Support Vector Machines and Kernel Methods

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Overview

Why do people care about SVMs?

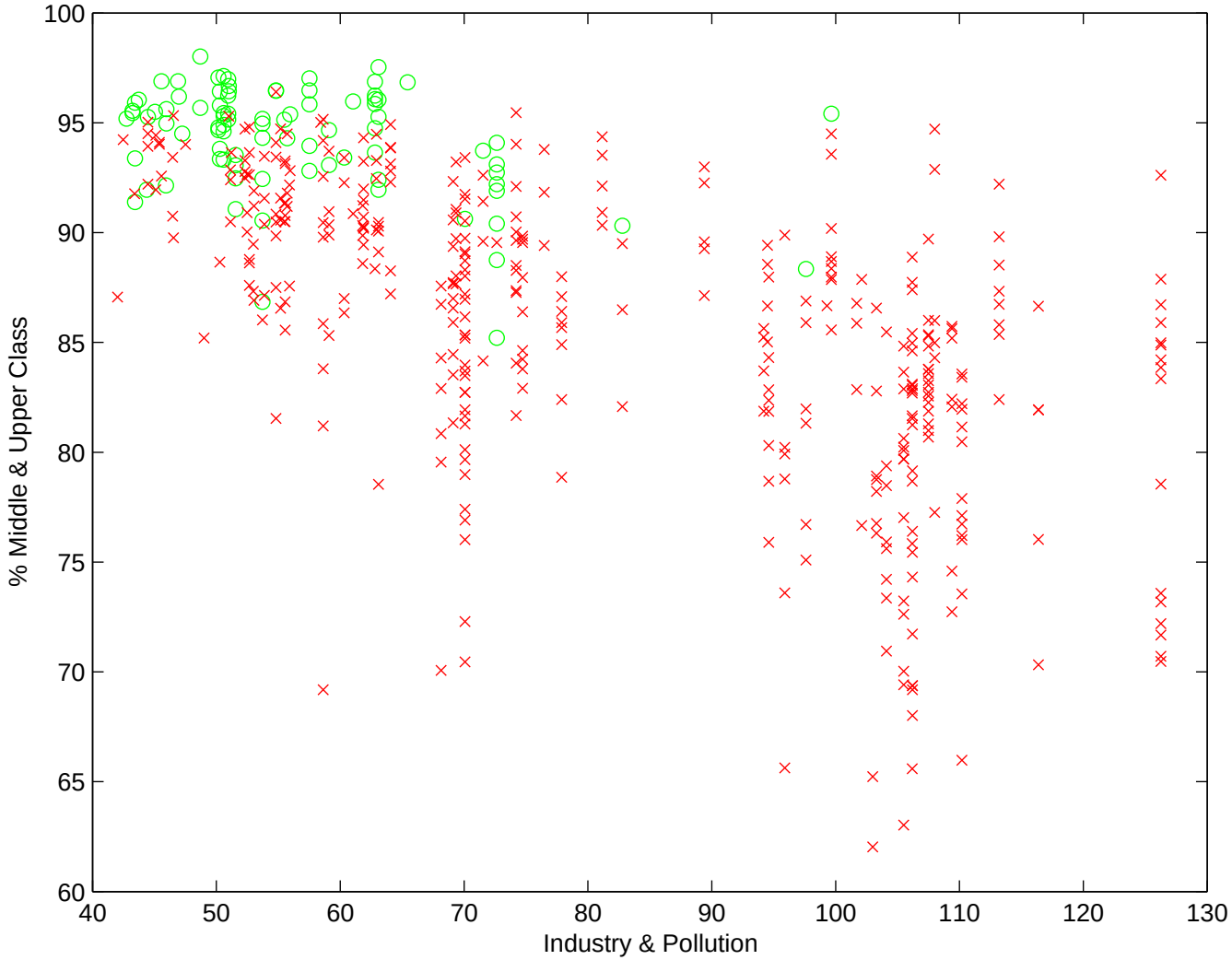
- Classification problems
- SVMs often produce good results over a wide range of problems
- SVMs can be easy to use

What are SVMs?

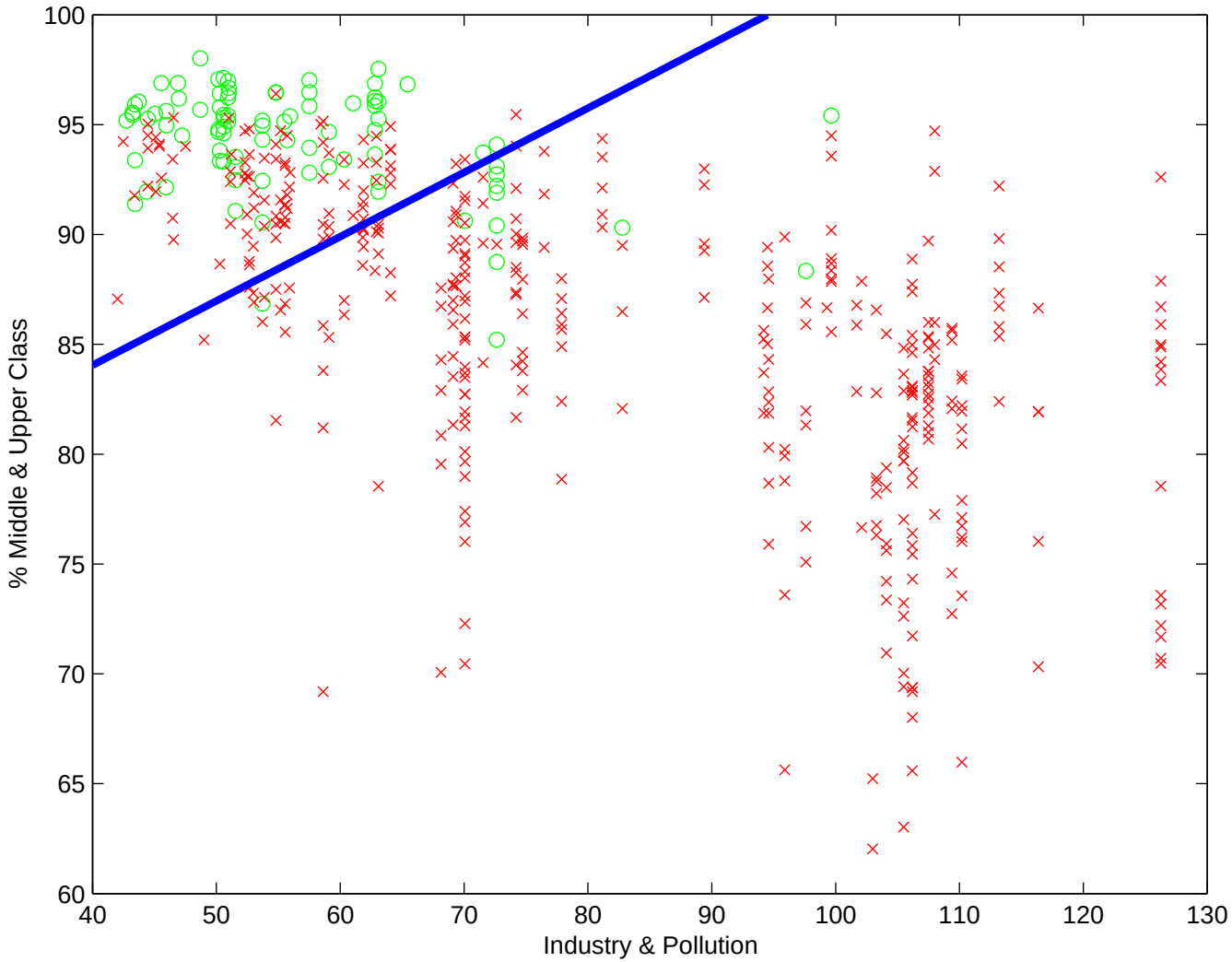
- Perceptrons
- Margins
- Feature expansion
- The “kernel trick”

Summary

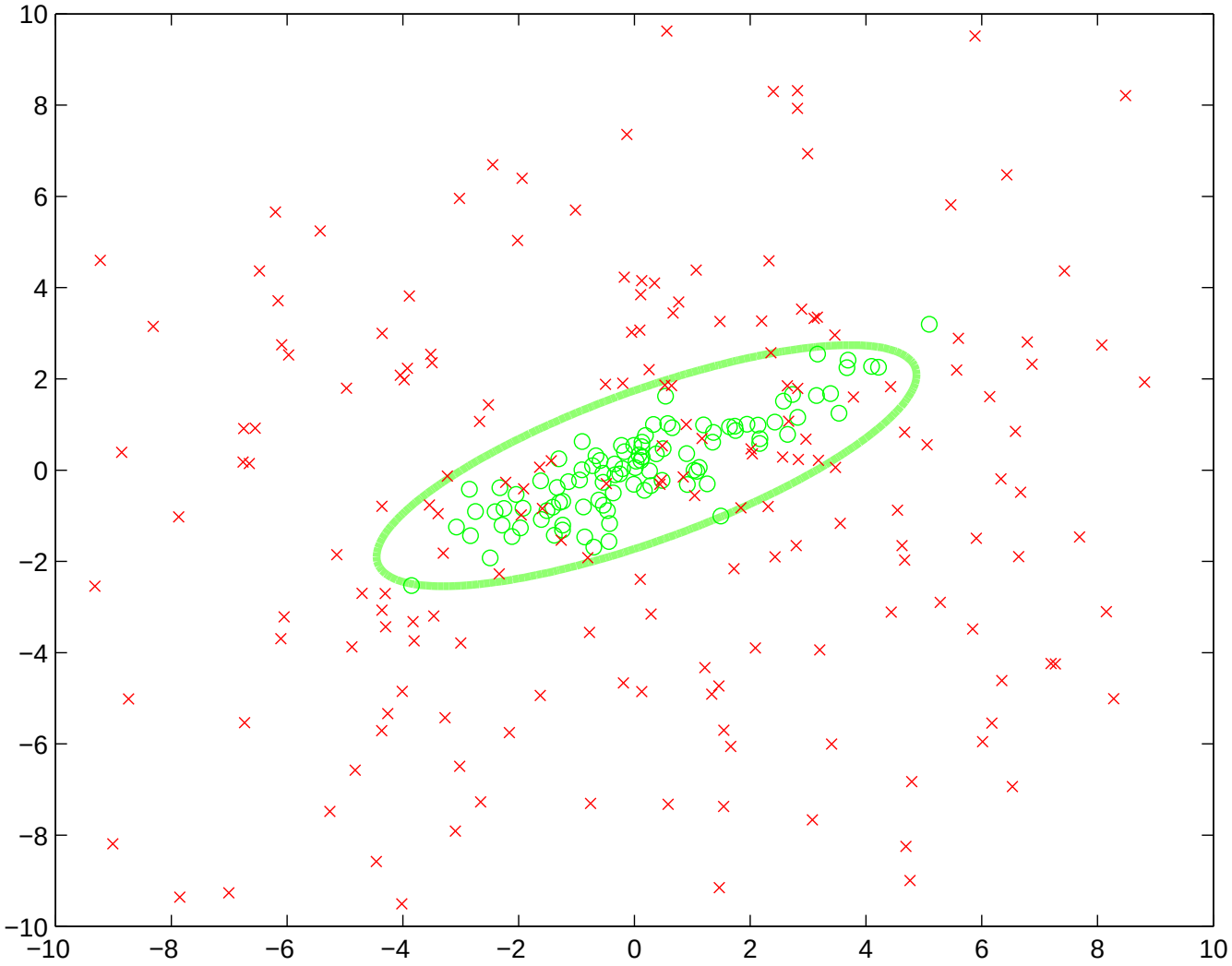
Example—Boston housing data



A good linear classifier



Sometimes a nonlinear classifier is better



Getting fancy

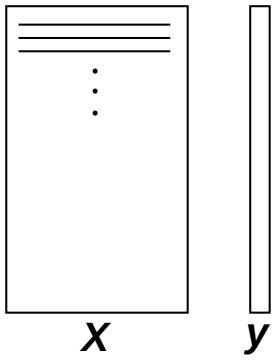
More features (tax level, units per building)

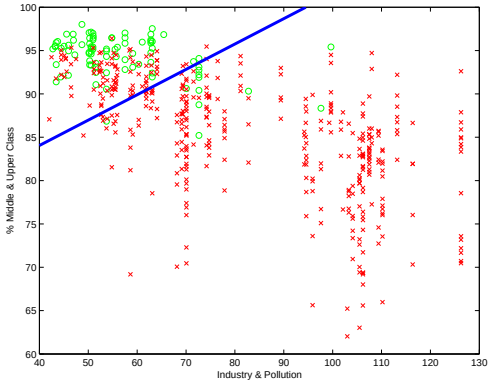
Lots more features (sine of tax level, hyperbolic tangent of sum of income and units)

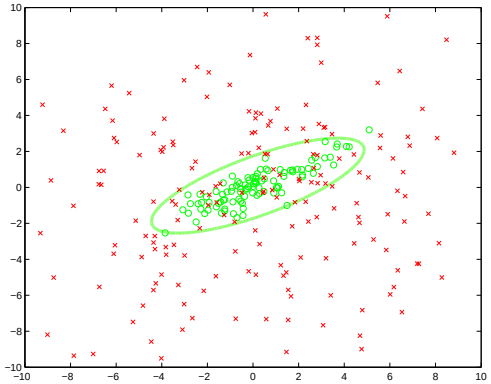
Text? Hyperlinks? Relational database records?

- difficult to featurize w/ reasonable number of features
- but what if we could handle large or infinite feature sets?

Classification problem







Data points $X = [\mathbf{x}_1; \mathbf{x}_2; \mathbf{x}_3; \ldots]$ with $\mathbf{x}_i \in \mathbb{R}^n$

Labels $\mathbf{y} = [y_1; y_2; y_3; \ldots]$ with $y_i \in \{-1, 1\}$

Solution is a subset of $\mathbb{R}^n$, the “classifier”

Often represented as a test $f(\mathbf{x}, \text{learnable parameters}) \geq 0$

Define: decision surface, linear separator, linearly separable

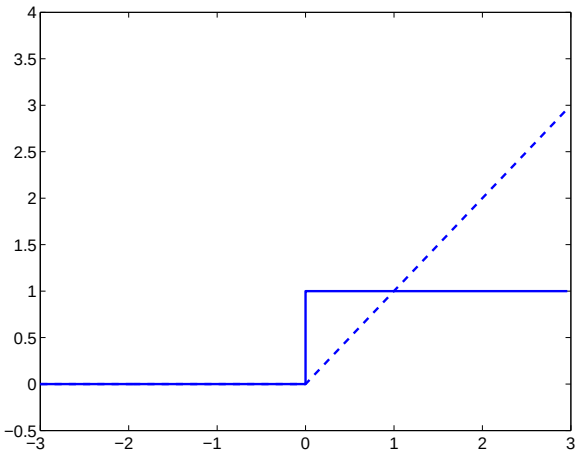
What is goal?

Classify new data with fewest possible mistakes

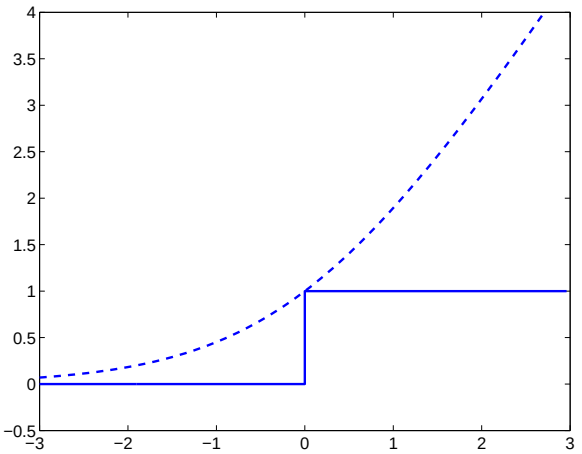
Proxy: minimize some function on training data

$$\min_{\mathbf{w}} \sum_i l(y_i f(\mathbf{x}_i; \mathbf{w})) + l_0(\mathbf{w})$$

That's $l(f(\mathbf{x}))$ for +ve examples, $l(-f(x))$ for -ve

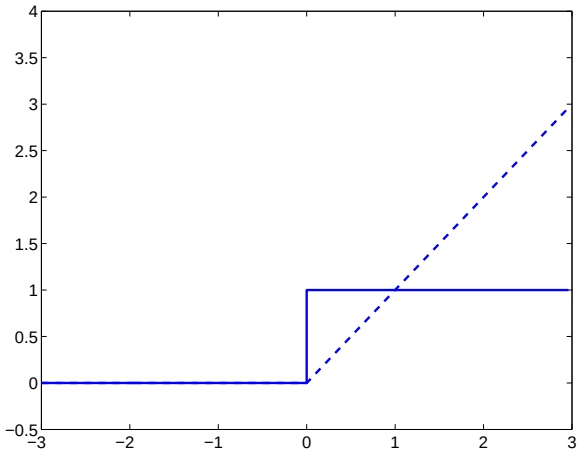


piecewise linear loss



logistic loss

Perceptrons



Weight vector $\mathbf{w}$, bias c

Classification rule: sign$(f(\mathbf{x}))$ where $f(\mathbf{x}) = \mathbf{x} \cdot \mathbf{w} + c$

Penalty for mispredicting: $l(yf(\mathbf{x})) = [yf(\mathbf{x})]_-$

This penalty is convex in $\mathbf{w}$, so all minima are global

Note: unit-length $\mathbf{x}$ vectors

Training perceptrons

Perceptron learning rule: on mistake,

$$\begin{aligned} \mathbf{w} &\texttt{ += } y\mathbf{x} \\ c &\texttt{ += } y \end{aligned}$$

That is, gradient descent on $l(yf(\mathbf{x}))$, since

$$\nabla_w \, [y(\mathbf{x} \cdot \mathbf{w} + c)]_- = \begin{cases} -y\mathbf{x} & \text{if } y(\mathbf{x} \cdot \mathbf{w} + c) < 0 \\ 0 & \text{otherwise} \end{cases}$$

Training perceptrons, cont'd

Solve linear inequalities (for separable case):

$$y(\mathbf{x} \cdot \mathbf{w} + c) \geq 0$$

That's

$\mathbf{x} \cdot \mathbf{w} + c \geq 0$	for positive examples
$\mathbf{x} \cdot \mathbf{w} + c \leq 0$	for negative examples

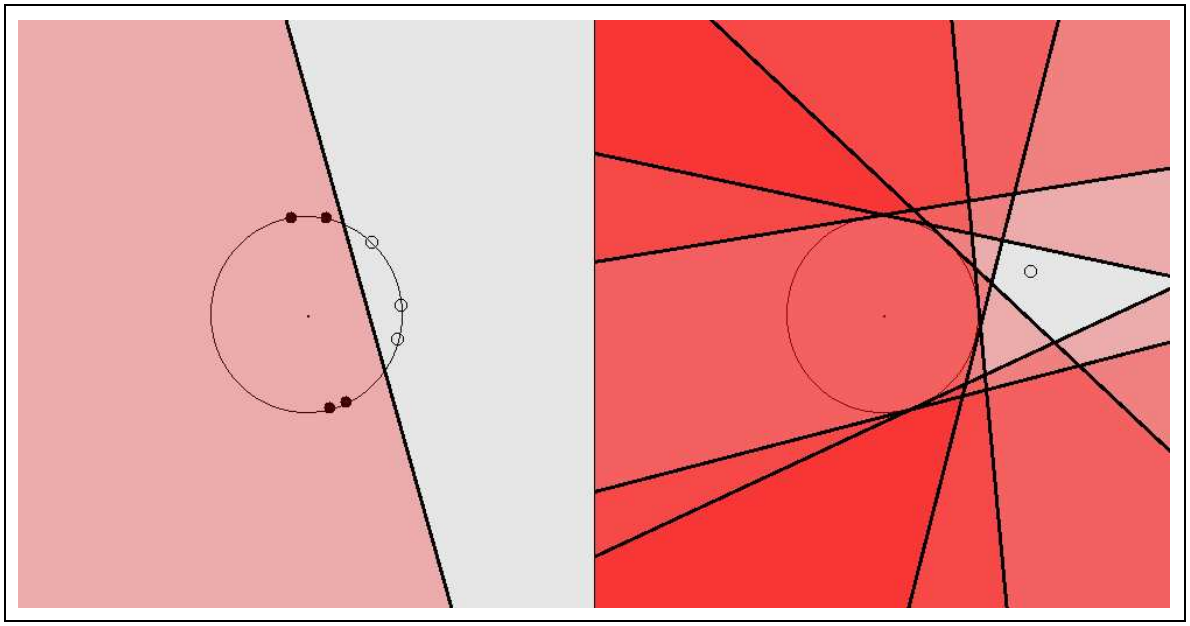
i.e., ensure correct classification of training examples

Linear program (for general case):

$$\min_{\mathbf{s} \geq 0, \mathbf{w}, c} \sum_i s_i \text{ subject to}$$

$$(y_i \mathbf{x}_i) \cdot \mathbf{w} + y_i c + s_i \geq 0$$

Version space



$$\mathbf{x} \cdot \mathbf{w} + c = 0$$

As a fn of $\mathbf{x}$: hyperplane w/ normal $\mathbf{w}$ at distance $c/||\mathbf{w}||$ from origin

As a fn of $\mathbf{w}$: hyperplane w/ normal $\mathbf{x}$ at distance $c/||\mathbf{x}||$ from origin

Problems with perceptrons

Slow learning (data inefficient)

Vulnerable to overfitting (especially when many input features)

Not very expressive (XOR)

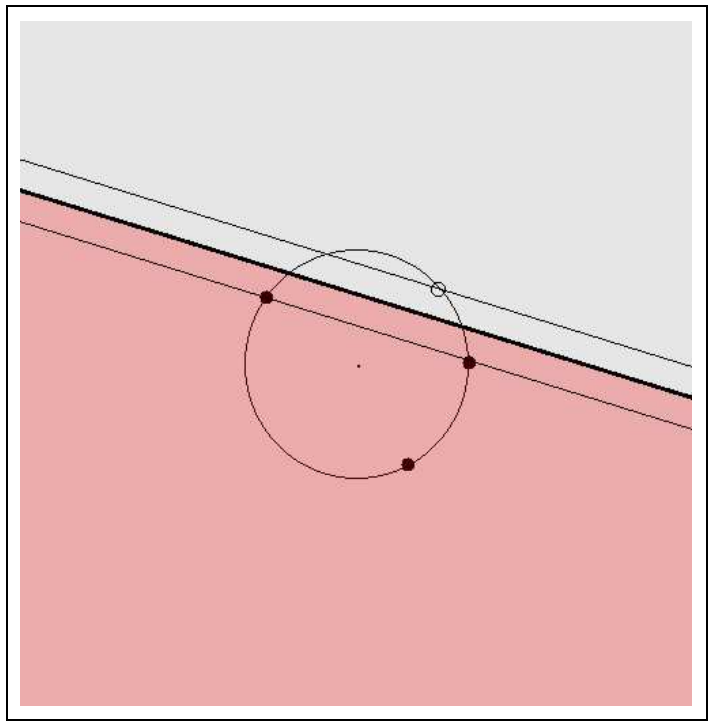
Modernizing the perceptron

Three extensions:

- Margins
- Feature expansion
- Kernel trick

Result is called a Support Vector Machine (reason given below)

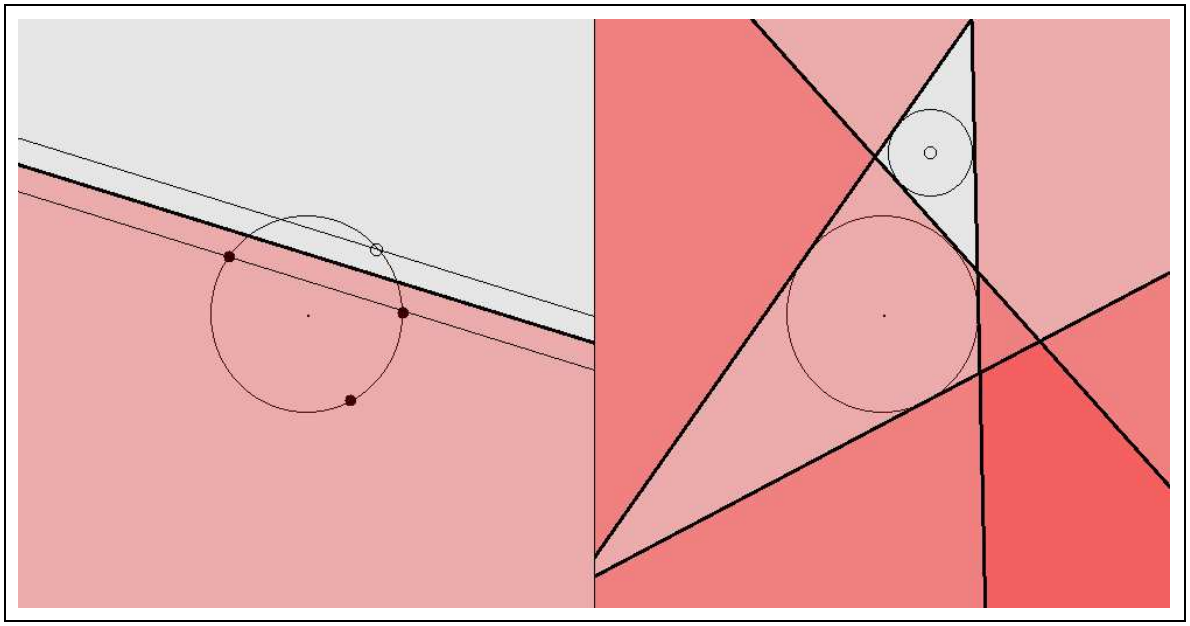
Margins



Margin is the signed $\perp$ distance from an example to the decision boundary

+ve margin points are correctly classified, -ve margin means error

SVMs are maximum margin



Maximize minimum distance from data to separator

“Ball center” of version space (caveats)

Other centers: analytic center, center of mass, Bayes point

Note: if not linearly separable, must trade margin vs. errors

Why do margins help?

If our hypothesis is near the boundary of decision space, we don’t necessarily learn much from our mistakes

If we’re far away from any boundary, a mistake has to eliminate a large volume from version space

Why margins help, explanation 2

Occam's razor: "simple" classifiers are likely to do better in practice

Why? There are fewer simple classifiers than complicated ones, so we are less likely to be able to fool ourselves by finding a really good fit by accident.

What does "simple" mean? Anything, as long as you tell me before you see the data.

Explanation 2 cont'd

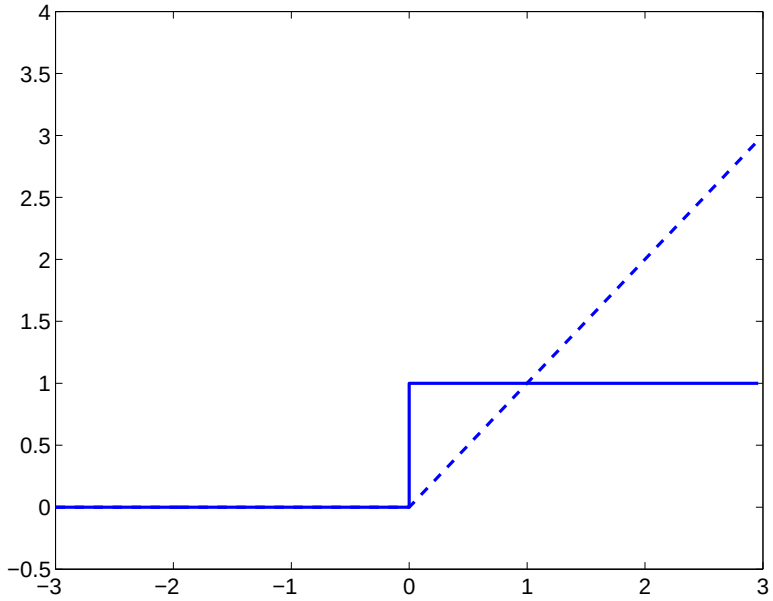
"Simple" can mean:

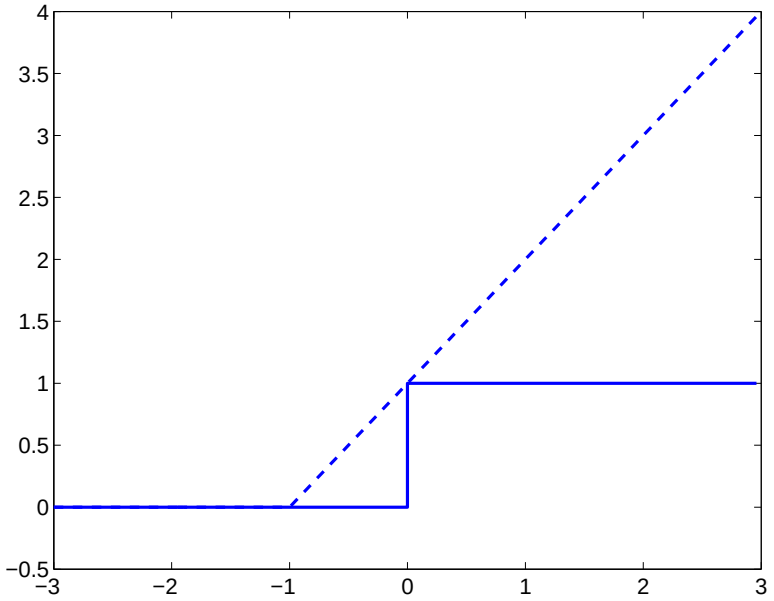
- Low-dimensional
- Large margin
- Short description length

For this lecture we are interested in large margins and compact descriptions

By contrast, many classical complexity control methods (AIC, BIC) rely on low dimensionality alone

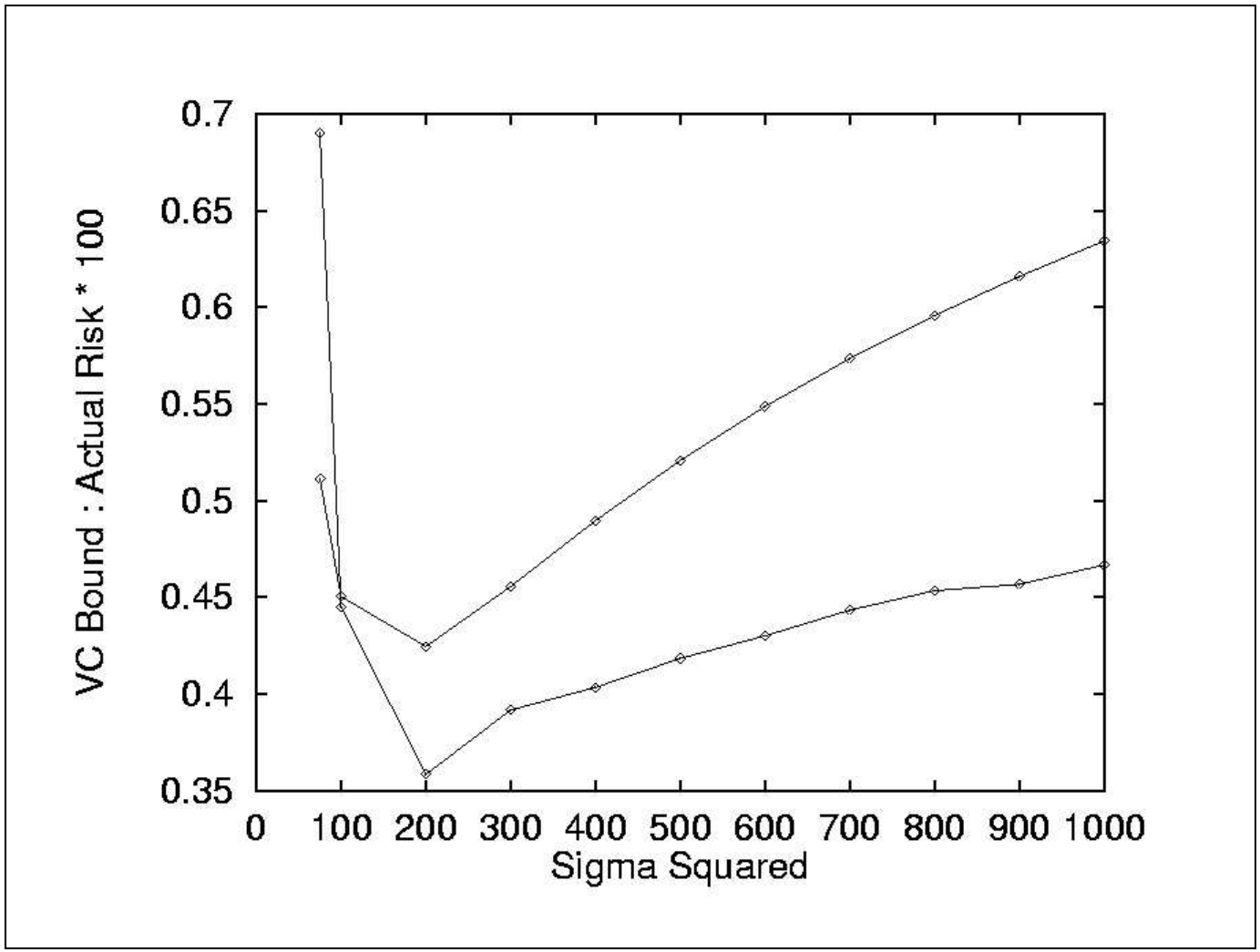
Why margins help, explanation 3





Margin loss is an upper bound on number of mistakes

Why margins help, explanation 4



Optimizing the margin

Most common method: convex quadratic program

Efficient algorithms exist (essentially the same as some interior point LP algorithms)

Because QP is strictly* convex, *unique* global optimum

Next few slides derive the QP. Notation:

- Assume w.l.o.g. $\|\mathbf{x}_i\|_2 = 1$
- Ignore slack variables for now (i.e., assume linearly separable)

*if you ignore the intercept term

Optimizing the margin, cont'd

Margin M is $\perp$ distance to decision surface:

$$\begin{aligned} y((\mathbf{x} - M\mathbf{w}/\|\mathbf{w}\|) \cdot \mathbf{w} + c) &= 0 \\ y(\mathbf{x} \cdot \mathbf{w} + c) &= M\mathbf{w} \cdot \mathbf{w}/\|\mathbf{w}\| = M\|\mathbf{w}\| \end{aligned}$$

SVM maximizes $M > 0$ such that all margins are $\geq M$:

$\max_{M>0,\mathbf{w},c} \; M$ subject to
$(y_i\mathbf{x}_i) \cdot \mathbf{w} + y_i c \geq M\|\mathbf{w}\|$

Notation: $\mathbf{z}_i = y_i\mathbf{x}_i$ and $Z = [\mathbf{z}_1; \mathbf{z}_2; \ldots]$, so that:

$$Z\mathbf{w} + \mathbf{y}c \geq M\|\mathbf{w}\|$$

Note $\lambda w, \lambda c$ is a solution if w, c is

Optimizing the margin, cont'd

Divide by $M\|\mathbf{w}\|$ to get $(Z\mathbf{w} + \mathbf{y}c)/M\|\mathbf{w}\| \geq 1$

Define $\mathbf{v} = \frac{\mathbf{w}}{M\|\mathbf{w}\|}$ and $d = \frac{c}{M\|\mathbf{w}\|}$, so that $\|\mathbf{v}\| = \frac{\|\mathbf{w}\|}{M\|\mathbf{w}\|} = \frac{1}{M}$

$\max_{\mathbf{v},d}\ 1/\|\mathbf{v}\|$ subject to
$Z\mathbf{v} + \mathbf{y}d \geq 1$

Maximizing $1/\|\mathbf{v}\|$ is minimizing $\|\mathbf{v}\|$ is minimizing $\|\mathbf{v}\|^2$

$\min_{\mathbf{v},d}\ \|\mathbf{v}\|^2$ subject to
$Z\mathbf{v} + \mathbf{y}d \geq 1$

Add slack variables to handle non-separable case:

$\min_{\mathbf{s}\geq 0,\mathbf{v},d}\ \|\mathbf{v}\|^2 + C\sum_i s_i$ subject to
$Z\mathbf{v} + \mathbf{y}d + \mathbf{s} \geq 1$

Feature expansion

Given an example $\mathbf{x} = [a\ b\ ...]$

Could add new features like a^2, ab, a^7b^3, $\sin(b)$, ...

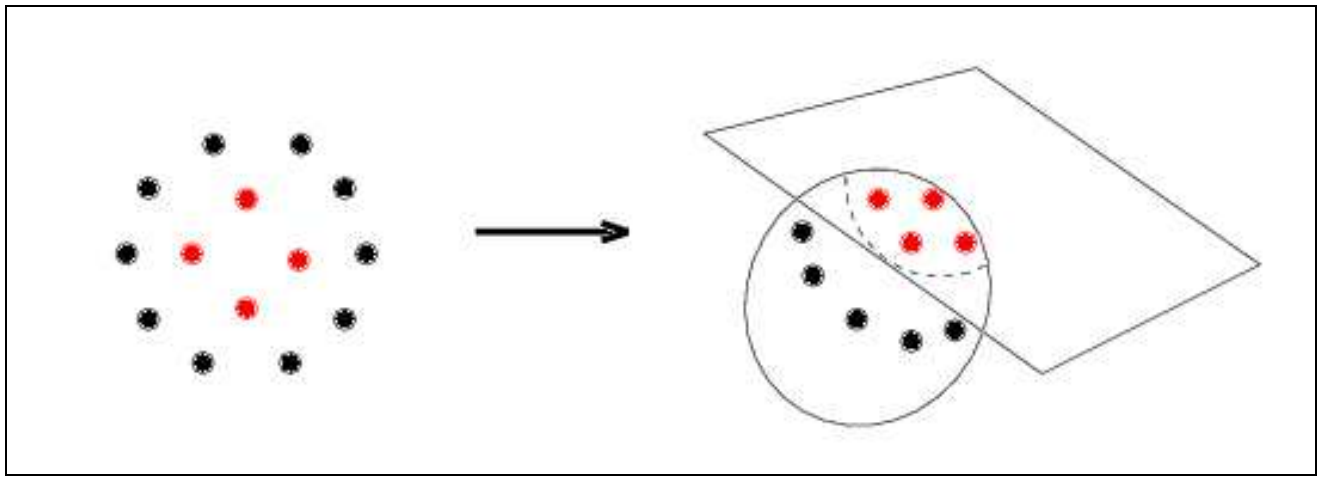
Same optimization as before, but with longer $\mathbf{x}$ vectors and so longer $\mathbf{w}$ vector

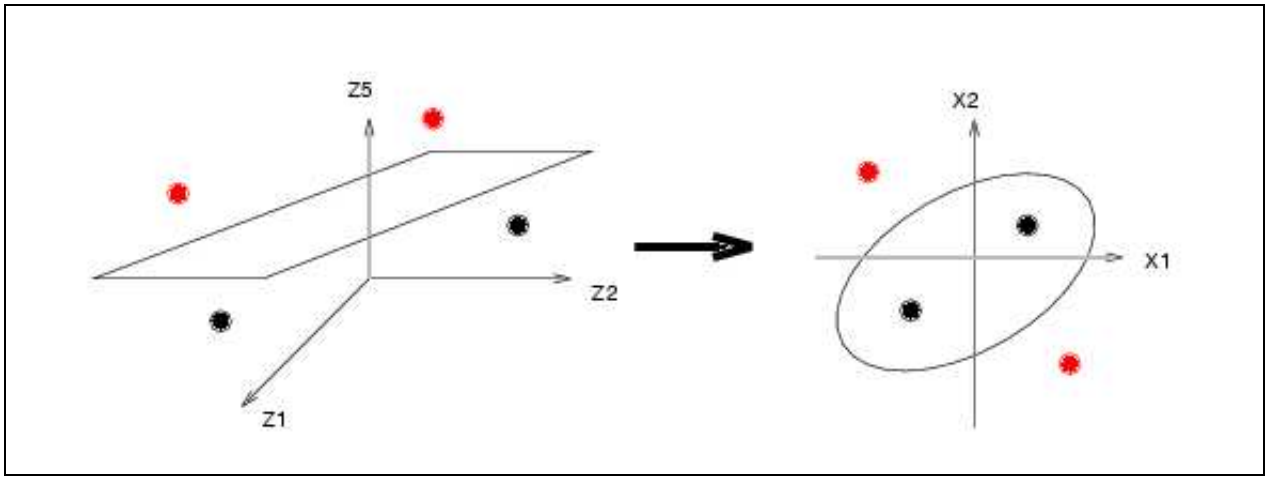
Classifier: "is $3a + 2b + a^2 + 3ab - a^7b^3 + 4\sin(b) \geq 2.6$?"

This classifier is nonlinear in original features, but linear in expanded feature space

We have replaced $\mathbf{x}$ by $\phi(\mathbf{x})$ for some nonlinear ϕ, so decision boundary is nonlinear surface $\mathbf{w} \cdot \phi(\mathbf{x}) + c = 0$

Feature expansion example





Some popular feature sets

Polynomials of degree k

$$1, a, a^2, b, b^2, ab$$

Neural nets (sigmoids)

$$\tanh(3a + 2b - 1), \tanh(5a - 4), \ldots$$

RBFs of radius σ

$$\exp\left(-\frac{1}{\sigma^2}((a - a_0)^2 + (b - b_0)^2)\right)$$

Feature expansion problems

Feature expansion techniques yield *lots* of features

E.g. polynomial of degree k on n original features yields $O(n^k)$ expanded features

E.g. RBFs yield infinitely many expanded features!

Inefficient (`for i = 1 to infinity do ...`)

Overfitting (VC-dimension argument)

How to fix feature expansion

We have already shown we can handle the overfitting problem: even if we have lots of parameters, large margins make simple classifiers

“All” that’s left is efficiency

Lagrange multipliers, then kernel trick

Lagrange Multipliers

Way to phrase constrained optimization problem as a game

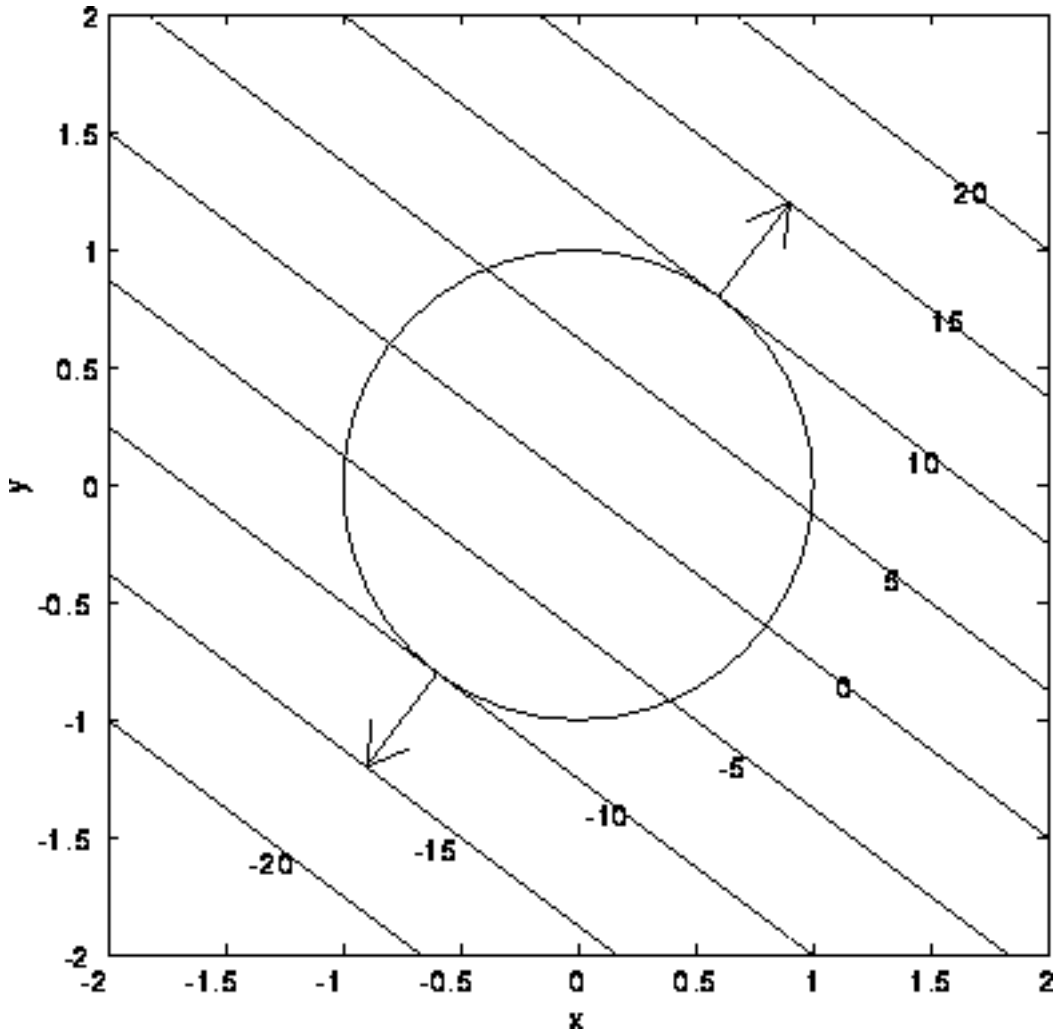
$\max_{\mathbf{x}} f(\mathbf{x})$ subject to $g(\mathbf{x}) \geq 0$

$\max_{\mathbf{x}} \min_{a \geq 0} \quad f(\mathbf{x}) + a g(\mathbf{x})$

If $\mathbf{x}$ plays $g(\mathbf{x}) < 0$, then a wins: playing big numbers makes payoff approach $-\infty$

If $\mathbf{x}$ plays $g(\mathbf{x}) \geq 0$, then a must play 0

Lagrange Multipliers: the picture



Lagrange Multipliers: the caption

Problem: maximize

$$f(x, y) = 6x + 8y$$

subject to

$$g(x, y) = x^2 + y^2 - 1 \geq 0$$

Using a Lagrange multiplier a,

$$\max_{xy} \min_{a \geq 0} \; f(x, y) + a g(x, y)$$

At optimum,

$$0 = \nabla f(x, y) + a \nabla g(x, y) = \begin{pmatrix} 6 \\ 8 \end{pmatrix} + 2a \begin{pmatrix} x \\ y \end{pmatrix}$$

Kernel trick

Way to make optimization efficient when there are lots of features

Compute one Lagrange multiplier per training example instead of one weight per feature (part I)

Use kernel function to avoid representing w ever (part II)

Will mean we can handle infinitely many features!

Kernel trick, part I

$\min_{\mathbf{w},c} \quad |\mathbf{w}|^2/2 \quad$ subject to $\quad Z\mathbf{w} + \mathbf{y}c \geq 1$

$\min_{\mathbf{w},c} \max_{\mathbf{a} \geq 0} \quad \mathbf{w}^\mathsf{T}\mathbf{w}/2 + \mathbf{a} \cdot (1 - Z\mathbf{w} - \mathbf{y}c)$

Minimize wrt $\mathbf{w}, c$ by setting derivatives to 0

$0 = \mathbf{w} - Z^\mathsf{T}\mathbf{a} \qquad 0 = \mathbf{a} \cdot \mathbf{y}$

Substitute back in for $\mathbf{w}, c$

$\max_{\mathbf{a} \geq 0} \quad \mathbf{a} \cdot 1 - \mathbf{a}^\mathsf{T} Z Z^\mathsf{T} \mathbf{a}/2 \quad$ subject to $\quad \mathbf{a} \cdot \mathbf{y} = 0$

Note: to allow slacks, add an upper bound $\mathbf{a} \leq C$

What did we just do?

$\max_{0 \le \mathbf{a} \le C} \quad \mathbf{a} \cdot 1 - \mathbf{a}^\mathsf{T} Z Z^\mathsf{T} \mathbf{a}/2 \quad$ subject to $\quad \mathbf{a} \cdot \mathbf{y} = 0$

Now we have a QP in $\mathbf{a}$ instead of $\mathbf{w}, c$

Once we solve for $\mathbf{a}$, we can find $\mathbf{w} = Z^\mathsf{T} \mathbf{a}$ to use for classification

We also need c which we can get from complementarity:

$$y_i \mathbf{x}_i \cdot \mathbf{w} + y_i c = 1 \qquad \Leftrightarrow \qquad a_i > 0$$

or as dual variable for $\mathbf{a} \cdot \mathbf{y} = 0$

Representer theorem

Optimal $\mathbf{w} = Z^\top \mathbf{a}$ is a linear combination of rows of Z

I.e., $\mathbf{w}$ is a linear combination of (signed) training examples

I.e., $\mathbf{w}$ has a finite representation even if there are infinitely many features

Surprising and useful fact; consequence of the Representer Theorem

Support vectors

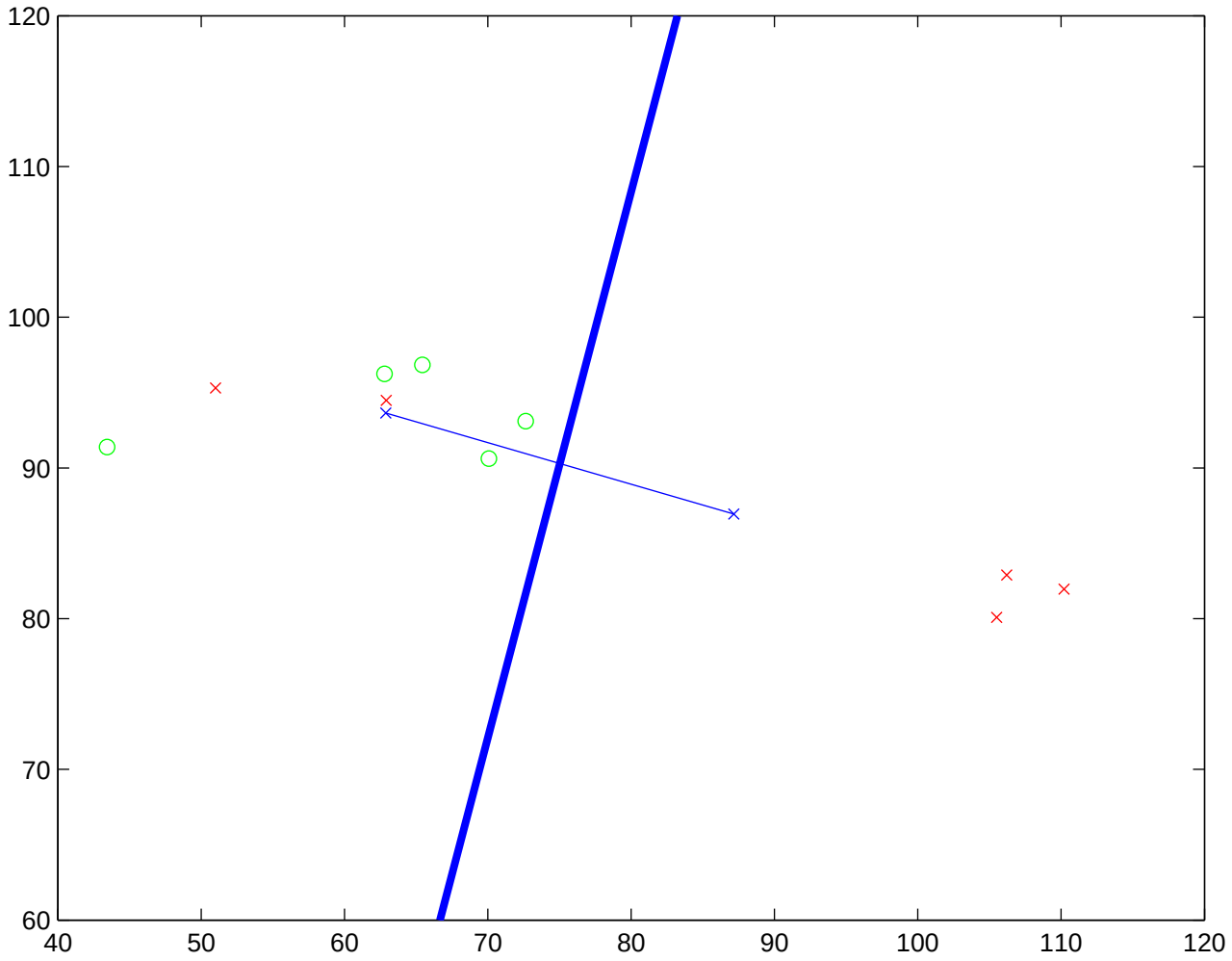
Examples with $a_i > 0$ are called support vectors

"Support vector machine" = learning algorithm ("machine") based on support vectors

Often many fewer than number of training examples ($\mathbf{a}$ is sparse)

This is the "short description" of an SVM mentioned above

Intuition for support vectors



Partway through optimization

Suppose we have 5 positive support vectors and 5 negative, all with equal weights

Best $\mathbf{w}$ so far is $Z^\top \mathbf{a}$: diff between mean of +ve SVs, mean of -ve

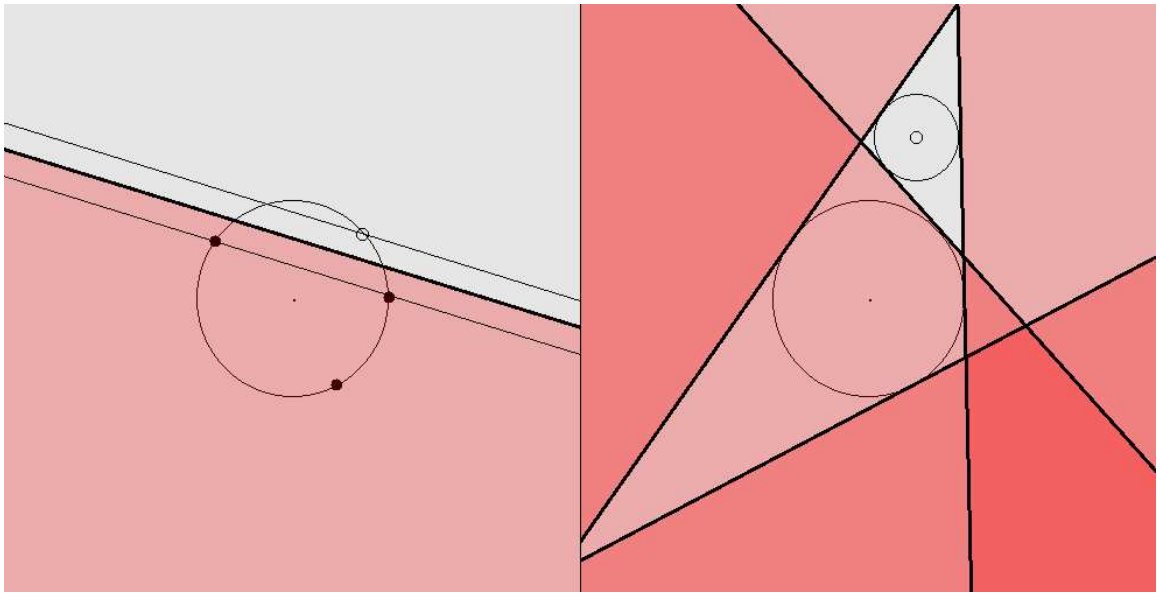
Averaging $\mathbf{x}_i \cdot \mathbf{w} + c = y_i$ for all SVs yields

$$c = -\bar{\mathbf{x}} \cdot \mathbf{w}$$

That is,

- Compute mean of +ve SVs, mean of -ve SVs
- Draw the line between means, and its perpendicular bisector
- This bisector is current classifier

At end of optimization



Gradient wrt a_i is $1 - y_i(\mathbf{x}_i \cdot \mathbf{w} + c)$

Increase a_i if (scaled) margin < 1, decrease if margin > 1

Stable iff ($a_i = 0$ AND margin ≥ 1) OR margin $= 1$

How to avoid writing down weights

Suppose number of features is really big or even infinite?

Can't write down X, so how do we solve the QP?

Can't even write down $\mathbf{w}$, so how do we classify new examples?

Solving the QP

$\max_{0 \leq \mathbf{a} \leq C} \quad \mathbf{a} \cdot 1 - \mathbf{a}^\mathsf{T} Z Z^\mathsf{T} \mathbf{a}/2 \quad$ subject to $\quad \mathbf{a} \cdot \mathbf{y} = 0$

Write $G = ZZ^\mathsf{T}$ (called Gram matrix)

That is, $G_{ij} = y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$

$\max_{0 \leq \mathbf{a} \leq C} \quad \mathbf{a} \cdot 1 - \mathbf{a}^\mathsf{T} G \mathbf{a}/2 \quad$ subject to $\quad \mathbf{a} \cdot \mathbf{y} = 0$

With m training examples, G is $m \times m$ — (often) small enough for us to solve the QP even if we can't write down X

Can we compute G directly, without computing X?

Kernel trick, part II

Yes, we can compute G directly—sometimes!

Recall that $\mathbf{x}_i$ was the result of applying a nonlinear feature expansion function ϕ to some shorter vector (say $\mathbf{q}_i$)

Define $K(\mathbf{q}_i, \mathbf{q}_j) = \phi(\mathbf{q}_i) \cdot \phi(\mathbf{q}_j)$

Mercer kernels

K is called a (Mercer) kernel function

Satisfies Mercer condition: $K(\mathbf{q}, \mathbf{q}') \geq 0$

Mercer condition for a function K is analogous to nonnegative definiteness for a matrix

In many cases there is a simple expression for K even if there isn't one for ϕ

In fact, it sometimes happens that we know K without knowing ϕ

Example kernels

Polynomial (typical component of ϕ might be $17q_1^2q_2^3q_4$)

$$K(\mathbf{q}, \mathbf{q}') = (1 + \mathbf{q} \cdot \mathbf{q}')^k$$

Sigmoid (typical component $\tanh(q_1 + 3q_2)$)

$$K(\mathbf{q}, \mathbf{q}') = \tanh(a\mathbf{q} \cdot \mathbf{q}' + b)$$

Gaussian RBF (typical component $\exp(-\frac{1}{2}(q_1 - 5)^2)$)

$$K(\mathbf{q}, \mathbf{q}') = \exp(-\|\mathbf{q} - \mathbf{q}'\|^2/\sigma^2)$$

Detail: polynomial kernel

Suppose $\mathbf{x} = \begin{pmatrix} 1 \\ \sqrt{2}q \\ q^2 \end{pmatrix}$

Then $\mathbf{x}' \cdot \mathbf{x} = 1 + 2qq' + q^2(q')^2$

From previous slide,

$$K(q, q') = (1 + qq')^2 = 1 + 2qq' + q^2(q')^2$$

Dot product + addition + exponentiation vs. $O(n^k)$ terms

The new decision rule

Recall original decision rule: sign$(\mathbf{x} \cdot \mathbf{w} + c)$

Use representation in terms of support vectors:

$$\text{sign}(\mathbf{x} \cdot Z^{\mathsf{T}} \mathbf{a} + c) = \text{sign}\left(\sum_i \mathbf{x} \cdot \mathbf{x}_i y_i a_i + c\right) = \text{sign}\left(\sum_i K(\mathbf{q}, \mathbf{q}_i) y_i a_i + c\right)$$

Since there are usually not too many support vectors, this is a reasonably fast calculation

Summary of SVM algorithm

Training:

- Compute Gram matrix $G_{ij} = y_i y_j K(\mathbf{q}_i, \mathbf{q}_j)$
- Solve QP to get $\mathbf{a}$
- Compute intercept c by using complementarity or duality

Classification:

- Compute $k_i = K(\mathbf{q}, \mathbf{q}_i)$ for support vectors $\mathbf{q}_i$
- Compute $f = c + \sum_i a_i k_i y_i$
- Test sign(f)

Advanced kernels

String kernels

Path kernels

Tree kernels

Graph kernels

String kernels

Pick $\lambda \in (0, 1)$

$\texttt{cat} \mapsto \texttt{c, a, t, } \lambda\ \texttt{ca, } \lambda\ \texttt{at, } \lambda^2\ \texttt{ct, } \lambda^2\ \texttt{cat}$

Strings are similar if they share lots of nearly-contiguous substrings

Works for words in phrases too: “man bites dog” similar to “man bites hot dog,” less similar to “dog bites man”

There is an efficient dynamic-programming algorithm to evaluate this kernel (Lodhi et al, 2002)

Summary

Perceptrons are a simple, popular way to learn a classifier

They suffer from inefficient use of data, overfitting, and lack of expressiveness

SVMs fix these problems using margins and feature expansion

In order to make feature expansion computationally feasible, we need the kernel trick

Kernel trick avoids writing out high-dimensional feature vectors by use of Lagrange multipliers and representer theorem

SVMs are popular classifiers because they usually achieve good error rates and can handle unusual types of data

References

`http://www.cs.cmu.edu/~ggordon/SVMs`
these slides, together with code

`http://svm.research.bell-labs.com/SVMdoc.html`
Burges's SVM tutorial

`http://citeseer.nj.nec.com/burges98tutorial.html`
Burges's paper "A Tutorial on Support Vector Machines for Pattern Recognition" (1998)

References

Huma Lodhi, Craig Saunders, Nello Cristianini, John Shawe-Taylor, Chris Watkins. “Text Classification using String Kernels.” 2002.

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Slides by Stitson & Weston

`http://oregonstate.edu/dept/math/CalculusQuestStudyGuides/vcalc/lagrang/lagrang.html`
Lagrange Multipliers

`http://svm.research.bell-labs.com/SVT/SVMsvt.html`
on-line SVM applet