Support Vector Machines (SVM) in bioinformatics

Day 1:
Introduction to SVM

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3 days outline

- Day 1: Introduction to SVM
- Day 2: Applications in bioinformatics
- Day 3: Advanced topics and current research

Today's outline

1. SVM: A brief overview (FAQ)
2. Simplest SVM: linear classifier for separable data
3. More useful SVM: linear classifiers for general data
4. Even more useful SVM: non-linear classifiers for general data
5. Remarks

Part 1

SVM: a brief overview (FAQ)

What is a SVM?

- a family of learning algorithm for classification of objects into two classes (works also for regression)
- Input: a training set

$$\mathcal{S} = \{(x_1, y_1), \ldots, (x_N, y_N)\}$$

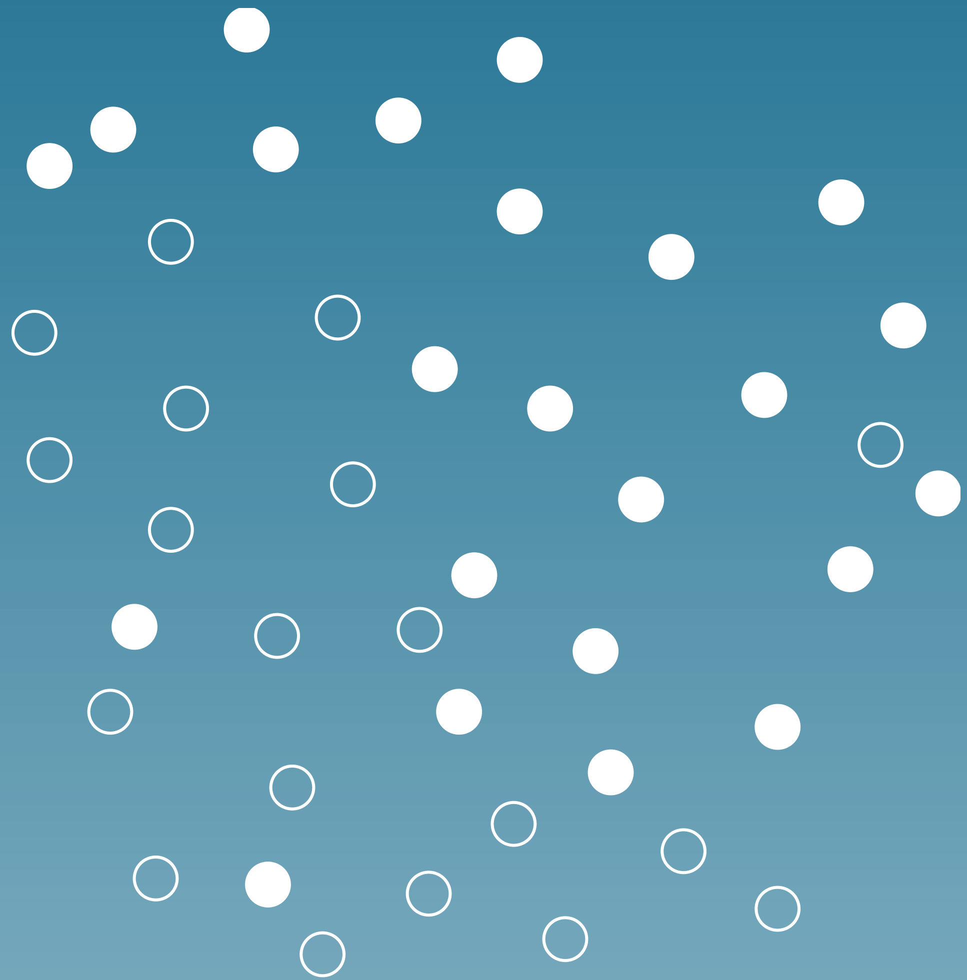
of objects $x_i \in \mathcal{X}$ and their known classes $y_i \in \{-1, +1\}$.

- Output: a classifier $f : \mathcal{X} \to \{-1, +1\}$ which predicts the class $f(x)$ for any (new) object $x \in \mathcal{X}$.

Examples of classification tasks (more tomorrow)

- Optical character recognition: x is an image, y a character.
- Text classification: x is a text, y is a category (topic, spam / non spam...)
- Medical diagnosis: x is a set of features (age, sex, blood type, genome...), y indicates the risk.
- Protein secondary structure prediction: x is a string, y is a secondary structure

Pattern recognition example



Are there other methods for classification?

- Bayesian classifier (based on maximum a posteriori probability)
- Fisher linear discriminant
- Neural networks
- Expert systems (rule-based)
- Decision tree
- ...

Why is it gaining popularity

- Good performance in real-world applications
- Computational efficiency (no local minimum, sparse representation...)
- Robust in high dimension (e.g., images, microarray data, texts)
- Sound theoretical foundations

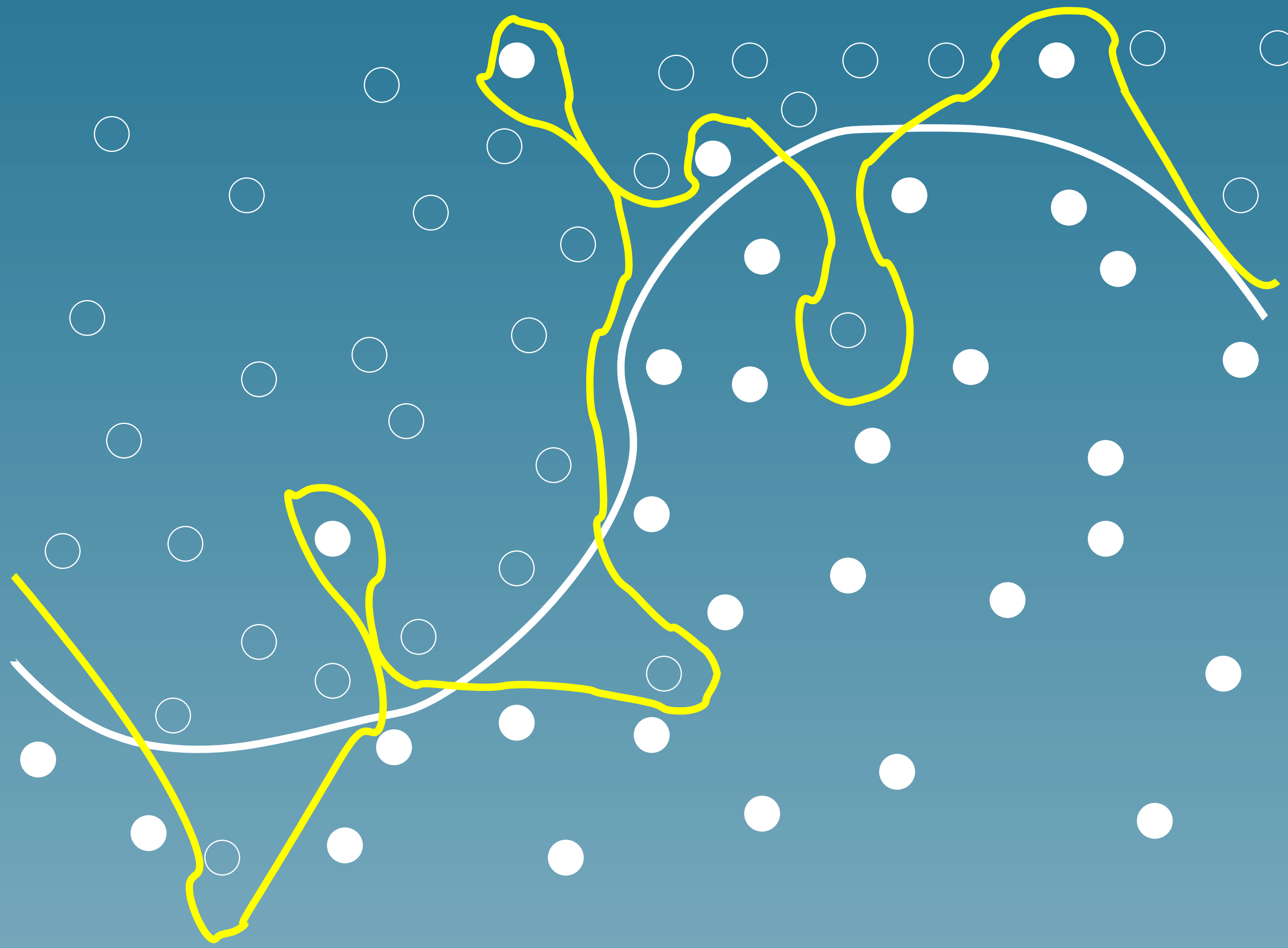
Why is it so efficient?

- Still a research subject
- Always try to classify objects with large confidence, which prevent from overfitting
- No strong hypothesis on the data generation process (contrary to Bayesian approaches)

What is overfitting?

- There is always a trade-off between good classification of the training set, and good classification of future objects (generalization performance)
- Overfitting means fitting too much the training data, which degrades the generalization performance
- Very important in large dimensions, or with complex non-linear classifiers.

Overfitting example



What is Vapnik's Statistical Learning Theory

- The mathematical foundation of SVM
- Gives conditions for a learning algorithm to generalize well
- The "capacity" of the set of classifiers which can be learned must be controlled

Why is it relevant for bioinformatics?

- Classification problems are very common (structure, function, localization prediction; analysis of microarray data; ...)
- Small training sets in high dimension is common
- Extensions of SVM to non-vector objects (strings, graphs...) is natural

Part 2

Simplest SVM:
Linear SVM for separable training sets

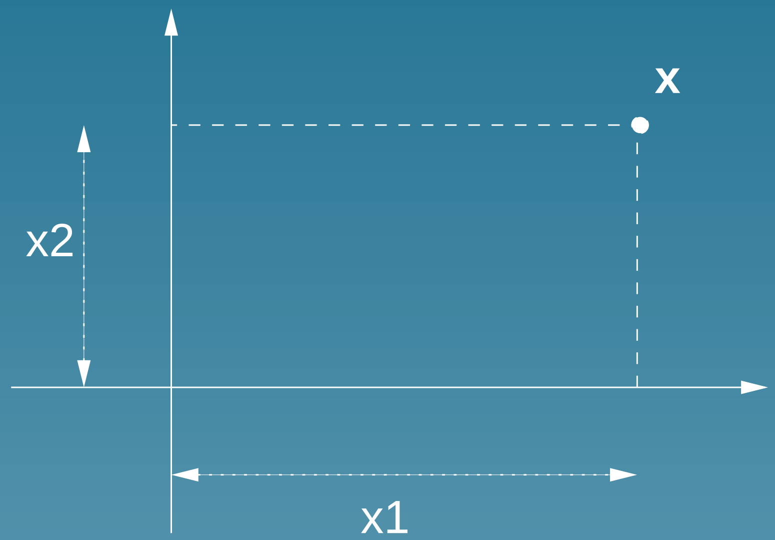
Framework

- We suppose that the object are finite-dimensional real vectors: $\mathcal{X} = \mathbb{R}^n$ and an object is:

$$\vec{x} = (x_1, \ldots, x_m).$$

- x_i can for example be a feature of a more general object
- Example: a protein sequence can be converted to a 20-dimensional vector by taking the amino-acid composition

Vectors and inner product

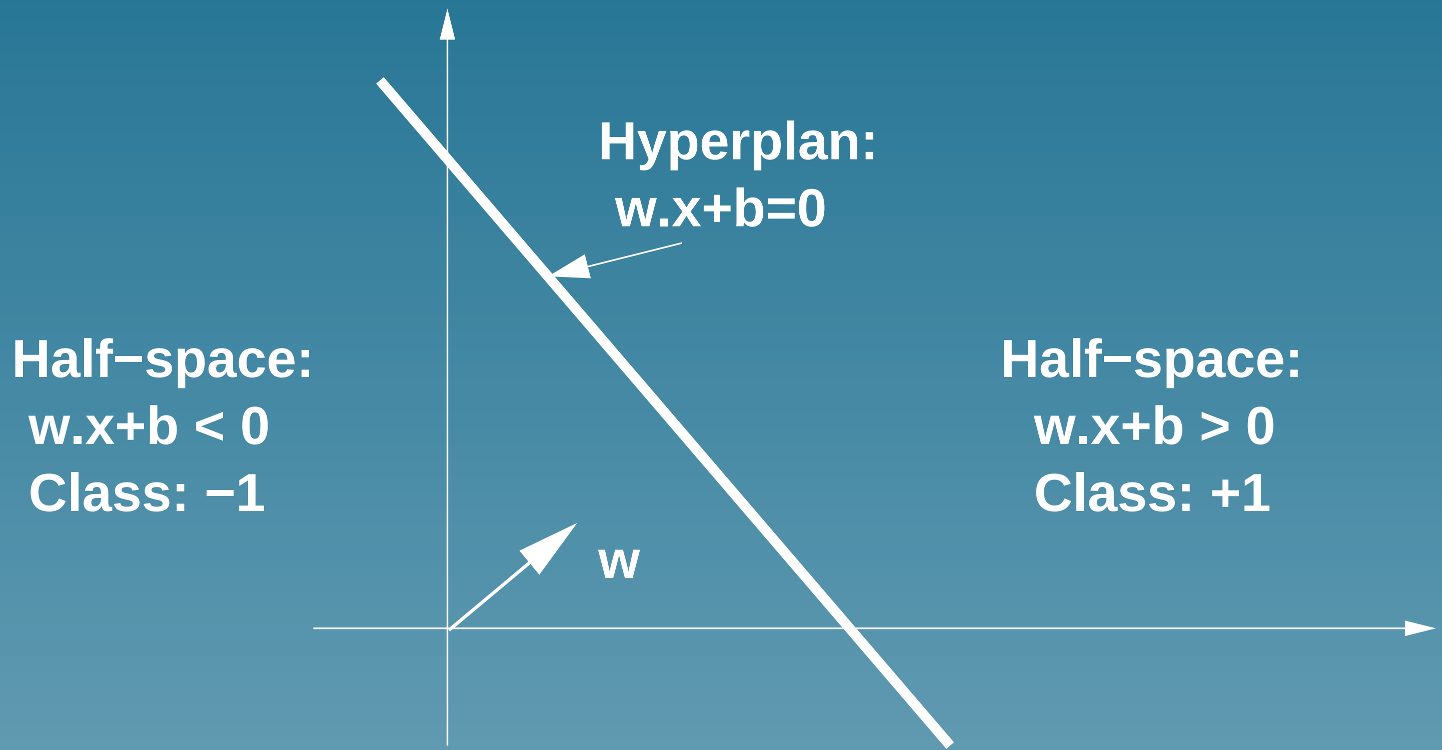


inner product:

$$\vec{x}.\vec{x'} = x_1 x'_1 + x_2 x'_2 \quad (+ \ldots + x_m x'_m) \tag{1}$$

$$= ||\vec{x}||.||\vec{x'}||.\cos(\vec{x}, \vec{x'}) \tag{2}$$

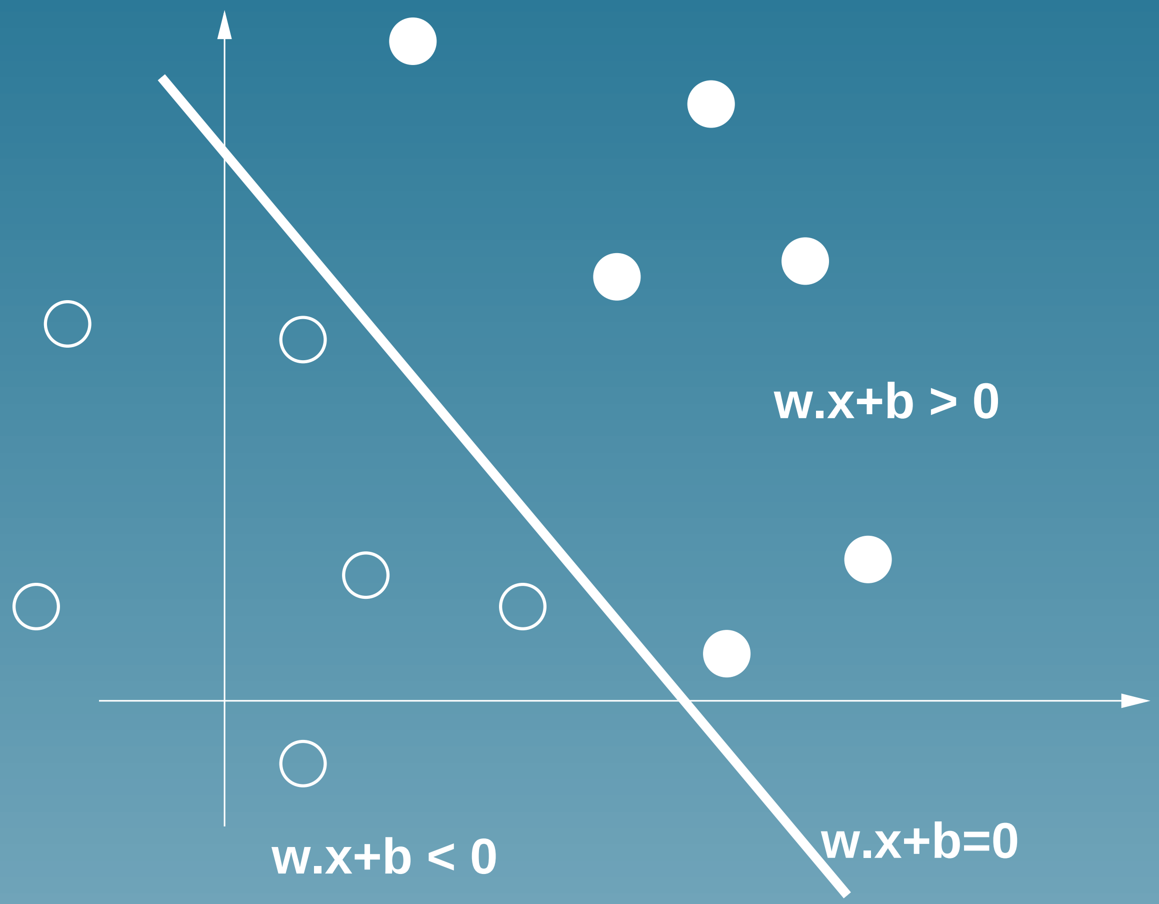
Linear classifier



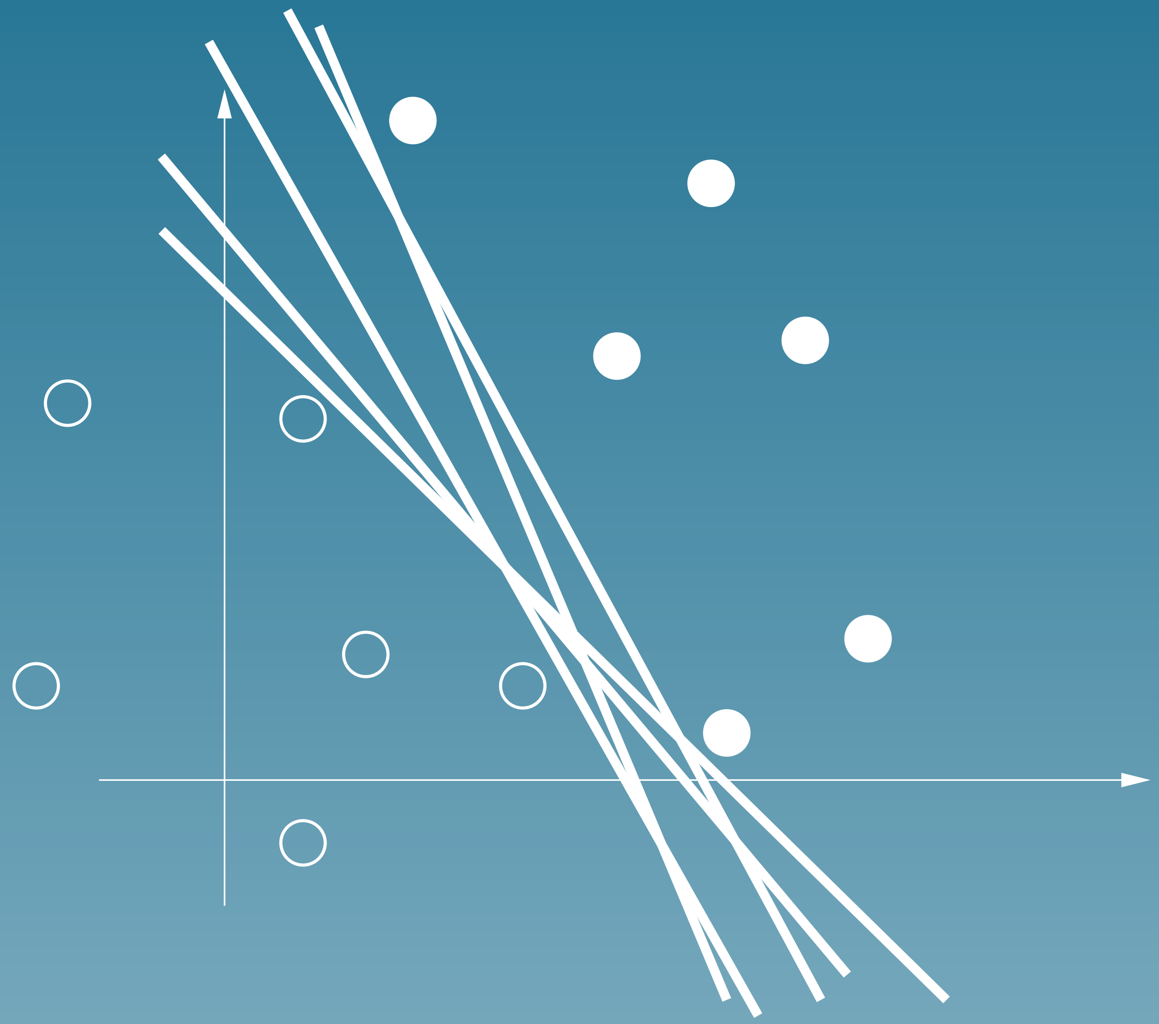
Classification is base on the sign the decision function:

$$f_{\vec{w},b}(\vec{x}) = \vec{w}.\vec{x} + b$$

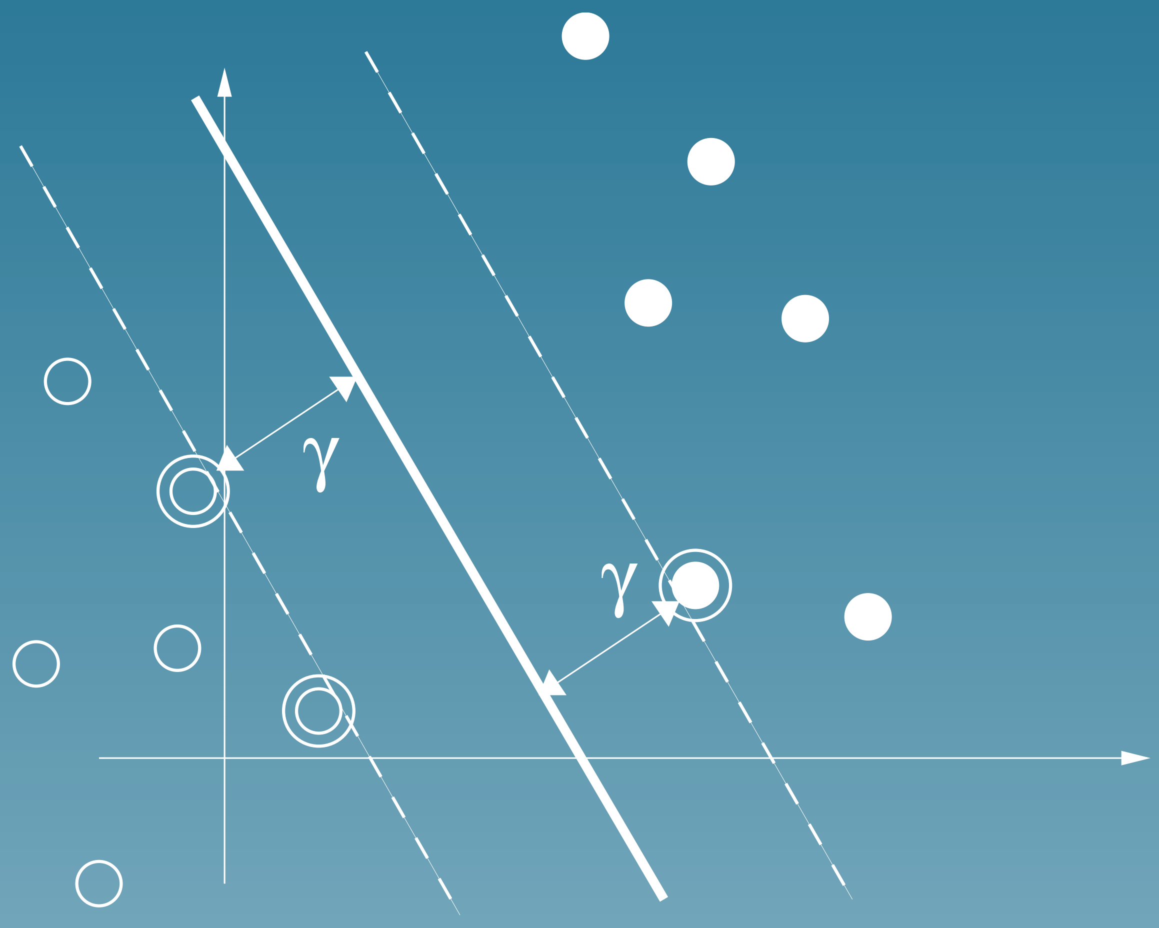
Linearly separable training set



Which one is the best?

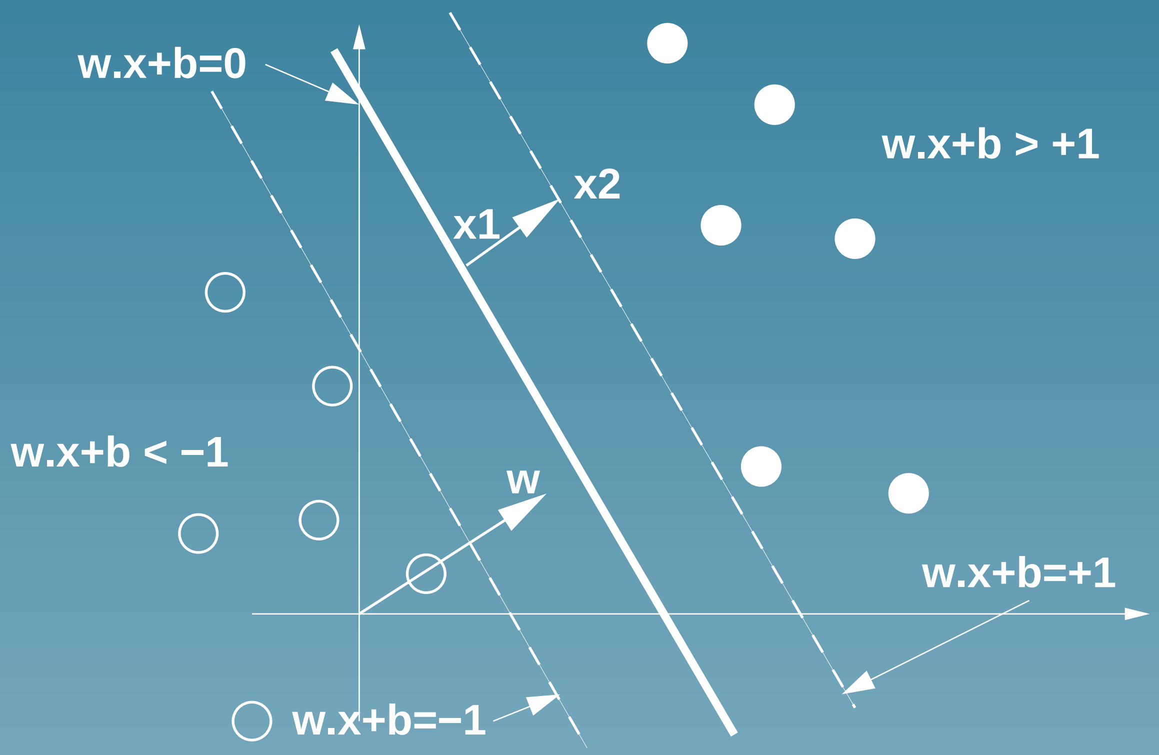


Vapnik's answer : LARGEST MARGIN



How to find the optimal hyperplane?

For a given linear classifier $f_{\vec{w},b}$ consider the tube defined by the values -1 and $+1$ of the decision function:



The width of the tube is $1/||\vec{w}||$

Indeed, the points $\vec{x}_1$ and $\vec{x_2}$ satisfy:

$$\begin{cases} \vec{w}.\vec{x}_1 + b = 0, \\ \vec{w}.\vec{x}_2 + b = 1. \end{cases}$$

By subtracting we get $\vec{w}.(\vec{x}_2 - \vec{x}_1) = 1$, and therefore:

$$\gamma = ||\vec{x}_2 - \vec{x}_1|| = \frac{1}{||\vec{w}||}.$$

All training points should be on the right side of the tube

For positive examples ($y_i = 1$) this means:

$$\vec{w}.\vec{x}_i + b \geq 1$$

For negative examples ($y_i = -1$) this means:

$$\vec{w}.\vec{x}_i + b \leq -1$$

Both cases are summarized as follows:

$$\forall i = 1, \ldots, N, \qquad y_i \left(\vec{w}.\vec{x}_i + b\right) \geq 1$$

Finding the optimal hyperplane

The optimal hyperplane is defined by the pair $(\vec{w}, b)$ which solves the following problem:

Minimize:

$$||\vec{w}||^2$$

under the constraints:

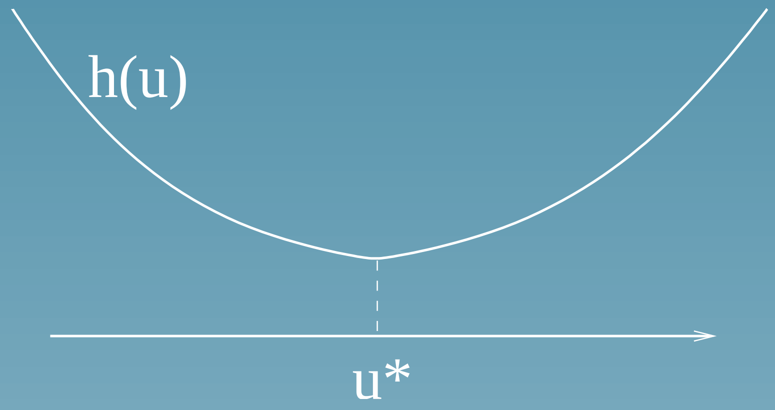
$$\forall i = 1, \ldots, N, \qquad y_i \left(\vec{w}.\vec{x}_i + b \right) - 1 \geq 0.$$

This is a classical quadratic program.

How to find the minimum of a convex function?

If $h(u_1, \ldots, u_n)$ is a convex and differentiable function of n variable, then $\vec{u}^*$ is a minimum if and only if:

$$\nabla h(u^*) = \begin{pmatrix} \frac{\partial h}{\partial u_1}(\vec{u}^*) \\ \vdots \\ \frac{\partial h}{\partial u_1}(\vec{u}^*) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$$



How to find the minimum of a convex function with linear constraints?

Suppose that we want the minimum of $h(u)$ under the constraints:

$$g_i(\vec{u}) \geq 0, \quad i = 1, \ldots, N,$$

where each function $g_i(\vec{u})$ is affine.

We introduce one variable α_i for each constraint and consider the Lagrangian:

$$L(\vec{u}, \vec{\alpha}) = h(\vec{u}) - \sum_{i=1}^{N} \alpha_i g_i(\vec{u}).$$

Lagrangian method (ctd.)

For each $\vec{\alpha}$ we can look for $\vec{u}_\alpha$ which minimizes $L(\vec{u}, \vec{\alpha})$ (with no constraint), and note the dual function:

$$L(\vec{\alpha}) = \min_{\vec{u}} L(\vec{u}, \vec{\alpha}).$$

The dual variable $\vec{\alpha}^*$ which maximizes $L(\vec{\alpha})$ gives the solution of the primal minimization problem with constraint:

$$\vec{u}^* = \vec{u}_{\alpha^*}.$$

Application to optimal hyperplane

In order to minimize:

$$\frac{1}{2}||\vec{w}||^2$$

under the constraints:

$$\forall i = 1, \ldots, N, \qquad y_i \left(\vec{w}.\vec{x}_i + b \right) - 1 \geq 0.$$

we introduce one dual variable α_i for each constraint, i.e., for each training point. The Lagrangian is:

$$L(\vec{w}, b, \vec{\alpha}) = \frac{1}{2}||\vec{w}||^2 - \sum_{i=1}^{N} \alpha_i \left(y_i \left(\vec{w}.\vec{x}_i + b \right) - 1 \right).$$

Solving the dual problem

The dual problem is to find α^* maximize

$$L(\vec{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \vec{x}_i . \vec{x}_j,$$

under the (simple) constraints $\alpha_i \geq 0$ (for $i = 1, \ldots, N$), and

$$\sum_{i=1}^{N} \alpha_i y_i = 0.$$

$\vec{\alpha}^*$ can be easily found using classical optimization softwares.

Recovering the optimal hyperplane

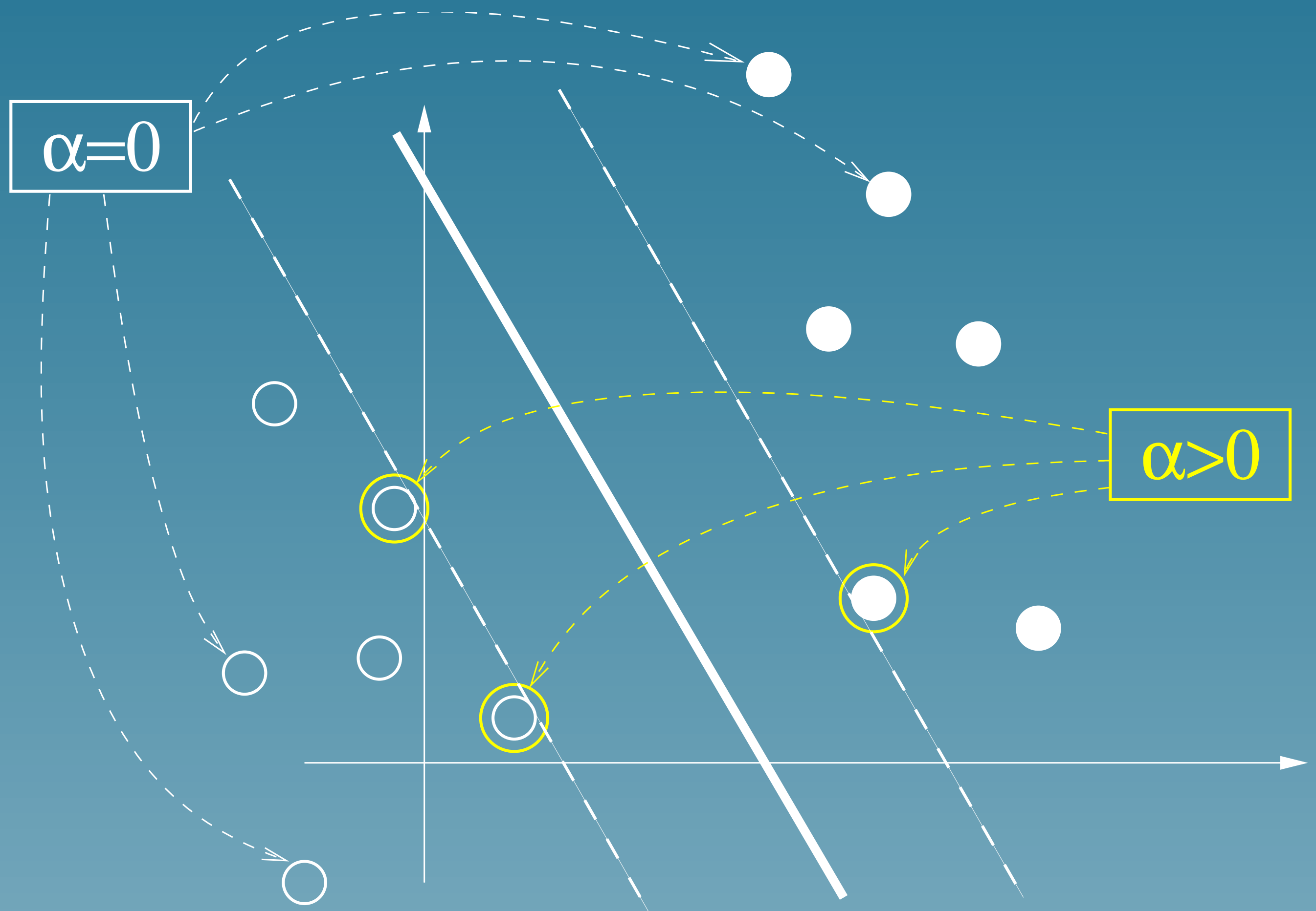
Once $\vec{\alpha}^*$ is found, we recover $(\vec{w}^*, b^*)$ corresponding to the optimal hyperplane. w^* is given by:

$$\vec{w}^* = \sum_{i=1}^{N} \alpha_i \vec{x}_i,$$

and the decision function is therefore:

$$\begin{aligned} f^*(\vec{x}) &= \vec{w}^* . \vec{x} + b^* \\ &= \sum_{i=1}^{N} \alpha_i \vec{x}_i . \vec{x} + b^*. \end{aligned} \tag{3}$$

Interpretation : support vectors



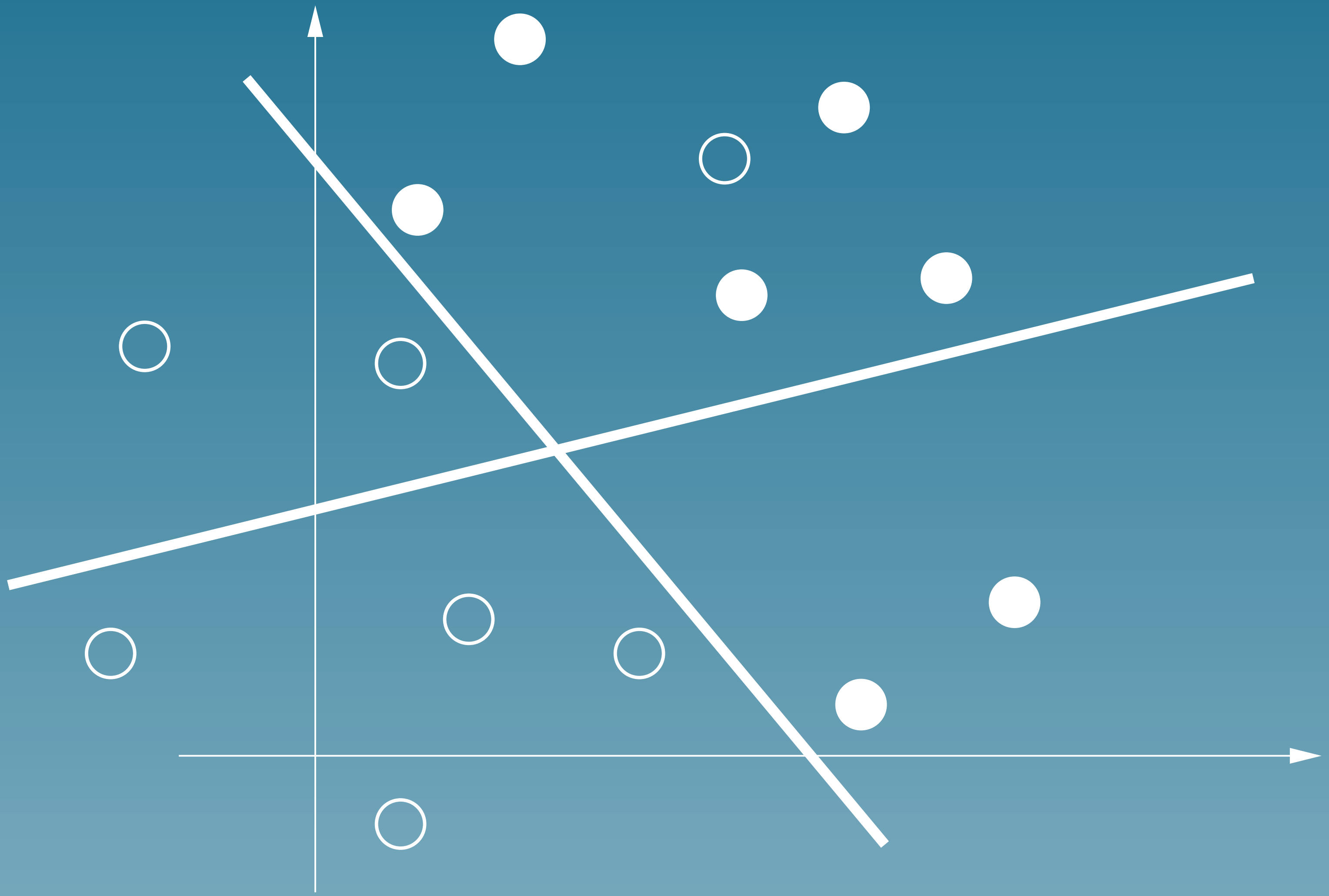
Simplest SVM: conclusion

- Finds the optimal hyperplane, which corresponds to the largest margin
- Can be solved easily using a dual formulation
- The solution is sparse: the number of support vectors can be very small compared to the size of the training set
- Only support vectors are important for prediction of future points. All other points can be forgotten.

Part 3

More useful SVM: Linear SVM for general training sets

In general, training sets are not linearly separable



What goes wrong?

The dual problem, maximize

$$L(\vec{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \vec{x}_i . \vec{x}_j,$$

under the constraints $\alpha_i \geq 0$ (for $i = 1, \ldots, N$), and

$$\sum_{i=1}^{N} \alpha_i y_i = 0,$$

has no solution: the larger some α_i, the larger the function to maximize.

Forcing a solution

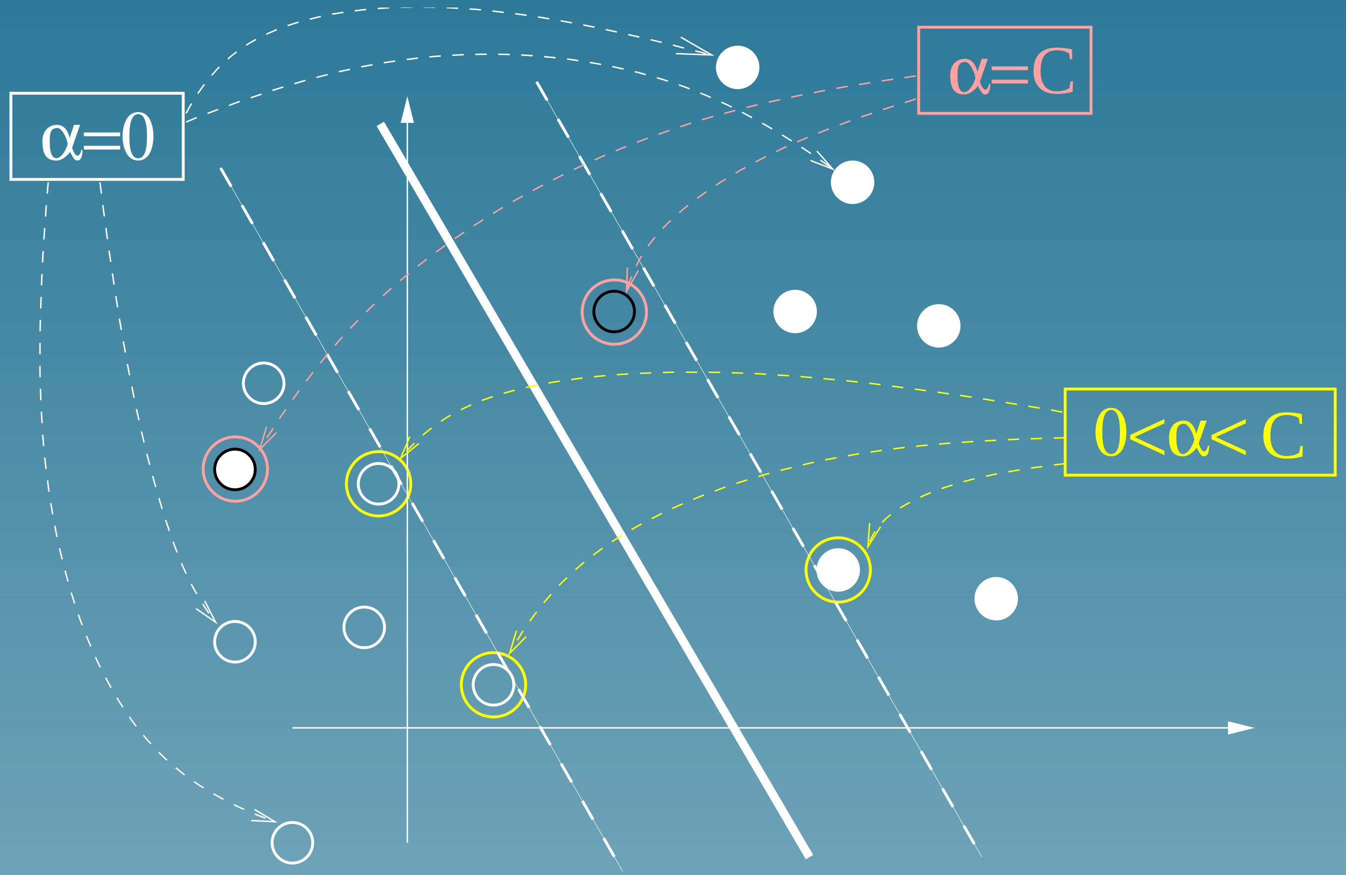
One solution is to limit the range of $\vec{\alpha}$, to be sure that one solution exists. For example, maximize

$$L(\vec{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \vec{x}_i . \vec{x}_j,$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \ldots, N \\ \sum_{i=1}^{N} \alpha_i y_i = 0. \end{cases}$$

Interpretation



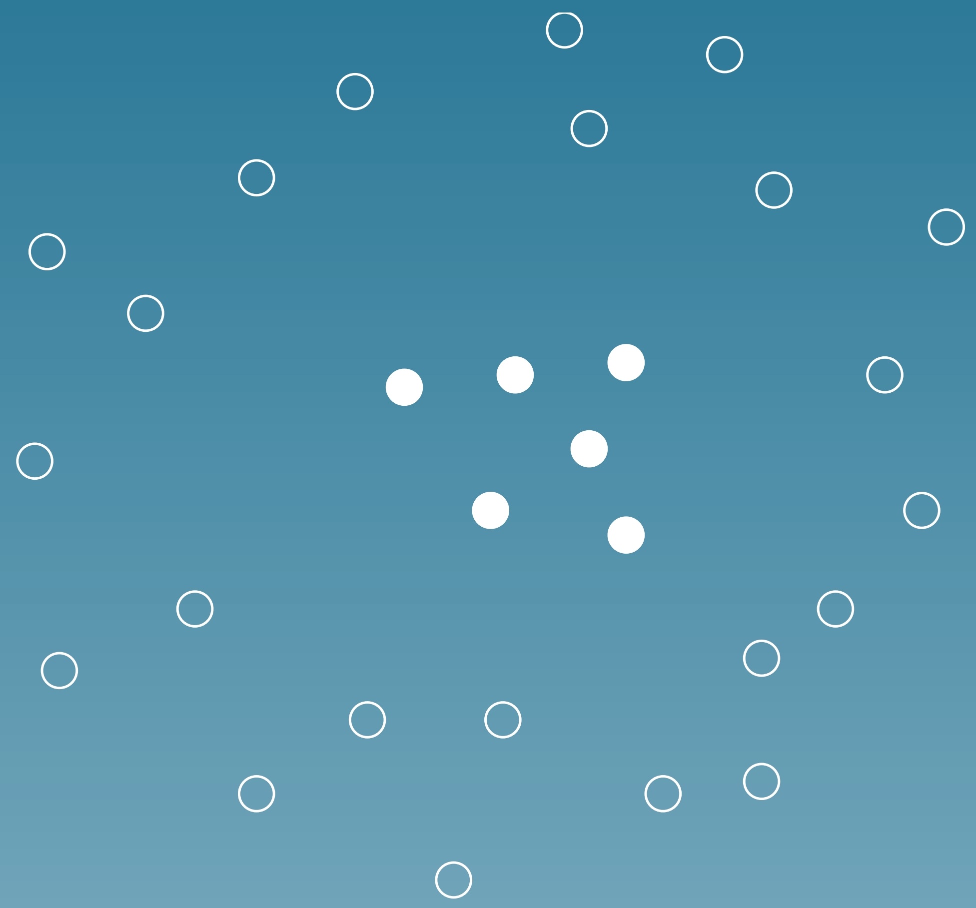
Remarks

- This formulation finds a trade-off between:
  - ⋆ minimizing the training error
  - ⋆ maximizing the margin
- Other formulations are possible to adapt SVM to general training sets.
- All properties of the separable case are conserved (support vectors, sparseness, computation efficiency...)

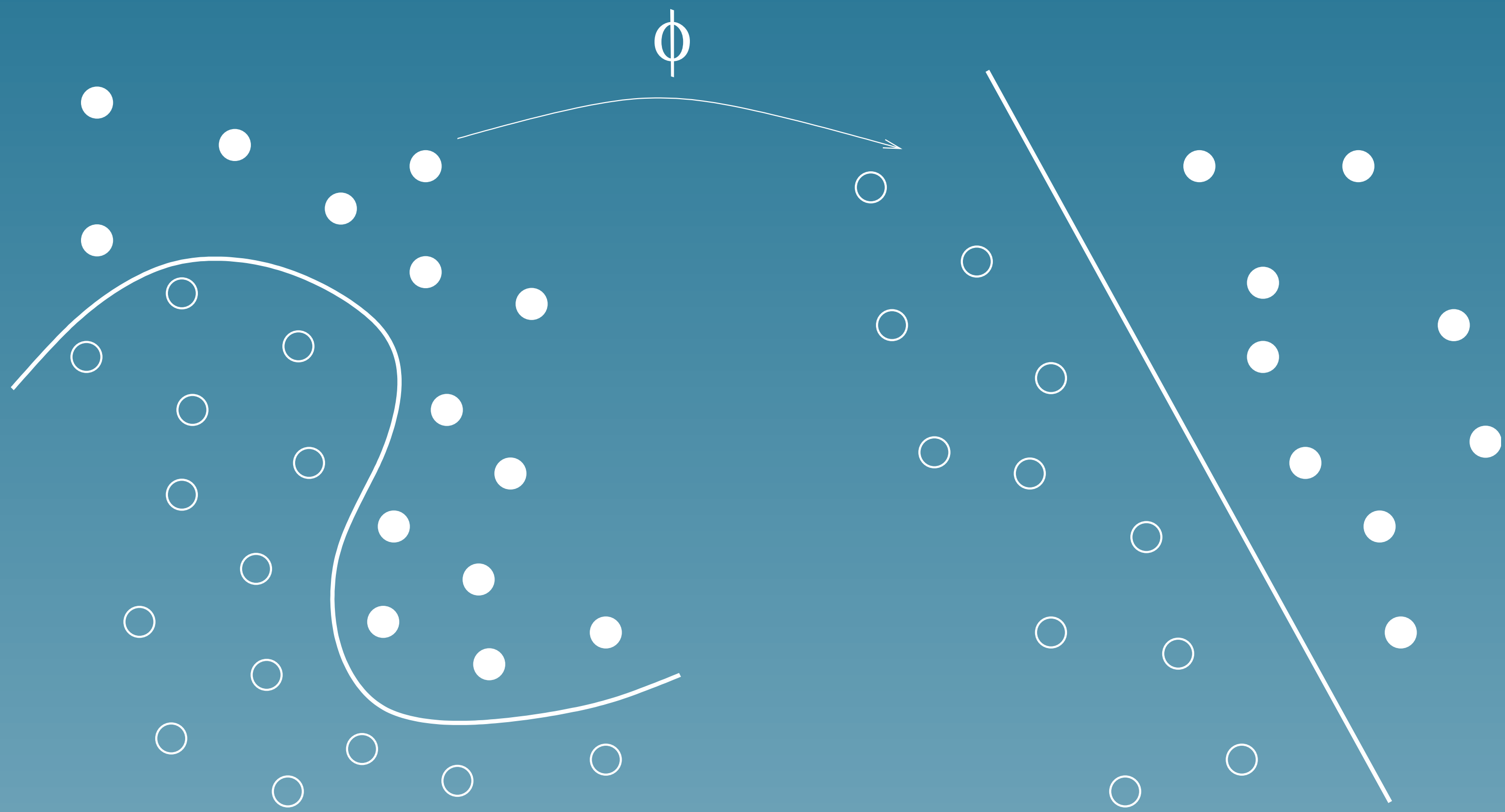
Part 4

General SVM: Non-linear classifiers for general training sets

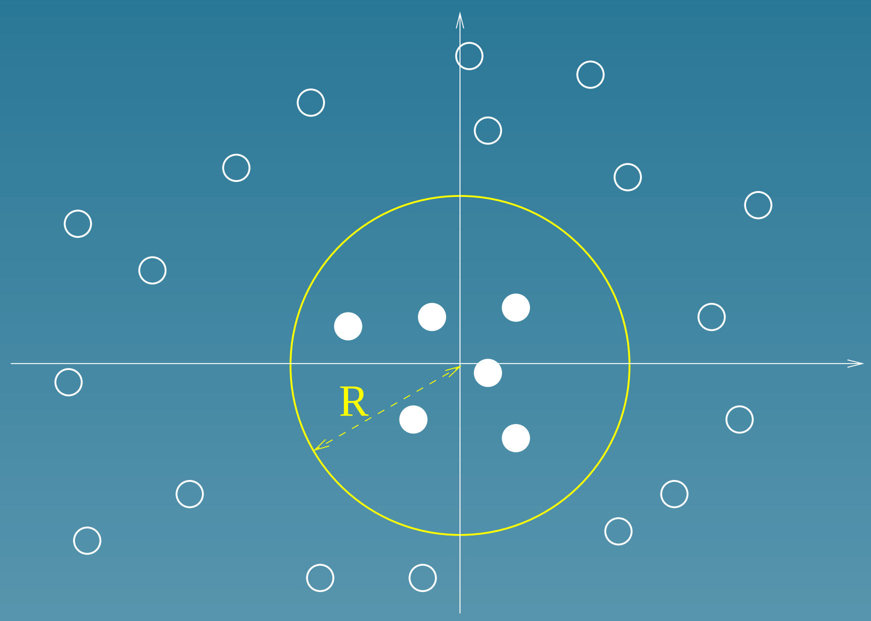
Sometimes linear classifiers are not interesting



Solution: non-linear mapping to a feature space



Example



Let $\Phi(\vec{x}) = (x_1^2, x_2^2)'$, $\vec{w} = (1,1)'$ and $b = 1$. Then the decision function is:

$$f(\vec{x}) = x_1^2 + x_2^2 - R^2 = \vec{w}.\Phi(\vec{x}) + b,$$

Kernel (*simple but important*)

For a given mapping Φ from the space of objects $\mathcal{X}$ to some feature space, the kernel of two objects x and x' is the inner product of their images in the features space:

$$\forall x, x' \in \mathcal{X}, \quad K(x, x') = \vec{\Phi}(x).\vec{\Phi}(x').$$

Example: if $\vec{\Phi}(\vec{x}) = (x_1^2, x_2^2)'$, *then*

$$K(\vec{x}, \vec{x}') = \vec{\Phi}(\vec{x}).\vec{\Phi}(\vec{x}') = (x_1)^2(x_1')^2 + (x_2)^2(x_2')^2.$$

Training a SVM in the feature space

Replace each $\vec{x}.\vec{x}'$ in the SVM algorithm by $K(x, x')$

The dual problem is to maximize

$$L(\vec{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j K(x_i, x_j),$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \ldots, N \\ \sum_{i=1}^{N} \alpha_i y_i = 0. \end{cases}$$

Predicting with a SVM in the feature space

The decision function becomes:

$$\begin{aligned} f(x) &= \vec{w}^{*}.\vec{\Phi}(x) + b^{*} \\ &= \sum_{i=1}^{N} \alpha_i K(x_i, x) + b^{*}. \end{aligned} \tag{4}$$

The kernel trick

- The explicit computation of $\vec{\Phi}(x)$ is not necessary. The kernel $K(x, x')$ is enough. SVM work implicitly in the feature space.

- It is sometimes possible to easily compute kernels which correspond to complex large-dimensional feature spaces.

Kernel example

For any vector $\vec{x} = (x_1, x_2)'$, consider the mapping:

$$\Phi(\vec{x}) = \left(x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1\right)'.$$

The associated kernel is:

$$\begin{aligned} K(\vec{x}, \vec{x}') &= \Phi(\vec{x}).\Phi(\vec{x}') \\ &= (x_1x_1' + x_2x_2' + 1)^2 \\ &= (\vec{x}.\vec{x}' + 1)^2 \end{aligned}$$

Classical kernels for vectors

- Polynomial:

$$K(x, x') = (x.x' + 1)^d$$

- Gaussian radial basis function

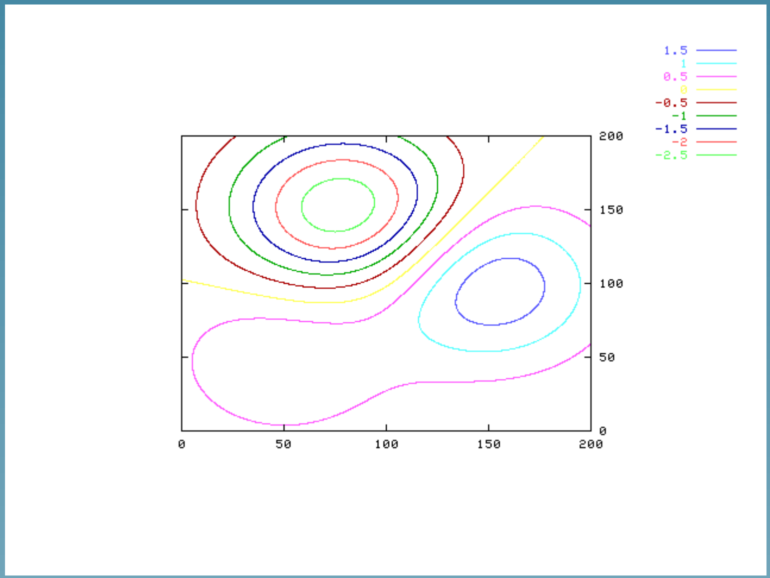
$$K(x, x') = \exp\left(\frac{||x - x'||^2}{2\sigma^2}\right)$$

- Sigmoid

$$K(x, x') = \tanh(\kappa x.x' + \theta)$$

Example: classification with a Gaussian kernel

$$f(\vec{x}) = \sum_{i=1}^{N} \alpha_i \exp\left(\frac{||\vec{x} - \vec{x}_i||^2}{2\sigma^2}\right)$$



Part 4

Conclusion (day 1)

Conclusion

- SVM is a simple but extremely powerful learning algorithm for binary classification
- The freedom to choose the kernel offers wonderful opportunities (see day 3: one can design kernels for non-vector objects such as strings, graphs...)
- More information : `http://www.kernel-machines.org`
- Lecture notes (draft) on my homepage