HUST

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HANOI UNIVERSITY OF SCIENCE AND TECHNOLOGY

ONE LOVE. ONE FUTURE.

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Machine Learning

IT3190E

Lecture: Introduction

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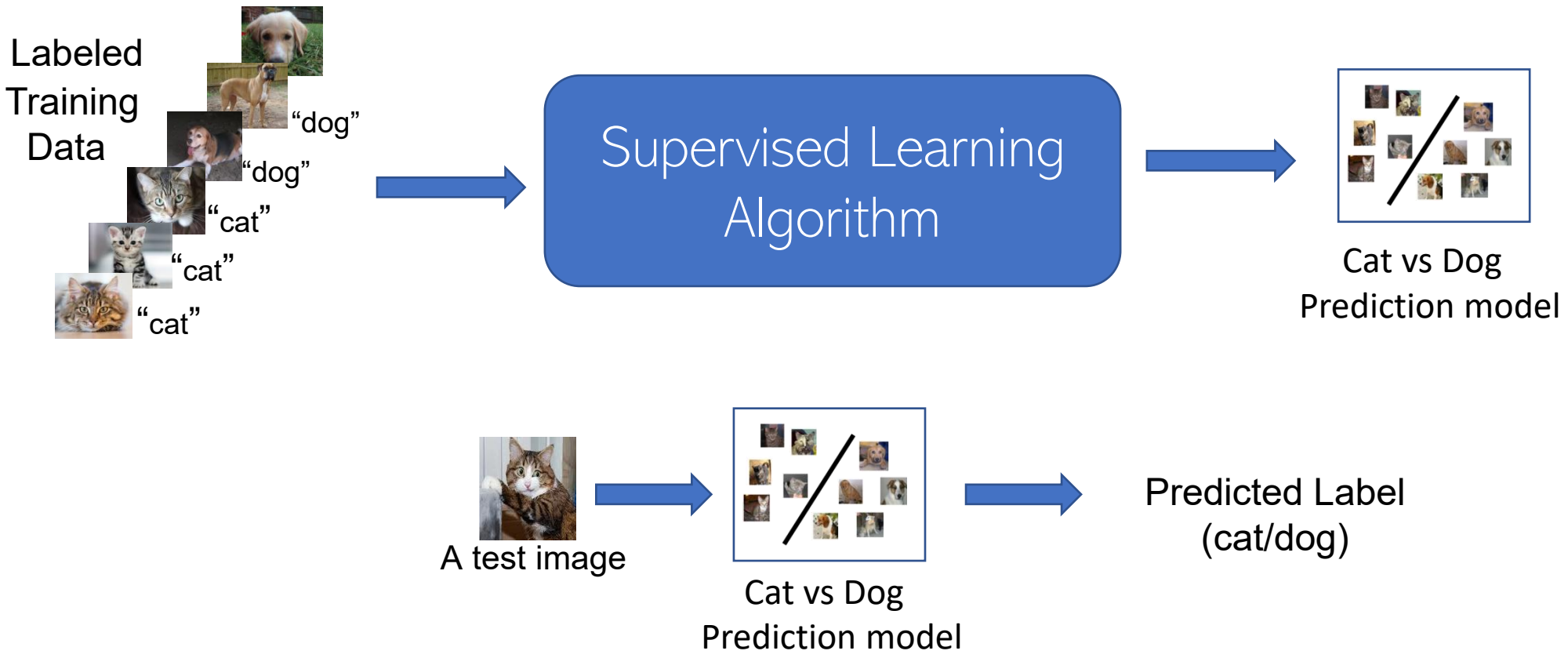
Contents

Learning with Prototypes

Supervised Learning



Some Types of Supervised Learning Problems

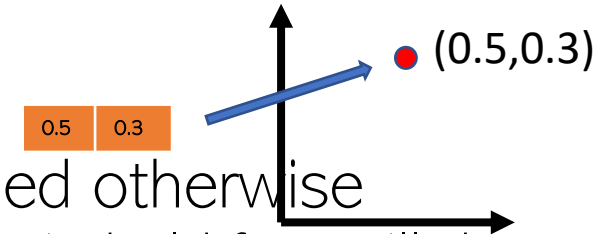
- Consider building an ML module for an e-mail client
- Some tasks that we may want this module to perform
  - Predicting whether an email of spam or normal: Binary Classification
  - Predicting which of the many folders the email should be sent to: Multi-class Classification
  - Predicting all the relevant tags for an email: Tagging or Multi-label Classification
  - Predicting what's the spam-score of an email: Regression
  - Predicting which email(s) should be shown at the top: Ranking
  - Predicting which emails are work/study-related emails: One-class Classification
- These predictive modeling tasks can be formulated as supervised learning problems
- Today: A very simple supervised learning model for binary/multi-class classification
  - This model doesn't require any fancy maths – just computing means and distances

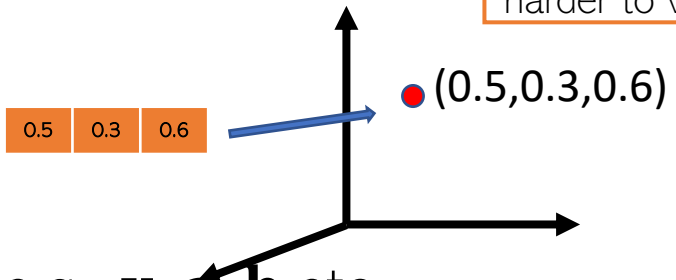
Some Notation and Conventions

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

- 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

Likewise for higher dimensions, even though harder to visualize





- 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

Some Notation and Conventions

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

- Unless specified otherwise, vectors will be assumed to be column vectors
  - So we will assume $\mathbf{x} = [x_1, x_2, \dots, x_D]$ 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 $\mathbf{x} = [x_1, x_2, \dots, x_D]$ 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 $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_\mathrm{N}$, 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 ($i = 1,2, \dots, D$) of the n^{th} image

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 $\{\mathbf{x}_n\}_{n=1}^N$

$$\mu = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n \in \mathbb{R}^D$$ (of the same size as each $\mathbf{x}_n$)

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

$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \boldsymbol{a}^\top \boldsymbol{b} = \sum_{i=1}^{D} a_i b_i$$ (a real-valued number denoting how "similar" $\boldsymbol{a}$ and $\boldsymbol{b}$ are)

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

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

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

Computing Distances

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

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

Sqrt of Inner product of the difference vector

Another expression in terms of inner products of individual vectors

- Weighted Euclidean distance between two vectors $\boldsymbol{a} \in \mathbb{R}^D$ and $\boldsymbol{b} \in \mathbb{R}^D$

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

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

- Absolute (L1 norm) distance between two vectors $\boldsymbol{a} \in \mathbb{R}^D$ and $\boldsymbol{b} \in \mathbb{R}^D$

L1 norm distance is also known as the Manhattan distance or Taxicab norm (it's a very natural notion of distance between two points in some vector space)

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

Our First Supervised Learner

Prelude: A Very Primitive Classifier

- 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

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

$d($ Test image ,  $) < d($ Test image ,  $)$? Predict cat else 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 Mahalanobis distance where you learn the W matrix (instead of using a predefined W), using "distance metric learning" techniques

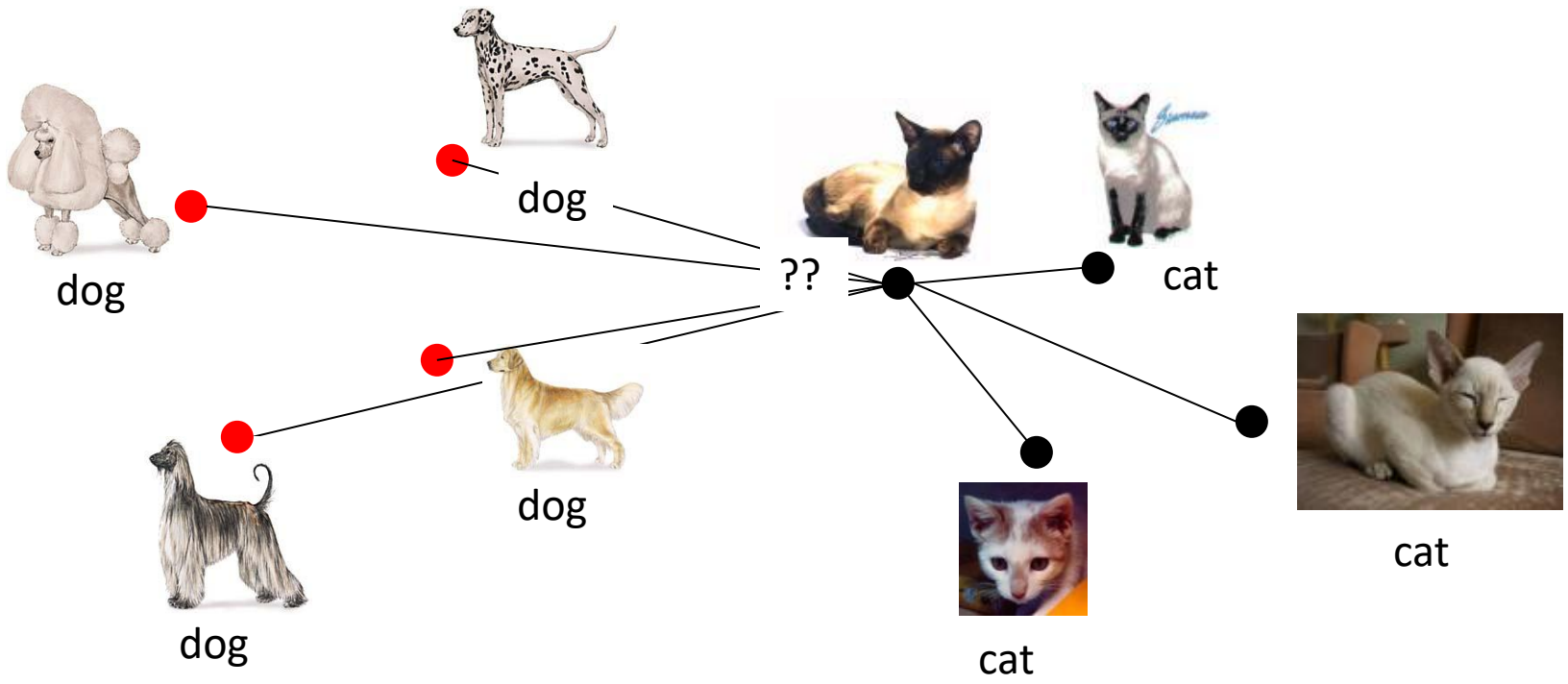
Even this simple model can be learned. For example, for the feature extraction/selection part and/or for the distance computation part

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

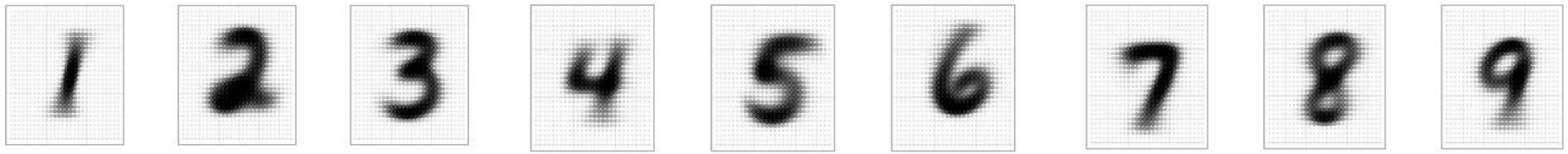
- We will consider two approaches to do th
  - Learning with Prototypes (LwP)
  - Nearest Neighbors (NN)
- Both LwP and NN will use multiple inputs per class but in different ways

Learning to predict categories



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

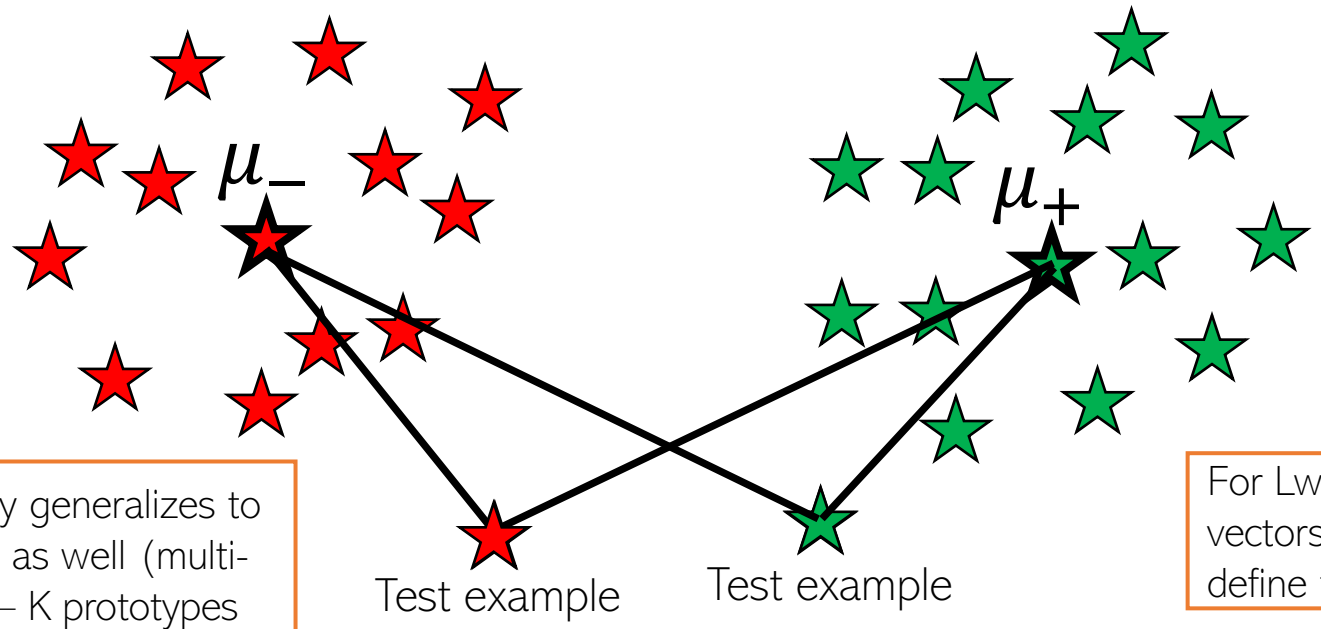
- Predict label of each test input based on its distances from the class prototypes
  - Predicted label will be the class that is the closest to the test input
- How we compute distances can have an effect on the accuracy of this model (may need to try Euclidean, weight Euclidean, Mahalanobis, or something else)

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

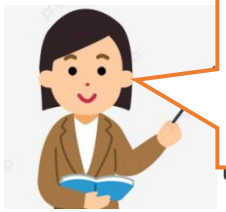
Learning with Prototypes (LwP): An Illustration

- 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"

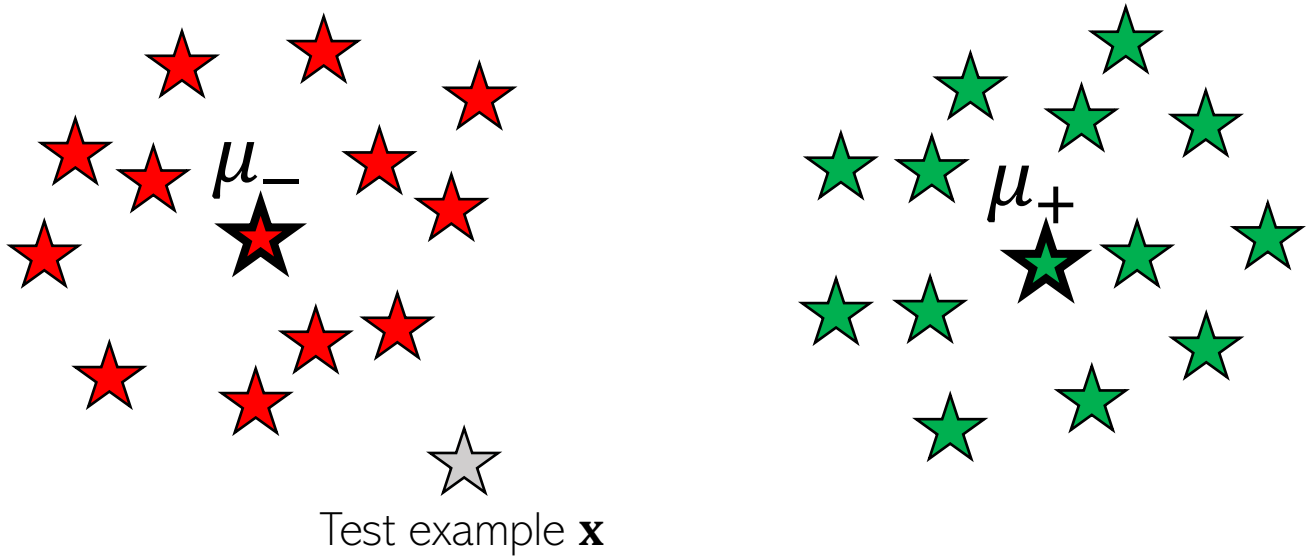
LwP: The Prediction Rule, Mathematically

- 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

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

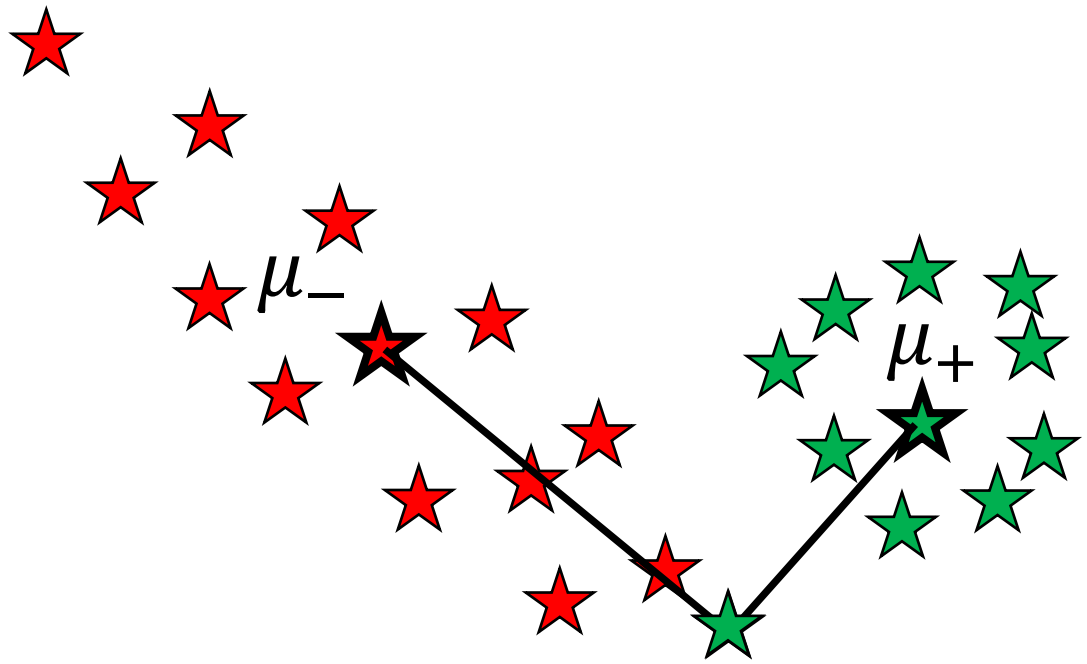
- Thus LwP with Euclidean distance is equivalent to a linear model with
  - Weight vector $\mathbf{w} = 2(\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-)$
  - Bias term $b = \left|\left|\boldsymbol{\mu}_-\right|\right|^2 - \left|\left|\boldsymbol{\mu}_+\right|\right|^2$

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

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

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)

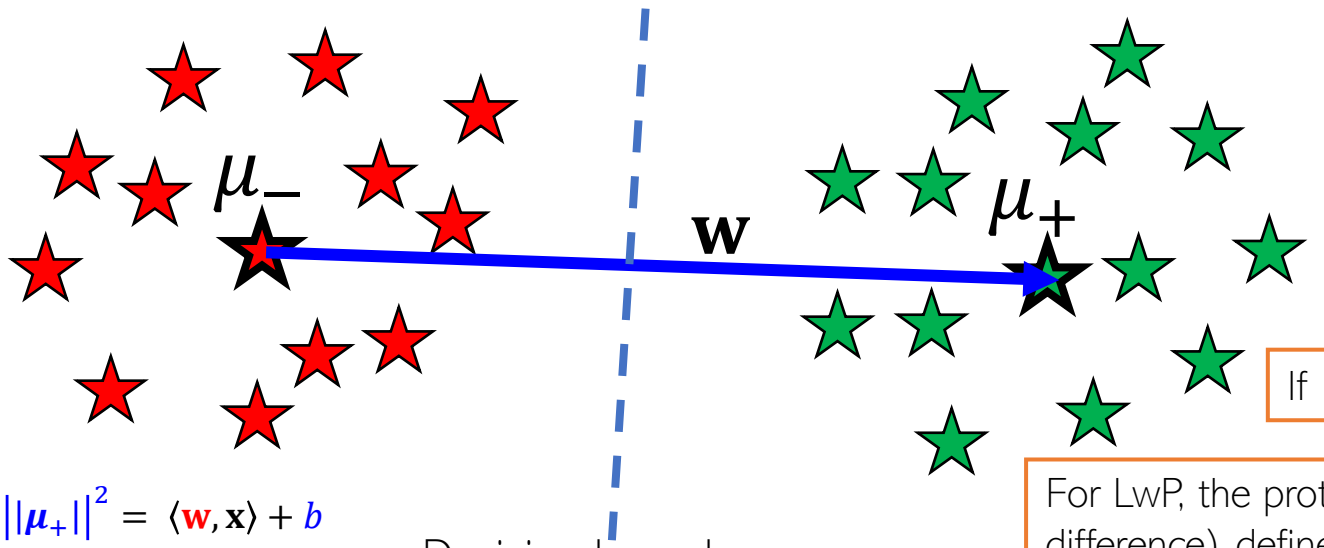
- In general, if classes are not equisized and spherical, LwP with Euclidean distance will usually not work well (but improvements possible; will discuss later)

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")

Learning with Prototypes (LwP)

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



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

$$\mathbf{w} = \boldsymbol{\mu}_+ - \boldsymbol{\mu}_-$$

If Euclidean distance used

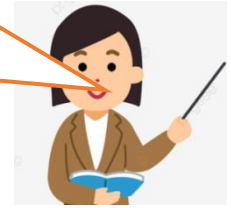
Prediction rule for LwP (for binary classification with Euclidean distance)

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

($f(\mathbf{x}) > 0$ then predict +1 otherwise -1)

Decision boundary (perpendicular bisector of line joining the class prototype vectors)

For LwP, the prototype vectors (or their difference) define the "model". $\boldsymbol{\mu}_+$ and $\boldsymbol{\mu}_-$ (or just $\mathbf{w}$ in the Euclidean distance case) are the model parameters.



Exercise: Show that for the bin. classfn case

$$f(\mathbf{x}) = \sum_{n=1}^{N} \alpha_n \langle \mathbf{x}_n, \mathbf{x} \rangle + b$$

Note: Even though $f(\mathbf{x})$ can be expressed in this form, if $N > D$, this may be more expensive to compute (O(N) time) as compared to $\langle \mathbf{w}, \mathbf{x} \rangle + b$ (O(D) time).

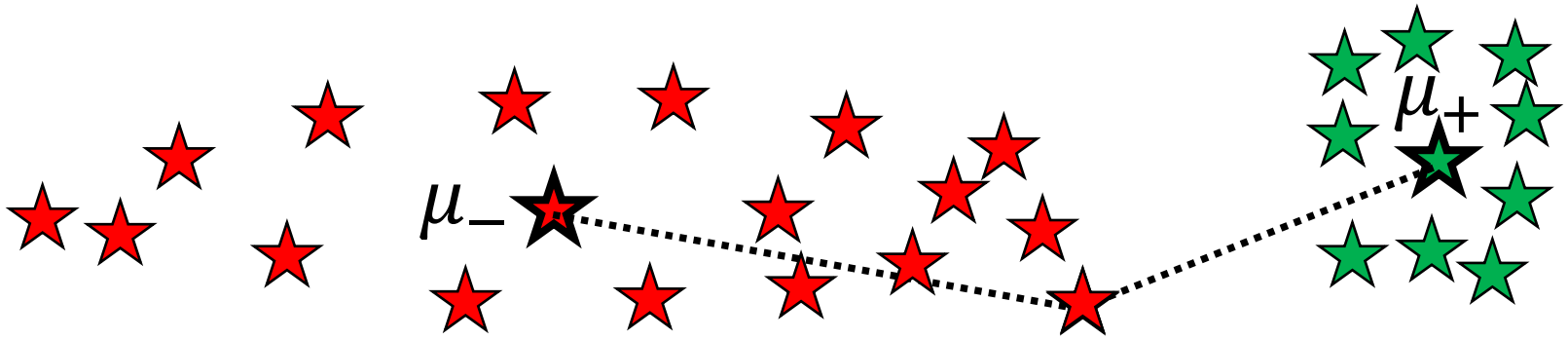
Can throw away training data after computing the prototypes and just need to keep the model parameters for the test time in such "parametric" models

So the "score" of a test point $\mathbf{x}$ is a weighted sum of its similarities with each of the N training inputs. Many supervised learning models have $f(\mathbf{x})$ in this form as we will see later

However the form $f(\mathbf{x}) = \sum_{n=1}^{N} \alpha_n \langle \mathbf{x}_n, \mathbf{x} \rangle + b$ is still very useful as we will see later when we discuss kernel methods

Improving LwP when classes are complex-shaped

- Using weighted Euclidean or Mahalanobis distance can sometimes help



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

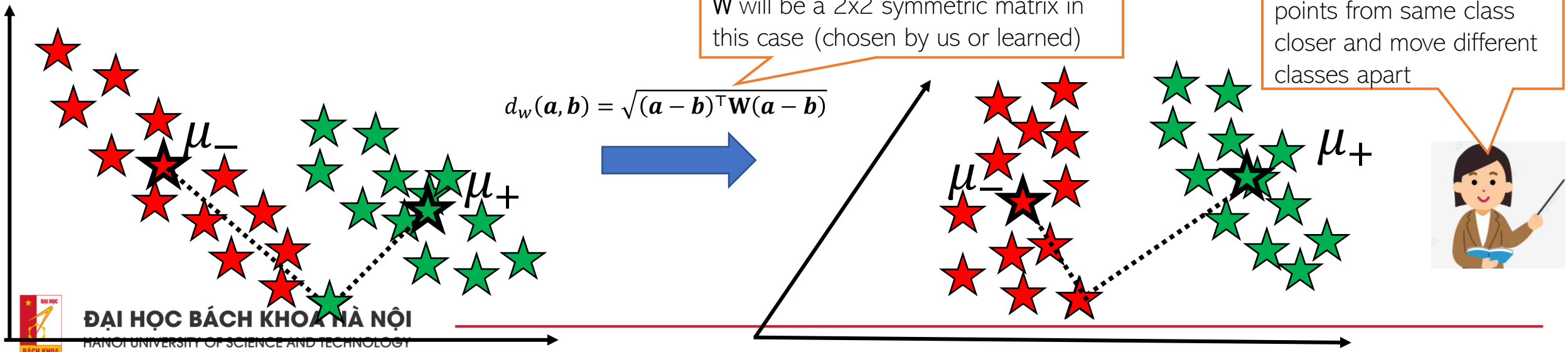
Use a smaller w_i for the horizontal axis feature in this example

- Note: Mahalanobis distance also has the effect of rotating the axes which helps

W will be a 2x2 symmetric matrix in this case (chosen by us or learned)

$$d_w(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{(\boldsymbol{a} - \boldsymbol{b})^\top \mathbf{W} (\boldsymbol{a} - \boldsymbol{b})}$$

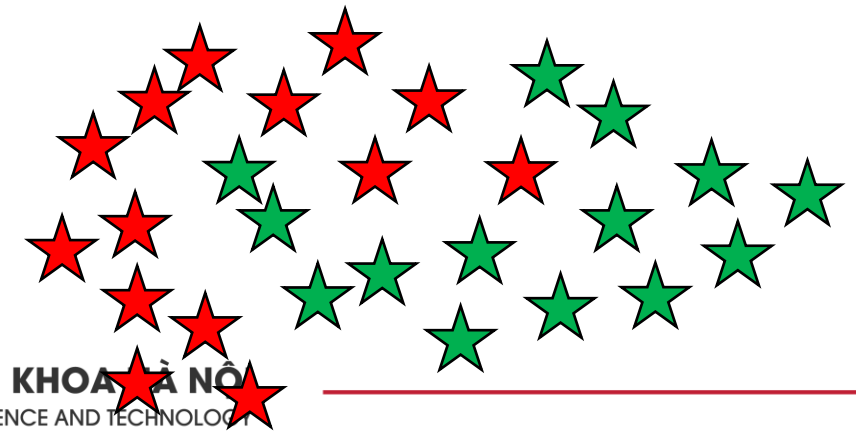
A good W will help bring points from same class closer and move different classes apart



Improving LwP when classes are complex-shaped

- Even with weighted Euclidean or Mahalanobis dist, LwP still a linear classifier ☹
- **Exercise:** Prove the above fact. You may use the following hint
  - Mahalanobis dist can be written as $d_{\boldsymbol{w}}(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{(\boldsymbol{a}-\boldsymbol{b})^{\top}\mathbf{W}(\boldsymbol{a}-\boldsymbol{b})}$
  - $\mathbf{W}$ is a symmetric matrix and thus can be written as $\mathbf{A}\mathbf{A}^{\top}$ for any matrix $\mathbf{A}$
  - Showing for Mahalabonis is enough. Weighted Euclidean is a special case with diag $\mathbf{W}$

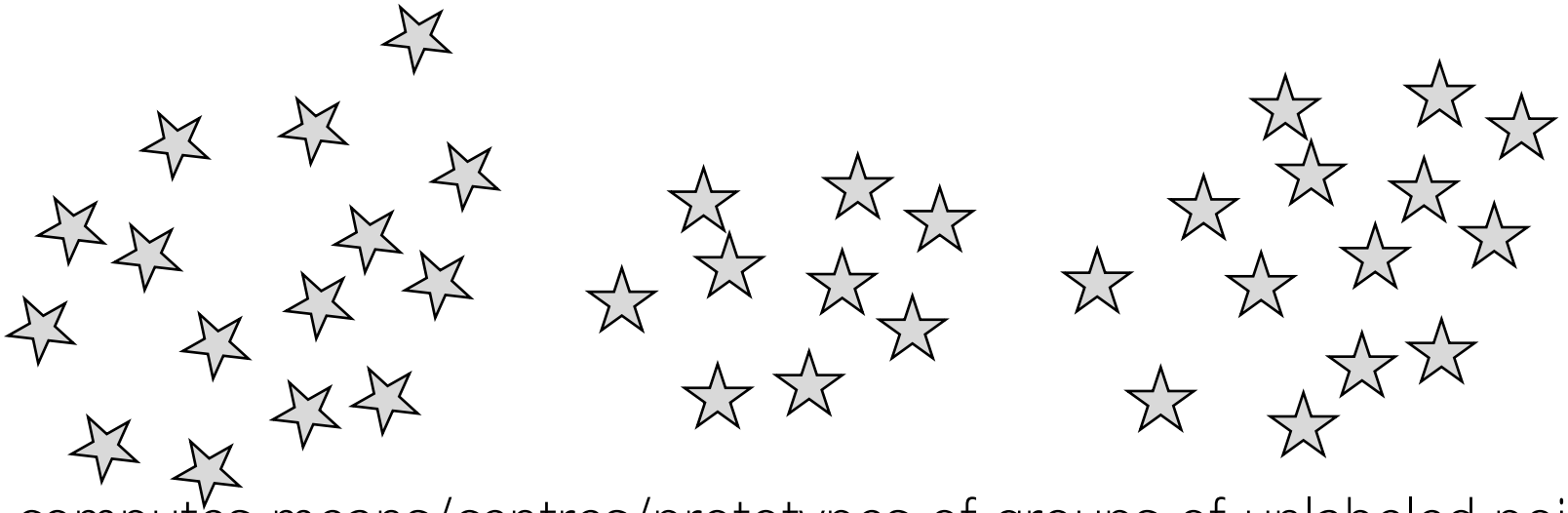
- LwP can be extended to learn nonlinear decision boundaries if we use nonlinear distances/similarities (more on this when we talk about kernels)



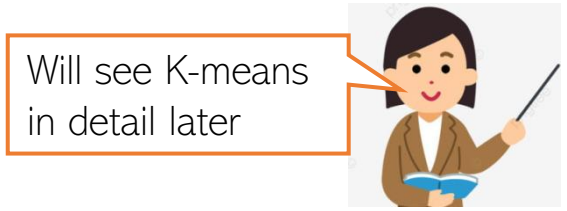
Note: Modeling each class by not just a mean by a probability distribution can also help in learning nonlinear decision boundaries. More on this when we discuss probabilistic models for classification

LwP as a subroutine in other ML models

- For data-clustering (unsupervised learning), *K*-means clustering is a popular algo



- *K*-means also computes means/centres/prototypes of groups of unlabeled points
- Harder than LwP since labels are unknown. But we can do the following
  - Guess the label of each point, compute means using guess labels
  - Refine labels using these means (assign each point to the current closest mean)
  - Repeat until means don't change anymore
- Many other models also use LwP as a subroutine



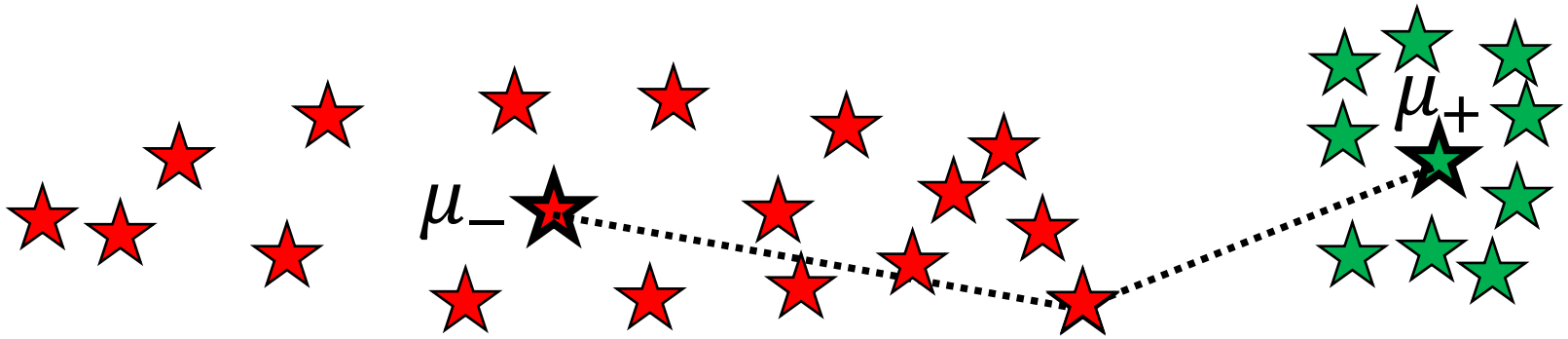
Next Lecture

- Nearest Neighbors

Exotic distances and nearest neighbors

Improving LwP when classes are complex-shaped

- Using weighted Euclidean or Mahalanobis distance can sometimes help



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

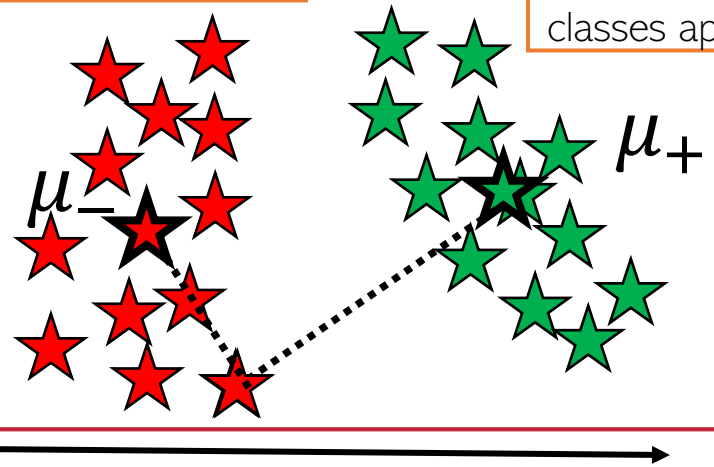
Use a smaller w_i for the horizontal axis feature in this example

- Note: Mahalanobis distance also has the effect of rotating the axes which helps

W will be a 2x2 symmetric matrix in this case (chosen by us or learned)

$$d_w(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{(\boldsymbol{a} - \boldsymbol{b})^\top \mathbf{W} (\boldsymbol{a} - \boldsymbol{b})}$$

A good W will help bring points from same class closer and move different classes apart



What is Mahalanobis Distance?

- Recall

$$\text{Euclidean } D(\mathbf{a},\mathbf{b}) = \sqrt{(\mathbf{a}-\mathbf{b})^T(\mathbf{a}-\mathbf{b})}$$

- And its generalization
  - Where W is a diagonal matrix

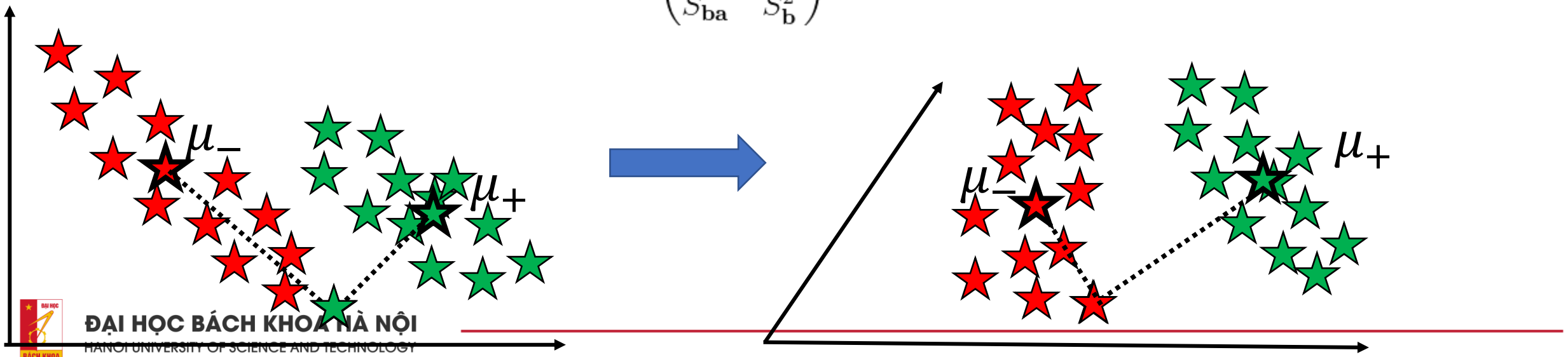
$$\text{Weighted Euclidean } D(\mathbf{a},\mathbf{b}) = \sqrt{(\mathbf{a}-\mathbf{b})^T\mathbf{W}(\mathbf{a}-\mathbf{b})}$$

- The Mahalanobis distance further generalizes the weighted Euclidean distance

- Here, S is the covariance ma

$$\text{Mahalanobis } D(\mathbf{a},\mathbf{b}) = \sqrt{(\mathbf{a}-\mathbf{b})^T\mathbf{S}^{-1}(\mathbf{a}-\mathbf{b})}$$

$$\begin{pmatrix} S_{\mathbf{a}}^2 & S_{\mathbf{ab}} \\ S_{\mathbf{ba}} & S_{\mathbf{b}}^2 \end{pmatrix}$$



Supervised Learning using Nearest Neighbors

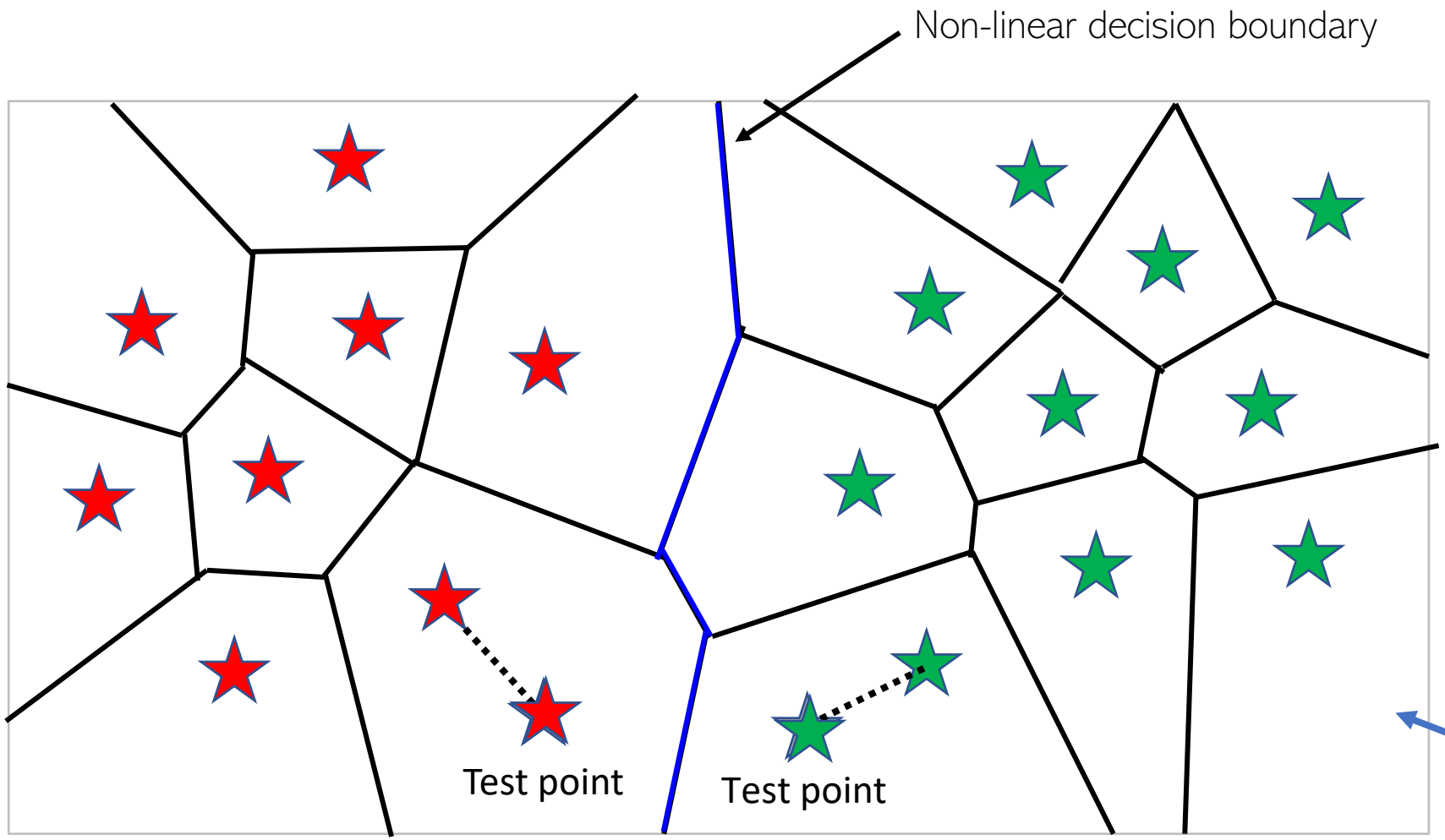
Nearest Neighbors

- Another supervised learning technique based on computing distances
- Very simple idea. Simply do the following at test time
  - Compute distance of the test point from all the training points
  - Sort the distances to find the "nearest" input(s) in training data
  - Predict the label using majority or avg label of these inputs
- Can use Euclidean or other dist (e.g., Mahalanobis). Choice important just like LwP
- Unlike LwP which does prototype based comparison, nearest neighbors method looks at the labels of individual training inputs to make prediction
- Applicable to both classification as well as regression (LwP only works for classification)

Nearest Neighbors for Classification

Reference material

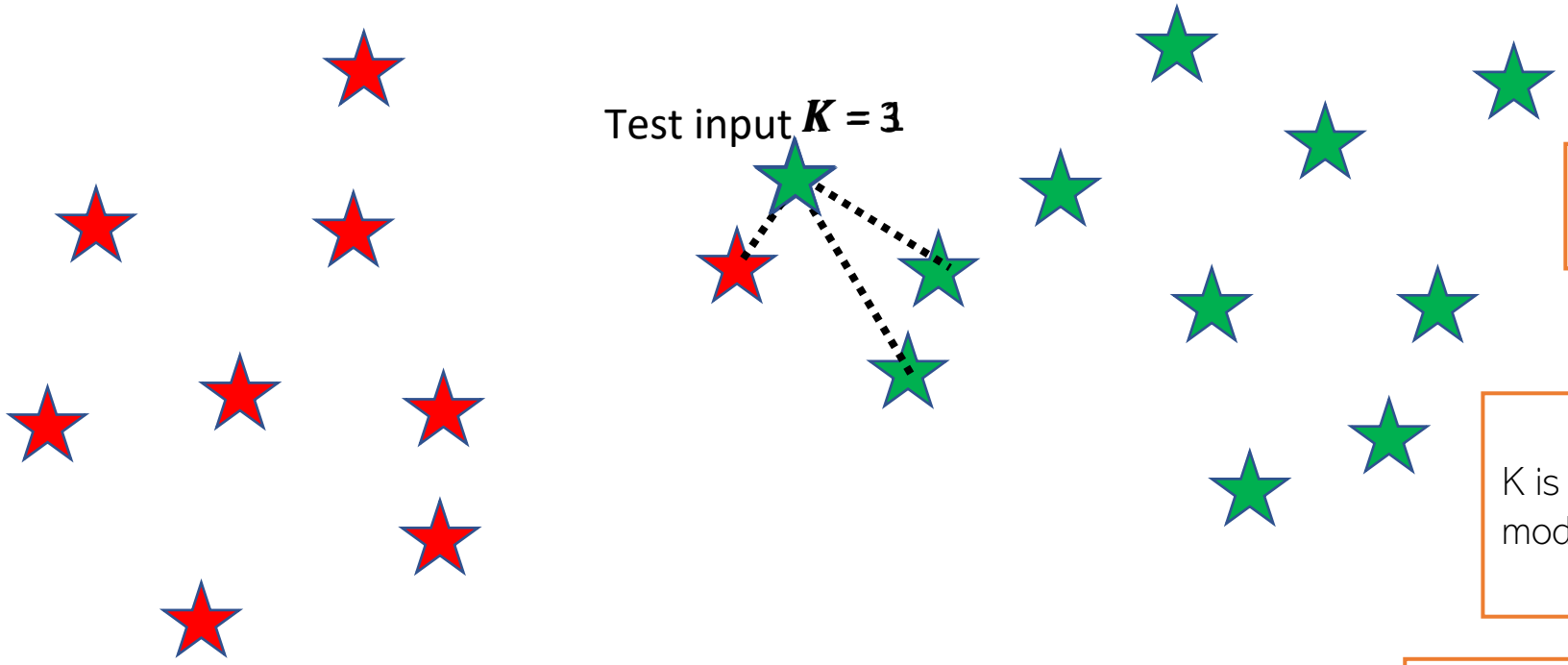
Nearest Neighbor (or "One" Nearest Neighbor)



Nearest neighbour approach induces a Voronoi tessellation/partition of the input space (all test points falling in a cell will get the label of the training input in that cell)

K Nearest Neighbors (*K*NN)

- In many cases, it helps to look at not one but $K > 1$ nearest neighbors



How to pick the "right" K value?

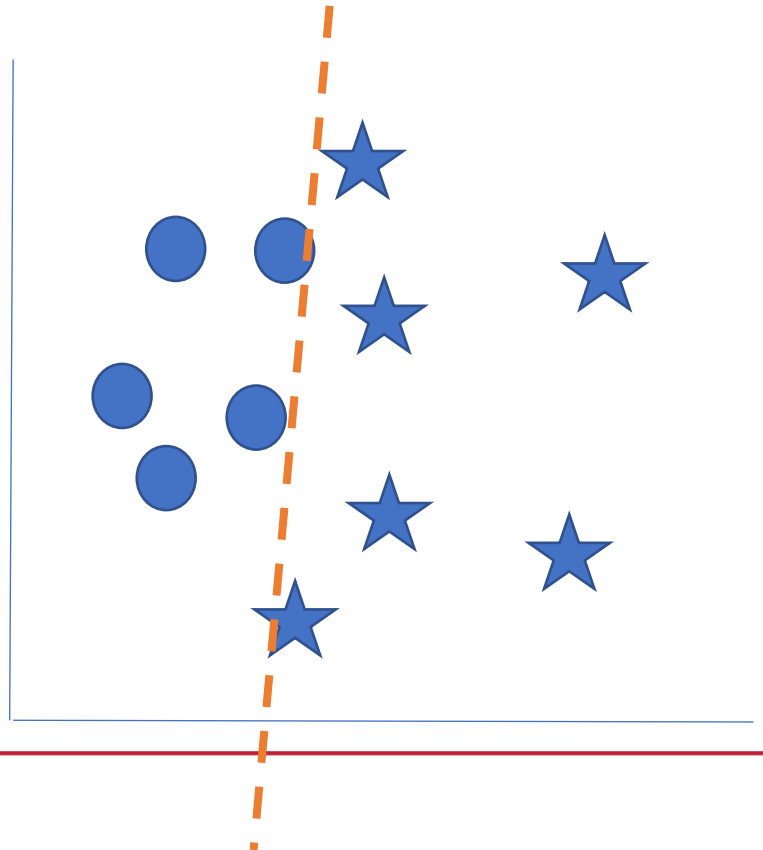
K is a free parameter in the model

Also, K should ideally be an odd number to avoid ties

- Essentially, taking more votes helps!
  - Also leads to smoother decision boundaries (less chances of overfitting on training data)

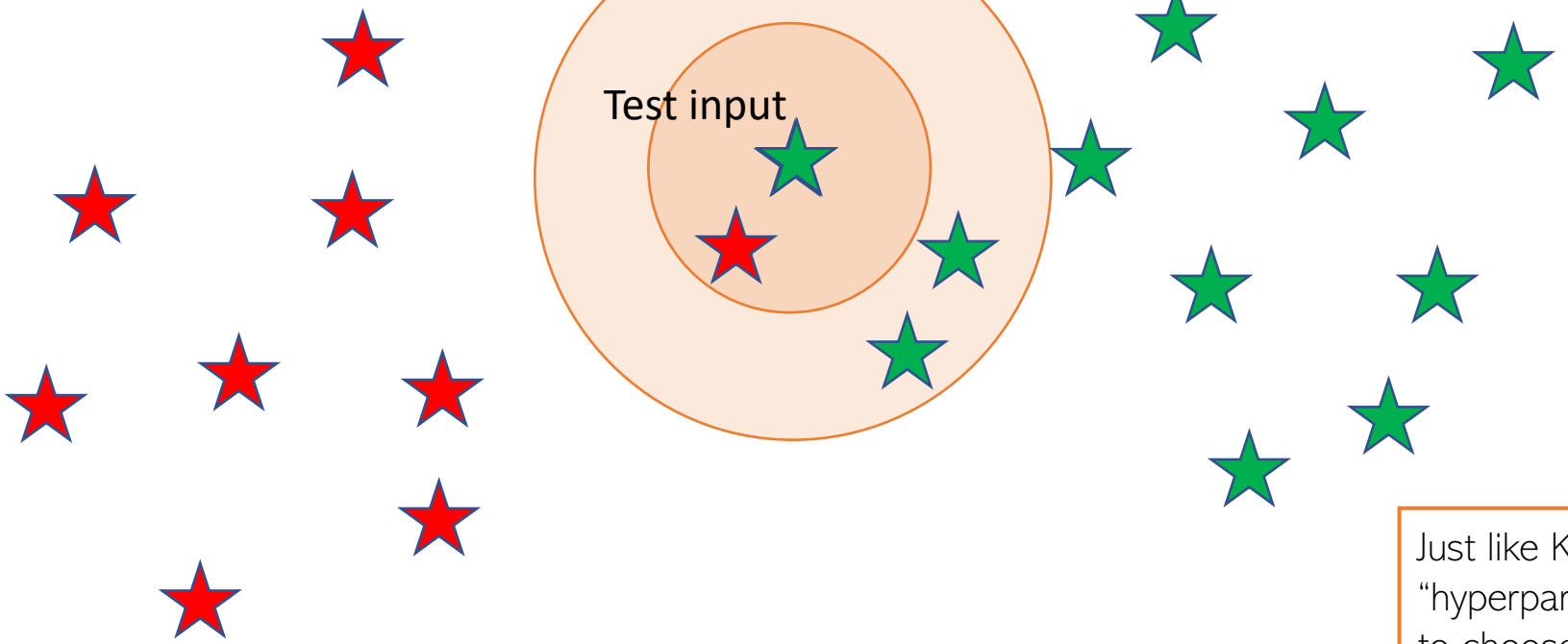
Setting parameter values

- The black magic of machine learning
  - “Predictions are hard, especially about the future” – Yogi Berra
- Basic idea: find parameter values for which you make the fewest possible mistakes on training data
- Pray that training data is representative
- If it’s not, your model will work badly
- We will see some nice math that helps
- Soon!



ϵ-Ball Nearest Neighbors (ϵ-NN)

- Rather than looking at a fixed number K of neighbors, can look inside a ball of a given radius ϵ, around the test input

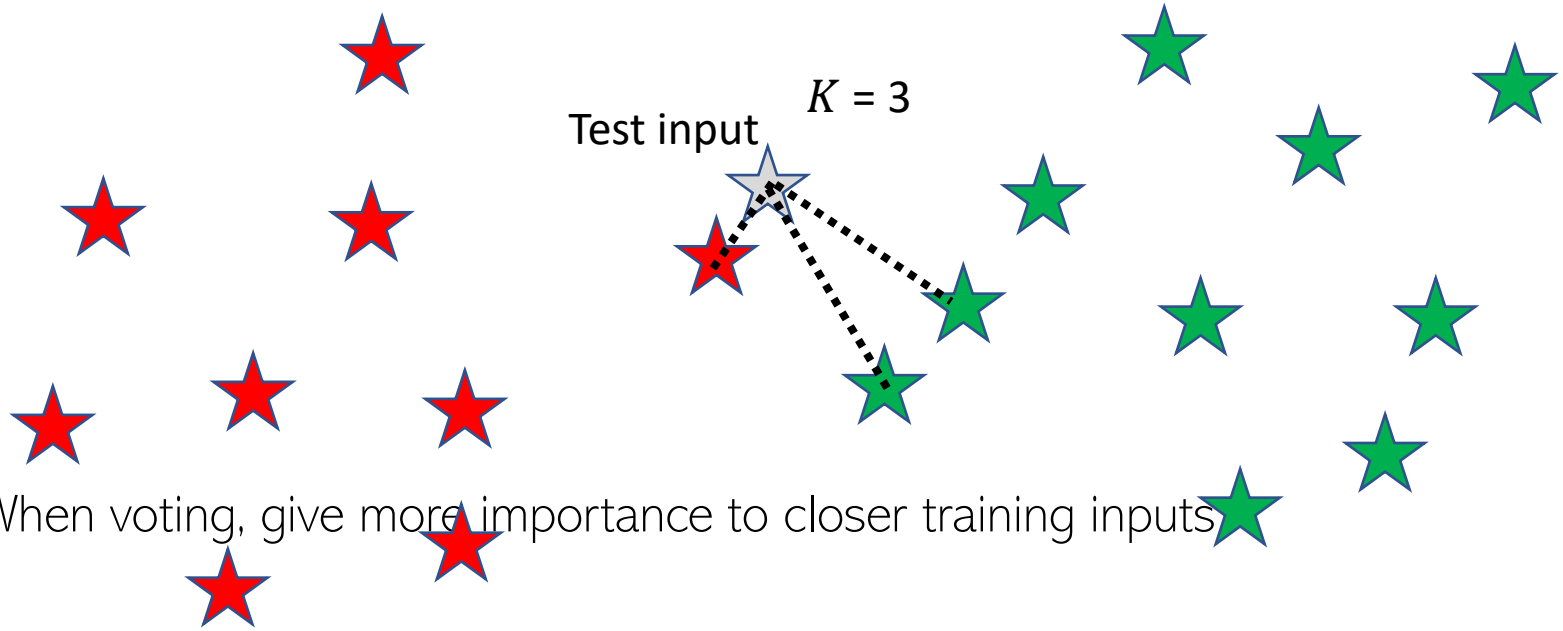


So changing ϵ may change the prediction. How to pick the "right" ϵ value?

Just like K, ϵ is also a "hyperparameter". One way to choose it is using "cross-validation" (will see shortly)

Distance-weighted *K*NN and ϵ-NN

- The standard KNN and ϵ-NN treat all nearest neighbors equally (all vote equally)

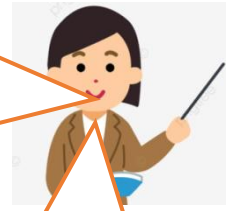


- An improvement: When voting, give more importance to closer training inputs

Unweighted KNN prediction: $\frac{1}{3}$ ★ + $\frac{1}{3}$ ★ + $\frac{1}{3}$ ★ = ★

Weighted KNN prediction: $\frac{3}{5}$ ★ + $\frac{1}{5}$ ★ + $\frac{1}{5}$ ★ = ★

In weighted approach, a single red training input is being given 3 times more importance than the other two green inputs since it is sort of "three times" closer to the test input than the other two green inputs

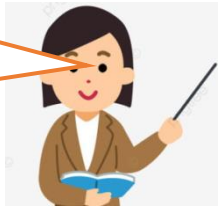


ϵ-NN can also be made weighted likewise

KNN/ϵ-NN for Other Supervised Learning Problems

- Can apply KNN/ϵ-NN for other supervised learning problems as well, such as
  - Multi-class classification
  - Regression
  - Tagging/multi-label learning

We can also try the weighted versions for such problems, just like we did in the case of binary classification



- For multi-class, simply used the same majority rule like in binary classfication case
  - Just a simple difference that now we have more than 2 classes
- For regression, simply compute the average of the outputs of nearest neighbors
- For multi-label learning, each output is a binary vector (presence/absence of tag)
  - Just compute the average of the binary vectors
  - Result won't be a binary vector but we can report the best tags based on magnitudes

KNN Prediction Rule: The Mathematical Form

- Let's denote the set of K nearest neighbors of an input $\mathbf{x}$ by $N_K(\mathbf{x})$

- The unweighted KNN prediction $\mathbf{y}$ for a test input $\mathbf{x}$ can be written as

$$\mathbf{y} = \frac{1}{K} \sum_{i \in N_K(\mathbf{x})} \mathbf{y}_i$$

For discrete labels with 5 possible values, the one-hot representation will be an all zeros vector of size 5, except a single 1 denoting the value of the discrete label, e.g., if label = 3 then one-hot vector = [0,0,1,0,0]

- This form makes direct sense of regression and for cases where the each output is a vector (e.g., multi-class classification where each output is a discrete value which can be represented as a one-hot vector, or tagging/multi-label classification where each output is a binary vector)
  - For binary classification, assuming labels as +1/-1, we predict $\mathbf{sign}(\frac{1}{K} \sum_{i \in N_K(\mathbf{x})} \mathbf{y}_i)$

Nearest Neighbours: Some Comments

- An old, classic but still very widely used algorithm
  - Competitive with state-of-the-art approaches most of the time
- Can work very well in practice with the right distance function
  - How do we pick the right distance function?
- Requires lots of storage (need to keep all the training data at test time)
- Prediction step can be slow at test time
  - For each test point, need to compute its distance from all the training points
- Clever data-structures or data-summarization techniques can provide speed-ups

Thanks