

DASC 4113 Machine Learning

Lecture 9 Ukash Nakarmi

Support Vector Machines



Learning Objectives

In this class, we will learn:

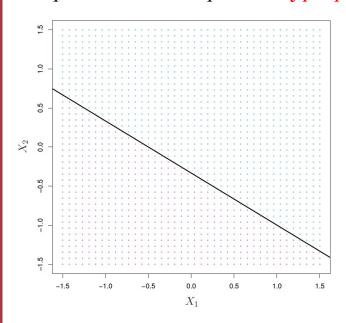
- A different approach to Classification termed "Maximal Marginal Classifier".
- Limitations of Maximal Marginal Classifier(MMC)
- An alternative: Support Vector Classifier that overcomes of MMC.
- A general approach termed "Support Vector Machines" that are able to handle non-linear Class Boundaries.
- Connection between Logistic Regression and Support Vector Machines.



Maximal Marginal Classifier

Hyperplane:

In a p-dimensional space, a hyperplane is a flat, affine subspace of a dimension p-1.



Example: A line in a 2 D space

2 Dimensions: X1 and X2

Hyperplane: A line, $1 + 2X_1 + 3X_2 = 0$.

Flat: Can use Euclidean Geometry/Linear Algebra. Affine: Does not have to contain an origin.



Hyperplane:

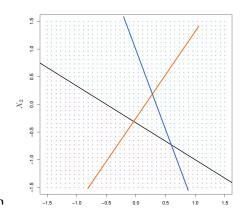
Expression for a Hyperplane in:

• A 2D space:

$$eta_o + eta_1 X_1 + eta_2 X_2 = 0$$
 Line, that does not pass-through origin

• A 3D space:

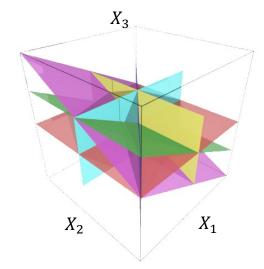
$$eta_o + eta_1 X_1 + eta_2 X_2 + eta_3 X_3 = 0$$
 Plane, that does not pass-through origin



• A p-D space:

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

(p-1)dimension, flat, affine subspace.





Hyperplane and Points in Space

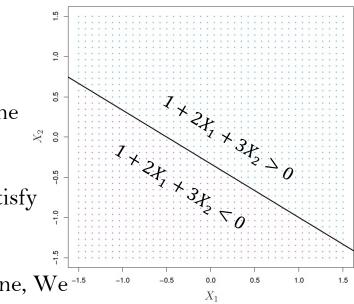
$$\beta_o + \beta_1 X_1 + \beta_2 X_2 = 0$$

There are set of points $X = (X_1, X_2)^T$ that satisfy the equation of the hyperplane. (The Points on the line)

And set of other points $X = (X_1, X_2)^T$ that do not satisfy the equation of the hyperplane.

For points that do not satisfy equation of a Hyperplane, We^{-1.5} $\stackrel{-1.0}{\text{We}}$ $\stackrel{-0.5}{=}$ $\stackrel{0.0}{=}$ $\stackrel{0.5}{=}$ $\stackrel{1.0}{=}$ $\stackrel{1.0}{=}$ get:

$$eta_o + eta_1 X_1 + eta_2 X_2 < 0$$
, or Purple Region
$$or \qquad \qquad \text{(The Points on either side of the line)}$$
 $eta_o + eta_1 X_1 + eta_2 X_2 > 0 \qquad \qquad \text{Blue Region}$





Hyperplane and Points in Space

For p - dimension space, a p dimension point(vector), $X = (X_1, X_2, X_3, ..., X_p)^T$,

Lies on the hyperplane:

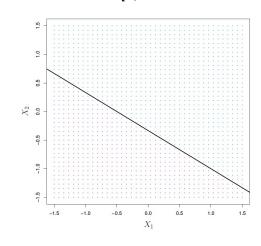
If:

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

Lies on the either side of a hyperplane:

If:

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



Conclusion: A hyperplane divides/separates a p-dimensional space into two halves.



Example:

- We measured p different tissue properties that plays role in whether a tissue is cancerous or not.
- We collected data from n different patients (samples).

So, we have a data matrix X of size $n \times p$.

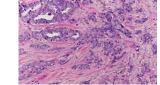
We can also say, we have n training observation in p dimensional space.

Task:

• We want to classify the observations into:

Cancerous
$$(Y = +1)$$
 or Non-cancerous $(Y = -1)$





Task:

• We want to classify the observations into:

Cancerous
$$(Y = +1)$$
 or
Non-cancerous $(Y = -1)$

n Inputs/samples each of p dimension

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

If we can find a hyperplane,

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p = 0$$
Such that:

For All Cancerous Samples, i.e., For Samples (x_i) whose response is $y_i = 1$,

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} > 0$$

n responses, either sample is from class -1 or class 1

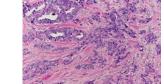
$$y_1,\ldots,y_n \in \{-1,1\}$$

For All Non-cancerous Samples, i.e., For Samples (x_i) whose response is $y_i = -1$,

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} < 0$$

Job is Done!





For All Cancerous Samples,
i.e., For Samples
$$(x_i)$$
 whose response is $y_i = 1$,

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} > 0$$

For All Non-cancerous Samples, i.e., For Samples (x_i) whose response is $y_i = -1$,

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} < 0$$

Equivalently, our separating hyperplane should be such that:

$$y_i(\beta_0+\beta_1x_{i1}+\beta_2x_{i2}+\cdots+\beta_px_{ip})>0$$
 , $\forall i=1,2,3,...n$

Then for any Test Samples: (x^*) ,

We can evaluate: $f(x^*)$, Sign of f(x) tells us the class, Magnitude tells us how far the sample is from the hyperplane

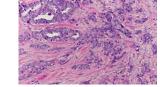
If:

$$f(x^*) > 0$$
: Test Sample belongs to class $Y = 1$, (Cancerous Tissue)

Else:

$$f(x^*) < 0$$
: Test Sample belongs to class $Y = -1$, (Non – Cancerous)





Example in a 2D space:

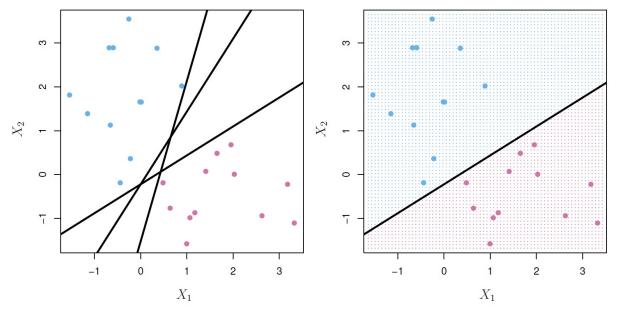
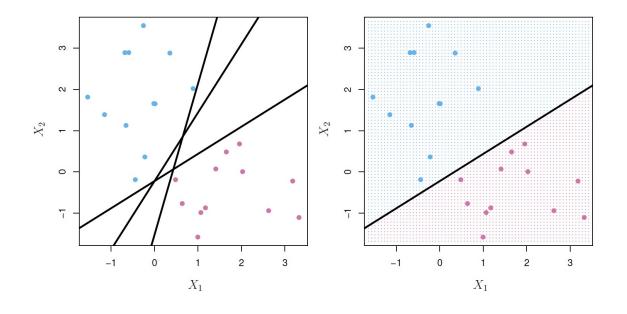


Fig: 9.2, X_1 and X_2 are 2 input features. Left: Some observation Samples (training) and MANY separating hyperplanes. Right: One of the separating hyperplanes and training and test samples in either side of hyperplane.





We could get many separating hyperplanes. Which one shall we choose?

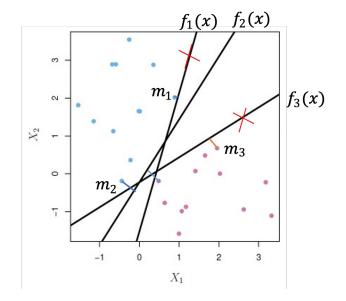


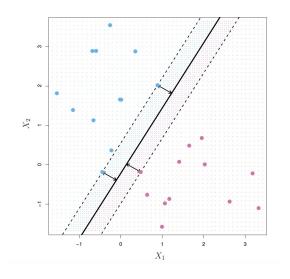
Which one shall we choose?

- Maximal Marginal Hyperplane/Optimal Separating Hyperplane
- A Hyperplane Farthest from the training observations.
- We can calculate perpendicular distance from each observation/training sample to the given hyperplane.
- The smallest of such distance is termed Margin.
- We want a hyperplane for which the Margin is Maximum. (Hence the term, Maximum Margin Classifier)



We want a hyperplane for which the Margin is Maximum.



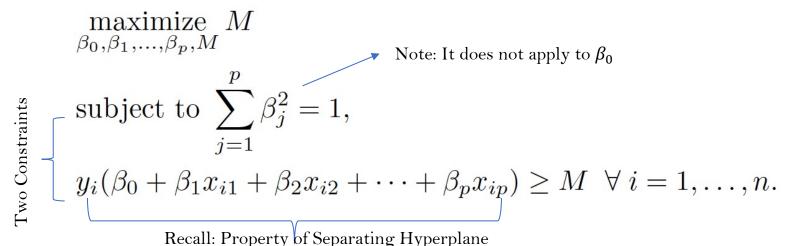


- Three separating hyperplanes, $f_1(x)$, $f_1(x)$, $f_1(x)$ with corresponding minimum margins m_1 , m_2 and m_3 , respectively.
- $m_2 > m_3 > m_1$, m_2 is maximum among all minimum margins.

i.e., $f_2(x)$ is a maximal minimum margin Separating Hyperplane



Construction:



What do these constraints enforce?

- Why \geq M? Why not \geq 0?, as given by property of Hyperplane?
- Why we need the first constraint?

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}) > 0$$
Property of Hyperplane

What do these constraints enforce?

- Why \geq M? Why not 0?
- Why we need the first constraint?

Let's first look at the second constraint:

$$y_i(eta_0+eta_1x_{i1}+eta_2x_{i2}+\cdots+eta_px_{ip})>0$$
 Why \geq M? Why not 0?

Property of Hyperplane: >0: Enforces each samples are on the correct side of the Hyperplane.

Adding Constraint, $\geq M$ (M is positive number)

Enforces: the minimum distance from the sample is at least M.



wo Constraints

The Maximal Margin Classifier

What do these constraints enforce?

- Why \geq M? Why not 0?
- Why we need the first constraint?

Subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1$$
,
$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}) \ge M \quad \forall i = 1, \dots, n.$$

First constraint:

Its not a necessary condition, but allows us to calculate the perpendicular distance from any sample to the hyperplane as:

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip})$$

if
$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} = 0$$
, Then, for any $k \neq 0$ $k(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}) = 0$;, as well.



First constraint:

Its not a necessary condition, but allows us to calculate the perpendicular distance from any sample to the hyperplane as:

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip})$$

Example:

$$1 + 2X_1 + 3X_2 = 0 : Hyperplane$$

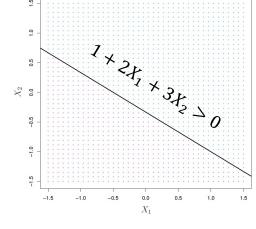
$$\beta_0 = 1$$
, $\beta_1 = 2$, $\beta_2 = 3$

Point: (1,-1) lies on this hyperplane

$$k = 5$$
, => New $\beta = 5 * old \beta$, i. e., β_0 , = 5, $\beta_1 = 10$, $\beta_2 = 15$

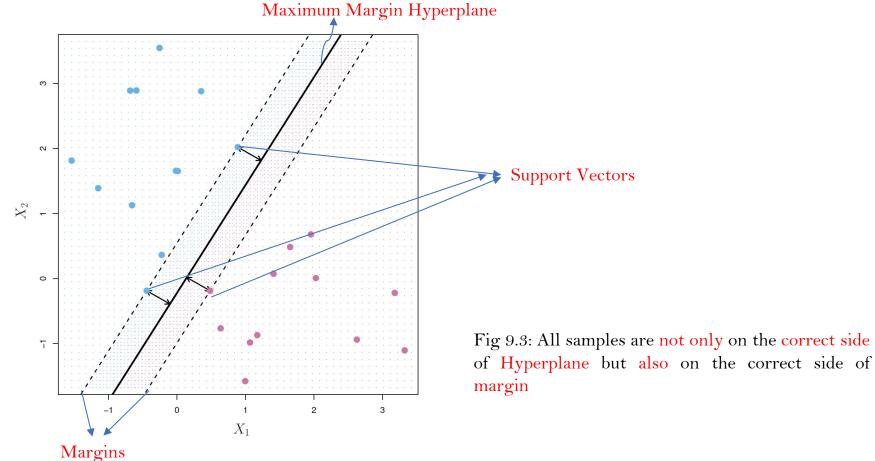
$$5 + 10X_1 + 15X_2 = 0 : New Hyperplane$$

Our Point: (1,-1) still lies on this New hyperplane.



No matter which hyperplane we had chosen, it would still correctly separate our data. So, not a necessary condition.

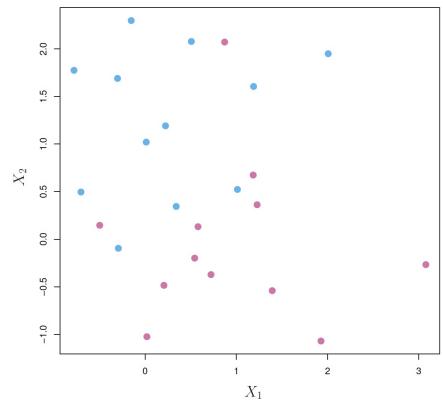






The Non-Separable Case

Data are not always linearly separable.

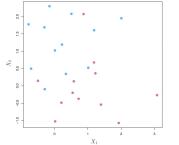


Example: Data not linearly separable. The separating Hyperplane does not exist.



Support Vector Classifier (SVC)

- Data are not always linearly separable. Separating hyperplane might not exist.
- Even when it exists, Perfectly separating Hyperplane may overfit the data, Not stable Learning Model.



SVCs

Introduce Some Tolerance.

i.e., Allow some misclassifications for some samples.

The process is called Support Vector Classifier (Soft margin)

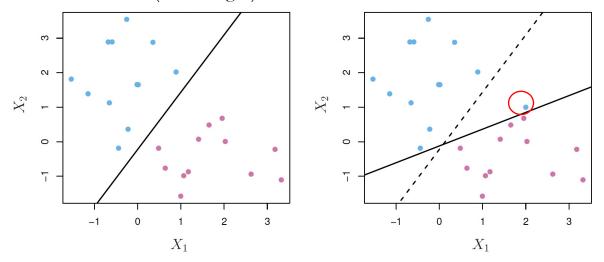


Fig: Left, A perfect separating Hyperplane. Right: Illustration: Just one extra sample point changed the separating hyperplane from a solid line on left to the solid line on right fig. Not stable learning.

Support Vector Classifier

subject to
$$\sum_{j=1}^{p} \beta_j^2 = 1,$$
$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}) \ge M(1 - \epsilon_i),$$
$$\epsilon_i \ge 0, \quad \sum_{j=1}^{n} \epsilon_i \le C,$$

- $\epsilon_i, \epsilon_2 \cdots \epsilon_n$, are called slack variables that allows individual sample to be on the wrong side of margin or even wrong side of the separating hyperplane.
- C is a non-negative tuning parameter.

Once we know model parameters β , Then to classify Test Samples:

Compute:
$$f(x^*) = \beta_0 + \beta_1 x_1^* + \dots + \beta_p x_p^*$$
 And Check Sign of $f(x^*)$ $f(x^*) > 0 \Rightarrow Class \ 1 \text{ or } f(x^*) < 0 \Rightarrow Class \ -1$,

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Support Vector Classifier

Consequence of Slack Variable ϵ :

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

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

 X_1

- When $\epsilon_i = 0$, Sample x_i is on the correct side of the margin.
- When $\epsilon_i > 0$, Sample x_i is on the wrong side of the margin, but on the correct side of separating hyperplane.
- When $\epsilon_i > 1$, Sample x_i is not only the wrong side of the margin, but also on the wrong side of the separating hyperplane.



Support Vector Classifier

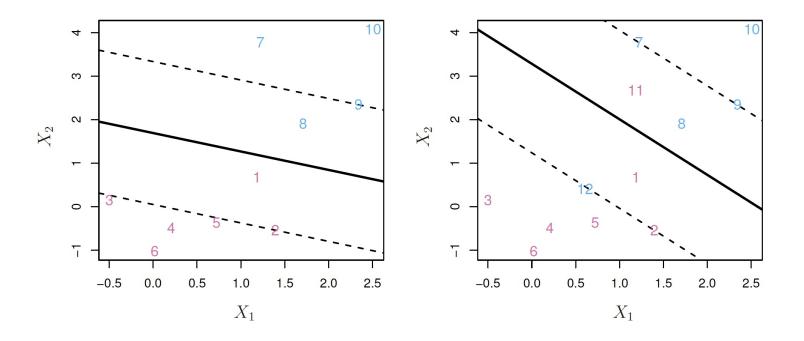


Figure 9.6, Support vector classifier. Left: some Samples only on the wrong side of margin (Still all correct classification), Right: some samples on wrong side of both margin and hyperplane (misclassification)



Support Vector Machines



Support Vector Machines



Recall: In Polynomial Regression/Regression with interaction variables:

We created transformation of input features/interaction variables as new variables.

Similarly,

Instead of fitting support vector classifiers using p features, $X_1, X_2, ..., X_p$, We could fit a support vector classifier using 2p features, $X_1, X_1, X_2, ..., X_p, X_p^2$,



Then, the Support Vector Classifier Model

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

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

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

Becomes



$$\max_{\beta_0,\beta_{11},\beta_{12},...,\beta_{p1},\beta_{p2},\epsilon_1,...,\epsilon_n,M} M$$
subject to $y_i \left(\beta_0 + \sum_{j=1}^p \beta_{j1} x_{ij} + \sum_{j=1}^p \beta_{j2} x_{ij}^2 \right) \ge M(1 - \epsilon_i),$

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



$$\max_{\beta_0,\beta_{11},\beta_{12},\dots,\beta_{p1},\beta_{p2},\epsilon_1,\dots,\epsilon_n,M} M$$
subject to $y_i \left(\beta_0 + \sum_{j=1}^p \beta_{j1} x_{ij} + \sum_{j=1}^p \beta_{j2} x_{ij}^2\right) \ge M(1 - \epsilon_i),$

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

Interesting Points:

- 1. The decision Boundary is nonlinear in the original input feature space.
- 2. But the decision Boundary is linear in the modified, enlarged (high-dimensional) feature space.

Interesting Questions:

- 1. Why do we enlarge the feature space only with degree of 2?
- 2. Do we always know what is the best enlarging method?



Interesting Questions:

- 1. Why do we enlarge the feature space only with degree of 2? We do not have to do only with degree of 2. We can use many ways to enlarge the feature space.
- 2. Do we always know what is the best feature space enlarging method? No, we can use different methods to enlarge feature dimension, but we do not generally know which one is the best.

Support Vector Machines provide efficient computational tool to expand feature space (dimension of feature space) by use of *kernels*.



Support Vector Machines provide efficient computational tool to expand feature space (dimension of feature space) by use of *kernels*.

The Linear Support Vector Classifier is expressed as:

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

 x_i : Training Samples

x: Test sample, new sample

 α_i : Coeff of Support Vector Model

Inner Product



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

What is interesting about this classifier?

1. To estimate parameters α_i , i = 1, 2, ..., n, we only need to compute $\binom{n}{2}$ inner products $\langle x_i, x_i' \rangle$ between all training samples.

$$\binom{n}{2} = \frac{n(n-1)}{2}$$

Note: We have not discussed how to calculate solve the optimization to compute α_i

2. In support vector classifier, only training observation that are support vectors (sample that lie on margin) are significant.

So, if S is a set of support vectors, Then:

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



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

Conclusion:

To do classification using Support Vector, all we need is inner product.

$$\max_{\beta_0,\beta_{11},\beta_{12},...,\beta_{p1},\beta_{p2},\epsilon_1,...,\epsilon_n,M} M$$
subject to $y_i \left(\beta_0 + \sum_{j=1}^p \beta_{j1} x_{ij} + \sum_{j=1}^p \beta_{j2} x_{ij}^2 \right) \ge M(1 - \epsilon_i),$

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



Inner Product, Dot Product and kernels

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

Let K be the kernel that generalize the inner product $\langle x_i, x_i' \rangle$

i.e.
$$K(x_i, x_i') = \langle x_i, x_i' \rangle$$

One popular inner product we know is a dot product:

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



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

When we choose inner product to be the dot product

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

We get support vector classifier, and it is known as a linear kernel. But, we could choose many different kernels.



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

We could choose many different kernels.

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

Polynomial Kernel

$$K(x_i, x_{i'}) = \exp(-\gamma \sum_{i=1}^{p} (x_{ij} - x_{i'j})^2).$$

Radial kernel



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

Question: Why not expand the features itself using many polynomials and then solve regression/classification?

Ans: Computational advantages. Using kernels:

- 1. We do not need to find explicit representation in new feature space.
- 2. Feature dimension can be very large (for example the implicit feature dimension of radial kernel is infinite).
- 3. All computations can be represented as inner product.



SVM and Relation to Regression

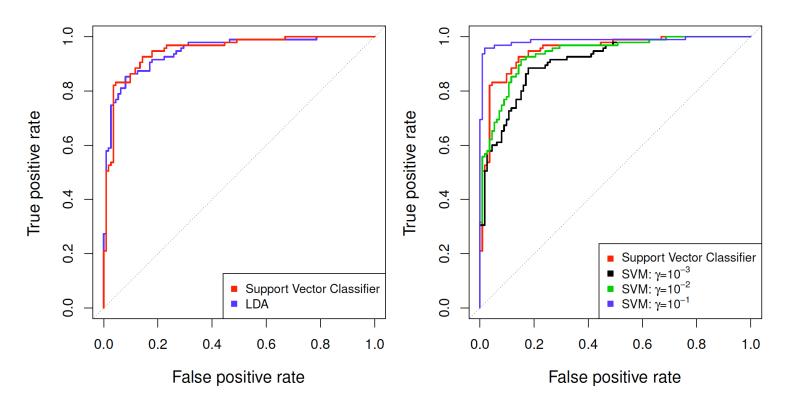
SVM has equivalent form of loss + penalty similar to Ridge Regression

$$\underset{\beta_0,\beta_1,\ldots,\beta_p}{\text{minimize}} \left\{ \sum_{i=1}^n \max\left[0,1-y_i f(x_i)\right] + \lambda \sum_{j=1}^p \beta_j^2 \right\}$$



SVM Example

Heart Disease Data

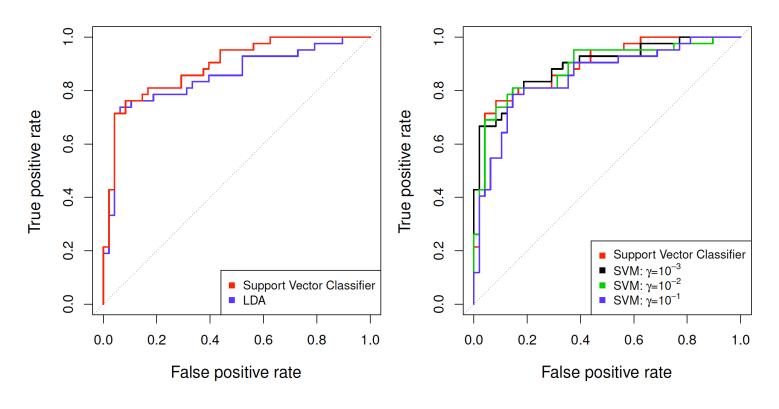


Performance for Training Data



SVM Example

Heart Disease Data



Performance for Test Data



What does it tell us? What is it?

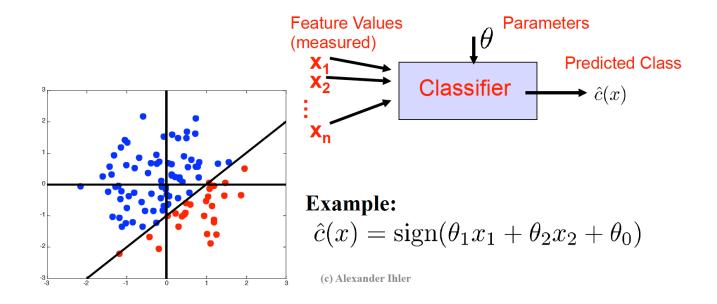


- Captures the complexity of learning model.
- How well the model can represent the data?

Rest of the Slides are based on Alexander Ihler and Andrew Moore's Slides

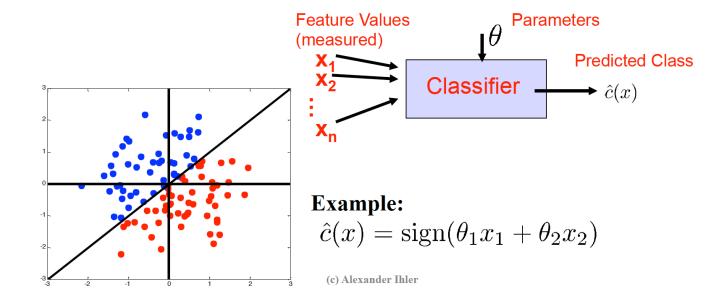


- We've seen many versions of underfit/overfit trade-off
 - Complexity of the learner
 - "Representational Power"
- Different learners have different power



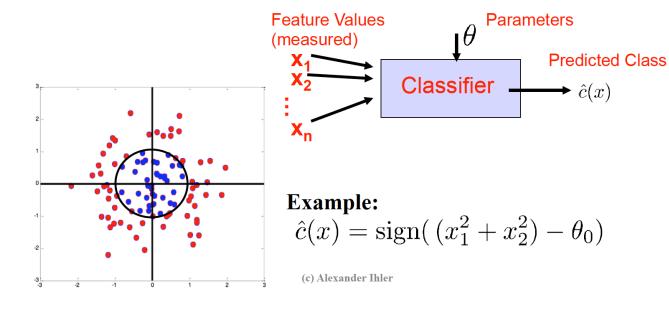


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- We've seen many versions of underfit/overfit trade-off
 - Complexity of the learner
 - "Representational Power"
- Different learners have different power
- Usual trade-off:
 - More power = represent more complex systems, might overfit
 - Less power = won't overfit, but may not find "best" learner
- How can we quantify representational power?
 - Not easily...
 - One solution is VC (Vapnik-Chervonenkis) dimension



Some notation

- Assume training data are iid from some distribution p(x,y)
- Define "risk" and "empirical risk"
 - These are just "long term" test and observed training error

$$R(\theta) = \text{TestError} = \mathbb{E}[\mathbb{1}[c \neq \hat{c}(x; \theta)]]$$

$$R^{\text{emp}}(\theta) = \text{TrainError} = \frac{1}{m} \sum_{i} \mathbb{1}[c^{(i)} \neq \hat{c}(x^{(i)}; \theta)]$$

- How are these related? Depends on overfitting...
 - Underfitting domain: pretty similar...
 - Overfitting domain: test error might be lots worse!



VC Dimension and Risk

- Given some classifier, let H be its VC dimension
 - Represents "representational power" of classifier

$$R(\theta) = \text{TestError} = \mathbb{E}[\mathbb{1}[c \neq \hat{c}(x; \theta)]]$$

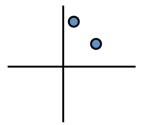
$$R^{\text{emp}}(\theta) = \text{TrainError} = \frac{1}{m} \sum_{i} \mathbb{1}[c^{(i)} \neq \hat{c}(x^{(i)}; \theta)]$$

• With "high probability" (1- η), Vapnik showed

TestError
$$\leq$$
 TrainError $+\sqrt{\frac{H\log(2m/H)+H-\log(\eta/4)}{m}}$



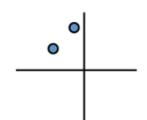
- We say a classifier f(x) can shatter points x⁽¹⁾...x^(h) iff For all y⁽¹⁾...y^(h), f(x) can achieve zero error on training data (x⁽¹⁾,y⁽¹⁾), (x⁽²⁾,y⁽²⁾), ... (x^(h),y^(h))
 (i.e., there exists some θ that gets zero error)
- Can $f(x;\theta) = sign(\theta_0 + \theta_1x_1 + \theta_2x_2)$ shatter these points?



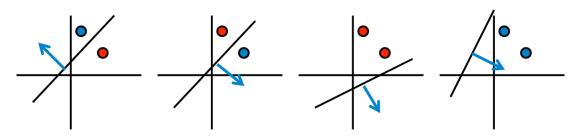
Some line that does not pass-through origin



We say a classifier f(x) can shatter points x⁽¹⁾...x^(h) iff For all y⁽¹⁾...y^(h), f(x) can achieve zero error on training data (x⁽¹⁾,y⁽¹⁾), (x⁽²⁾,y⁽²⁾), ... (x^(h),y^(h))
 (i.e., there exists some θ that gets zero error)

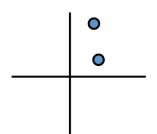


- Can $f(x;\theta) = sign(\theta_0 + \theta_1x_1 + \theta_2x_2)$ shatter these points?
- Yes: there are 4 possible training sets...





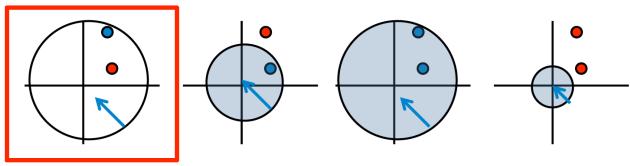
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 (i.e., there exists some θ that gets zero error)
- Can $f(x;\theta) = sign(x_1^2 + x_2^2 \theta)$ shatter these points?



Our classifier now is a Circle with radius of θ



- We say a classifier f(x) can shatter points x⁽¹⁾...x^(h) iff For all y⁽¹⁾...y^(h), f(x) can achieve zero error on training data (x⁽¹⁾,y⁽¹⁾), (x⁽²⁾,y⁽²⁾), ... (x^(h),y^(h))
 (i.e., there exists some θ that gets zero error)
- Can $f(x;\theta) = sign(x_1^2 + x_2^2 \theta)$ shatter these points?
- Nope!



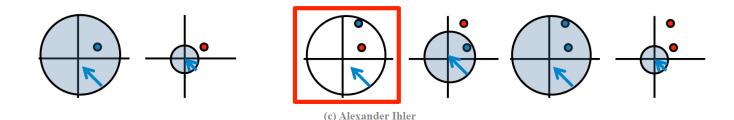
(c) Alexander Ihler



The VC dimension H is defined as

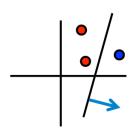
The maximum number of points h that can be arranged so that f(x) can shatter them

- Example: what's the VC dimension of the (zero-centered) circle, $f(x;\theta) = sign(x_1^2 + x_2^2 \theta)$?
- VCdim = 1 : can arrange one point, cannot arrange two (previous example was general)

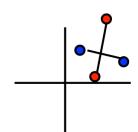




- Example: what's the VC dimension of the two-dimensional line, $f(x;\theta) = sign(\theta_1 x_1 + \theta_2 x_2 + \theta_0)$?
- VC dim >= 3? Yes



VC dim >= 4? No...
 Any line through these points must split one pair (by crossing one of the lines)



In General, for linear classifier in a d dimension with a constant term:

VC dimension = d+1.