

CS 383/613 – Machine Learning

Support Vector Machines

Slides adapted from material created by E. Alpaydin Prof. Mordohai, Prof. Greenstadt, Pattern Classification (2nd Ed.), Pattern Recognition and Machine Learning



Objectives

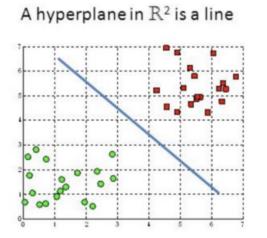
- Support Vector Machines
 - Large Margin Intuition
 - Optimization Objective Function
 - Non-Linear SVMs

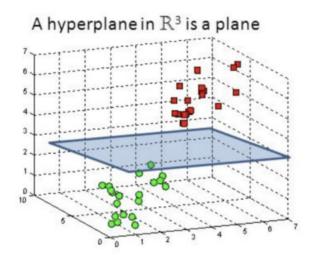


SVMs

• Support Vector Machines (SVMs) are a linear classification algorithm that have shown to be quite successful in pattern recognition.

https://towardsdatascience.com

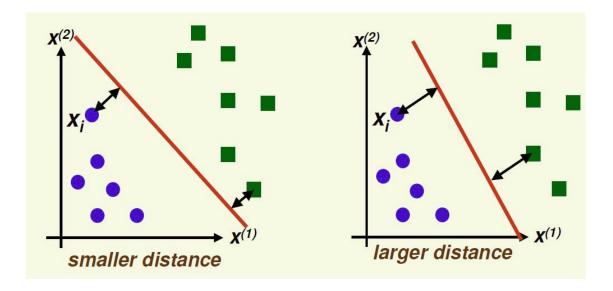






SVM Intuition

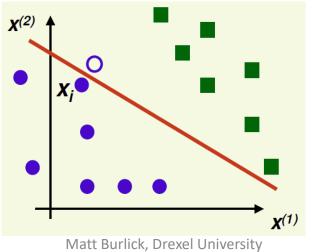
- Idea: Maximize distance to closest example (of each type)
 - For now, we'll assume total separability





SVM Intuition

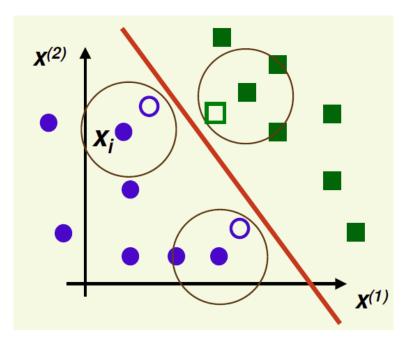
- Training data is just a subset of all possible data
 - Suppose hyperplane is close to sample X_i (open circle)
 - The *margin* is small
 - ullet If we see a new sample close to $oldsymbol{X}_i$ it may be on the wrong side of the hyperplane
- Therefore, poor generalization





SVM Intuition

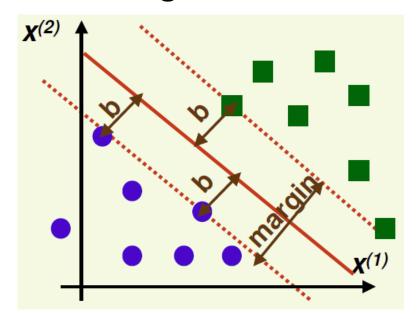
- Intuition: We want hyperplane as far as possible from any sample
- New samples close to old samples will then be classified correctly
- Good generalization





SVM – Linearly Separable Case

- Definition: Margin
 - ullet The margin is twice the absolute value of distance b of the closest example to the hyperplane
- Our goal is to maximize the margin



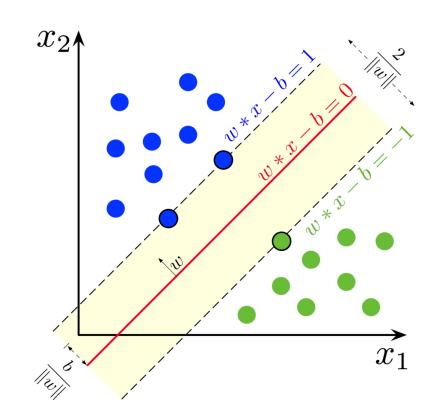


Linear Discriminant Function

- The general equation for a line is $Ax_1 + Bx_2 + C = 0$
- This equation holds for any point (x_1, x_2) on the line.
- We can write this as a discriminant function:

$$g(\mathbf{x}) = Ax_1 + Bx_2 + C$$

- Then:
 - g(x) = 0 for any point x on the line.
 - g(x) > 0 for any point above the line
 - $g(\mathbf{x}) < 0$ for any point below the line.





Linear Discriminant Function

$$g(\mathbf{x}) = Ax_1 + Bx_2 + C$$

• A and B are just weights (and C is a bias), so let's write this as:

$$w = \begin{bmatrix} A \\ B \end{bmatrix}, b = C$$

Now we have

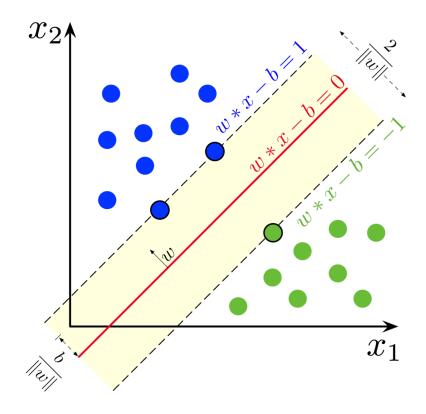
$$g(x) = xw + b$$

- Can we just add a bias feature to our data (like in linear and logistic regression), so the bias is not separate?
- Yes!
- Let

$$\mathbf{w} = \begin{bmatrix} A \\ B \\ C \end{bmatrix}, \mathbf{x} = [x_1, x_2, 1]$$

Now

$$g(x) = xw$$

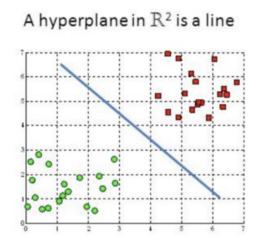


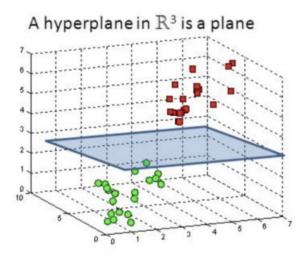


Linear Discriminant Function

$$g(x) = xw$$

- If x and w have more than three elements, then this is the discriminant function for a hyperplane.
 - If $g(\mathbf{x}) = 0$ then we're on the hyperplane.
 - If $g(\mathbf{x}) > 0$ then we're on one side of the hyperplane
 - If $g(\mathbf{x}) < 0$ then we're on the other side of it.



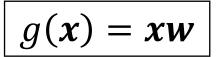


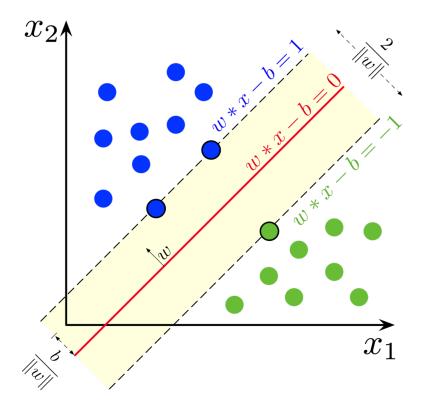


Hyperplanes and Support Vectors

- We want the separating hyperplane to be equidistant from the toughest to classify samples.
- These toughest samples are called the **support** vectors, and we'll designate them as x_+^* and x_-^*
- To provide a standard/canonical model we will want our feature vectors to project to be 1 one unit from the hyperplane.

$$x_+^* w = 1$$
$$x_-^* w = -1$$







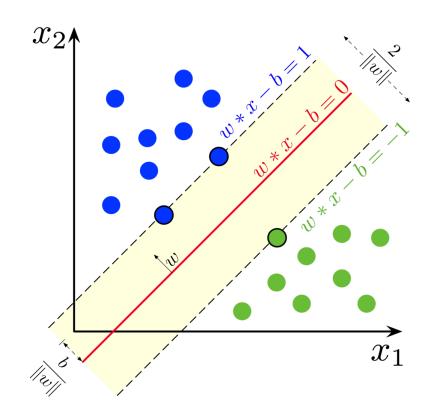
Hyperplanes and Margin

$$g(\mathbf{x}) = \mathbf{x}\mathbf{w} + b$$

 Geometrically, the distance between the planes containing the support vectors is:

$$\frac{2}{|w|}$$

- We call this the margin
 - And it's what we want to maximize!





Margin

$$g(\mathbf{x}) = \mathbf{x}\mathbf{w}$$

$$margin = \frac{2}{|w|}$$

• |w| is just the magnitude of w and thus be computed as:

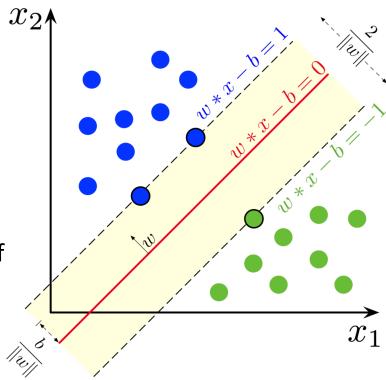
$$margin = \frac{2}{\sqrt{\mathbf{w}^T \mathbf{w}}}$$

• However, maximizing the square of this is suffice:

$$margin = \frac{2}{\mathbf{w}^T \mathbf{w}}$$

• And finally, people typically attempt to *minimize* the reciprocal of this:

$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$



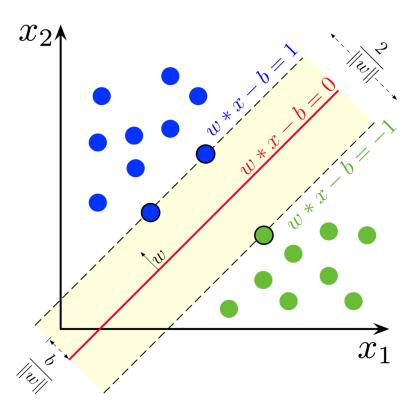


Margin Formula

$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

 But what about wanting all the observations ending up on the correct side and outside the margin? i.e

$$x_+ w \ge 1$$
, $x_- w \le -1$



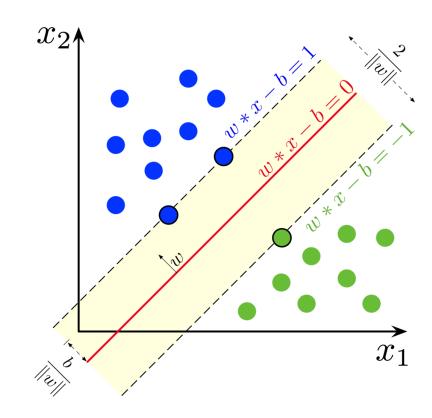


Primal vs Lagrangian Dual Problem

$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

$$s. t \quad x_+ \mathbf{w} \ge 1, \quad x_- \mathbf{w} \le -1$$

- There's two common ways to include these conditions:
 - Primal Form
 - Lagrangian Dual Form.
- We're going to look at the Lagrangian Dual Problem
 - It is more flexible/general and typically provides better results.



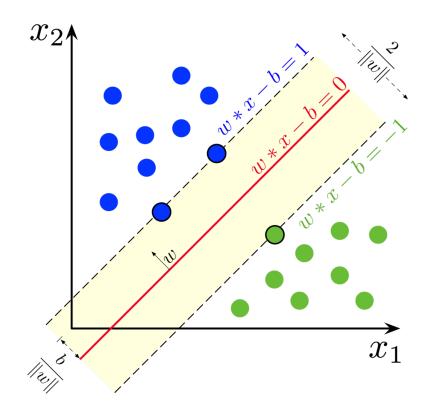


$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$
s. t $x_+ \mathbf{w} \ge 1$, $x_- \mathbf{w} \le -1$

- Given that $y \in \{-1, +1\}$, we want $yxw 1 \ge 0$
 - Support vectors will have yxw 1 = 0
 - Things not at ideal locations will have yxw 1 < 0
- Lagrange multipliers are scalers, one per term, that establish costs (or importance) for different terms.
- Let α_i be the Lagrange multiplier for observation i.
- We then want to maximize

$$J_L = \sum_{i=1}^{N} (\alpha_i (Y_i X_i \mathbf{w} - 1))$$

• Note, that we'll also want to ensure that $\alpha_i>0$





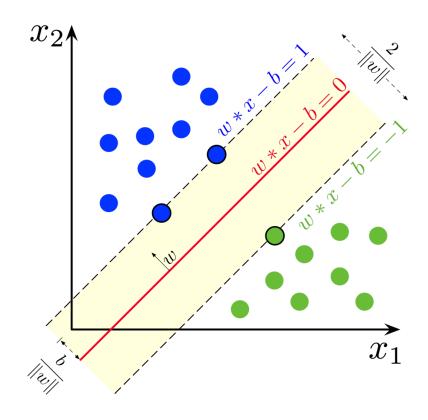
Minimize:
$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

Maximize:
$$J_L = \sum_{i=1}^{N} (\alpha_i (Y_i X_i \mathbf{w} - 1))$$

- One thing to minimize (reciprocal of margin), one thing to maximize (things being on the correct side).
 - Hence, the dual problem!
- We could write this as a single objective by turning the maximization part into minimization (by negating it):

$$J = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} - \sum_{i=1}^{N} (\alpha_{i} (Y_{i} X_{i} \mathbf{w} - 1))$$

$$s. t \alpha_{i} \geq 0 \forall i = 1, ..., N$$

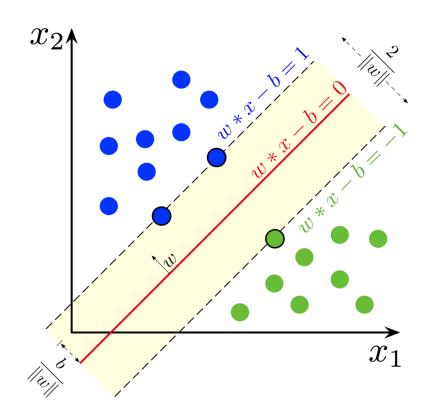




$$J = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} - \sum_{i=1}^{N} (\alpha_{i} (Y_{i} X_{i} \mathbf{w} - 1))$$

$$s. t \alpha_{i} \ge 0 \forall i = 1, ..., N$$

- This minimization will also want non-support (but correctly located) vectors to have $\alpha_i = 0$.
- Thus:
 - Thing in the wrong location will have $\alpha_i < 0$
 - Which we'll force to $\alpha_i = 0$
 - Things passed the margin (but on the correct side) will get minimized to $\alpha_i=0$
- Therefore, only our support vectors will have $\alpha_i > 0$!





$$g(x) = xw$$

$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^{N} (\alpha_i (Y_i X_i \mathbf{w} - 1))$$

$$s. t \alpha_i \ge 0 \forall i = 1, ..., N$$

- We're going to use calculus to find the values of w and α .
- Doing so will be easier if we can write this second term more concisely using linear algebra.
- Let's start by expending the equation out a bit....

$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \left(\sum_{i=1}^N \alpha_i Y_i X_i \mathbf{w} - \sum_{i=1}^N \alpha_i \right)$$



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Lagrangian Dual Problem

$$g(x) = xw$$

$$J = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \left(\sum_{i=1}^{N} \alpha_i Y_i X_i \mathbf{w} - \sum_{i=1}^{N} \alpha_i \right)$$

$$s. t \alpha_i \ge 0 \ \forall i = 1, ..., N$$

- Now to eliminate those summations via matrix multiplications...
- We can do this as:

$$J = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} - \left(\boldsymbol{\alpha}^{T} diag(Y) X \mathbf{w} - trace \left(diag(\boldsymbol{\alpha}) \right) \right)$$

Recall that the trace operator is sum of elements on the diagonal.



$$J = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} - \left(\boldsymbol{\alpha}^{T} \operatorname{diag}(Y) X \mathbf{w} - \operatorname{trace}(\operatorname{diag}(\boldsymbol{\alpha})) \right)$$

$$s. \ t \ \alpha_{i} \ge 0 \ \forall i = 1, ..., N$$

- So, how do we use calculus to find w and α ?
- This is most easily done via a combination of direct and gradient based solutions.
- We'll use a direct solution to find w in terms of α , find α via a gradient-based approach
 - The gradient approach for α is needed to impose the $\alpha_i \geq 0$ constraint.



Finding Hyperplane

$$J = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} - \left(\boldsymbol{\alpha}^{T} diag(Y) X \mathbf{w} - trace \left(diag(\boldsymbol{\alpha}) \right) \right)$$

s. $t \alpha_{i} \geq 0 \ \forall i = 1, ..., N$

- To find the w, we'll take the derivative with respect to it
- Doing this we get:

$$\frac{\partial J}{\partial \mathbf{w}} = \mathbf{w} - (\mathbf{\alpha}^T \operatorname{diag}(Y)X)^T = \mathbf{w} - X^T \operatorname{diag}(Y)\mathbf{\alpha}$$

Set this to zero and solve for w

$$\mathbf{w} = X^T diag(Y)\mathbf{\alpha}$$



Finding Hyperplane

$$J = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} - \left(\boldsymbol{\alpha}^{T} \operatorname{diag}(Y) X \mathbf{w} + b \boldsymbol{\alpha}^{T} Y - \operatorname{trace}(\operatorname{diag}(\boldsymbol{\alpha})) \right)$$
$$\mathbf{w} = X^{T} \operatorname{diag}(Y) \boldsymbol{\alpha}$$
$$s. \ t \ \alpha_{i} \ge 0 \ \forall i = 1, ..., N$$

- To find α , let's establish a gradient rule, $\frac{\partial J}{\partial \alpha}$
- First let's do a substitution to get J solely in terms of lpha

$$J = \frac{1}{2} (X^T \operatorname{diag}(Y) \boldsymbol{\alpha})^T (X^T \operatorname{diag}(Y) \boldsymbol{\alpha}) - \left(\boldsymbol{\alpha}^T \operatorname{diag}(Y) X X^T \operatorname{diag}(Y) \boldsymbol{\alpha} - \operatorname{trace} \left(\operatorname{diag}(\boldsymbol{\alpha}) \right) \right)$$

Simplifying

$$J = trace(diag(\boldsymbol{\alpha})) - \frac{1}{2}\boldsymbol{\alpha}^T diag(Y)XX^T diag(Y)\boldsymbol{\alpha}$$

• Now $\frac{\partial J}{\partial \alpha}$...

$$\frac{\partial J}{\partial \boldsymbol{\alpha}} = ones(size(Y)) - diag(Y)XX^T diag(Y)\boldsymbol{\alpha}$$



Finding Hyperplane

$$J = \frac{1}{2} \mathbf{w}^{T} \mathbf{w} - (\boldsymbol{\alpha}^{T} \operatorname{diag}(Y) X \mathbf{w} - \operatorname{trace}(\operatorname{diag}(\boldsymbol{\alpha})))$$
$$\frac{\partial J}{\partial \boldsymbol{\alpha}} = \operatorname{ones}(\operatorname{size}(Y)) - \operatorname{diag}(Y) X X^{T} \operatorname{diag}(Y) \boldsymbol{\alpha}$$
$$\mathbf{w} = X^{T} \operatorname{diag}(Y) \boldsymbol{\alpha}$$
$$s.t \ \alpha_{i} \geq 0 \ \forall i = 1, ..., N$$

- A few caveats....
 - 1. $\frac{\partial J}{\partial \alpha}$ is actually the partial of the part of J that we want to **maximize**.
 - 2. During gradient **ascent** we'll need to set any $\alpha_i < 0$ to zero
- Pseudocode!
 - Initialize $\alpha = 0$
 - While minimal change in α
 - $\frac{\partial J}{\partial \alpha} = ones(size(Y)) diag(Y)XX^T diag(Y)\alpha$
 - $\alpha += \eta \frac{\partial J}{\partial \alpha}$
 - $\alpha(\alpha < 0) = 0$
 - $\alpha > 0$ are our support vectors!
 - $w = X^T diag(Y)\alpha$



Simple Example

Given data

$$X = \begin{bmatrix} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix} \quad Y = \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \end{bmatrix}$$

- It is typically beneficial to zscore our data in SVMs since we're computing the dot product between observations.
- And we'll also want to add a bias feature.
- So, our new observations are:

$$X = \begin{bmatrix} -0.866 & -0.866 & 1 \\ -0.866 & 0.866 & 1 \\ 0.866 & -0.866 & 1 \\ 0.866 & 0.866 & 1 \end{bmatrix} \qquad Y = \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \end{bmatrix}$$



Simple Example

$$X = \begin{bmatrix} -0.866 & -0.866 & 1 \\ -0.866 & 0.866 & 1 \\ 0.866 & -0.866 & 1 \\ 0.866 & 0.866 & 1 \end{bmatrix} \qquad Y = \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \end{bmatrix}$$

• Doing gradient ascent to learn α , we arrive at:

$$\alpha = \begin{bmatrix} 0.325 \\ 0.325 \\ 0.325 \\ 0.325 \end{bmatrix}$$

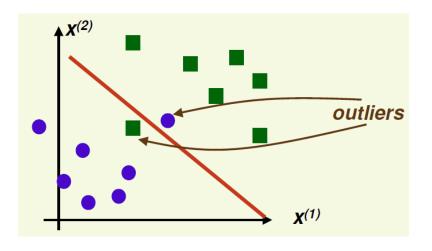
- All support vectors!
- And *w* as

$$w = X^T diag(Y)\alpha = \begin{bmatrix} 1.1547 \\ 0 \\ 0 \end{bmatrix}$$



Non-Separable Situations

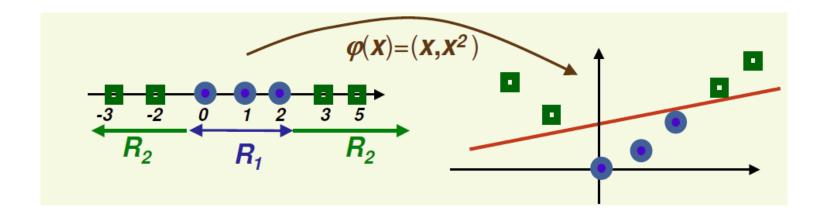
- Data is most likely to be not linearly separable
 - But linear classifier may still be appropriate
- Idea:
 - Move the data to a *higher* dimensionality where it may be separable





Mapping Functions

- A mapping function, $\phi(x)$, takes use from the feature space of x to some higher dimensional feature space
- A higher dimensional space is more easily linearly separable.
 - But don't forget about some of the issues with too many features!
- For instance, imagine the mapping function $\phi(x) = [x_1, x_1^2]$ on the data below:





Non-Separable SVM

So, where in our equations do we need the mapped observations?

$$\frac{\partial J}{\partial \boldsymbol{\alpha}} = ones(size(Y)) - diag(Y)\boldsymbol{X}\boldsymbol{X}^T diag(Y)\boldsymbol{\alpha}$$
$$\mathbf{w} = \boldsymbol{X}^T diag(Y)\boldsymbol{\alpha}$$



Non-Separable SVM

In our new space this is

$$\frac{\partial J}{\partial \alpha} = ones(size(Y)) - diag(Y)\phi(X)\phi(X)^T diag(Y)\alpha$$
$$\mathbf{w} = \phi(X)^T diag(Y)\alpha$$

We can make predictions as:

$$g(\mathbf{x}) = \phi(\mathbf{x})\mathbf{w} = \phi(\mathbf{x})\phi(X)^T diag(Y)\alpha$$



Cosine Similarty

$$\alpha = (diag(Y)XX^Tdiag(Y))^{-1}$$
ones(size(α), 1)

• Note that the two places that we need $\phi(x)$ involve $\phi(x)\phi(x)^T$:

$$\frac{\partial J}{\partial \alpha} = ones(size(Y)) - diag(Y)\phi(X)\phi(X)^T diag(Y)\alpha$$
$$g(x) = \phi(x)\phi(X)^T diag(Y)\alpha + b$$

- The computation $\phi(a)\phi(b)^T$ is known as the *cosine similarity* between observation a and b.
- There is a group of functions, known as *kernel functions*, that can compute $\phi(a)\phi(b)^T$ without explicitly mapping to the higher dimensional space.



Kernels

Commonly used kernels include:

- Linear: $\kappa(\boldsymbol{a},\boldsymbol{b}) = \boldsymbol{a}\boldsymbol{b}^T$
- Polynomial (degree is p): $\kappa(\boldsymbol{a}, \boldsymbol{b}) = (\boldsymbol{a}\boldsymbol{b}^T + 1)^p$
- Radial Basis Function (RBF): $\kappa(\boldsymbol{a}, \boldsymbol{b}) = e^{-\frac{(\boldsymbol{a}-\boldsymbol{b})(\boldsymbol{a}-\boldsymbol{b})^{T}}{2\sigma^{2}}}$



Example: The Kernel Trick

• As an example, let's show that using a quadratic kernel, $\kappa(\boldsymbol{a}, \boldsymbol{b}) = (\boldsymbol{a}\boldsymbol{b}^T + 1)^2$, when a and b are 1-D feature vectors is equivalent to $\kappa(\boldsymbol{a}, \boldsymbol{b}) = \phi(\boldsymbol{a})\phi(\boldsymbol{b})^T$ where $\phi(\boldsymbol{x}) = \begin{bmatrix} x_1^2 & \sqrt{2}x_1 & 1 \end{bmatrix}$?



Kernels

Quadratic Polynomial Kernel:

$$\kappa(\boldsymbol{a},\boldsymbol{b}) = \left(\boldsymbol{a}\boldsymbol{b}^T + 1\right)^2$$

Observational data:

$$x = [x_1]$$

• Therefore,
$$\kappa(\boldsymbol{a}, \boldsymbol{b}) = \left(\boldsymbol{a}\boldsymbol{b}^T + 1\right)^2 = (a_1b_1 + 1)^2$$

= $(a_1b_1)^2 + 2(a_1b_1) + 1$
= $a_1^2b_1^2 + 2a_1b_1 + 1$

• What is $\phi(x)$ in order to write:

$$\kappa(\mathbf{a}, \mathbf{b}) = a_1^2 b_1^2 + 2a_1 b_1 + 1 = \phi(\mathbf{a}) \phi(\mathbf{b})^T$$



Kernel Trick

$$\kappa(\boldsymbol{a}, \boldsymbol{b}) = \begin{bmatrix} a_1^2, \sqrt{2}a_1, 1 \end{bmatrix} \begin{bmatrix} b_1^2\\ \sqrt{2}b_1\\ 1 \end{bmatrix}$$

Therefore

$$\phi(\mathbf{x}) = \begin{bmatrix} x_1^2 & \sqrt{2}x_1 & 1 \end{bmatrix}$$

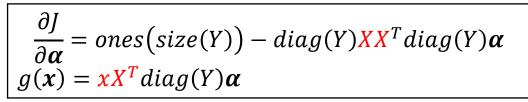
 We just showed that using the polynomial kernel of degree two on observations with a single feature is equivalent to compute the cosine similarity on observations in 3D space!



Kernels

Commonly used kernels include:

- Linear: $\kappa(\boldsymbol{a}, \boldsymbol{b}) = \boldsymbol{a}\boldsymbol{b}^T$
- Polynomial (degree is p): $\kappa(\boldsymbol{a}, \boldsymbol{b}) = (\boldsymbol{a}\boldsymbol{b}^T + 1)^p$
- Radial Basis Function (RBF): $\kappa(\boldsymbol{a}, \boldsymbol{b}) = e^{-\frac{(\boldsymbol{a}-\boldsymbol{b})(\boldsymbol{a}-\boldsymbol{b})^T}{2\sigma^2}}$
- Which should we use?
 - Start with linear, and if underfitting, move up to quadratic, etc...
 - Try to find one that give you the balance between over and underfitting.
 - Note: RBF kernel does the computations in the highest possible dimensionality.





Non-Separable SVM

- Let K(A,B) be a pairwise similarity matrix comparing the rows of A and B using a kernel function $\kappa(a,b)$.
 - K(A,B) will be of size of size $M \times N$ where M is the number of rows (observations) in A and B is the number of rows (observations) in B
- We can now compute the gradient of α using the kernel trick as:

$$\frac{\partial J}{\partial \boldsymbol{\alpha}} = ones(size(Y)) - diag(Y)\kappa(X,X)diag(Y)\boldsymbol{\alpha}$$

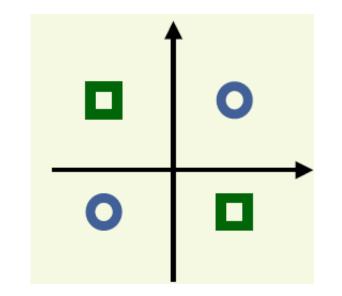
• And then apply the discriminant to an observation (without actually solving for \boldsymbol{w}) as:

$$g(\mathbf{x}) = \mathbf{K}(\mathbf{x}, \mathbf{X}) diag(Y) \boldsymbol{\alpha}$$





- Class 1 (positive): X1=[1,-1], X2=[-1,1]
- Class 2 (negative): X3=[1,1], X4=[-1,-1]
- Therefore, our data set is:



$$X = \begin{bmatrix} 1 & -1 \\ -1 & 1 \\ 1 & 1 \\ -1 & -1 \end{bmatrix}, Y = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}$$

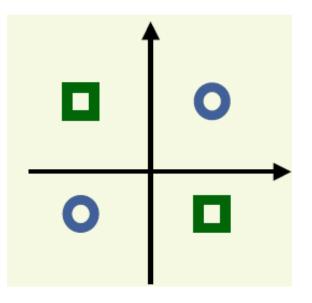
• We will once again prepare our data by zscoring and adding a bias feature: $\begin{bmatrix} 0.866 & -0.866 & 1 \end{bmatrix}$

$$X \rightarrow \begin{bmatrix} 0.866 & -0.866 & 1 \\ -0.866 & 0.866 & 1 \\ 0.866 & 0.866 & 1 \\ -0.866 & -0.866 & 1 \end{bmatrix}$$



SVM Example: XOR

- In this current space our data is not separable!
- Going through the gradient ascent to learn α will never terminate! \otimes





SVM Example: XOR

$$\frac{\partial J}{\partial \boldsymbol{\alpha}} = ones(size(Y)) - diag(Y)\boldsymbol{X}\boldsymbol{X}^T diag(Y)\boldsymbol{\alpha}$$

- So, we could explicitly do everything in a higher space, if we know of a good mapping function.
- Instead let's use our kernel trick and instead of computing $\phi(\mathbf{X}_i)^T\phi(\mathbf{X}_j)$ in our equation for J let's use $\kappa(\mathbf{X}_i,\mathbf{X}_j)$!
- If we choose to use a quadratic kernel, $\kappa(\mathbf{a}, \mathbf{b}) = (ab^T + 1)^2$ then we'd eventually get to:

$$\alpha = \begin{bmatrix} 0.2222 \\ 0.2222 \\ 0.2222 \\ 0.2222 \end{bmatrix}$$

Now they're all support vectors!



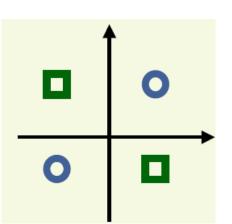
SVM Example: XOR

$$X \to \begin{bmatrix} 0.866 & -0.866 & 1 \\ -0.866 & 0.866 & 1 \\ 0.866 & 0.866 & 1 \\ -0.866 & -0.866 & 1 \end{bmatrix} \quad Y = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}$$

 $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0.2222$

- Let's do a sanity check!
 - Predict the value for x = [1, -1]
- Thanks to the kernel trick we just need to compute: $g(\mathbf{x}) = \kappa(\mathbf{x}, X) diag(Y) \alpha$
- Recall we chose $\kappa(\boldsymbol{a},\boldsymbol{b}) = (\boldsymbol{a}\boldsymbol{b}^T + 1)^2$
- Therefore

$$g([1,-1]) = [12.25, 0.25, 4, 4] \begin{pmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0.222 \\ 0.222 \\ 0.222 \end{bmatrix} \end{pmatrix} = 1$$





Resources

- https://towardsdatascience.com/support-vector-machine-introduction-to-machine-learning-algorithms-934a444fca47
- https://www.saedsayad.com/support vector machine.htm
- https://svivek.com/teaching/lectures/slides/svm/svm-sgd.pdf
- https://www.youtube.com/watch?v= PwhiWxHK8o
- https://www.cs.rpi.edu/~stewart/lec23-post/svms.pdf
- https://kuleshov-group.github.io/aml-book/contents/lecture13-svm-dual.html
- https://web.mit.edu/6.034/wwwbob/svm-notes-long-08.pdf
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