBINE



posterior probability of ENTAILED

Scoring Our Clues

score(

s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.

, ENTAILED) =

(ignore the feature indexing for now)

score_1(, ENTAILED) +

score_2(, ENTAILED) +

score_3(, ENTAILED) +

…

A linear scoring model!

Scoring Our Clues

score(s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago. , ENTAILED) =

score$_1$(, ENTAILED) +

score$_2$(, ENTAILED) +

score$_3$(, ENTAILED) +

...

A linear scoring model!

Learn these scores… but how?

What do we optimize?

Turning Scores into Probabilities (More Generally)

$$\text{score}(x, y_1) > \text{score}(x, y_2)$$

$$\Rightarrow$$

$$p(y_1 | x) > p(y_2 | x)$$

KEY IDEA

Maxent Modeling

$$p\left(\textsc{Entailed} \;\middle|\; \boxed{\begin{array}{l}\text{s: Michael Jordan, coach Phil}\\ \text{Jackson and the star cast,}\\ \text{including Scottie Pippen, took}\\ \text{the Chicago Bulls to six}\\ \text{National Basketball Association}\\ \text{championships.}\\ \text{h: The Bulls basketball team is}\\ \text{based in Chicago.}\end{array}}\right) \propto$$

$$\exp\left(\underbrace{\text{score}\left(\boxed{\begin{array}{l}\text{s: Michael Jordan, coach Phil}\\ \text{Jackson and the star cast, including}\\ \text{Scottie Pippen, took the Chicago}\\ \text{Bulls to six National Basketball}\\ \text{Association championships.}\\ \text{h: The Bulls basketball team is based}\\ \text{in Chicago.}\end{array}}, \textsc{Entailed}\right)}_{\text{A linear scoring model!}}\right)$$

Maxent Modeling

p(ENTAILED |

s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.

) $\propto$

exp(

score$_1$(, ENTAILED) +

score$_2$(, ENTAILED) +

score$_3$(, ENTAILED) +

...

))

Maxent Modeling

p(ENTAILED |

s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.

) ∝

exp(

score_1(, ENTAILED) +

score_2(, ENTAILED) +

score_3(, ENTAILED) +

…

))

Learn the scores (but we'll declare what combinations should be looked at)

Maxent Modeling

$$p(\text{ENTAILED} \mid$$

s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.

$$) \propto$$

$$\exp(\text{weight}_1 * \text{applies}_1(🗎, \text{ENTAILED}) + \text{weight}_2 * \text{applies}_2(🗎, \text{ENTAILED}) + \text{weight}_3 * \text{applies}_3(🗎, \text{ENTAILED}) +))$$

Maxent Modeling

p(ENTAILED | s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.) $\propto$

exp($\text{weight}_1 * \text{applies}_1$(, ENTAILED) +
$\text{weight}_2 * \text{applies}_2$(, ENTAILED) +
$\text{weight}_3 * \text{applies}_3$(, ENTAILED) +
…))

K different weights…

for K different features

Maxent Modeling

p(ENTAILED | s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.) ∝

exp(
weight$_1$ * applies$_1$(🗎, ENTAILED) +
weight$_2$ * applies$_2$(🗎, ENTAILED) +
weight$_3$ * applies$_3$(🗎, ENTAILED) +
…
))

K different weights…

for K different features…

multiplied and then summed

Maxent Modeling

p(ENTAILED | s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.) $\propto$

exp(Dot_product of weight_vec feature_vec(🗎, ENTAILED))

K different weights…

for K different features…

multiplied and then summed

Maxent Modeling

p(ENTAILED |

s: Michael Jordan, coach Phil Jackson and the star cast, including Scottie Pippen, took the Chicago Bulls to six National Basketball Association championships.
h: The Bulls basketball team is based in Chicago.

) ∝

$$\exp\left(\theta^T f\left(\right. \right.$$

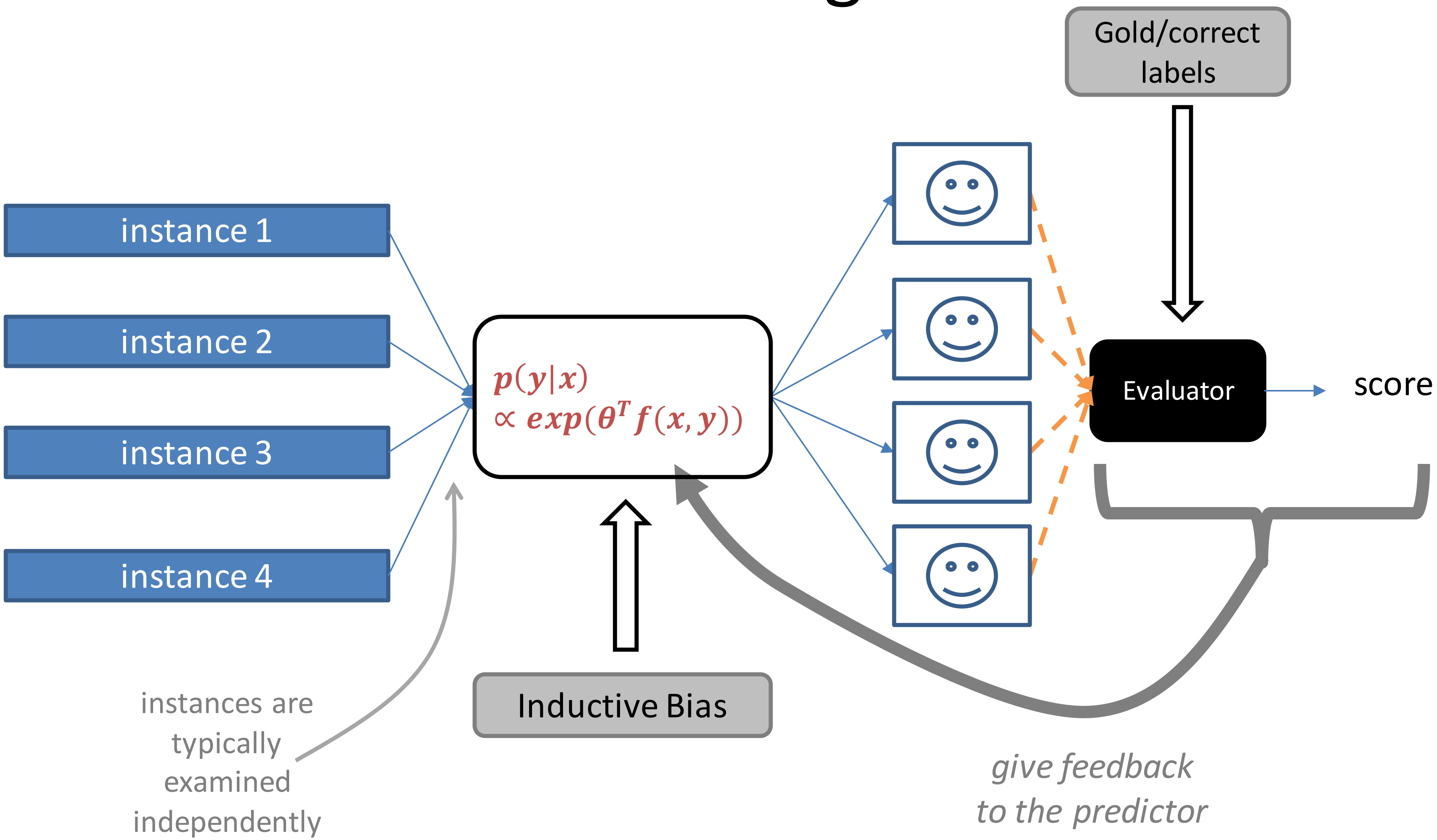
$$\left. \left. , \text{ENTAILED} \right) \right)$$

K different weights…

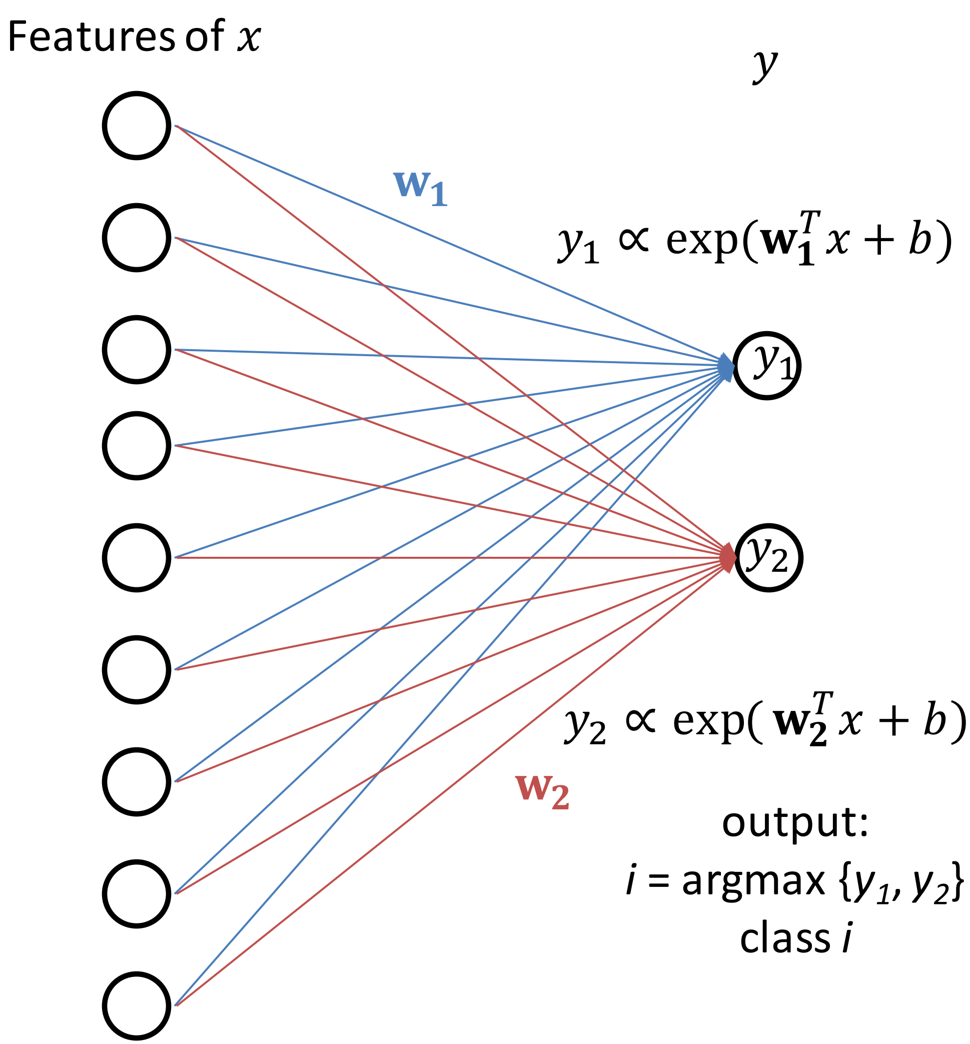
for K different features…

multiplied and then summed

Machine Learning Framework: Learning

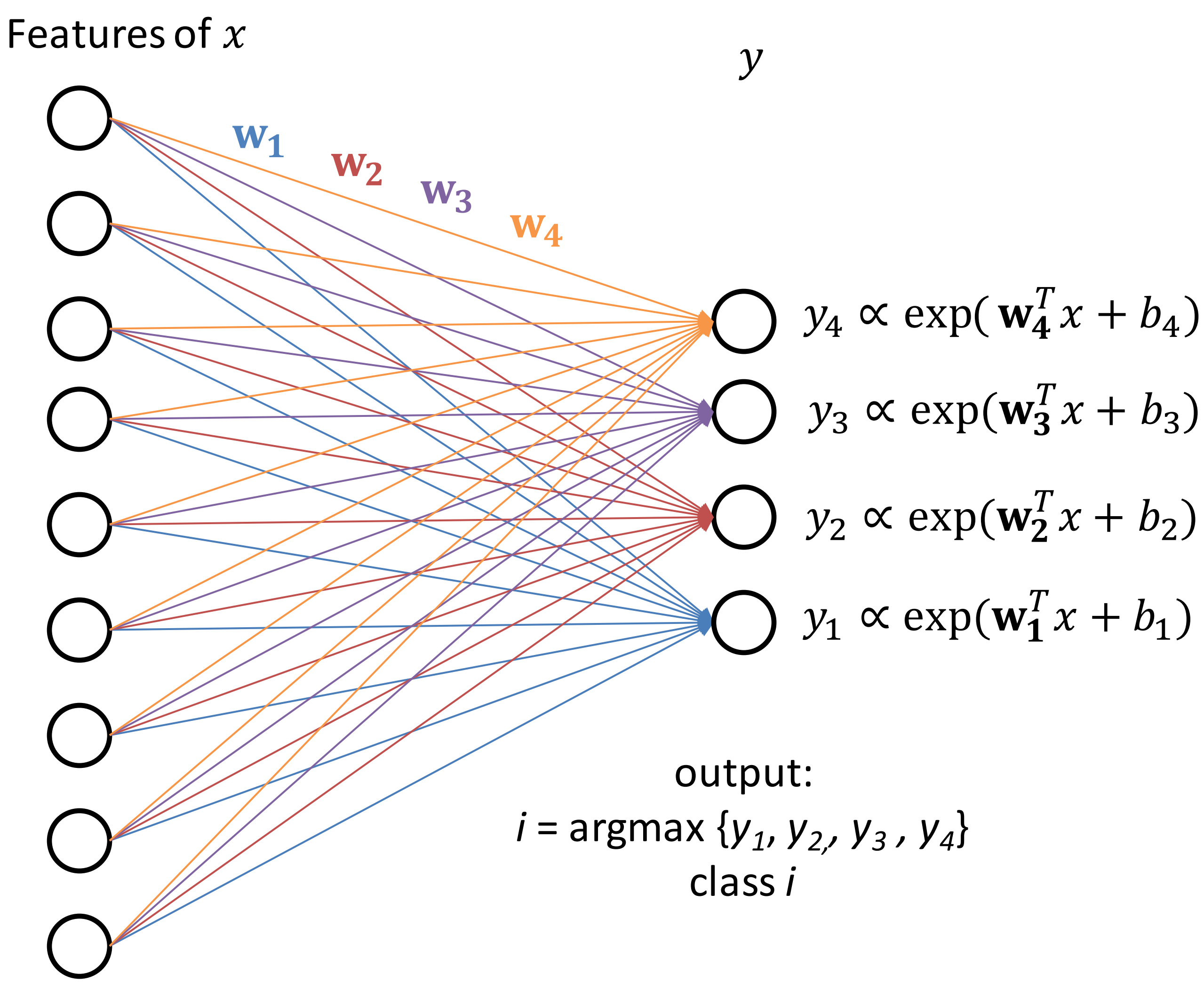


A Graphical View of Logistic Regression/Classification (2 classes)



output:
i = argmax $\{y_1, y_2\}$
class i

A Graphical View of Logistic Regression/Classification (4 classes)



output:
i = argmax $\{y_1, y_2, y_3, y_4\}$
class i

sklearn.linear_model.LogisticRegression ¶

class `sklearn.linear_model.LogisticRegression`(*penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None*) [source]

Logistic Regression (aka logit, MaxEnt) classifier.

In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi_class' option is set to 'ovr', and uses the cross-entropy loss if the 'multi_class' option is set to 'multinomial'. (Currently the 'multinomial' option is supported only by the 'lbfgs', 'sag', 'saga' and 'newton-cg' solvers.)

This class implements regularized logistic regression using the 'liblinear' library, 'newton-cg', 'sag', 'saga' and 'lbfgs' solvers. **Note that regularization is applied by default**. It can handle both dense and sparse input. Use C-ordered arrays or CSR matrices containing 64-bit floats for optimal performance; any other input format will be converted (and copied).

The 'newton-cg', 'sag', and 'lbfgs' solvers support only L2 regularization with primal formulation, or no regularization. The 'liblinear' solver supports both L1 and L2 regularization, with a dual formulation only for the L2 penalty. The Elastic-Net regularization is only supported by the 'saga' solver.

Read more in the User Guide.

Parameters:

penalty : ***{'l1', 'l2', 'elasticnet', 'none'}, default='l2'***

Used to specify the norm used in the penalization. The 'newton-cg', 'sag' and 'lbfgs' solvers support only l2 penalties. 'elasticnet' is only supported by the 'saga' solver. If 'none' (not supported by the liblinear solver), no regularization is applied.

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html