

Support Vector Machines



- Support Vector Machines are one of the more complex algorithms we will learn, but it all begins with a simple premise:
 - Does a hyperplane exist that can effectively separate classes?



- Section Overview
 - Intuition and Theory for SVM
 - SVM Classification Example
 - SVM Regression Example
 - SVM Project Exercise and Solutions



- Relevant Reading in ISLR
 - Chapter 9 covers Support Vector Machine Classification
 - Wikipedia has a section on Support Vector Machine Regression.



Support Vector Machines

Theory and Intuition - Hyperplanes and Margins



- We will slowly build up to SVMs:
 - Maximum Margin Classifier
 - Support Vector Classifier
 - Support Vector Machines
 - Let's begin by understanding what a hyperplane is...

- In an N-dimensional space, a hyperplane is a flat affine subspace of hyperplane dimension N – 1.
- For example:
 - 1-D Hyperplane is a single point
 - 2-D Hyperplane is a line
 - 3-D Hyperplane is flat plane



1-D Hyperplane is a single point





1-D Hyperplane is a single point





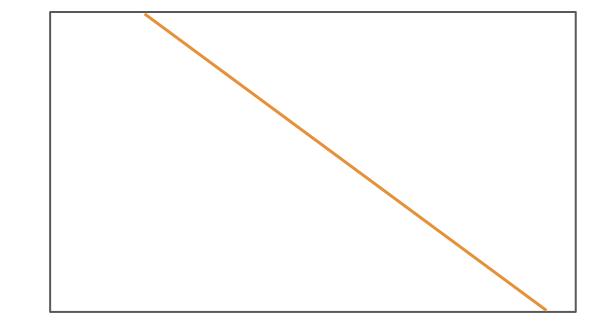
• 2-D Hyperplane is a line

X2



• 2-D Hyperplane is a line

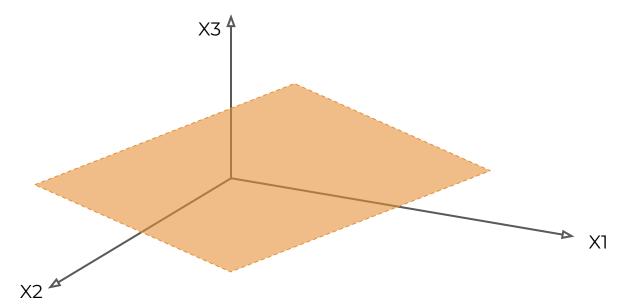
X2



X1

Support Vector Machines

• 3-D Hyperplane is a flat plane



- The main idea behind SVM is that we can use Hyperplanes to create a separation between classes.
- Then new points will fall on one side of this separating hyperplane, which we can then use to assign a class.



- Imagine a data set with one feature and one binary target label.
- For example:
 - A weight feature for baby chicks
 - Classified by Male or Female
- What would this look like visualized?



Place points along feature.







 Notice in this case, classes are perfectly separable. This is unlikely in real world datasets.



WEIGHT





 Idea behind SVM is to create a separating hyperplane between the classes.







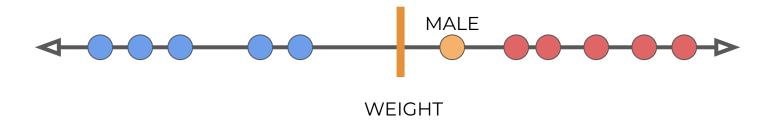
 A new point would be classified based on what side of the point they land on.







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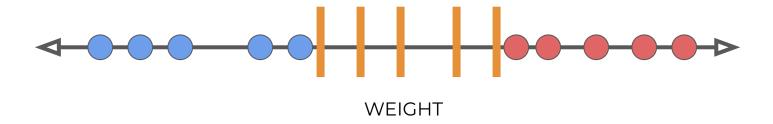
 How do we choose where to put this separating hyperplane?







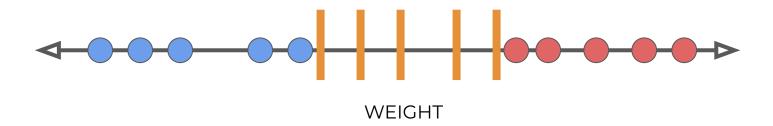
 Note there are many options that perfectly separate out these classes:







 Which of these is the "best" separator between the classes?







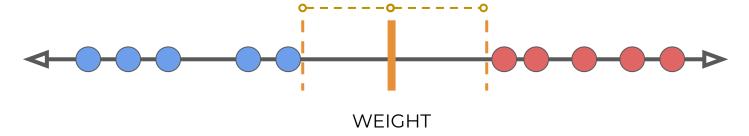
 We could use the separator that maximizes the margins between the classes.







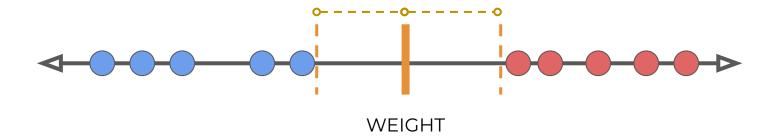
 We could use the separator that maximizes the margins between the classes.







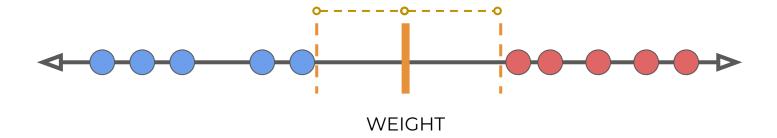
 This is known as a Maximal Margin Classifier.







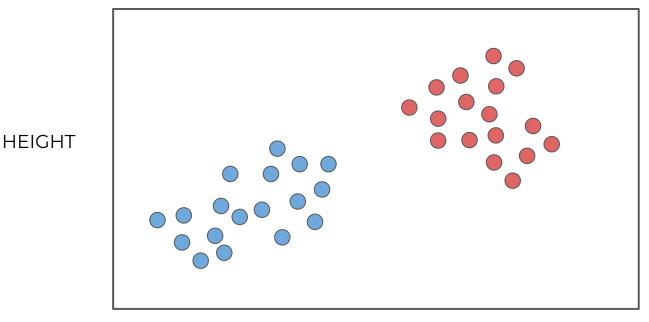
 This same idea of maximum margins applies to N-dimensions.

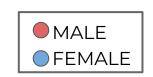






Imagine a 2 dimensional feature space:

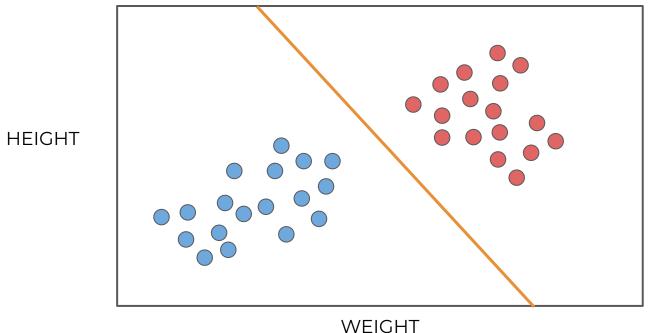




WEIGHT

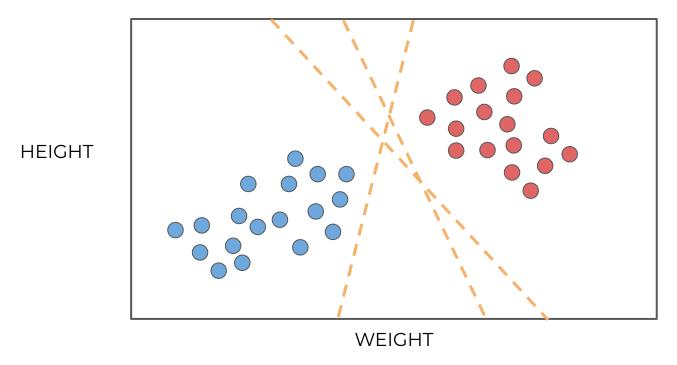


Separating hyperplane is a line.



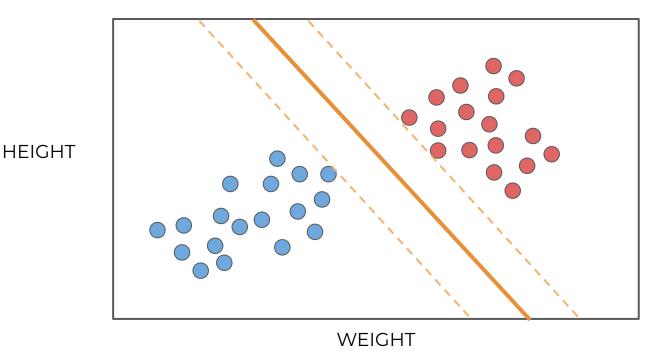


Multiple possible hyperplanes:



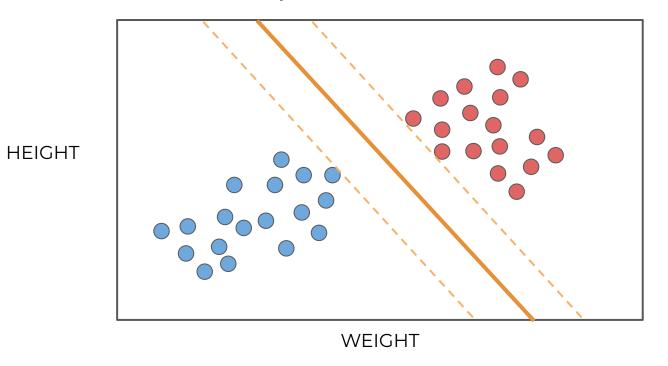


• Choose to maximize margins:



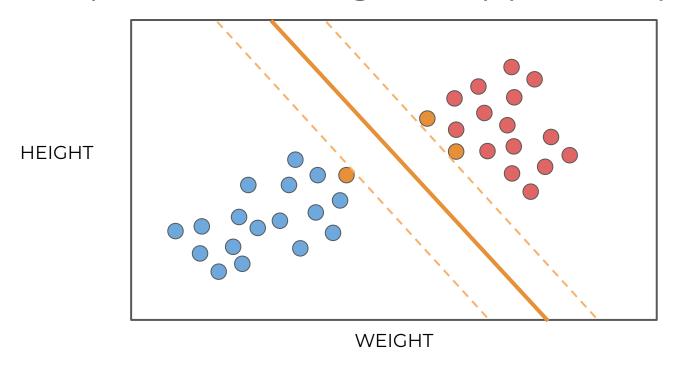


Note each data point is a 2D vector:



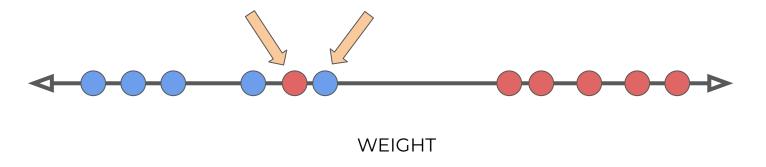


Data points at margin "support" separator:





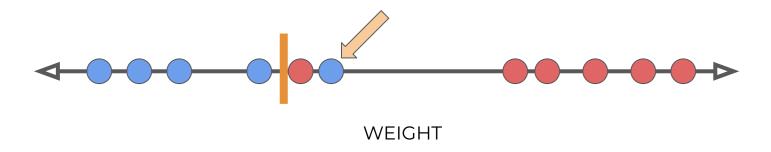
 What happens if classes are not perfectly separable?







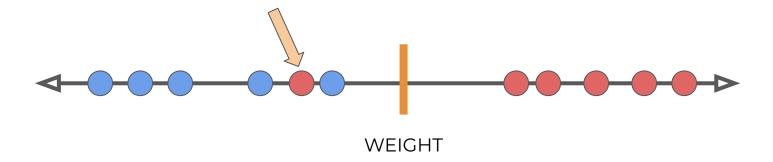
 We are not be able to separate without allowing for misclassifications.







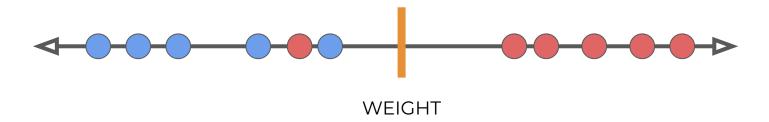
 We are not be able to separate without allowing for misclassifications.







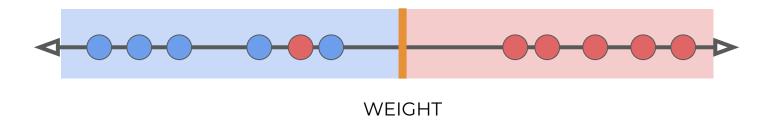
 We will have a bias-variance trade-off depending where we place this separator:







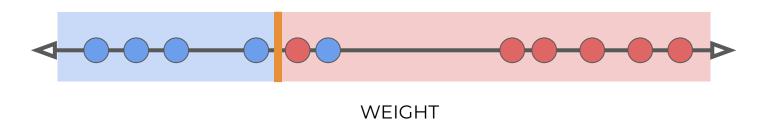
 For one feature this classifier creates ranges for male and female:







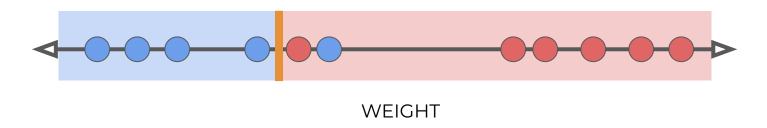
 This fit only misclassified one female training point as male:







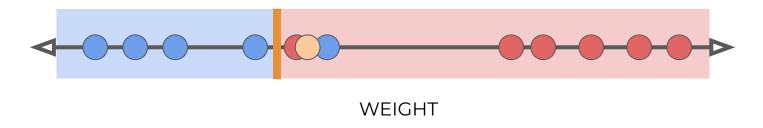
 This looks like a high variance fit to training data, picking too much noise from Female:







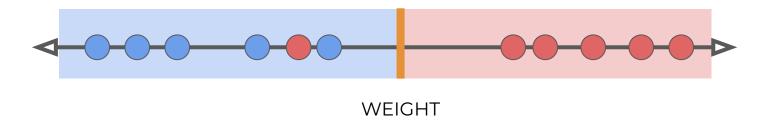
 A new test point close to existing female weights could get classified as male:







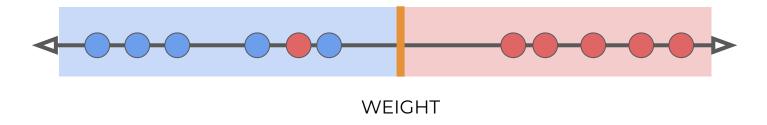
 We will have a bias-variance trade-off depending where we place this separator:







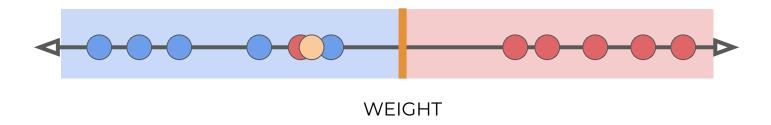
 Here we allow more bias to lead to better long term results on future data:







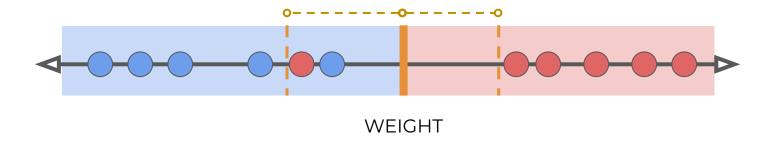
 Here we allow more bias to lead to better long term results on future data:







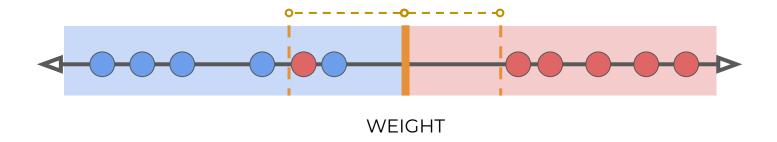
 Distance between threshold and the observations is a soft margin:







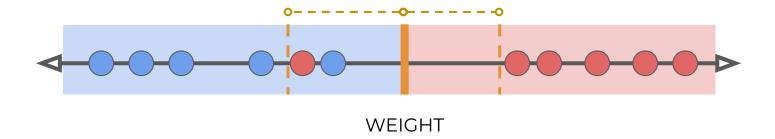
 Soft margin allows for misclassification inside the margins.







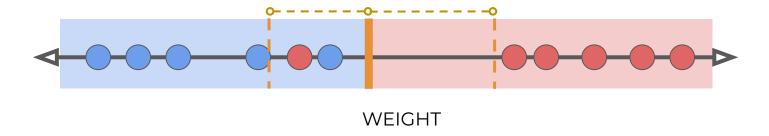
• There are many possible threshold splits if we allow for soft margins.







 We can use cross validation to determine the optimal size of the margins.

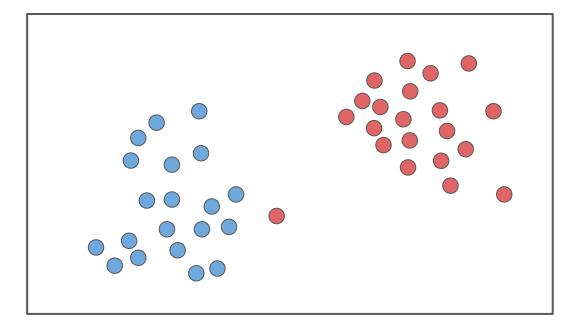






HEIGHT

• 2D soft margin example:



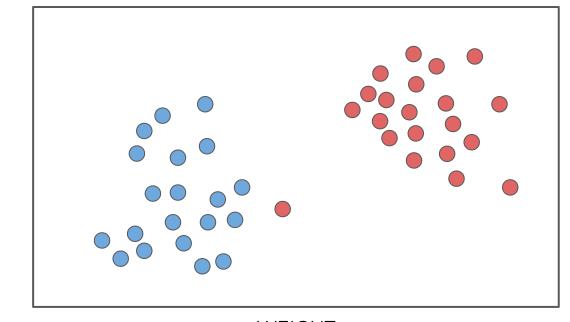
MALE FEMALE

WEIGHT



HEIGHT

Data set is technically perfectly separable

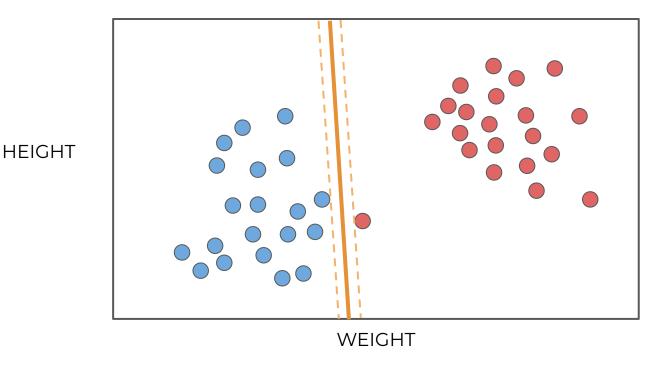


MALE FEMALE

WEIGHT



Maximal Margin Classifier

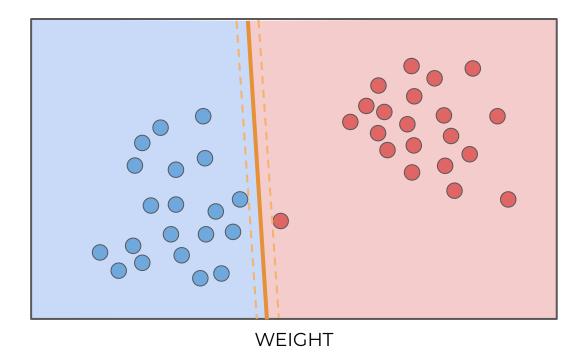


MALE FEMALE



Maximal Margin Classifier

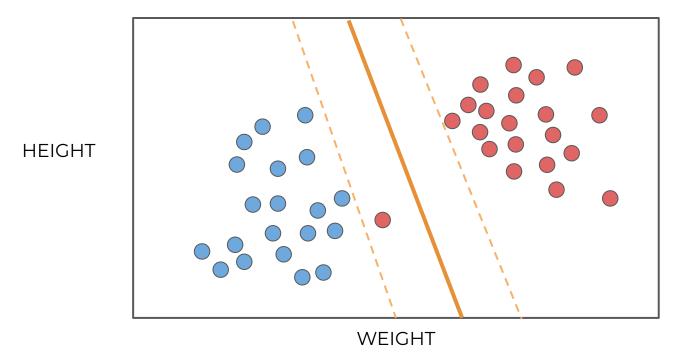
HEIGHT







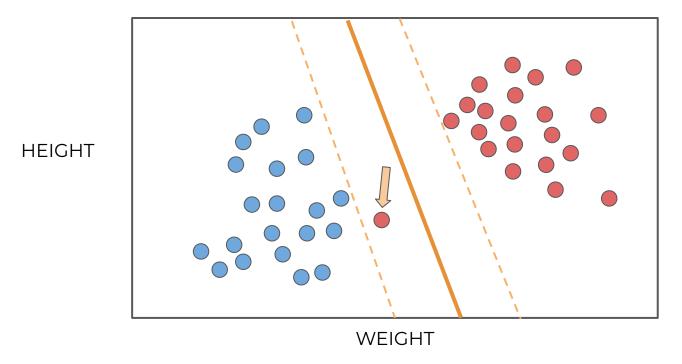
Support Vector Classifier (Soft Margins)



MALE FEMALE



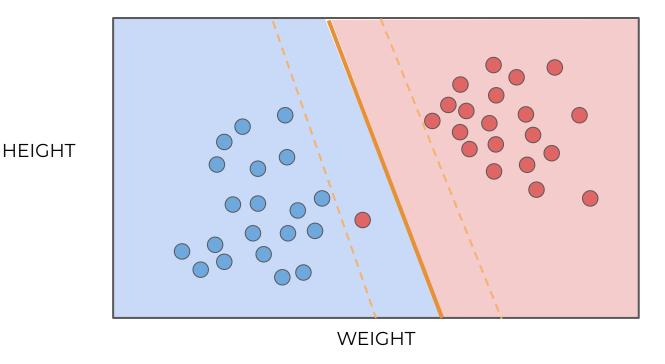
Support Vector Classifier (Soft Margins)



MALE FEMALE



Support Vector Classifier (Soft Margins)

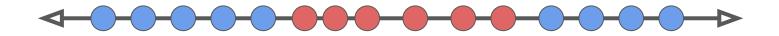






- We've only visualized cases where the classes are easily separated by the hyperplane in the original feature space.
- Allowing for some misclassifications still resulted in reasonable results.
- What would happen in a case where a hyperplane performs poorly, even when allowing for misclassifications?





FEATURE

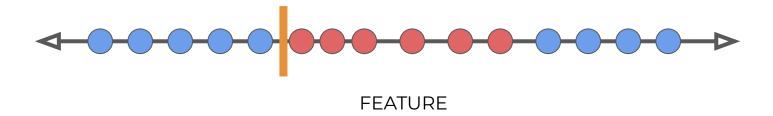






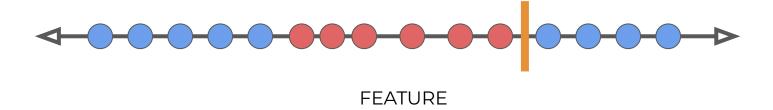










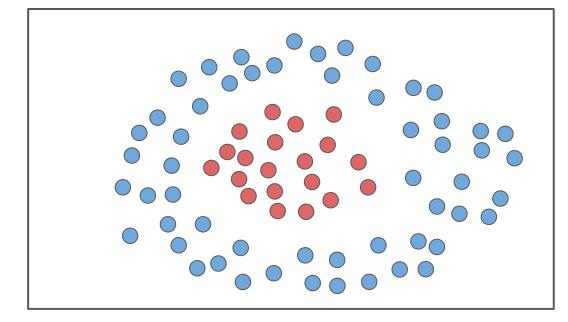


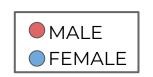




FEATURE

Can't split classes with hyperplane line:





FEATURE



- To solve these cases, we move on from Support Vector Classifier, to Support Vector Machines.
- SVMs use **kernels** to project the data to a higher dimension, in order to use a hyperplane in this higher dimension to separate the data.



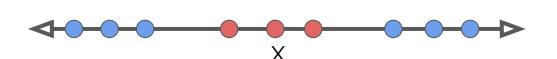
Theory and Intuition - Kernels



- Kernels allow us to move beyond a Support Vector Classifier and use Support Vector Machines.
- There are a variety of kernels we can use to "project" the features to a higher dimension.
- Let's explore how this works through some visual examples...



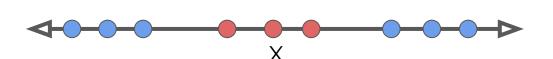
 Recall our 1D example of classes not easily separated by a single hyperplane:





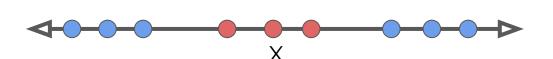


 Let's explore how using a kernel could project this feature onto another dimension.



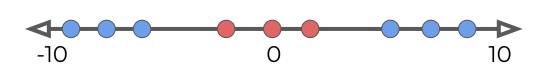






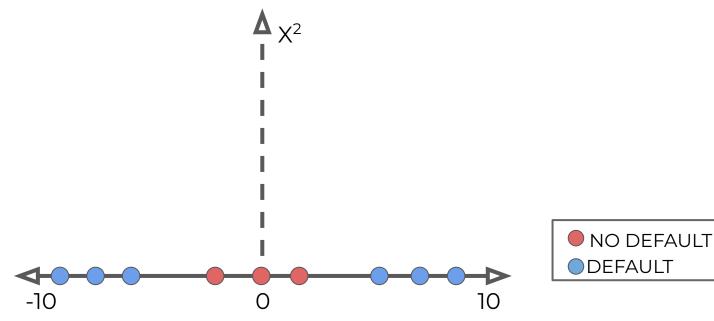




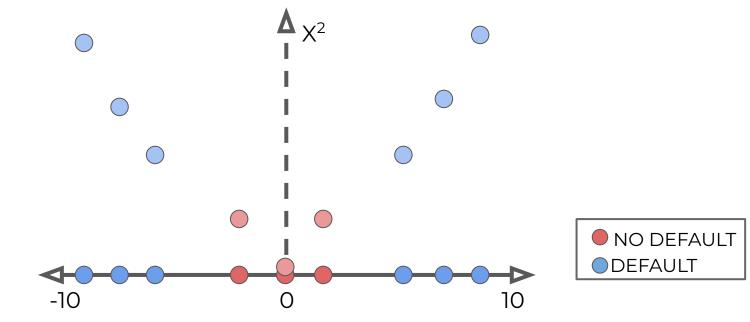






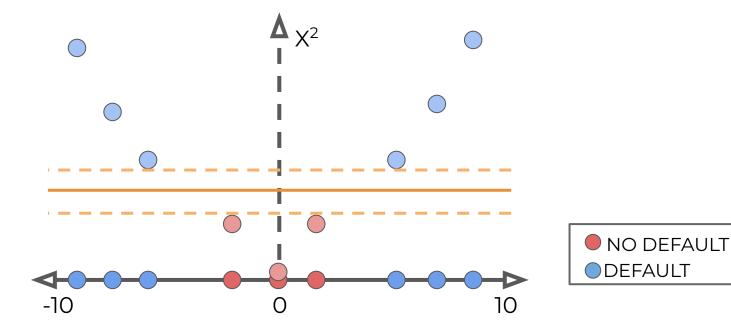






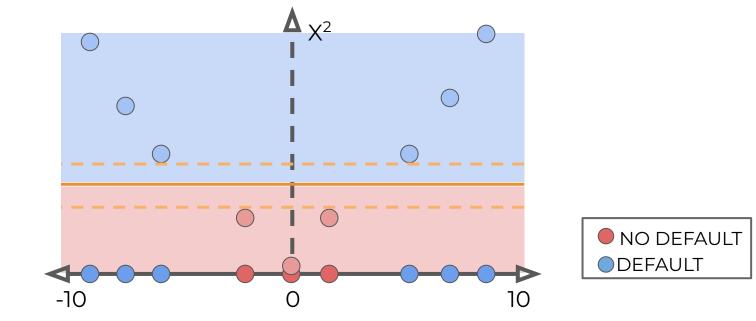


• Create a hyperplane after this projection:

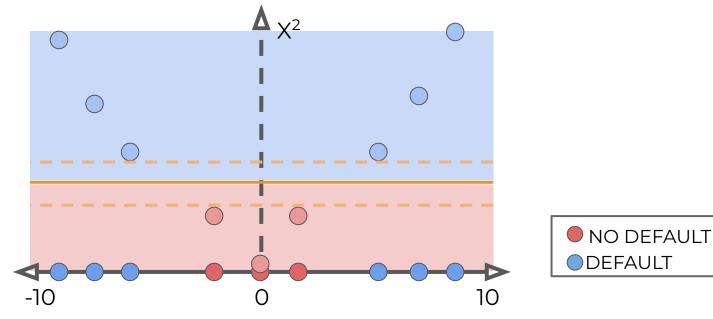




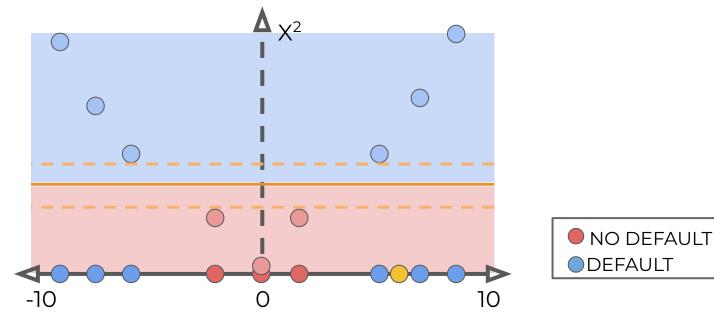
• Create a hyperplane after this projection:



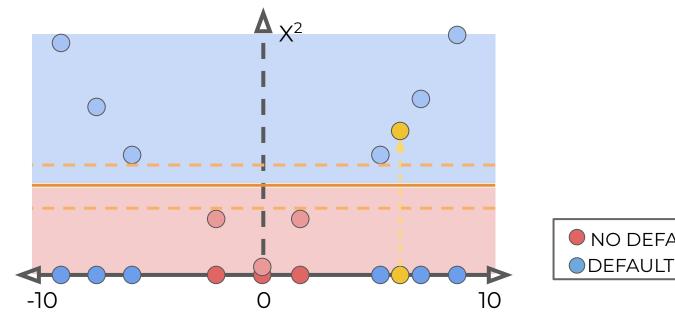






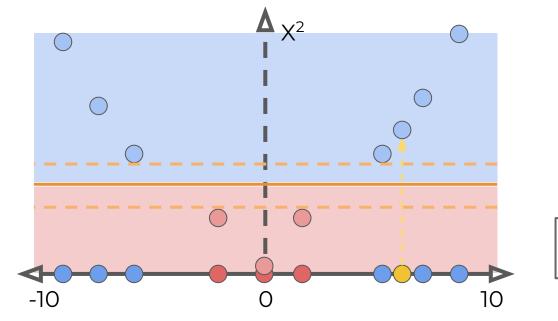






NO DEFAULT



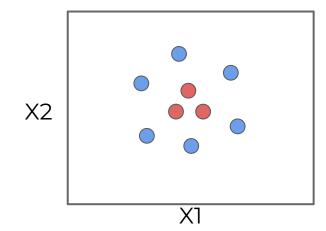


NO DEFAULT

DEFAULT

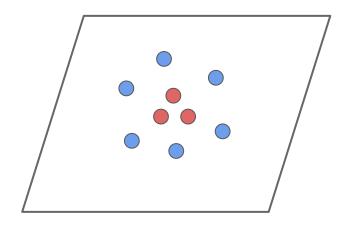


 Imagine a 2D feature space where a hyperplane can not separate effectively, even with soft margins.



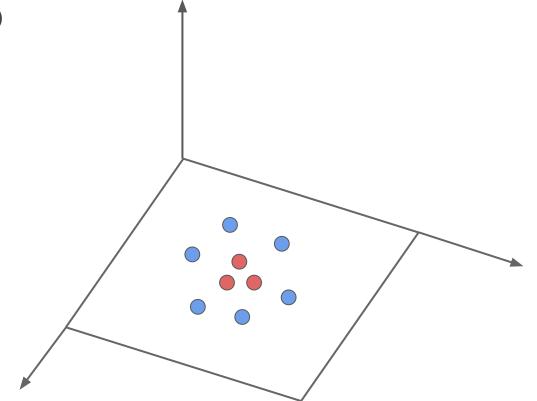


 We use Support Vector Machines to enable the use of a kernel transformation to project to a higher dimension.



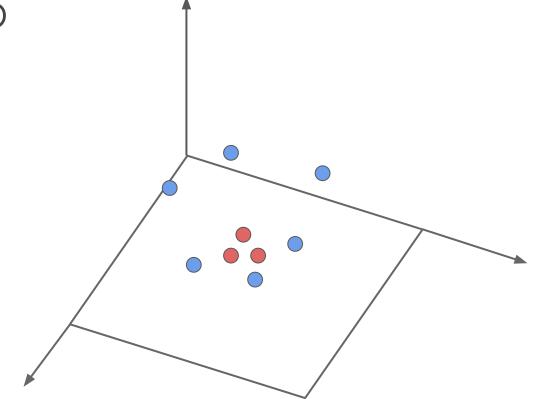


2D to 3D

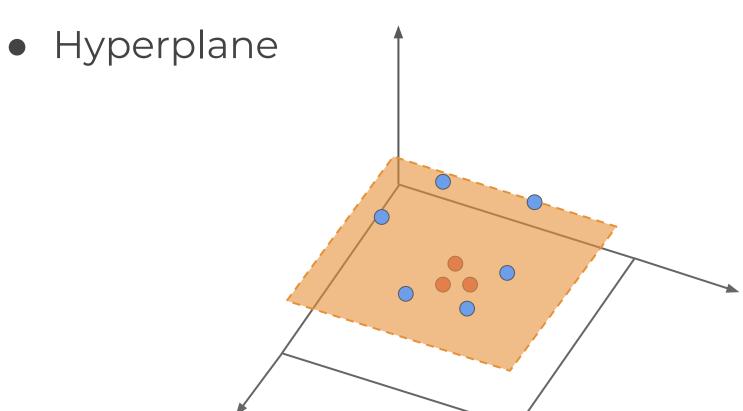




2D to 3D









- You may have heard of the use of kernels in SVM as the "kernel trick".
- We previously visualized transforming data points from one dimension into a higher dimension.
- Mathematically, the kernel trick actually avoids recomputing the points in a higher dimensional space!



- How does the kernel trick achieve this?
- It takes advantage of dot products of the transpositions of the data.



Theory and Intuition - Kernel Trick and Math

- Let's briefly go over some of the general mathematics of SVM and how it is related to the Scikit-Learn class calls.
- We'll begin with a brief review of using margin based classifiers, and how they can be described with equations.
 - Note: Feel free to consider this an "optional" concept.



- Relative Reading:
 - o Background in Chapter 9 of ISLR.
 - For a comprehensive overview of everything discussed, check out:
 - Cortes, Corinna; Vapnik, Vladimir N. (1995). "Support-vector networks".
 Machine Learning.



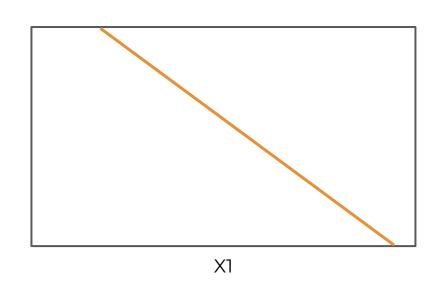
Hyperplanes Defined



X1



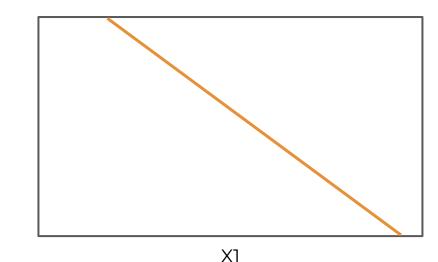
Hyperplanes Defined





Hyperplanes Defined

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 = 0$$

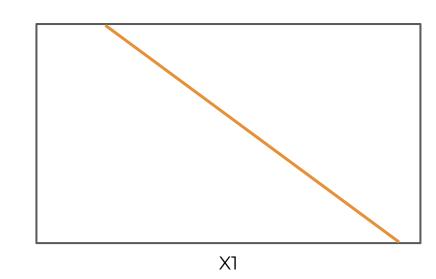




Hyperplanes Defined

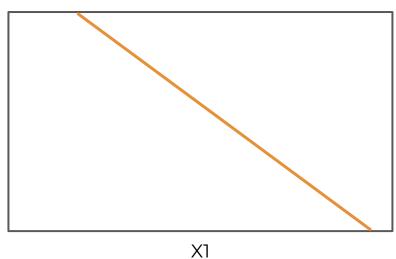
$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 = 0$$

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p = 0$$



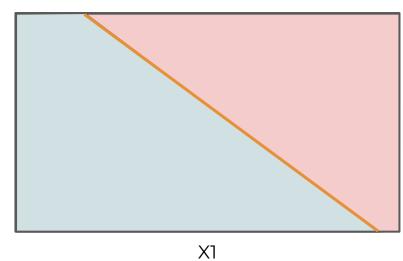


Separating Hyperplanes





Separating Hyperplanes





Separating Hyperplanes



X1

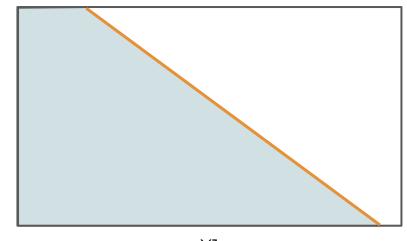
$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p > 0$$



Separating Hyperplanes



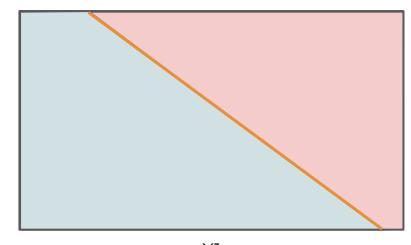
$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p < 0$$





Separating Hyperplanes

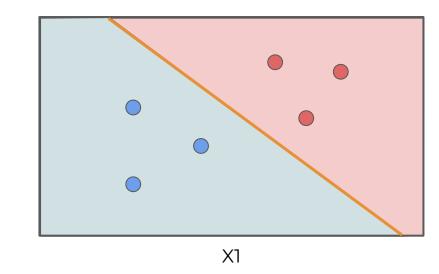
$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p > 0$$
 $\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p < 0$





Data Points

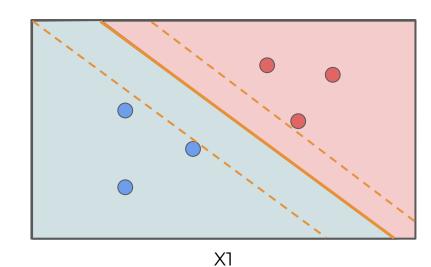
$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$
 $\times 2$





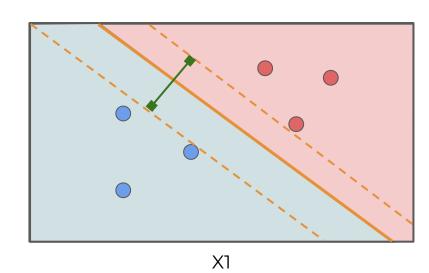
X2

 $\underset{\beta_0,\beta_1,...,\beta_p,M}{\text{maximize}} M$





$$\underset{\beta_0,\beta_1,...,\beta_p,M}{\text{maximize}} \underline{\underline{M}}$$





 $\max_{\beta_0,\beta_1,\ldots,\beta_p,M} \sup_{j=1}^{p} \beta_j^2 = 1$ $y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \geq M \ \forall i = 1,\ldots,n.$



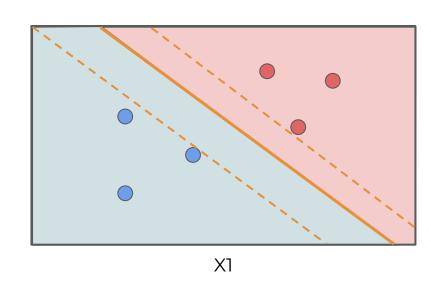
Max Margin Classifier

$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

 $\underset{\beta_0,\beta_1,...,\beta_p,M}{\text{maximize}} M$

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M \ \forall i = 1, \ldots, n.$$



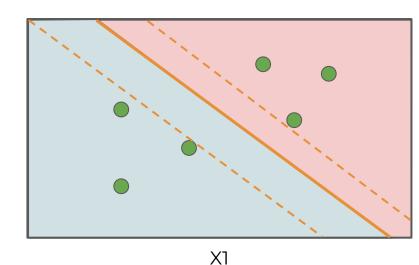


Max Margin Classifier

$$\begin{bmatrix} x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix} \end{bmatrix}$$

X2

 $\begin{aligned} & \underset{\beta_0,\beta_1,...,\beta_p,M}{\text{maximize}} & M \\ & \text{subject to} & \sum_{j=1}^p \beta_j^2 = 1 \end{aligned}$



$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M \ \forall \ i = 1, \ldots, n.$$

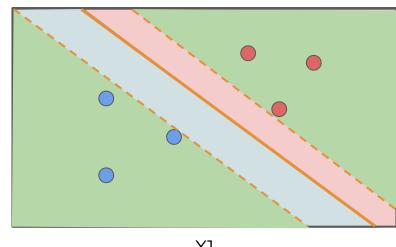


Max Margin Classifier

$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

maximize M $\beta_0, \beta_1, \dots, \beta_p, M$

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$



$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M$$
 $\forall i = 1, \ldots, n.$



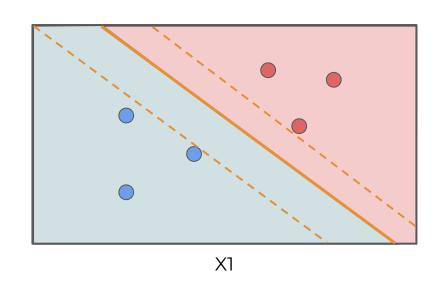
Max Margin Classifier

$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

 $\underset{\beta_0,\beta_1,...,\beta_p,M}{\text{maximize}} M$

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M \ \forall i = 1, \ldots, n.$$





X1

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$
$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip})$$



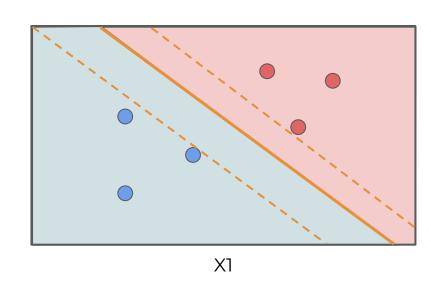
Max Margin Classifier

$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

 $\underset{\beta_0,\beta_1,...,\beta_p,M}{\text{maximize}} M$

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M \ \forall i = 1, \ldots, n.$$

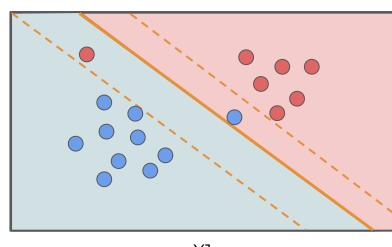




Support Vector Classifier

$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

X2

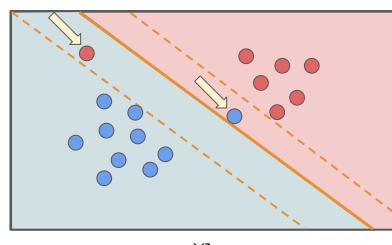




Support Vector Classifier

$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

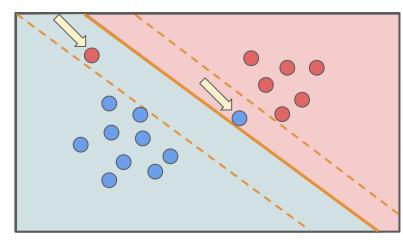
X2





Support Vector Classifier

$$\max_{\beta_0,\beta_1,...,\beta_p,\epsilon_1,...,\epsilon_n,M} M$$
 subject to
$$\sum_{j=0}^{p} \beta_j^2 = 1$$
 x2

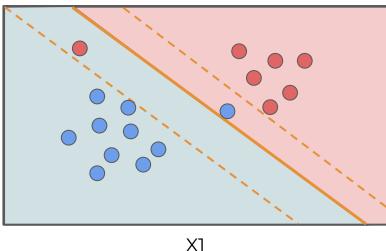




Support Vector Classifier

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$

$$\epsilon_i \ge 0, \quad \sum_{i=1}^n \epsilon_i \le C$$



$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M(1 - \epsilon_i)$$



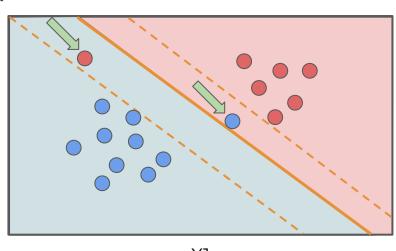
X2

Support Vector Classifier

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$

$$\epsilon_i \ge 0, \ \sum_{i=1}^n \epsilon_i \le C$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M(1 - \epsilon_i)$$





Note on Scikit-Learn's SVC!

C: float, default=1.0

Regularization parameter. The strength of the regularization is inversely proportional to C. Must be strictly positive. The penalty is a squared I2 penalty.

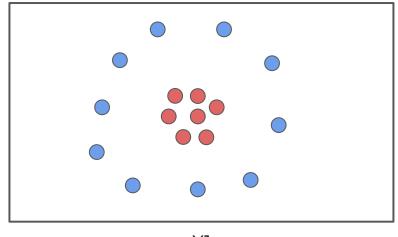
$$\epsilon_i \ge 0, \quad \sum_{i=1}^n \epsilon_i \le C$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \ge M(1 - \epsilon_i)$$



$$X_1, X_2, \ldots, X_p,$$

X2



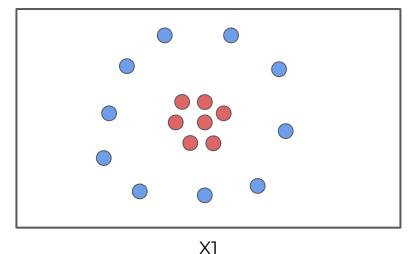


Support Vector Machines

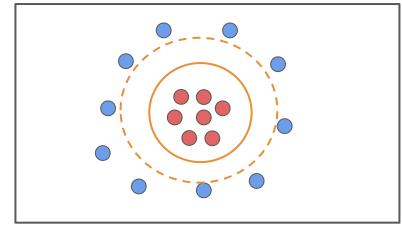
$$X_1, X_2, \dots, X_p,$$

$$X_1, X_1, X_2, X_2, \dots, X_p, X_p^2$$

$$X_1, X_1, X_2, X_2, \dots, X_p, X_p^2$$







XΊ



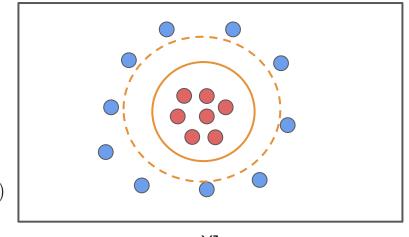
X2

Support Vector Machines

$$X_1, X_1^2, X_2, X_2^2, \dots, X_p, X_p^2$$

subject to
$$y_i \left(\beta_0 + \sum_{j=1}^p \beta_{j1} x_{ij} + \sum_{j=1}^p \beta_{j2} x_{ij}^2 \right) \ge M(1 - \epsilon_i)$$

$$\sum_{i=1}^{n} \epsilon_i \le C, \quad \epsilon_i \ge 0, \quad \sum_{i=1}^{p} \sum_{k=1}^{2} \beta_{jk}^2 = 1.$$

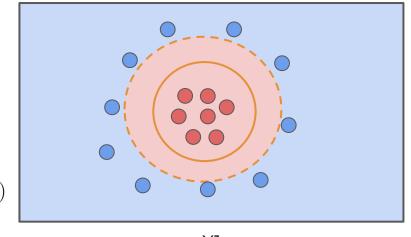




$$X_1, X_1^2, X_2, X_2^2, \dots, X_p, X_p^2$$

subject to
$$y_i \left(\beta_0 + \sum_{j=1}^p \beta_{j1} x_{ij} + \sum_{j=1}^p \beta_{j2} x_{ij}^2 \right) \ge M(1 - \epsilon_i)$$

$$\sum_{i=1}^{n} \epsilon_i \le C, \quad \epsilon_i \ge 0, \quad \sum_{i=1}^{p} \sum_{k=1}^{2} \beta_{jk}^2 = 1.$$

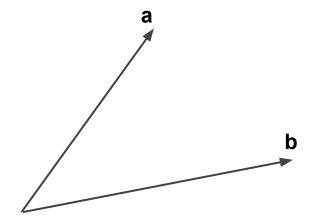




- How to deal with very large feature space?
- As polynomial order grows larger, the number of computations necessary to solve for margins also grows!
- The answer lies in the **kernel trick** which makes use of the **inner product** of vectors, also known as the **dot product**.

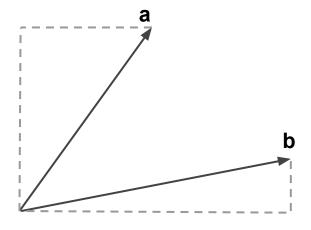


$$\langle a, b \rangle = \sum_{i=1}^{r} a_i b_i$$



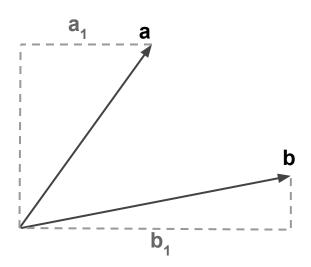


$$\langle a, b \rangle = \sum_{i=1}^{r} a_i b_i$$

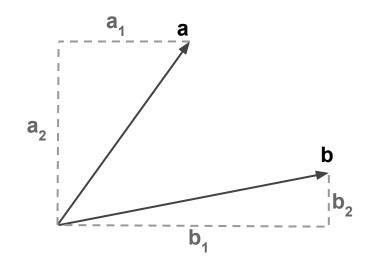




$$\langle a, b \rangle = \sum_{i=1}^{r} a_i b_i$$



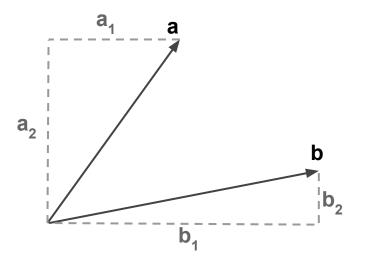
$$\langle a, b \rangle = \sum_{i=1}^{r} a_i b_i$$





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

$$a \cdot b = a_1 b_1 + a_2 b_2$$

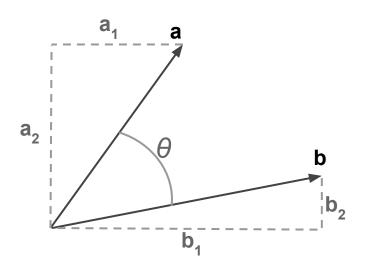




$$\langle a, b \rangle = \sum_{i=1}^{r} a_i b_i$$

$$a \cdot b = a_1 b_1 + a_2 b_2$$

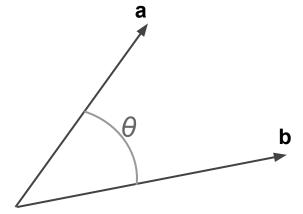
$$a \cdot b = |a||b|cos(\theta)$$





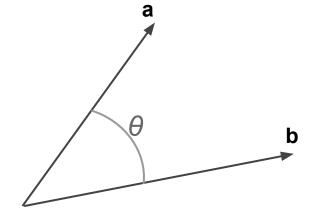
 Notice how the dot product can be thought of as a **similarity** between the vectors.

$$a \cdot b = |a||b|cos(\theta)$$



- $cos(0^{\circ}) = 1$
- $cos(90^\circ) = 0$
- $cos(180^\circ) = -1$

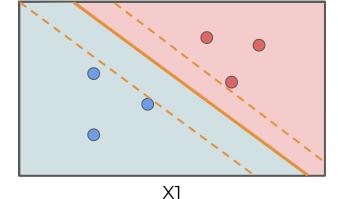
$$a \cdot b = |a||b|cos(\theta)$$





Linear Support Vector Classifier rewritten:

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$

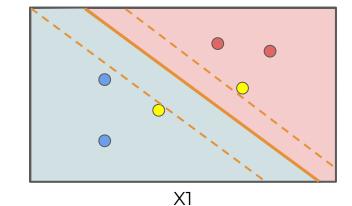


Calculating the inner products of all pairs of training observations



Linear Support Vector Classifier rewritten:

$$f(x) = \beta_0 + \sum_{i=1}^{\infty} \alpha_i \langle x, x_i \rangle$$



Only non-zero for the support vectors.



Linear Support Vector Classifier rewritten:

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$

$$\int f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$



Linear Support Vector Classifier rewritten:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle$$

S collection of indices of these support points



Kernel Function

$$K(x_i, x_{i'}) = \sum_{j=1}^{p} x_{ij} x_{i'j}$$

A kernel is a function that quantifies the similarity of two observations.



Kernel Function

$$K(x_i, x_{i'}) = \sum_{i=1}^{p} x_{ij} x_{i'j} \qquad f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle$$



Kernel Function

$$K(x_i, x_{i'}) = \sum_{j=1}^{p} x_{ij} x_{i'j} \qquad f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle$$

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



Kernel Function

$$K(x_i, x_{i'}) = \sum_{j=1}^{p} x_{ij} x_{i'j} \qquad f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i K(x, x_i)$$

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



Polynomial Kernel

$$K(x_i, x_{i'}) = (1 + \sum_{j=1}^{p} x_{ij} x_{i'j})^d \qquad f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle$$

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



Radial Basis Kernel

$$K(x_i, x_{i'}) = \exp(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2) \qquad f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle$$

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



- The use of kernels as a replacement is known as the kernel trick.
- Kernels allow us to avoid computations in the enlarged feature space, by only needing to perform computations for each distinct pair of training points (details in 9.3.2 in ISLR).



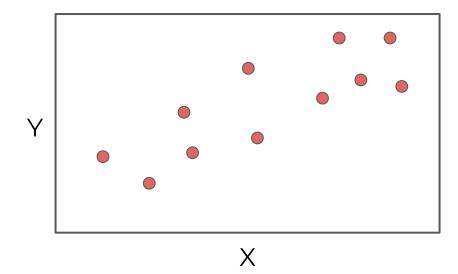
- Intuitively we've already seen inner products act as a measurement of similarity between vectors.
- The use of kernels can be thought of as a measure of similarity between the original feature space and the enlarged feature space.



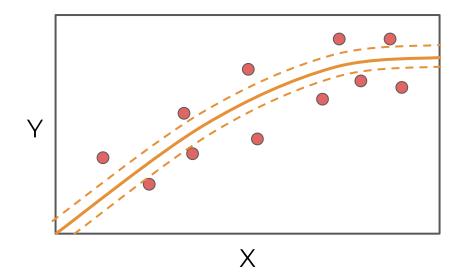
 Now that we understand the theory and intuition behind SVMs, let's move on to actually using them with code!



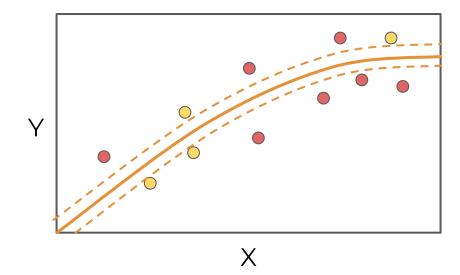
Regression with Scikit-Learn



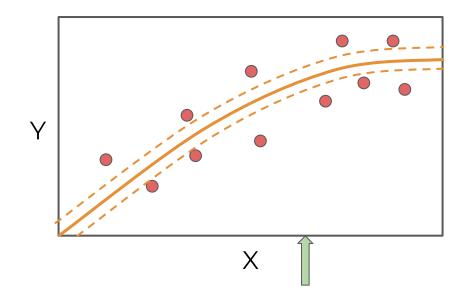




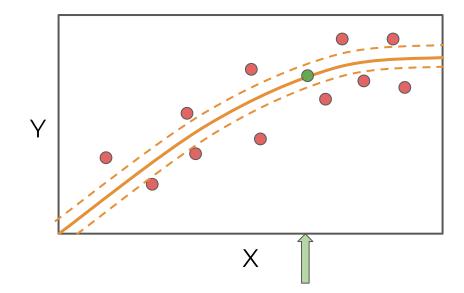




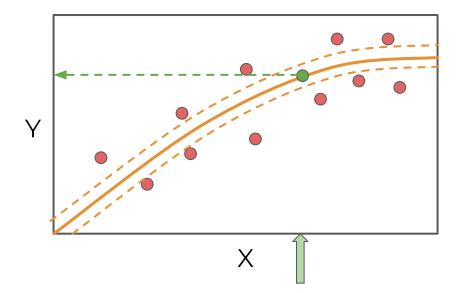






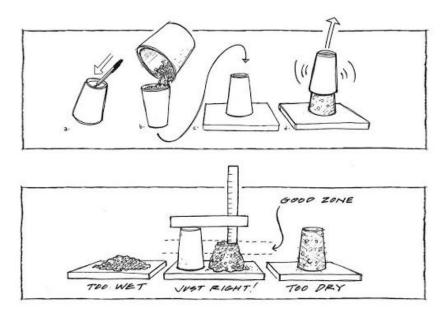








Concrete Slump Test





Concrete Slump Test





