Tufts

Class #09:
Support Vector Machines (SVMs)
and Kernel Functions

Machine Learning (COMP 135)

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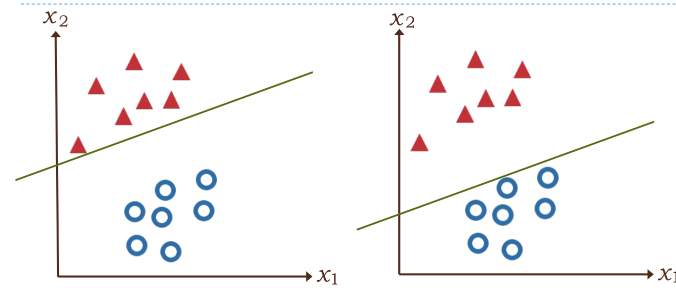
Data Separation



- Linear classification with a perceptron or logistic function looks for a dividing line in the data (or a plane, or other linearly defined structure)
  - Often ***multiple*** lines are possible
  - Essentially, the algorithms are ***indifferent***: they don't care which line we pick

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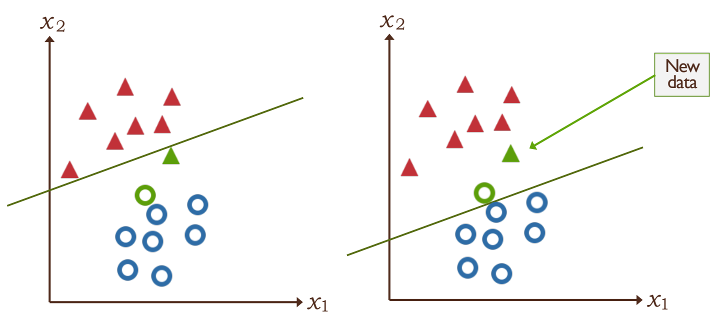
"Fragile" Separation



- As more data comes in, these classifiers may start to fail
  - A separator that is too close to one cluster or the other now makes mistakes
  - May happen even if new data follows same distribution seen in the training set

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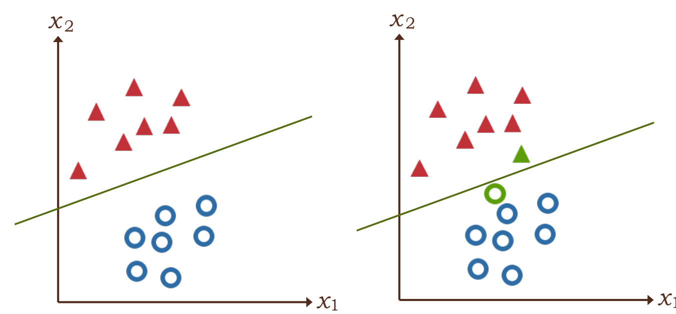
"Robust" Separation



- What we want is a large margin separator: a separation that has the largest distance possible from each part of our data-set
- This will often give much better performance when used on new data

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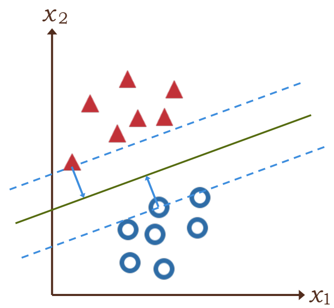
Large Margin Separation



This is sometimes called the "widest road" approach

A support vector machine (SVM) is a technique that finds this road

The points that define the edges of the road are knows as the support vectors

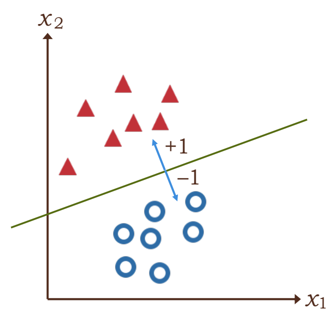
- A new learning problem: ***find*** the separator with the largest margin
- This will be measured from the data points, on opposite sides, that are ***closest together***

Linear Classifiers and SVMs

Linear	
Weight equation	$\mathbf{w} \cdot \mathbf{x} = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n$
Threshold function	$h_{\mathbf{w}} = \begin{cases} 1 & \mathbf{w} \cdot \mathbf{x} \geq 0 \\ 0 & \mathbf{w} \cdot \mathbf{x} < 0 \end{cases}$

SVM	
Weight equation	$\mathbf{w} \cdot \mathbf{x} + b = (w_1 x_1 + w_2 x_2 + \cdots + w_n x_n) + b$
Threshold function	$h_{\mathbf{w}} = \begin{cases} +1 & \mathbf{w} \cdot \mathbf{x} \geq 0 \\ -1 & \mathbf{w} \cdot \mathbf{x} < 0 \end{cases}$

Large Margin Separation



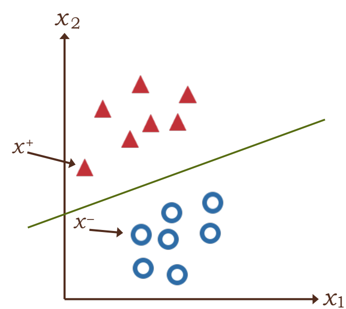
$$\mathbf{w} \cdot \mathbf{x} + b = 0$$

A key difference: the SVM is going to do this ***without*** learning and remembering weight vector $\mathbf{w}$.

Instead, it will use features of the ***data-items themselves***.

- Like a linear classifier, the SVM separates at the line where its learned vector of weights is zero

Mathematics of SVMs



$$\mathbf{w} \cdot \mathbf{x}^+ + b = +1$$
$$\mathbf{w} \cdot \mathbf{x}^- + b = -1$$

$$\mathbf{w} \cdot (\mathbf{x}^+ - \mathbf{x}^-) = 2$$
$$\frac{\mathbf{w}}{||\mathbf{w}||} \cdot (\mathbf{x}^+ - \mathbf{x}^-) = \frac{2}{||\mathbf{w}||}$$

$$||\mathbf{w}|| = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}$$

- It turns out that the weight-vector $\mathbf{w}$ for the largest margin separator has some important properties relative to the closest data-points on each side (x^+ and x^-)

Mathematics of SVMs

- Through the magic of mathematics (Lagrangian multipliers, to be specific), we can derive a quadratic programming problem

1. We start with our data-set:

$$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)\} \qquad [\forall i,\ y_i \in \{+1, -1\}]$$

2. We then solve a constrained optimization problem:

$$W(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i\, \alpha_j\, y_i\, y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\forall i,\ \alpha_i \geq 0$$

$$\sum_i \alpha_i\, y_i = 0$$

The goal: based on ***known*** values $(\mathbf{x}_i, y_i)$ ***find*** the values we ***don't know*** (α_i) that:

1. Will maximize value of margin $W(\alpha)$
2. Satisfy the two numerical constraints

Mathematics of SVMs

- Although complex, a constrained optimization problem like this can be algorithmically solved to get the α_i values we want:

$$W(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i\, \alpha_j\, y_i\, y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\forall i,\ \alpha_i \geq 0$$

$$\sum_i \alpha_i\, y_i = 0$$

A note about notation: these equations involve two different, necessary products:

1. The usual application of ***weights*** to ***points***:
   $\mathbf{w} \cdot \mathbf{x}_i = w_1 x_{i,1} + w_2 x_{i,2} + \cdots + w_n x_{i,n}$
2. Products of ***points*** and ***other points***:
   $\mathbf{x}_i \cdot \mathbf{x}_j = x_{i,1} x_{j,1} + x_{i,2} x_{j,2} + \cdots + x_{i,n} x_{j,n}$

- Once done, we can find the weight-vector and bias term if we want:

$$\mathbf{w} = \sum_i \alpha_i\, y_i\, \mathbf{x}_i \qquad b = -\frac{1}{2}\left(\max_{i \,|\, y_i = -1} \mathbf{w} \cdot \mathbf{x}_i + \min_{j \,|\, y_j = +1} \mathbf{w} \cdot \mathbf{x}_j\right)$$

The Dual Formulation

- It turns out that we don't need to use the weights at all
- Instead, we can simply use the α_i values ***directly***:

$$\mathbf{w} \cdot \mathbf{x}_i + b = \sum_j \alpha_j y_j (\mathbf{x}_i \cdot \mathbf{x}_j) + b$$

What we ***usually*** look for in a parametric method: the weights, $\mathbf{w}$, and offset, b, defining the classifier

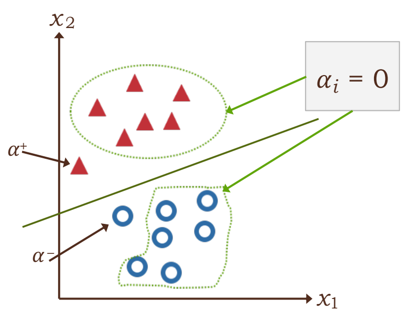
What we can use ***instead***: we compute an ***equivalent*** result based upon the α parameters, the outputs y, and products between data-points themselves (along with the standard offset)

The Dual Formulation

$$\mathbf{w} \cdot \mathbf{x}_i + b = \sum_j \alpha_j y_j (\mathbf{x}_i \cdot \mathbf{x}_j) + b$$

- Now, if we had to sum over ***every*** data-point as on the right-hand side of this equation, this would look very bad for a large data-set
- It turns out that these α_i values have a special property, however, that makes it feasible to use them as part of our classification function…

Sparseness of SVMs



So, when we do the calculation:

$$\sum_j \alpha_j y_j (\mathbf{x}_i \cdot \mathbf{x}_j) + b$$

We only have to sum over points $\mathbf{x}_j$ that are in the set of support vectors, ***ignoring*** all others, since the related α values are all 0.

Thus, an SVM need only remember and use the values for a few support vectors, not those for all the rest of the data.

- The α_i values are 0 ***everywhere except*** at the support vectors (the points closest to the separator)

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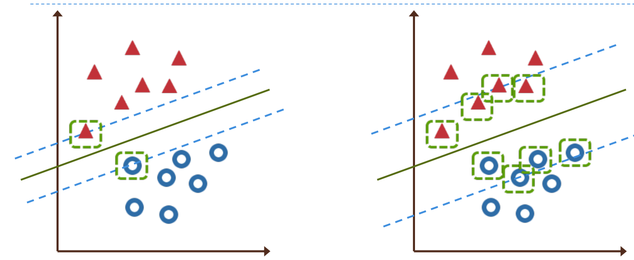
Hard and Soft Margins



- We have slightly simplified one detail of how most SVMs actually work
- It is ***not always true*** that the support vectors lie on the margins, with nothing else in between them
- This is only true in the hard margin case

- SVMs can have soft margins, instead (and usually do) to deal with noisier data
- We weaken the requirement that no points lie between the margins
  - ***All points*** within the margins then become the support vectors for classification

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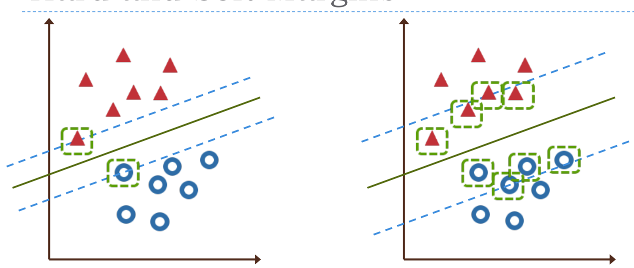
Hard and Soft Margins



- In upcoming exercises, we see how to vary margin strength in `sklearn`
- SVM models come with a regularization parameter (C, as in the case of classifiers) that can be:
  1. ***Increased*** to enforce a ***harder*** margin
  2. ***Decreased*** to allow a ***softer*** margin

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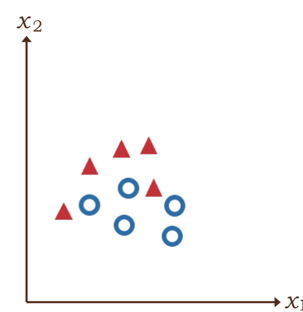
Another Nice Trick



$$\sum_j \alpha_j y_j (\mathbf{x}_i \cdot \mathbf{x}_j) + b$$

Using a kernel "trick", we can find a function that ***transforms*** the data into another form, where it is actually possible to separate it in a linear manner

- The dual formulation uses dot-products of data-points with each other (instead of with weights)
- Combining this with the idea of a kernel will allow us to deal with data that is not linearly separable

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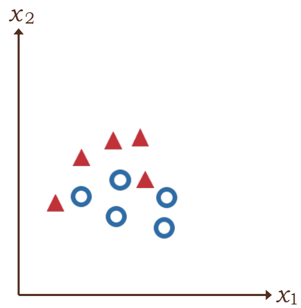
Transforming Non-Separable Data



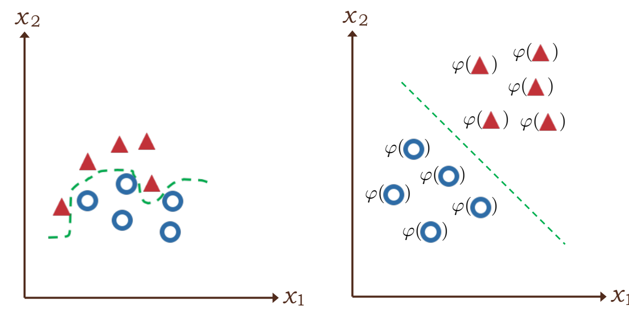
A transformation function:

$\varphi(\mathbf{x}) \qquad \varphi : \mathbb{R}^n \rightarrow \mathbb{R}^m$

maps data-vectors to new vectors, of either the same dimensionality ($m = n$) or a different one ($m \neq n$)

- If data that is not linearly separable, we can ***transform*** it
  - We ***change*** features used to represent our data
  - As usual, we ***don't care*** what the data feature are, so long as we can get classification to work

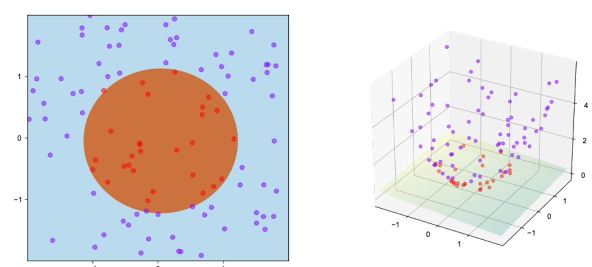
Transforming Non-Separable Data



$\varphi(\mathbf{x}) \qquad \varphi : \mathbb{R}^n \rightarrow \mathbb{R}^m$

$$\sum_j \alpha_j y_j (\varphi(\mathbf{x}_i) \cdot \varphi(\mathbf{x}_j)) + b$$

The "Kernel Trick"



$$\varphi(x_1, x_2) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

Simplifying the Transformation Function

- We can derive a simpler (2-dimensional) equation, ***equivalent to*** the cross-product needed when doing SVM computations in the transformed (3-dimensional) space:

$$\varphi(\mathbf{x}) \cdot \varphi(\mathbf{z}) = (x_1^2,\ x_2^2,\ \sqrt{2}x_1x_2) \cdot (z_1^2,\ z_2^2,\ \sqrt{2}z_1z_2) \longleftarrow \text{Needed}$$

$$= x_1^2z_1^2 + x_2^2z_2^2 + \sqrt{2}x_1x_2\sqrt{2}z_1z_2$$

$$= \boxed{x_1^2z_1^2 + x_2^2z_2^2 + 2x_1x_2z_1z_2} \longleftarrow \text{10 multiplications, 2 additions}$$

$$= \boxed{(x_1z_1 + x_2z_2)^2} \longleftarrow \text{3 multiplications, 1 addition}$$

$$= (\mathbf{x} \cdot \mathbf{z})^2$$

Used instead

The Kernel Function

$$k(\mathbf{x}, \mathbf{z}) = \varphi(\mathbf{x}) \cdot \varphi(\mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^2$$

- This final function (right side) is what the SVM will actually use to compute dot-products in its equations
- This is called the kernel function
- To make SVMs really useful we look for a kernel that:

1. Separates the data usefully
2. Is relatively efficient to calculate

Another Reason to Use Kernel Functions

$$\mathbf{w} \cdot \mathbf{x}_i + b = \sum_j \alpha_j y_j (\varphi(\mathbf{x}_i) \cdot \varphi(\mathbf{x}_j)) + b$$

- The SVM formulation generally uses dot-products of data-points (perhaps run through some kernel) rather than the standard product of features and weights
- We have cases where the kernel-data approach is ***possible***, but the weights-based one is ***not***
  - Some useful kernels, that are easy to compute, correspond to weight-equations applied to ***very high dimensional*** transforms of the original data
  - In some common cases, equivalent weight-data vectors are ***infinite-***dimensional, and simply cannot be used in computation