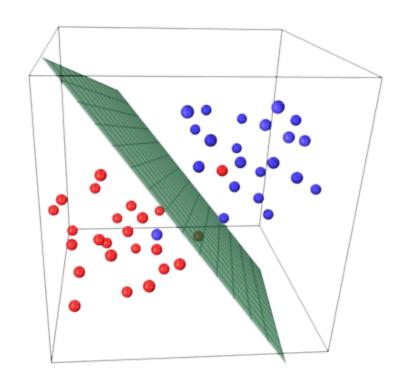


# Support Vector Machines

DSI SEA5, jf.omhover, Sep 30 2016

a priori version (for "solutions" use a posteriori version)





# Support Vector Machines

DSI SEA5, jf.omhover, Sep 30 2016

#### **STANDARDS**

- Compute a hyperplane as a decision boundary in SVC
- Explain what a support vector is in plain english
- Tune a SVC or SVM using their hyperparameters
- State what happens to bias and variance if we tune these hyperparameters
- State how "one-vs-one" and "one-vs-rest" approaches for multi-class problems are implemented.



# Support Vector Machines

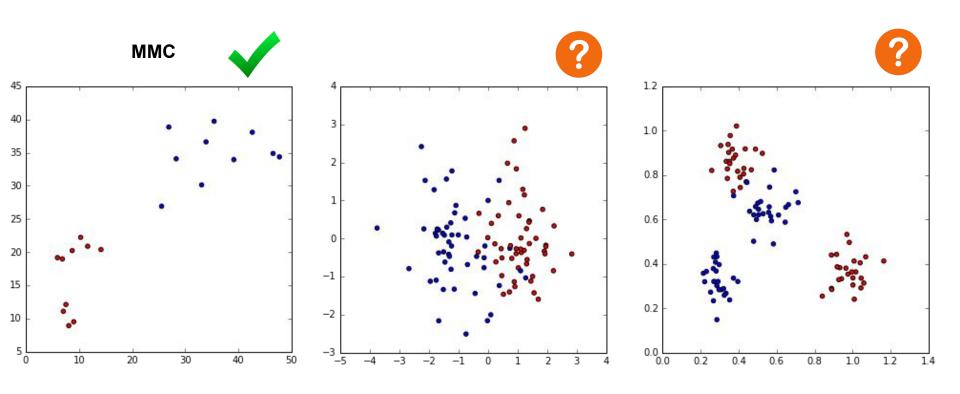
DSI SEA5, jf.omhover, Sep 30 2016

#### **OBJECTIVES**

- Understand the notion of decision boundaries
- Describe the function and parameters of SVMs
- Investigate some of the maths behind SVMs
- Extend SVMs by soft margins and kernel tricks
- Investigate how SVMs perform in terms of Bias-Variance
- Get your mind blown

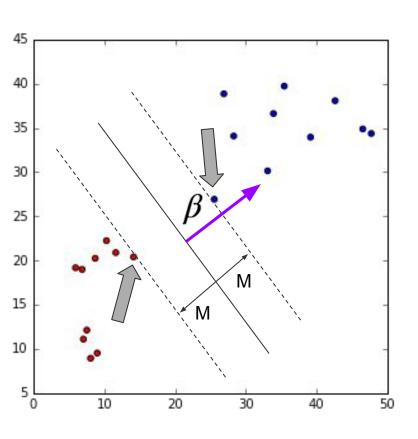
## Brainstorm: what's a good decision boundary?





#### Maximum Margin Classification





$$max_{\beta_0,\dots,\beta_p}M$$

subject to 
$$\sum_{j=1}^{p} \beta_j^2 = 1$$

$$y_i.(\beta_0 + \beta_1.x_{i,1} + \dots + +\beta_p.x_{i,p}) \ge M$$

$$y_i.(\beta_0 + x_i^T.\beta) \ge M$$

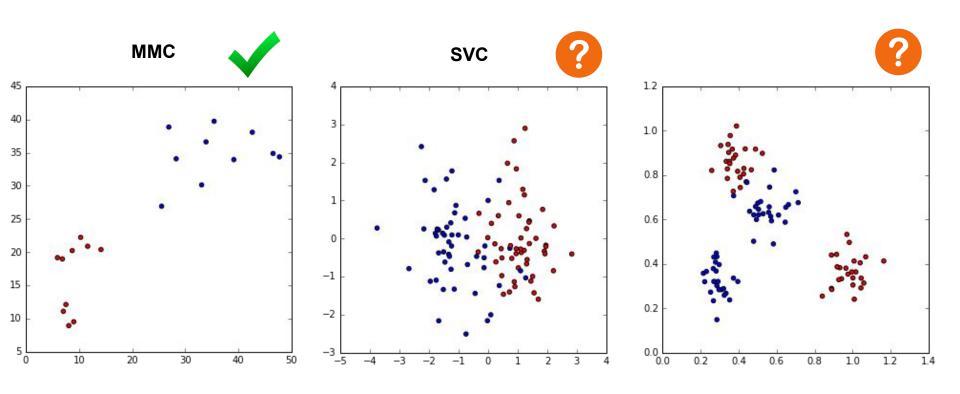
Points that condition the margin.

Points that have a direct influence on the margin.

Points that end up being the closest to the hyperplane.

## Brainstorm: what's a good decision boundary?





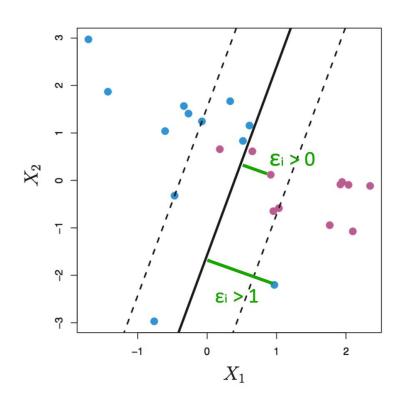


## Support Vectors Classifier

introducing soft margins

#### Soft Margins / Support Vectors Classifier





Relax the constraints for a limited number of vectors

C : our "budget" to spend on relaxing this constraint

Each vector can expense  $\epsilon_i$  on the margin (slack)

$$max_{\beta_0,\cdots,\beta_p,\epsilon_1,\cdots,\epsilon_p}M$$

subject to 
$$\sum_{i=1}^{p} \beta_i^2 = 1$$

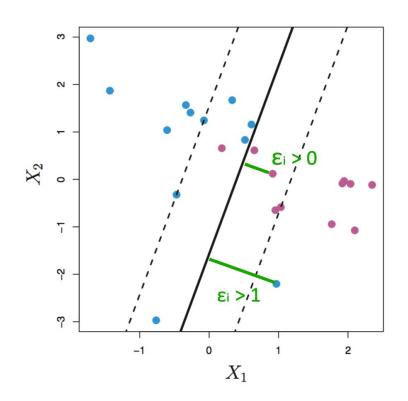
$$y_i.(\beta_0 + \beta_1.x_{i,1} + \dots + + \beta_p.x_{i,p}) \ge M(1 - \epsilon_i)$$

$$y_i.(\beta_0 + x_i^T.\beta) \ge M(1 - \epsilon_i)$$

subject to 
$$\forall i, \ e_i \geq 0$$
 and  $\sum_{i=1}^n e_i \leq C$ 

#### How to solve that?





Namedropping: Lagrange dual objective function

$$L_D = \sum_{i=1}^{n} \alpha_i - 1/2 \sum_{i=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} < x_i, x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_i y_i y_{i'} < x_i y_i x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_i y_i y_i y_{i'} < x_i y_i x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_i y_i y_i y_i' < x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_i y_i y_i y_i' < x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i x_i y_i y_i' < x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i x_i y_i y_i' < x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i x_i y_i y_i' < x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i x_i' y_i y_i' < x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1}^{n} \alpha_i x_i y_i y_i' < x_i' > 1/2 \sum_{i'=1}^{n} \sum_{i'=1$$

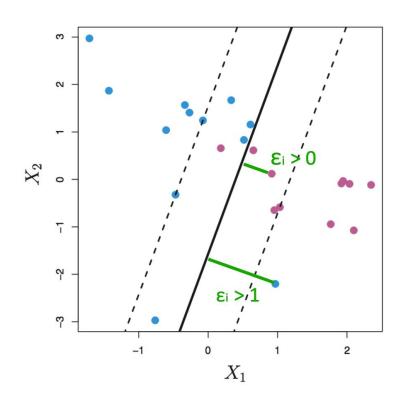
 $f_{\beta_0,\beta_1,\cdots,\beta_p}$  is a solution to that maximization problem

$$f_{\beta_0,\beta_1,\dots,\beta_p}(x) = \beta_0 + \sum_{i=1}^p \alpha_i < x, x_i >$$

Alpha is non zero only for support vectors

#### Soft Margins / Support Vectors





# "Support vectors": Only the observations that lie on the margin or violate it will affect the hyperplane

Large C : many support vectors Small C : few support vectors

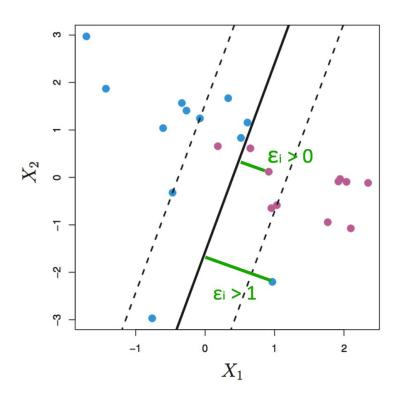
 $f_{eta_0,eta_1,...,eta_p}$  is a solution to that maximization problem

$$f_{\beta_0,\beta_1,\dots,\beta_p}(x) = \beta_0 + \sum_{i=1}^p \alpha_i < x, x_i > 0$$

Alpha is non zero only for support vectors

#### Soft Margins / SVC / Hyperparameter C





Relax the constraints for a limited number of vectors

C : our "budget" to spend on relaxing this constraint

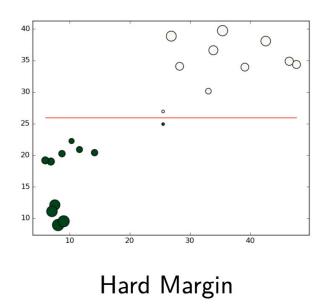
Each vector can expense  $\epsilon_i$  on the margin (slack)

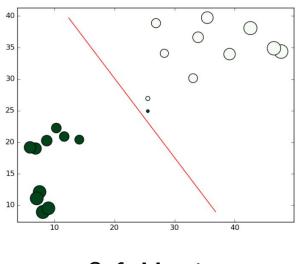
Small C: narrow margins, highly fit, low bias, high variance

Large C: wider margins, fitting less hard, high bias, low variance

## Soft Margins / Hard Margins



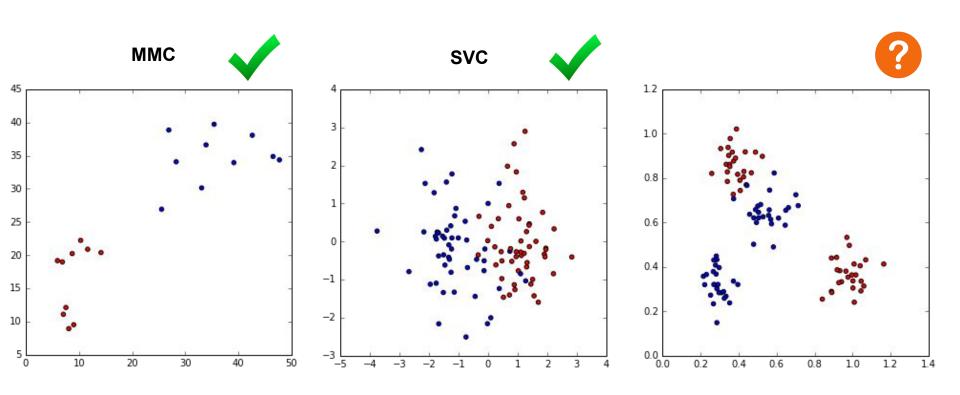




Soft Margin

## Brainstorm: what's a good decision boundary?





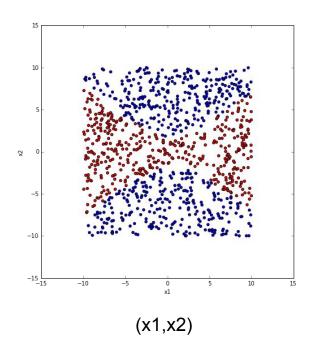


# Support Vectors Machines

introducing kernels

### The Kernel Song

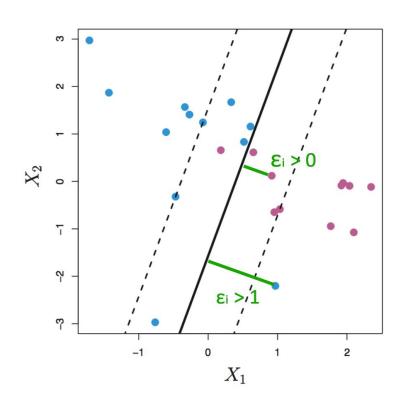




First I was afraid, I was petrified
That my linearity routine would fail me hard that time...

#### Sol 1: Expending in the polynomial realm...





Adding to the input space...

$$max_{\beta_0,\dots,\beta_p,,\beta_{2,1},\dots,\beta_{2,p},\epsilon_1,\dots,\epsilon_p}M$$

subject to 
$$\sum_{j=1}^p \beta_j^2 + \sum_{j=1}^p \beta_{2,j}^2 = 1$$

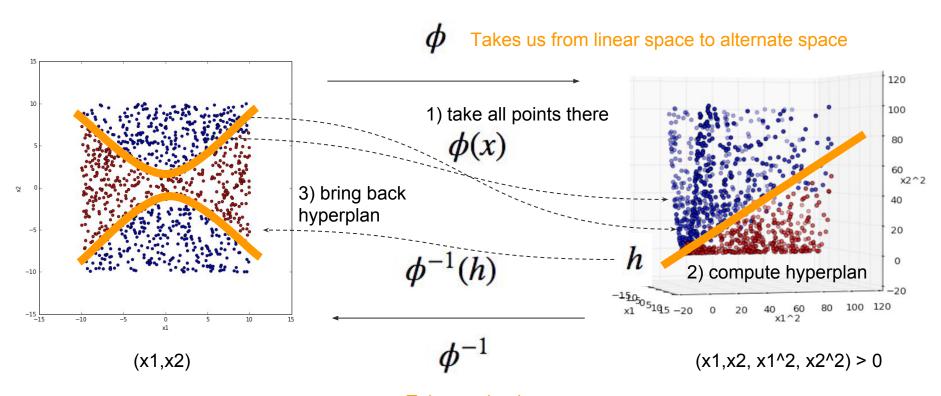
$$y_i.(\beta_0 + \sum_{j=1}^p \beta_j.x_{i,j} + \sum_{j=1}^p \beta_2,j.x_{i,j}^2) \ge M(1 - \epsilon_i)$$

$$y_i.(\beta_0 + x_i^T.\beta) \ge M(1 - \epsilon_i)$$

subject to 
$$\forall i, \ \epsilon_i \geq 0$$
 and  $\sum_{i=1}^n \epsilon_i \leq C$ 

#### Sol 2: Let's devise an alternate space

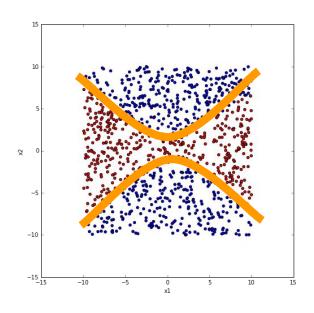




Takes us back

#### How to solve that?





Namedropping : Lagrange dual objective function

$$L_{D} = \sum_{i}^{n} \alpha_{i} - 1/2 \sum_{i}^{n} \sum_{i'}^{n} \alpha_{i} \alpha_{i'} y_{i} y_{i'} K(x_{i}, x_{i'}')$$

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

 $f_{eta_0,eta_1,\cdots,eta_p}$  is a solution to that maximization problem

$$f_{\beta_0,\beta_1,\dots,\beta_p}(x) = \beta_0 + \sum_{i=1}^p \alpha_i < \phi(x), \phi(x_i) >$$

Alpha is non zero only for support vectors

#### Kernels we use...



#### Solution to SVC only involves inner product of observations

$$\begin{split} \langle x_i, x_{i'} \rangle &= \sum_{i=1}^p x_{ij} x_{i'j} \\ f(x) &= \beta_0 + \sum_{i=1}^n \alpha_i \langle x, x_i \rangle \quad \leftarrow \text{SVC} \\ f(x) &= \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle \quad \leftarrow \text{Only requires support vectors} \end{split}$$

#### More generally, instead of just taking inner product, we can use \*Kernels\*

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i K(x, x_i) \quad \leftarrow \text{SVM, since using Kernels now}$$
 
$$K(x_i, x_{i'}) = \sum_{j=1}^p x_{ij} x_{i'j}, \quad \text{Linear Kernel}$$
 
$$K(x_i, x_{i'}) = (1 + \sum_{j=1}^p x_{ij} x_{i'j})^d \quad \text{Polynomial Kernel}$$
 
$$K(x_i, x_{i'}) = \exp(-\gamma \sum_{j=1}^p (x_{ij} - x_{i'j})^2) \quad \text{Radial Basis Function Kernel ("Gaussian")}$$

#### Polynomial Kernel

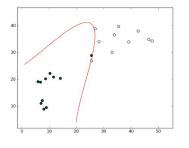


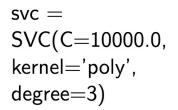
$$K(x^{(i)}, x^{(j)}) = (1 + x^{(i)} \cdot x^{(j)})^d$$

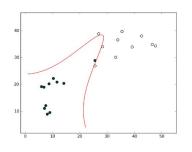
- ightharpoonup equivalent to the dot product in the d-order  $\phi$  space
- ► requires an extra hyper-parameter, d, for "degree"

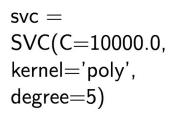
#### Polynomial Kernel

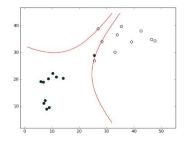












### RBF Kernel (Radial Basis Function)

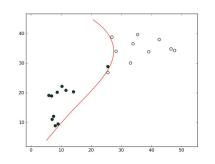


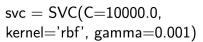
$$K(x^{(i)}, x^{(j)}) = \exp(-\gamma ||x^{(i)} - x^{(j)}||^2)$$

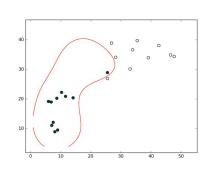
- equivalent to the dot product in the Hilbert space of infinite dimensions
- ightharpoonup requires an extra hyper-parameter,  $\gamma$ , "gamma"

## RBF Kernel (Radial Basis Function)

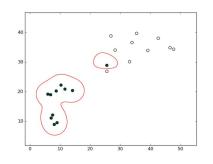




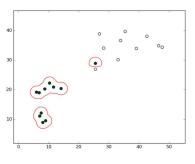




svc = SVC(C=10000.0, kernel='rbf', gamma=0.01)



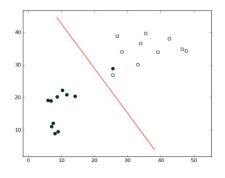
svc = SVC(C=10000.0, kernel='rbf', gamma=0.1)

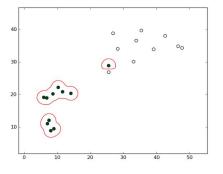


svc = SVC(C=10000.0, kernel='rbf', gamma=1.0)

#### Best fit?







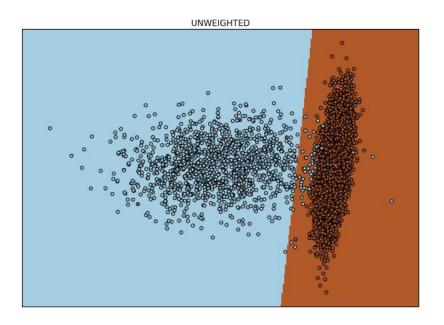


# Adaptation of SVM to real-world problems

#### Unbalanced classes



Adjusting weights (beta) so that they are inversely proportional to class representativity



#### Multiple classes



#### One-versus-One:

Train a classifier on all pairs of classes

Use each pair for determining the class of an observation (aggregating)

#### One-versus-All / One-versus-Rest:

Train a classifier on each class (+1), considering all other as the rest (-1)

Use this classifier for determining if an observation fits in that class



# Pair Assignment

#### Snippets...



from sklearn.svm import SVC

```
svm = SVC(kernel='linear').fit(X, y)
svm = SVC(kernel='linear', C=x).fit(X,y)
svm = SVC(kernel='poly', C=c, degree=5).fit(X,y)
svm = SVC(kernel='rbf', C=c, gamma=0.5).fit(X,y)
```