Support Vector Machines

Ryan Henning

Galvanize

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Objectives

Support Vector Machines (SVMs) Lecture

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Support Vector Machines (SVMs) Lecture

1. Gain an intuition about the *purpose* and *power* of SVMs.
2. Explore (some) of the mathematics behind SVMs.
3. Supercharge SVMs with kernels and soft margins.
4. Gain an intuition about the Bias-Variance tradeoff while using SVMs.

Support Vector Machines

A rough history

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Maximum Margin Classifier: (morning lecture)
1963: Vapnik, Chervonenkis

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Support Vector Machines

A rough history

Maximum Margin Classifier: (morning lecture)
1963: Vapnik, Chervonenkis

Soft Margins and the "Kernel Trick": (afternoon lecture)
1992-1995: Vapnik, Boser, Guyon, Cortes
This is the modern Support Vector Machine (SVM).

Outline

Supervised Learning

High level: What is supervised learning?

Supervised Learning

High level:

Learn an unknown function from a set of **labeled** training data.

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- Our training data is limited and finite. A useful algorithm must generalize well to "unseen" data.

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High level:

Learn an unknown function from a set of **labeled** training data.

- Our training data is limited and finite. A useful algorithm must generalize well to "unseen" data.
- Example: Children learning colors.
- Support Vector Machines (SVMs) are a *supervised* learning algorithm.

Outline

Notation

Goal:

Learn a model of a function $F : X \to Y$ from a training set D.

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Learn a model of a function $F : X \to Y$ from a training set D.

$D = \{(x^{(1)}, t^{(1)}), \ldots, (x^{(m)}, t^{(m)})\}$, where

- $x^{(j)} \in X$ is often called the "input".
- $t^{(j)} \in Y$ is often called the "label" or "target".

Notation (cont.)

$F : X \to Y$

- Often, $X = \mathbb{R}^n$
- Often, Y is a finite set (i.e. a classification task)

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We want our learned model to *generalize* well.
Explain the concept of "generalization error".

Notation (cont.)

$F : X \to Y$

- Often, $X = \mathbb{R}^n$
- Often, Y is a finite set (i.e. a classification task)

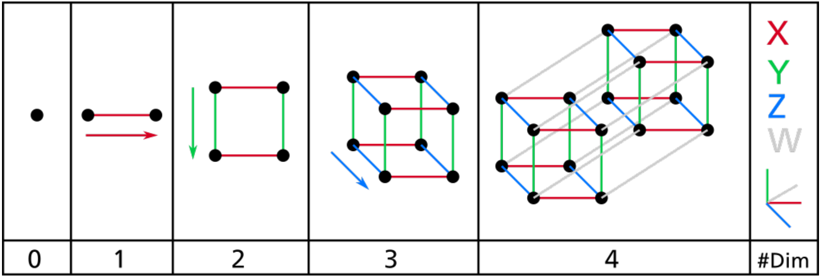
We want our learned model to *generalize* well.

Generalization error is a measure of the model's performance on all possible "unseen" data.

Outline

Dimensions

Basic stuff, I know.



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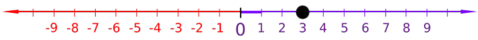
1D

How do you split this space?



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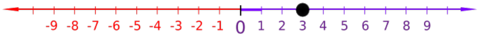
How do you split this space?



Split a line (1D) with a point (0D).

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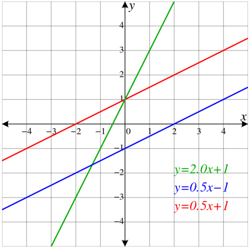
2D

How do you split this space?



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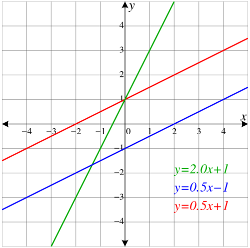
2D

How do you split this space?



Split a plane (2D) with a line (1D).

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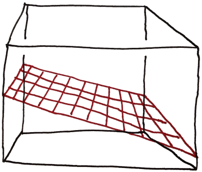
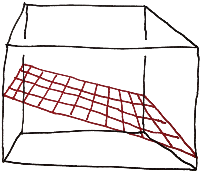
3D

How do you split this space?



3D

How do you split this space?



Split space (3D) with a plane (2D).

4D, 5D, etc...

Hard to visualize... :/

In general, an n-dimensional space can be separated by an $(n-1)$-dimensional *hyperplane*.

4D, 5D, etc...

Hard to visualize... :/

In general, an n-dimensional space can be separated by an $(n-1)$-dimensional *hyperplane*.

In an n-dimensional space any hyperplane can be defined by $w \in \mathbb{R}^n$ and $b \in \mathbb{R}$. The hyperplane includes all $x \in \mathbb{R}^n$ where:

$$w_0 x_0 + w_1 x_1 + \ldots + w_{n-1} x_{n-1} - b = 0$$

4D, 5D, etc...

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usually written:

$$w \cdot x - b = 0$$

How to interpret w and b

So, w and b define a hyperplane. Is there an interpretation of w and b that can help us visualize this hyperplane?

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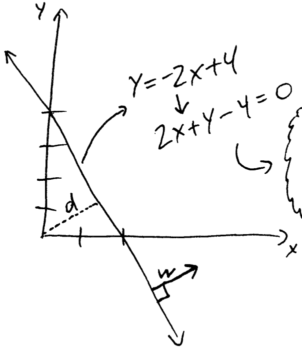
- $\frac{w}{||w||}$ is the hyperplane's normal vector.
- $\frac{b}{||w||}$ is the hyperplane's distance from the origin.

Example in 2D



$$y = -2x + 4$$
$$\downarrow$$
$$2x + y - 4 = 0$$

$$w = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$
$$b = 4$$

$$d = \frac{4}{\sqrt{2^2 + 1^2}} = 1.79$$

Outline

Binary Classification

A supervised learning problem

Recall, we're trying to learn $F : X \to Y$.

- Let, $X = \mathbb{R}^n$
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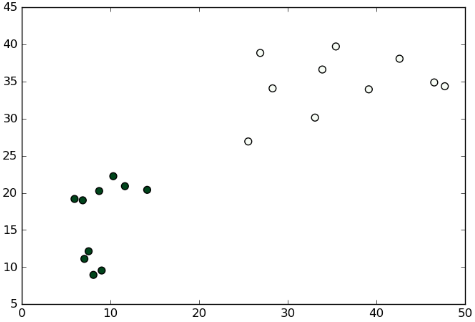
Recall, we're trying to learn $F : X \to Y$.

- Let, $X = \mathbb{R}^n$
- For binary classification, $Y = \{-1, 1\}$
  We're using -1 instead of 0 for future mathematical convenience.

Big idea: Let's have our model find a hyperplane that splits our n-dimensional data X into the set where $y = -1$ and the set where $y = 1$.

Binary Classification: Example

How many ways can we use a hyperplane to classify this dataset correctly?

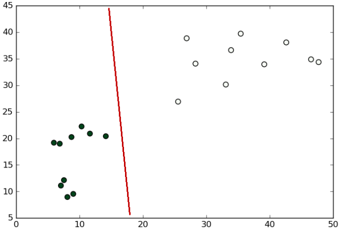


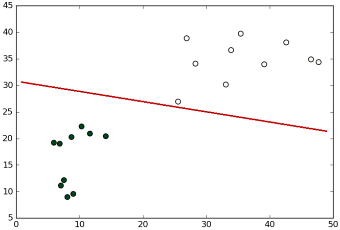
$$X = \mathbb{R}^2$$

$$Y = \{-1, 1\}$$

Binary Classification: Example

Two Example Solutions





Outline

Defining Margin

The distance from the hyperplane to the nearest training-data point.

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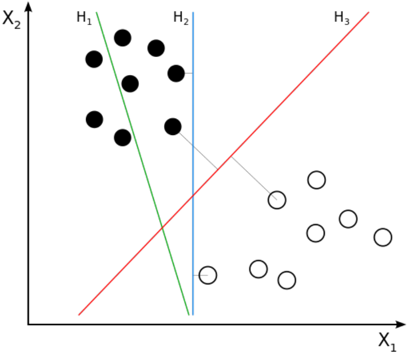

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Why Maximize the Margin?

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Large margin means better generalization.

- Intuitively, this makes sense (see previous slide)
- As margin increases, VC-dimension decreases, meaning variance decreases

Outline

Maximum Margin Classifier

Goal

Goal: Calculate w and b of the hyperplane:

$$w \cdot x - b = 0$$

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... such that the classes are split correctly and the margin is maximized.

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Goal: Calculate w and b of the hyperplane:

$$w \cdot x - b = 0$$

... such that the classes are split correctly and the margin is maximized.

First, some house cleaning: What happens to the hyperplane when we scale w and b by some factor c?

Maximum Margin Classifier

Setup

We need to define a "canonical" w and b. This will help later.

Let

$$|w \cdot x^{(i)} - b| = 1$$

where $x^{(i)}$ is the closest point to the hyperplane.

Maximum Margin Classifier

Setup

We need to define a "canonical" w and b. This will help later.

Let

$$|w \cdot x^{(i)} - b| = 1$$

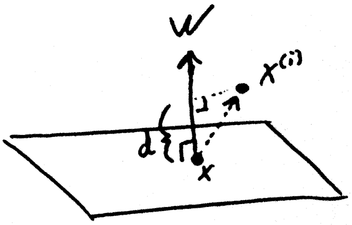
where $x^{(i)}$ is the closest point to the hyperplane.

There will be a unique scaled w and b to achieve this.

Maximum Margin Classifier

Margin

Now, if $x^{(i)}$ is the closest point to the hyperplane, then the distance from $x^{(i)}$ to the hyperplane is our margin. What is that distance?



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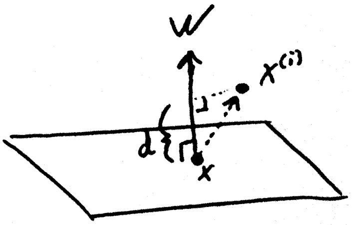
$$\left| \frac{w}{||w||} \cdot (x^{(i)} - x) \right| = d$$



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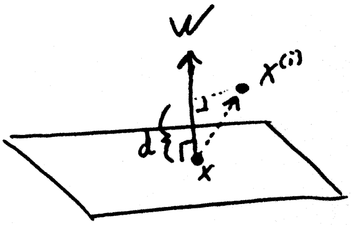
$$\frac{|w \cdot x^{(i)} - w \cdot x|}{||w||} = d$$



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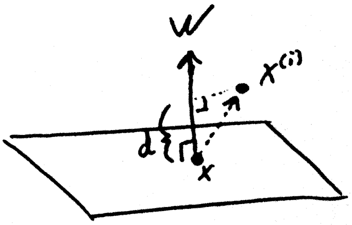
$$\frac{|w \cdot x^{(i)} - w \cdot x|}{||w||} = d$$

$$\frac{|w \cdot x^{(i)} - b - w \cdot x + b|}{||w||} = d$$



Maximum Margin Classifier

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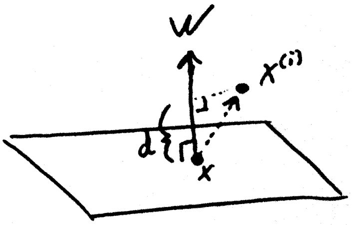
$$\left|\frac{w}{||w||}\cdot(x^{(i)} - x)\right| = d$$

$$\frac{|w\cdot x^{(i)} - w\cdot x|}{||w||} = d$$

$$\frac{|w\cdot x^{(i)} - b - w\cdot x + b|}{||w||} = d$$

$$\frac{1}{||w||} = d = margin$$



Maximum Margin Classifier

First Attempt

Maximize $\frac{1}{||w||}$

subject to:

$$|w \cdot x^{(i)} - b| \geq 1,$$

$$\text{for all } x^{(i)} \in D$$

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First Attempt

Maximize $\frac{1}{||w||}$

subject to:

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$$\text{for all } x^{(i)} \in D$$

... but we don't know how to solve this optimization problem. Let's reformulate.

Maximum Margin Classifier

Reformulated

Minimize $\frac{1}{2}||w||^2$

subject to:

$$y^{(i)}(w \cdot x^{(i)} - b) \geq 1,$$

$$\text{for all } (y^{(i)}, x^{(i)}) \in D$$

Maximum Margin Classifier

Reformulated

Minimize $\frac{1}{2}||w||^2$

subject to:

$$y^{(i)}(w \cdot x^{(i)} - b) \geq 1,$$

$$\text{for all } (y^{(i)}, x^{(i)}) \in D$$

... plus more steps... and we eventually get a quadratic programming formulation.

Support Vectors

The maximum margin hyperplane is defined only by the points that touch the margin. These are called the "support vectors".

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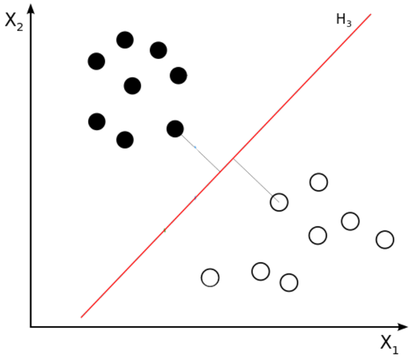

`sklearn`'s interface

LogisticRegression vs SVC

LogisticRegression:

Link

SVC:

Link

(end of morning lecture)

Outline

Soft Margin Motivation

What if:

1. Your data isn't linearly separable?
2. Your data is noisy / has outliers?

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What if:

1. Your data isn't linearly separable?
2. Your data is noisy / has outliers?

Soft Margins address these problems.

Soft Margin

The C hyperparameter

An extension to Maximum Margin Classifiers adds a C constant that gives the misclassification error penalty.

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Large C: Harder margins: value classification accuracy over a large margin

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The C hyperparameter

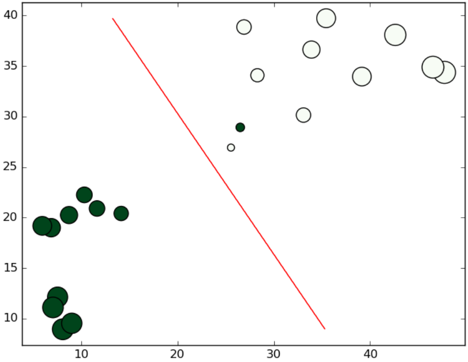
An extension to Maximum Margin Classifiers adds a C constant that gives the misclassification error penalty.

Large C: Harder margins: value classification accuracy over a large margin

Small C: Softer margins: value a large margin over classification accuracy

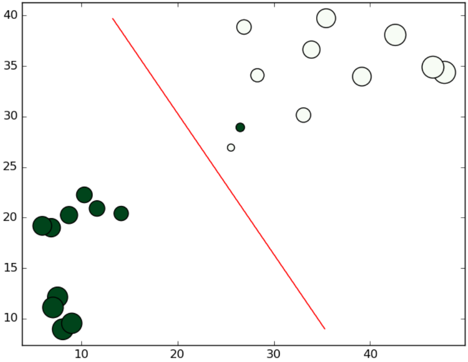
Soft Margins

Inseparable Data



Soft Margins

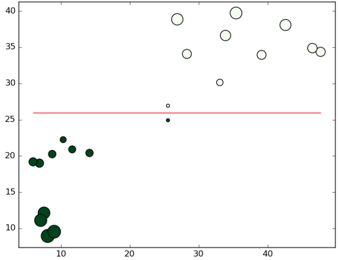
Inseparable Data



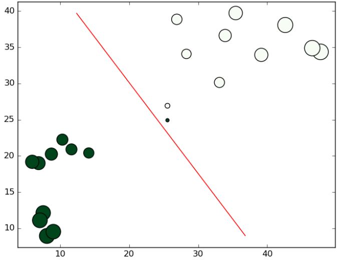
Only possible with a soft margin.

Soft Margins

Outliers in Data



Hard Margin



Soft Margin

Soft Margins

scikit-learn code

```
from sklearn.svm import SVC
...
svc = SVC(C=1.0, kernel='linear')
svc.fit(x, y)
```

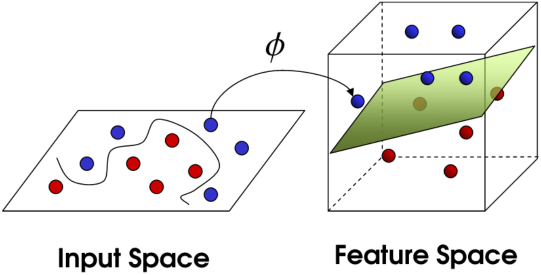
SVC supports the C parameter as the soft-margin hyperparameter.

Outline

The "Kernel Trick"

The idea...

Idea: If data is inseparable in its input space, maybe it will be separable in a higher-dimensional space.



[1]Unknown source

The "Kernel Trick"

Back to the math...

In our optimization problem to maximize the margin, we eventually end up optimizing a vector alpha $\alpha^{(i)}, i \in [1, m]$ in the following equation:

The "Kernel Trick"

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In our optimization problem to maximize the margin, we eventually end up optimizing a vector alpha $\alpha^{(i)}, i \in [1, m]$ in the following equation:

$$\mathcal{L}(\alpha) = \sum_{i=1}^{m} \alpha^{(i)} - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} y^{(i)} y^{(j)} \alpha^{(i)} \alpha^{(j)} (x^{(i)} \cdot x^{(j)})$$

The "Kernel Trick"

Back to the math...

In our optimization problem to maximize the margin, we eventually end up optimizing a vector alpha $\alpha^{(i)}, i \in [1, m]$ in the following equation:

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$$\mathcal{L}(\alpha) = \sum_{i=1}^{m} \alpha^{(i)} - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} y^{(i)} y^{(j)} \alpha^{(i)} \alpha^{(j)} (\phi(x^{(i)}) \cdot \phi(x^{(j)}))$$

The "Kernel Trick"

Creating a kernel...

$$\phi(x^{(i)}) \cdot \phi(x^{(j)}) \in \mathbb{R}$$

... this is just a real number.

The "Kernel Trick"

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What if we never applied ϕ and we never took the dot product, but we instead replaced this whole thing with a "kernel function".

The "Kernel Trick"

Creating a kernel...

$$\phi(x^{(i)}) \cdot \phi(x^{(j)}) \in \mathbb{R}$$

... this is just a real number.

What if we never applied ϕ and we never took the dot product, but we instead replaced this whole thing with a "kernel function".

$$K(x^{(i)}, x^{(j)}) = \phi(x^{(i)}) \cdot \phi(x^{(j)}) \in \mathbb{R}$$

The "Kernel Trick"

Why is this so cool?

- Saves some computation. We never need to compute ϕ.
- Opens new possibilities. A kernel can operate in infinite dimensions!

The "Kernel Trick"

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- Saves some computation. We never need to compute ϕ.
- Opens new possibilities. A kernel can operate in infinite dimensions!

You can use any $K(x^{(i)}, x^{(j)})$ as long as there **exists** some ϕ such that

$$K(x^{(i)}, x^{(j)}) = \phi(x^{(i)}) \cdot \phi(x^{(j)})$$

... but you don't have to know what ϕ actually **is**!

The Polynomial Kernel

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

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- equivalent to the dot product in the d-order ϕ space

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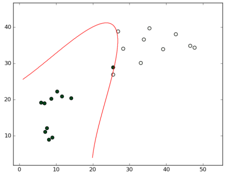
$$K(x^{(i)}, x^{(j)}) = (1 + x^{(i)} \cdot x^{(j)})^d$$

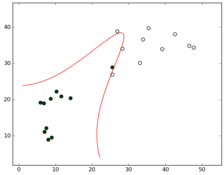
- equivalent to the dot product in the d-order ϕ space
- requires an extra hyper-parameter, d, for "degree"

The Polynomial Kernel

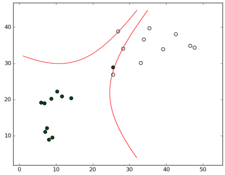
Example



svc = SVC(C=10000.0, kernel='poly', degree=3)



svc = SVC(C=10000.0, kernel='poly', degree=5)



svc = SVC(C=10000.0, kernel='poly', degree=10)

The RBF Kernel

(Radial Basis Function)

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

The RBF Kernel

(Radial Basis Function)

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

- equivalent to the dot product in the Hilbert space of infinite dimensions

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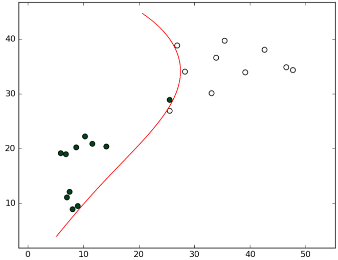
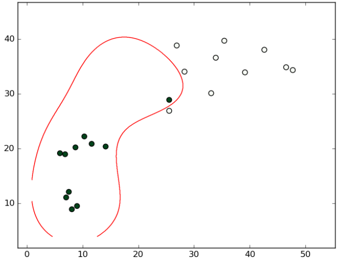
- equivalent to the dot product in the Hilbert space of infinite dimensions
- requires an extra hyper-parameter, γ, “gamma”

The RBF Kernel

Examples



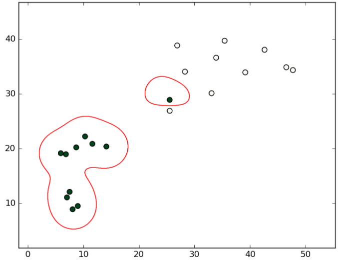
svc = SVC(C=10000.0, kernel='rbf', gamma=0.001)



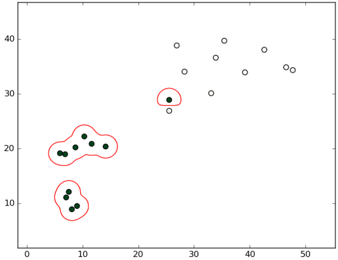
svc = SVC(C=10000.0, kernel='rbf', gamma=0.01)

The RBF Kernel

More Examples



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



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

Bias-Variance tradeoff

Explanation

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Variance

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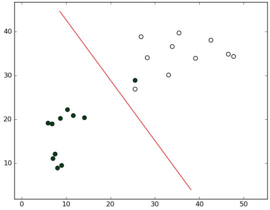
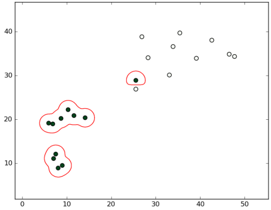
Example



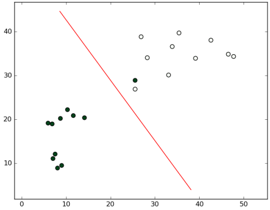


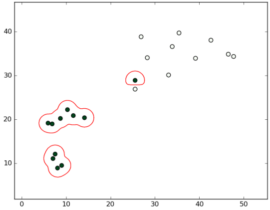
svc = SVC(C=0.01, kernel="linear")

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

Bias-Variance tradeoff

Example





svc = SVC(C=0.01, kernel="linear")

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

Which is a better fit for this dataset?

Outline

Grid Search

Hyperparameter Tuning

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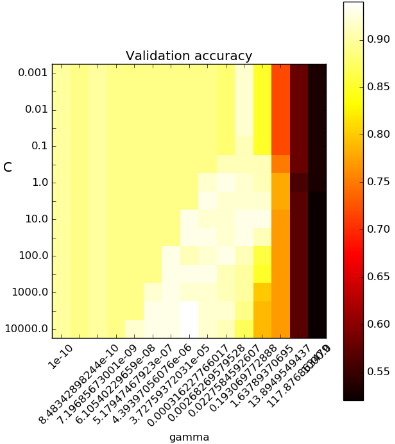

Grid Search

code

```
svc_rbf = SVC(kernel='rbf')

param_space = {'C':     np.logspace(-3, 4, 15),
               'gamma': np.logspace(-10, 3, 15)}

grid_search = GridSearchCV(svc_rbf, param_space,
                           scoring='accuracy', cv=10)
grid_search.fit(x, y)

print grid_search.grid_scores_
print grid_search.best_params_
print grid_search.best_score_
print grid_search.best_estimator_
```