Support Vector Machine

(and Statistical Learning Theory)

Tutorial

Jason Weston

NEC Labs America

4 Independence Way, Princeton, USA.

jasonw@nec-labs.com

1 Support Vector Machines: history

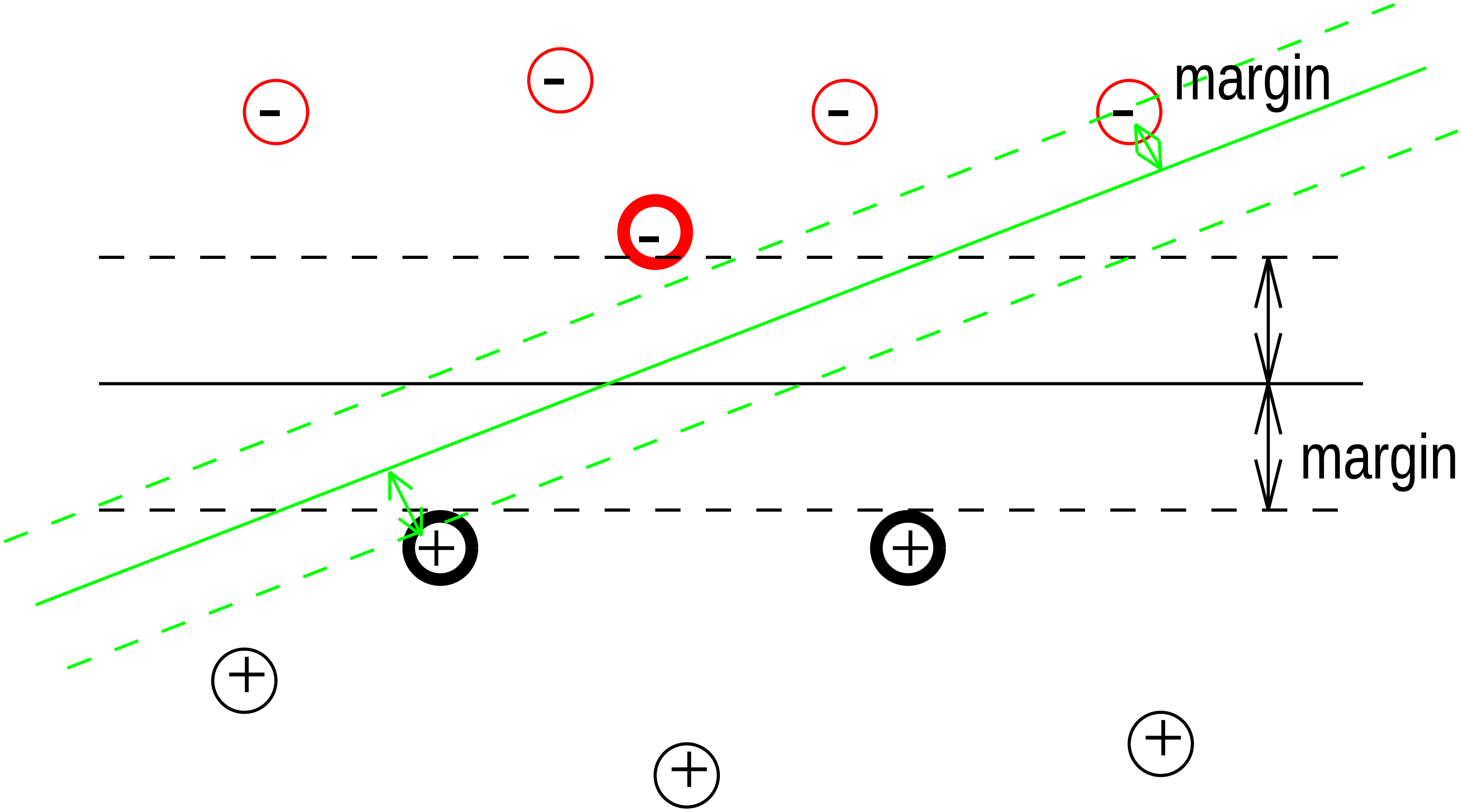
- SVMs introduced in COLT-92 by Boser, Guyon & Vapnik. Became rather popular since.
- Theoretically well motivated algorithm: developed from Statistical Learning Theory (Vapnik & Chervonenkis) since the 60s.
- Empirically good performance: successful applications in many fields (bioinformatics, text, image recognition, . . .)

2 Support Vector Machines: history II

- Centralized website: `www.kernel-machines.org`.
- Several textbooks, e.g. ”An introduction to Support Vector Machines” by Cristianini and Shawe-Taylor is one.
- A large and diverse community work on them: from machine learning, optimization, statistics, neural networks, functional analysis, etc.

3 Support Vector Machines: basics

[Boser, Guyon, Vapnik ’92],[Cortes & Vapnik ’95]



Nice properties: convex, theoretically motivated, nonlinear with kernels..

4 Preliminaries:

- Machine learning is about learning structure from data.
- Although the class of algorithms called ”SVM”s can do more, in this talk we focus on pattern recognition.
- So we want to learn the mapping: $\mathcal{X} \mapsto \mathcal{Y}$, where $x \in \mathcal{X}$ is some object and $y \in \mathcal{Y}$ is a class label.
- Let’s take the simplest case: 2-class classification. So: $x \in R^n$, $y \in \{\pm 1\}$.

5 Example:

Suppose we have 50 photographs of elephants and 50 photos of tigers.

vs.

We digitize them into 100 x 100 pixel images, so we have $x \in R^n$ where $n = 10,000$.

Now, given a new (different) photograph we want to answer the question: **is it an elephant or a tiger?** [we assume it is one or the other.]

6 Training sets and prediction models

- input/output sets $\mathcal{X}$, $\mathcal{Y}$
- training set $(x_1, y_1), \ldots, (x_m, y_m)$
- ”generalization”: given a previously seen $x \in \mathcal{X}$, find a suitable $y \in \mathcal{Y}$.
- i.e., want to learn a classifier: $y = f(x, \alpha)$, where α are the parameters of the function.
- For example, if we are choosing our model from the set of hyperplanes in R^n, then we have:

$$f(x, \{w, b\}) = \text{sign}(w \cdot x + b).$$

7 Empirical Risk and the true Risk

- We can try to learn $f(x,\alpha)$ by choosing a function that performs well on training data:

$$R_{emp}(\alpha) = \frac{1}{m}\sum_{i=1}^{m} \ell(f(x_i,\alpha),y_i) = \text{Training Error}$$

where ℓ is the zero-one *loss function*, $\ell(y,\hat{y}) = 1$, if $y \neq \hat{y}$, and 0 otherwise. R_{emp} is called the *empirical risk*.

- By doing this we are trying to minimize the overall risk:

$$R(\alpha) = \int \ell(f(x,\alpha),y)dP(x,y) = \text{Test Error}$$

where P(x,y) is the (unknown) joint distribution function of x and y.

8 Choosing the set of functions

What about $f(x, \alpha)$ allowing *all* functions from $\mathcal{X}$ to $\{\pm 1\}$?

Training set $(x_1, y_1), \ldots, (x_m, y_m) \in \mathcal{X} \times \{\pm 1\}$

Test set $\bar{x}_1, \ldots, \bar{x}_{\bar{m}} \in \mathcal{X}$,

such that the two sets do not intersect.

For any f there exists f^*:

1. $f^*(x_i) = f(x_i)$ for all i
2. $f^*(x_j) \neq f(x_j)$ for all j

Based on the training data alone, there is no means of choosing which function is better. On the test set however they give different results. So generalization is not guaranteed.

$\Longrightarrow$ a restriction must be placed on the functions that we allow.

9 Empirical Risk and the true Risk

Vapnik & Chervonenkis showed that an upper bound on the true risk can be given by the empirical risk + an additional term:

$$R(\alpha) \leq R_{emp}(\alpha) + \sqrt{\frac{h(log(\frac{2m}{h}+1) - log(\frac{\eta}{4})}{m}}$$

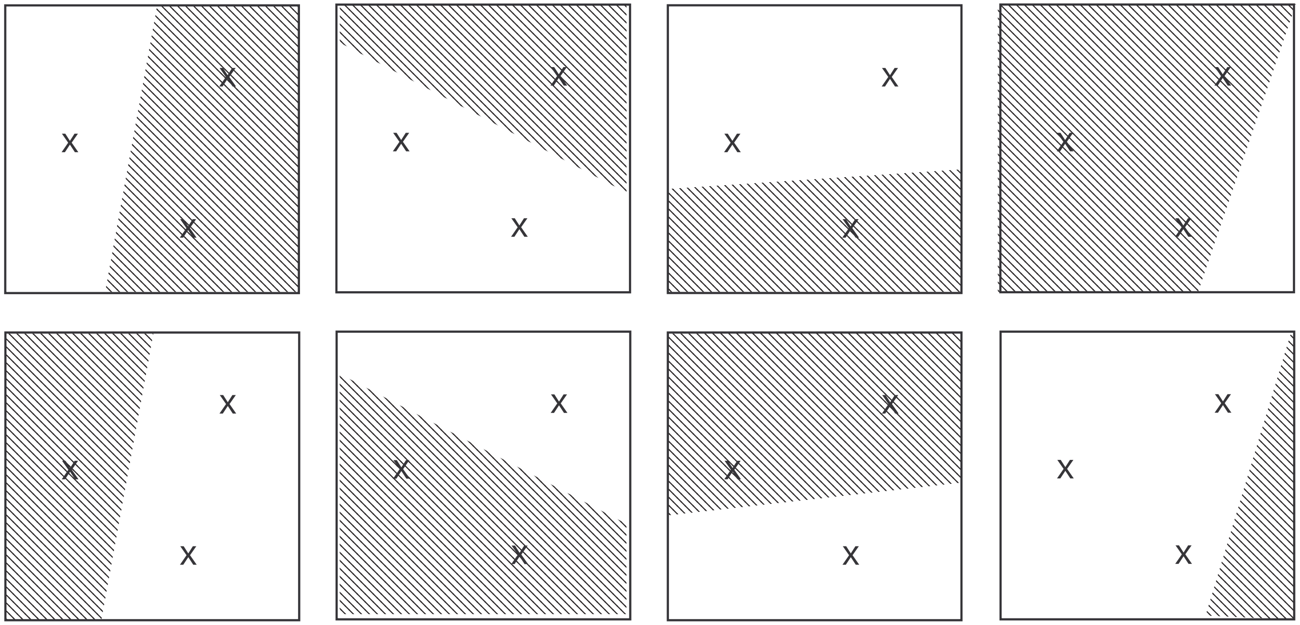
where h is the VC dimension of the set of functions parameterized by α.

- The VC dimension of a set of functions is a measure of their *capacity* or complexity.
- If you can describe a lot of different phenomena with a set of functions then the value of h is large.

[VC dim = the maximum number of points that can be separated in all possible ways by that set of functions.]

10 VC dimension:

The VC dimension of a set of functions is the maximum number of points that can be separated in all possible ways by that set of functions. For hyperplanes in R^n, the VC dimension can be shown to be $n + 1$.



11 VC dimension and capacity of functions

Simplification of bound:

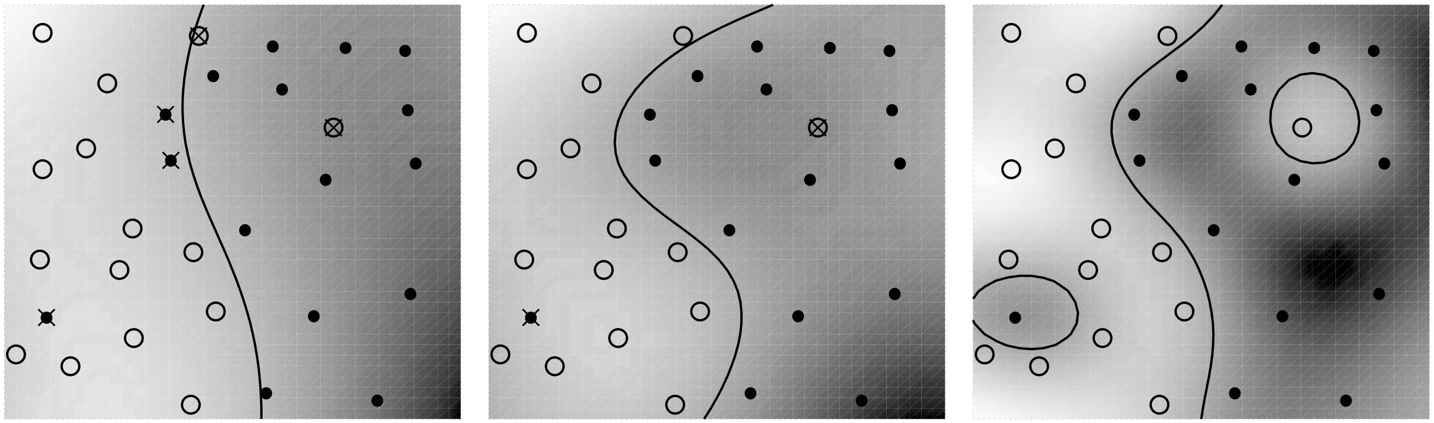
Test Error $\leq$ Training Error + Complexity of set of Models

- Actually, a lot of bounds of this form have been proved (different measures of capacity). The complexity function is often called a regularizer.

- If you take a high capacity set of functions (explain a lot) you get low training error. But you might ”overfit”.

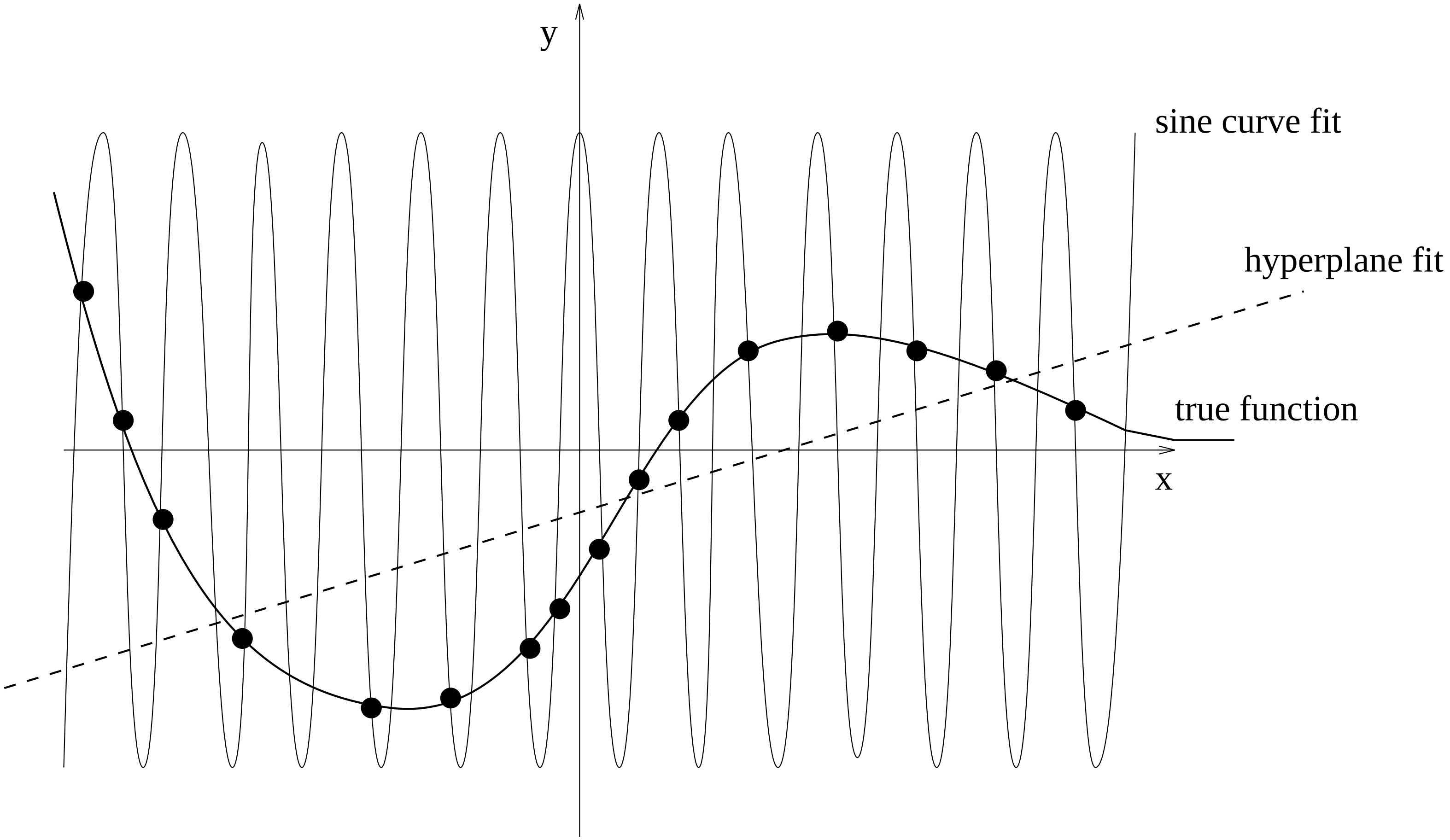
- If you take a very simple set of models, you have low complexity, but won’t get low training error.

12 Capacity of a set of functions *(classification)*

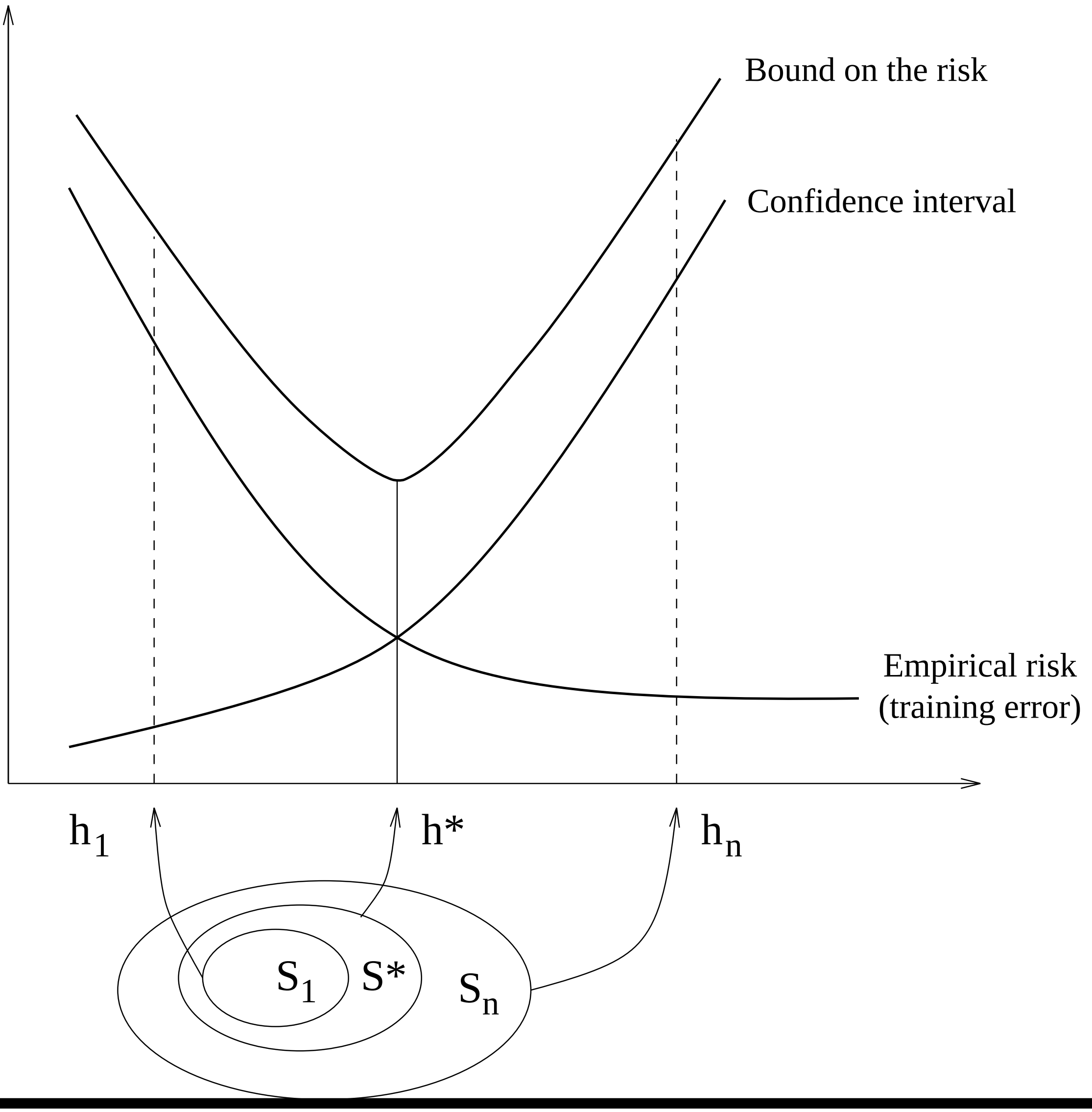


[Images taken from a talk by B. Schoelkopf.]

13 Capacity of a set of functions *(regression)*



14 Controlling the risk: model complexity



15 Capacity of hyperplanes

Vapnik & Chervonenkis also showed the following:

Consider hyperplanes $(w \cdot x) = 0$ *where* w *is normalized w.r.t a set of points* X^* *such that:* $\min_i |w \cdot x_i| = 1$.

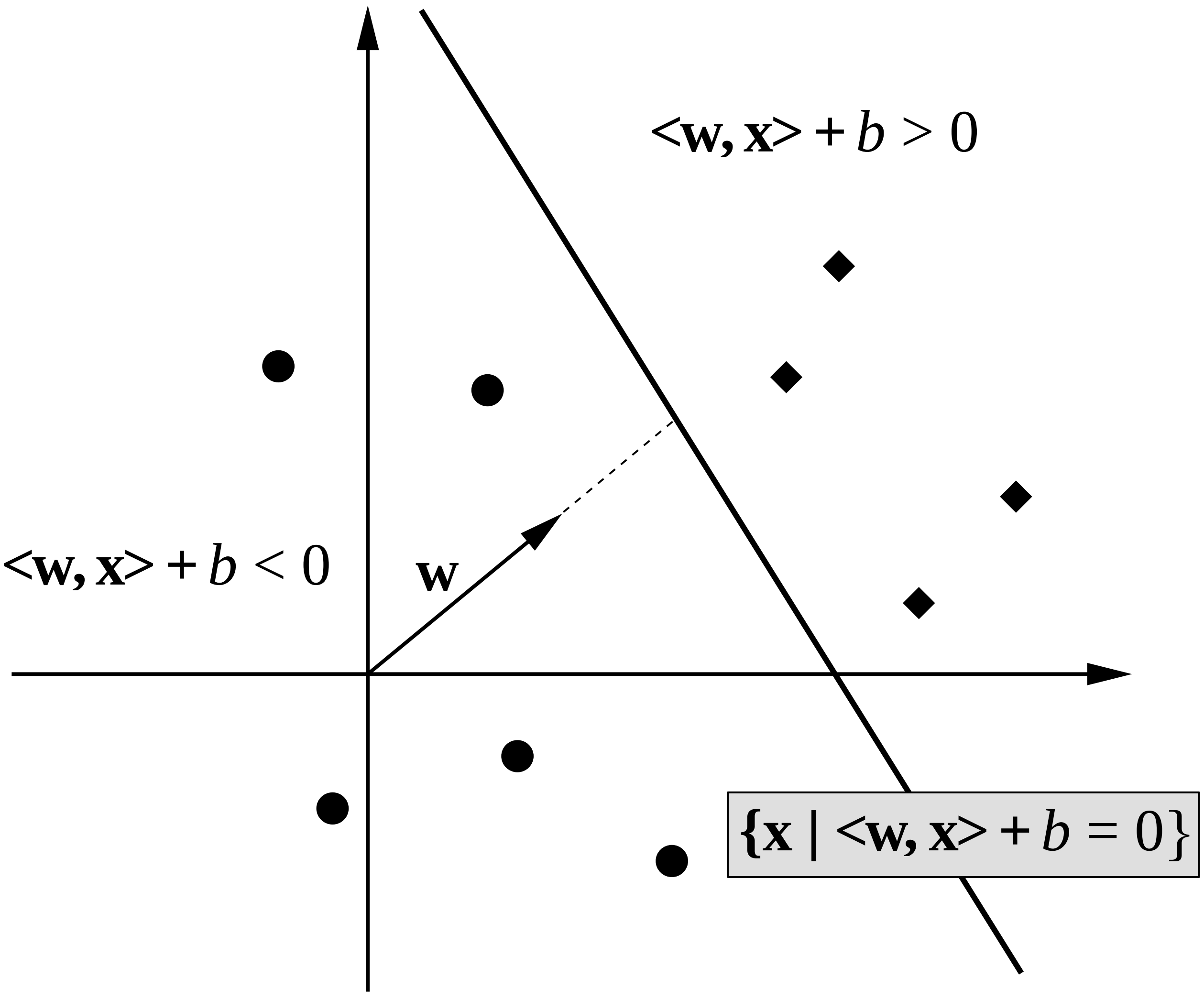
The set of decision functions $f_w(x) =$ *sign*$(w \cdot x)$ *defined on* X^* *such that* $||w|| \leq A$ *has a VC dimension satisfying*

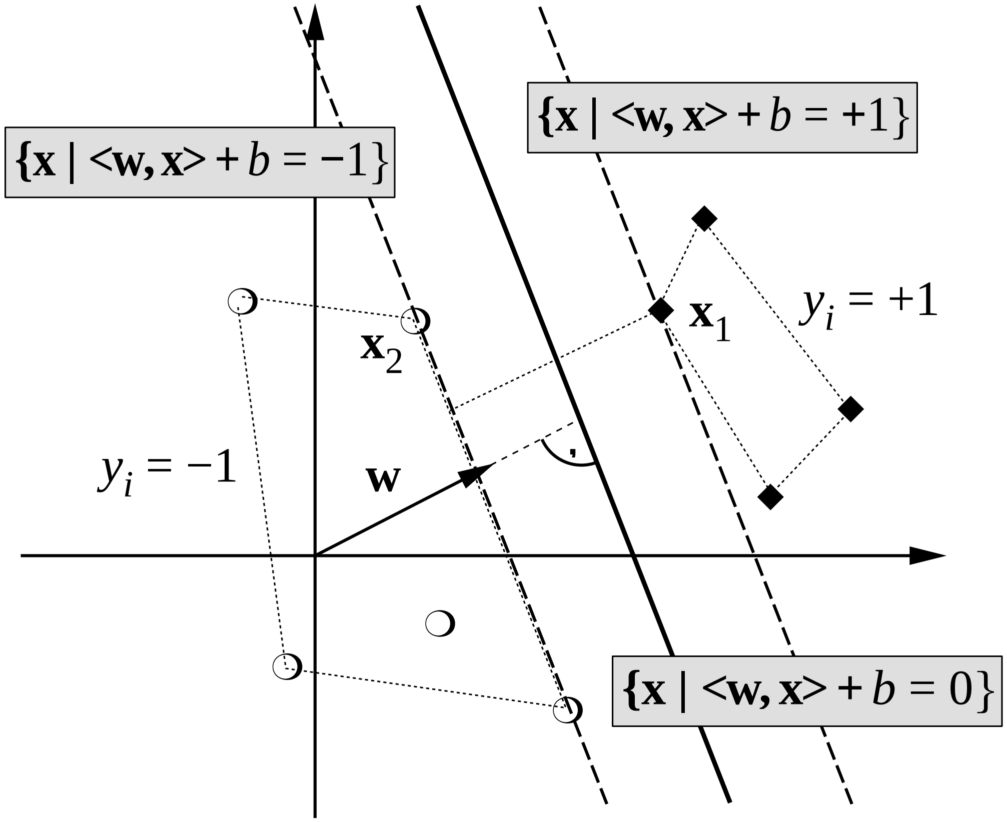
$$h \leq R^2 A^2.$$

where R *is the radius of the smallest sphere around the origin containing* X^*.

$\Longrightarrow$ minimize $||w||^2$ and have low capacity

$\Longrightarrow$ minimizing $||w||^2$ equivalent to obtaining a large margin classifier


$<\mathbf{w},\mathbf{x}> + b > 0$
$<\mathbf{w},\mathbf{x}> + b < 0$
$\mathbf{w}$
$\{\mathbf{x} \mid <\mathbf{w},\mathbf{x}> + b = 0\}$


$\{\mathbf{x} \mid \langle\mathbf{w},\mathbf{x}\rangle + b = -1\}$
$\{\mathbf{x} \mid \langle\mathbf{w},\mathbf{x}\rangle + b = +1\}$
$\mathbf{x}_1$
$y_i = +1$
$\mathbf{x}_2$
$y_i = -1$
$\mathbf{w}$
$\{\mathbf{x} \mid \langle\mathbf{w},\mathbf{x}\rangle + b = 0\}$

Note:

$$\langle\mathbf{w},\mathbf{x}_1\rangle + b = +1$$
$$\langle\mathbf{w},\mathbf{x}_2\rangle + b = -1$$

$$\Rightarrow \quad \langle\mathbf{w},(\mathbf{x}_1 - \mathbf{x}_2)\rangle = 2$$

$$\Rightarrow \quad \left\langle \frac{\mathbf{w}}{\|\mathbf{w}\|}, (\mathbf{x}_1 - \mathbf{x}_2) \right\rangle = \frac{2}{\|\mathbf{w}\|}$$

16 Linear Support Vector Machines (at last!)

So, we would like to find the function which minimizes an objective like:

Training Error + Complexity term

We write that as:

$$\frac{1}{m}\sum_{i=1}^{m}\ell(f(x_i,\alpha),y_i) + \text{Complexity term}$$

For now we will choose the set of hyperplanes (we will extend this later), so $f(x) = (w \cdot x) + b$:

$$\frac{1}{m}\sum_{i=1}^{m}\ell(w \cdot x_i + b, y_i) + ||w||^2$$

subject to $\min_i |w \cdot x_i| = 1$.

17 Linear Support Vector Machines II

That function before was a little difficult to minimize because of the step function in $\ell(y, \hat{y})$ (either 1 or 0).

Let's assume we can separate the data perfectly. Then we can optimize the following:

Minimize $||w||^2$, subject to:

$$(w \cdot x_i + b) \geq 1, \quad \text{if} \quad y_i = 1$$

$$(w \cdot x_i + b) \leq -1, \quad \text{if} \quad y_i = -1$$

The last two constraints can be compacted to:

$$y_i(w \cdot x_i + b) \geq 1$$

This is a quadratic program.

18 SVMs : non-separable case

To deal with the non-separable case, one can rewrite the problem as:

Minimize:

$$||w||^2 + C \sum_{i=1}^{m} \xi_i$$

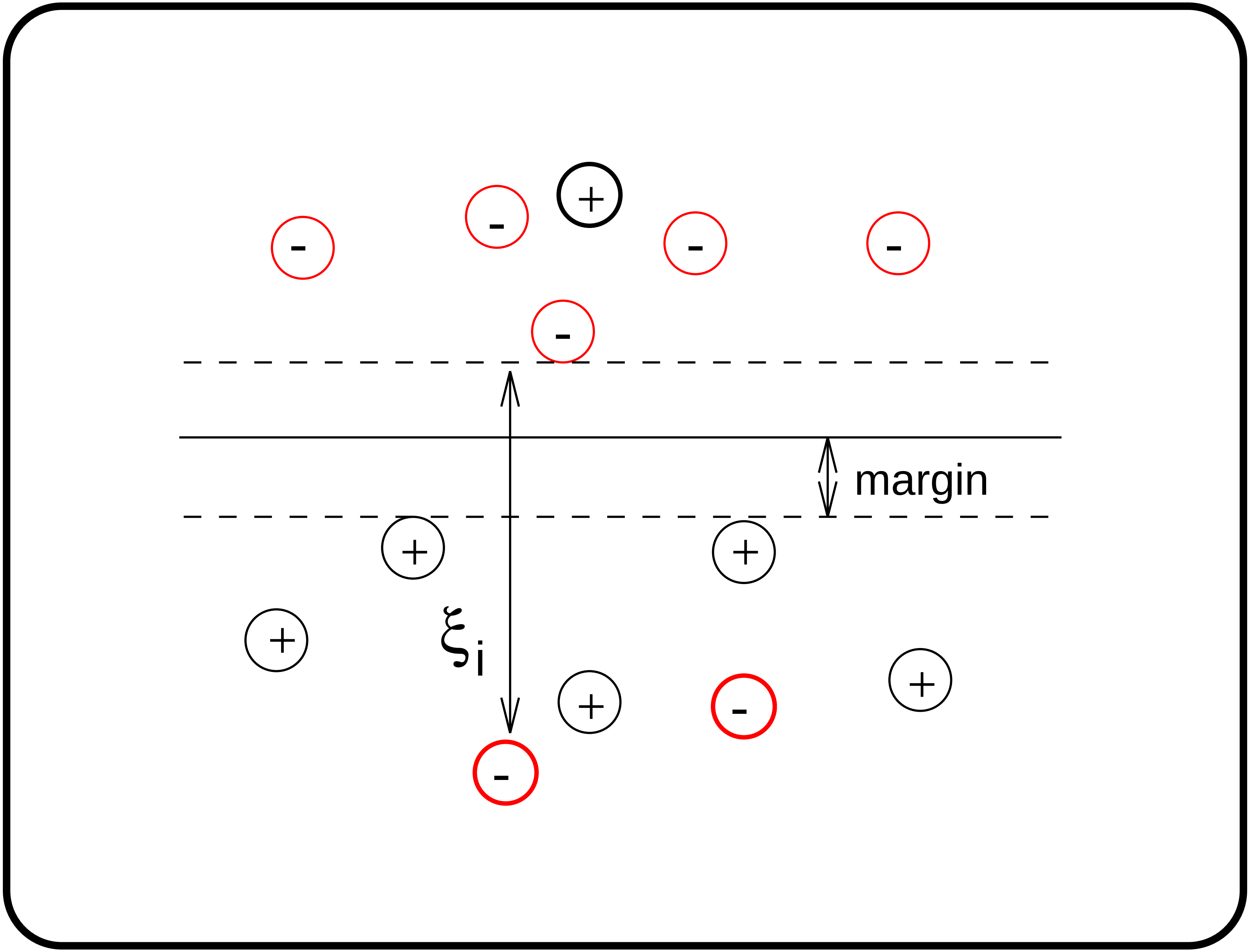
subject to:

$$y_i(w \cdot x_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$$

This is just the same as the original objective:

$$\frac{1}{m} \sum_{i=1}^{m} \ell(w \cdot x_i + b, y_i) + ||w||^2$$

except ℓ is no longer the zero-one loss, but is called the ”hinge-loss”: $\ell(y, \hat{y}) = \max(0, 1 - y\hat{y})$. This is still a quadratic program!


-
-
+
-
-
-
margin
+
+
ξ_i
+
+
-
+
-

19 Support Vector Machines - Primal

- **Decision function:**

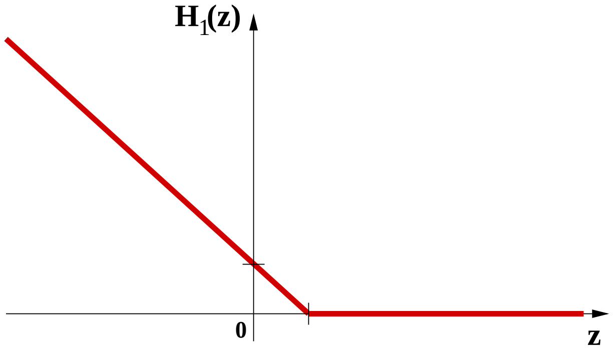
$$f(\boldsymbol{x}) = \boldsymbol{w} \cdot \boldsymbol{x} + b$$

- **Primal formulation:**

$$\min P(\boldsymbol{w}, b) = \underbrace{\frac{1}{2} \|\boldsymbol{w}\|^2}_{\text{maximize margin}} + \underbrace{C \sum_i H_1[\, y_i\, f(\boldsymbol{x}_i)\,]}_{\text{minimize training error}}$$

Ideally H_1 would count the number of errors, approximate with:

Hinge Loss $H_1(z) = \max(0, 1 - z)$



20 SVMs : non-linear case

Linear classifiers aren't complex enough sometimes. SVM solution:

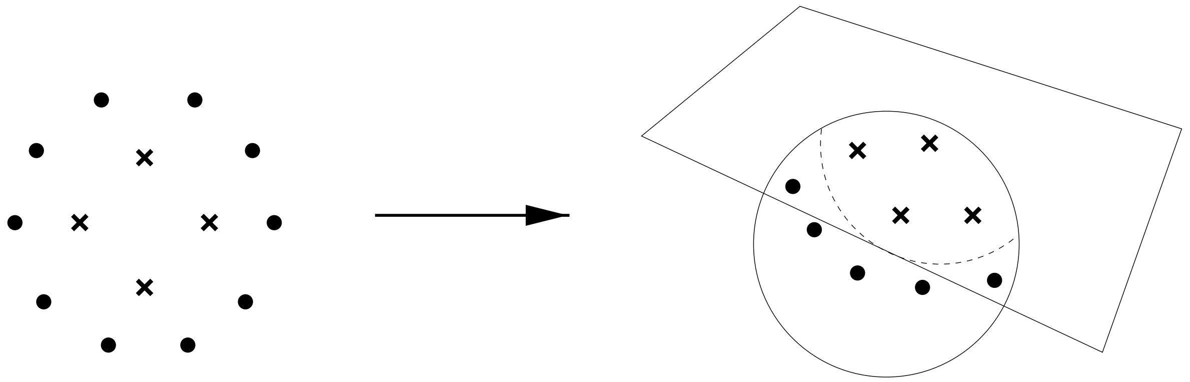
Map data into a richer feature space including nonlinear features, then construct a hyperplane in that space so all other equations are the same!

Formally, preprocess the data with:

$$x \mapsto \Phi(x)$$

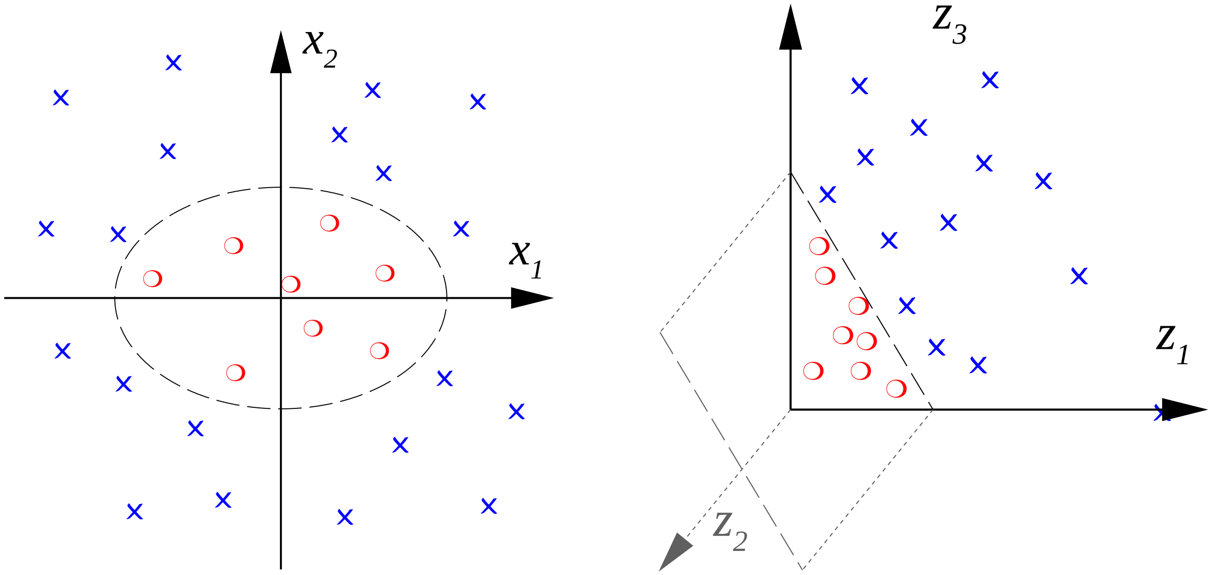
and then learn the map from $\Phi(x)$ to y:

$$f(x) = w \cdot \Phi(x) + b.$$



21 SVMs : polynomial mapping

$$\Phi : R^2 \longrightarrow R^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{(}2)x_1x_2, x_2^2)$$



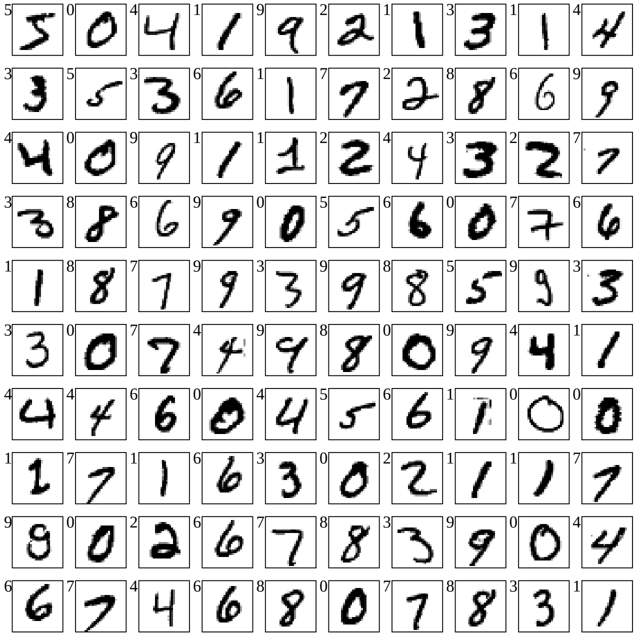
22 SVMs : non-linear case II

For example MNIST hand-writing recognition.

60,000 training examples, 10000 test examples, 28x28.

Linear SVM has around 8.5% test error.

Polynomial SVM has around 1% test error.



23 SVMs : full MNIST results

Classifier	Test Error
linear	8.4%
3-nearest-neighbor	2.4%
RBF-SVM	1.4 %
Tangent distance	1.1 %
LeNet	1.1 %
Boosted LeNet	0.7 %
Translation invariant SVM	0.56 %

Choosing a good mapping $\Phi(\cdot)$ (encoding prior knowledge + getting right complexity of function class) for your problem improves results.

24 SVMs : the kernel trick

Problem: the dimensionality of $\Phi(x)$ can be very large, making w hard to represent explicitly in memory, and hard for the QP to solve.

The Representer theorem (Kimeldorf & Wahba, 1971) shows that (for SVMs as a special case):

$$w = \sum_{i=1}^{m} \alpha_i \Phi(x_i)$$

for some variables α. Instead of optimizing w directly we can thus optimize α.

The decision rule is now:

$$f(x) = \sum_{i=1}^{m} \alpha_i \Phi(x_i) \cdot \Phi(x) + b$$

We call $K(x_i, x) = \Phi(x_i) \cdot \Phi(x)$ the *kernel function*.

25 Support Vector Machines - kernel trick II

We can rewrite all the SVM equations we saw before, but with the $w = \sum_{i=1}^{m} \alpha_i \Phi(x_i)$ equation:

- **Decision function:**

$$f(x) = \sum_i \alpha_i \Phi(\boldsymbol{x_i}) \cdot \Phi(\boldsymbol{x}) + b$$

$$= \sum_i \alpha_i K(\boldsymbol{x}_i, \boldsymbol{x}) + b$$

- **Dual formulation:**

$$\min P(\boldsymbol{w},\, b) = \underbrace{\frac{1}{2} \| \sum_{i=1}^{m} \alpha_i \Phi(x_i) \|^2}_{\text{maximize margin}} + \underbrace{C \sum_i H_1[\, y_i\, f(\boldsymbol{x}_i)\,]}_{\text{minimize training error}}$$

26 Support Vector Machines - Dual

But people normally write it like this:

- **Dual formulation:**

$$\min_{\boldsymbol{\alpha}} \; D(\boldsymbol{\alpha}) = \frac{1}{2} \sum_{i,j} \alpha_i \, \alpha_j \, \Phi(\boldsymbol{x}_i) \cdot \Phi(\boldsymbol{x}_j) - \sum_i y_i \, \alpha_i \quad \text{s.t.} \; \left\{ \begin{array}{l} \sum_i \alpha_i = 0 \\ 0 \leq y_i \, \alpha_i \leq C \end{array} \right.$$

- **Dual Decision function:**

$$f(x) = \sum_i \alpha_i K(\boldsymbol{x}_i, \boldsymbol{x}) + b$$

- **Kernel function** $K(\cdot, \cdot)$ is used to make (implicit) nonlinear feature map, e.g.
  - Polynomial kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x} \cdot \boldsymbol{x}' + 1)^d$.
  - RBF kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\gamma ||\boldsymbol{x} - \boldsymbol{x}'||^2)$.

27 Polynomial-SVMs

The kernel $K(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x} \cdot \boldsymbol{x}')^d$ gives the same result as the explicit mapping + dot product that we described before:

$$\Phi : R^2 \rightarrow R^3 \quad (x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt(2)x_1x_2, x_2^2)$$

$$\Phi((x_1, x_2) \cdot \Phi((x_1', x_2') = (x_1^2, \sqrt(2)x_1x_2, x_2^2) \cdot ({x'}_1^2, \sqrt(2){x'}_1{x'}_2, {x'}_2^2)$$

$$= x_1^2{x'}_1^2 + 2x_1{x'}_1x_2{x'}_2 + x_2^2{x'}_2^2$$

is the same as:

$$K(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x} \cdot \boldsymbol{x}')^2 = ((x_1, x_2) \cdot ({x'}_1, {x'}_2))^2$$

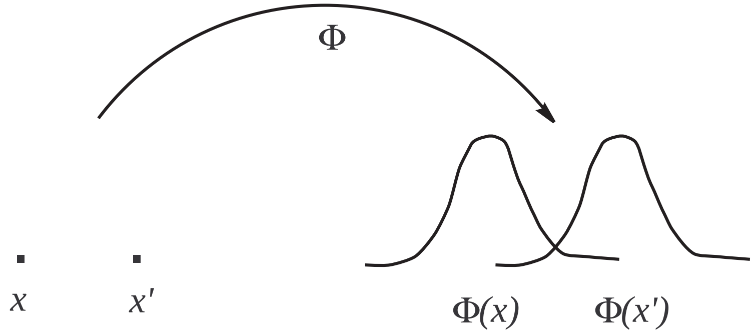
$$= (x_1{x'}_1 + x_2{x'}_2)^2 = x_1^2{x'}_1^2 + x_2^2{x'}_2^2 + 2x_1{x'}_1x_2{x'}_2$$

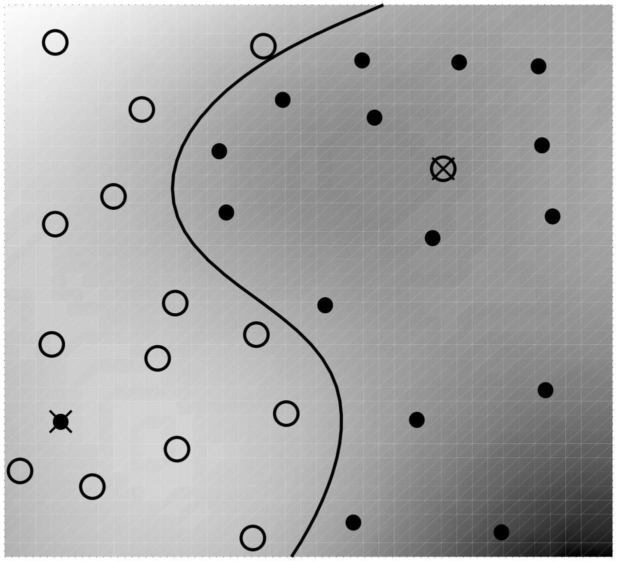
Interestingly, if d is large the kernel is still only requires n multiplications to compute, whereas the explicit representation may not fit in memory!

28 RBF-SVMs

The RBF kernel $K(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\gamma ||\boldsymbol{x} - \boldsymbol{x}'||^2)$ is one of the most popular kernel functions. It adds a ”bump” around each data point:

$$f(\boldsymbol{x}) = \sum_{i=1}^{m} \alpha_i \exp(-\gamma ||\boldsymbol{x}_i - \boldsymbol{x}||^2) + b$$





Using this one can get state-of-the-art results.

29 SVMs : more results

There is much more in the field of SVMs/ kernel machines than we could cover here, including:

- Regression, clustering, semi-supervised learning and other domains.
- Lots of other kernels, e.g. string kernels to handle text.
- Lots of research in modifications, e.g. to improve generalization ability, or tailoring to a particular task.
- Lots of research in speeding up training.

Please see text books such as the ones by Cristianini & Shawe-Taylor or by Schoelkopf and Smola.

30 SVMs : software

Lots of SVM software:

- LibSVM (C++)
- SVMLight (C)

As well as complete machine learning toolboxes that include SVMs:

- Torch (C++)
- Spider (Matlab)
- Weka (Java)

All available through `www.kernel-machines.org`.