Lecture #19: Support Vector Machines

CS 109A, STAT 121A, AC 209A: Data Science

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Lecture Outline

Review

Extension to Non-linear Boundaries

A User’s Guide to Support Vector Machines

Review

Classifiers and Decision Boundaries

Last time, we derived a linear classifier based on the intuition that a good classifier should

- maximize the distance between the points and the decision boundary (maximize margin)
- misclassify as few points as possible

SVC as Optimization

With the help of geometry, we translated our wish list into an optimization problem

$$\begin{cases} \min\limits_{\xi_n \in \mathbb{R}^+, w, b} \|w\|^2 + \lambda \sum\limits_{n=1}^{N} \xi_n \\ \text{such that } y_n(w^\top x_n + b) \geq 1 - \xi_n,\ n = 1, \ldots, N \end{cases}$$

where ξ_n quantifies the error at x_n.

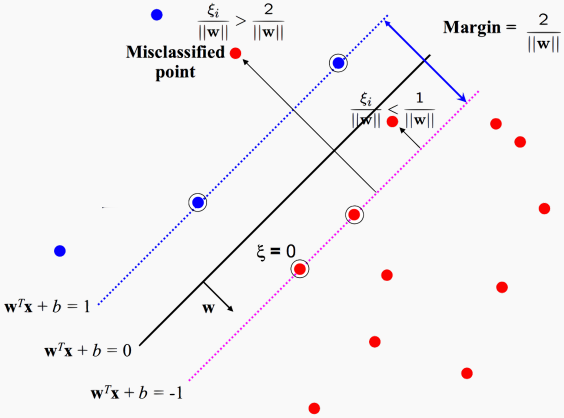
The SVC optimization problem is often solved in an alternate form (the dual form)

$$\max_{\alpha_n \geq 0, \sum_n \alpha_n y_n = 0} \sum_n \alpha_n - \frac{1}{2} \sum_{n,m=1}^{N} y_n y_m \alpha_n \alpha_m x_n^\top x_m$$

Later that this alternate form allows us to use SVC with non-linear boundaries.

Decision Boundaries and Support Vectors

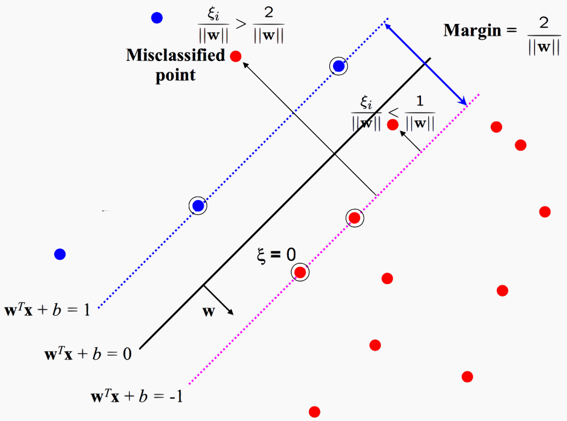
If we remember how the error terms ξ_n's were defined, we see that the points where $\xi_n = 0$ are precisely the support vectors



$\frac{\xi_i}{||\mathbf{w}||} > \frac{2}{||\mathbf{w}||}$
Misclassified point
Margin = $\frac{2}{||\mathbf{w}||}$
$\frac{\xi_i}{||\mathbf{w}||} < \frac{1}{||\mathbf{w}||}$
$\xi = 0$
$\mathbf{w}$
$\mathbf{w}^T\mathbf{x} + b = 1$
$\mathbf{w}^T\mathbf{x} + b = 0$
$\mathbf{w}^T\mathbf{x} + b = -1$

Decision Boundaries and Support Vectors

It’s intuitive to see that to re-construct the decision boundary, ***only the support vectors are needed!***



$\frac{\xi_i}{||\mathbf{w}||} > \frac{2}{||\mathbf{w}||}$
Misclassified point
Margin = $\frac{2}{||\mathbf{w}||}$
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$\xi = 0$
$\mathbf{w}^T\mathbf{x} + b = 1$
$\mathbf{w}$
$\mathbf{w}^T\mathbf{x} + b = 0$
$\mathbf{w}^T\mathbf{x} + b = -1$

Decision Boundaries and Support Vectors

- The decision boundary of an SVC is given by

$$\hat{w}^\top x + \hat{b} = \sum_{x_n \text{ is a support vector}} \hat{\alpha}_n y_n (x_n^\top x_n) + b$$

  where $\hat{\alpha}_n$ and the set of support vectors are found by solving the optimization problem.

- To classify a test point x_{test}, we predict

$$\hat{y}_{test} = \text{sign}\left(\hat{w}^\top x + \hat{b}\right)$$

Extension to Non-linear Boundaries

Polynomial Regression: Two Perspectives

Given a training set

$$\{(x_1, y_1), \ldots, (x_N, y_N)\}$$

with a single real-valued predictor, we can view fitting a 2nd degree polynomial model

$$w_0 + w_1 x + w_2 x^2$$

on the data as the process of finding the best quadratic curve that fits the data. But in practice, we first expand the feature dimension of the training set

$$x_n \mapsto (x_n^0, x_n^1, x_n^2)$$

and train a ***linear model*** on the expanded data

$$\{(x_n^0, x_n^1, x_N^2, y_1), \ldots, (x_N^0, x_N^1, x_N^2, y_N)\}$$

Transforming the Data

The key observation is that training a polynomial model is just training a linear model on data with transformed predictors.

In our previous example, transforming the data to fit a 2nd degree polynomial model requires a map

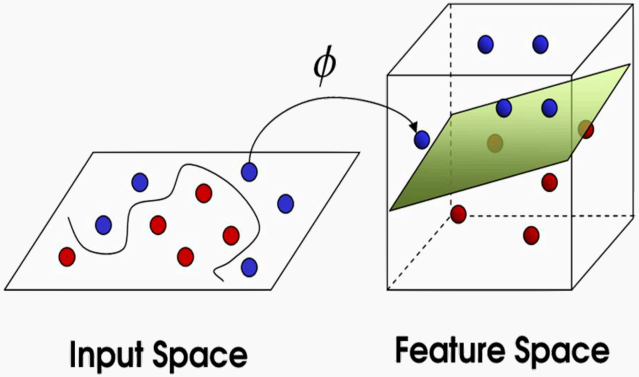
$$\phi : \mathbb{R} \to \mathbb{R}^3$$
$$\phi(x) = (x^0, x^1, x^2)$$

where $\mathbb{R}$ called the ***input space***, $\mathbb{R}^3$ is called the ***feature space***.

While the data is does not have a linear correlation in the input space $\mathbb{R}$, it may have one in the feature space $\mathbb{R}^3$.

SVC with Non-Linear Decision Boundaries

The same insight applies to classification: while the data may not be linear separable in the input space, it may be in a feature space after a fancy transformation:



SVC with Non-Linear Decision Boundaries

The motto: instead of tweaking the definition of SVC to accommodate non-linear decision boundaries. We map the data into a feature space in which the classes are linearly separable:

- Apply transform $\phi : \mathbb{R}^J \to \mathbb{R}^{J'}$ on training data

  $$x_n \mapsto \phi(x_n)$$

  where typically J' is much larger than J.
- Train an SVC on the transformed data

  $$\{(\phi(x_1), y_1), \ldots, (\phi(x_N), y_N)\}$$

The Kernel Trick

Since the feature space $\mathbb{R}^{J'}$ is extremely high dimensional, computing ϕ explicitly can be costly.

Instead, we note that computing ϕ is unnecessary.

Recall that training an SVC involves solving the optimization problem

$$\max_{\alpha_n \geq 0,\, \sum_n \alpha_n y_n = 0} \sum_n \alpha_n - \frac{1}{2} \sum_{n,m=1}^{N} y_n y_m \alpha_n \alpha_m \phi(x_n)^\top \phi(x_m)$$

In the above, ***we are only interested in computing inner products*** $\phi(x_n)^\top \phi(x_m)$ ***in the feature space*** and not the quantities $\phi(x_n)$.

The Kernel Trick

The ***inner product*** between two vectors is a measure of the similarity of the two vectors.

Definition

Given a transformation $\phi : \mathbb{R}^J \to \mathbb{R}^{J'}$, from input space $\mathbb{R}^J$ to feature space $\mathbb{R}^{J'}$, the function $K : \mathbb{R}^J \times \mathbb{R}^J \to \mathbb{R}$ defined by

$$K(x_n, x_m) = \phi(x_n)^\top \phi(x_m), \quad x_n, x_m \in \mathbb{R}^J$$

is called the ***kernel function*** of ϕ.

Generally, ***kernel function*** may refer to any function $K : \mathbb{R}^J \times \mathbb{R}^J \to \mathbb{R}$ that measure the similarity of vectors in $\mathbb{R}^J$, without explicitly defining a transform ϕ.

The Kernel Trick

For a choice of kernel K,

$$K(x_n, x_m) = \phi(x_n)^\top \phi(x_m)$$

we train an SVC by solving

$$\max_{\alpha_n \geq 0,\, \sum_n \alpha_n y_n = 0} \sum_n \alpha_n - \frac{1}{2} \sum_{n,m=1}^{N} y_n y_m \alpha_n \alpha_m K(x_n, x_m)$$

Computing $K(x_n, x_m)$ can be done without computing the mappings $\phi(x_n), \phi(x_m)$.

This way of training a SVC in feature space while without explicitly working with the mapping ϕ is called ***the kernel trick***.

Transforming Data: An Example

Example

Let's define $\phi : \mathbb{R}^2 \to \mathbb{R}^6$ by

$$\phi\left([x_1, x_2]\right) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

The inner product in the feature space is

$$\phi\left([x_{11}, x_{12}]\right)^\top \phi\left([x_{21}, x_{22}]\right) = (1 + x_{11}x_{21} + x_{12}x_{22})^2$$

Thus, we can directly define a kernel function $K : \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}$ by

$$K(x_1, x_2) = (1 + x_{11}x_{21} + x_{12}x_{22})^2.$$

Notice that we need not compute $\phi\left([x_{11}, x_{12}]\right)$, $\phi\left([x_{21}, x_{22}]\right)$ to compute $K(x_1, x_2)$.

Kernel Functions

Common kernel functions include:

- **Polynomial Kernel**

$$K(x_1, x_2) = (x_1^\top x_2 + 1)^d$$

  where d is a hyperparameter

- **Radial Basis Function Kernel**

$$K(x_1, x_2) = \text{exp}\left\{-\frac{\|x_1 - x_2\|^2}{2\sigma^2}\right\}$$

  where σ is a hyperparameter

- **Sigmoid Kernel**

$$K(x_1, x_2) = \text{tanh}(\kappa x_1^\top x_2 + \theta)$$

  where κ and θ are hyperparameters.

A User's Guide to Support Vector Machines

Why Does SVM Work?

[Not filling these in until it’s clear that this lecture is needed]

Choosing the Kernel Function

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Strengths and Weaknesses of SVM

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