Kernel Methods

COMP9417 Machine Learning and Data Mining

Term 2, 2019

Acknowledgements

Material derived from slides for the book
"Elements of Statistical Learning (2nd Ed.)" by T. Hastie,
R. Tibshirani & J. Friedman. Springer (2009)
http://statweb.stanford.edu/~tibs/ElemStatLearn/

Material derived from slides for the book
"Machine Learning: A Probabilistic Perspective" by P. Murphy
MIT Press (2012)
http://www.cs.ubc.ca/~murphyk/MLbook

Material derived from slides for the book
"Machine Learning" by P. Flach
Cambridge University Press (2012)
http://cs.bris.ac.uk/~flach/mlbook

Material derived from slides for the book
"Bayesian Reasoning and Machine Learning" by D. Barber
Cambridge University Press (2012)
http://www.cs.ucl.ac.uk/staff/d.barber/brml

Material derived from slides for the book
"Machine Learning" by T. Mitchell
McGraw-Hill (1997)
http://www-2.cs.cmu.edu/~tom/mlbook.html

Material derived from slides for the course
"Machine Learning" by A. Srinivasan
BITS Pilani Goa Campus, India (2016)

Aims

This lecture will develop your understanding of kernel methods in machine learning. Following it you should be able to:

- describe learning with the dual perceptron
- outline the idea of learning in a dual space
- describe the concept of maximising the margin in linear classification
- outline the typical loss function for maximising the margin
- describe the method of support vector machines (SVMs)
- describe the concept of kernel functions
- outline the idea of using a kernel in a learning algorithm
- outline non-linear classification with kernel methods

Predictive machine learning scenarios

Task	*Label space*	*Output space*	*Learning problem*
Classification	$\mathcal{L} = \mathcal{C}$	$\mathcal{Y} = \mathcal{C}$	learn an approximation $\hat{c} : \mathcal{X} \to \mathcal{C}$ to the true labelling function c
Scoring and ranking	$\mathcal{L} = \mathcal{C}$	$\mathcal{Y} = \mathbb{R}^{\lvert\mathcal{C}\rvert}$	learn a model that outputs a score vector over classes
Probability estimation	$\mathcal{L} = \mathcal{C}$	$\mathcal{Y} = [0,1]^{\lvert\mathcal{C}\rvert}$	learn a model that outputs a probability vector over classes
Regression	$\mathcal{L} = \mathbb{R}$	$\mathcal{Y} = \mathbb{R}$	learn an approximation $\hat{f} : \mathcal{X} \to \mathbb{R}$ to the true labelling function f

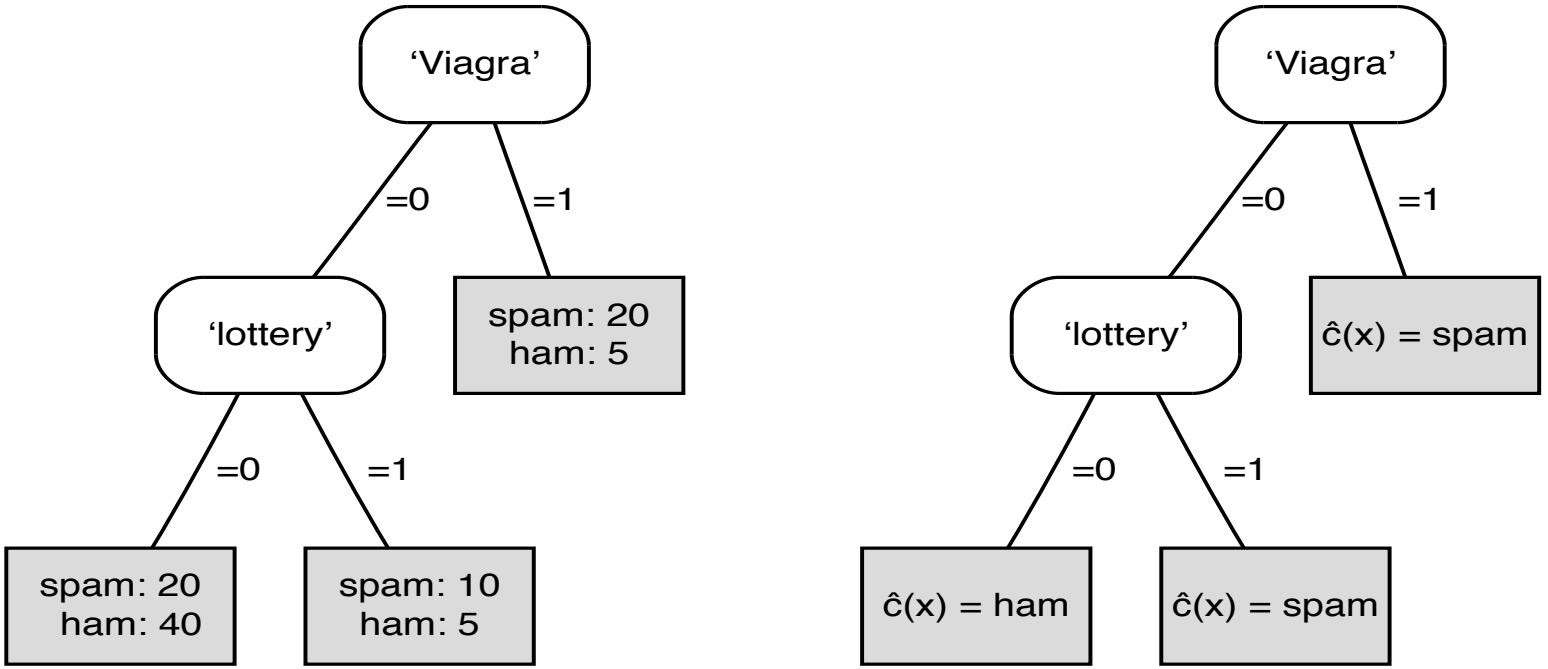
Classification

A **classifier** is a mapping $\hat{c} : \mathcal{X} \to \mathcal{C}$, where $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ is a finite and usually small set of **class labels**. We will sometimes also use C_i to indicate the set of examples of that class.

We use the 'hat' to indicate that $\hat{c}(x)$ is an estimate of the true but unknown function $c(x)$. Examples for a classifier take the form $(x, c(x))$, where $x \in \mathcal{X}$ is an instance and $c(x)$ is the true class of the instance (sometimes contaminated by noise).

Learning a classifier involves constructing the function $\hat{c}$ such that it matches c as closely as possible (and not just on the training set, but ideally on the entire instance space $\mathcal{X}$).

A decision tree



(left) A tree with the training set class distribution in the leaves.

(right) A tree with the majority class prediction rule in the leaves.

Scoring classifier

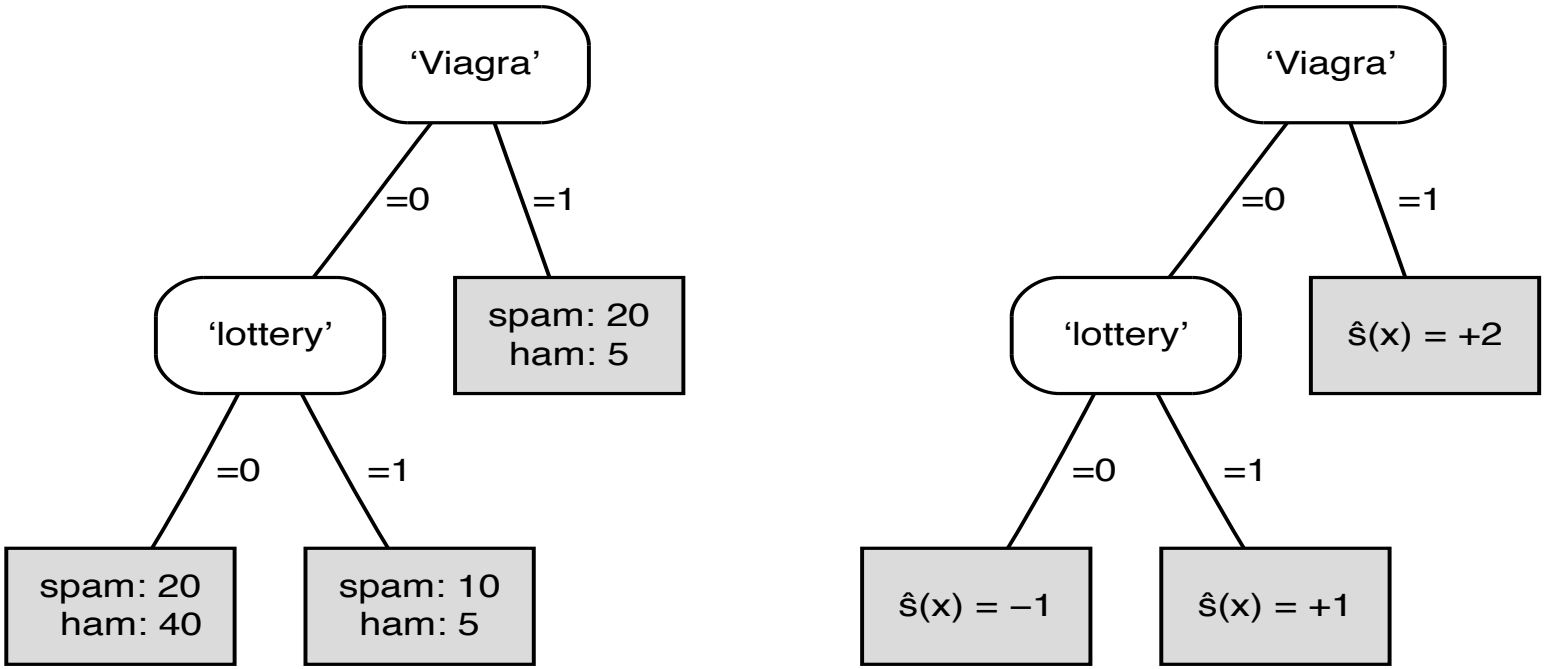
A **scoring classifier** is a mapping $\hat{\mathbf{s}} : \mathcal{X} \to \mathbb{R}^k$, i.e., a mapping from the instance space to a k-vector of real numbers.

The boldface notation indicates that a scoring classifier outputs a vector $\hat{\mathbf{s}}(x) = (\hat{s}_1(x), \ldots, \hat{s}_k(x))$ rather than a single number; $\hat{s}_i(x)$ is the score assigned to class C_i for instance x.

This score indicates how likely it is that class label C_i applies.

If we only have two classes, it usually suffices to consider the score for only one of the classes; in that case, we use $\hat{s}(x)$ to denote the score of the positive class for instance x.

A scoring tree



(left) A tree with the training set class distribution in the leaves.

(right) A tree using the logarithm of the class ratio as scores; spam is taken as the positive class.

Margins and loss functions

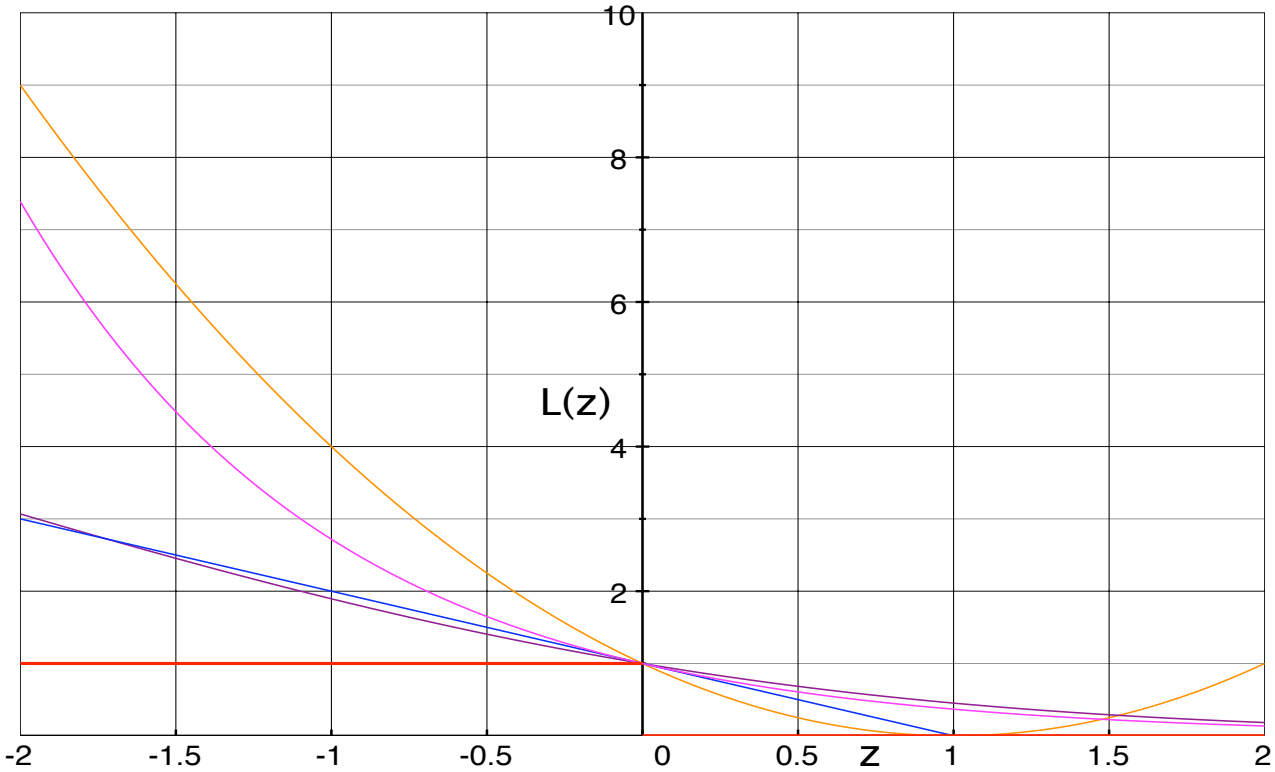
If we take the true class $c(x)$ as $+1$ for positive examples and -1 for negative examples, then the quantity $z(x) = c(x)\hat{s}(x)$ is positive for correct predictions and negative for incorrect predictions: this quantity is called the **margin** assigned by the scoring classifier to the example.

We would like to reward large positive margins, and penalise large negative values. This is achieved by means of a so-called **loss function** $L : \mathbb{R} \mapsto [0, \infty)$ which maps each example's margin $z(x)$ to an associated loss $L(z(x))$.

We will assume that $L(0) = 1$, which is the loss incurred by having an example on the decision boundary. We furthermore have $L(z) \geq 1$ for $z < 0$, and usually also $0 \leq L(z) < 1$ for $z > 0$.

The average loss over a test set Te is $\frac{1}{|Te|} \sum_{x \in Te} L(z(x))$.

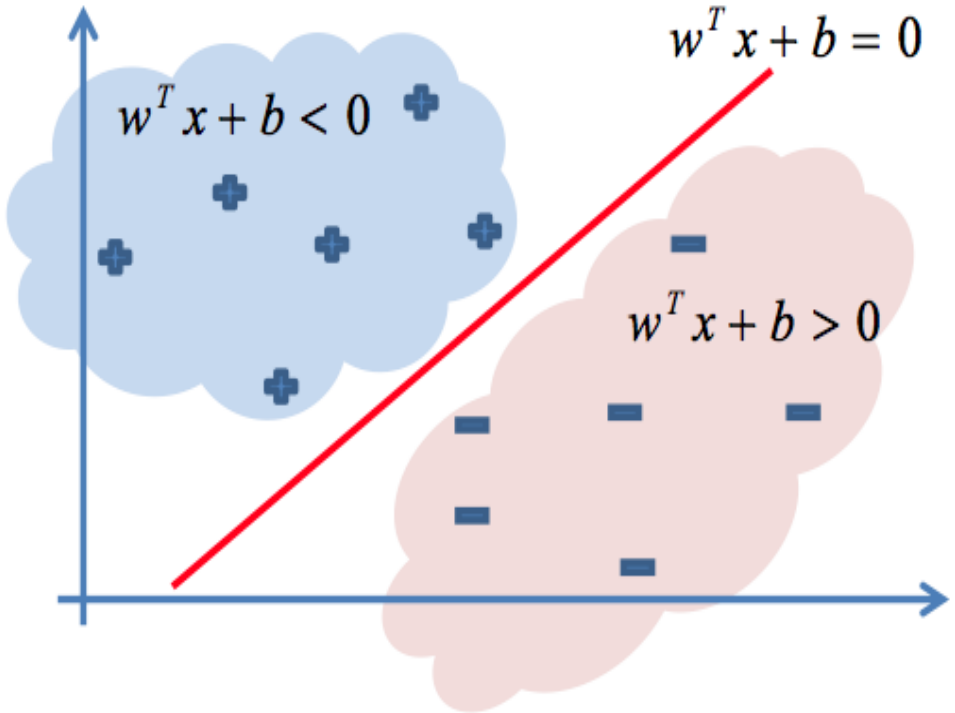
Loss functions



From bottom-left: (i) 0–1 loss $L_{01}(z) = 1$ if $z \leq 0$, and $L_{01}(z) = 0$ if $z > 0$; (ii) hinge loss $L_{\mathrm{h}}(z) = (1 - z)$ if $z \leq 1$, and $L_{\mathrm{h}}(z) = 0$ if $z > 1$; (iii) logistic loss $L_{\log}(z) = \log_2(1 + \exp(-z))$; (iv) exponential loss $L_{\exp}(z) = \exp(-z)$; (v) squared loss $L_{\mathrm{sq}}(z) = (1 - z)^2$ (can be set to 0 for $z > 1$, just like hinge loss).

Review: Linear classification

- Two-class classifier "separates" instances in feature space: $f(x) = sign(w^T x + b)$

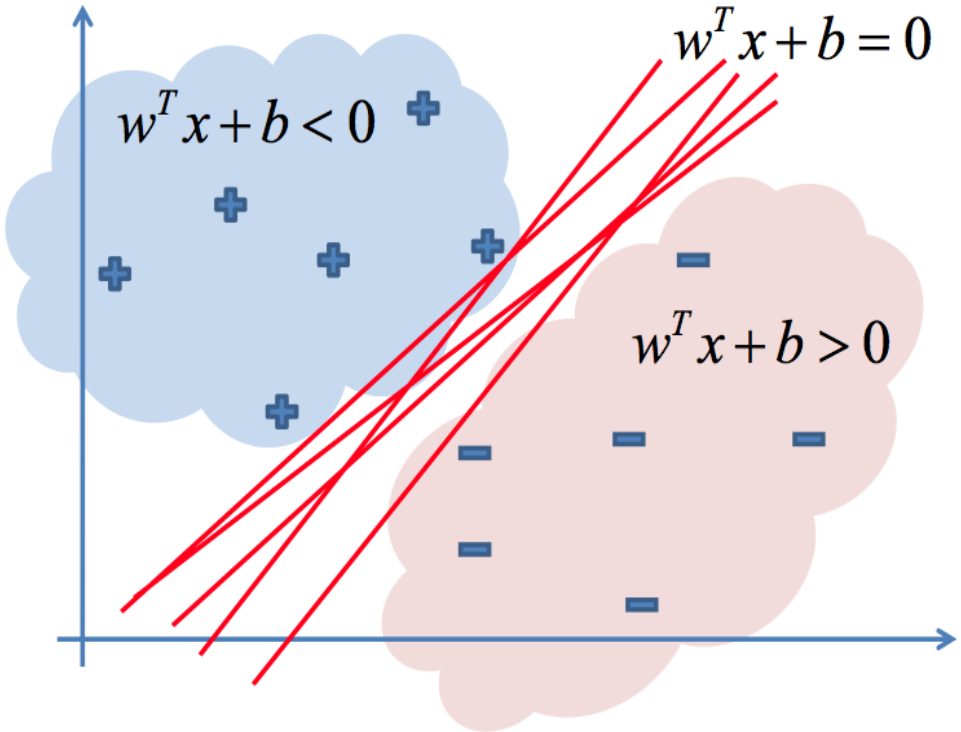


Issues in linear classification

- Define a decision boundary by a hyperplane in feature space
- A linear model can be used for classification

Issues in linear classification

- Many possible linear decision boundaries: which one to choose ?



Issues in linear classification

Different classification learning algorithms use different criteria:

- Basic linear classifier finds class means (centroids), joins them by a straight line, and its perpendicular bisector is the separating hyperplane
- Nearest-neighbour, naive Bayes, logistic regression all use different criteria
- Perceptron training uses iterative reweighting (gradient descent)
- Perceptron may find different models depending on starting conditions

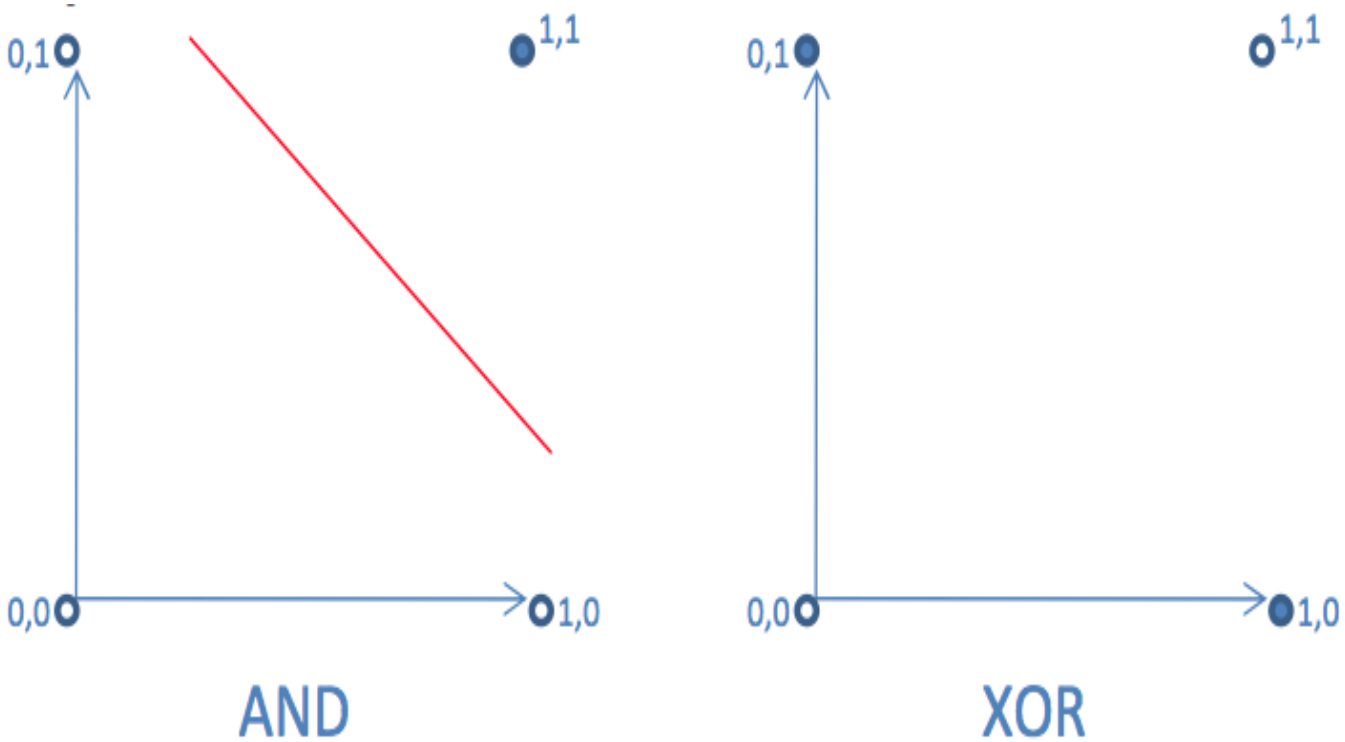
Issues in linear classification

Is there an optimal linear classification learning method ?

- one approach is to define the *empirical risk*, or error on the data
- the maximum *margin* separating hyperplane
- unique solution
- minimises empirical risk
- is there a way to trade-off minimising risk with model complexity?
- answer: yes, under Vapnik's framework for statistical learning
  - *structural risk minimization*

Issues in linear classification

- May not be possible to find a linear separating hyperplane



- filled / empty circles are in / out of the target concept
- AND is linearly separable – but not XOR

Extending linear classification

- Linear classifiers can't model nonlinear class boundaries
- Simple trick to allow them to do that:
  - Nonlinear mapping: map attributes into new space consisting of combinations of attribute values
  - For example: all products with n factors that can be constructed from the attributes (*feature construction* or *basis expansion*)
- e.g., for 2 attributes, all products with $n = 3$ factors

$$y = w_1 x_1^3 + w_2 x_1^2 x_2 + w_3 x_1 x_2^2 + w_4 x_2^3$$

- y is predicted output for instances with two attributes x_1 and x_2

Two main problems

- efficiency:
  - With 10 attributes and $n = 5$ have to learn more than 2000 coefficients (weights)
  - Linear regression (with attribute selection) running time is cubic in the number of attributes
- overfitting:
  - "Too nonlinear" – number of coefficients large relative to number of training instances
  - *Curse of dimensionality* applies ...

Linear classifiers in dual form

Every time an example $\mathbf{x}_i$ is misclassified, add $y_i\mathbf{x}_i$ to the weight vector.

- After training has completed, each example has been misclassified zero or more times. Denoting this number as α_i for example $\mathbf{x}_i$, the weight vector can be expressed as

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

- In the dual, instance-based view of linear classification we are learning instance weights α_i rather than feature weights w_j. An instance $\mathbf{x}$ is classified as

$$\hat{y} = \text{sign}\left(\sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \cdot \mathbf{x}\right)$$

- During training, the only information needed about the training data is all pairwise dot products: the n-by-n matrix $\mathbf{G} = \mathbf{X}\mathbf{X}^{\mathrm{T}}$ containing these dot products is called the **Gram matrix**.

Perceptron training in dual form

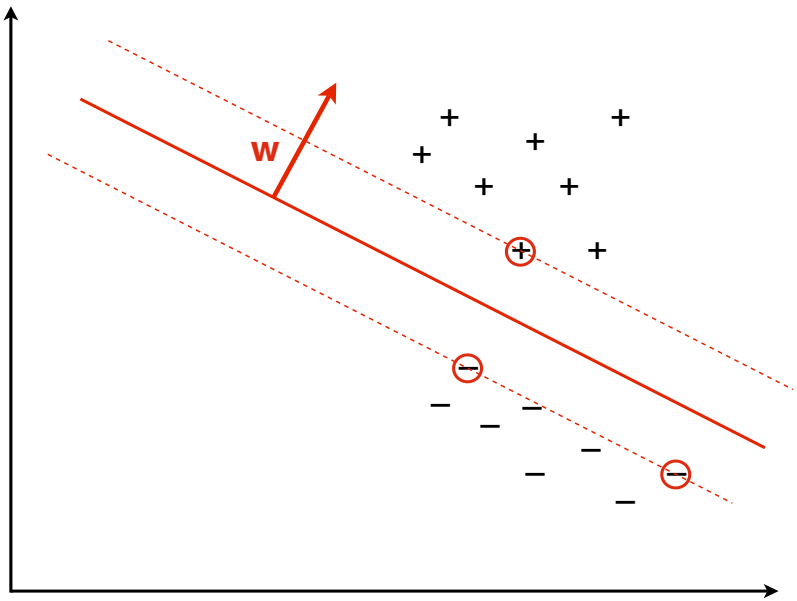
Algorithm DualPerceptron(D) // perceptron training in dual form

Input: labelled training data D in homogeneous coordinates

Output: coefficients α_i defining weight vector $\mathbf{w} = \sum_{i=1}^{|D|} \alpha_i y_i \mathbf{x}_i$

```
1  α_i ← 0 for 1 ≤ i ≤ |D|
2  converged←false
3  while converged = false do
4  |   converged←true
5  |   for i = 1 to |D| do
6  |   |   if y_i Σ_{j=1}^{|D|} α_j y_j x_i · x_j ≤ 0 then
7  |   |   |   α_i ← α_i + 1
8  |   |   |   converged←false
9  |   |   end
10 |   end
11 end
```

Support vector machine



The decision boundary learned by a support vector machine maximises the margin, which is indicated by the dotted lines. The circled data points are the support vectors.

Support vector machines

- Support vector machines (*machine* $\equiv$ *algorithm*) learn linear classifiers
- Can avoid overfitting – learn a form of decision boundary called the *maximum margin hyperplane*
- Fast for mappings to nonlinear spaces
  - employ a mathematical trick to avoid the actual creation of new "pseudo-attributes" in transformed instance space
  - i.e. the nonlinear space is created *implicitly*

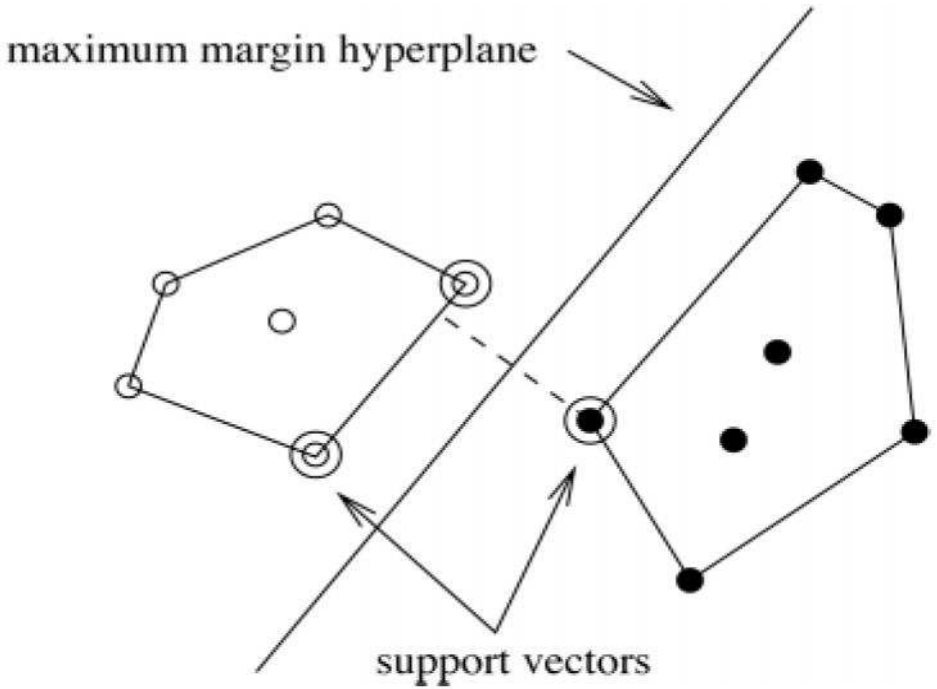
The kernel trick

Let $\mathbf{x}_1 = (x_1, y_1)$ and $\mathbf{x}_2 = (x_2, y_2)$ be two data points, and consider the mapping $(x, y) \mapsto (x^2, y^2, \sqrt{2}xy)$ to a three-dimensional feature space. The points in feature space corresponding to $\mathbf{x}_1$ and $\mathbf{x}_2$ are $\mathbf{x}'_1 = (x_1^2, y_1^2, \sqrt{2}x_1y_1)$ and $\mathbf{x}'_2 = (x_2^2, y_2^2, \sqrt{2}x_2y_2)$. The dot product of these two feature vectors is

$$\mathbf{x}'_1 \cdot \mathbf{x}'_2 = x_1^2x_2^2 + y_1^2y_2^2 + 2x_1y_1x_2y_2 = (x_1x_2 + y_1y_2)^2 = (\mathbf{x}_1 \cdot \mathbf{x}_2)^2$$

That is, by squaring the dot product in the original space we obtain the dot product in the new space *without actually constructing the feature vectors*! A function that calculates the dot product in feature space directly from the vectors in the original space is called a *kernel* – here the kernel is $\boldsymbol{\kappa}(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2)^2$.

Training a support vector machine



Training a support vector machine

- learning problem: fit maximum margin hyperplane, i.e. a kind of linear model
- for a linearly separable two-class data set the maximum margin hyperplane is the classification surface which
  - correctly classifies all examples in the data set
  - has the greatest *separation* between classes
- "convex hull" of instances in each class is tightest enclosing convex polygon
- for a linearly separable two-class data set convex hulls do not overlap
- maximum margin hyperplane is orthogonal to shortest line connecting convex hulls, intersects with it halfway
- the more "separated" the classes, the larger the margin, the better the generalization

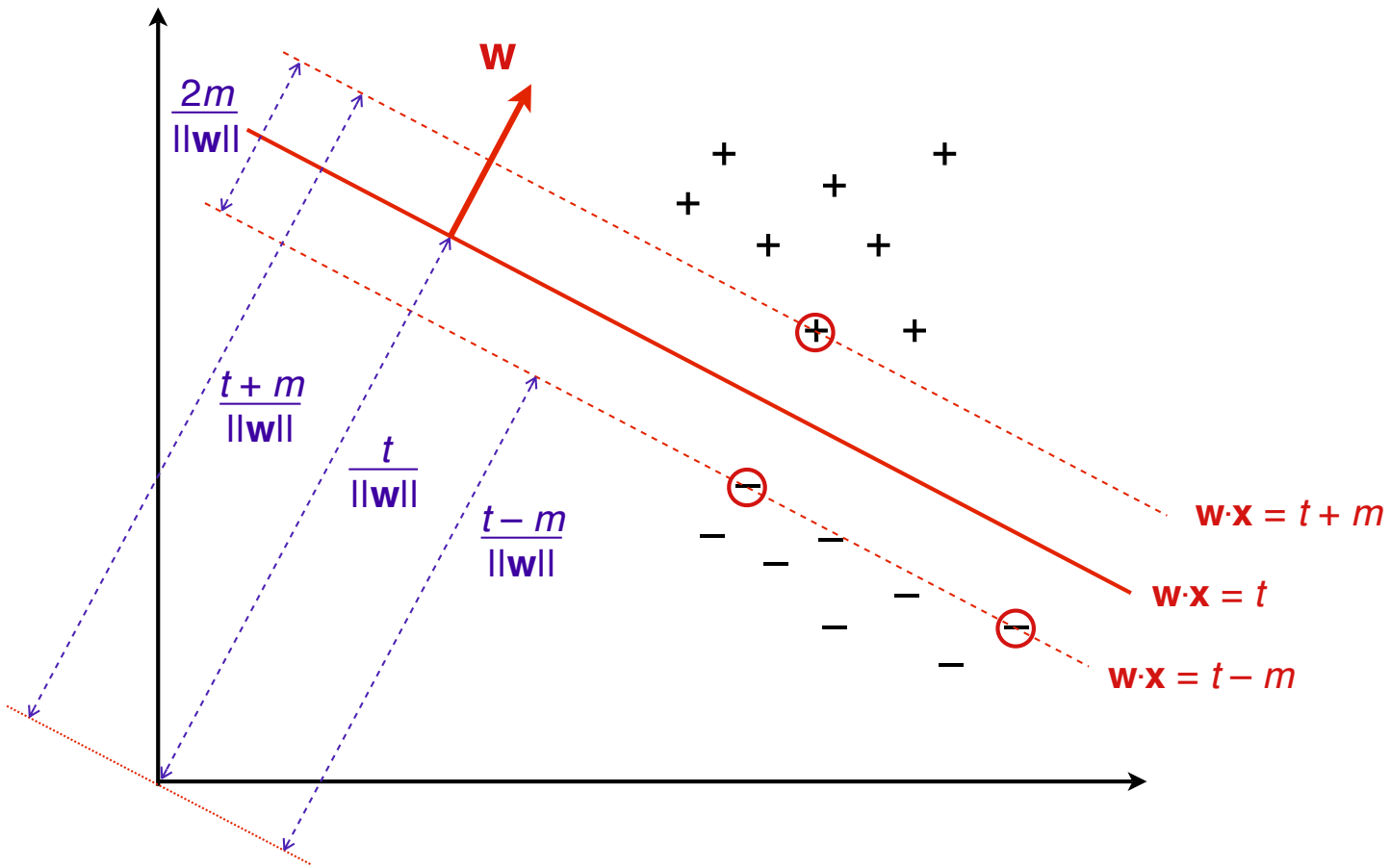
Support vectors

- Instances closest to maximum margin hyperplane are *support vectors*
- Important observation: support vectors define maximum margin hyperplane!
  - All other instances can be deleted without changing position and orientation of the hyperplane!

Finding support vectors

- Determining parameters is a constrained quadratic optimization problem
  - standard algorithms, or
  - special-purpose algorithms are faster, e.g. Platt's sequential minimal optimization (SMO), or LibSVM
- Note: all this assumes separable data!

Support vector machine



The geometry of a support vector classifier. The circled data points are the support vectors, which are the training examples nearest to the decision boundary. The support vector machine finds the decision boundary that maximises the margin $m/||\mathbf{w}||$.

Maximising the margin

Since we are free to rescale t, $||\mathbf{w}||$ and m, it is customary to choose $m = 1$. Maximising the margin then corresponds to minimising $||\mathbf{w}||$ or, more conveniently, $\frac{1}{2}||\mathbf{w}||^2$, provided of course that none of the training points fall inside the margin.

This leads to a quadratic, constrained optimisation problem:

$$\mathbf{w}^*, t^* = \arg\min_{\mathbf{w},t} \frac{1}{2}||\mathbf{w}||^2 \qquad \text{subject to } y_i(\mathbf{w} \cdot \mathbf{x}_i - t) \geq 1, 1 \leq i \leq n$$

Using the method of Lagrange multipliers, the dual form of this problem can be derived.

Deriving the dual problem

Adding the constraints with multipliers α_i for each training example gives the Lagrange function

$$\begin{aligned}
\Lambda(\mathbf{w}, t, \alpha_1, \ldots, \alpha_n) &= \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{n} \alpha_i (y_i(\mathbf{w} \cdot \mathbf{x}_i - t) - 1) \\
&= \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{n} \alpha_i y_i (\mathbf{w} \cdot \mathbf{x}_i) + \sum_{i=1}^{n} \alpha_i y_i t + \sum_{i=1}^{n} \alpha_i \\
&= \frac{1}{2}\mathbf{w} \cdot \mathbf{w} - \mathbf{w} \cdot \left(\sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \right) + t \left(\sum_{i=1}^{n} \alpha_i y_i \right) + \sum_{i=1}^{n} \alpha_i
\end{aligned}$$

- By taking the partial derivative of the Lagrange function with respect to t and setting it to 0 we find $\sum_{i=1}^{n} \alpha_i y_i = 0$.
- Similarly, by taking the partial derivative of the Lagrange function with respect to $\mathbf{w}$ and setting to 0 we obtain $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$ – the same expression as we derived for the perceptron.

Deriving the dual problem

- For the perceptron, the instance weights α_i are non-negative integers denoting the number of times an example has been misclassified in training. For a support vector machine, the α_i are non-negative reals.
- What they have in common is that, if $\alpha_i = 0$ for a particular example $\mathbf{x}_i$, that example could be removed from the training set without affecting the learned decision boundary. In the case of support vector machines this means that $\alpha_i > 0$ only for the support vectors: the training examples nearest to the decision boundary.

These expressions allow us to eliminate $\mathbf{w}$ and t and lead to the dual Lagrangian

$$\begin{aligned}\Lambda(\alpha_1, \ldots, \alpha_n) &= -\frac{1}{2}\left(\sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i\right) \cdot \left(\sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i\right) + \sum_{i=1}^{n} \alpha_i \\ &= -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i\end{aligned}$$

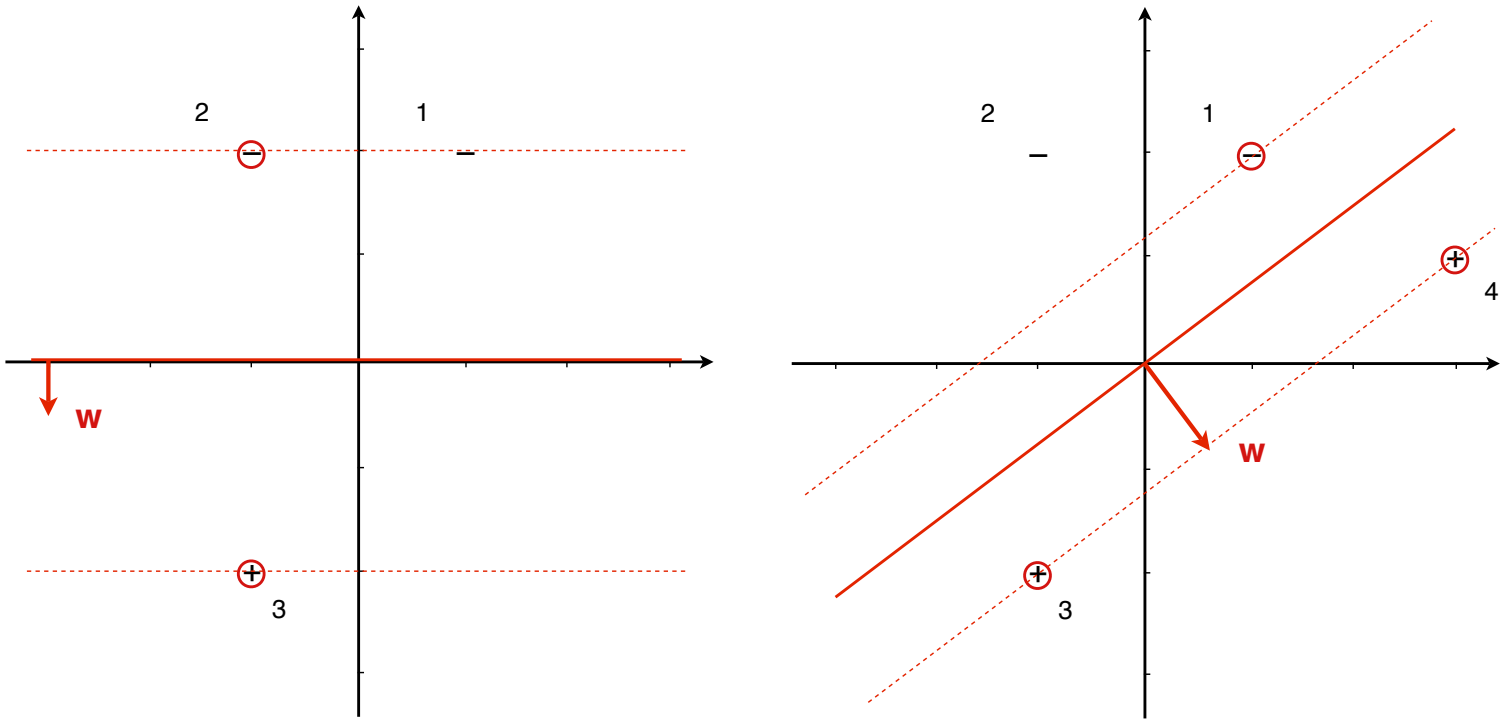
SVM in dual form

The dual optimisation problem for support vector machines is to maximise the dual Lagrangian under positivity constraints and one equality constraint:

$$\alpha_1^*, \ldots, \alpha_n^* = \underset{\alpha_1,\ldots,\alpha_n}{\arg\max} -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j + \sum_{i=1}^{n}\alpha_i$$

$$\text{subject to} \quad \alpha_i \geq 0, \quad 1 \leq i \leq n \quad \text{and} \quad \sum_{i=1}^{n}\alpha_i y_i = 0$$

Two maximum-margin classifiers



(left) A maximum-margin classifier built from three examples, with $\mathbf{w} = (0, -1/2)$ and margin 2. The circled examples are the support vectors: they receive non-zero Lagrange multipliers and define the decision boundary. (right) By adding a second positive the decision boundary is rotated to $\mathbf{w} = (3/5, -4/5)$ and the margin decreases to 1.

Two maximum-margin classifiers

$$\mathbf{X} = \begin{pmatrix} 1 & 2 \\ -1 & 2 \\ -1 & -2 \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} -1 \\ -1 \\ +1 \end{pmatrix} \qquad \mathbf{X}' = \begin{pmatrix} -1 & -2 \\ 1 & -2 \\ -1 & -2 \end{pmatrix}$$

The matrix $\mathbf{X}'$ on the right incorporates the class labels; i.e., the rows are $y_i \mathbf{x}_i$. The Gram matrix is (without and with class labels):

$$\mathbf{X}\mathbf{X}^{\mathrm{T}} = \begin{pmatrix} 5 & 3 & -5 \\ 3 & 5 & -3 \\ -5 & -3 & 5 \end{pmatrix} \qquad \mathbf{X}'\mathbf{X}'^{\mathrm{T}} = \begin{pmatrix} 5 & 3 & 5 \\ 3 & 5 & 3 \\ 5 & 3 & 5 \end{pmatrix}$$

The dual optimisation problem is thus

$$\begin{aligned} &\arg\max_{\alpha_1,\alpha_2,\alpha_3} -\frac{1}{2}\left(5\alpha_1^2 + 3\alpha_1\alpha_2 + 5\alpha_1\alpha_3 + 3\alpha_2\alpha_1 + 5\alpha_2^2 + 3\alpha_2\alpha_3 + 5\alpha_3\alpha_1 + 3\alpha_3\alpha_2 + 5\alpha_3^2\right) + \alpha_1 + \\ &= \arg\max_{\alpha_1,\alpha_2,\alpha_3} -\frac{1}{2}\left(5\alpha_1^2 + 6\alpha_1\alpha_2 + 10\alpha_1\alpha_3 + 5\alpha_2^2 + 6\alpha_2\alpha_3 + 5\alpha_3^2\right) + \alpha_1 + \alpha_2 + \alpha_3 \end{aligned}$$

subject to $\alpha_1 \geq 0, \alpha_2 \geq 0, \alpha_3 \geq 0$ and $-\alpha_1 - \alpha_2 + \alpha_3 = 0$.

Two maximum-margin classifiers

- Using the equality constraint we can eliminate one of the variables, say α_3, and simplify the objective function to

$$\arg\max_{\alpha_1,\alpha_2,\alpha_3} -\frac{1}{2}\left(20\alpha_1^2 + 32\alpha_1\alpha_2 + 16\alpha_2^2\right) + 2\alpha_1 + 2\alpha_2$$

- Setting partial derivatives to 0 we obtain $-20\alpha_1 - 16\alpha_2 + 2 = 0$ and $-16\alpha_1 - 16\alpha_2 + 2 = 0$ (notice that, because the objective function is quadratic, these equations are guaranteed to be linear).
- We therefore obtain the solution $\alpha_1 = 0$ and $\alpha_2 = \alpha_3 = 1/8$. We then have $\mathbf{w} = 1/8(\mathbf{x}_3 - \mathbf{x}_2) = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix}$, resulting in a margin of $1/||\mathbf{w}|| = 2$.
- Finally, t can be obtained from any support vector, say $\mathbf{x}_2$, since $y_2(\mathbf{w} \cdot \mathbf{x}_2 - t) = 1$; this gives $-1 \cdot (-1 - t) = 1$, hence $t = 0$.

Two maximum-margin classifiers

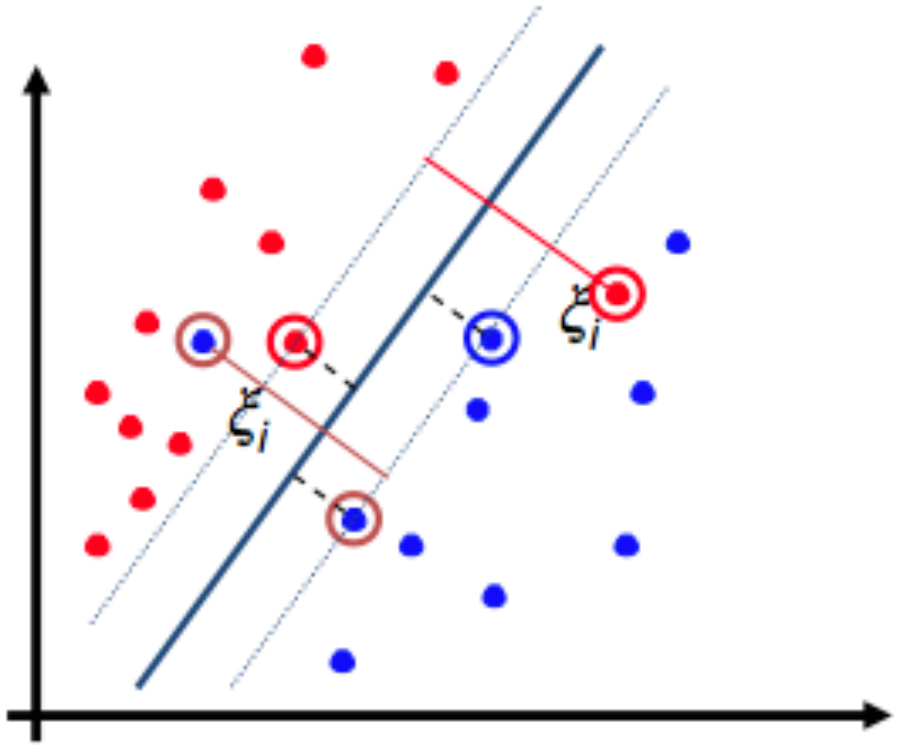
We now add an additional positive at $(3, 1)$. This gives the following data matrices:

$$\mathbf{X}' = \begin{pmatrix} -1 & -2 \\ 1 & -2 \\ -1 & -2 \\ 3 & 1 \end{pmatrix} \qquad \mathbf{X}'\mathbf{X}'^{\mathrm{T}} = \begin{pmatrix} 5 & 3 & 5 & -5 \\ 3 & 5 & 3 & 1 \\ 5 & 3 & 5 & -5 \\ -5 & 1 & -5 & 10 \end{pmatrix}$$

- It can be verified by similar calculations to those above that the margin decreases to 1 and the decision boundary rotates to $\mathbf{w} = \begin{pmatrix} 3/5 \\ -4/5 \end{pmatrix}$.
- The Lagrange multipliers now are $\alpha_1 = 1/2$, $\alpha_2 = 0$, $\alpha_3 = 1/10$ and $\alpha_4 = 2/5$. Thus, only $\mathbf{x}_3$ is a support vector in both the original and the extended data set.

Noise

- Misclassified examples may break the separability assumption



- Introduce "slack" variables ξ_i to allow misclassification of instances
- Minimise $\Phi(w) = w^T w + C \sum \xi_i$

Noise

- "soft margin" SVMs to handle noisy data
- Parameter C bounds influence of any one training instance on decision boundary
- Constraint $0 \leq \alpha_i \leq C$
- Still a quadratic optimization problem
- C has to be found by, e.g., cross-validation

Allowing margin errors

The idea is to introduce *slack variables* ξ_i, one for each example, which allow some of them to be inside the margin or even at the wrong side of the decision boundary. We will call these *margin errors*. Thus, we change the constraints to $\mathbf{w} \cdot \mathbf{x}_i - t \geq 1 - \xi_i$ and add the sum of all slack variables to the objective function to be minimised, resulting in the following *soft margin* optimisation problem:

$$\mathbf{w}^*, t^*, \xi_i^* = \arg\min_{\mathbf{w}, t, \xi_i} \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n} \xi_i$$
$$\text{subject to } y_i(\mathbf{w} \cdot \mathbf{x}_i - t) \geq 1 - \xi_i \text{ and } \xi_i \geq 0, 1 \leq i \leq n$$

Allowing margin errors

- C is a user-defined parameter trading off margin maximisation against slack variable minimisation: a high value of C means that margin errors incur a high penalty, while a low value permits more margin errors (possibly including misclassifications) in order to achieve a large margin.
- If we allow more margin errors we need fewer support vectors, hence C controls to some extent the 'complexity' of the SVM and hence is often referred to as the *complexity parameter*.

Allowing margin errors

The Lagrange function is then as follows:

$$\begin{aligned}\Lambda(\mathbf{w}, t, \xi_i, \alpha_i, \beta_i) &= \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i(y_i(\mathbf{w}\cdot\mathbf{x}_i - t) - (1-\xi_i)) - \sum_{i=1}^{n}\beta_i\xi_i \\ &= \Lambda(\mathbf{w}, t, \alpha_i) + \sum_{i=1}^{n}(C - \alpha_i - \beta_i)\xi_i\end{aligned}$$

- For an optimal solution every partial derivative with respect to ξ_i should be 0, from which it follows that the added term vanishes from the dual problem.
- Furthermore, since both α_i and β_i are positive, this means that α_i cannot be larger than C:

Three cases for the training instances

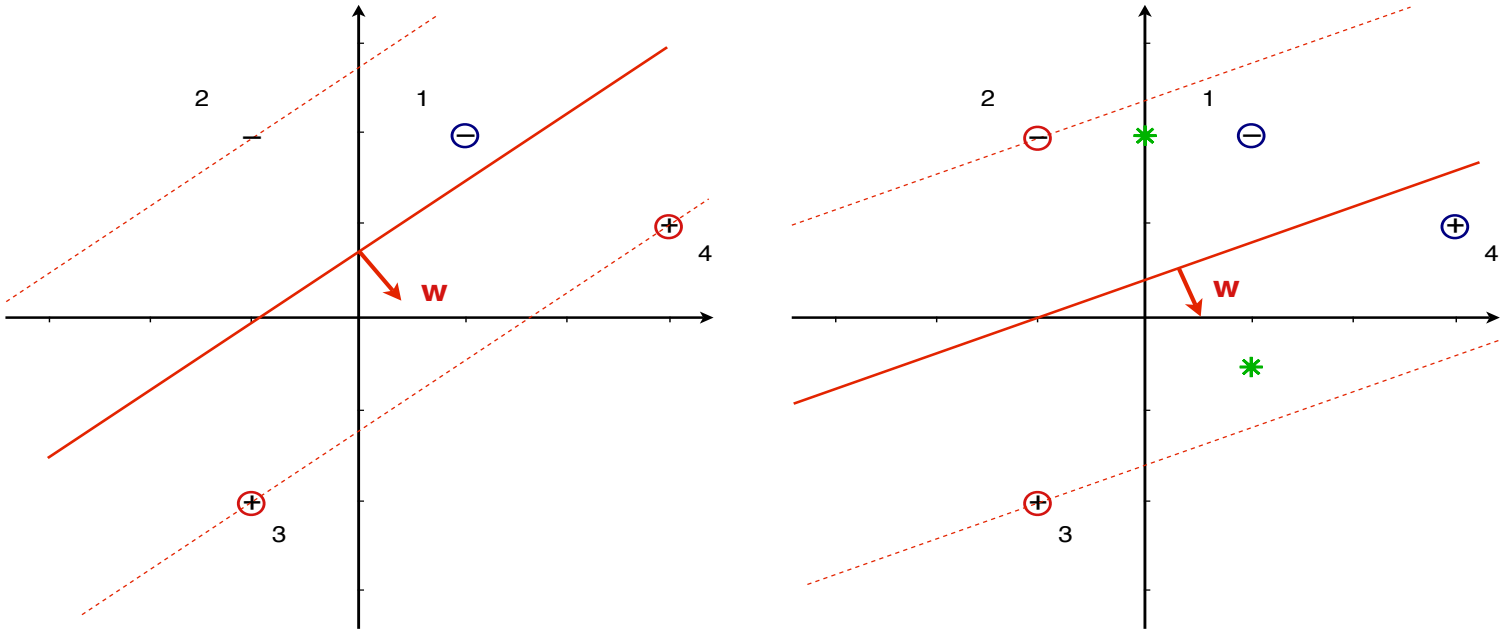
What is the significance of the upper bound C on the α_i multipliers?

- Since $C - \alpha_i - \beta_i = 0$ for all i, $\alpha_i = C$ implies $\beta_i = 0$. The β_i multipliers come from the $\xi_i \geq 0$ constraint, and a multiplier of 0 means that the lower bound is not reached, i.e., $\xi_i > 0$ (analogous to the fact that $\alpha_j = 0$ means that $\mathbf{x}_j$ is not a support vector and hence $\mathbf{w} \cdot \mathbf{x}_j - t > 1$).
- In other words, a solution to the soft margin optimisation problem in dual form divides the training examples into three cases:

$$\begin{aligned} \alpha_i = 0 &\quad \text{these are outside or on the margin;} \\ 0 < \alpha_i < C &\quad \text{these are the support vectors on the margin;} \\ \alpha_i = C &\quad \text{these are on or inside the margin.} \end{aligned}$$

- Notice that we still have $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$, and so both second and third case examples participate in spanning the decision boundary.

Soft margins



(left) The soft margin classifier learned with $C = 5/16$, at which point $\mathbf{x}_2$ is about to become a support vector. (right) The soft margin classifier learned with $C = 1/10$: all examples contribute equally to the weight vector. The asterisks denote the class means, and the decision boundary is parallel to the one learned by the basic linear classifier.

Soft margins

- Recall that the Lagrange multipliers for the classifier above are $\alpha_1 = 1/2$, $\alpha_2 = 0$, $\alpha_3 = 1/10$ and $\alpha_4 = 2/5$. So α_1 is the largest multiplier, and as long as $C > \alpha_1 = 1/2$ no margin errors are tolerated.
- For $C = 1/2$ we have $\alpha_1 = C$, and hence for $C < 1/2$ we have that $\mathbf{x}_1$ becomes a margin error and the optimal classifier is a soft margin classifier. Effectively, with decreasing C the decision boundary and the upper margin move upward, while the lower margin stays the same.
- The upper margin reaches $\mathbf{x}_2$ for $C = 5/16$, at which point we have $\mathbf{w} = \begin{pmatrix} 3/8 \\ -1/2 \end{pmatrix}$, $t = 3/8$ and the margin has increased to 1.6. Furthermore, we have $\xi_1 = 6/8, \alpha_1 = C = 5/16, \alpha_2 = 0, \alpha_3 = 1/16$ and $\alpha_4 = 1/4$.

Soft margins

- If we now decrease C further, the decision boundary starts to rotate clockwise, so that $\mathbf{x}_4$ becomes a margin error as well, and only $\mathbf{x}_2$ and $\mathbf{x}_3$ are support vectors. The boundary rotates until $C = 1/10$, at which point we have $\mathbf{w} = \begin{pmatrix} 1/5 \\ -1/2 \end{pmatrix}$, $t = 1/5$ and the margin has increased to 1.86. Furthermore, we have $\xi_1 = 4/10$ and $\xi_4 = 7/10$, and all multipliers have become equal to C.
- Finally, when C decreases further the decision boundary stays where it is, but the norm of the weight vector gradually decreases and all points become margin errors.

Soft margins

NOTE: a minimal-complexity soft margin classifier summarises the classes by their class means in a way very similar to the basic linear classifier.

Sparse data

- SVM algorithms can be sped up dramatically if the data is *sparse* (i.e. many values are 0)
- Why? Because they compute lots and lots of dot products
- With sparse data dot products can be computed very efficiently
  - Just need to iterate over the values that are non-zero
- SVMs can process sparse datasets with tens of thousands of attributes

Nonlinear SVMs

- Apply same trick: "pseudo attributes" representing attribute combinations
- Overfitting not (such) a (big) problem because the maximum margin hyperplane is stable (only replacement of "support vectors" changes decision boundary)
  - usually few support vectors relative to the size of the training set
  - error bounded by number of support vectors, irrespective of dimensionality
- Efficiency problem remains ?
  - Every time dot product is computed need to go through all the "pseudo attributes"

Kernel trick

- Can avoid computing the "pseudo attributes"!
- Can compute the dot product *before* the nonlinear mapping is performed
- All computatation done in original low-dimensional space
- Instead of computing

$$x = b + \sum_{i \text{ is a support vector}} \alpha_i y_i \mathbf{a}(i) \bullet \mathbf{a}$$

we can compute

$$x = b + \sum_{i \text{ is a support vector}} \alpha_i y_i (\mathbf{a}(i) \bullet \mathbf{a})^n$$

where n is number of factors

Kernel trick

- Corresponds to a map into the instance space spanned by all products of n attributes
- bound α_i to prevent overfitting

This mathematical trick is a general approach to solve non-linearly separable problems by an implicit mapping into the (possibly very) high-dimensional *feature* space. Applies as long as certain conditions are satisfied.
E.g., polynomial *kernel* function

$$K(x, y) = (1 + x \bullet y)^d$$

Next slide: classic example for 2 attributes x_1, x_2 where $d = 2$.

Kernel trick

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right)$$

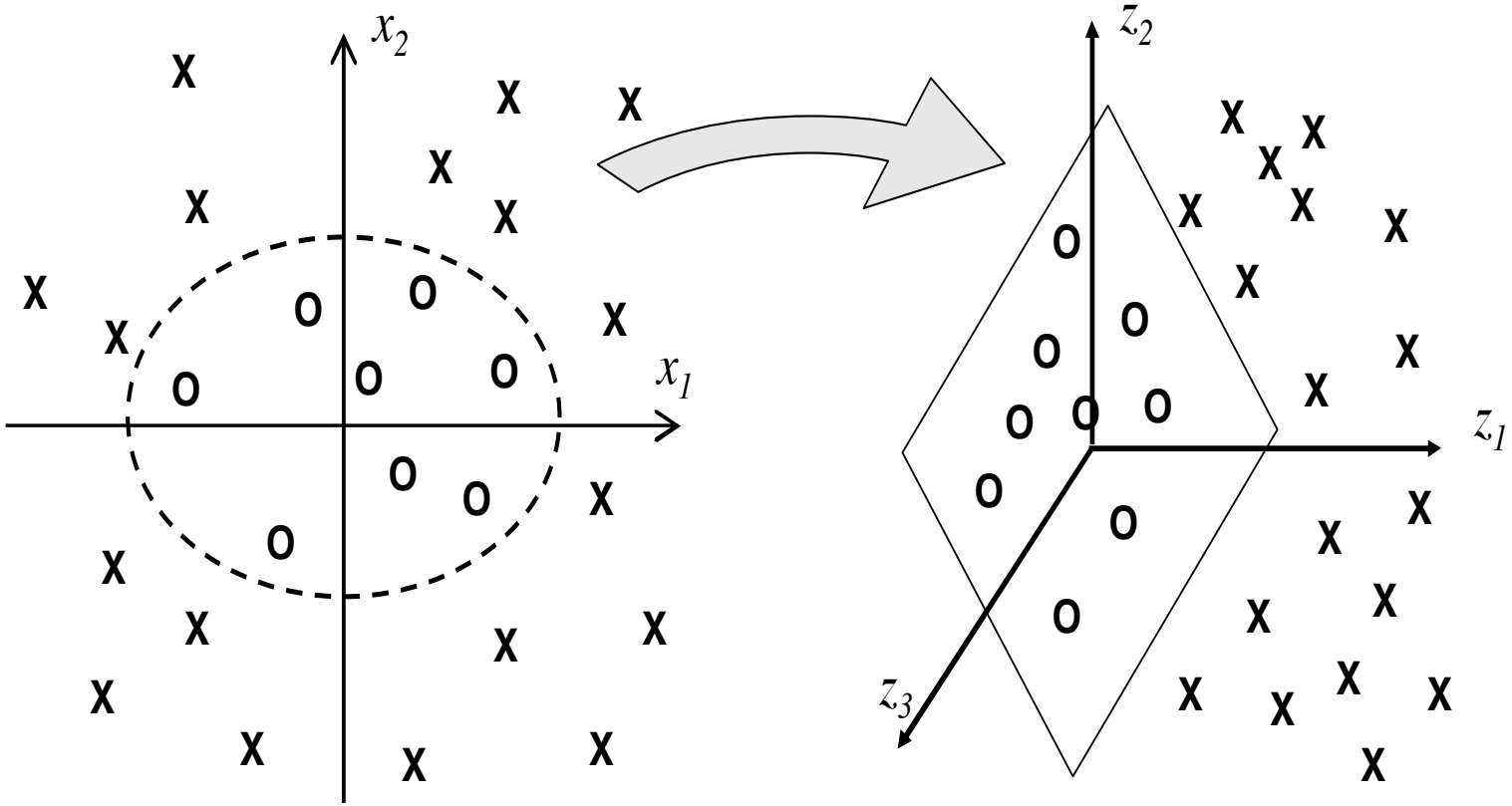


Figure by Avrim Blum, CS Dept, CMU.

Kernel functions

- The mapping is performed by the kernel function
- $(\mathbf{x} \bullet \mathbf{y})^n$ computes dot product of vectors $\mathbf{x}$ and $\mathbf{y}$ and raises them to power n
  - *polynomial kernel*
- Can use other kernel functions than polynomial kernel

$$x = b + \sum_{i \text{ is a support vector}} \alpha_i y_i K(\mathbf{a}(i) \bullet \mathbf{a})$$

- Requirement: $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i) \bullet \phi(\mathbf{x}_j)$
  - must satisfy matrix conditions to be a Mercer kernel

Kernel functions

- Common choices for kernel functions include:
- polynomial kernel of degree d

$$K(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \bullet \mathbf{x}_j + 1)^d$$

- radial basis function kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) = e\frac{-(\mathbf{x}_i \bullet \mathbf{x}_j + 1)^2}{2\sigma^2}$$

- sigmoid kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta \mathbf{x}_i \bullet \mathbf{x}_j + b)$$

'Kernelising' the perceptron

The perceptron algorithm is a simple counting algorithm – the only operation that is somewhat involved is testing whether example $\mathbf{x}_i$ is correctly classified by evaluating $y_i \sum_{j=1}^{|D|} \alpha_j y_j \mathbf{x}_i \cdot \mathbf{x}_j$.

- The key component of this calculation is the dot product $\mathbf{x}_i \cdot \mathbf{x}_j$.
- Assuming bivariate examples $\mathbf{x}_i = (x_i, y_i)$ and $\mathbf{x}_j = (x_j, y_j)$ for notational simplicity, the dot product can be written as $\mathbf{x}_i \cdot \mathbf{x}_j = x_i x_j + y_i y_j$.
- The corresponding instances in the quadratic feature space are $\left(x_i^2, y_i^2\right)$ and $\left(x_j^2, y_j^2\right)$, and their dot product is $\left(x_i^2, y_i^2\right) \cdot \left(x_j^2, y_j^2\right) = x_i^2 x_j^2 + y_i^2 y_j^2$.
- This is almost equal to $(\mathbf{x}_i \cdot \mathbf{x}_j)^2 = (x_i x_j + y_i y_j)^2 = (x_i x_j)^2 + (y_i y_j)^2 + 2 x_i x_j y_i y_j$, but not quite because of the third term of cross-products.
- We can capture this term by extending the feature vector with a third feature $\sqrt{2}xy$.

'Kernelising' the perceptron

This gives the following feature space:

$$\phi(\mathbf{x}_i) = \left(x_i^2, y_i^2, \sqrt{2}x_i y_i\right) \qquad \phi(\mathbf{x}_j) = \left(x_j^2, y_j^2, \sqrt{2}x_j y_j\right)$$

$$\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j) = x_i^2 x_j^2 + y_i^2 y_j^2 + 2x_i x_j y_i y_j = (\mathbf{x}_i \cdot \mathbf{x}_j)^2$$

- We now define $\boldsymbol{\kappa}(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j)^2$, and replace $\mathbf{x}_i \cdot \mathbf{x}_j$ with $\boldsymbol{\kappa}(\mathbf{x}_i, \mathbf{x}_j)$ in the dual perceptron algorithm to obtain the *kernel perceptron*
- This would work for many other kernels satisfying certain conditions.

'Kernelising' the perceptron

Algorithm KernelPerceptron(D, η) // perceptron training algorithm using a ker

Input: labelled training data D in homogeneous coordinates, plus kernel function κ

Output: coefficients α_i defining non-linear decision boundary

$\alpha_i \leftarrow 0$ for $1 \leq i \leq |D|$
converged$\leftarrow$false
while *converged* $=$ false **do**
    converged$\leftarrow$true
    for $i = 1$ to $|D|$ **do**
        if $y_i \sum_{j=1}^{|D|} \alpha_j y_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \leq 0$ **then**
            $\alpha_i \leftarrow \alpha_i + 1$
            converged$\leftarrow$false
        end
    end
end

Other kernels

We can define a polynomial kernel of any degree p as $\boldsymbol{\kappa}(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j)^p$. This transforms a d-dimensional input space into a high-dimensional feature space, such that each new feature is a product of p terms (possibly repeated).

If we include a constant, say $\boldsymbol{\kappa}(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j + 1)^p$, we would get all lower-order terms as well. So, for example, in a bivariate input space and setting $p = 2$ the resulting feature space is

$$\phi(\mathbf{x}) = \left(x^2, y^2, \sqrt{2}xy, \sqrt{2}x, \sqrt{2}y, 1\right)$$

with linear as well as quadratic features.

Other kernels

An often-used kernel is the *Gaussian kernel*, defined as

$$\boldsymbol{\kappa}(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(\frac{-||\mathbf{x}_i - \mathbf{x}_j||^2}{2\sigma^2}\right)$$

where σ is a parameter known as the *bandwidth*.

Notice that the soft margin optimisation problem (above) is defined in terms of dot products between training instances and hence the 'kernel trick' can be applied to SVMs:

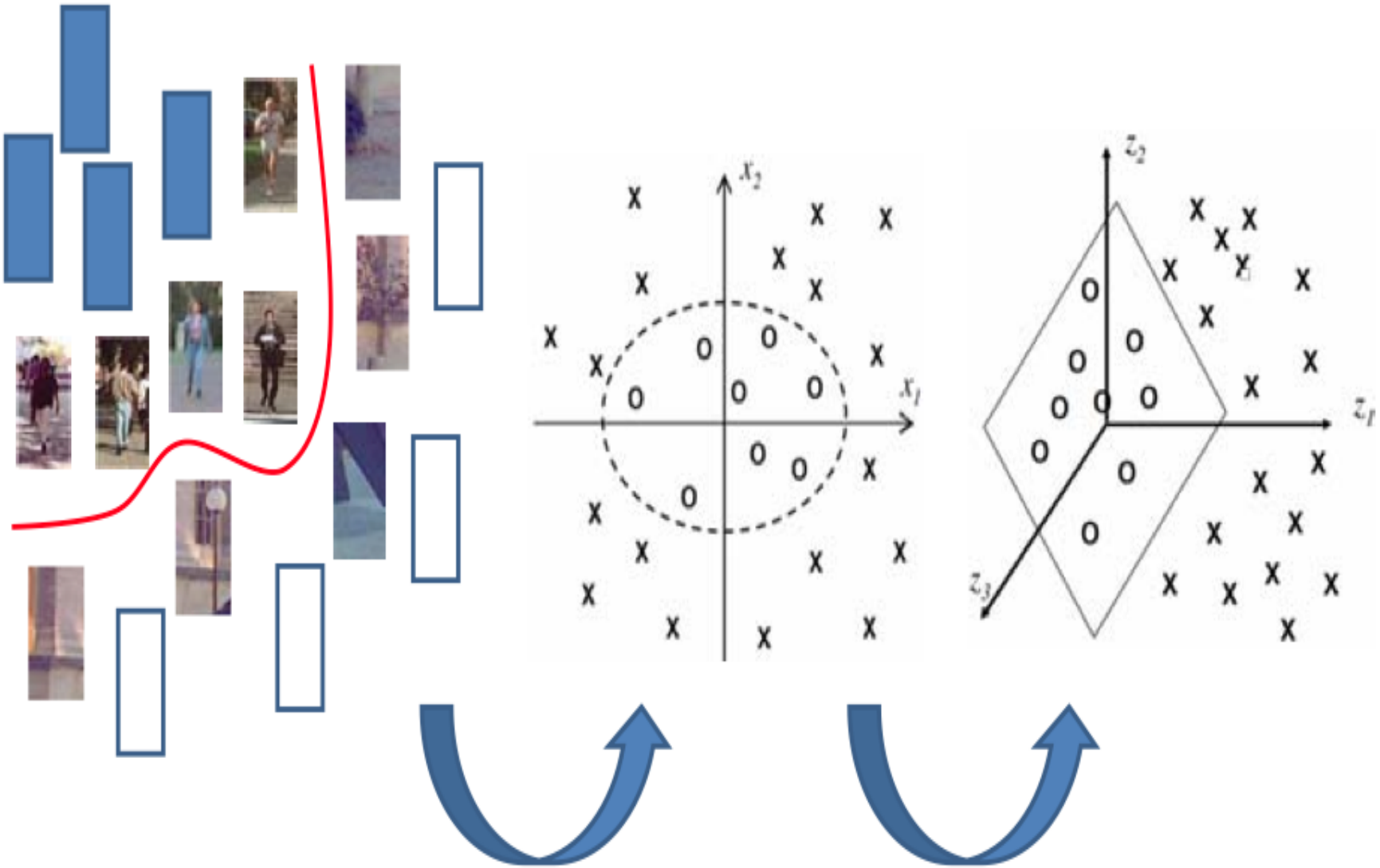
Other kernels

- The decision boundary learned with a non-linear kernel cannot be represented by a simple weight vector in input space. Thus, in order to classify a new example $\mathbf{x}$ we need to evaluate $y_i \sum_{j=1}^{n} \alpha_j y_j \boldsymbol{\kappa}(\mathbf{x}, \mathbf{x}_j)$ which is an $O(n)$ computation involving all training examples, or at least the ones with non-zero multipliers α_j.
- This is why support vector machines are a popular choice as a kernel method, since they naturally promote sparsity in the support vectors.
- Although we have restricted attention to numerical features here, kernels can be defined over discrete structures, including trees, graphs, and logical formulae, opening the way to extending geometric models to non-numerical data.

SVM Applications

- Machine vision: e.g face identification
  - Prior to deep learning, achieves lowest error
- Handwritten digit recognition:
  - Comparable to best alternative
- Bioinformatics: e.g. prediction of protein secondary structure, microarray classification
- Text classification
- Algorithm can be modified to deal with numeric prediction problems – support vector regression

Example - pedestrian detection



Example - classification from gene expression

Data set	# of Samples	Class –1	Class +1
AML vs. ALL (train)	38	27 ALL	11 AML
AML vs. ALL (test)	35	21 ALL	14 AML
B-cell vs. T-cell	23	15 B-cell	8 T-cell
FSC vs. DLCL	77	19 FSC	58 DLCL
GL vs. MD	41	14 GL	27 MD
Lymphoma outcome	58	20 Low risk	38 High ris
Medullo outcome	50	38 Low risk	12 High ris

		Errors			
Data set	Method	Total	Class 1	Class –1	# of genes used
AML vs. ALL	WVA	2	1	1	50
	kNN	3	1	2	10
	SVM	0	0	0	40
B-cell vs. T-cell	WVA	0	0	0	9
	kNN	0	0	0	10
	SVM	0	0	0	10
FSC vs. DLCL	WVA	6	1	5	30
	kNN	3	1	2	200
	SVM	4	2	2	250
GL vs. MD	WVA	1	1	0	3
	kNN	0	0	0	5
	SVM	1	1	0	100
Lymphoma outcome	WVA	15	5	10	12
	KNN	15	8	7	15
	SVM	13	3	10	100
Medullo outcome	WVA	13	6	7	6
	kNN	10	6	4	5
	SVM	7	6	1	50

Summary: Learning with Kernel Methods

- Kernel methods around for a long time in statistics
- Main example of the "optimisation" approach to machine learning
- Kernelisation a "modular" approach to machine learning
- Algorithms that can be kernelised can learn different model classes simply by changing the kernel, e.g., string kernels for sequence data
- SVMs exemplify this – mostly for classification (but also regression, "one-class' classification, etc.)
- SVMs one of the most widely used "off-the-shelf" classifier learning methods, especially for "small n (examples), large p (dimensionality)" classification problems