Support Vector Machines

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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.

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

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

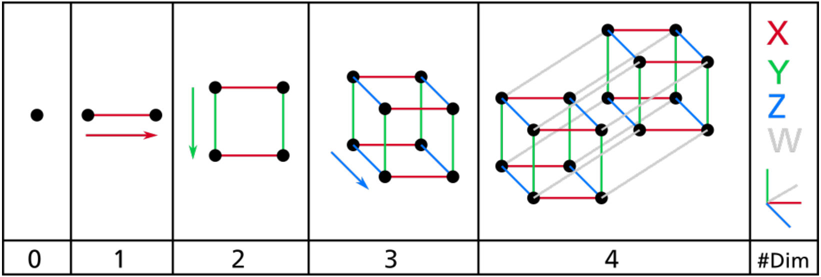
We want our learned model to *generalize* well.

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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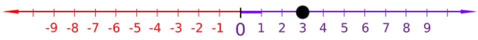
1D

How do you split this space?



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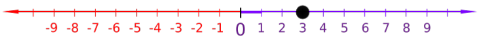
How do you split this space?



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

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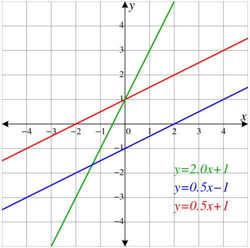
2D

How do you split this space?



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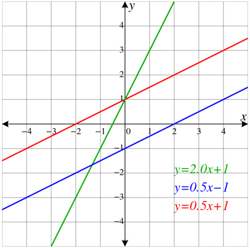
2D

How do you split this space?



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

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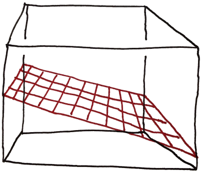
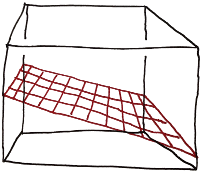
3D

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:

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

4D, 5D, etc...

Hard to visualize... :/

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

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.

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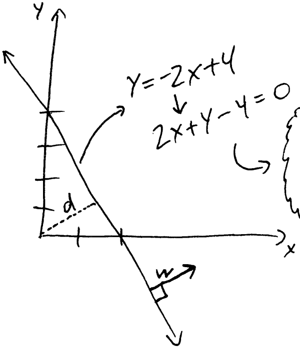
- $\frac{w}{||w||}$ is the hyperplane's normal vector.
- $\frac{b}{||w||}$ is the hyperplane's distance from the origin.

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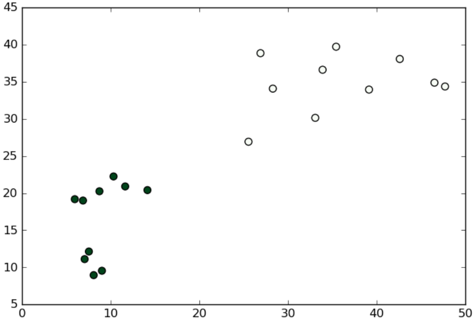
- Let, $X = \mathbb{R}^n$
- For binary classification, $Y = \{-1, 1\}$
  We're using -1 instead of 0 for future mathematical convenience.

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?

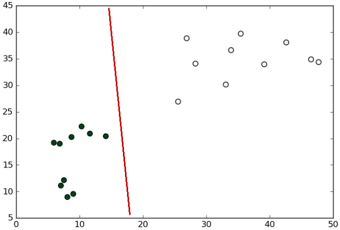


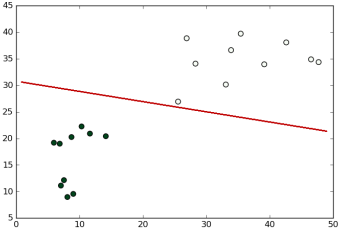
$$X = \mathbb{R}^2$$

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

Binary Classification: Example

Two Example Solutions





Outline

Defining Margin

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

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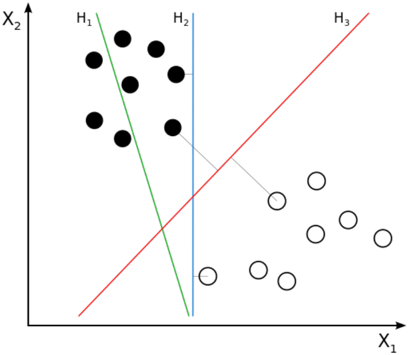

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Large margin means better generalization.

- 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

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

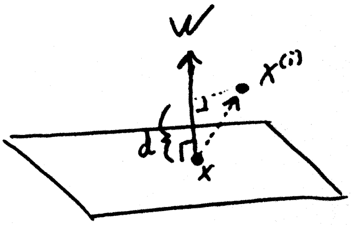
where $x^{(i)}$ is the closest point to the hyperplane.

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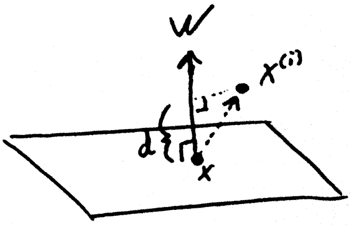
Now, if $x^{(i)}$ is the closest point to the hyperplane, then the distance from $x^{(i)}$ to the hyperplane is our margin. What is that distance?

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



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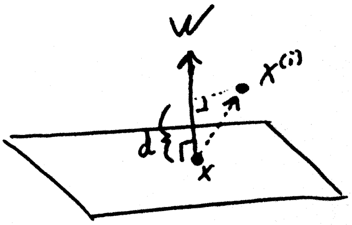
$$\frac{|w \cdot x^{(i)} - w \cdot x|}{||w||} = d$$



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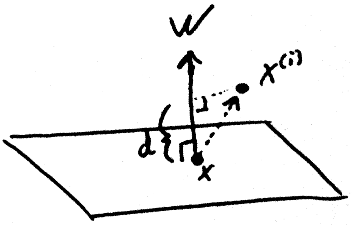
$$\frac{|w \cdot x^{(i)} - w \cdot x|}{||w||} = d$$

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



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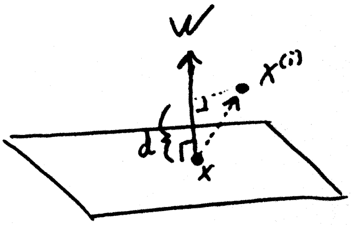
$$\frac{|w \cdot x^{(i)} - w \cdot x|}{||w||} = d$$

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

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



Maximum Margin Classifier

First Attempt

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

subject to:

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

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

Maximum Margin Classifier

First Attempt

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

subject to:

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

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

... 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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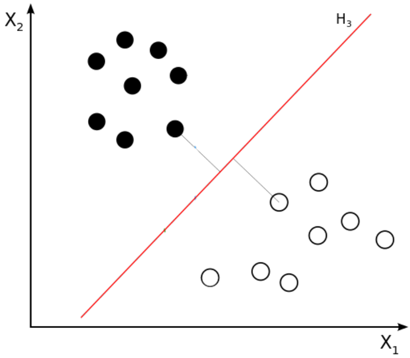

sklearn's interface

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?

Soft Margin Motivation

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

Soft Margin

The C hyperparameter

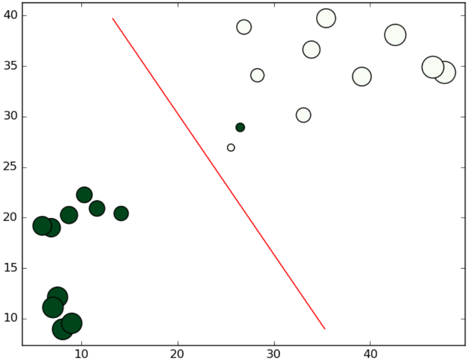
An extension to Maximum Margin Classifiers adds a C constant that gives the misclassification error penalty.

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

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

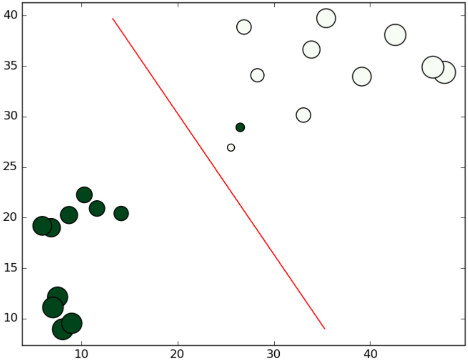
Soft Margins

Inseparable Data



Soft Margins

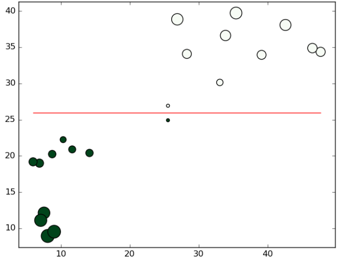
Inseparable Data



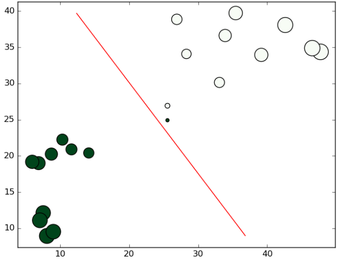
Only possible with a soft margin.

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)
```

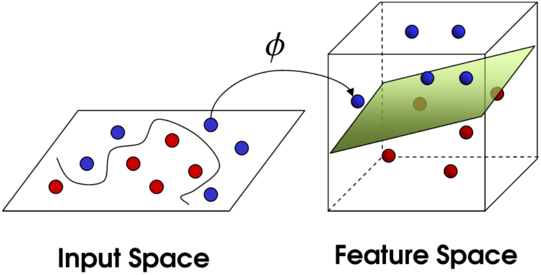
SVC supports the C parameter as the soft-margin hyperparameter.

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"

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:

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

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!

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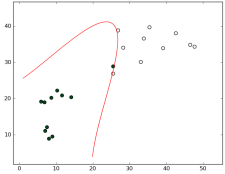
$$K(x^{(i)}, x^{(j)}) = (1 + x^{(i)} \cdot x^{(j)})^d$$

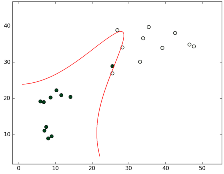
- equivalent to the dot product in the d-order ϕ space
- requires an extra hyper-parameter, d, for “degree”

The Polynomial Kernel

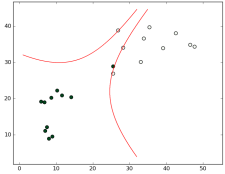
Example



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)

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

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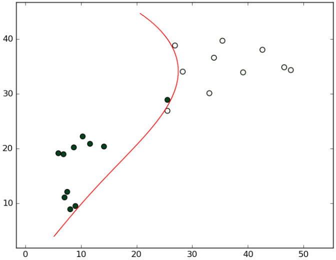
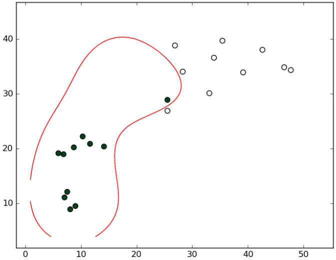
- requires an extra hyper-parameter, γ, "gamma"

The RBF Kernel

Examples



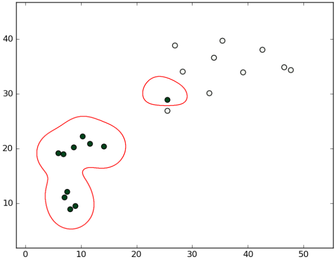


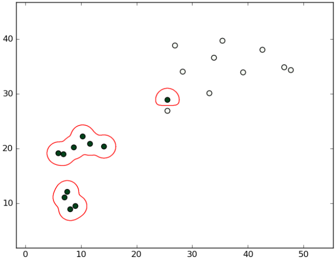
svc = SVC(C=10000.0, kernel='rbf', gamma=0.001)

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

The RBF Kernel

More Examples





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Bias-Variance tradeoff

Explanation

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Variance

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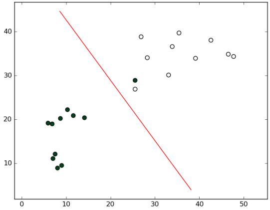
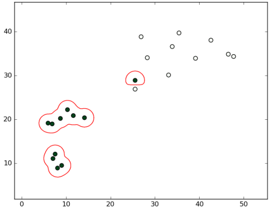


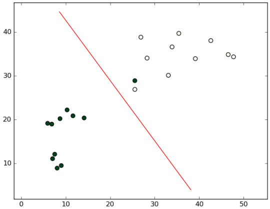
svc = SVC(C=0.01, kernel="linear")



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

Bias-Variance tradeoff

Example



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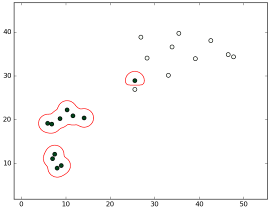

svc = SVC(C=10000.0, kernel='rbf', gamma=1.0)

Which is a better fit for this dataset?

Outline

SVMs vs Logistic Regression

(some rules of thumb)

1. Logistic Regression maximizes the *Binomial Log Likelihood* function.
2. SVMs maximize the *margin*.
3. When classes are nearly separable, SVMs tends to do better than Logistic Regression.
4. Otherwise, Logistic Regression (with Ridge) and SVMs are similar.
5. However, if you want to estimate probabilities, Logistic Regression is the better choice.
6. With kernels, SVMs work well. Logistic Regression works fine with kernels but can get computationally too expensive.

Grid Search

Hyperparameter Tuning

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Let's find C and *gamma* by searching through values we expect might work well.

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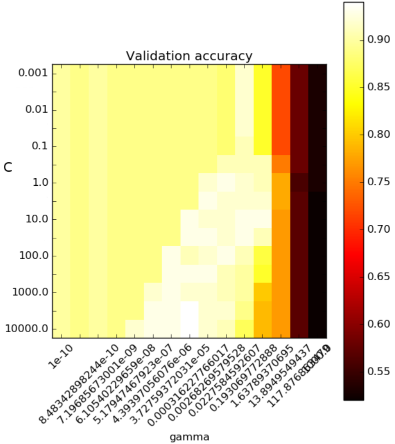

Grid Search

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_
```