Mathematics For Data Science

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Who am I?

- PhD from University of Utah in 2014 (Geometric Group Theory)
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Objectives

- Learn some fun mathematics
  - Kernel trick for support vector machines
  - VC Generalization Bound (why machine learning works!)
- See how understanding how machine learning is working “under the hood” can improve your intuition about model selection and hyper-parameter choice

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.

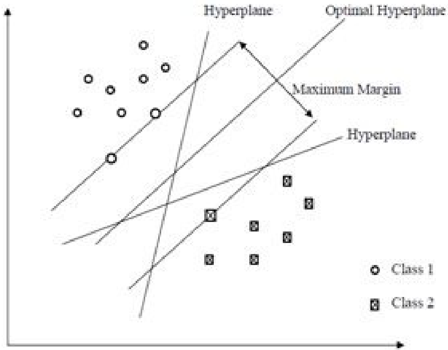


Figure 1:Maximal Margin

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

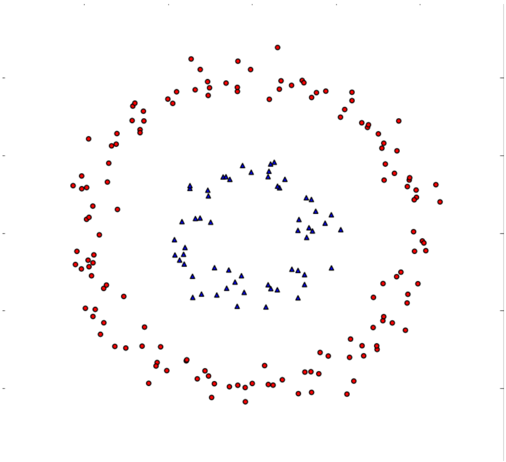


Figure 2:Oh.

The solution

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

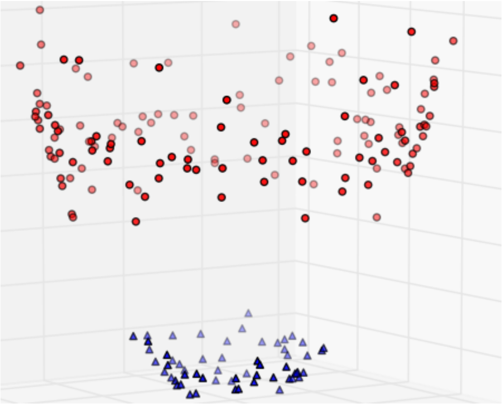


Figure 3:Yay!

Issue 1: Memory

- Even for polynomial transformations, the numbers of dimensions (features) in the target space can grow very quickly
- Consider the transformation $\phi : \mathbb{R}^2 \to \mathbb{R}^5$ 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 $\phi_d : \mathbb{R}^N \to \mathbb{R}^{\binom{N+d}{d}}$ 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 $N, d >> 0$

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

What is a kernel function?

A *kernel function* is a continuous function

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

which satisfies

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

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

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

This definition is a little opaque, but the idea is that a kernel function generalizes the idea of an inner product (also known as a linear kernel).

Mercer's Theorem

Mercer's Theorem says that if $K : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$ is a kernel function, then there exists a vector space with an inner product (a *Hilbert space*) V and a mapping $\phi : \mathbb{R}^N \to V$ 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 (sometimes infinite!) 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
- Find c and d by cross-validation
- Comes from the polynomial transformation ϕ_d (ignoring some constants)

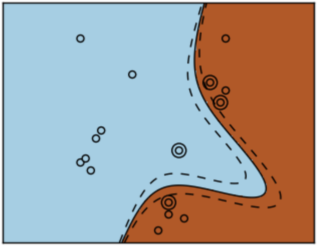


Figure 4:Polynomial Kernel

Example: RBF (Gaussian) kernel

- $K(x, y) = e^{-\gamma ||x-y||^2}$
- γ is chosen *a priori* by the user
- Largest when x and y are close, decays exponentially
- With the RBF kernel, SVM looks for clusters of similarly labeled points
- Can learn much more complicated decision boundaries compared to polynomial or linear kernels (watch for overfitting, adjust γ)

More RBF kernel

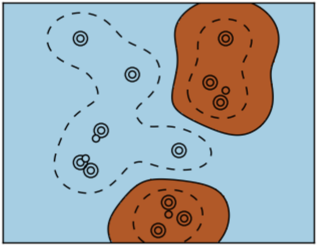


Figure 5:RBF Kernel

More RBF kernel

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

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

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

- With a little algebra one gets

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

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

Overview

- Understand how the kernel trick works
- Pick the right kernel for what you think the decision boundary might look like
- Questions?

VC Dimension and the VC Generalization Bound

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 $X_1, \ldots, X_n$ are iid random variables and let

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

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
- $E_{gen}(h)$ = true error rate of h

$E_{gen}(h)$ 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:

1. We have a finite hypothesis set $\{h_1, \ldots, h_M\}$
2. 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?

- 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
- A *dichotomy* is a choice of label $+1$ or -1 for each point in a data set
- For any finite data set $\{x_1, \ldots, x_N\}$, each $h \in \mathcal{H}$ gives a dichotomy $h(x_1), \ldots, h(x_N) \in \{+1, -1\}^N$
- Define

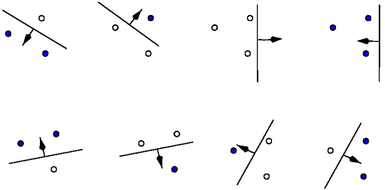
$$m_{\mathcal{H}(N)} = \max_{x_1,\ldots,x_N} |\{h(x_1), \ldots, h(x_N)|h \in \mathcal{H}\}|$$

Shattering

- $m_{\mathcal{H}}(N) \leq 2^N$
- $\mathcal{H}$ *shatters* $x_1, \ldots, x_N$ if $|\{h(x_1), \ldots, h(x_N) | h \in \mathcal{H}\}| = 2^N$
- In this case $m_{\mathcal{H}}(N) = 2^N$
- In other words, $\mathcal{H}$ shatters a set of points if it could obtain zero training error on that set

Examples

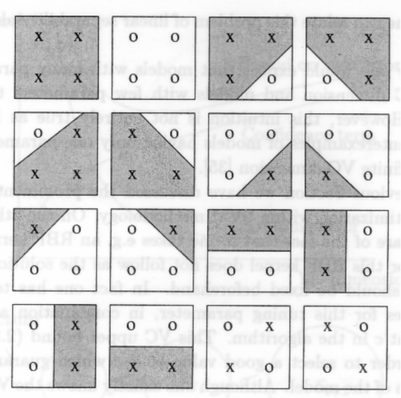
- Linear decision boundaries shatter 3 points in $\mathbb{R}^2$



- Convex polgons 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

$$d_{VC} \geq N$$

$$\Leftrightarrow$$

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

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

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

- VC Dimension is a measure of complexity of a hypothesis

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 $\delta > 0$

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

with probability $1 - \delta$

What does this tell us?

1. 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
2. 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

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

- So

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

- $N \sim 30,000$
- In general, $N \sim 10,000 \times d_{VC}$
- Empirically, $N \sim 10 \times d_{VC}$ (VC bound badly overestimates)

Conclusion

- The VC Generalization Bound is the theorem that tells you machine learning actually works!
- Obtain statistical guarantees about how well your model generalizes
- Extremely slack bound, but better than nothing

Sketch of Proof (optional)

Theorem (VC Generalization Bound)

$$\mathbb{P}\left(\sup_h |E_{train}(h) - E_{gen}(h)| > \epsilon\right) \leq 4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N}$$

Proof

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

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

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

Sketch Part 2

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

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

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

Sketch Part 3

3. Use the Hoeffding bound to show

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

Conclusion

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- Extremely slack bound, but better than nothing

References

Books

- Y. S. Abu-Mostafa, M. Magdon-Ismail, H.-T. Lin *Learning From Data: A Short Course*
- V. Vapnik, *The Nature of Statistical Learning Theory*

Papers

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- Eduardo Sontag, *VC Dimension of Neural Networks*, http://www.mit.edu/~esontag/FTP_DIR/vc-expo.pdf

Images

- http://www.svms.org/vc-dimension/