Stats 102B - Week 7, Lecture 3

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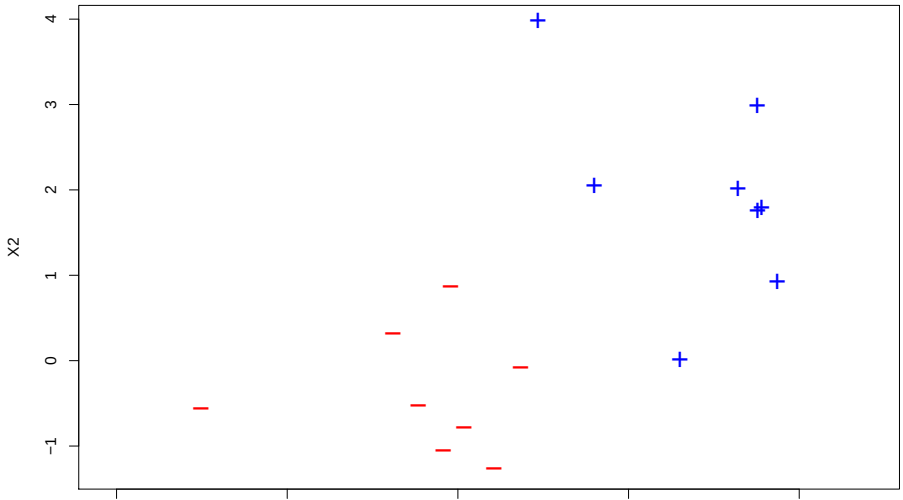
Week 7 Friday

UCLA

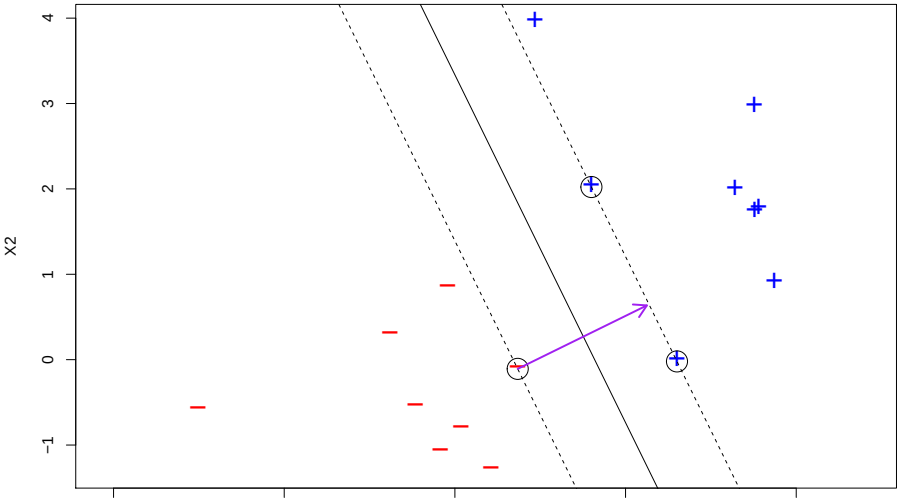
Section 1

Support Vector Machines

Support Vector Machines - Maximum Margin Classifier



Maximizing the Margin



Maximizing the Margin

Recap of Lecture 7-1:

Our boundary is a linear hyperplane. It is the set of points $\mathbf{x}$ that satisfy:

$$\mathbf{w}^T\mathbf{x} - b = 0$$

Where $\mathbf{w}$ is a vector normal (perpendicular) to the hyperplane.

We want to find the $\mathbf{w}$ that maximizes the margin (the distance to the nearest point in either group).

Maximizing the Margin

If we dot the vector $(\mathbf{x}_1 - \mathbf{x}_2)$ with the direction perpendicular to the margin, we will get the length of the margin.

$$2\gamma = \frac{1}{||\mathbf{w}||}\mathbf{w}^T(\mathbf{x}_1 - \mathbf{x}_2)$$

With a bit of math (Lecture 7-1 slide 10), we showed that

$$\gamma = \frac{1}{||\mathbf{w}||}$$

Maximizing the Margin Mathematically

Because $||\mathbf{w}||$ is in the denominator, maximizing the distance γ now becomes equivalent to minimizing $||\mathbf{w}||$.

We wish to minimize $||\mathbf{w}||$, subject to the constraint $t_n(\mathbf{w}^T\mathbf{x}_n - b) \geq 1$ for all i.

Optimizing a function subject to a constraint can be achieved using Lagrange multipliers. With the Lagrange multipliers, the objective function can be written as:

$$\underset{\mathbf{w},\alpha}{\text{argmin}} \ \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{n=1}^{N} \alpha_n(t_n(\mathbf{w}^T\mathbf{x}_n - b) - 1)$$

$$\text{subject to } \alpha_n > 0, \text{for all } n$$

I left it here after saying there is no closed form solution.

Maximizing the margin

The function we wish to minimize is:

$$\frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{n=1}^{N} \alpha_n(t_n(\mathbf{w}^T\mathbf{x}_n - b) - 1)$$

At the minimum the derivatives of this function with respect to $\mathbf{w}$ and b will be equal to zero.

$$\frac{\partial}{\partial \mathbf{w}} = \mathbf{w} - \sum_{n=1}^{N} \alpha_n t_n \mathbf{x}_n = 0$$

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n t_n \mathbf{x}_n$$

$$\frac{\partial}{\partial b} = -\sum_{n=1}^{N} \alpha_n t_n = 0$$

Maximizing the margin

We can plug in the value of $\mathbf{w}$ from the previous page ($\mathbf{w} = \sum \alpha_n t_n \mathbf{x}_n$) into the function we wish to optimize.

$$= \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{n=1}^{N} \alpha_n (t_n(\mathbf{w}^T\mathbf{x}_n - b) - 1)$$

$$= \frac{1}{2}\left(\sum_{m=1}^{N} \alpha_m t_m \mathbf{x}_m^T\right)\left(\sum_{n=1}^{N} \alpha_n t_n \mathbf{x}_n\right) - \sum_{n=1}^{N} \alpha_n \left(t_n \left(\sum_{m=1}^{N} \alpha_m t_m \mathbf{x}_m^T \mathbf{x}_n - b\right) - 1\right)$$

$$= \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N} \alpha_m t_m \mathbf{x}_m^T \alpha_n t_n \mathbf{x}_n - \sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n t_n \alpha_m t_m \mathbf{x}_m^T \mathbf{x}_n + \sum_{n=1}^{N} \alpha_n t_n b + \sum_{n=1}^{N} \alpha_n$$

$$= \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N} \alpha_m \alpha_n t_m t_n \mathbf{x}_m^T \mathbf{x}_n - \sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_m \alpha_n t_m t_n \mathbf{x}_m^T \mathbf{x}_n + 0 \times b + \sum_{n=1}^{N} \alpha_n$$

$$= \sum_{n=1}^{N} \alpha_n - \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N} \alpha_m \alpha_n t_m t_n \mathbf{x}_m^T \mathbf{x}_n$$

Maximizing the margin

$$\sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1}^{N} \alpha_m \alpha_n t_m t_n \mathbf{x}_m^T \mathbf{x}_n$$

We need to find the optimum of the above, subject to:

$$\alpha_n \geq 0, \sum_{n=1}^{N} \alpha_n t_n = 0$$

Though there is no closed form solution, but the optimum can be found via quadratic programming.

It's worth noting that the optimization problem does not contain $\mathbf{w}$ itself.

Maximizing the margin

At the solution, $\mathbf{w}$ can be expressed as:

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n t_n \mathbf{x}_n$$

At the solution, the support vectors (i.e. the $\mathbf{x}$ points that define the margin) will have α_n values that are not 0, while the non-support vectors have $\alpha_n = 0$. (The non-support vectors have no influence on the value of $\mathbf{w}$)

We can think of α as a measure of how much influence a particular value in the training data has on defining $\mathbf{w}$

Identifying $\mathbf{w}$ is a matter of finding the correct values of α_n.

Soft-Margins

The maximum-margin classifier uses the following constraint.

$$t_n(\mathbf{w}^T\mathbf{x}_n - b) \geq 1$$

The value 1 represents the distance from the boundary (center line) to the nearest point (dotted lines). The constraint is called a "hard margin" because all of the data points in the data set must satisfy the property that its distance is at least 1.

We can relax the constraint and allow for some points to be closer to the boundary (center line) than 1. If we say $\xi_n \geq 0$, we can have the following constraint instead:

$$t_n(\mathbf{w}^T\mathbf{x}_n - b) \geq 1 - \xi_n$$

If $0 < \xi_n \leq 1$, then the point i is within the margins.

If $1 < \xi_n$, then the point i is on the wrong side of the boundary.

Soft Margins

With soft-margins the optimization problem changes slightly. We still want to optimize:

$$\sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1}^{N} \alpha_m \alpha_n t_m t_n \mathbf{x}_m^T \mathbf{x}_n$$

But there is now an upper bound C on the what α can be in the constraint.

$$\text{subject to } \sum_{n=1}^{N} \alpha_n t_n = 0, 0 \leq \alpha_n \leq C \text{ , for all n}$$

Effectively, the upper bound limits the amount of influence that a single point can have on defining the boundary.

Non-linear boundaries with Kernel functions

We can find linear boundaries by maximizing this function.

$$\sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1}^{N} \alpha_m \alpha_n t_m t_n \mathbf{x}_m^T \mathbf{x}_n$$

We can find non-linear boundaries by optimizing a very similar function that uses a kernel function.

$$\sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m=1}^{N} \sum_{n=1}^{N} \alpha_m \alpha_n t_m t_n k(\mathbf{x}_m, \mathbf{x}_n)$$

The difference here is that we have replaced the dot product of two points $\mathbf{x}_m^T \mathbf{x}_n$ with a kernel function $k(\mathbf{x}_m, \mathbf{x}_n)$

What is a Kernel function?

A kernel function is an inner product (or dot product) of vectors after we have applied some kind of transformation function $\phi()$ to the original vector.

$$k(\mathbf{x}_m, \mathbf{x}_n) = \langle \varphi(\mathbf{x}_m), \varphi(\mathbf{x}_n) \rangle$$

Transformation Functions

The Kernel function returns the inner product after we apply a transformation ϕ.

For example, the function φ can project a two dimensional point into three dimensions.

$$\varphi(\mathbf{x}) = \varphi([x_1, x_2]) = [x_1, x_2, x_1^2 + x_2^2]$$

Example:

Let's say we have transformation function $\varphi(\mathbf{x}) = \varphi([x_1, x_2]) = [x_1, x_2, x_1^2 + x_2^2]$

and vectors: $\mathbf{x}_n = [1, 1]$ and $\mathbf{x}_m = [5, 1]$

When we apply the transformation function to our vectors, we get:

$\varphi(\mathbf{x}_n) = [1, 1, 1^2 + 1^2] = [1, 1, 2]$

$\varphi(\mathbf{x}_m) = [5, 1, 5^2 + 1^2] = [5, 1, 26]$

The dot product of these vectors is then:

$$k(\mathbf{x}_m, \mathbf{x}_n) = \langle \varphi(\mathbf{x}_m), \varphi(\mathbf{x}_n) \rangle = \langle [1, 1, 2], [5, 1, 26] \rangle = (1 \cdot 5 + 1 \cdot 1 + 2 \cdot 26) = 58$$

The Kernel function

It is not necessary to actually use φ to project the data into higher dimensions.

We can use the Kernel function directly to get the resulting inner product.

In this case, if $\varphi(\mathbf{x}) = \varphi([x_1, x_2]) = [x_1, x_2, x_1^2 + x_2^2]$, the kernel function is:

$$k(\mathbf{x}_m, \mathbf{x}_n) = \mathbf{x}_m^T \mathbf{x}_n + ||\mathbf{x}_m||^2 ||\mathbf{x}_n||^2$$

The Kernel function

$\mathbf{x}_n = [1, 1], \mathbf{x}_m = [5, 1]$

We can use φ to transform the vectors first and take the inner product:

$$k(\mathbf{x}_m, \mathbf{x}_n) = \langle \varphi(\mathbf{x}_m), \varphi(\mathbf{x}_n) \rangle = \langle [1, 1, 2], [5, 1, 26] \rangle = (1 \cdot 5 + 1 \cdot 1 + 2 \cdot 26) = 58$$

Or we can use the kernel function directly on the input vectors:

$$k(\mathbf{x}_m, \mathbf{x}_n) = \mathbf{x}_m^T \mathbf{x}_n + ||\mathbf{x}_m||^2 ||\mathbf{x}_n||^2 = \langle [1, 1], [5, 1] \rangle + (1^2 + 1^2)(5^2 + 1^2) = (1 \cdot 5 + 1 \cdot 1) + 2 \cdot 26 = 58$$

The Kernel 'trick' for SVM

When using a kernel function, it is equivalent to using the φ function to project the data into a higher dimensional space.

After projecting the data, we can use SVM to find a linear hyperplane that separates the points.

Animation:

https://www.youtube.com/watch?v=3liCbRZPrZA

Kernel Functions

Many possible kernel functions exist.

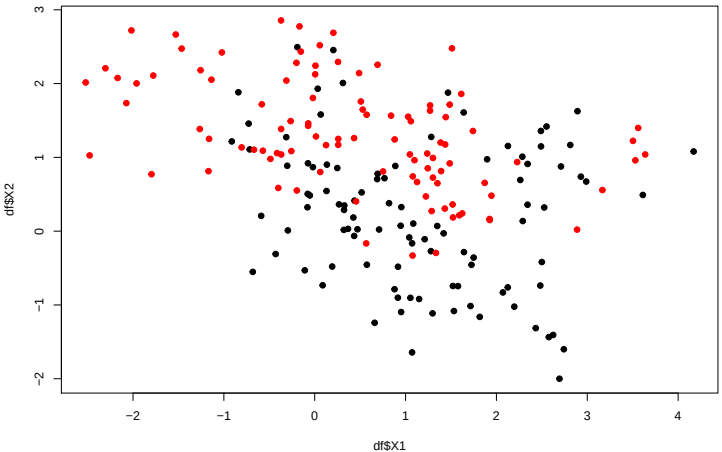
https://en.wikipedia.org/wiki/Positive-definite_kernel

Commonly used ones are the Gaussian and Polynomial Kernel

For some Kernel functions, the corresponding transformation function transforms the 2D vector into a very high dimensional vector. The Gaussian kernel actually transforms the vector into an infinite dimensional vector. (It's based on the Taylor expansion of the exp function.)

Again, it is not necessary to actually transform the original vectors. You can use the Kernel function directly.

Data to be classified (from Elements of Statistical Learning)



svm() in R

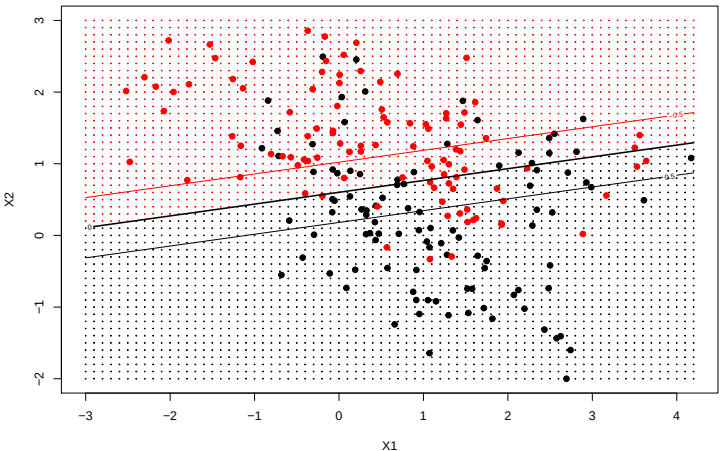
We will use the `svm()` function available in package `e1071`.

There are a few options you can use that will affect the SVM fit.

You can choose the kernel. Here we use a linear kernel.

```
library(e1071)
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "linear")
```

Linear Kernel



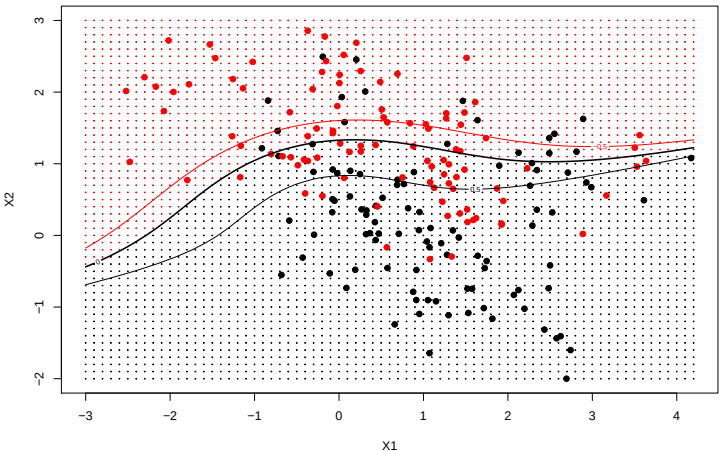
Polynomial Kernel

You can use a polynomial kernel. There will be another argument for the Polynomial degree. The default is 3.

You can also choose a gamma parameter.

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "polynomial",
             degree = 3, gamma = 0.5)
```

Polynomial Kernel, degree 3

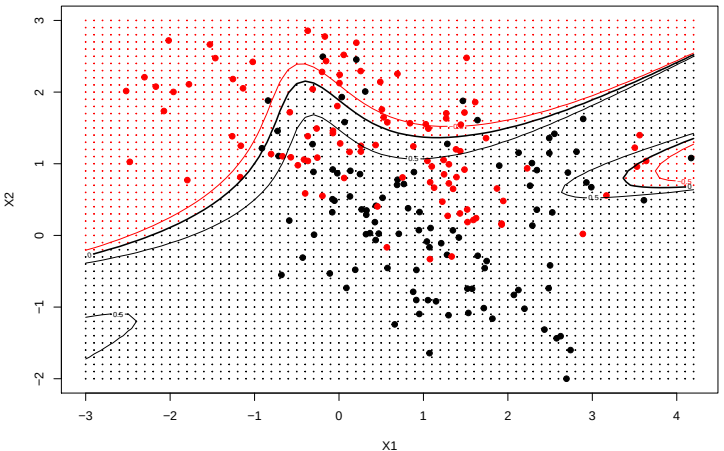


Polynomial Kernel

A degree 5 polynomial

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "polynomial",
             degree = 5, gamma = 0.5)
```

Polynomial Kernel, degree 5



Gaussian Kernel

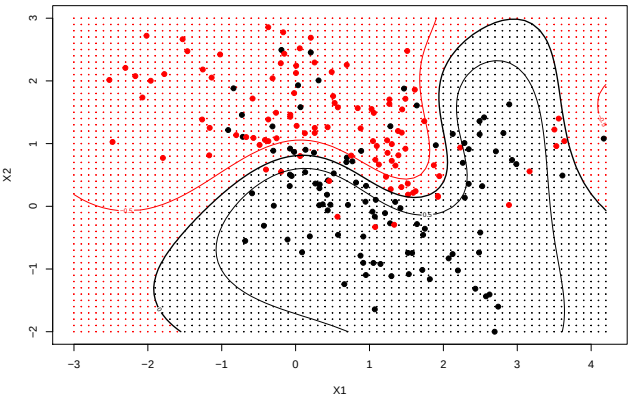
Radial Basis Functions (Gaussian kernels) are very popular for SVM because of the flexibility it offers.

When specifying the Radial basis kernel, you can select the parameters for gamma and cost.

For your homework assignment, I want you to study the effect of using different parameters.

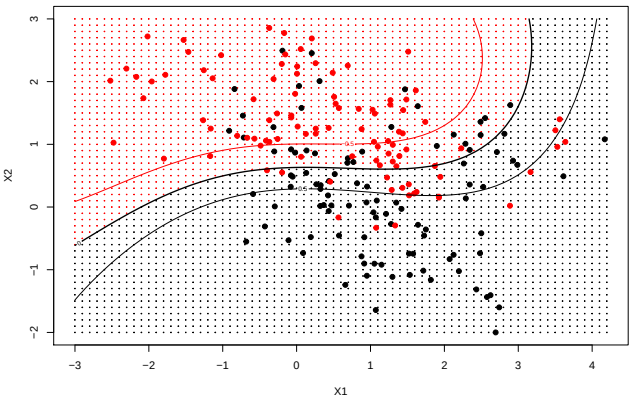
```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial",
             gamma = 0.5, cost = 1)
```

Gaussian Kernel



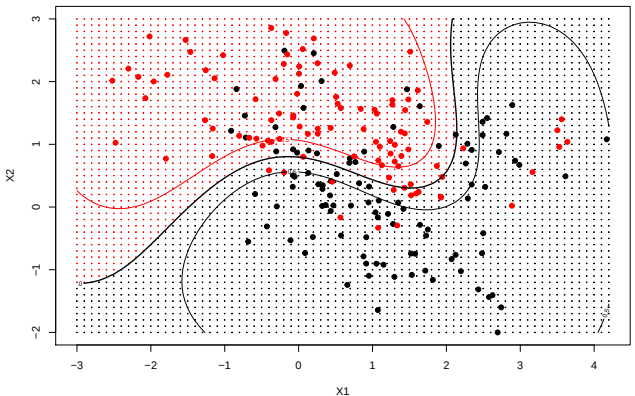
Gaussian Kernel - altering gamma, keep cost = 1

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.1, cost = 1)
```



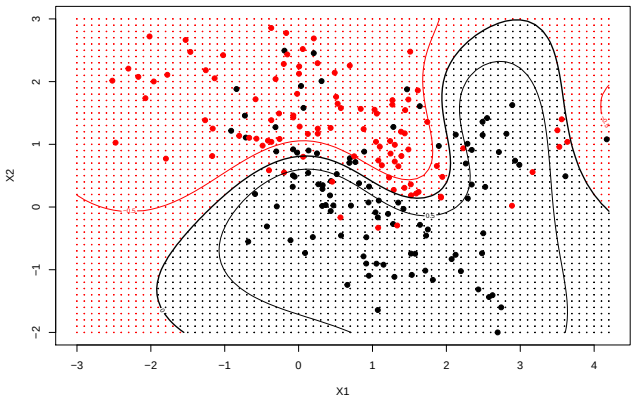
Gaussian Kernel - altering gamma, keep cost = 1

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.3, cost = 1)
```



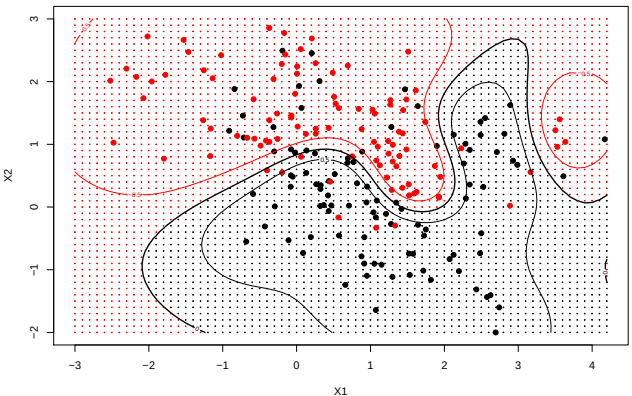
Gaussian Kernel - altering gamma, keep cost = 1

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.5, cost = 1)
```



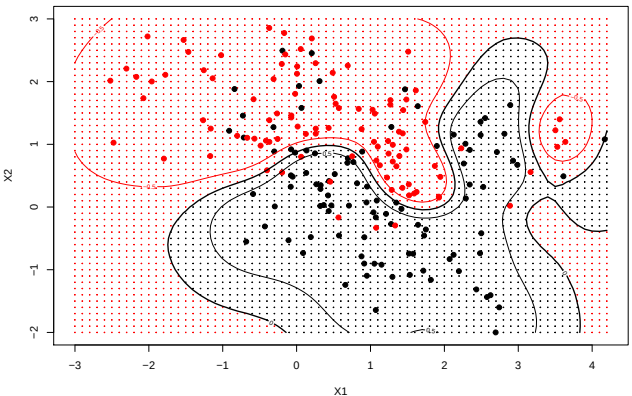
Gaussian Kernel - altering gamma, keep cost = 1

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 1, cost = 1)
```



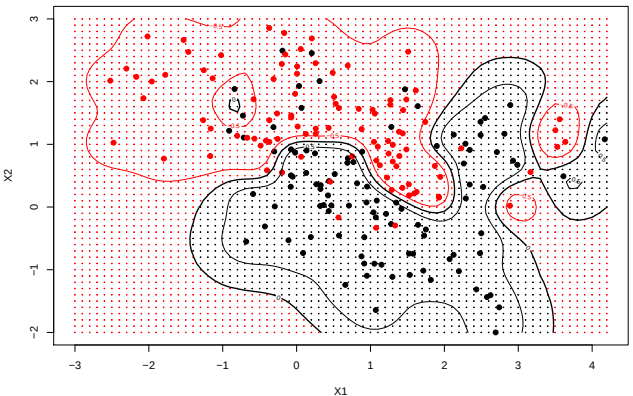
Gaussian Kernel - altering gamma, keep cost = 1

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 2, cost = 1)
```



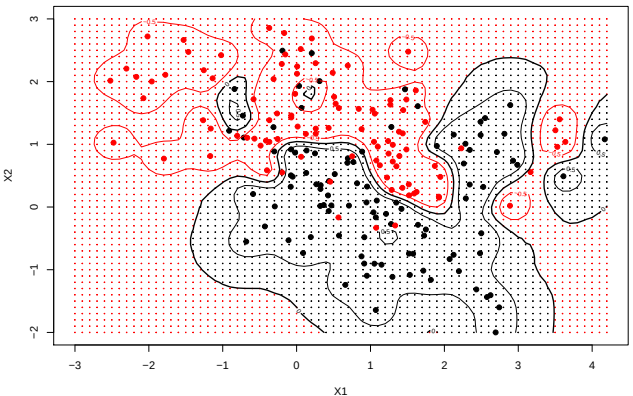
Gaussian Kernel - altering gamma, keep cost = 1

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 5, cost = 1)
```



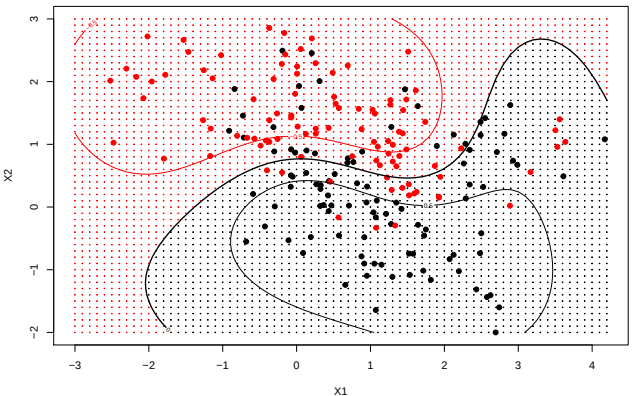
Gaussian Kernel - altering gamma, keep cost = 1

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 10, cost = 1)
```



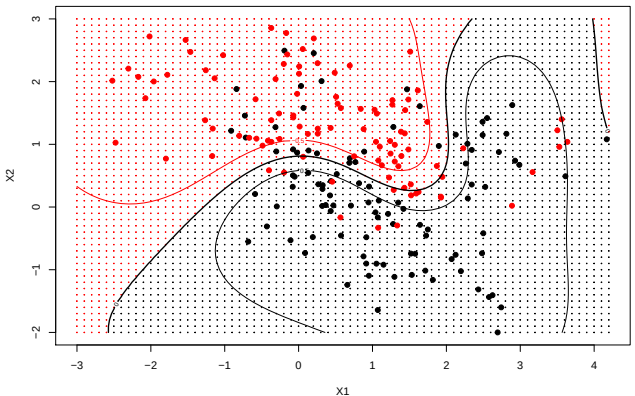
Gaussian Kernel - altering cost, keep gamma = 0.5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.5, cost = 0.1)
```



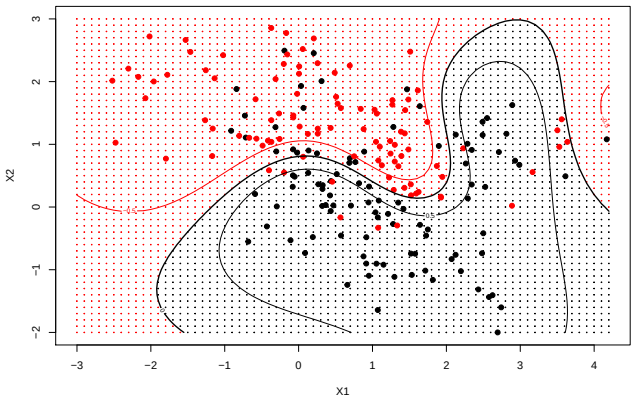
Gaussian Kernel - altering cost, keep gamma = 0.5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.5, cost = 0.5)
```



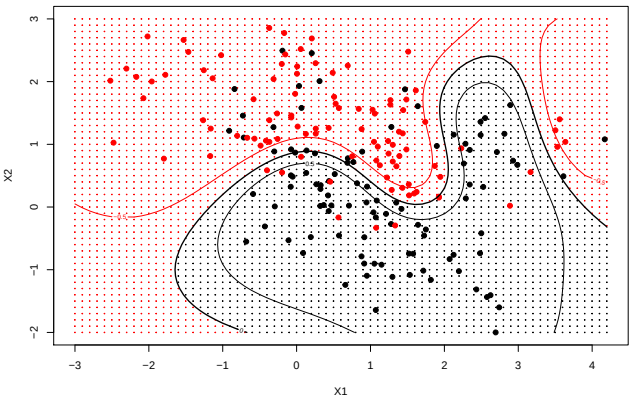
Gaussian Kernel - altering cost, keep gamma = 0.5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.5, cost = 1)
```



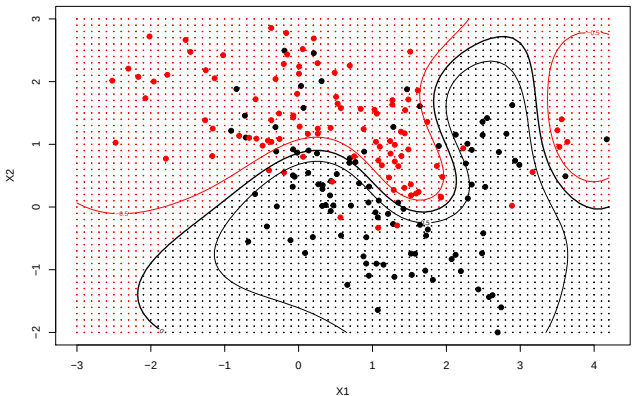
Gaussian Kernel - altering cost, keep gamma = 0.5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.5, cost = 2)
```



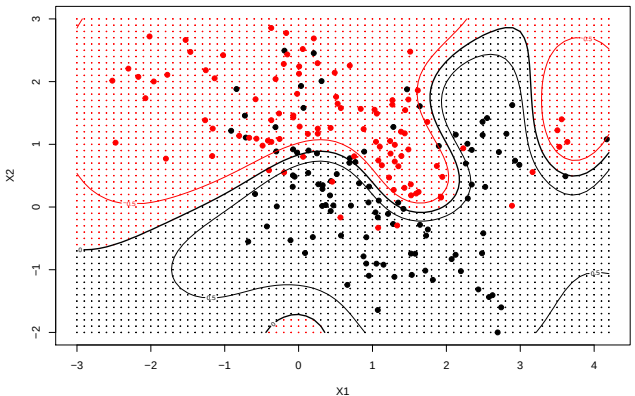
Gaussian Kernel - altering cost, keep gamma = 0.5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.5, cost = 5)
```



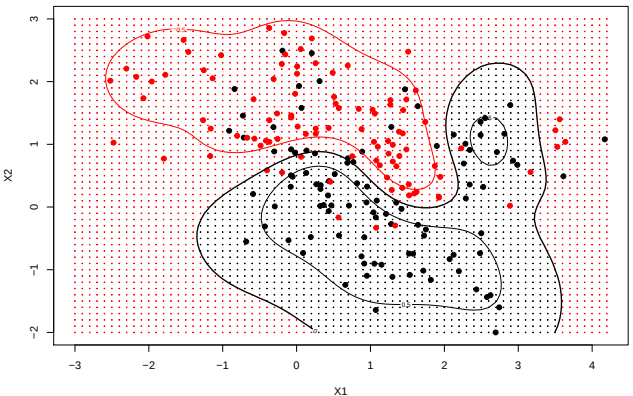
Gaussian Kernel - altering cost, keep gamma = 0.5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 0.5, cost = 10)
```



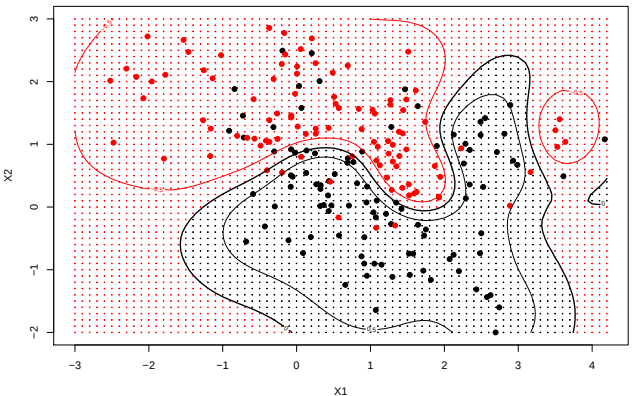
Gaussian Kernel - altering cost, keep gamma = 2

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 2, cost = 0.1)
```



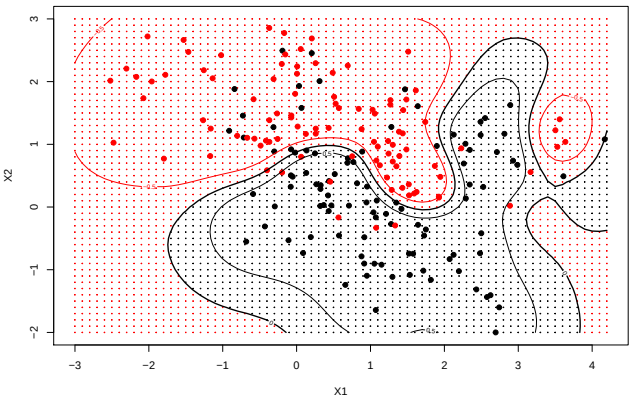
Gaussian Kernel - altering cost, keep gamma = 2

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 2, cost = 0.5)
```



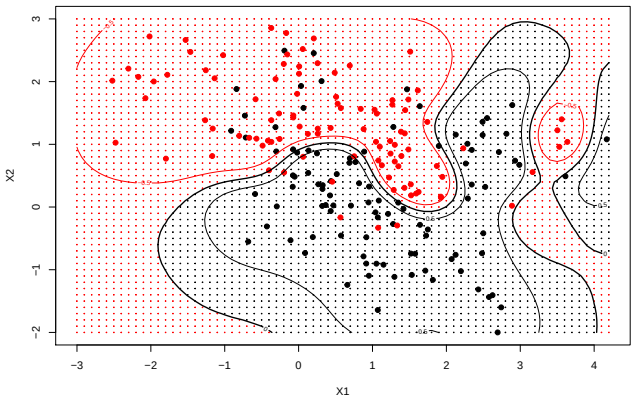
Gaussian Kernel - altering cost, keep gamma = 2

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 2, cost = 1)
```



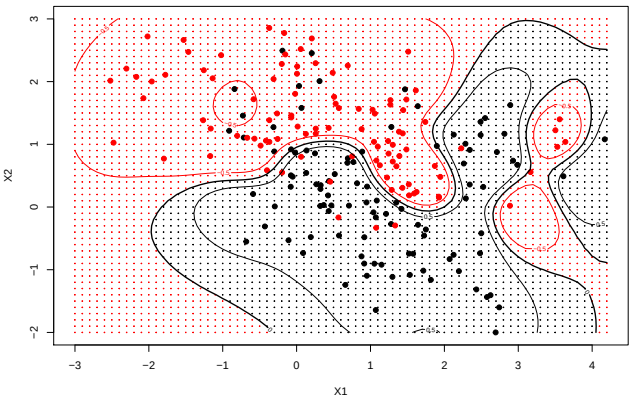
Gaussian Kernel - altering cost, keep gamma = 2

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 2, cost = 2)
```



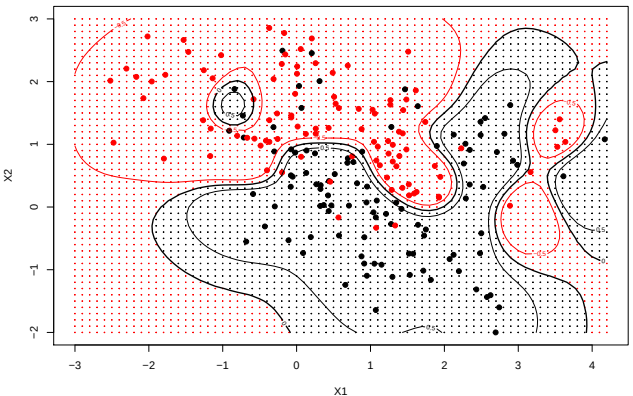
Gaussian Kernel - altering cost, keep gamma = 2

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 2, cost = 5)
```



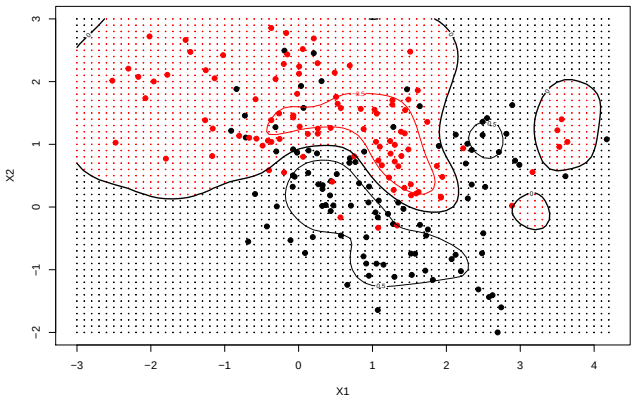
Gaussian Kernel - altering cost, keep gamma = 2

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 2, cost = 10)
```



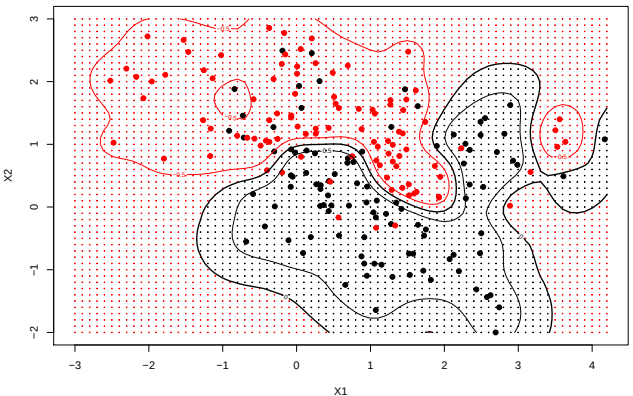
Gaussian Kernel - altering cost, keep gamma = 5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 5, cost = 0.1)
```



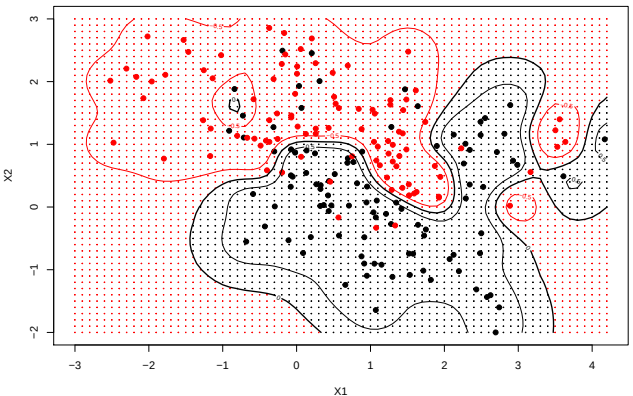
Gaussian Kernel - altering cost, keep gamma = 5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 5, cost = 0.5)
```



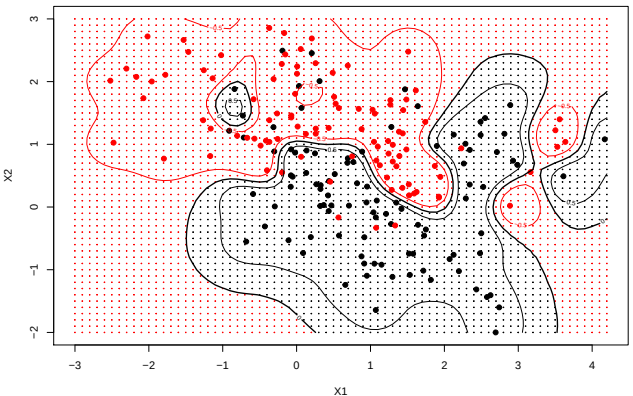
Gaussian Kernel - altering cost, keep gamma = 5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 5, cost = 1)
```



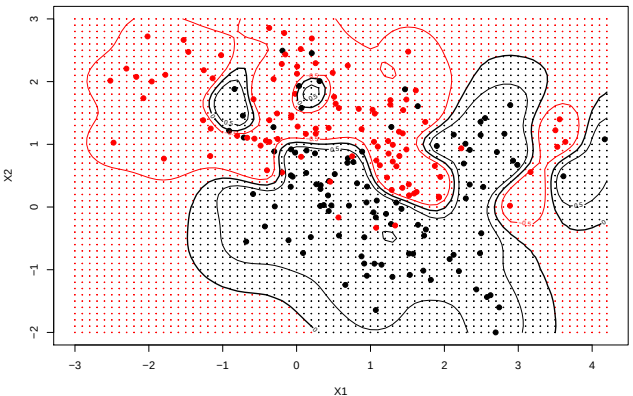
Gaussian Kernel - altering cost, keep gamma = 5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 5, cost = 2)
```



Gaussian Kernel - altering cost, keep gamma = 5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 5, cost = 5)
```



Gaussian Kernel - altering cost, keep gamma = 5

```
model <- svm(y ~ . , data = df, scale = FALSE, kernel = "radial", gamma = 5, cost = 10)
```