

Mathematics For Data Science

Brian J. Mann

Feb 10-11, 2016

Who am I?

- PhD from University of Utah in 2014 (Geometric Group Theory)
- Worked for **Amazon Web Services** doing supply chain optimization and forecasting
- Now at **Galvanize** teaching data science and consulting
- **Slides**
- brian.mann@galvanize.com

Support Vector Machines (SVM)

- Idea: try to separate classes by an optimal hyperplane
- Here *optimal* means that the minimum distance from the hyperplane to any of the training points (the *margin*) is maximal.

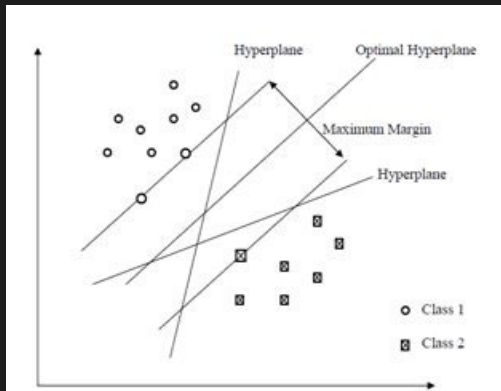


Figure 1:Maximal Margin

Ok, that sounds great. What's the problem?

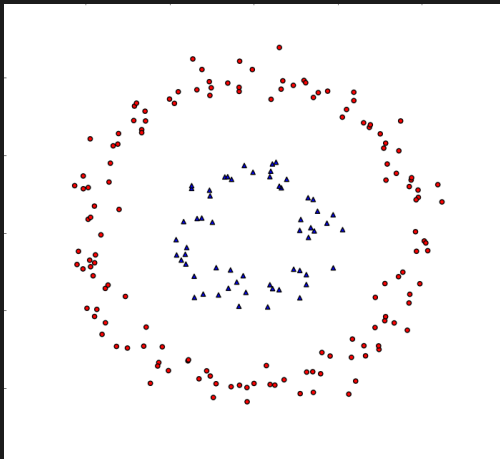


Figure 2: Well, shit.

The solution

- Map our data to a higher dimensional space where it's (almost) linearly separable

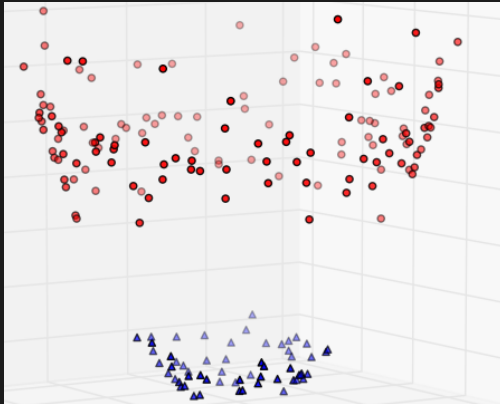


Figure 3:Yay!

Talk's over, right?

- Not quite, there's still some problems

Issue 1: Memory

- Even for polynomial transformations, the numbers of dimensions (features) in the target space can grow very quickly
- Consider the transformation $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^5$ given by

$$(x_1, x_2) \mapsto (x_1^2, x_1 x_2, x_2^2, x_1, x_2, 1)$$

- More generally, a mapping $\phi_d : \mathbb{R}^N \rightarrow \mathbb{R}^{\binom{N+d}{d}}$ that maps a vector to the vector of all monomial terms in N variables of degree $\leq d$
- $\binom{N+d}{d}$ grows very quickly as $d \gg 0$

Issue 2: Computation

- The optimal hyperplane for the transformed data is

$$f(x) = \sum_i a_i \cdot \langle \phi(x_i), \phi(x) \rangle + b = 0$$

- Need to compute the dot product of high-dimensional vectors (in fact, sometimes they might be infinite dimensional!)

A solution

- What if there was a way to compute $\langle \phi(x), \phi(y) \rangle$ directly without ever computing $\phi(x)$ or $\phi(y)$?
- There is!
- This is what *kernel functions* do for us

Kernels

- Make ϕ implicit
- This implicit ϕ might have an infinite dimensional target vector space

What is a kernel function?

A *kernel function* is a continuous function

$$K : \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}$$

which satisfies

- $K(x, y) = K(y, x)$ (symmetric)
- K is positive-semidefinite i.e.

$$\sum_i \sum_j K(x_i, x_j) c_i c_j > 0$$

for all finite sequences x_1, \dots, x_n and all $c_i, c_j \in \mathbb{R}$

Mercer's Theorem

Mercer's Theorem says that if $K : \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}$ is a kernel function, then there exists a vector space with an inner product (a *Hilbert space*) V and a mapping $\phi : \mathbb{R}^N \rightarrow V$ so that

$$K(x, y) = \langle \phi(x), \phi(y) \rangle$$

- In English, if K is a kernel function, it consists of a transformation followed by an inner product in some higher dimensional space V .
- Kernels allow us to compute high-dimensional inner products in V in terms of our original inputs in \mathbb{R}^N .

Example: Polynomial kernel

- $K(x, y) = (\langle x, y \rangle + c)^d$
- c and d are chosen *a priori* by the user, not trained
- Comes from the polynomial transformation ϕ_d (ignoring some constants)

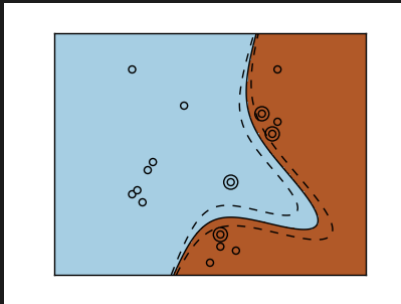


Figure 4: Polynomial Kernel

Example: RBF (Gaussian) kernel

- $K(x, y) = \exp(-\gamma \|x - y\|^2)$
- γ is chosen *a priori* by the user

More RBF kernel

What are ϕ and the dimension of V in this case?

- Let $\gamma = 1/2$ for ease of computation, then

$$K(x, y) = \sum_{j=0}^{\infty} \frac{\langle x, y \rangle^j}{j!} \exp\left(-\frac{\|x\|^2}{2}\right) \exp\left(-\frac{\|y\|^2}{2}\right)$$

- With a little algebra one gets

$$\phi(x) = \left(\frac{e^{-\frac{\|x\|^2}{2j}}}{\sqrt{j!}^{1/j}} \binom{j}{n_1, \dots, n_k} \right)^{1/2} \Bigg|_{j=0, \dots, \infty, \sum_{i=1}^k n_i = j}$$

- V is infinite dimensional ($V = l^2$ the space of square-summable sequences)

More RBF kernel

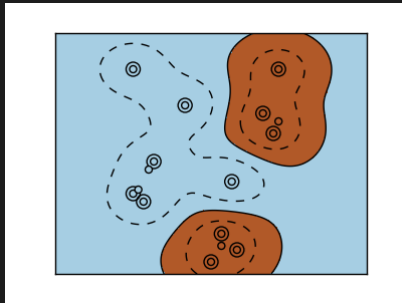


Figure 5:RBF Kernel

Questions?

VC Dimension and the VC Bound Theorem

Question?

- Why should you expect that your training error tells you anything about the error of your model on new data? In other words, why/how do you know that your model will generalize at all?

We need to start somewhere

Theorem (Hoeffding Inequality)

Suppose X_1, \dots, X_n are iid random variables and let

$$\bar{X} = \frac{X_1 + X_2 + \dots + X_N}{N}$$

then

$$\mathbb{P}(|\bar{X} - \mathbb{E}(\bar{X})| > \epsilon) \leq 2e^{-2\epsilon^2 N}$$

In English

- For any threshold value ϵ , if you sample a random variable enough times, the probability that the sample mean differs from the true mean by more than ϵ is nearly 0.
- i.e. If you flip a fair coin enough times, you expect the ratio of heads to tails get arbitrarily close to 1:1 with high probability.

Assumptions

- For the purposes of this talk, we'll focus on binary classification problems
- All of this can be extended to other supervised learning problems
- Positive and negative classes will be represented as $+1$ and -1

What does this have to do with machine learning?

- Suppose h is some hypothesis (a function that classifies observations as either $+1$ or -1)
- $E_{train}(h)$ = error rate on your training set
- $E_{gen}(h)$ = h 's true error rate

$E_{gen}(h)$ and $E_{train}(h)$ are random variables that satisfy the hypotheses of the Hoeffding Inequality so

$$\mathbb{P}(|E_{train}(h) - E_{gen}(h)| > \epsilon) \leq 2e^{-2\epsilon^2 N}$$

Naive error generalization bound

Suppose:

- We have a finite hypothesis set $\{h_1, \dots, h_M\}$
- Given some training data, we apply some learning procedure to find the optimal hypothesis g

It is NOT TRUE that

$$\mathbb{P}(|E_{train}(g) - E_{gen}(g)| > \epsilon) \leq 2e^{-2\epsilon^2 N}$$

since g is chosen after the data is generated

Naive error generalization bound

However, the event

$$|E_{train}(g) - E_{gen}(g)| > \epsilon$$

is in the union of the events

$$|E_{train}(h_i) - E_{gen}(h_i)| > \epsilon$$

so

$$\mathbb{P}(|E_{train}(g) - E_{gen}(g)| > \epsilon) \leq 2Me^{-2\epsilon^2 N}$$

Problem with this naive bound

- The bound

$$\mathbb{P}(|E_{train}(g) - E_{gen}(g)| > \epsilon) \leq 2Me^{-2\epsilon^2 N}$$

only works for finite hypothesis sets

- Not really useful for any real-world examples

Can we do better?

- How do we make this idea work?
 - Even with finitely many hypothesis functions the bound is still quite bad since the events

$$|E_{train}(h_i) - E_{gen}(h_i)| > \epsilon$$

probably have large overlaps

- In fact, they overlap enough to allow us to work with infinite hypothesis sets (i.e. hyperplanes in \mathbb{R}^N)

Shattering

- Let \mathcal{H} be our hypotheses set
 - \mathcal{H} might be all separating hyperplanes in \mathbb{R}^N
 - or the set of all of the possible decision functions you can get with a neural network of some fixed topology
- For any finite data set $\{x_1, \dots, x_N\}$, each $h \in \mathcal{H}$ gives a dichotomy $h(x_1), \dots, h(x_N) \in \{+1, -1\}^N$
- Define

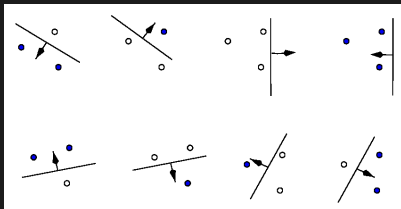
$$m_{\mathcal{H}}(N) = \max_{x_1, \dots, x_N} |\{h(x_1), \dots, h(x_N) | h \in \mathcal{H}\}|$$

Shattering

- $m_{\mathcal{H}}(N) \leq 2^N$
- \mathcal{H} shatters x_1, \dots, x_N if $|\{h(x_1), \dots, h(x_N) | h \in \mathcal{H}\}| = 2^N$
- In this case $m_{\mathcal{H}}(N) = 2^N$

Examples

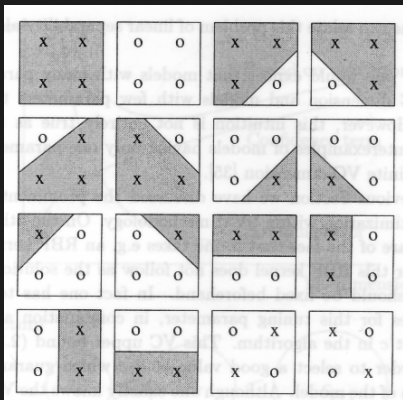
- Linear decision boundaries shatter 3 points in \mathbb{R}^2



- Convex polygons in \mathbb{R}^2 shatter arbitrarily many points
 - Choose N points on the unit circle
 - Take the convex hull of the +1's

Non-example

- Linear decision boundaries do not shatter any 4 points in \mathbb{R}^2



Vapnik-Chervonenkis (VC) Dimension

- The VC Dimension d_{VC} of \mathcal{H} is defined to be the largest N for which $m_{\mathcal{H}}(N) = 2^N$
- Said another way

$$d_{VC} \geq N$$

$$\Leftrightarrow$$

there exists a data set of size N such that \mathcal{H} shatters it

- The VC Dimension gives a polynomial upper bound on $m_{\mathcal{H}}(N)$

$$m_{\mathcal{H}}(N) \leq N^{d_{VC}} + 1$$

Examples

- For linear decision boundaries in \mathbb{R}^2 , $d_{VC} = 3$
- For linear decision boundaries in \mathbb{R}^N , $d_{VC} = N + 1$
 - Choose $N + 1$ points which do not live on the same hyperplane
 - Can get any dichotomy on these points, so $d_{VC} \geq N + 1$
 - With $N + 2$ points, can find hyperplane through N points with the remaining two points on either side
 - Labelling points on this hyperplane -1 , others $+1 \Rightarrow$ impossible dichotomy
 - $d_{VC} = N + 1$
- Convex polygons in \mathbb{R}^2 have $d_{VC} = \infty$

The VC Bound

The VC generalization bound states that for any $\delta > 0$

$$E_{gen}(g) \leq E_{train}(g) + \sqrt{\frac{8}{N} \ln \frac{4m_{\mathcal{H}}(2N)}{\delta}}$$

with probability $1 - \delta$

What does this tell us?

- Since $m_{\mathcal{H}}(N)$ is bounded by a polynomial of degree d_{VC} in N , the RHS of

$$E_{gen}(g) \leq E_{train}(g) + \sqrt{\frac{8}{N} \ln \frac{4m_{\mathcal{H}}(2N)}{\delta}}$$

- $\rightarrow E_{train}(g)$ as the size of the training set increases
- Since $m_{\mathcal{H}}(N)$ or d_{VC} is a measure of model complexity, more complicated models make the bound worse (overfitting!!!!)

Examples

Suppose we want $E_{gen}(g)$ to be within 10% of $E_{train}(g)$ with 90% confidence for a model with $d_{VC} = 3$. How much data do we need?

- From the VC Bound

$$\sqrt{\frac{8}{N} \ln \frac{4m_{\mathcal{H}}(2N)}{0.9}} \leq 0.1$$

- So

$$N \geq \frac{8}{0.1^2} \ln \left(\frac{4(2N)^3 + 4}{0.1} \right)$$

- $N \sim 30,000$
- It turns out that $N \sim 10,000 \times d_{VC}$
- Empirically, $N \sim 10 \times d_{VC}$ (VC bound badly overestimates)

Sketch of Proof

- Instead of working with the space of all possible observations, pick a second test set the same size as the training set

$$\mathbb{P} \left(\sup_h |E_{train}(h) - E_{gen}(h)| > \epsilon/2 \right) \leq$$
$$2\mathbb{P} \left(\sup_h |E_{train}(h) - E_{test}(h)| > \epsilon/2 \right)$$

- Replace the infinite hypothesis set with the number of dichotomies that the hypothesis set can have on a finite set S of points giving

$$\mathbb{P} \left(\sup_h |E_{train}(h) - E_{test}(h)| > \epsilon/2 \right) \leq$$
$$m_{\mathcal{H}}(2N) \times \sup_S \sup_h \mathbb{P} (|E_{train}(h) - E_{test}(h)| > \epsilon/2 | S)$$

Sketch Part 2

- Use the Hoeffding bound to show

$$\mathbb{P}(|E_{train}(h) - E_{test}(h)| > \epsilon/2 | S) \leq 2e^{-\frac{1}{8}\epsilon^2 N}$$

References

- Yaser S. Abu-Mostafa, Malik Magdon-Ismail, Hsuan-Tien Lin
Learning From Data: A Short Course
- Eduardo Sontag, *VC Dimension of Neural Networks*,
http://www.mit.edu/~esontag/FTP_DIR/vc-expo.pdf
- Images: <http://www.svms.org/vc-dimension/>