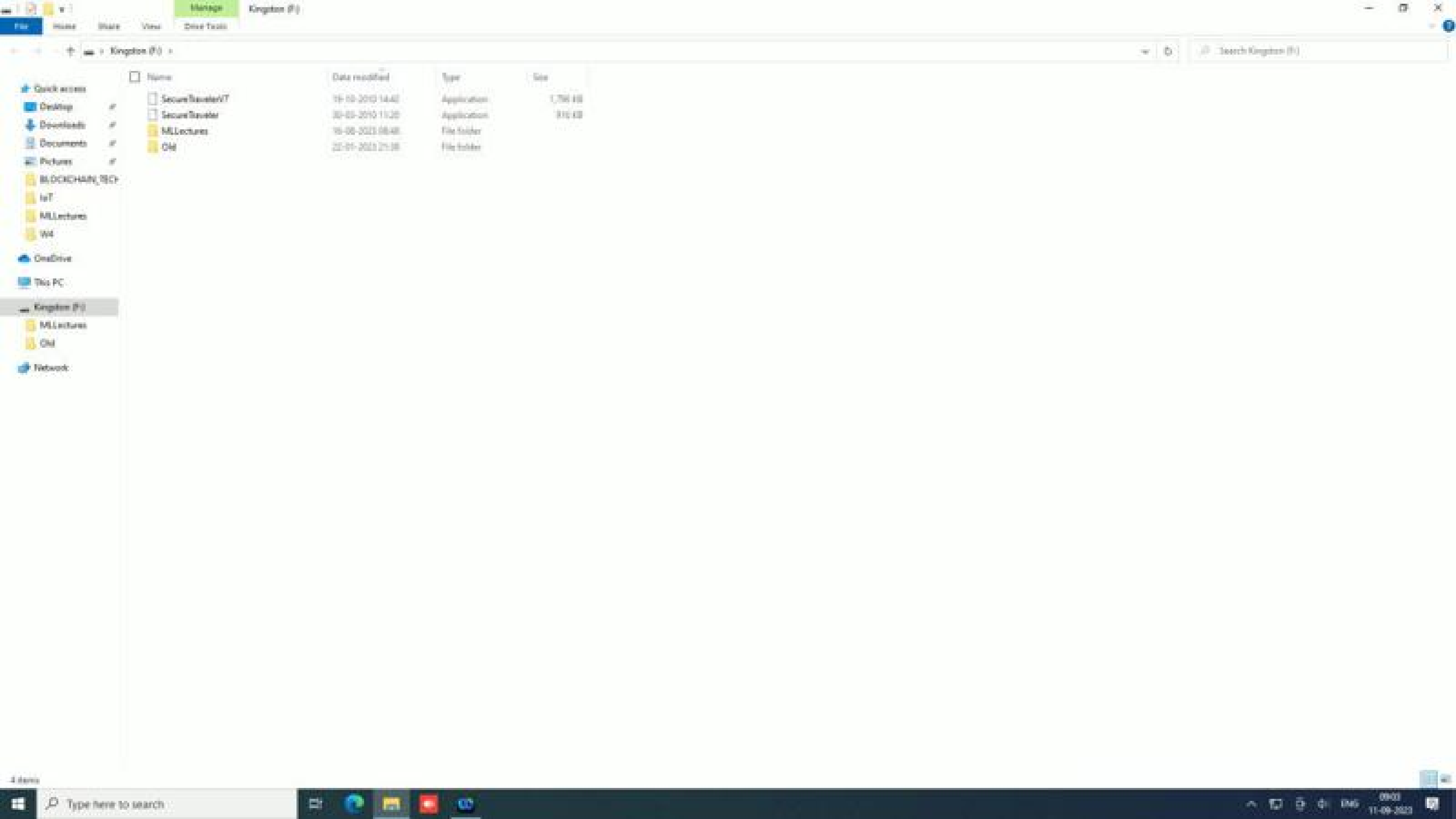

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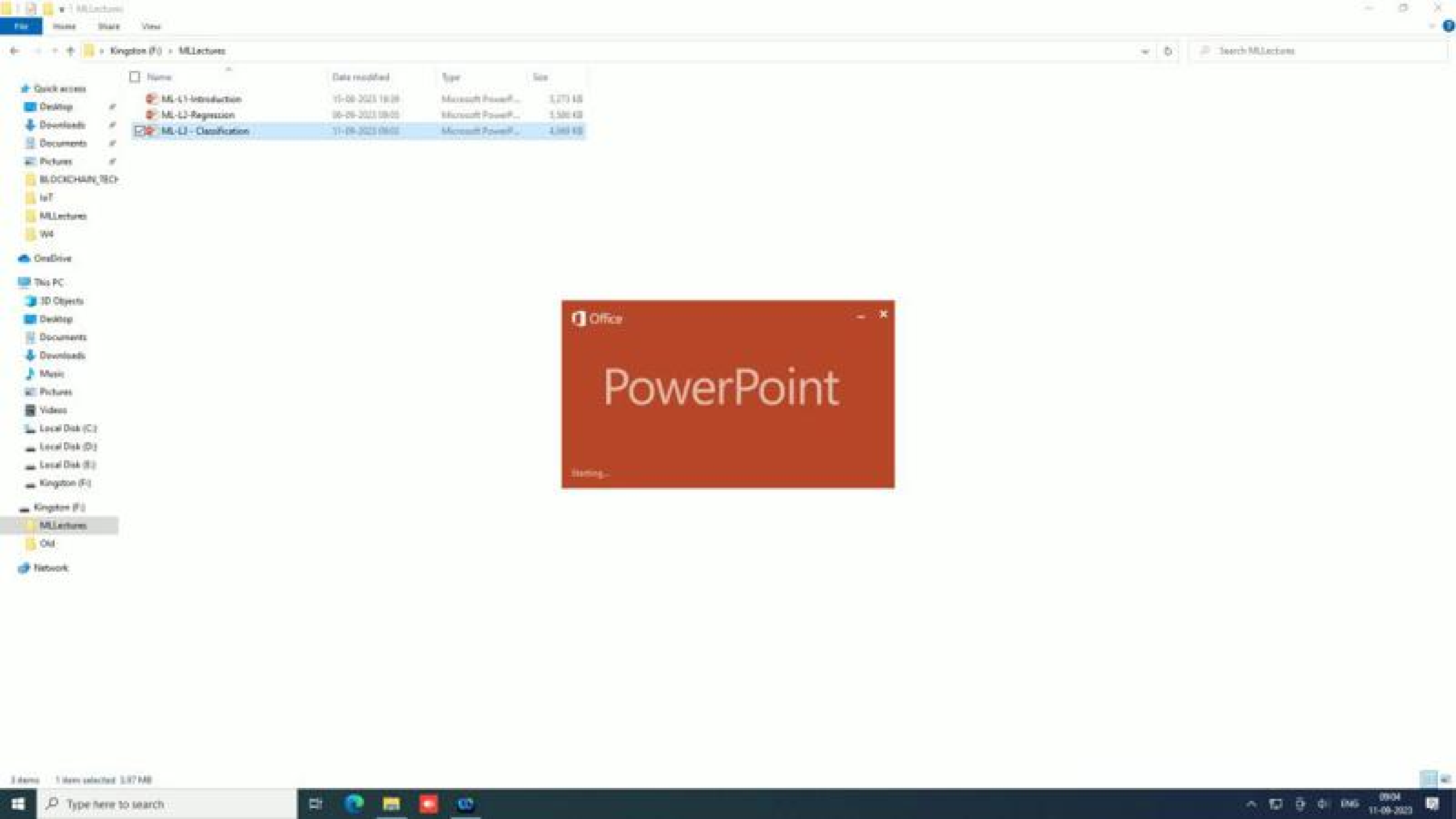

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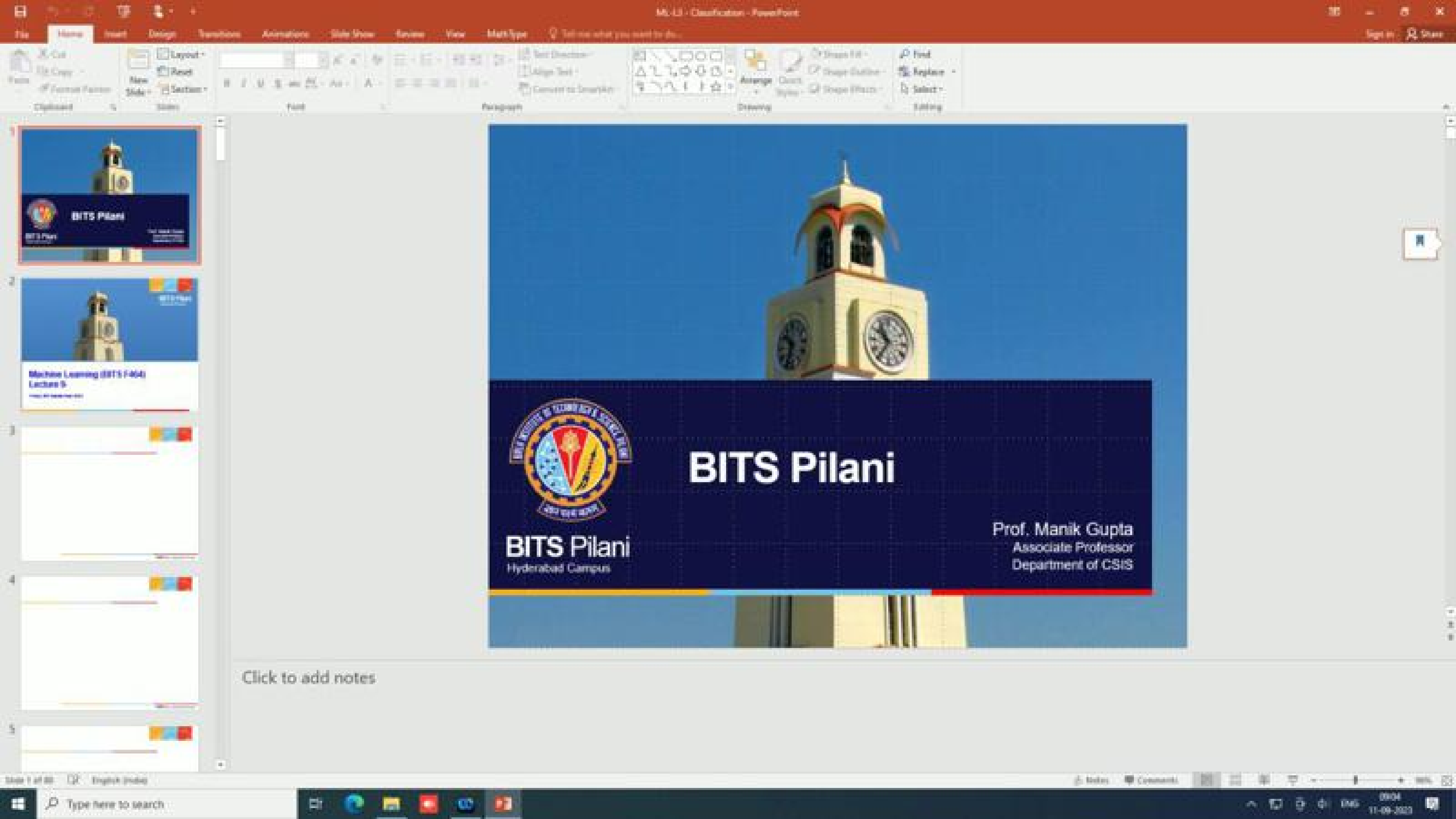
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Department of CSIS
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Agenda

Linear Models for Classification

- Discriminant Functions
- Least square classification
- Fishers Linear Discriminant
- Perceptron

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Linear Models for Classification

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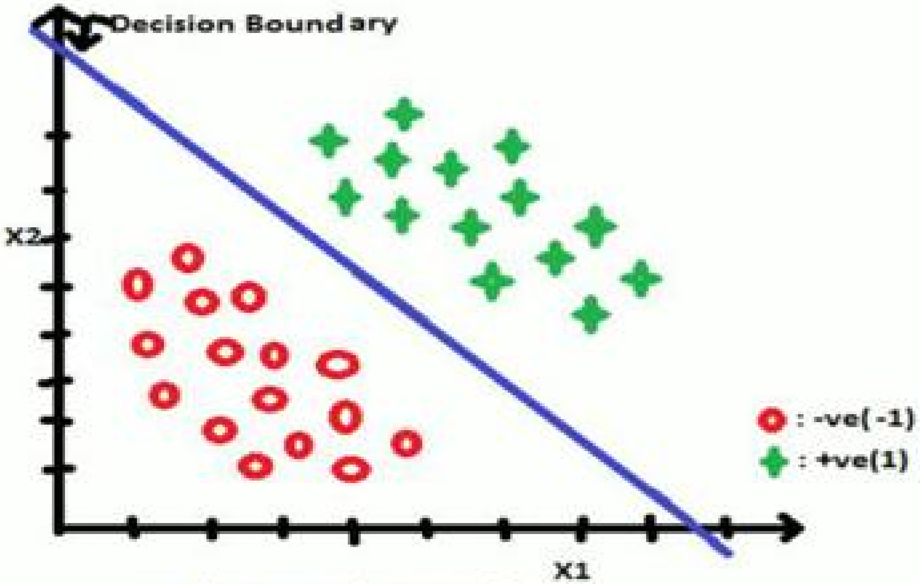
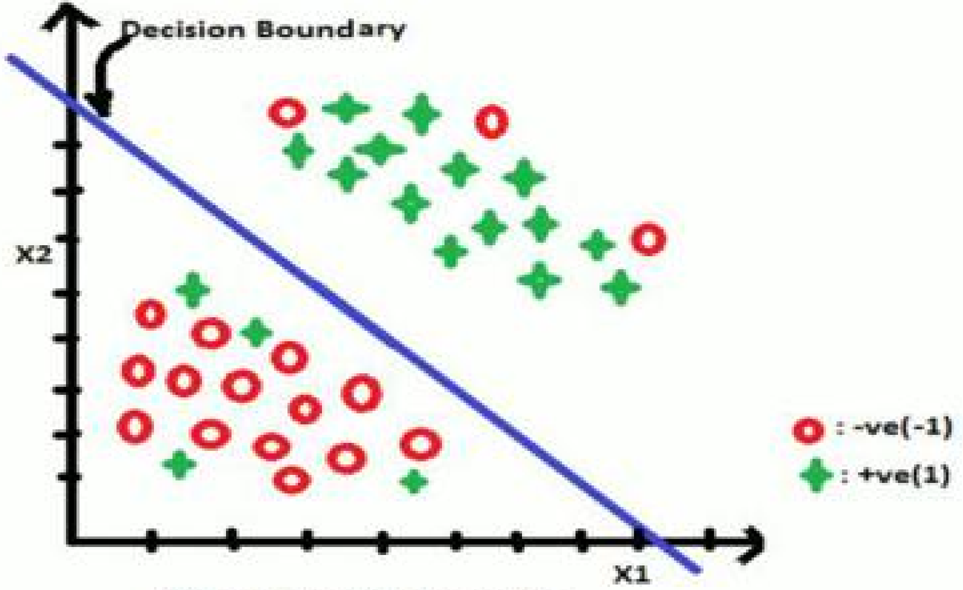
Introduction

- The goal in classification is to take an input vector $\boldsymbol{x}$ and to assign it to one of K discrete classes C_k where $k = 1, \ldots, K$.
- In the most common scenario, the classes are taken to be disjoint, so that each input is assigned to one and only one class.
- The input space is thereby divided into *decision regions* whose boundaries are called *decision boundaries* or *decision surfaces*.

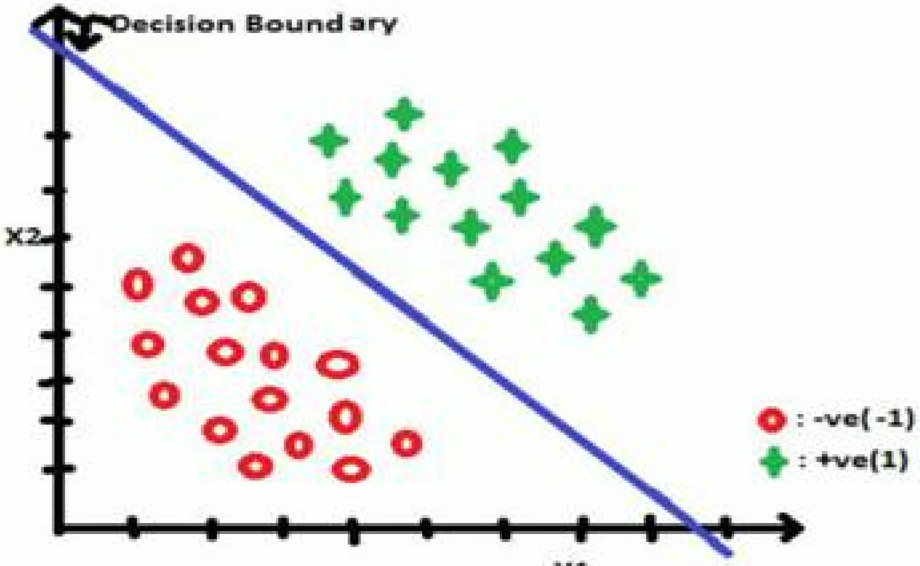
- We will consider linear models for classification, by which we mean that the decision surfaces are linear functions of the input vector $\boldsymbol{x}$ and hence are defined by $(D-1)$-dimensional hyperplanes within the D-dimensional input space.
- Datasets whose classes can be separated exactly by linear decision surfaces are said to be *linearly separable*.



Perfect Linearly separable



Almost Linearly Separable



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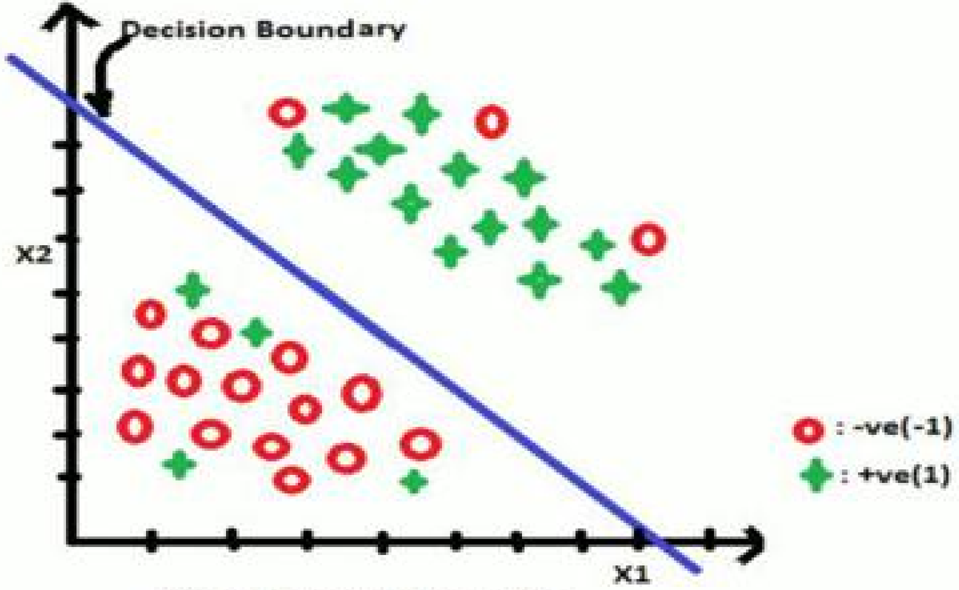


Almost Linearly Separable

- For regression problems, the target variable $\boldsymbol{t}$ was simply the vector of real numbers whose values we wish to predict.
- In the case of classification, there are various ways of using target values to represent class labels.
- For probabilistic models, the most convenient, in the case of two-class problems –
  - Binary representation in which there is a single target variable $t \in \{0, 1\}$ such that $t = 1$ represents class C_1 and $t = 0$ represents class C_2.
  - We can interpret the value of t as the probability that the class is C_1, with the values of probability taking only the extreme values of 0 and 1.

- For $K > 2$ classes, it is convenient to use a $1 - of - K$ coding scheme in which $\boldsymbol{t}$ is a vector of length K such that if the class is C_j , then all elements t_k of $\boldsymbol{t}$ are zero except element tj , which takes the value 1.
- For instance, if we have $K = 5$ classes, then a pattern from class 2 would be given the target vector

$$\mathbf{t} = (0, 1, 0, 0, 0)^{\mathrm{T}}.$$

Generalized linear models

- In the linear regression models considered, the model prediction $y(\boldsymbol{x}, \boldsymbol{w})$ was given by a linear function of the parameters $\boldsymbol{w}$.
- In the simplest case, the model is also linear in the input variables and therefore takes the form $y(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + w_0$, so that y is a real number.

- For classification problems, however, we wish to predict discrete class labels, or more generally posterior probabilities that lie in the range (0, 1).

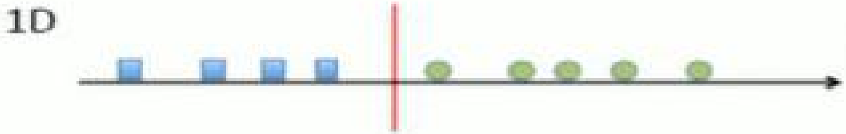
- To achieve this, we consider a generalization of this model in which we transform the linear function of $\boldsymbol{w}$ using a nonlinear function

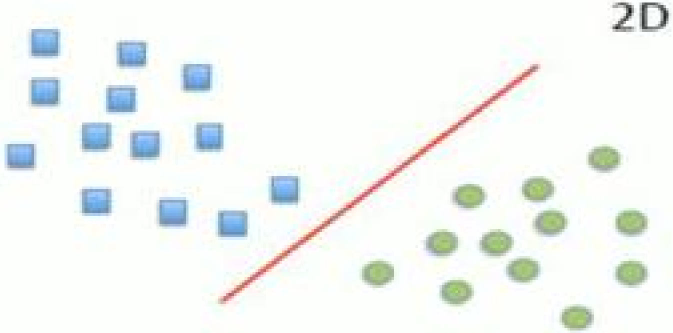
$f(\cdot)$ so that

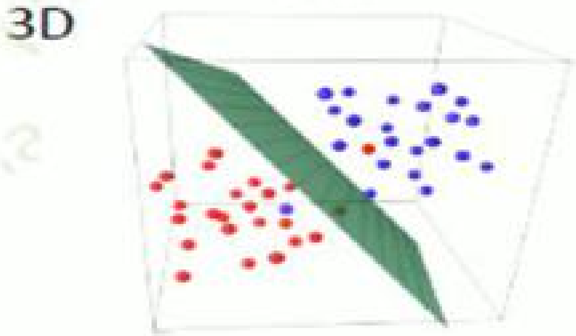
$$y(\mathbf{x}) = f\left(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0\right).$$

- In the machine learning literature, $f(\cdot)$ is known as an *activation function*, whereas its inverse is called a *link function* in the statistics literature.
- The decision surfaces correspond to $y(\boldsymbol{x}) = constant$, so that $\boldsymbol{w}^T\boldsymbol{x} + w_0 = constant$ and hence the decision surfaces are linear functions of $\boldsymbol{x}$, even if the function $f(\cdot)$ is nonlinear.
- For this reason, this class of models are called *generalized linear models*

Constant decision surfaces







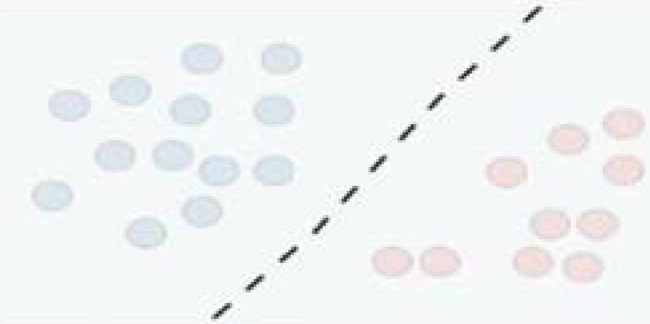
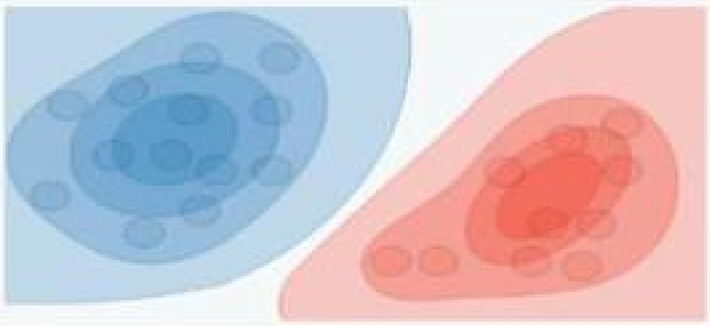
$$w_0 + \mathbf{w}^T \mathbf{x} = 0$$

All are linear boundaries

- Three distinct approaches to the classification problem.
  - The simplest involves constructing a **discriminant function** that directly assigns each vector $\boldsymbol{x}$ to a specific class.
  - A more powerful approach, however, models the conditional probability distribution $p(C_k|\boldsymbol{x})$ in an inference stage, and then subsequently uses this distribution to make optimal decisions.

- There are two different approaches to determining the conditional probabilities $p(C_k|\boldsymbol{x})$.

- There are two different approaches to determining the conditional probabilities $p(C_k|\boldsymbol{x})$.
  - One technique is to model them directly, for example by representing them as parametric models and then optimizing the parameters using a training set
  - Alternatively, we can adopt a generative approach in which we model the **class-conditional densities** given by $p(x|C_k)$, together with the **prior probabilities** $p(C_k)$ for the classes, and then we compute the required posterior probabilities using Bayes' theorem.

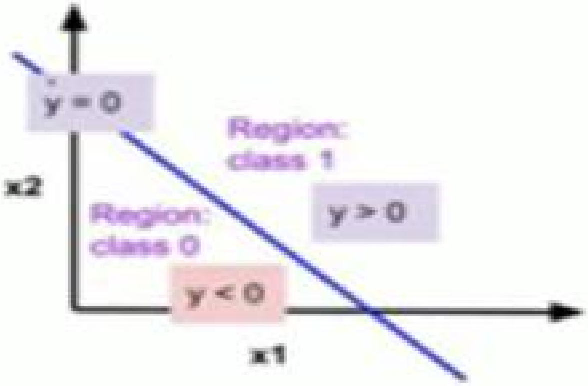
	Discriminative model	Generative model
Goal	Directly estimate $P(y\|x)$	Estimate $P(x\|y)$ to then deduce $P(y\|x)$
What's learned	Decision boundary	Probability distributions of the data
Illustration		
Examples	Regressions, SVMs	GDA, Naive Bayes

Discriminant Functions

- A discriminant is a function that takes an input vector $\boldsymbol{x}$ and assigns it to one of K classes, denoted C_k.

Discriminant functions learn direct mapping between feature vector $\mathbf{x}$ and label y.

- An input vector $\boldsymbol{x}$ is assigned to class C_1 if $y(\boldsymbol{x}) >= 0$ and to class C_2 otherwise.
- The corresponding decision boundary is therefore defined by the relation $y(\boldsymbol{x}) = 0$, which corresponds to a $(D-1)$-dimensional hyperplane within the D $-$dimensional input space.



- The simplest representation of a linear discriminant function is obtained by taking a linear function of the input vector so that

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

where w is the weight vector and w_0 is a bias.

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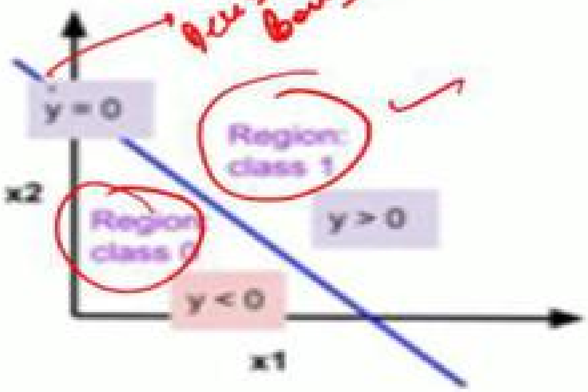
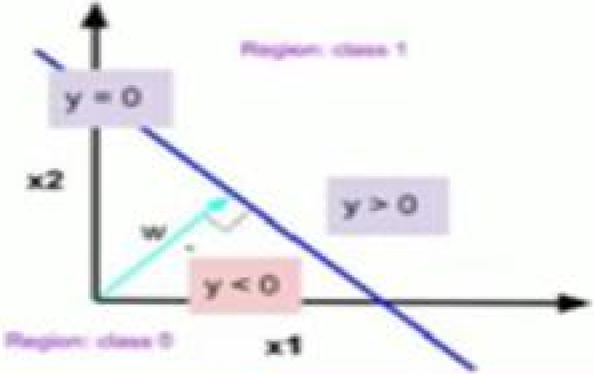
decision boundary



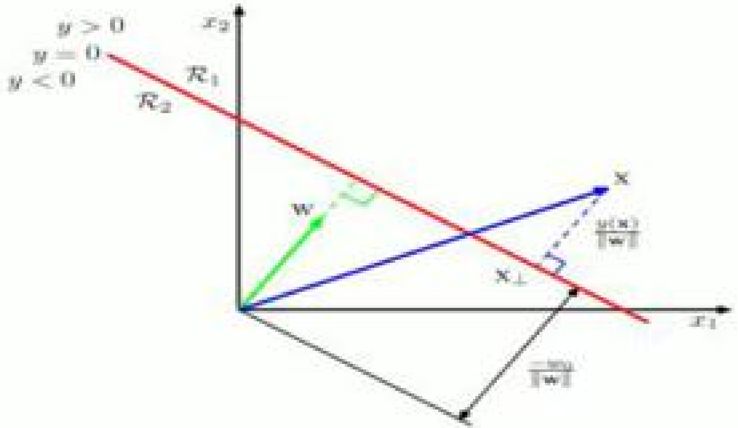
- Consider two points $\boldsymbol{x}_A$ and $\boldsymbol{x}_B$ both of which lie on the decision surface.
- Because $y(\boldsymbol{x}_A) = y(\boldsymbol{x}_B) = 0$, we have $\boldsymbol{w}^T(\boldsymbol{x}_A - \boldsymbol{x}_B) = 0$ and hence the vector $\boldsymbol{w}$ is orthogonal to every vector lying within the decision surface, and so $\boldsymbol{w}$ **determines the orientation of the decision surface.**
- Similarly, if $\boldsymbol{x}$ is a point on the decision surface, then $y(\boldsymbol{x}) = 0$, and so the normal distance from the origin to the decision surface is given by

$$\frac{\mathbf{w}^{\mathrm{T}}\mathbf{x}}{\|\mathbf{w}\|} = -\frac{w_0}{\|\mathbf{w}\|}.$$



- **Value of $y(x)$ gives a signed measure of the perpendicular distance r of the point x from the decision surface.**
- Consider an arbitrary point x and let $x_{\perp}$ be its orthogonal projection onto the decision surface, so that

$$\mathbf{x} = \mathbf{x}_{\perp} + r\frac{\mathbf{w}}{\|\mathbf{w}\|}.$$

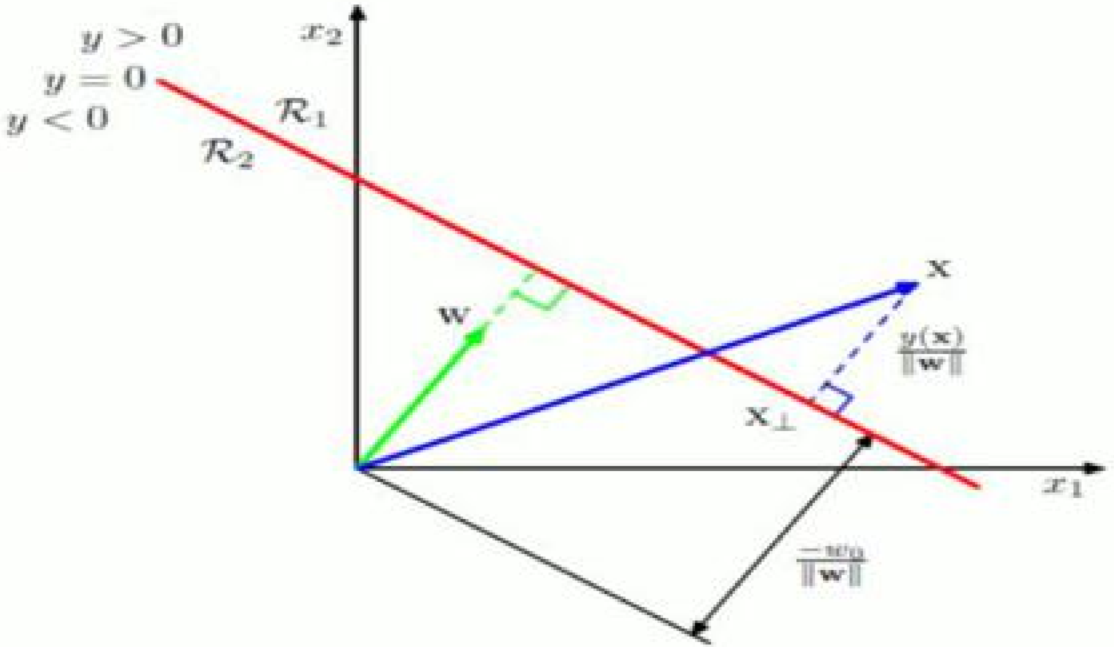


- Multiplying both sides of this result by w^T and adding w_0, and making use of $y(x) = w^T x + w_0$ and $y(x_{\perp}) = w^T x_{\perp} + w_0 = 0$, we have

$$r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}.$$

Geometry of discriminant function in 2D

- w_0 determines the location of the decision surface.
- $\mathbf{w}$ determines the orientation of the decision surface.
- y gives signed measure of perpendicular distance of the point $\mathbf{x}$ from the decision surface.
- Decision surface divides feature space into two regions.



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- Consider an arbitrary point $\boldsymbol{x}$ and let $\boldsymbol{x}_{\perp}$ be its orthogonal projection onto the decision surface, so that

$$\mathbf{x} = \mathbf{x}_{\perp} + r\frac{\mathbf{w}}{\|\mathbf{w}\|}.$$

- Multiplying both sides of this result by $\boldsymbol{w}^T$ and adding w_0, and making use of $y(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + w_0$ and $y(\boldsymbol{x}_{\perp}) = \boldsymbol{w}^T\boldsymbol{x}_{\perp} + w_0 = 0$, we have

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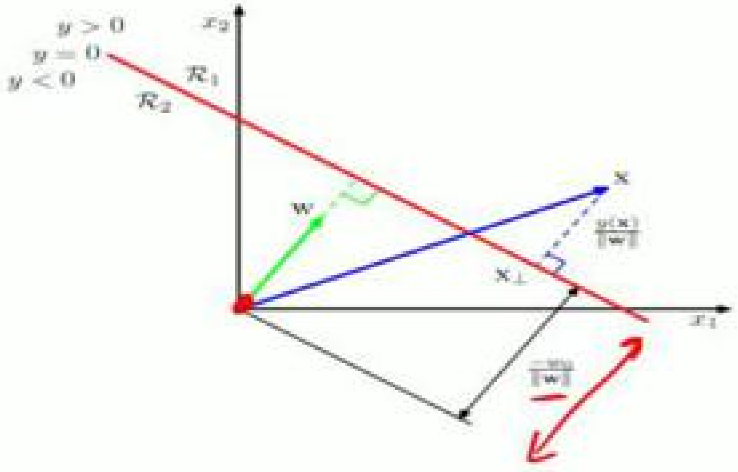

$-\frac{w_0}{\|w\|}$

Geometry of discriminant function in 2D

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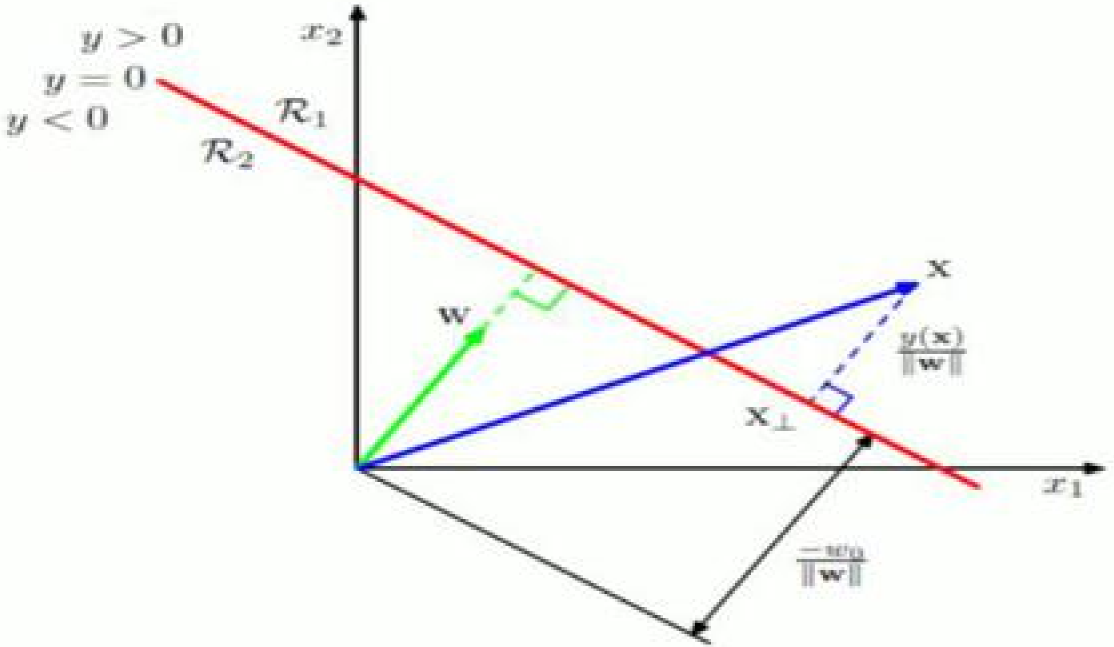

Agenda

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- Discriminant Functions
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- Fishers Linear Discriminant
- Perceptron

Click to add notes

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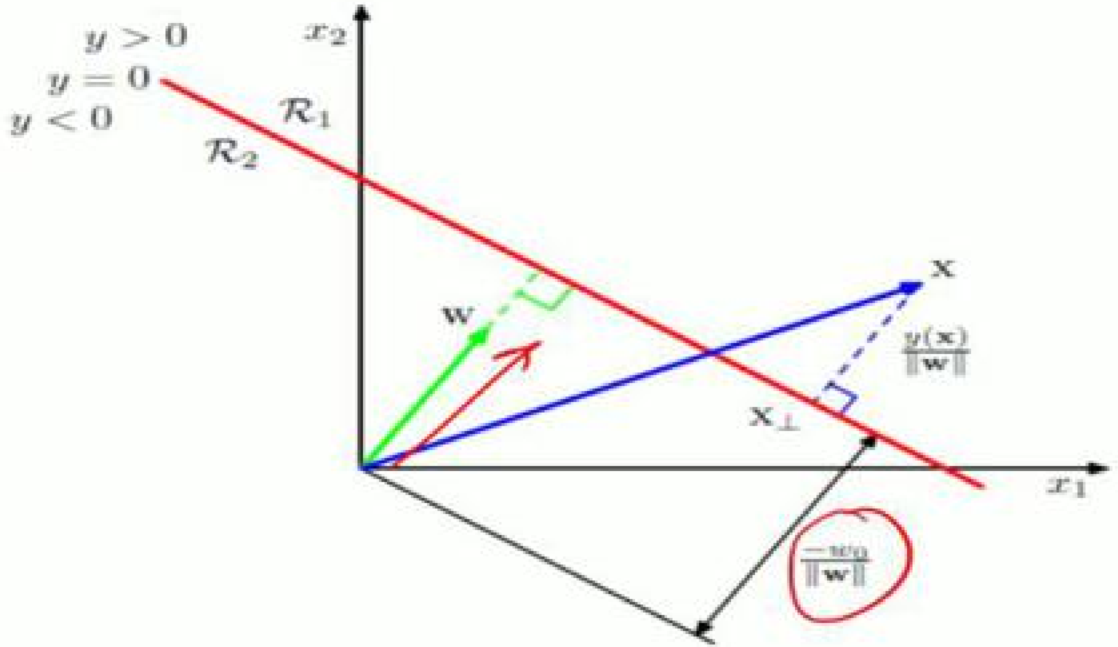


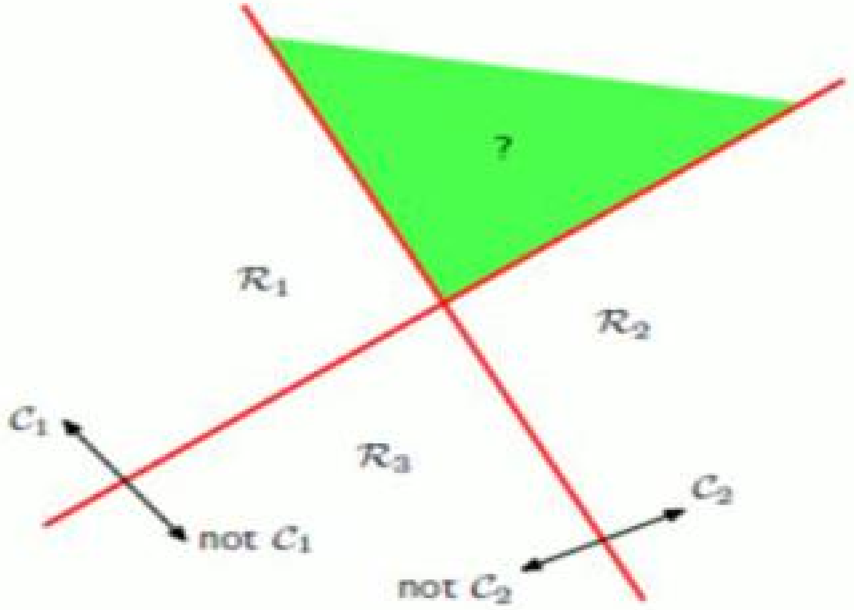
Multiple Classes

- Assuming the number of classes to be K>2, the discriminant functions can be build in two ways by combining a number of two-class discriminant functions

  - **One vs rest** – build K-1 discriminant functions. Each discriminant function solves a two class classification problem.

  - **One vs one** – one discriminant function per pair of classes. Each point is then classified according to a majority vote amongst the discriminant functions.

Issues with one-vs-rest



Issues with one-vs-rest

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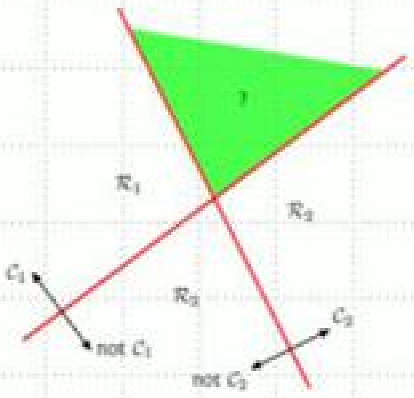

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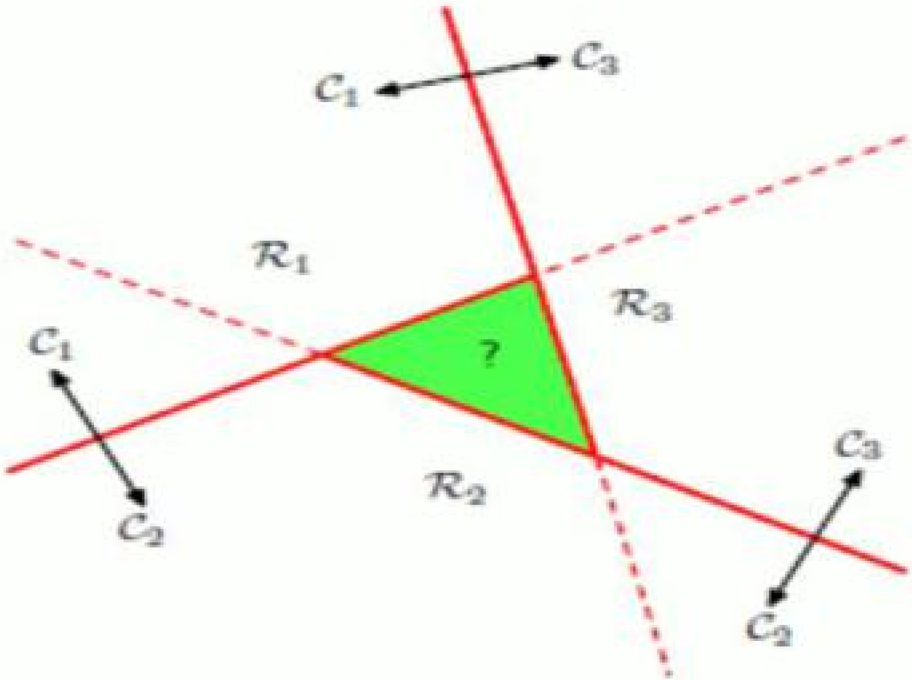
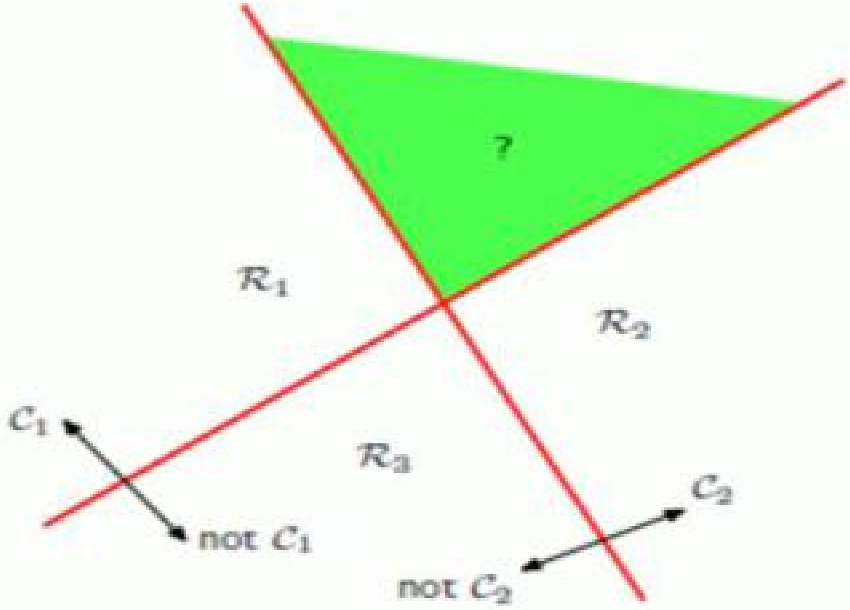
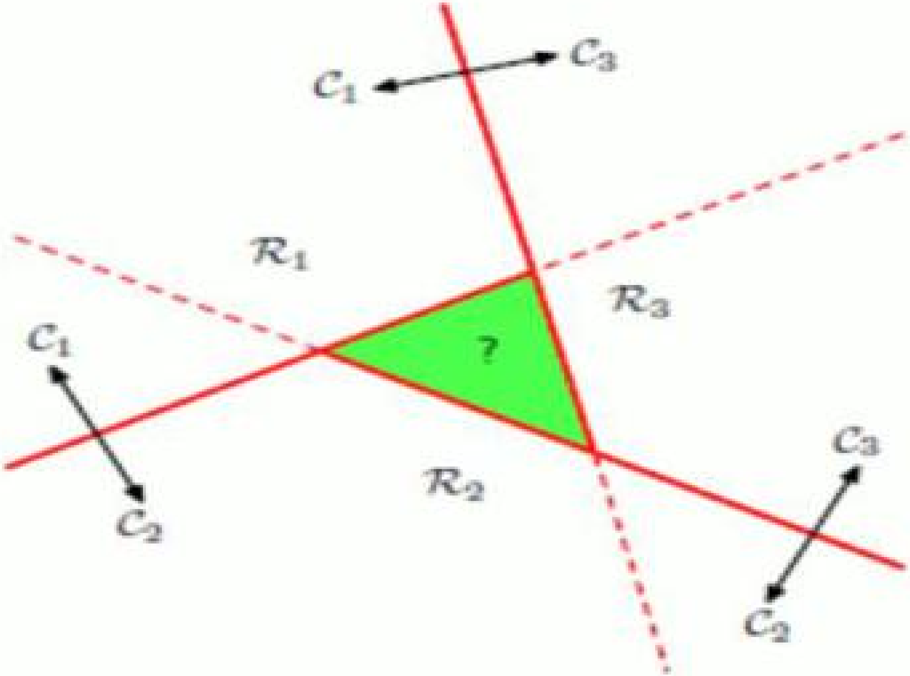
Issues with one-vs-one



Issues with one-vs-rest



Issues with one-vs-one



- Considering a single K-class discriminant comprising K linear functions of the form

$$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$

and then assigning a point $\boldsymbol{x}$ to class C_k if $y_k(\boldsymbol{x}) > y_j(\boldsymbol{x})$ for all $j \neq k$.

- The decision boundary between class C_k and class C_j is therefore given by $y_k(\boldsymbol{x}) = y_j(\boldsymbol{x})$ and hence corresponds to a $(D-1)$-dimensional hyperplane defined by

$$(\mathbf{w}_k - \mathbf{w}_j)^{\mathrm{T}}\mathbf{x} + (w_{k0} - w_{j0}) = 0.$$

- Three approaches to learning the parameters of linear discriminant functions, based on
  - Least Squares
  - Fisher's Linear Discriminant
  - Perceptron Algorithm

Least square classification

- Consider a classification problem with K classes, with a 1-of-K binary coding scheme for the target vector t.
- Each class C_k has its own linear model.
- Each class C_k is described by its own linear model so that

$$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$

- This can be rewritten as

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}}\widetilde{\mathbf{x}}$$

where , $\widetilde{\boldsymbol{W}}$ is a matrix whose k^{th} column comprises the D + 1-dimensional vector $\widetilde{\boldsymbol{w}}_k = (w_{k0}, \boldsymbol{w}_{\boldsymbol{k}}^{\boldsymbol{T}})^{\mathrm{T}}$ and $\widetilde{\boldsymbol{x}}$ is the corresponding augmented input vector $(1, \boldsymbol{x}^T)^T$ with a dummy input $x_0 = 1$.

$$\widetilde{W} = \begin{bmatrix} w_1^0 & \cdots & w_K^0 \\ \vdots & \vdots & \vdots \\ w_1^D & \cdots & w_K^D \end{bmatrix}$$

- A new input $\boldsymbol{x}$ is then assigned to the class for which the output $y_k = \widetilde{w}_k^T \widetilde{x}$ is largest.

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- We now determine the parameter matrix , $\widetilde{\boldsymbol{W}}$ by minimizing a sum-of-squares error function
- Consider a training data set $\{\boldsymbol{x}_n, \boldsymbol{t}_n\}$ where $n = 1, \ldots, N$, and define a matrix $\boldsymbol{T}$ whose n^{th} row is the vector $\boldsymbol{t}_{\boldsymbol{n}}^{\boldsymbol{T}}$, together with a matrix $\boldsymbol{X}$ whose n^{th} row is $\boldsymbol{x}_{\boldsymbol{n}}^{\boldsymbol{T}}$

$$T = \begin{bmatrix} t_1^1 & \dots & t_1^K \\ \vdots & \vdots & \vdots \\ t_N^1 & \dots & t_N^K \end{bmatrix}, \tilde{X} = \begin{bmatrix} x_1^0 & \dots & x_1^D \\ \vdots & \vdots & \vdots \\ x_N^0 & \dots & x_N^D \end{bmatrix}$$

- The sum-of-squares error function can then be written as

$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}.$$

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3 4

$$T = \begin{array}{cc} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} & \begin{array}{l} \to c1 \\ \to c2 \\ \to c3 \\ \to c4 \end{array} \end{array}$$

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$$\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$$

(D+1) × K matrix whose kth column comprises of D+1 dimensional vector:

$$\tilde{\mathbf{w}}_k = (w_{k0}, \mathbf{w}_k^T)^T.$$

corresponding augmented input vector:

$$\tilde{\mathbf{x}} = (1, \mathbf{x}^T)^T.$$

$$\tilde{\mathbf{W}} = (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T \mathbf{T}$$

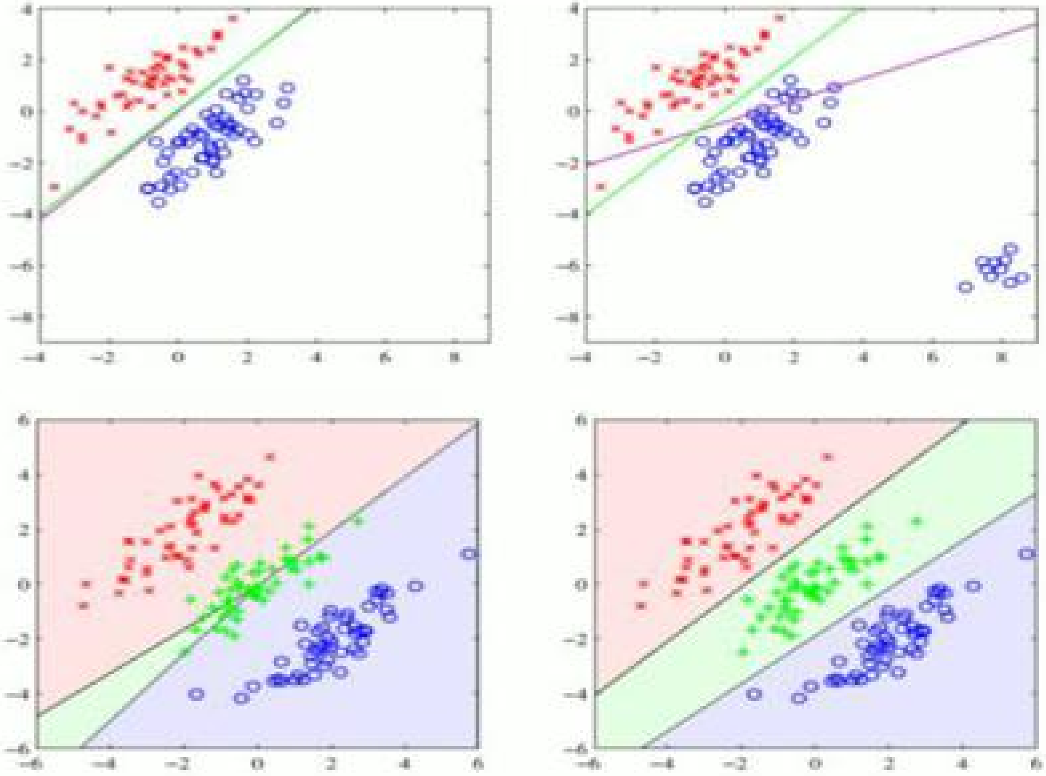
Optimal weights

N × (D+1) input matrix whose n^{th} row is $\tilde{\mathbf{x}}_n^T$.

N × K target matrix whose n^{th} row is $\mathbf{t}_n^T$.

Issues with LSC

- Least-squares solutions lack robustness to outliers and can give poor results.

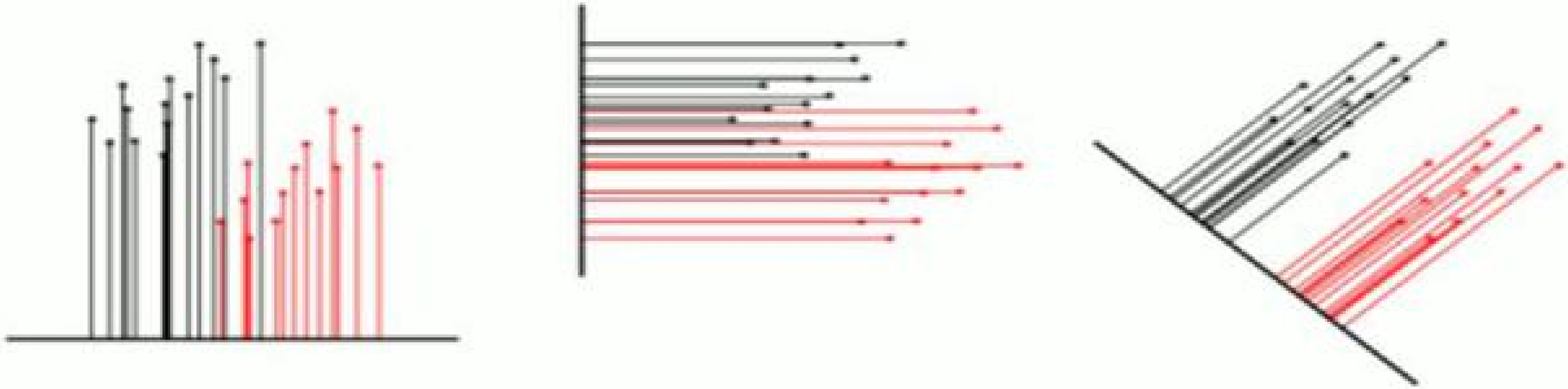


Fisher's linear discriminant

- One way to view a linear classification model is in terms of dimensionality reduction.
- Suppose we take a D-dim input vector and project it down to one dimension using $y = \boldsymbol{w}^T \boldsymbol{x}$

- Main Idea: Find the projection that maximizes the class separation.

Projection of data from two classes onto various lines



Projection of data from two classes onto various lines

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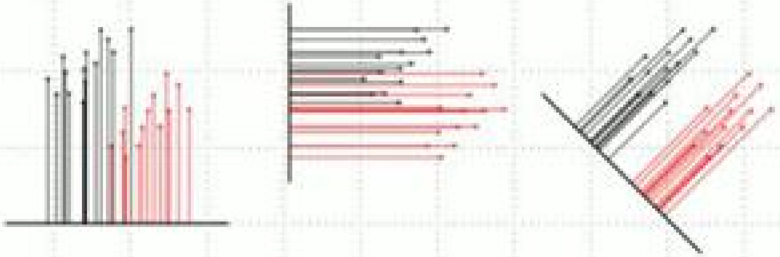

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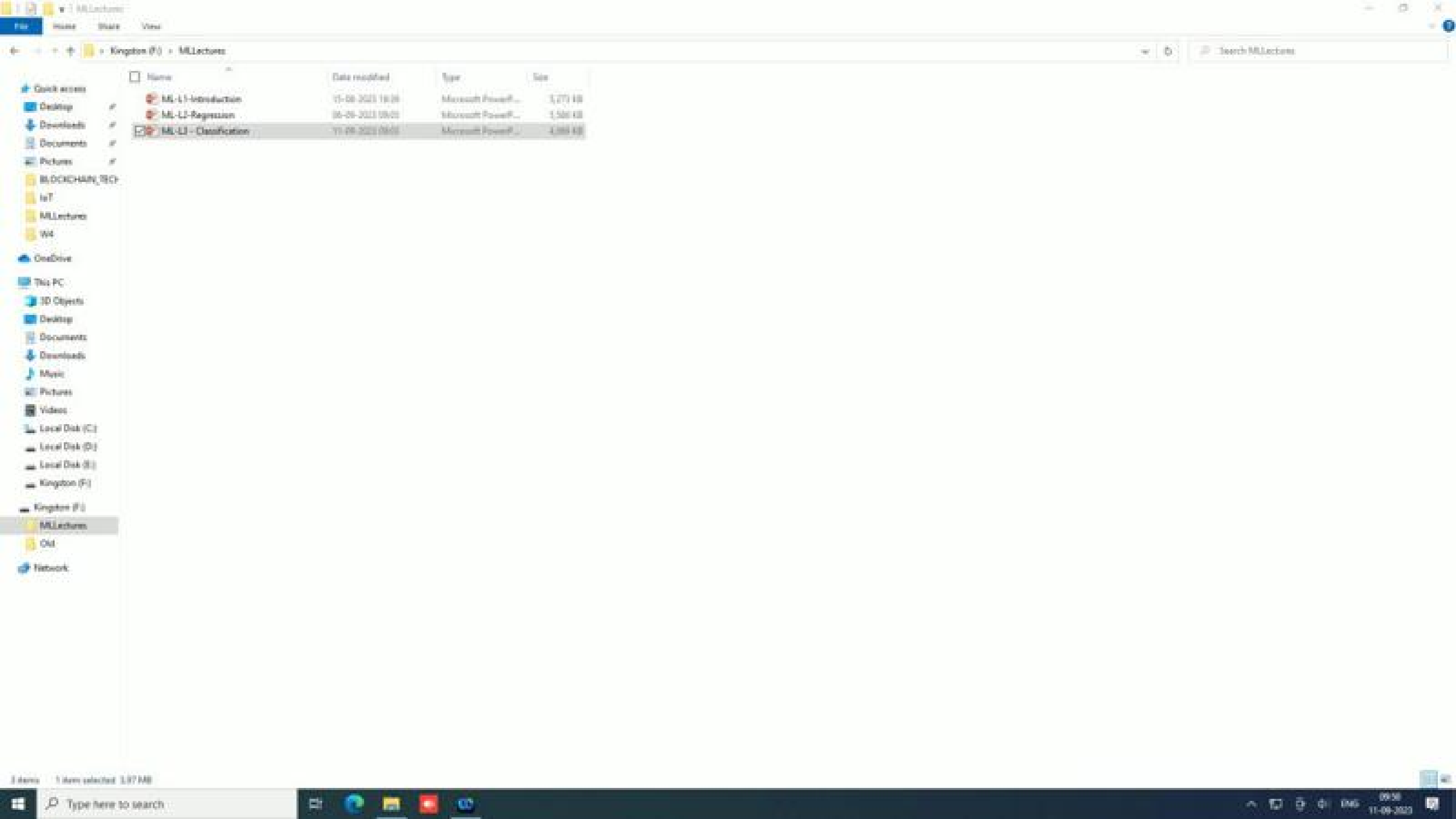
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