Kernel-Based Learning & Multivariate Modeling

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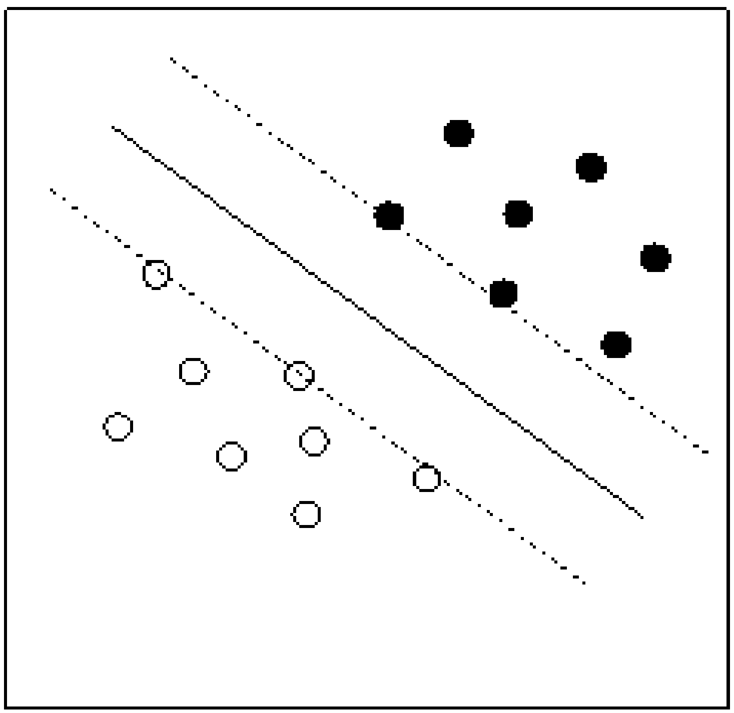
Kernel-Based Learning & Multivariate Modeling

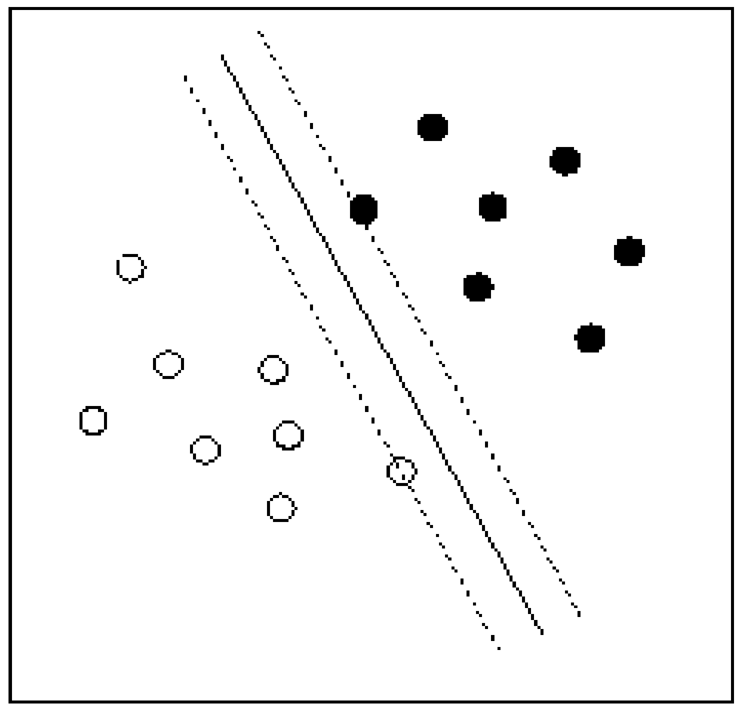
Syllabus

Sep 10 Introduction to kernel-based learning
Sep 17 The SVM for classification, regression & novelty detection (I)
Oct 01 The SVM for classification, regression & novelty detection (II)
Oct 08 Kernel design (I): theoretical issues
Oct 15 Kernel design (II): practical issues
Oct 22 Kernelizing ML & stats algorithms
Oct 29 Advanced topics

Support Vector Machines

Preliminaries


(a) Larger margin


(b) Smaller margin

Which solution is more likely to lead to better **generalization**?

Support Vector Machines

Preliminaries

- Criterion for building a two-class classifier:

  Maximize the **margin = width of the separation** between the classes, defined by the distance to the nearest training examples

- **Working Hypotheses**:

  1. The data are linearly separable ("linsep") –very unlikely, but see later

  2. The larger the margin, the better the generalization (a first intuition)

Goal: find the separating hyperplane with the **largest margin**

Support Vector Machines

Preliminaries

For a two-class classifier, the **VC dimension** ϑ is the maximum number of points that can be separated in all possible 2^{ϑ} ways (**shattered**) by using functions representable by the classifier.

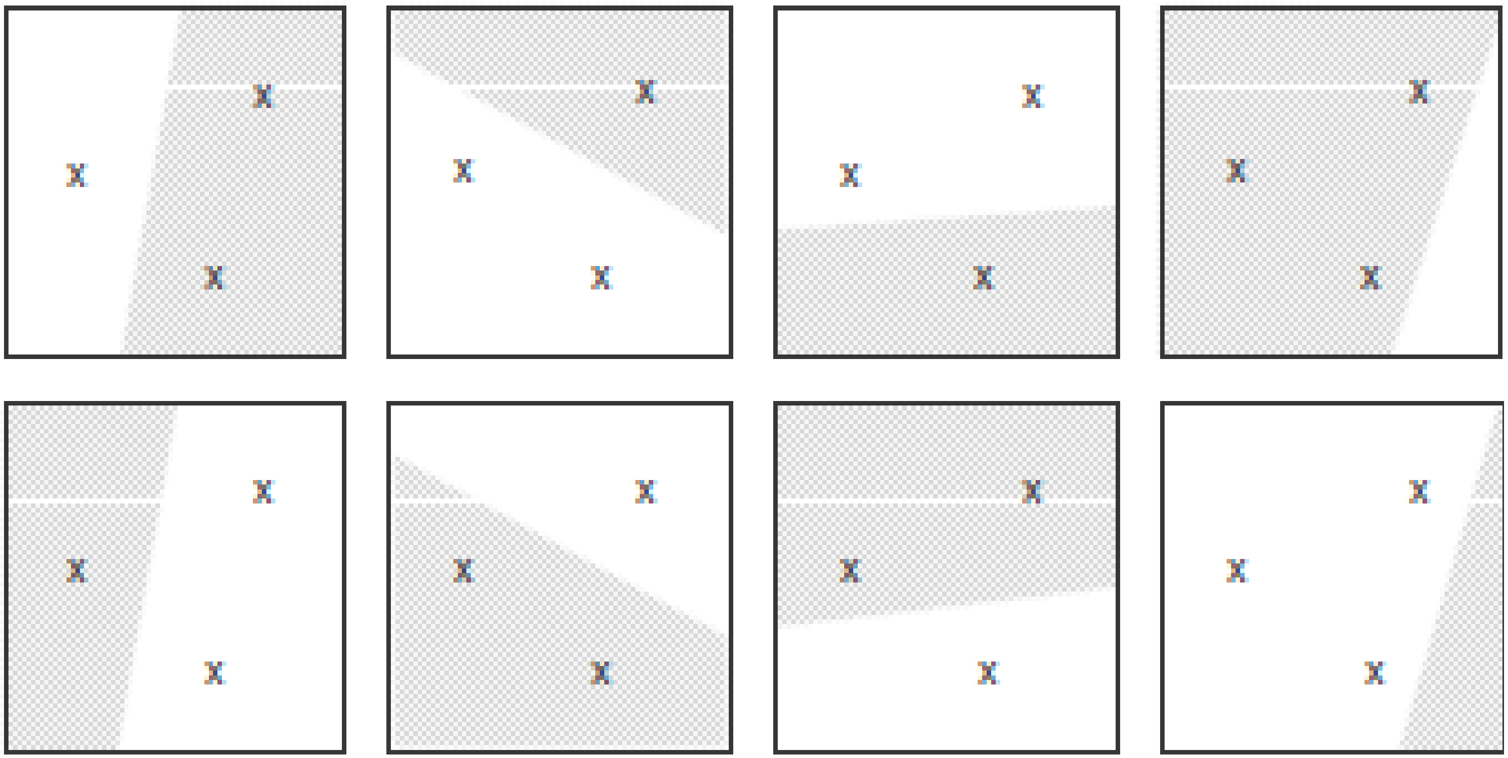
- Note it is *sufficient* that one set of ϑ points exists that can be shattered for the VC dimension to be at least ϑ

- If the VC dimension of a class is ϑ, this means there is at least one set of ϑ points that can be shattered by members of the class. It does not mean that every set of ϑ points can be shattered

- If no set of $\vartheta + 1$ points can be shattered by members of the class, then the VC dimension of the class is at most ϑ

Support Vector Machines

An example



- In $\mathbb{R}^2$ we can shatter these three points (VC dim is ≥ 3)

- No set of four or more points can be shattered (VC dim is < 4)

Support Vector Machines

Why is the VC dimension relevant?

Theorem (Vapnik and Chervonenkis, 1974). Let D be an i.i.d data sample of size n and $\mathcal{Y}$ a class of parametric binary classifiers. Let ϑ denote the VC dimension of $\mathcal{Y}$. Take $y \in \mathcal{Y}$ with empirical error $R_n(y)$ on D. For all $\eta > 0$ it holds true that, with probability at least $1 - \eta$, the true error of y is bounded by:

$$R(y) \leq R_n(y) + H(n, \vartheta, \eta)$$

where

$$H(n, \vartheta, \eta) = \sqrt{\frac{\vartheta(\ln(2n/\vartheta) + 1) - \ln(\eta/4)}{n}}$$

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Formalisation

We have a data set $D = \{(\boldsymbol{x}_1, t_1), \ldots, (\boldsymbol{x}_n, t_n)\}$, with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $t_i \in \{-1, +1\}$, describing a two-class problem.

We wish to find a linear function f which best models D:

- Set up an **affine function** $g(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b$

- Obtain a **linear discriminant** as $f(\boldsymbol{x}) = \text{sgn}(g(\boldsymbol{x}))$

- We would like to find $\boldsymbol{w}, b$ such that:

  $\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b > 0$, when $t_i = +1$
  $\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b < 0$, when $t_i = -1$

  that is $t_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) > 0$ or simply $t_i \, g(\boldsymbol{x}_i) > 0 \qquad (1 \le i \le n)$

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Formalisation

- The quantity $t_i\, g(\boldsymbol{x}_i)$ is called the **functional margin** of $\boldsymbol{x}_i$ (there will be an "error" whenever $t_i\, g(\boldsymbol{x}_i) < 0$)

- Define the **loss** $L(t_i, \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle) := \max(1 - t_i\, g(\boldsymbol{x}_i), 1)$

- Given the plane $\pi : g(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b = 0$, the distance $d(\boldsymbol{x}, \pi) = \frac{|g(\boldsymbol{x})|}{\|\boldsymbol{w}\|}$ is called the **geometrical margin** of $\boldsymbol{x}$.

- The **optimal separating hyperplane** (OSH) for linsep data is the one that maximizes the geometrical margin:

$$\max_{\boldsymbol{w},b} \left\{ \min_{1 \le i \le n} d(\boldsymbol{x}_i, \pi) \right\} \qquad \text{subject to } t_i\,(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) > 0 \ (1 \le i \le n)$$

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Formalisation

- Rescaling $\boldsymbol{w}, b$ such that $|\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b| = 1$ for the points closest to the hyperplane, we obtain $|\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b| \geq 1$. The **support vectors** (SVs) are those $\{\boldsymbol{x}_i \ / \ |\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b| = 1\}$.

- The new loss is $\max(1 - t_i\, g(\boldsymbol{x}_i), 0) =: (1 - t_i\, g(\boldsymbol{x}_i))_+$ (**hinge loss**)

- The **margin** is twice the distance of any SV to the plane π:

  $2\, d(\boldsymbol{x}_{\mathsf{SV}}, \pi) = 2/\|\boldsymbol{w}\|$, since $|g(\boldsymbol{x}_{\mathsf{SV}})| = 1$

- Therefore we find the **canonical** OSH by solving

$$\max_{\boldsymbol{w}, b} \left\{ \frac{2}{\|\boldsymbol{w}\|} \quad / \quad t_i\, (\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \geq 1, \qquad 1 \leq i \leq n \right\}$$

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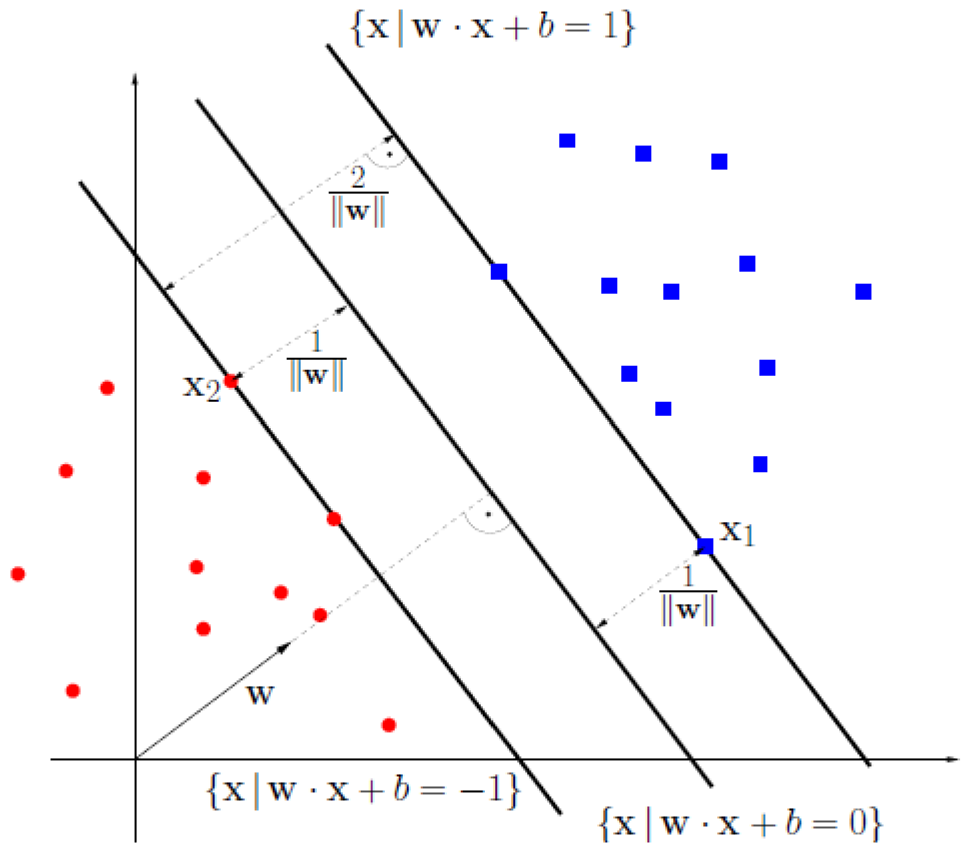
Geometrical view of the OSH



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A look on what's to come

1. The solution for $\boldsymbol{w}$ can be expressed as $\boldsymbol{w} = \sum_{i=1}^{n} t_i \alpha_i \boldsymbol{x}_i$, $\alpha_i \geq 0$.

   (as a consequence of the **Representer theorem**)

2. A fraction of the training data vectors will have $\alpha_i = 0$ (**sparsity**, as a consequence of the chosen error function)

3. The $\boldsymbol{x}_i$ for which $\alpha_i > 0$ will coincide with the **support vectors**

4. The **discriminant function** (classifier) is written

$$f_{\mathsf{SVM}}(\boldsymbol{x}) = \mathrm{sgn}(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b) = \mathrm{sgn}\left(\sum_{i=1}^{n} t_i \alpha_i \langle \boldsymbol{x}, \boldsymbol{x}_i \rangle + b \right)$$

Support Vector Machines

More than an intuition

- Separating hyperplanes in $\mathbb{R}^d$ have VC dimension $d+1$

- When we use a feature map into a very high dimension $D \in (\mathbb{N} \cup \{\infty\})$, VC dimension will grow accordingly

- If we bound the margin of the hyperplanes, we limit VC dimension (therefore, we have an explicit control on complexity)

Support Vector Machines

More than an intuition

Theorem. Consider canonical hyperplanes $f(\boldsymbol{x}) = \mathrm{sgn}(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b)$ and a data set $D = \{(\boldsymbol{x}_1, t_1), \ldots, (\boldsymbol{x}_n, t_n)\}$, with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $t_i \in \{-1, +1\}$. The **subclass** of linear classifiers with margin $m \geq m_0$ has VC dimension ϑ bounded by

$$\vartheta \leq \min\left(\left\lceil \frac{R^2}{m_0^2} \right\rceil, d\right) + 1$$

where R is the radius of the smallest sphere centered at the origin containing the $\boldsymbol{x}_i$.

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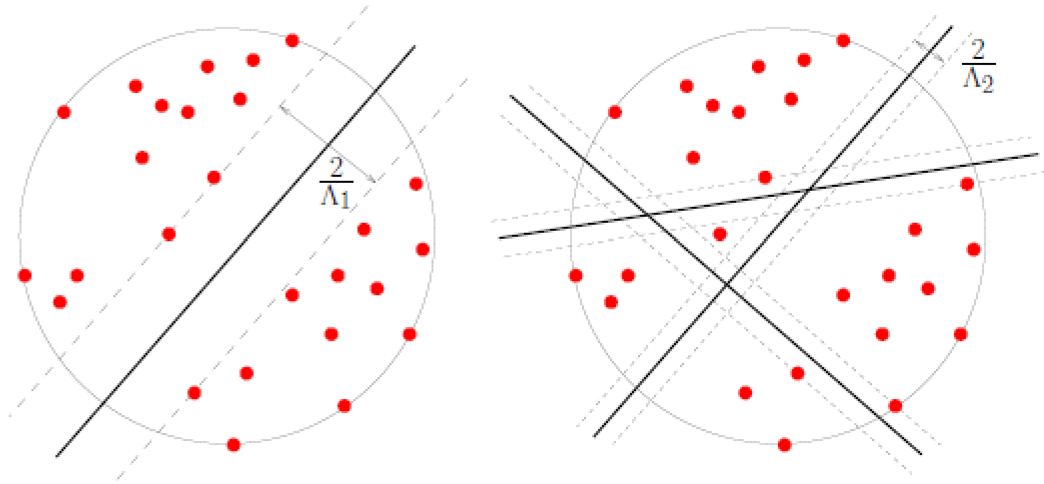
More than an intuition



- Left: hyperplanes with a large margin have reduced chances to separate the data (the VC dimension is small)

- Right: smaller margins allow more separating hyperplanes (the VC dimension is large)

Support Vector Machines

Formulation

$$\underset{\boldsymbol{w},b}{\textbf{minimize}} \qquad \frac{1}{2}\|\boldsymbol{w}\|^2$$

$$\textbf{subject to } t_i\left(\langle \boldsymbol{w}, \boldsymbol{x}_i\rangle + b\right) \geq 1, \qquad 1 \leq i \leq n$$

This is solved (numerically) by QP techniques:

- Quadratic (therefore convex) function subject to linear constraints
- Unique solution (or set of equivalent ones)
- Therefore, no local minima

Support Vector Machines

Formulation

For the set of constraints to be satisfied, the data set must be linsep; this is a very unrealistic requirement in practice

- We could aim at minimizing the **number of** violated constraints $|\{n \ \ / \ \ t_i\,(\langle \boldsymbol{w}, \boldsymbol{x}_i\rangle + b) < 1\}|$, but this turns out to be NP-hard ...

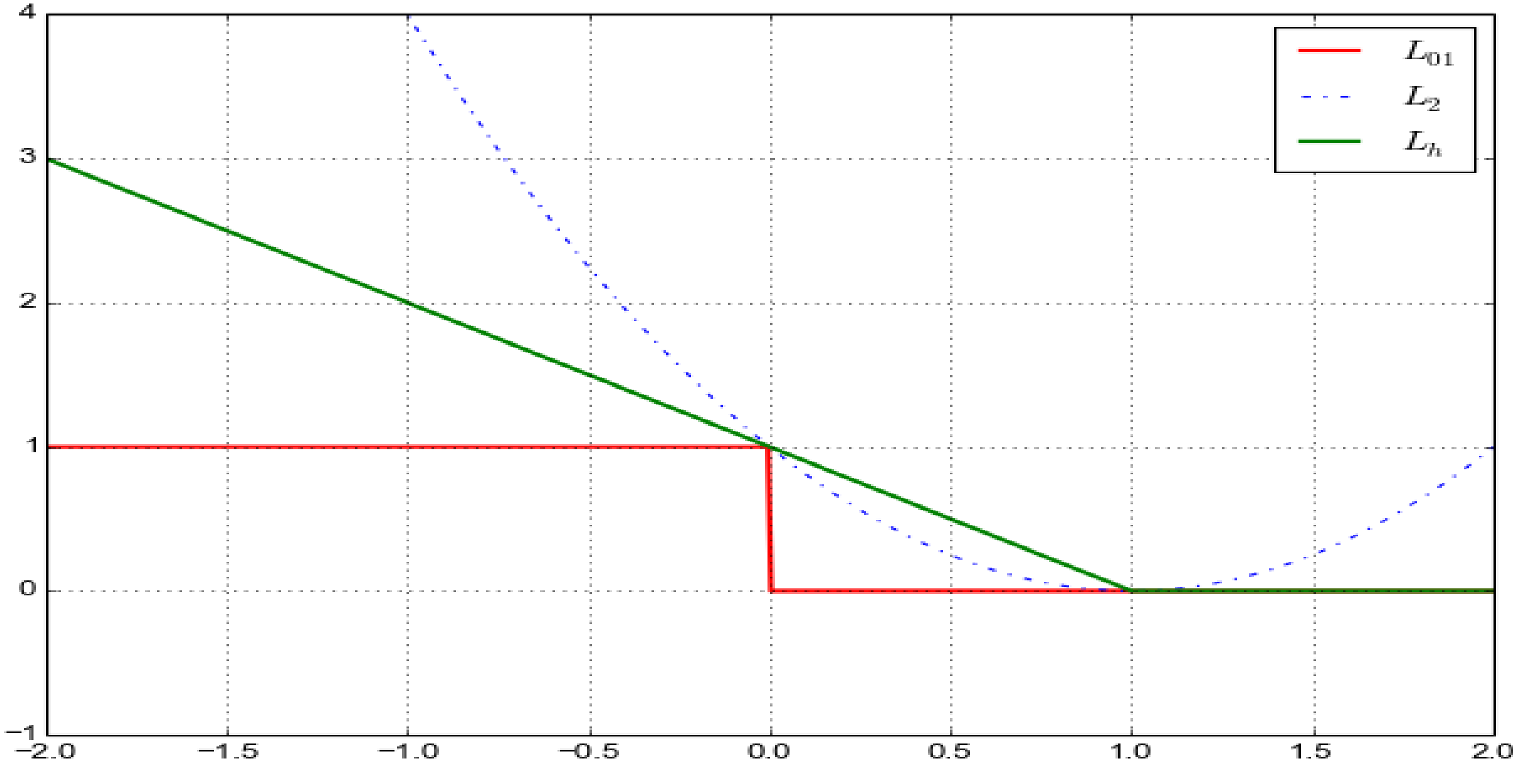
- Instead, we can minimize a convex function of $\boldsymbol{w}$:

$$\underset{\boldsymbol{w},b}{\textbf{minimize}} \qquad \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{n}(1 - t_i\, g(\boldsymbol{x}_i))_+, \qquad C > 0$$

- Yes, the new term is the total **hinge loss**!

Support Vector Machines

Formulation



L_{01} is the 0/1 loss; L_2 is the square loss; L_h is the hinge loss

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Margin violations

- This problem is rewritten as another QP, by introducing a set of margin violations ε_i –called **slack** variables–, for each $\boldsymbol{x}_i$:

$$\underset{\boldsymbol{w},b,\{\varepsilon_i\}}{\textbf{minimize}} \qquad \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{n}\varepsilon_i$$

$$\textbf{subject to } t_i\left(\langle \boldsymbol{w}, \boldsymbol{x}_i\rangle + b\right) \geq 1 - \varepsilon_i \textbf{ and } \varepsilon_i \geq 0 \ (1 \leq i \leq n)$$

- This is a **soft** margin ($\varepsilon_i > 0$ implying $\boldsymbol{x}_i$ would violate the original constraint)
- For a training error to occur $\varepsilon_i > 1$ and so $\sum_{i=1}^{n}\varepsilon_i$ is an upper bound on the number of training errors
- The optimal slacks satisfy $\varepsilon_i = (1 - t_i\, g(\boldsymbol{x}_i))_+$

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Excursion: Lagrange multipliers

The famous method of Lagrange multipliers allows the optimization of smooth functions subject to **equality constraints**.

The Karush, Kuhn and Tucker (KKT) theory extends Lagrange's method to include **inequality constraints**.

Consider the problem of minimizing $f(\boldsymbol{x})$ in a convex $\Omega \subset \mathbb{R}^d$, subject to:

- $g_j(\boldsymbol{x}) \leq 0$ affine functions, $1 \leq j \leq k$
- $h_j(\boldsymbol{x}) = 0$ affine functions, $1 \leq j \leq l$

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Excursion: Lagrange multipliers

Define the **Lagrangian** as:

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\boldsymbol{x}) + \sum_{j=1}^{k} \alpha_j g_j(\boldsymbol{x}) + \sum_{j=1}^{l} \beta_j h_j(\boldsymbol{x})$$

where f, g_j, h_j are continuously differentiable functions.

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Excursion: Lagrange multipliers

Theorem. Necessary and sufficient conditions for a point $\boldsymbol{x}^*$ to be an optimum are the existence of $\boldsymbol{\alpha}^* \in \mathbb{R}^k$ and $\boldsymbol{\beta}^* \in \mathbb{R}^l$ such that:

1. $\frac{\partial \mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)}{\partial \boldsymbol{x}} = 0$

2. $\frac{\partial \mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)}{\partial \boldsymbol{\beta}} = 0$

3. $\alpha_j^* g_j(\boldsymbol{x}^*) = 0, 1 \leq j \leq k$ (KKT complementarity conditions)

4. $g_j(\boldsymbol{x}^*) \leq 0, 1 \leq j \leq k$

5. $\alpha_j^* \geq 0, 1 \leq j \leq k$

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SVM Lagrangian (primal)

We construct the **Lagrangian**:

$$\mathcal{L} = \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{i=1}^{n} \alpha_i \Big\{ t_i \left(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b \right) - 1 + \varepsilon_i \Big\} + C \sum_{i=1}^{n} \varepsilon_i - \sum_{i=1}^{n} \mu_i \varepsilon_i$$

- The $\alpha_i, \mu_i \geq 0$ are the **Lagrange multipliers**; the μ_i ensure that $\varepsilon_i \geq 0$
- The solution is a **saddle point** of $\mathcal{L}$: minimum w.r.t. $\boldsymbol{w}, b$ and the ε_i and maximum w.r.t. the α_i and μ_i

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Lagrangian form

The gradient of $\mathcal{L}$ with respect to $\boldsymbol{w}, b$ and ε_i must vanish:

$$\frac{\partial \mathcal{L}}{\partial b} = \sum_{i=1}^{n} \alpha_i t_i = 0, \qquad \frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{i=1}^{n} \alpha_i t_i \, \boldsymbol{x}_i = 0, \qquad \frac{\partial \mathcal{L}}{\partial \varepsilon_i} = C - \alpha_i - \mu_i = 0$$

In addition, the KKT complementarity conditions must hold:

$$\alpha_i \Big(t_i \left(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b \right) - 1 + \varepsilon_i \Big) = 0$$

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Dual formulation

The Lagrangian $\mathcal{L}$ is convex; its optimization is equivalent to the maximization of its concave **dual problem** $\mathcal{L}_D$:

$$\underset{\boldsymbol{w},b,\{\alpha_i\}}{\textbf{minimize}} \qquad \mathcal{L}_D = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j t_i t_j \left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \right\rangle$$

$$\textbf{subject to } 0 \leq \alpha_i \leq C \ (1 \leq i \leq n), \qquad \textbf{and } \sum_{i=1}^{n} \alpha_i t_i = 0$$

- Neither $\mu_i, \varepsilon_i, \boldsymbol{w}, b$ appear in the dual form; maximization is only w.r.t. the α_i

- This optimization problem is expressed *only* in terms of inner products of the data points: the dual lends itself to kernelisation

- How many free parameters? n (independent of data dimension)

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Dual formulation

A closer look at the KKT complementarity conditions:

- $\alpha_i = 0$ implies $t_i\, g(\boldsymbol{x}_i) > 1$ and $\varepsilon_i = 0$ ($\boldsymbol{x}_i$ is **not a SV**)

- $\alpha_i \in (0, C)$ implies $t_i\, g(\boldsymbol{x}_i) = 1$ and $\varepsilon_i = 0$ ($\boldsymbol{x}_i$ is a **non-bound SV**)

- $\alpha_i = C$ implies $t_i\; g(\boldsymbol{x}_i) < 1$ and $\varepsilon_i > 0$ ($\boldsymbol{x}_i$ is a **bound SV**)

  (in particular, $\varepsilon_i > 1$ implies $\boldsymbol{x}_i$ is a **training error**)

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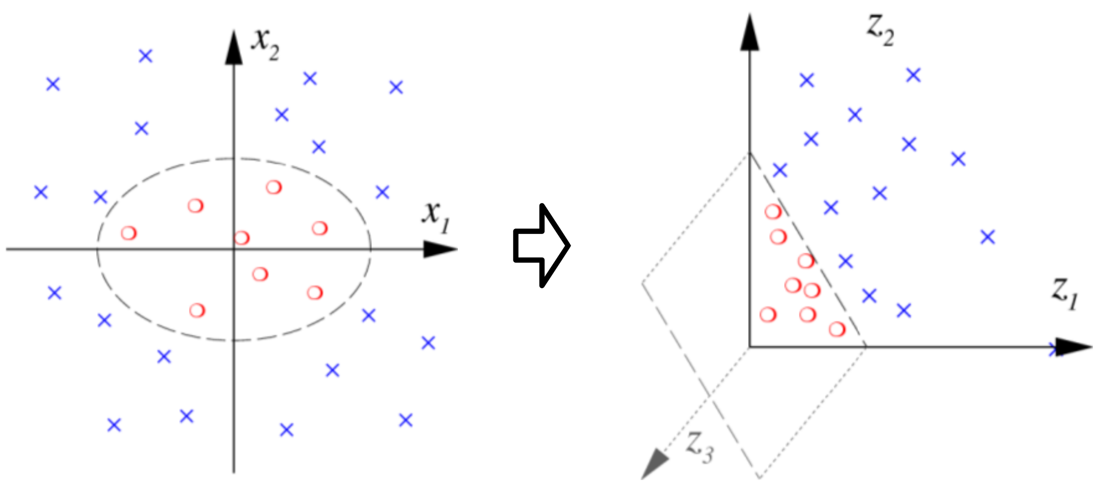
The SVM goes non-linear

Recall the idea of mapping input data into some Hilbert space (called the **feature space**) via a non-linear mapping $\phi : \mathcal{X} \to \mathcal{H}$

The associated kernel function is $k(\boldsymbol{x}, \boldsymbol{x}') = \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{x}') \rangle_{\mathcal{H}}, \;\; \boldsymbol{x}, \boldsymbol{x}' \in \mathcal{X}$



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SVM kernelization

- We now substitute $\boldsymbol{x}_i$ by $\phi(\boldsymbol{x}_i)$, then build the OSH in $\mathcal{H}$
- The dual of the new QP problem is formulated exactly as before, replacing $\left\langle \boldsymbol{x}_i, \boldsymbol{x}_j \right\rangle$ with $\left\langle \phi(\boldsymbol{x}_i), \phi(\boldsymbol{x}_j) \right\rangle_{\mathcal{H}} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$
- The discriminant function becomes:

$$f_{\mathsf{SVM}}(\boldsymbol{x}) = \operatorname{sgn}\left(\sum_{i=1}^{n} \alpha_i t_i k(\boldsymbol{x}, \boldsymbol{x}_i) + b \right)$$

Support Vector Machines

LOOCV bounds (I)

A rough but simple bound on LOOCV (leave-one-out CV) error can be computed as:

$$\text{LOOCV}(n) \leq \frac{1}{n}\mathbb{E}(n_{\text{SV}})$$

n_{SV} is the number of SVs for a given sample of size n
The $\mathbb{E}()$ is taken over all such samples

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LOO bounds (II)

Theorem. The LOOCV error of a stable SVM$^{(*)}$ on a set of training patterns $\boldsymbol{x}_i$ is bounded by $|\{i\,/\,(2\alpha_i R^2 + \varepsilon_i) \geq 1\}|/n$, where R^2 is an upper bound on $k(\boldsymbol{x}, \boldsymbol{x})$ and $k(\boldsymbol{x}, \boldsymbol{x}') \geq 0$.

- This quantity can be extracted easily from the solution

- This LOOCV error is an unbiased estimate of true error

$^{(*)}$ A SVM is stable if there is at least one non-bound SV (see *Estimating the Generalization Performance of a SVM Efficiently*. T. Joachims; In ICML, 2000)

Support Vector Machines

Final remarks (I)

- The fact that the **OSH** is determined only by the support vectors is most remarkable, since usually this number will be small

- The **support vectors** (SVs) are:

  1. the only training examples that define the solution

  2. the most difficult examples to classify

- This means all the **relevant information** in the data set is summarized by the SVs: we would have obtained the same result by using *only* the SVs from the outset

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Final remarks (II)

- The SVM is specially well suited for "large d, low n" problems, because:

  1. complexity grows with n (non-parametric model)

  2. space requirements (the kernel matrix) also grows with n

  3. generalization error does not depend on d

- The "architecture" is determined automatically by the method (not by experimentation, as in neural networks)

Support Vector Machines

Hot topics

- Choice of the **best kernel** is an open issue; **kernel design** is an active area of research

- More efficient algorithms for solving **big QP** problems are being developed

- Sometimes the **fraction of SVs** is very high (indicating a poor fit); it is possible to control this fraction directly (ν-SVMs)

- Performance usually depends on a careful choice of the external parameters: C and those of the kernel function; we need principled ways for **hyper-parameter** selection

Support Vector Machines

Where to look for more ...

- *An Introduction to Kernel-based Learning Algorithms*. K.-R. Mueller, S. Mika, G. Raetsch, K. Tsuda, and B. Schoelkopf, IEEE Neural Networks, 12(2):181-201, 2001.

- *A Tutorial on Support Vector Machines for Pattern Recognition*. Christopher Burges.
  `https://research.microsoft.com/en-us/um/people/cburges/papers/svmtutorial.pdf`

- *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*. Bernhard Schoelkopf and Alexander J. Smola, MIT Press, 2001.

- *An Introduction to Support Vector Machines and Other Kernel-based Learning Methods*. Nello Cristianini and John Shawe-Taylor, Cambridge University Press, 2000.

- *Kernel Methods for Pattern Analysis*. John Shawe-Taylor and Nello Cristianini, Cambridge University Press, 2004.

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