Course Logistics and Introduction

CS771: Introduction to Machine Learning

Course Logistics

- Timing and Venue: Mon/Thur 6:00-7:15pm, L-20
- Course website: https://tinyurl.com/cs771-a24 (slides, readings, etc)
- Online discussion/QA: Piazza (https://tinyurl.com/cs771-a24-piazzasignup)
- Instructor's contact email: piyush@cse.iitk.ac.in, office: RM-502 (CSE dept)
  - Prefix email subject with CS771, else might get ignored
  - Use of Piazza is encouraged for course-related matters (also has private messaging)
  - Office hours: By appointment
- TAs: Team of 20 TAs. Their contact and office hours details shared soon
- Unofficial auditors are welcome. However, can't participate in exams/quizzes
  - Can attempt homeworks, quizzes, exams on their own. Won't be graded

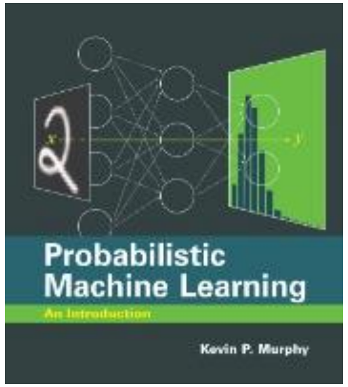
Workload and Grading Policy

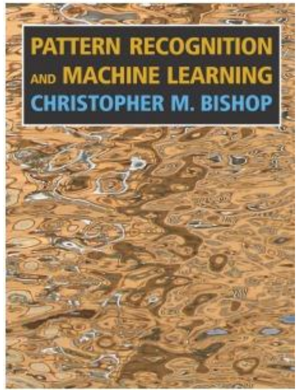
Quizzes will be closed-book. For exams, one A4 size cheat-sheet will be allowed

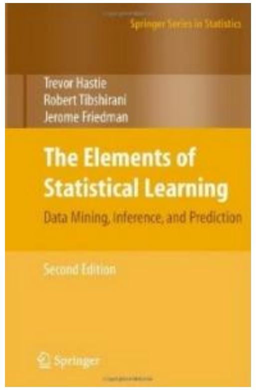
- 4 quizzes: 20%
- 2 homeworks/mini-projects: 30%
  - Writeups must be prepared in PDF using the provided LaTeX template
  - Knowledge of Python programming is assumed
  - To be done in groups of 5 students. Form your groups NOW
- Mid-sem exam: 20%
- End-sem exam: 30%
- Quiz dates (tentative): Aug 13, Sept 3, Oct 1, Oct 22 (duration: 30 mins)
  - Quiz timing and venue: will be announced closed to the quiz date
- HW/mini-project dates (tentative): Aug 19, Oct 3 (roughly 3 work-weeks given)
- Mid-sem and end-sem exam dates: As per DOAA announcements

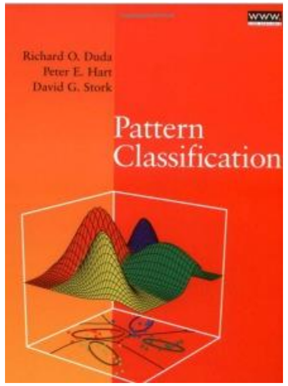
Textbook and References

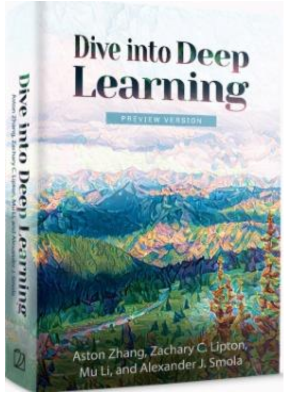
- Many excellent texts but none “required”. Some include:

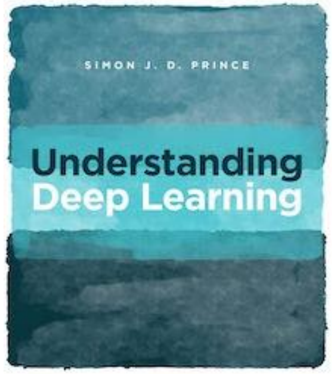












- See the course website for links and other relevant texts and references

- Different books might vary in terms of
  - Set of topics covered
  - Flavor (e.g., classical statistics, deep learning, probabilistic/Bayesian, theory)
  - Terminology and notation (beware of this especially)

- For each topic in the course, we will provide you recommended readings

Course Goals

- Introduction to the foundations of machine learning (ML)
- Focus on developing the ability to
  - Understand the underlying principles (and maths ☺) behind ML models and algos
  - Understand how to implement and evaluate them
  - Understand/develop intuition on choosing the right ML model/algo for your problem
- (Hopefully) inspire you to work on and learn more about ML
- Not an intro to popular software frameworks and libraries, such as scikit-learn, PyTorch, Tensorflow, etc
  - However, you are encouraged to explore these as the course progresses

Expectations from you

- Attend classes regularly (even though we have no attendance policy)

- Please make yourself acquainted with the maths required for the course
  - We will provide some refresher slides and reference material
  - Some of the maths will be introduced as and when it is needed

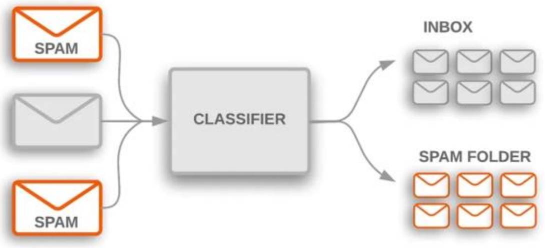
- Please ensure that you understand the maths on the slides
  - We won't do all the derivations on the slides
  - In class, our focus will be on key steps and intuition
  - If not obvious, you should try to work out the detailed steps at home (will be good practice for quizzes and exams) on your own or with classmates
  - If things are unclear, please do reach out to us (e.g., on Piazza or office hours)

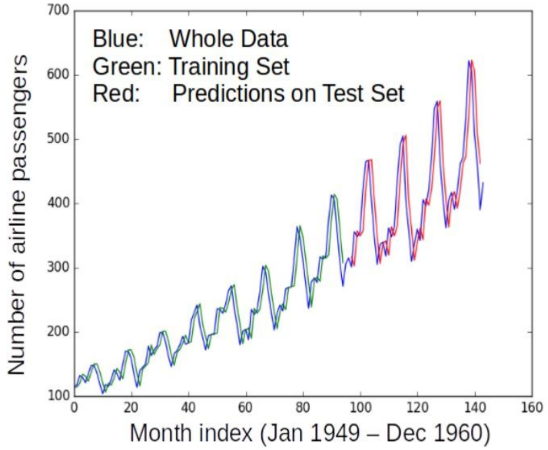
What Is Machine Learning?

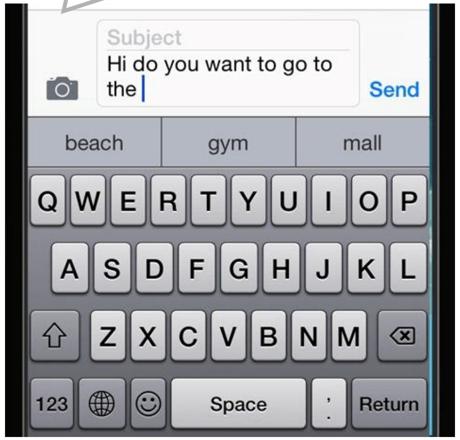
Machine Learning (ML)

- Designing algorithms that ingest data and learn a model of the data
- The learned model can be used to
  - Detect patterns/structures/themes/trends etc. in the data
  - Make predictions about future data and make decisions

Next word prediction (key task in large-language models like ChatGPT)



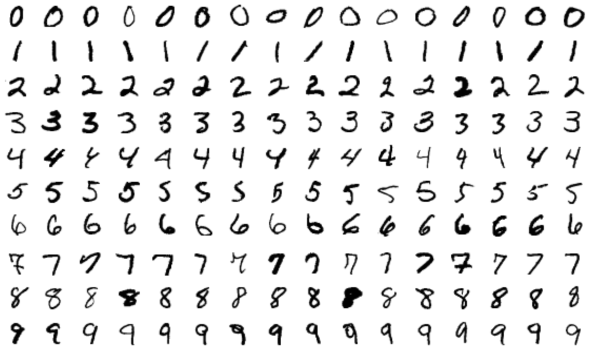




- Modern ML algorithms are heavily "data-driven"
  - No need to pre-define all the rules by humans (infeasible/impossible anyway)
  - The rules are not "static"; can adapt as the ML algo ingests more and more data

Where Should We Use ML?

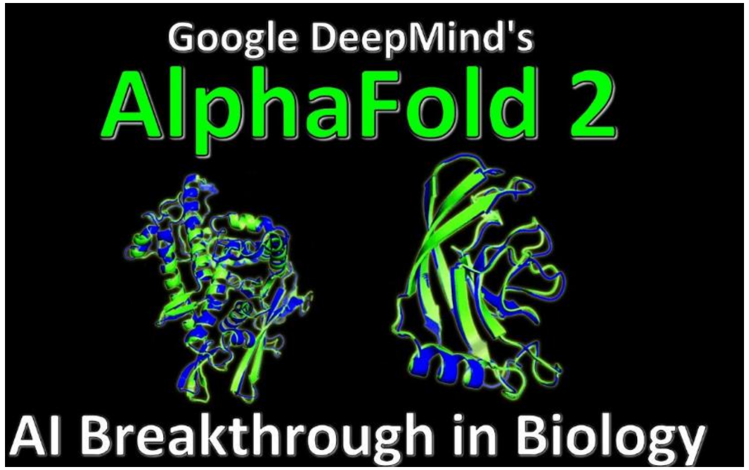
Handwritten digit recognition: Not too complex but still reasonably complex that an ML approach is desirable



- When the learning problem is very complex, e.g.,
  - Enumerating all rules is infeasible or too time-consuming
  - Rules might evolve with time
- In such cases, hard-coding the rules in a computer program may not work
  - Difficult to define and code all possible rules
  - Difficult to update the program if rules evolve
- ML replaces the idea of humans writing code by humans supplying data
  - The ML algorithm automatically learns the model (the rules) from the supplied data
  - The model can evolve with more and more data

ML: Some Success Stories

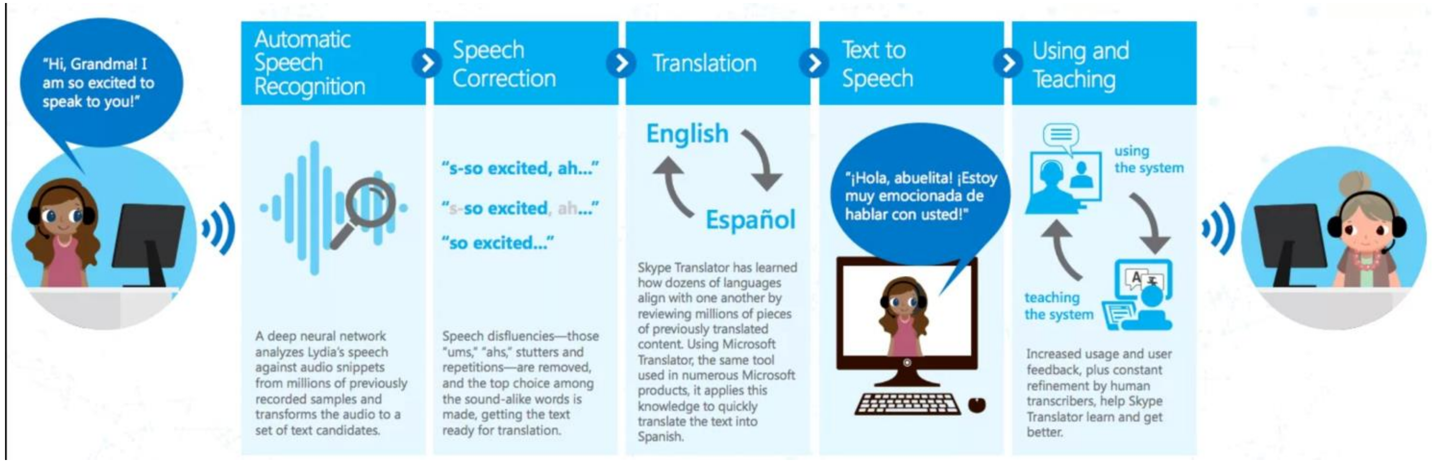
Protein Structure Prediction



Autonomous Driving

AI Generated Digital Art (Dall E 2)

Real-time Speech Translation

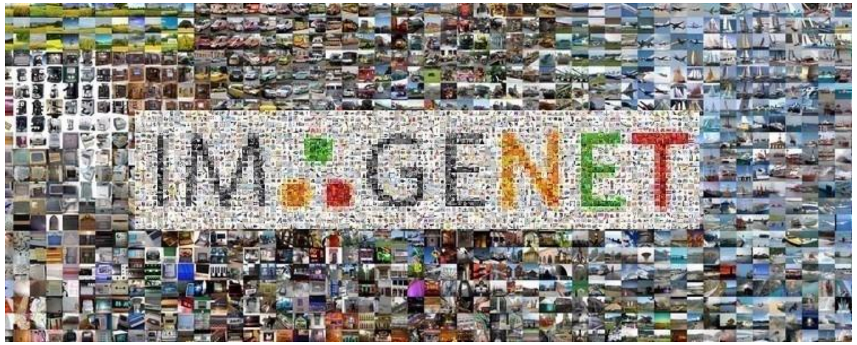


Conversational Systems

Digital art pic credit: David Schnurr

Key Enablers for Modern ML

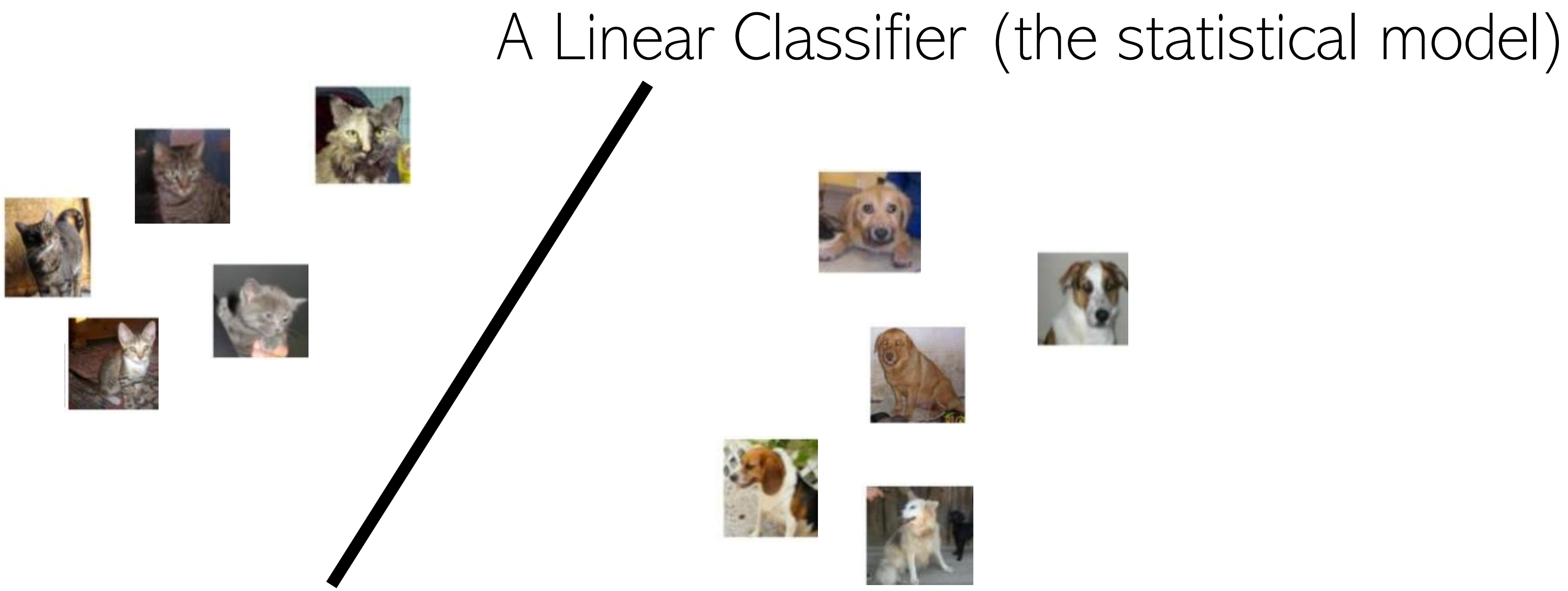
- Availability of large amounts of data to train ML models



- Increased computing power (e.g., GPUs)

ML: A Simple Illustration

- ML enables intelligent systems to be data-driven rather than rule-driven
- How: By supplying training data and building statistical models of data
- Pictorial illustration of an ML model for binary classification:



ML: A Simple Illustration

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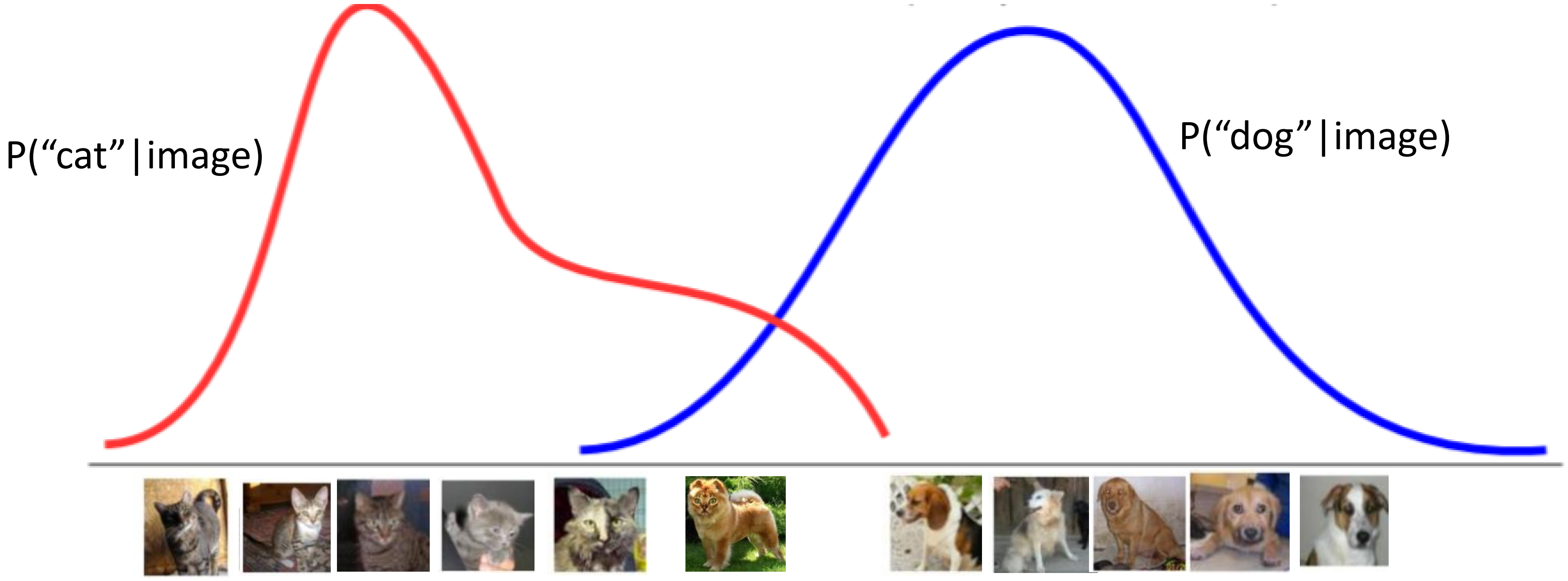
A Probabilistic Classifier (the statistical model)



ML: The Exam Analogy

- It's the performance on the D-day which matters

- In an exam, our success is measured based on how well we did on the questions in the test (not on the questions we practiced on)

- Likewise, in ML, success of the learned model is measured based on how well it predicts/fits the future test data (not the training data)

In Machine Learning, generalization performance on the test data matters (we should not "overfit" on training data)

A Loose Taxonomy of ML

“Labeled” means, during training, for each input, the corresponding output is available (i.e., the machine learner is explicitly told that a cat image is of a cat)

Learning using labeled data

Supervised Learning

Some examples of supervised learning problems

- Classification
- Regression
- Ranking

Learning using unlabeled data

Unsupervised Learning

Some examples of unsupervised learning problems

- Clustering
- Dimensionality Reduction
- Unsupervised Probability Density Estimation
- Generative Models (e.g., ChatGPT)

Machine Learning

Reinforcement Learning

RL doesn’t use “labeled” or “unlabeled” data in the traditional sense! In RL, an agent learns via its interactions with an environment

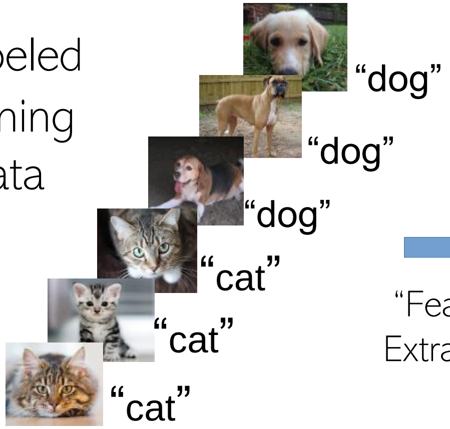
Many other specialized flavors of ML also exist, some of which include

- Semi-supervised Learning
- Self-supervised Learning (very popular these days)
- Active Learning
- Transfer Learning
- Multitask Learning
- Zero-Shot/Few-Shot Learning
- Continual learning

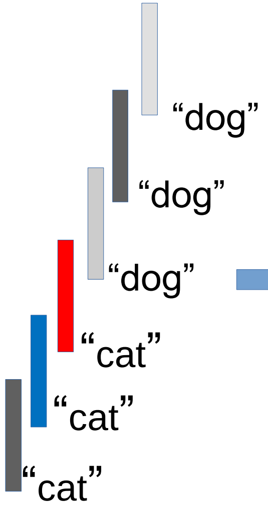
A Typical Supervised Learning Workflow

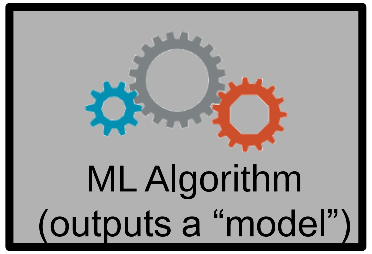
Note: This example is for the problem of binary classification, a supervised learning problem

Labeled Training Data



"Feature" Extraction



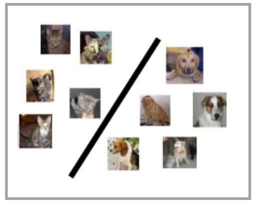


Is feature extraction done "manually" as a pre-processing step before the ML algo starts working? Can't we "automate" this part? Can't we "learn" good features directly from raw inputs?

Feature extraction converts raw inputs to a numeric representation that the ML algo can understand and work with. More on feature extraction later.

Test Image

"Feature" Extraction

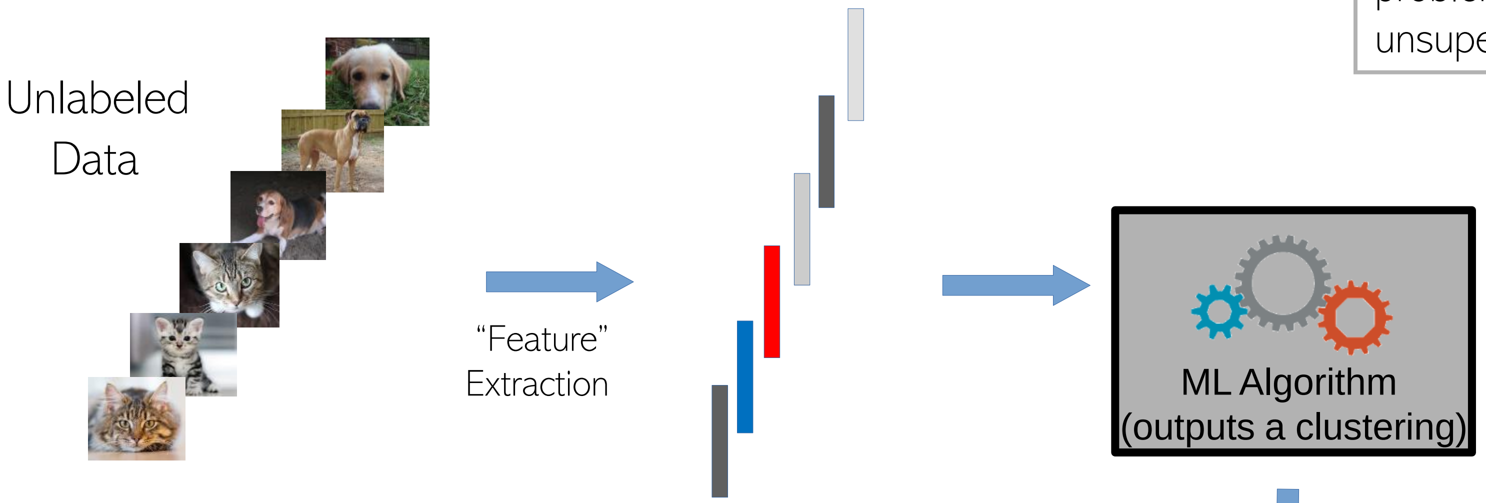


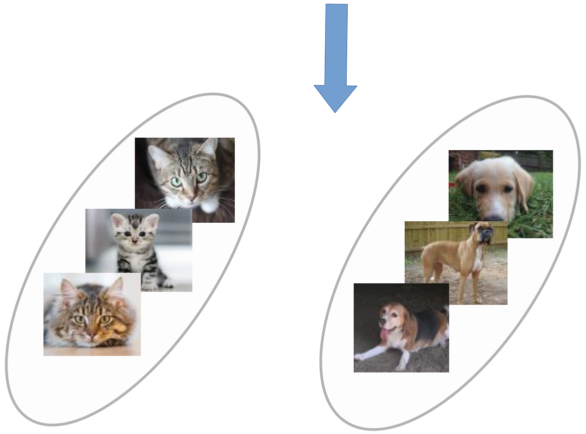
Cat vs Dog Prediction model

Predicted Label (cat/dog)

Indeed. Deep Learning algos do precisely that! (feature + model learning). More on Deep Learning later

A Typical Unsupervised Learning Workflow





Note: This example is for the problem of data clustering, an unsupervised learning problem

Yes. In this example, given a new "test" cat/dog image, we can assign it to the cluster with closer centroid

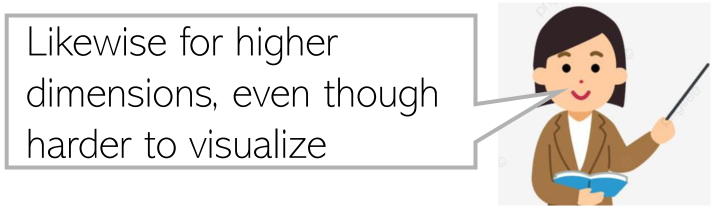
Does unsupervised learning also have a test phase? That is, can we also predict the cluster of a new test input?

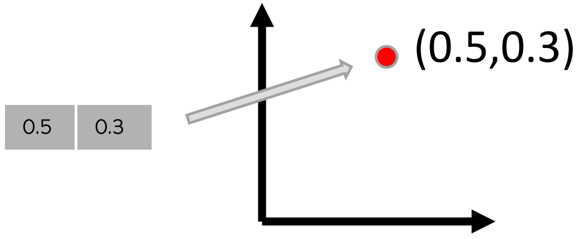
Notation and Convention

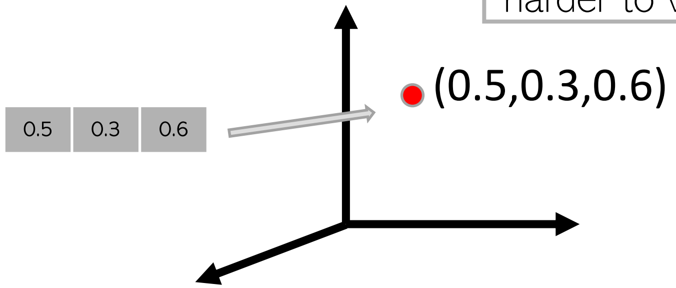
- In ML, inputs are usually represented by vectors
- A vector consists of an array of scalar values

0.5	0.3	0.6	0.1	0.2	0.5	0.9	0.2	0.1	0.5

- Geometrically, a vector is just a point in a vector space, e.g.,
  - A length 2 vector is a point in 2-dim vector space
  - A length 3 vector is a point in 3-dim vector space







- Unless specified otherwise
  - Small letters in bold font will denote vectors, e.g., $\mathbf{x}, \mathbf{a}, \mathbf{b}$ etc.
  - Small letters in normal font to denote scalars, e.g. x, a, b, etc
  - Capital letters in bold font will denote matrices (2-dim arrays), e.g., $\mathbf{X}, \mathbf{A}, \mathbf{B}$, etc

Notation and Convention

- A single vector will be assumed to be of the form $\mathbf{x} = [x_1, x_2, \ldots, x_D]$

- Unless specified otherwise, vectors will be assumed to be column vectors
  - So we will assume $\mathbf{x} = [x_1, x_2, \ldots, x_D]$ to be a column vector of size $D \times 1$
  - Assuming each element to be real-valued scalar, $\mathbf{x} \in \mathbb{R}^{D \times 1}$ or $\mathbf{x} \in \mathbb{R}^D$ ($\mathbb{R}$: space of reals)

- If $\mathbf{x} = [x_1, x_2, \ldots, x_D]$ is a feature vector representing, say an image, then
  - D denotes the dimensionality of this feature vector (number of features)
  - x_i (a scalar) denotes the value of i^{th} feature in the image

- For denoting multiple vectors, we will use a subscript with each vector, e.g.,
  - N images denoted by N feature vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_\mathrm{N}$, or compactly as $\{\mathbf{x}_n\}_{n=1}^{N}$
  - The vector $\mathbf{x}_n$ denotes the n^{th} image
  - x_{ni} (a scalar) denotes the i^{th} feature ($i = 1,2, \ldots, D$) of the n^{th} image

Notation and Convention

- Sup. learning requires training data as N input-output pairs $\{(\mathbf{x_n}, y_n)\}_{n=1}^{N}$
- Unsupervised learning requires training data as N inputs $\{\mathbf{x_n}\}_{n=1}^{N}$

RL and other flavors of ML problems also use similar notation

- Each input $\mathbf{x_n}$ is (usually) a vector containing the values of the features or attributes or covariates that encode properties of the object it represents, e.g.,
  - For a 7×7 image: $\mathbf{x_n}$ can be a 49×1 vector of pixel intensities

Size or length of the input $\mathbf{x_n}$ is commonly known as data/input dimensionality or feature dimensionality

- (In sup. learning) Each y_n is the output or response or label associated with input $\mathbf{x_n}$ (and its value is known for the training inputs)
  - Output can be a scalar, a vector of numbers, or even a structured object (more on this later)

Some Basic Operations on Vectors

- Addition/subtraction of two vectors gives another vector of the same size

- The mean $\boldsymbol{\mu}$ (average or centroid) of N vectors $\{\mathbf{x}_n\}_{n=1}^N$

$$\boldsymbol{\mu} = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}_n$$

(of the same size as each $\mathbf{x}_n$)

- The inner/dot product of two vectors $\boldsymbol{a} \in \mathbb{R}^D$ and $\boldsymbol{b} \in \mathbb{R}^D$

Assuming both $\boldsymbol{a}$ and $\boldsymbol{b}$ have unit Euclidean norm

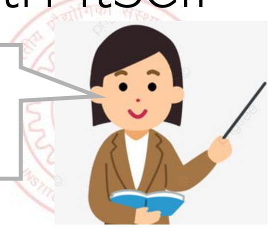
$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \boldsymbol{a}^\top \boldsymbol{b} = \sum_{i=1}^{D} a_i b_i$$

(a real-valued number denoting how "similar" $\boldsymbol{a}$ and $\boldsymbol{b}$ are)

- For a vector $\boldsymbol{a} \in \mathbb{R}^D$, its Euclidean norm is defined via its inner product with itself

$$||\boldsymbol{a}||_2 = \sqrt{\boldsymbol{a}^\top \boldsymbol{a}} = \sqrt{\sum_{i=1}^{d} a_i^2}$$

- Also the Euclidean distance of $\boldsymbol{a}$ from origin
- Note: Euclidean norm is also called L2 norm



Computing Distances

- Euclidean (L2 norm) distance between two vectors $\boldsymbol{a} \in \mathbb{R}^D$ and $\boldsymbol{b} \in \mathbb{R}^D$

$$d_2(\boldsymbol{a}, \boldsymbol{b}) = ||\boldsymbol{a} - \boldsymbol{b}||_2 = \sqrt{\sum_{i=1}^{D} (a_i - b_i)^2}$$

Another expression in terms of inner products of individual vectors

$$= \sqrt{(\boldsymbol{a} - \boldsymbol{b})^\top (\boldsymbol{a} - \boldsymbol{b})} = \sqrt{\boldsymbol{a}^\top \boldsymbol{a} + \boldsymbol{b}^\top \boldsymbol{b} - 2\boldsymbol{a}^\top \boldsymbol{b}}$$

- Other types of distances can be defined too, such as L1 norm

$$d_1(\boldsymbol{a}, \boldsymbol{b}) = ||\boldsymbol{a} - \boldsymbol{b}||_1 = \sum_{i=1}^{D} |a_i - b_i|$$

- Even more general type of distances can be defined

$\mathbf{W}$ is a DxD diagonal matrix with weights $\boldsymbol{w}_i$ on its diagonals. Weights may be known or even learned from data (in ML problems)

$$d_w(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{\sum_{i=1}^{D} w_i (a_i - b_i)^2} = \sqrt{(\boldsymbol{a} - \boldsymbol{b})^\top \mathbf{W} (\boldsymbol{a} - \boldsymbol{b})}$$

Computing Similarities

- Can also define similarity between two vectors $\boldsymbol{a} \in \mathbb{R}^D$ and $\boldsymbol{b} \in \mathbb{R}^D$

- Basically, opposite of distance

- For defining similarity, can use any function that gives
  - High value when $\boldsymbol{a}$ and $\boldsymbol{b}$ are close/similar
  - Small value when $\boldsymbol{a}$ and $\boldsymbol{b}$ are far/dissimilar

- Some examples
  - Dot product or cosine similarity
  - Kernel/similarity functions, such as the RBF ("radial basis function" or "Gaussian") kernel

Kernel functions like this provide a "nonlinear" similarity function unlike the standard dot product which is a linear similarity function (more on this later)

γ is called the bandwidth hyperparameter of this kernel function

$$k(\boldsymbol{a}, \boldsymbol{b}) = \exp(-\gamma ||\boldsymbol{a} - \boldsymbol{b}||^2)$$

Our First Supervised Learner

Prelude: A Very Primitive Classifier

The idea also applies to multi-class classification: Use one image per class, and predict label based on the distances of the test image from all such images

- Consider a binary classification problem – cat vs dog
- Assume training data with just 2 images – one  and one 
- Given a new test image (cat/dog), how do we predict its label?
- A simple idea: Predict using its distance from each of the 2 training images

d(Test image , ) < *d*(Test image , ) ? **Predict cat <u>else</u> dog**

Wait. Is it ML? Seems to be like just a simple "rule". Where is the "learning" part in this?

Some possibilities: Use a feature learning/selection algorithm to extract features, and use a weighted Euclidean distance where you learn the w_i's matrix (instead of using a predefined w_i's), using "distance metric learning" techniques

Excellent question! Glad you asked! Even this simple model can be <u>learned</u>. For example, for the feature extraction/selection part and/or for the distance computation part

Improving Our Primitive Classifier

- Just one input per class may not sufficiently capture variations in a class

- A natural improvement can be by using more inputs per class

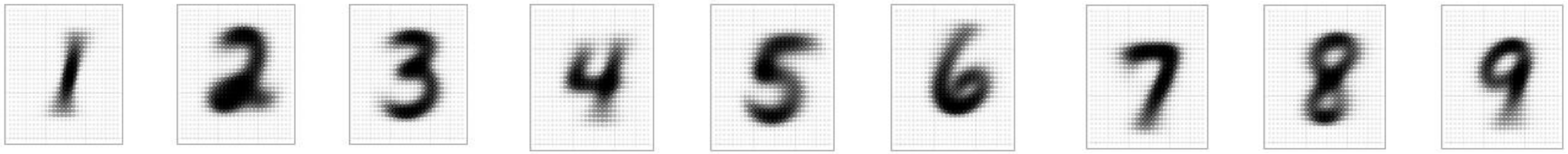
- We will consider two approaches to do this
  - Learning with Prototypes (LwP), also called “Nearest Class Mean” (NCM)
  - Nearest Neighbors (NN – not “neural networks”, at least not for now ☺)

- Both LwP and NN will use multiple inputs per class but in different ways

Learning with Prototypes (LwP)

- Basic idea: Represent each class by a "prototype" vector

- Class Prototype: The "mean" or "average" of inputs from that class



Averages (prototypes) of each of the handwritten digits 1-9

- Predict label of each test input based on its distances from the class prototypes
  - Predicted label will be the class that is the closest to the test input

- How we compute distances can have an effect on the accuracy of this model (may need to try Euclidean, weight Euclidean, or something else)

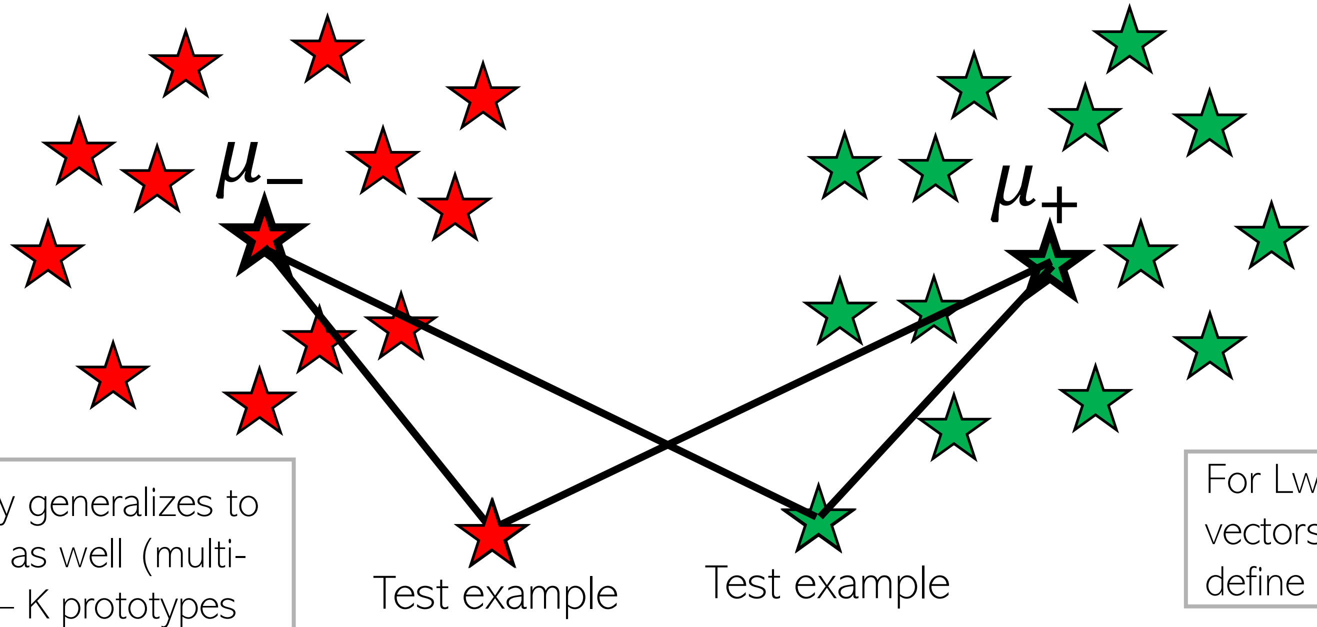
Pic from: https://www.reddit.com/r/dataisbeautiful/comments/3wgbv9/average_handwritten_digit_oc/

Learning with Prototypes (LwP): An Illustration

- Suppose the task is binary classification (two classes assumed pos and neg)

- Training data: N labelled examples $\{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$, $\mathbf{x}_n \in \mathbb{R}^D$, $y_n \in \{-1, +1\}$
  - Assume N_+ example from positive class, N_- examples from negative class
  - Assume green is positive and red is negative

$$\mu_- = \frac{1}{N_-} \sum_{y_n=-1} \mathbf{x}_n$$



$$\mu_+ = \frac{1}{N_+} \sum_{y_n=+1} \mathbf{x}_n$$

LwP straightforwardly generalizes to more than 2 classes as well (multi-class classification) – K prototypes for K classes

For LwP, the prototype vectors (μ_+ and μ_- here) define the "model"

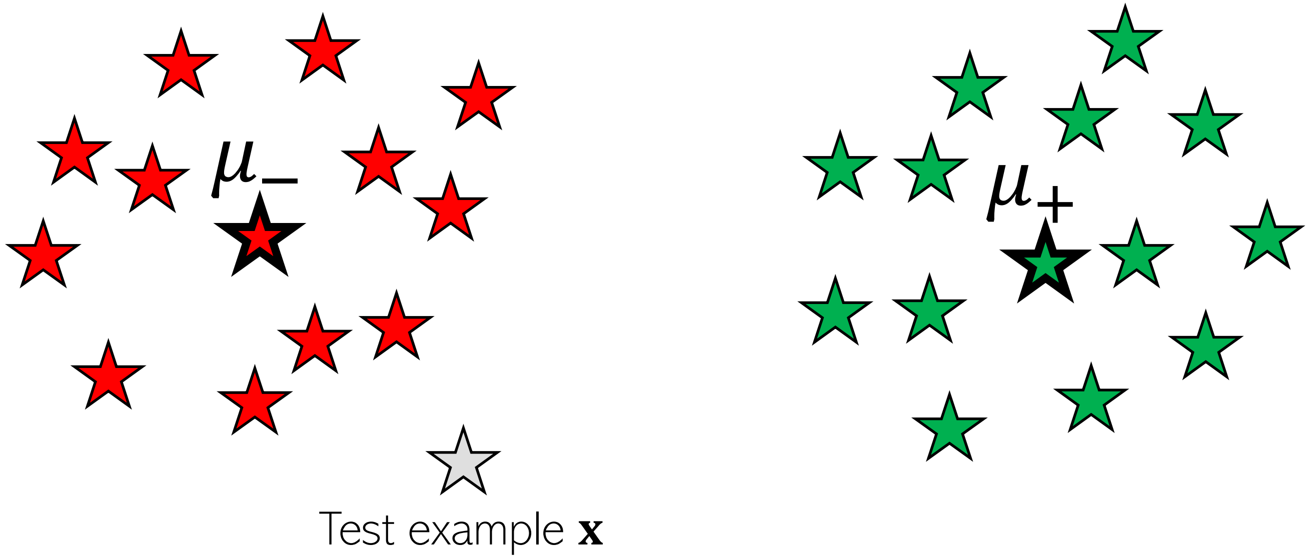
LwP: The Prediction Rule, Mathematically

- What does the prediction rule for LwP look like mathematically?

- Assume we are using Euclidean distances here

$$||\boldsymbol{\mu}_- - \mathbf{x}||^2 = ||\boldsymbol{\mu}_-||^2 + ||\mathbf{x}||^2 - 2\langle \boldsymbol{\mu}_-, \mathbf{x} \rangle$$

$$||\boldsymbol{\mu}_+ - \mathbf{x}||^2 = ||\boldsymbol{\mu}_+||^2 + ||\mathbf{x}||^2 - 2\langle \boldsymbol{\mu}_+, \mathbf{x} \rangle$$



Prediction Rule: Predict label as +1 if $f(\mathbf{x}) = ||\boldsymbol{\mu}_- - \mathbf{x}||^2 - ||\boldsymbol{\mu}_+ - \mathbf{x}||^2 > 0$ otherwise -1

LwP: The Prediction Rule, Mathematically

- Let's expand the prediction rule expression a bit more

$$
\begin{aligned}
f(\mathbf{x}) &= ||\boldsymbol{\mu}_- - \mathbf{x}||^2 - ||\boldsymbol{\mu}_+ - \mathbf{x}||^2 \\
&= ||\boldsymbol{\mu}_-||^2 + ||\mathbf{x}||^2 - 2\langle\boldsymbol{\mu}_-, \mathbf{x}\rangle - ||\boldsymbol{\mu}_+||^2 - ||\mathbf{x}||^2 + 2\langle\boldsymbol{\mu}_+, \mathbf{x}\rangle \\
&= 2\langle\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-, \mathbf{x}\rangle + ||\boldsymbol{\mu}_-||^2 - ||\boldsymbol{\mu}_+||^2 \\
&= \langle\mathbf{w}, \mathbf{x}\rangle + b
\end{aligned}
$$

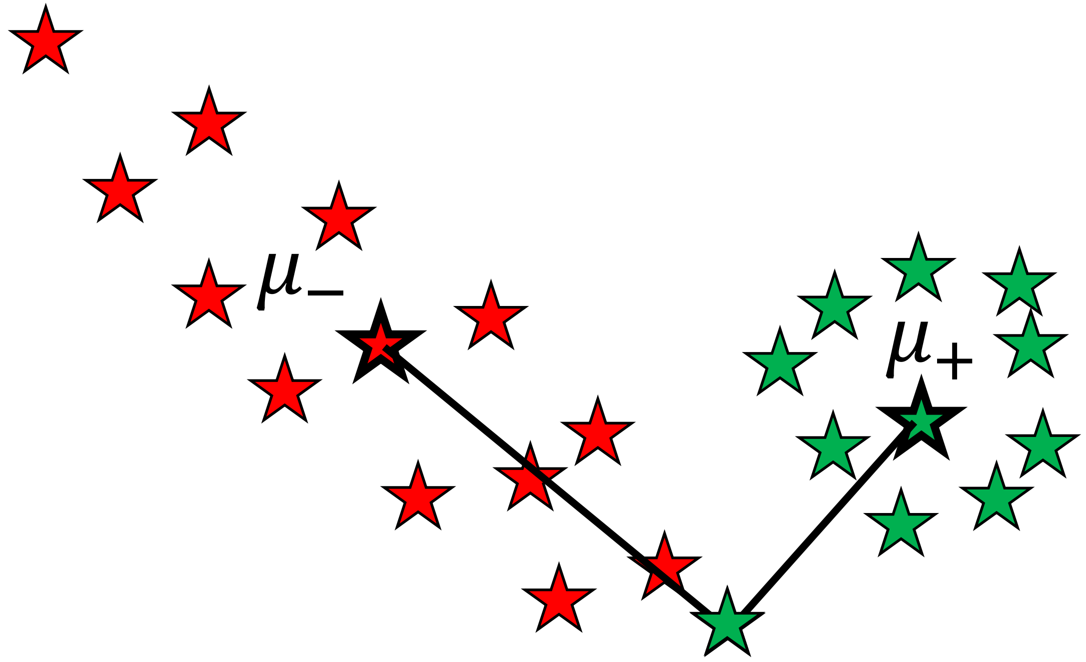
- Thus LwP with Euclidean distance is equivalent to a linear model with
  - Weight vector $\mathbf{w} = 2(\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-)$
  - Bias term $b = ||\boldsymbol{\mu}_-||^2 - ||\boldsymbol{\mu}_+||^2$

Will look at linear models more formally and in more detail later

- Prediction rule therefore is: Predict +1 if $\langle\mathbf{w}, \mathbf{x}\rangle + b > 0$, else predict -1

LwP: Some Failure Cases

- Here is a case where LwP with Euclidean distance may not work well



Can use feature scaling or use Mahalanobis distance to handle such cases (will discuss this in the next lecture)

- In general, if classes are not equisized and spherical, LwP with Euclidean distance will usually not work well. Can you think of how to fix this issue?

LwP: Some Key Aspects

- Very simple, interpretable, and lightweight model
  - Just requires computing and storing the class prototype vectors

- Works with any number of classes (thus for multi-class classification as well)

- Can be generalized in various ways to improve it further, e.g.,
  - Modeling each class by a probability distribution rather than just a prototype vector
  - Using distances other than the standard Euclidean distance (e.g., Mahalanobis)

- With a learned distance function, can work very well even with very few examples from each class (used in some "few-shot learning" models nowadays – if interested, please refer to "Prototypical Networks for Few-shot Learning")