CS189/CS289A
Introduction to Machine Learning
Lecture 3: Support Vector Machines

Peter Bartlett

January 27, 2015

Outline

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- Recall: linear classifiers, perceptron algorithm

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- Support vector machines

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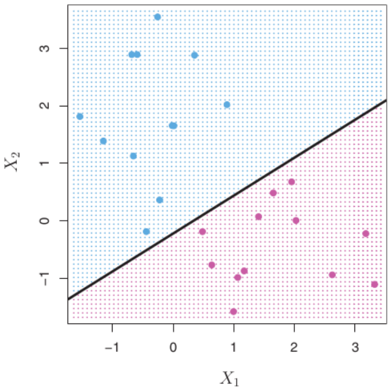
Linear classifiers

For a pattern $x \in \mathbb{R}^d$

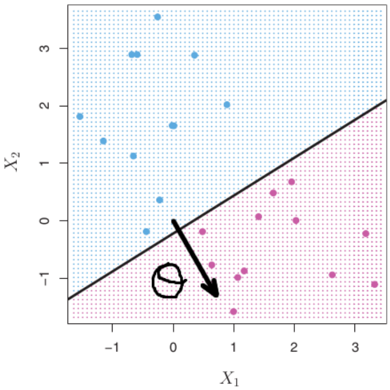


Linear classifiers

For a pattern $x \in \mathbb{R}^d$ and parameters $\theta \in \mathbb{R}^d$, $\theta_0 \in \mathbb{R}$, define

$$f(x) = \theta \cdot x + \theta_0,$$

$$\hat{y} = \begin{cases} 1 & \text{if } f(x) \geq 0, \\ -1 & \text{if } f(x) < 0. \end{cases}$$



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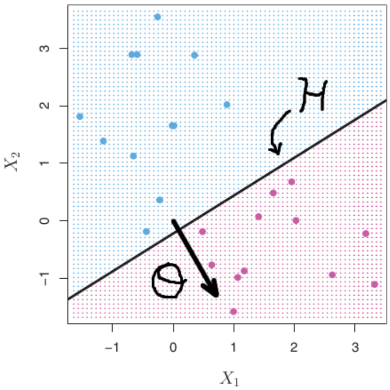

Decision boundary:

$$H = \left\{ x \in \mathbb{R}^d : f(x) = 0 \right\} = \left\{ x \in \mathbb{R}^d : \theta \cdot x + \theta_0 = 0 \right\}.$$

Methods for choosing linear classifiers

Methods for choosing linear classifiers

- Suppose we have a training set $(x_1, y_1), \ldots, (x_n, y_n)$.
  (For example, the $x_i \in \mathbb{R}^{400}$ might be grey-scale images of digits and the y_i their class label $y_i \in \{0, 1, \ldots, 9\}$.)

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- How do we use the data to choose a linear classifier?
- We consider three approaches:
  - The perceptron algorithm.
  - The hard margin support vector machine.
  - The (soft margin) support vector machine.
- (Later, we'll also look at other methods, including logistic regression and linear discriminant analysis.)

Perceptron algorithm

Perceptron algorithm:

Input: $(X_1, Y_1), \ldots, (X_n, Y_n) \in \mathbb{R}^d \times \{\pm 1\}$
while some $y^i \neq \mathrm{sign}(\theta \cdot x^i)$
    pick some misclassified (x^i, y^i)
    $\theta \leftarrow \theta + y^i x^i$
Return θ.

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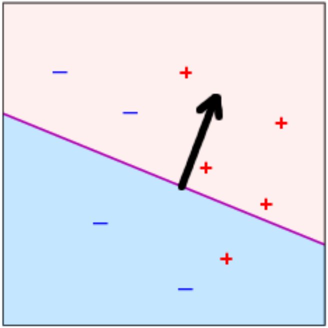

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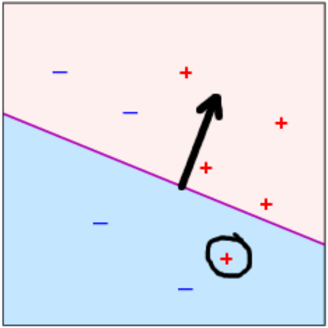

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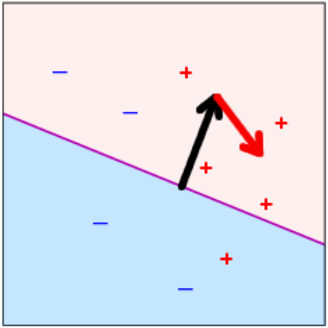

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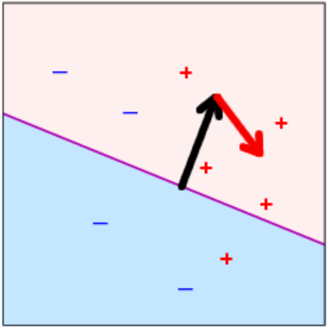

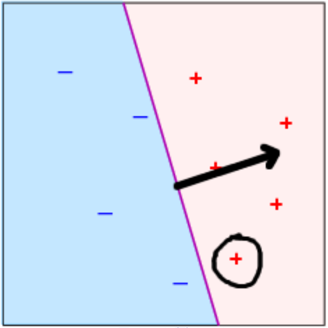

Perceptron algorithm

We can view the perceptron algorithm as a stochastic gradient method to minimize a cost function.

Perceptron algorithm

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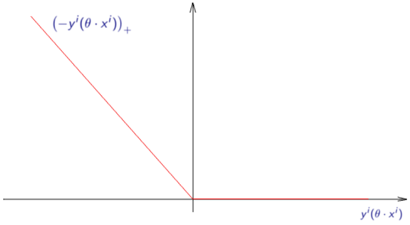
Margin cost function

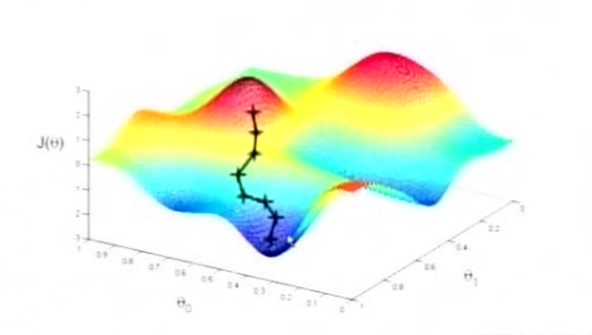
$$J(\theta) = \sum_i \left(-y^i(\theta \cdot x^i)\right)_+$$

$J(\theta) = 0 \Rightarrow$ all x^i classified correctly.



Perceptron algorithm

Gradient descent



Perceptron algorithm

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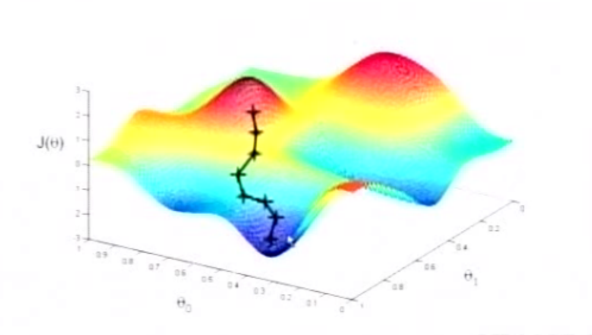
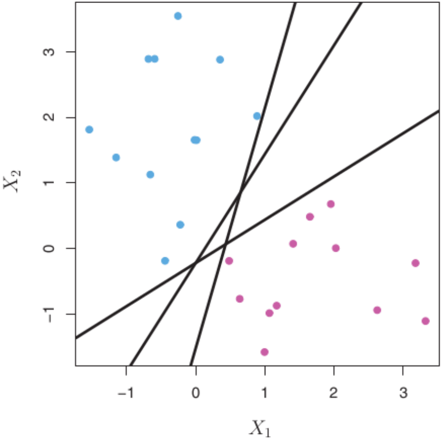


$$\theta \leftarrow \theta \underbrace{- \nabla J(\theta)}_{\text{downhill}}$$

Support vector machines

- There are always many linear classifiers that give identical classifications of the training data. Which is better?



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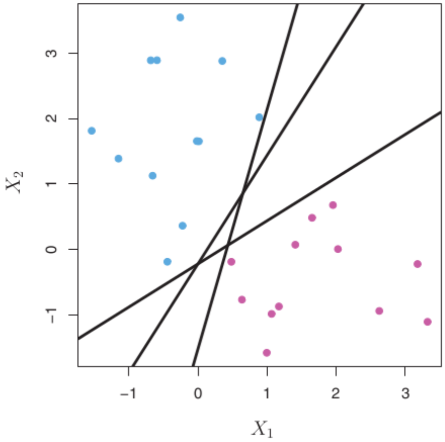
- *Support vector machines* choose the classifier that maximizes the *margin* on the training data, where the margin is the minimum over (x^i, y^i) pairs of the signed distance to the decision boundary,

$$\text{distance} := y^i \frac{\theta \cdot x^i}{\|\theta\|}.$$



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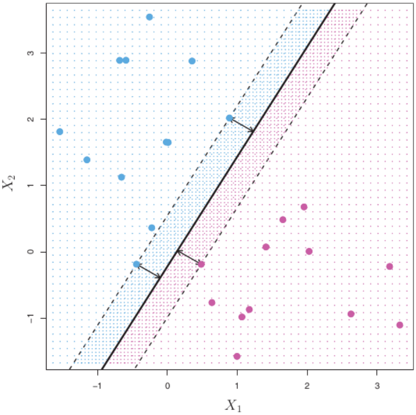

Support vector machines

Maximizing the margin:

$$\begin{aligned} \min_{\theta} \quad & \|\theta\|^2 \\ \text{such that} \quad & y^i \theta \cdot x^i \geq 1 \qquad (i = 1, \ldots, n) \end{aligned}$$

Support vector machines

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- This is a *quadratic program*: a minimization problem involving a convex quadratic criterion, subject to linear constraints).

Support vector machines

Maximizing the margin:

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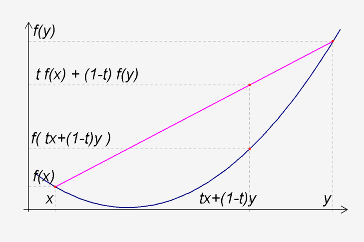
- This is a *quadratic program*: a minimization problem involving a convex quadratic criterion, subject to linear constraints).
- There are efficient algorithms for solving QPs.

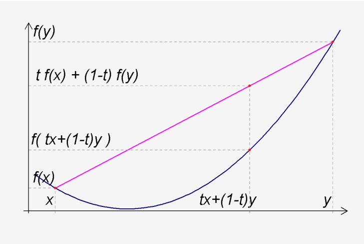
Convex vs non-convex minimization

Convex vs non-convex minimization



A convex function

Convex vs non-convex minimization



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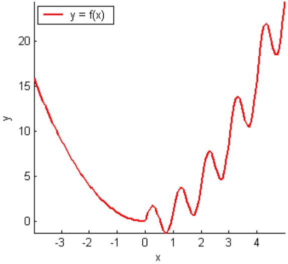

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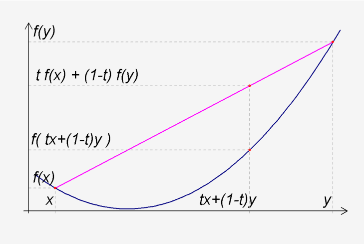

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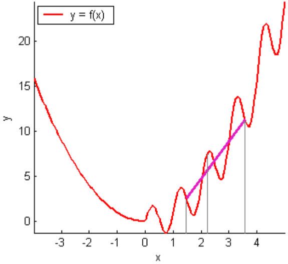

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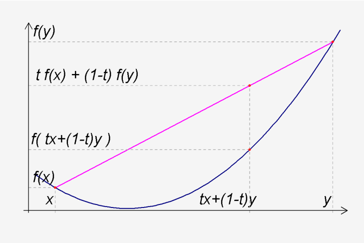

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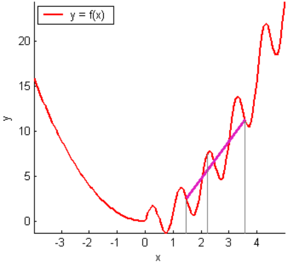

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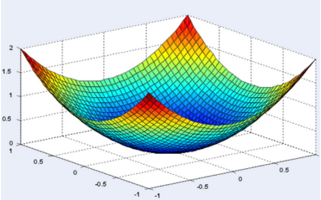

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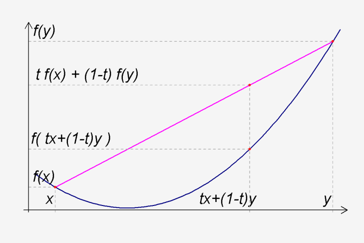

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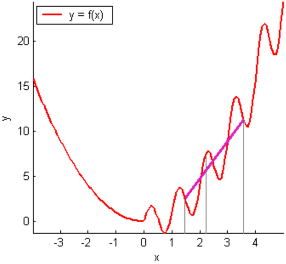

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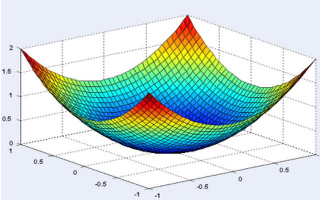

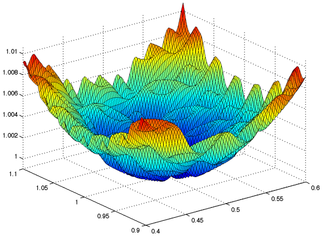

Support vector machines

Hard margin SVM

$$\begin{aligned} \min_{\theta} \quad & \|\theta\|^2 \\ \text{such that} \quad & y^i \theta \cdot x^i \geq 1 \qquad (i = 1, \ldots, n) \end{aligned}$$

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- The points that satisfy these constraints with equality are called *support vectors*.

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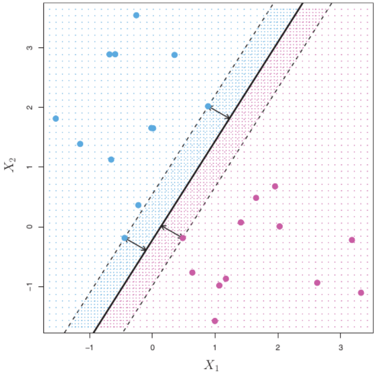

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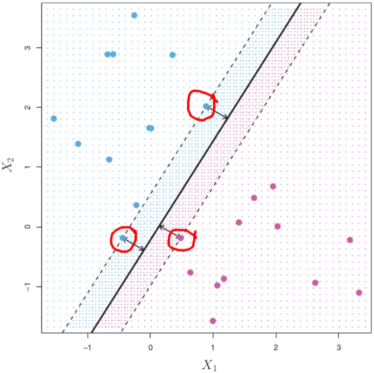

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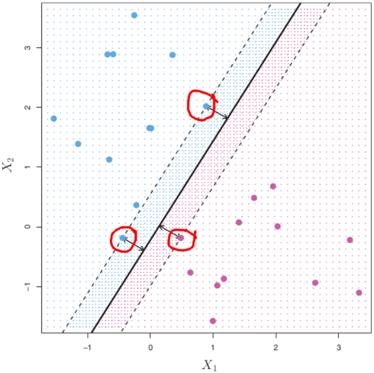

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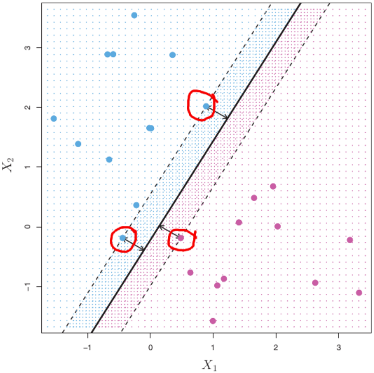
- The points that satisfy these constraints with equality are called *support vectors*.
- Small changes to any other data points will not affect the maximal margin hyperplane.
- We can think of the set of support vectors as a *compressed* version of the training data.



Support vector machines

Soft margin SVM

$$\min_{\theta} \quad \|\theta\|^2 + C\sum_{i=1}^{n}\left(1 - y^i\theta\cdot x^i\right)_+ .$$

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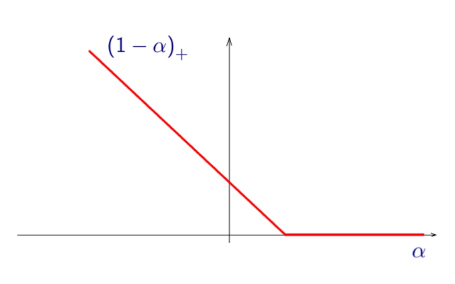
SVM margin cost function:



Support vector machines

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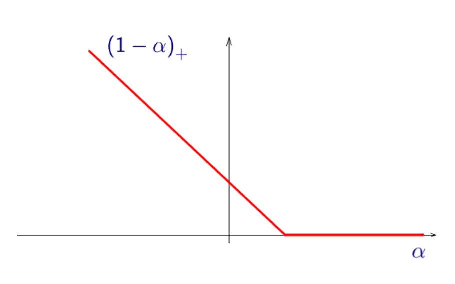

- Hard margin SVM: every term $(1 - y^i\theta\cdot x^i)_+ = 0$.

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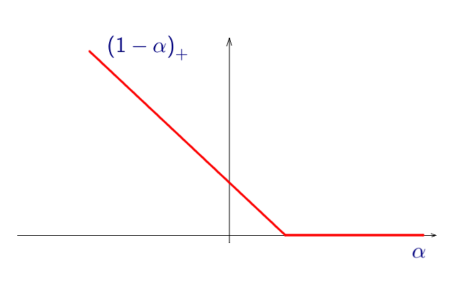

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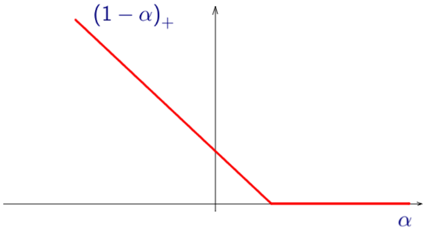
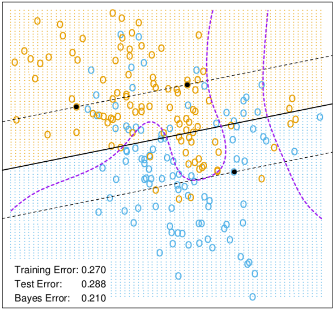


- Hard margin SVM: every term $(1 - y^i\theta\cdot x^i)_+ = 0$.
- Soft margin SVM: the constraints can be violated, but not too much.
- The parameter C adjusts the trade-off: $\|\theta\|^2$ versus fit to the data.

- Simulated data: (x, y) pairs chosen according to a known distribution.



$C = 10000$

Support vector machines

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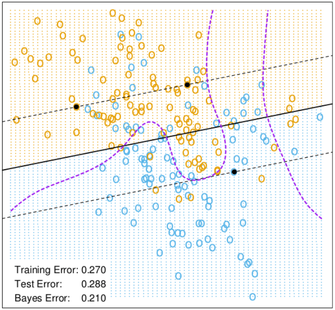
- (Purple line is the optimal decision boundary—'Bayes classifier'. It minimizes the probability of misclassification.)



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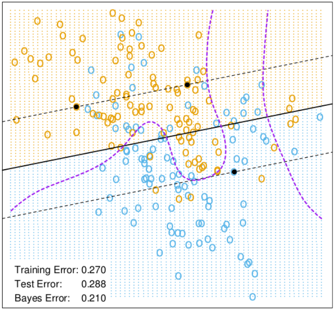

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Support vector machines

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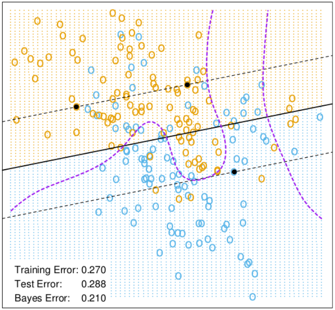
- Solid black line is the SVM decision boundary $\{x : \theta \cdot x = 0\}$.



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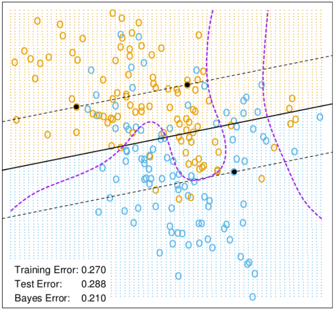
- Solid black line is the SVM decision boundary $\{x : \theta \cdot x = 0\}$.
- Dashed black lines represent $\{x : \theta \cdot x \in \{-1, 1\}\}$.



$C = 10000$

$$\min_{\theta} \quad \|\theta\|^2 + C \sum_{i=1}^{n} \left(1 - y^i \theta \cdot x^i\right)_+ .$$

Support vector machines

- Simulated data: (x, y) pairs chosen according to a known distribution.
- (Purple line is the optimal decision boundary—'Bayes classifier'. It minimizes the probability of misclassification.)
- Solid black line is the SVM decision boundary $\{x : \theta \cdot x = 0\}$.
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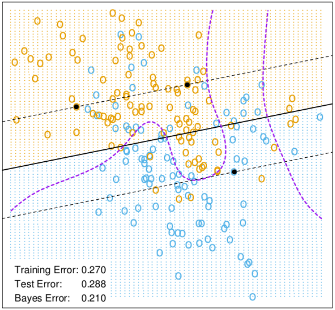

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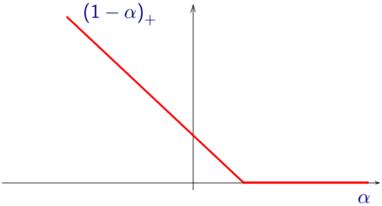

Outline

- Recall: linear classifiers, perceptron algorithm
- Support vector machines
- **Features**
- Features and overfitting
- Role of the regularization parameter C
- Regularization and overfitting
- Kernels

Features

- What if a linear decision boundary performs poorly?

Features

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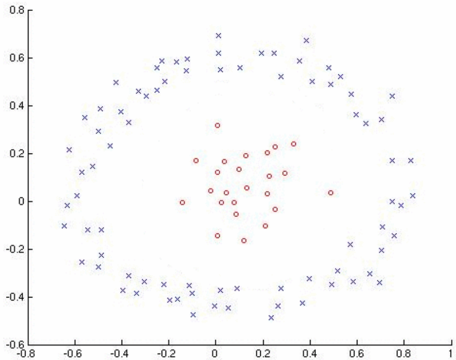

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- What if a linear decision boundary performs poorly?
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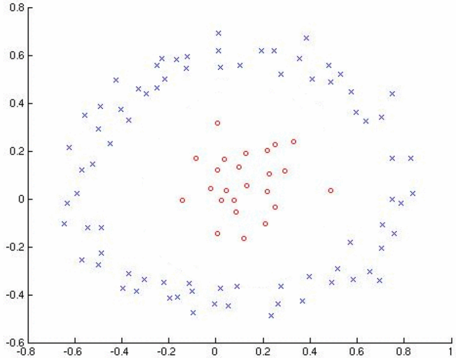
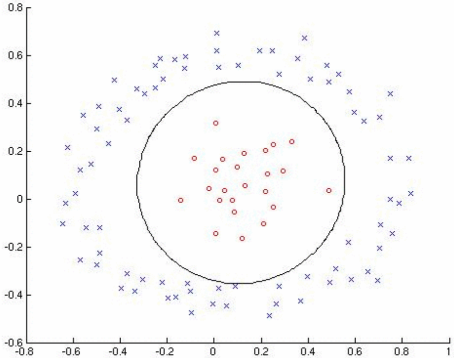
- No linear decision boundary can effectively separate “o”s from “x”s.



Features

- What if a linear decision boundary performs poorly?
- Consider this toy example.
- No linear decision boundary can effectively separate "o"s from "x"s.
- But a quadratic decision boundary can separate them.



Features

Quadratic classifier

$f(x) = \|x - c\|^2 - r^2$ (center $c \in \mathbb{R}^2$, radius r)

Features

$$\hat{y} = \begin{cases} 1 & \text{if } f(x) \geq 0, \\ -1 & \text{if } f(x) < 0. \end{cases}$$

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Recall: Linear classifier

$$f(x) = \theta \cdot x.$$

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$$\begin{aligned} f(x) &= \|x - c\|^2 - r^2 \qquad\qquad (\text{center } c \in \mathbb{R}^2, \text{ radius } r) \\ &= (x_1 - c_1)^2 + (x_2 - c_2)^2 - r^2 \end{aligned}$$

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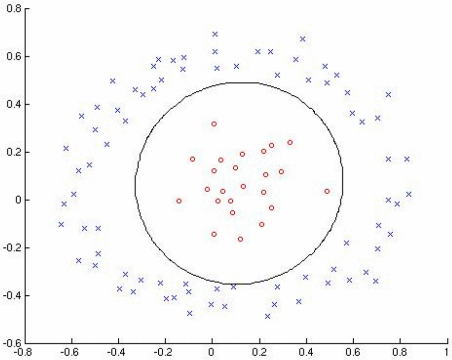
Features

- The quadratic decision boundary corresponds to a linear classifier with new features



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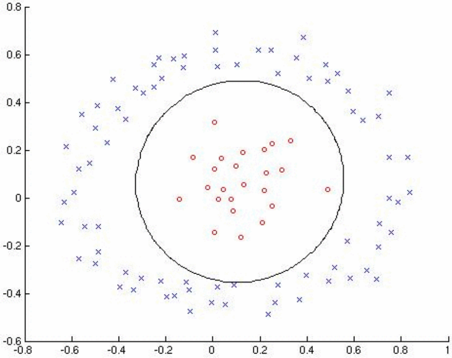

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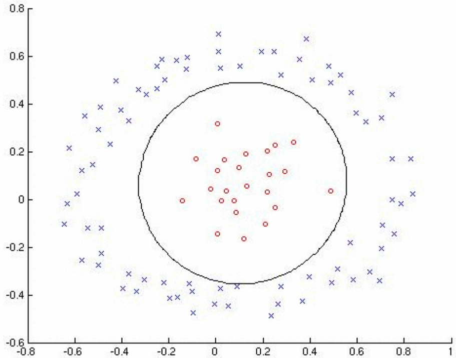

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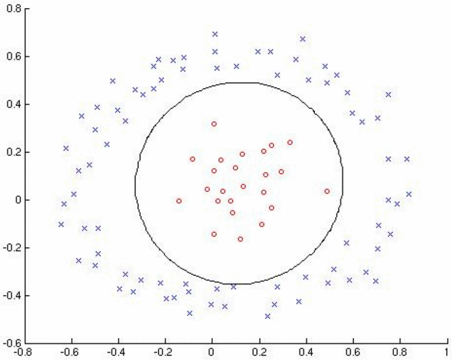
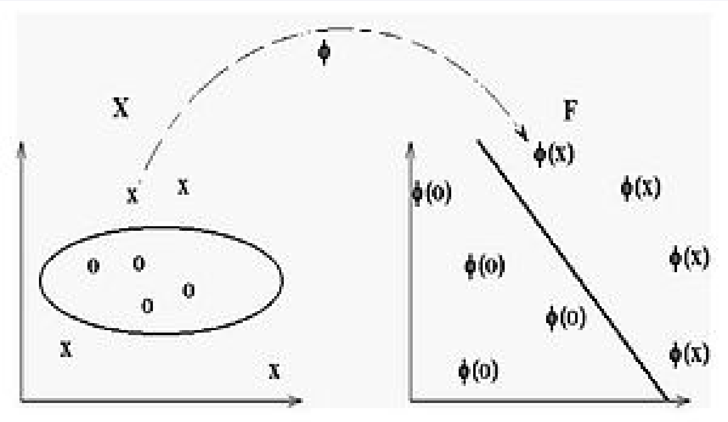
- The features we choose are very important!



Features

Feature map ϕ



An aside

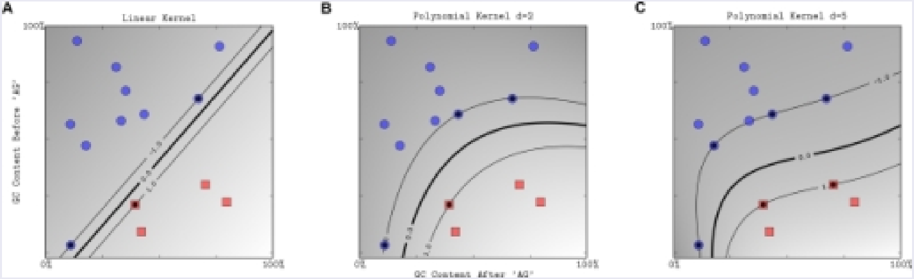
We used this idea earlier when we were simplifying notation to drop the offset θ_0: we transformed the pattern $x \in \mathbb{R}^d$ into a pattern $\tilde{x} \in \mathbb{R}^{d+1}$ with a constant component: to dispense with the offset θ_0:

$$\tilde{x} = \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix}, \qquad \tilde{\theta} = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_d \end{pmatrix}.$$

Then

$$\tilde{f}(\tilde{x}) := \tilde{\theta} \cdot \tilde{x} = \sum_{i=1}^{d} \theta_i x_i + \theta_0 = \theta \cdot x + \theta_0 = f(x).$$

SVMs with polynomial features of various degrees:



degree $= 1$ degree $= 2$ degree $= 5$

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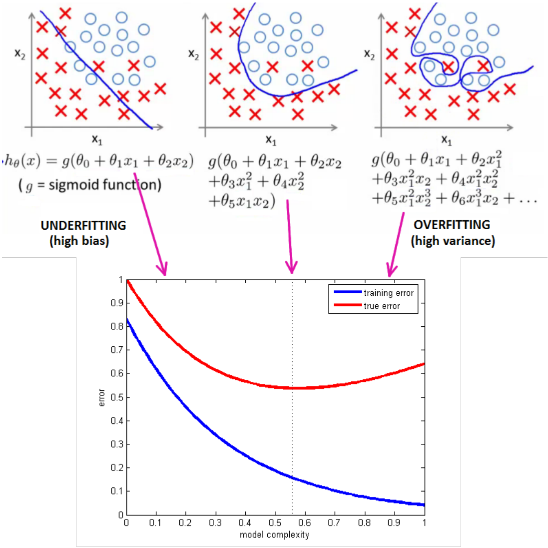
- The richer the set of features, the more likely we will encounter *overfitting*.
- It's a balancing act: we want our features to be as complex as necessary to represent the classifier, but no more complex.

Features and overfitting



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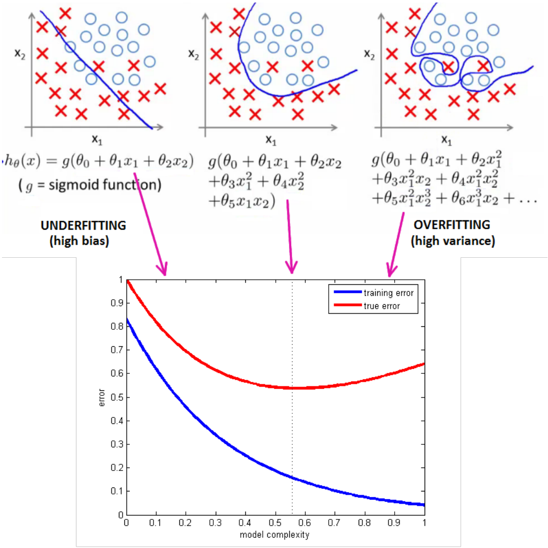


What happens to this picture as sample size grows?

Features

Digit recognition

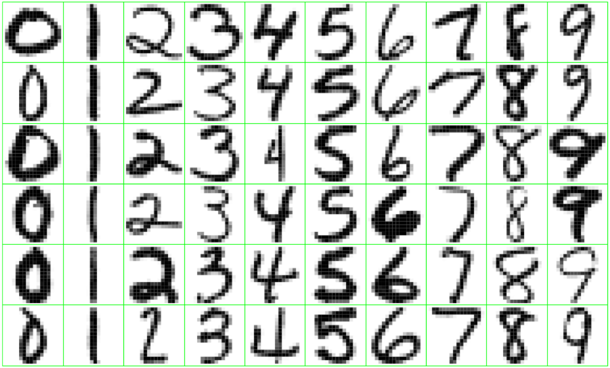
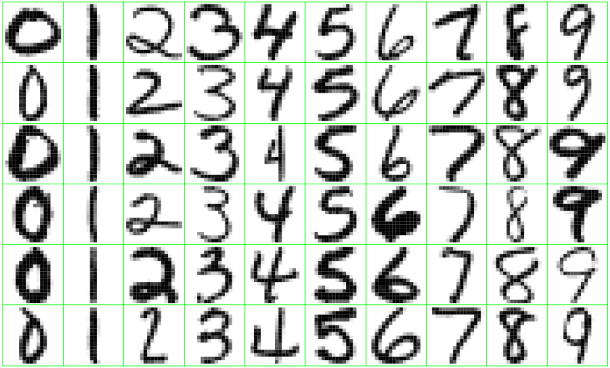


FIGURE 1.2. *Examples of handwritten digits from U.S. postal envelopes.*

Features

Digit recognition

- What features should we use?



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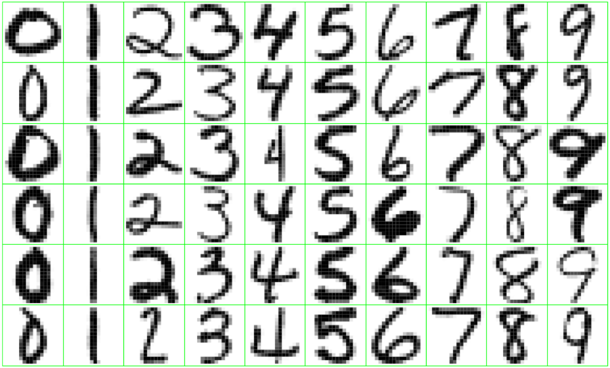
Digit recognition

- What features should we use?
  - Grey scale level for each pixel



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Features

Digit recognition

- What features should we use?
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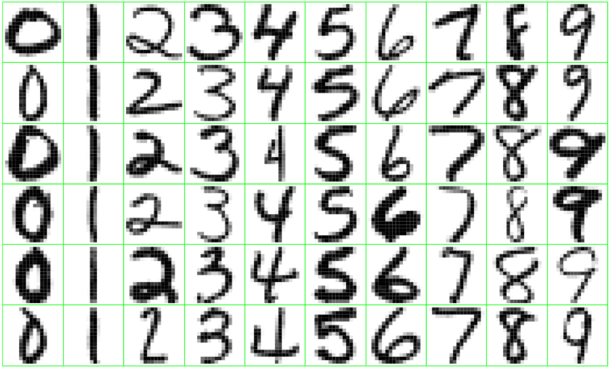

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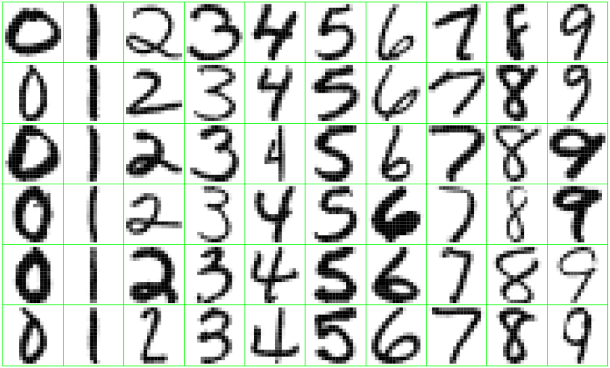
Features

Digit recognition

- What features should we use?
  - Grey scale level for each pixel
  - Orientation histograms
  - Polynomials of these



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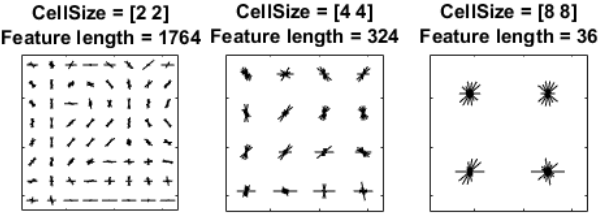
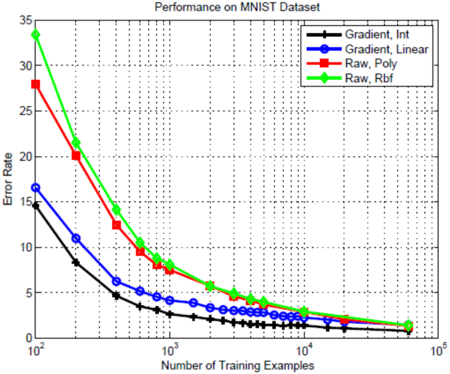
Histograms of Oriented Gradients

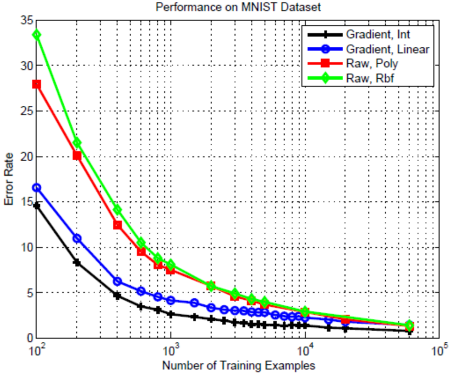


Support vector machines on MNIST data



(Maji and Malik, 2009)

Support vector machines on MNIST data



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- For large sample sizes, different features give similar performance.

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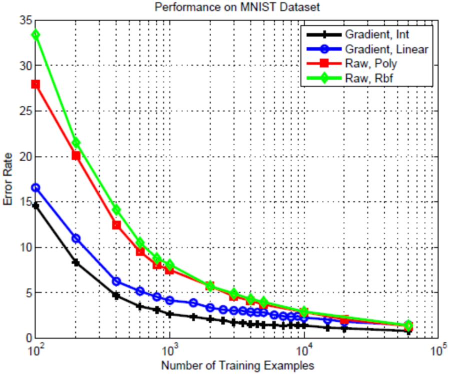

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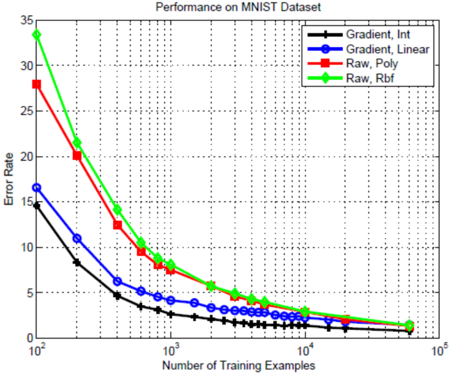

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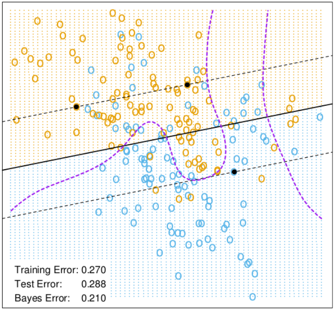
- For large sample sizes, different features give similar performance.
- For smaller sample sizes, there are significant differences.
- For some features, good classifiers are easier to find than for others.

Outline

- Recall: linear classifiers, perceptron algorithm
- Support vector machines
- Features
- Features and overfitting
- **Role of the regularization parameter** C
- Regularization and overfitting
- Kernels

Regularization and SVMs

- Simulated data: (x, y) pairs chosen according to a known distribution.



$C = 10000$

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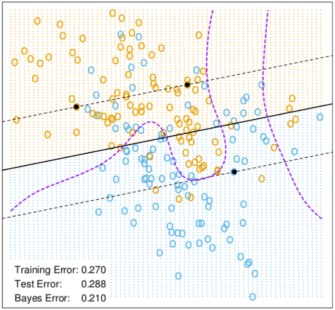

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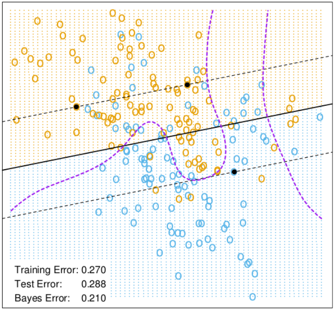

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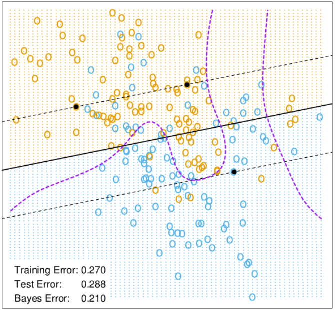

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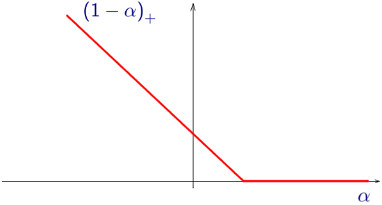

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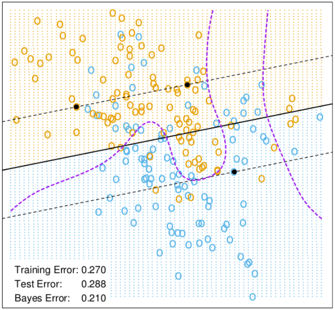

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Regularization and SVMs

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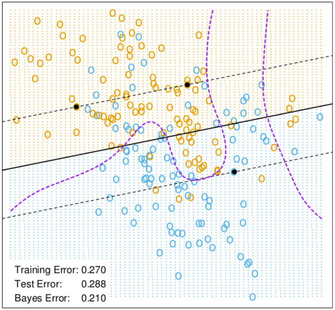
- C controls trade-off between margin $1/\|\theta\|$ and fit to data:



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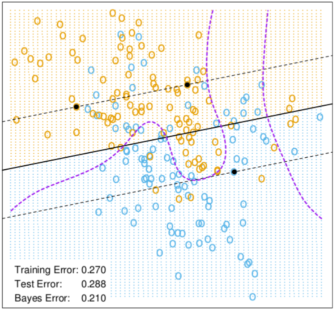

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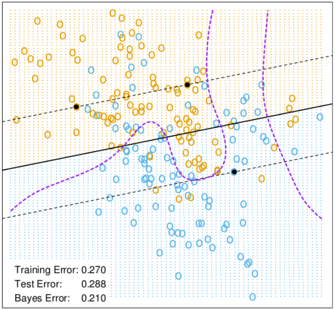

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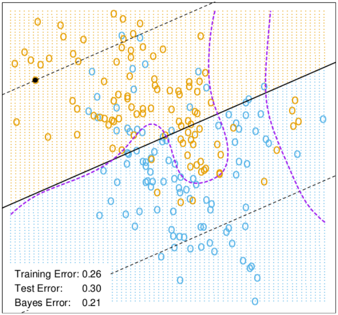

$C = 0.01$

Regularization and SVMs

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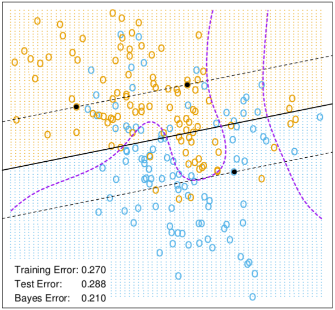
- C controls trade-off between margin $1/\|\theta\|$ and fit to data:
- Large C: focus on fit to data (small margin ok).
- Small C: focus on large margin.
- Overfitting increases with: less data, more features, C.

(Not apparent in this example with $d = 2$ and $n = 100$s.)



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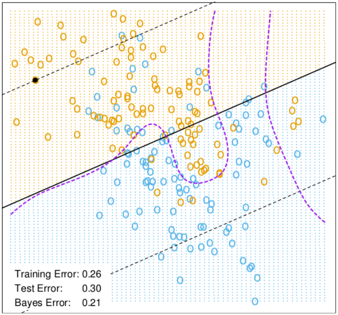

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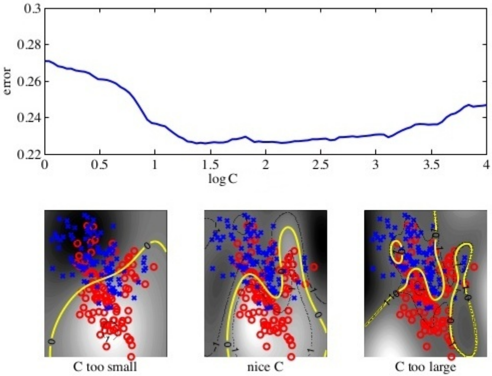
Regularization and SVMs

- Simulated data with *many features* $\phi(x)$.



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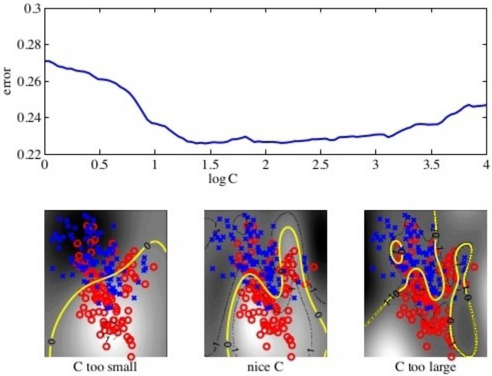

Regularization and SVMs

- Simulated data with *many features* $\phi(x)$.
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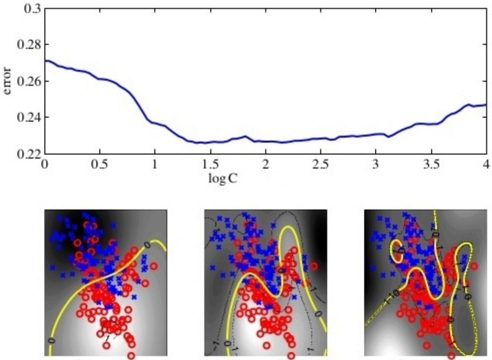

C too small   nice C   C too large

Regularization and SVMs

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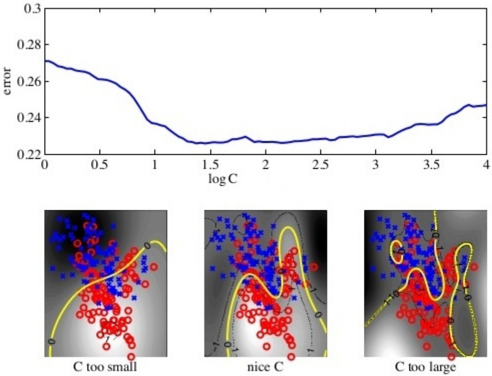

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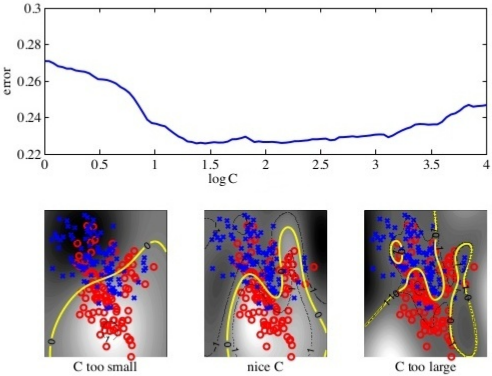
- Overfitting increases with: less data, more features.



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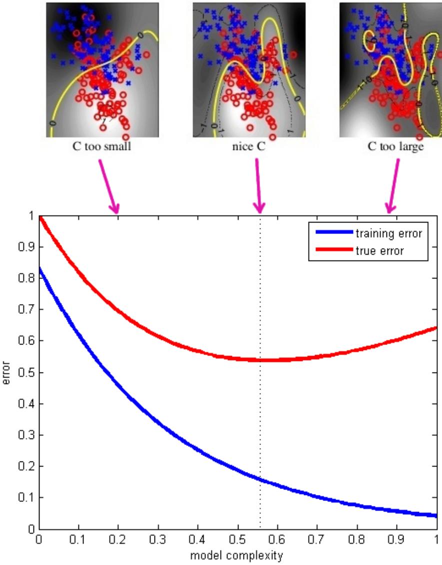

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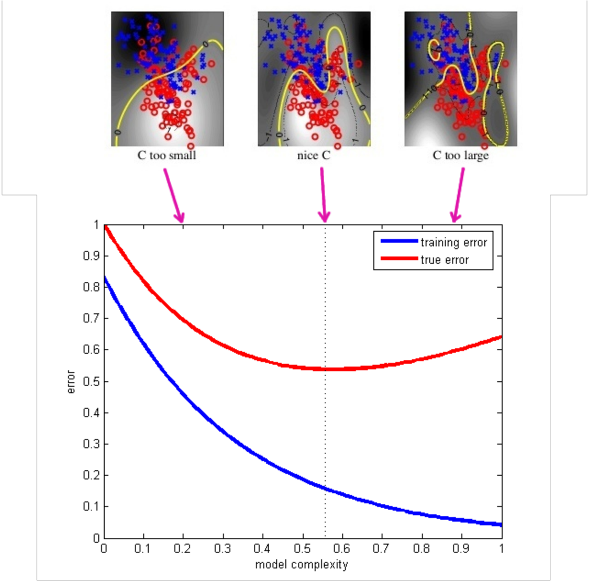
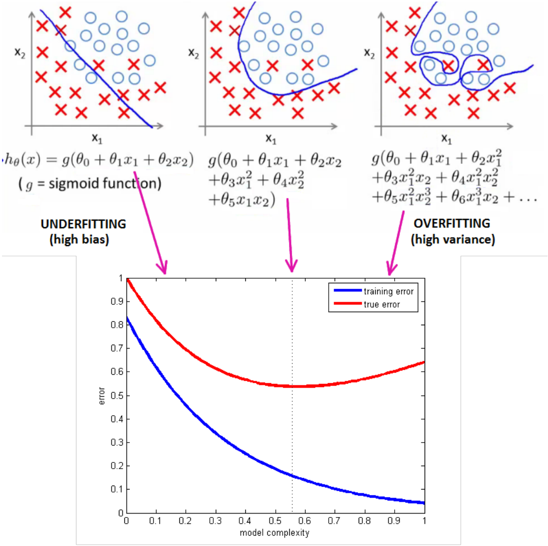


What happens to this picture as sample size grows?

c.f. Features and overfitting



Outline

- Recall: linear classifiers, perceptron algorithm
- Support vector machines
- Features
- Features and overfitting
- Role of the regularization parameter C
- Regularization and overfitting
- **Kernels**

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  - Soft margin SVM

Perceptron algorithm: only uses inner products

Perceptron algorithm:

Input: $(X_1, Y_1), \ldots, (X_n, Y_n) \in \mathbb{R}^d \times \{\pm 1\}$
while some $y^i \neq \mathrm{sign}(\theta \cdot x^i)$
  pick some misclassified (x^i, y^i)
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- As long as we can calculate the inner products $x^i \cdot x^j$ for training vectors x^i, x^j, that is all we need.

SVM: only uses inner products

Hard margin SVM

$$\begin{aligned} \min_{\theta} \quad & \|\theta\|^2 \\ \text{such that} \quad & y^i \theta \cdot x^i \geq 1 \qquad (i = 1, \ldots, n) \end{aligned}$$

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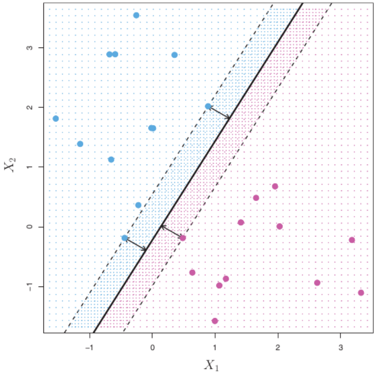

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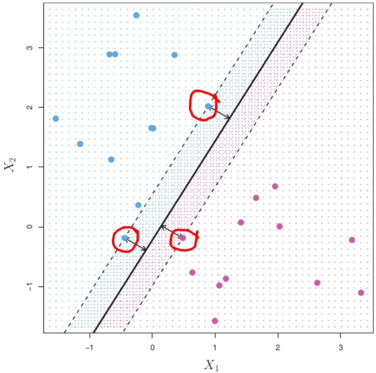

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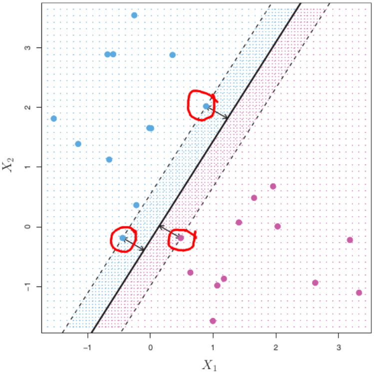

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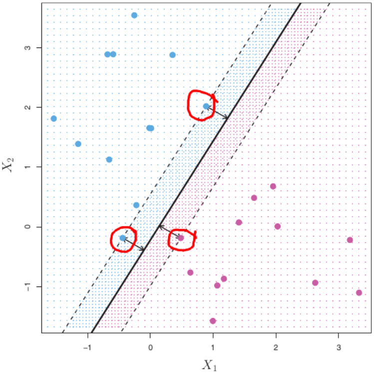

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$$\min_{\theta} \qquad \|\theta\|^2 + C\sum_{i=1}^{n}\left(1 - y^i\theta\cdot x^i\right)_+ .$$

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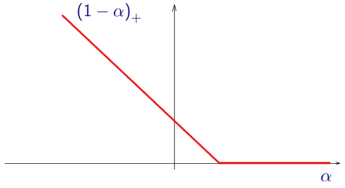

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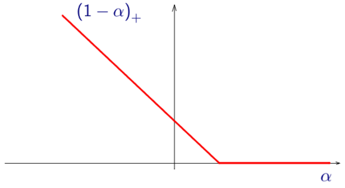

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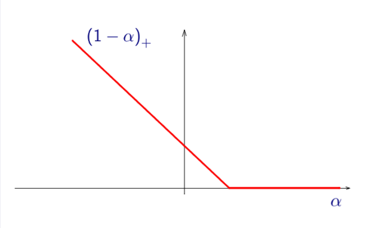

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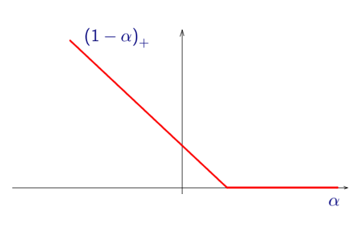

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- K is called a *kernel*.

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Kernels

Examples of Kernels for $x, \tilde{x} \in \mathbb{R}^d$

$$K_m(x, \tilde{x}) = (1 + x \cdot \tilde{x})^m$$ degree-m polynomial kernel

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&= \underbrace{\begin{pmatrix} 1 \\ x_1^2 \\ x_2^2 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ \sqrt{2}x_1x_2 \end{pmatrix}}_{\phi(x)} \cdot \underbrace{\begin{pmatrix} 1 \\ \tilde{x}_1^2 \\ \tilde{x}_2^2 \\ \sqrt{2}\tilde{x}_1 \\ \sqrt{2}\tilde{x}_2 \\ \sqrt{2}\tilde{x}_1\tilde{x}_2 \end{pmatrix}}_{\phi(\tilde{x})}
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This is equivalent to the polynomial features we considered earlier. But we can compute it via

$$\theta \cdot \phi(x) = \sum_j \alpha^j y^j K_2(x^j, x).$$

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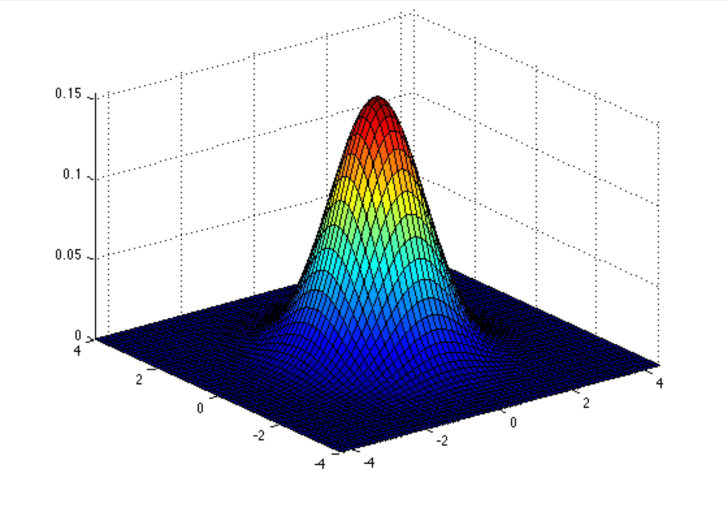
$$K_m(x, \tilde{x}) = (1 + x \cdot \tilde{x})^m \qquad \text{degree-}m \text{ polynomial kernel}$$

$$K_{rbf}(x, \tilde{x}) = \exp\left(-\gamma \|x - \tilde{x}\|^2\right) \qquad \text{radial basis function kernel}$$

Kernels

Gaussian radial basis function kernel (for fixed $\tilde{x} \in \mathbb{R}^2$)



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It turns out we can, but ϕ is infinite-dimensional.

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- Large values: rough decision boundary (only nearby points).

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- Large values: rough decision boundary (only nearby points).
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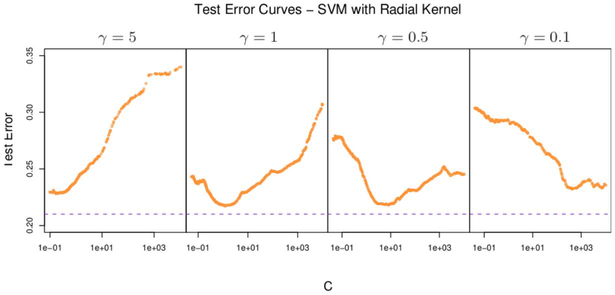

FIGURE 12.6. *Test-error curves as a function of the cost parameter C for the radial-kernel SVM classifier on the mixture data. At the top of each plot is the scale parameter γ for the radial kernel: $K_\gamma(x, y) = \exp -\gamma||x - y||^2$. The optimal value for C depends quite strongly on the scale of the kernel. The Bayes error rate is indicated by the broken horizontal lines.*

Kernels

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- Often this representation is considerably easier to compute. For example, the degree m polynomial kernel on $\mathbb{R}^d$ is an inner product involving $\binom{m+d}{m}$ features.

Outline

- Recall: linear classifiers, perceptron algorithm
- Support vector machines
- Features
- Features and overfitting
- Role of the regularization parameter C
- Regularization and overfitting
- Kernels