Support Vector Machines

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Introduction

- Consider a binary classification task
  - Support Vector Machines (SVM) try to find a plane that separates the two classes in the space of our predictive features
- If no such plane exists, there are two possible solutions
  - Relaxing what we mean by "separate"
  - Expanding our feature space to facilitate separation

Hyperplanes

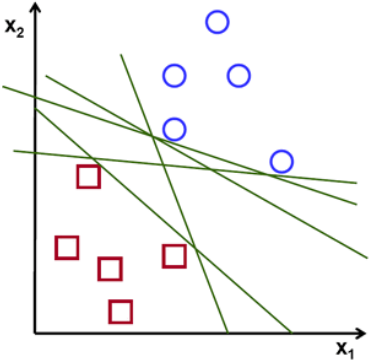
- A hyperplane is defined by a set of coefficients:

$$f(\mathbf{X}) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p$$

- Recognize that *multivariable linear regression* is a hyperplane
  - This hyperplane represents the expected value of a continuous outcome, Y, estimated via least squares for a set of predictors
- Support vector machines seek a *separating hyperplane*
  - $f(\mathbf{X}) > 0$ for one class, and $f(X) < 0$ for the other class

Separation in low dimensions

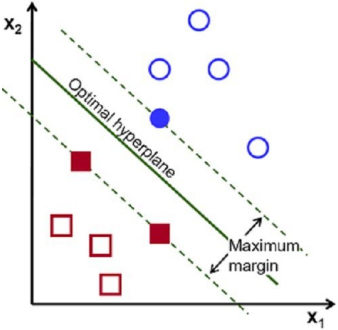
Consider 2 features, X_1 and X_2, and a binary outcome. It might be possible to draw several separating hyperplanes:



Which of these hyperplanes is the best classifier?

The maximum margin classifier

A *hard margin* SVM finds the "maximum margin" hyperplane:



This plane represents the "widest street" between classes, and it is characterized by "support vectors", or training data-points that would change this hyperplane if removed

Finding the maximum margin classifier

- Consider the constraint: $\sum_{j=1}^{p} \beta_j = 1$, which normalizes how our hyperplane is defined
  - This won't impact the direction of the plane, as $\{\beta_1 = 1, \beta_2 = 1\}$ and $\{\beta_1 = 3, \beta_2 = 3\}$ have the same orientation
- SVMs find $\beta_1, \ldots, \beta_p$ which maximize M in the expression: $y_i(\beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \beta_p x_{i,p}) \geq M$
  - Here the binary outcome, y_i, is encoded as $+1$ or -1, so the left side of this expression is the distance from the current hyperplane to the i^{th} data-point

Finding the maximum margin classifier

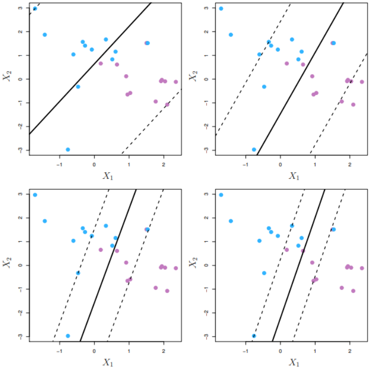
- The coefficients defining the SVM classifier can be found using the Lagrangian multiplier method
  - We will not cover this method in this course (as SVMs are the only classifier we'll study that use it)
- If you're interested in the mathematical details, I recommend Robert Berwick's (of MIT) "An Idiot's guide to support vector machines"

Non-separable data (soft margin)

- If the data are non-seperable, we can relax the maximum margin approach to find a *soft margin classifier*:
- Now we aim to find $\beta_1, \ldots, \beta_p$ that maximize M where $y_i(\beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \beta_p x_{i,p}) \geq M(1 - \epsilon_i)$
  - Subject to $\epsilon \geq 0$ and $\sum_{i=1}^{n} \epsilon_i < s$
    - $\epsilon_i = 0$ if a point is on the correct side of the margin
    - $0 < \epsilon_i < 1$ if a point is within the margin
    - $\epsilon_i > 1$ if a point is on the wrong side of the margin
  - s is controls the total amount of "slack" that is allowed, with larger values allowing for more "slack"
    - As s decreases the tolerance for data-points being on the wrong side of the hyperplane diminishes

Soft-margin examples

As s decreases (left to right), the margin M decreases:



A larger s yields a more stable classifier, so the bias-variance trade-off can be manipulated via the value of s.

Feature expansion

- Consider the features: $\{X_1, X_2\}$, and recall that the SVM classifier finds a decision boundary (separating hyperplane) of the form $\beta_0 + \beta_1 X_1 + \beta_2 X_2$
- We could apply transformations to create a new set of features: $\{X_1, X_2, X_1^2, X_2^2, X_1 X_2\}$
  - Now the decision boundary would have the form: $\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1 X_2$
- This corresponds to a *non-linear boundary* in the *original feature space*
  - *Kernel functions* allow for computationally efficient mappings of the original features to higher dimensions for the purpose of finding a non-linear decision boundary

Inner products

To fully understand kernel functions, we'll need to be familiar with the **inner product**:

$$\begin{aligned}\text{inner product of } \mathbf{x}_1, \mathbf{x}_2 &= \mathbf{x}_1^T \mathbf{x}_2 \\ &= \sum_{j=1}^{p} x_{1j} x_{2j}\end{aligned}$$

We will not go too far into the details, but SVM estimation can be re-framed in terms of the inner product of each pair of data-points:

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \mathbf{x}^T \mathbf{x}_i$$

Inner products (cont.)

In the previous formulation (repeated below), it turns out that many of the $\hat{\alpha}_i$ are zero

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \mathbf{x}^T \mathbf{x}_i$$

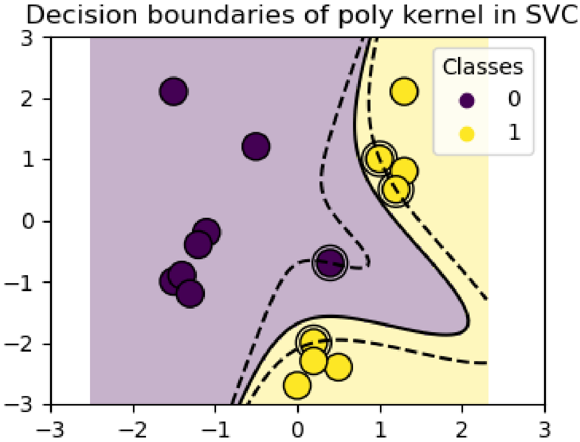
- This is a collection of $\binom{n}{2}$ inner products, corresponding to n different α_i parameters, but only those involving points on or inside the margin have non-zero values (ie: $\hat{\alpha}_i \neq 0$)
    - Various feature expansion approaches are more easily handled using this framework using the proper Kernel function $K()$

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$$

Kernel functions

1. Linear kernel - $K(\mathbf{x}, \mathbf{x}_i) = \mathbf{x}^T \mathbf{x}_i$
2. Polynomial kernel - $K(\mathbf{x}, \mathbf{x}_i) = (\gamma \mathbf{x}^T \mathbf{x}_i + 1)^d$
   - γ controls the influence of individual training samples, d is the degree of the polynomial expansion
3. Radial Basis Function (RBF) kernel - $K(\mathbf{x}, \mathbf{x}_i) = exp(-\gamma ||\mathbf{x} - \mathbf{x}_i||^2)$
   - γ controls the influence of individual training samples
4. Sigmoid kernel - $K(\mathbf{x}, \mathbf{x}_i) = tanh(\gamma \mathbf{x}^T \mathbf{x}_i + r)$
   - γ controls the influence of individual training samples, r is a bias term that allows the transformation to be shifted up or down

Polynomial kernel ($d = 3$, $\gamma = 2$)



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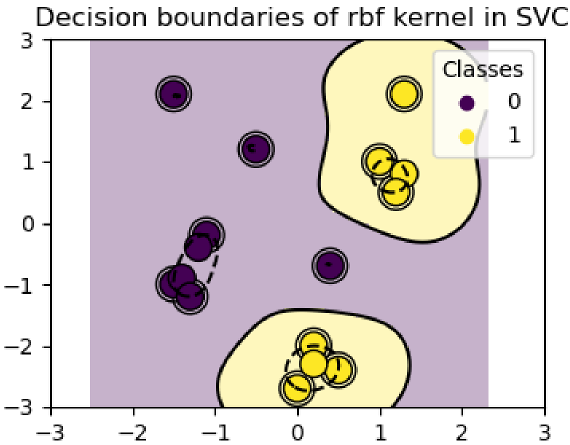
RBF kernel



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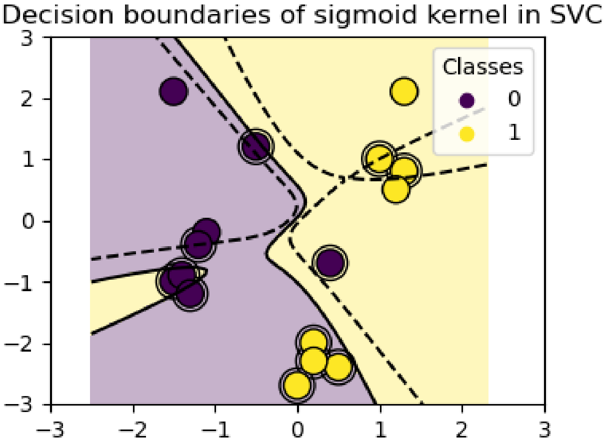
Sigmoid kernel



Practical guidance

- SVMs treat each feature equally, so standardization is an important data preparation step
- The kernel function (type of feature expansion) and "slack" parameter can be tuned via cross-validation to achieve optimal classification performance
  - `sklearn` represents "slack" using a parameter `C` that is inversely proportional to what we called s
  - Other hyperparameters affiliated with certain kernel functions, such as `\gamma` can also be tuned in this manner
- Support vector regression is also implemented in `sklearn`, the SVM lab will briefly cover this method
  - SVMs also have been generalized to multi-class tasks, and use a one-vs-one scheme in `sklearn`