Support Vector Machines and Kernel Methods – Part 2

UNC-CH COMP 755

Slides adapted from: A. Zisserman, B. Schölkopf, D. Sontag, L. Zettlemoyer, C. Guestrin, et al.

Dual SVM derivation (1) – the linearly separable case

Original optimization problem:

$$\text{minimize}_{\mathbf{w},b} \quad \frac{1}{2}\mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1, \ \ \forall j$$

Rewrite constraints

One Lagrange multiplier per example

Lagrangian:

$$L(\mathbf{w}, \alpha) = \frac{1}{2}\mathbf{w}.\mathbf{w} - \sum_j \alpha_j \left[\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j - 1\right]$$
$$\alpha_j \geq 0, \ \ \forall j$$

Our goal now is to solve: $\min_{\vec{w},b} \ \max_{\vec{\alpha}\geq 0} \ L(\vec{w}, \vec{\alpha})$

Dual SVM derivation (2) – the linearly separable case

(Primal) $$\min_{\vec{w},b} \max_{\vec{\alpha}\geq 0} \frac{1}{2}||\vec{w}||^2 - \sum_j \alpha_j \left[(\vec{w}\cdot\vec{x}_j + b)\, y_j - 1 \right]$$

Swap min and max

(Dual) $$\max_{\vec{\alpha}\geq 0} \min_{\vec{w},b} \frac{1}{2}||\vec{w}||^2 - \sum_j \alpha_j \left[(\vec{w}\cdot\vec{x}_j + b)\, y_j - 1 \right]$$

Slater's condition from convex optimization guarantees that these two optimization problems are equivalent!

Dual SVM derivation (3) – the linearly separable case

(Dual) $$\max_{\vec{\alpha}\geq 0} \min_{\vec{w},b} \frac{1}{2}||\vec{w}||^2 - \sum_j \alpha_j \left[(\vec{w}\cdot\vec{x}_j + b)\, y_j - 1\right]$$

Can solve for optimal **w**, b as function of α:

$$\frac{\partial L}{\partial w} = w - \sum_j \alpha_j y_j x_j \quad \rightarrow \quad \mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j$$

$$\frac{\partial L}{\partial b} = -\sum_j \alpha_j y_j \quad \rightarrow \quad \sum_j \alpha_j y_j = 0$$

Substituting these values back in (and simplifying), we obtain:

(Dual) $$\max_{\vec{\alpha}\geq 0,\, \sum_j \alpha_j y_j = 0} \sum_j \alpha_j - \frac{1}{2}\sum_{i,j} \underbrace{y_i y_j \alpha_i \alpha_j}_{\text{scalars}} \underbrace{(\vec{x}_i \cdot \vec{x}_j)}_{\text{dot product}}$$

Sums over all training examples

Dual SVM derivation (3) – the linearly separable case

(Dual) $$\max_{\vec{\alpha} \geq 0} \min_{\vec{w}, b} \frac{1}{2}||\vec{w}||^2 - \sum_j \alpha_j \left[(\vec{w} \cdot \vec{x}_j + b) \, y_j - 1 \right]$$

Can solve for optimal **w**, b as function of α:

$$\frac{\partial L}{\partial w} = w - \sum_j \alpha_j y_j x_j \quad \rightarrow \quad \mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j$$

$$\frac{\partial L}{\partial b} = -\sum_j \alpha_j y_j \quad \rightarrow \quad \sum_j \alpha_j y_j = 0$$

Substituting these values back in (and simplifying), we obtain:

(Dual) $$\max_{\vec{\alpha} \geq 0, \, \sum_j \alpha_j y_j = 0} \sum_j \alpha_j - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j \left(\vec{x}_i \cdot \vec{x}_j \right)$$

So, in dual formulation we will solve for α directly!

- **w** and b are computed from α (if needed)

Dual SVM derivation (3) – the linearly separable case

Lagrangian:

$$L(\mathbf{w},\alpha) = \frac{1}{2}\mathbf{w}.\mathbf{w} - \sum_j \alpha_j \left[\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j - 1\right]$$

$$\alpha_j \geq 0, \ \ \forall j$$

$\alpha_j > 0$ for some *j* implies constraint is tight. We use this to obtain *b*:

$$y_j \left(\vec{w} \cdot \vec{x}_j + b\right) = 1 \quad (1)$$

$$y_j y_j \left(\vec{w} \cdot \vec{x}_j + b\right) = y_j \quad (2)$$

$$\left(\vec{w} \cdot \vec{x}_j + b\right) = y_j \quad (3)$$

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

$$b = y_k - \mathbf{w}.\mathbf{x}_k$$

for any k where $\alpha_k > 0$

Classification rule using dual solution

$$y \leftarrow \mathrm{sign}(\vec{w} \cdot \vec{x} + b)$$

Using dual solution

$$y \leftarrow \mathrm{sign}\left[\sum_i \alpha_i y_i \underbrace{(\vec{x}_i \cdot \vec{x})} + b\right]$$

dot product of feature vectors of new example with support vectors

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

$$b = y_k - \mathbf{w}.\mathbf{x}_k$$

for any k where $C > \alpha_k > 0$

Dual for the non-separable case

Primal:

$$\text{minimize}_{\mathbf{w},b} \quad \tfrac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_j \xi_j$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j, \ \ \forall j$$
$$\xi_j \geq 0, \ \ \forall j$$

Solve for w,b, α:

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$
$$b = y_k - \mathbf{w}.\mathbf{x}_k$$

for any k where $C > \alpha_k > 0$

Dual:

$$\text{maximize}_{\alpha} \quad \sum_i \alpha_i - \tfrac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \mathbf{x}_j$$
$$\sum_i \alpha_i y_i = 0$$
$$C \geq \alpha_i \geq 0$$

What changed?

- Added upper bound of C on α_i!
- Intuitive explanation:
  - Without slack, $\alpha_i \rightarrow \infty$ when constraints are violated (points misclassified)
  - Upper bound of C limits the α_i, so misclassifications are allowed

Support vectors

- **Complementary slackness** conditions:

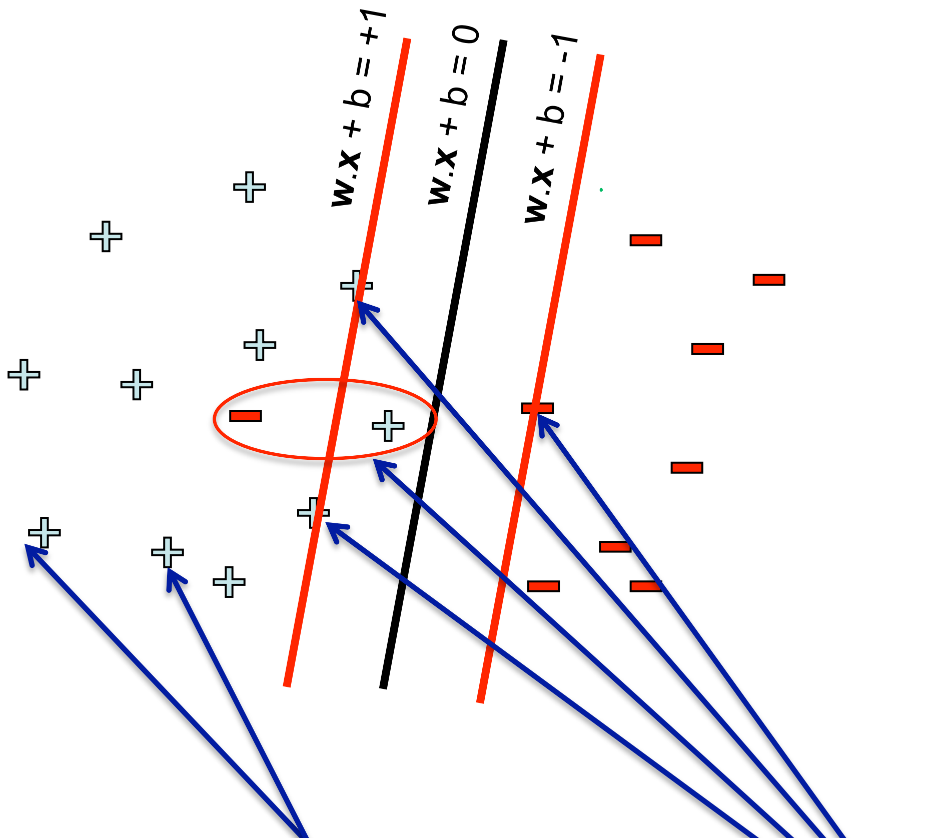
$$\alpha_j^* \left[y_j(\vec{w}^* \cdot \vec{x}_j + b) - 1 + \xi_j \right] = 0 \implies \alpha_j^* = 0 \ \vee \ y_j(\vec{w}^* \cdot \vec{x}_j + b) = 1 - \xi_j$$

$$\implies \alpha_j^* = 0 \ \vee \ y_j(\vec{w}^* \cdot \vec{x}_j + b) \leq 1$$

- **Support vectors**: points x_j such that $y_j(\vec{w}^* \cdot \vec{x}_j + b) \leq 1$ (includes all j such that $\alpha_j^* > 0$, but also additional points where $\alpha_j^* = 0 \wedge y_j(\vec{w}^* \cdot \vec{x}_j + b) \leq 1$)

- Note: the SVM dual solution may not be unique!

Dual SVM interpretation: Sparsity



$$\mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j$$

Final solution tends to be sparse

- α_j=0 for most j
- don't need to store these points to compute w or make predictions

Non-support Vectors:

- α_j=0
- moving them will not change w

Support Vectors:

- $\alpha_j \geq 0$

SVM with kernels

$$\text{maximize}_{\alpha} \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

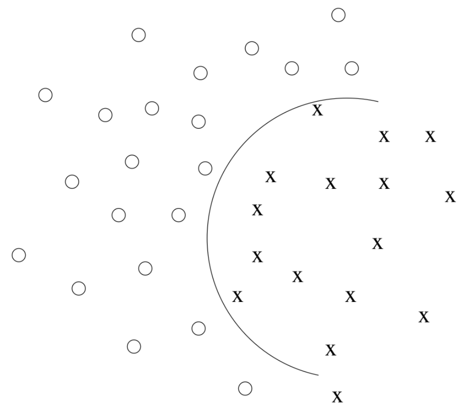
$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$$
$$\sum_i \alpha_i y_i = 0$$
$$C \geq \alpha_i \geq 0$$

- Never compute features explicitly!!!
  - Compute dot products in closed form
- $O(n^2)$ time in size of dataset to compute objective
  - much work on speeding up

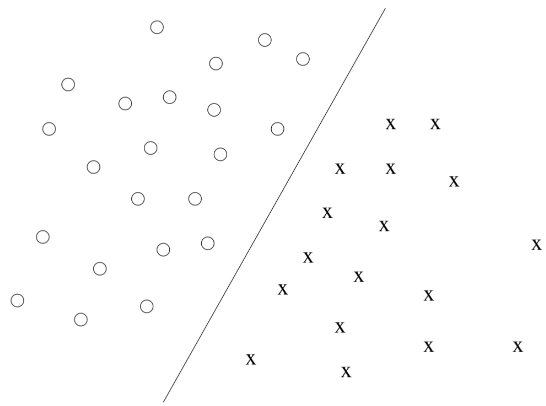
Predict with:

$$y \leftarrow \text{sign}\left[\sum_i \alpha_i y_i K(x_i, x) + b\right]$$

Quadratic kernel



Non-linear separator in the original $\mathbf{x}$-space



Linear separator in the feature ϕ-space

[Tommi Jaakkola]

Quadratic kernel

$$
\begin{aligned}
k(\mathbf{x},\mathbf{z}) &= (\mathbf{x}^T\mathbf{z}+c)^2 = \left(\sum_{j=1}^n x^{(j)}z^{(j)}+c\right)\left(\sum_{\ell=1}^n x^{(\ell)}z^{(\ell)}+c\right) \\
&= \sum_{j=1}^n\sum_{\ell=1}^n x^{(j)}x^{(\ell)}z^{(j)}z^{(\ell)} + 2c\sum_{j=1}^n x^{(j)}z^{(j)} + c^2 \\
&= \sum_{j,\ell=1}^n (x^{(j)}x^{(\ell)})(z^{(j)}z^{(\ell)}) + \sum_{j=1}^n (\sqrt{2c}x^{(j)})(\sqrt{2c}z^{(j)}) + c^2,
\end{aligned}
$$

Feature mapping given by:

$$\mathbf{\Phi}(\mathbf{x}) = [x^{(1)2}, x^{(1)}x^{(2)}, ..., x^{(3)2}, \sqrt{2c}x^{(1)}, \sqrt{2c}x^{(2)}, \sqrt{2c}x^{(3)}, c]$$

[Cynthia Rudin]

Common kernels

- Polynomials of degree exactly *d*

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^d$$

- Polynomials of degree up to *d*

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^d$$

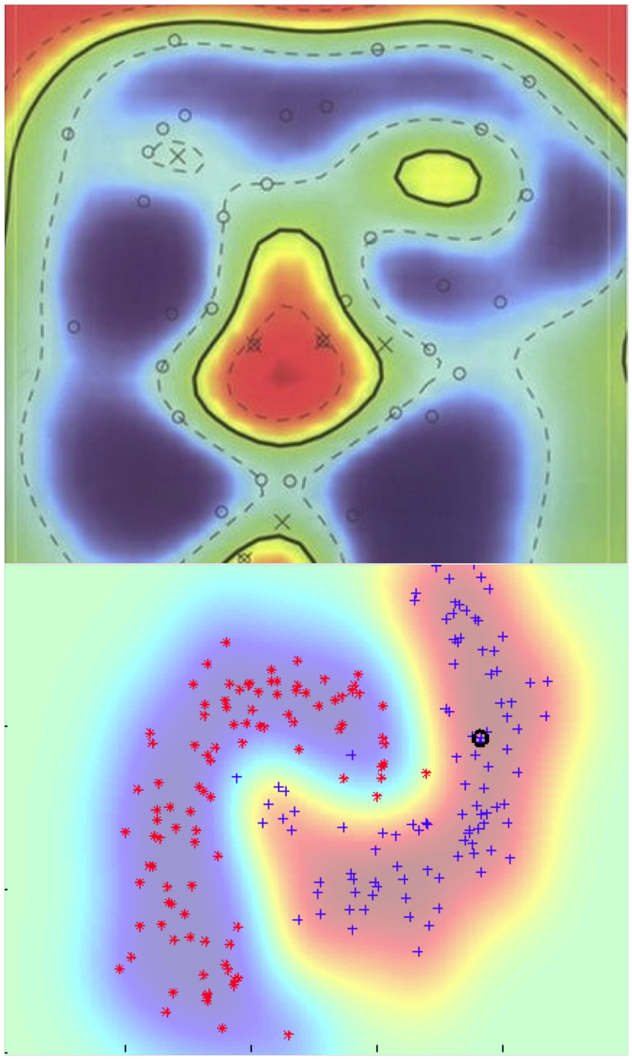
- Gaussian kernels

$$K(\vec{u}, \vec{v}) = \exp\left(-\frac{||\vec{u} - \vec{v}||_2^2}{2\sigma^2}\right)$$

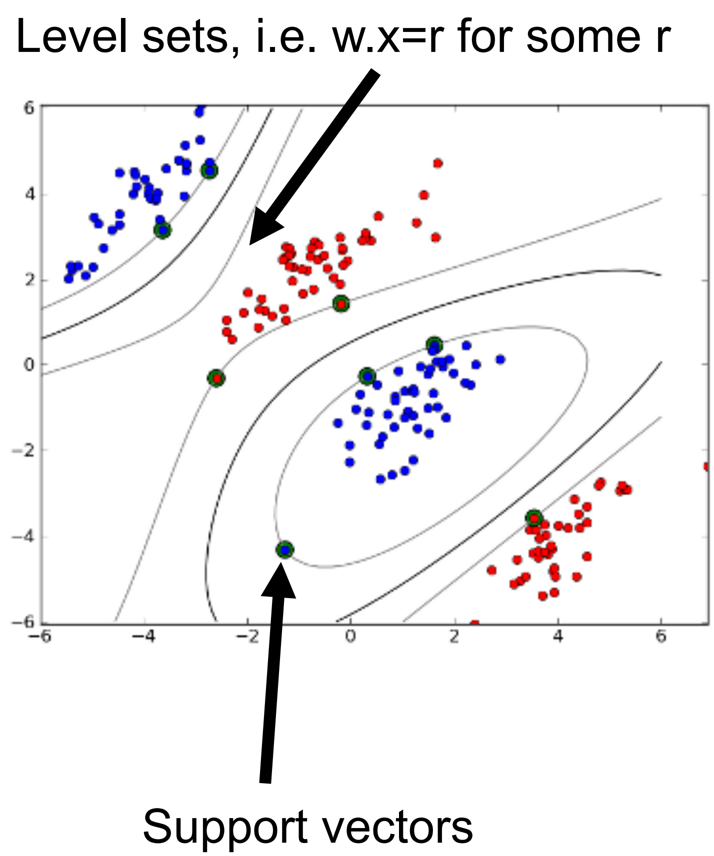
Euclidean distance, squared

- And many others: very active area of research! (e.g., structured kernels that use dynamic programming to evaluate, string kernels, …)

Gaussian kernel



[Cynthia Rudin]



[mblondel.org]

Kernel algebra

kernel composition	feature composition
a) $k(\mathbf{x},\mathbf{v}) = k_a(\mathbf{x},\mathbf{v}) + k_b(\mathbf{x},\mathbf{v})$	$\boldsymbol{\phi}(\mathbf{x}) = (\boldsymbol{\phi}_a(\mathbf{x}), \boldsymbol{\phi}_b(\mathbf{x})),$
b) $k(\mathbf{x},\mathbf{v}) = f k_a(\mathbf{x},\mathbf{v}),\ f > 0$	$\boldsymbol{\phi}(\mathbf{x}) = \sqrt{f}\boldsymbol{\phi}_a(\mathbf{x})$
c) $k(\mathbf{x},\mathbf{v}) = k_a(\mathbf{x},\mathbf{v}) k_b(\mathbf{x},\mathbf{v})$	$\phi_m(\mathbf{x}) = \phi_{ai}(\mathbf{x})\phi_{bj}(\mathbf{x})$
d) $k(\mathbf{x},\mathbf{v}) = \mathbf{x}^T A\mathbf{v}$, A positive semi-definite	$\boldsymbol{\phi}(\mathbf{x}) = L^T\mathbf{x}$, where $A = LL^T$.
e) $k(\mathbf{x},\mathbf{v}) = f(\mathbf{x}) f(\mathbf{v}) k_a(\mathbf{x},\mathbf{v})$	$\phi(\mathbf{x}) = f(\mathbf{x})\phi_a(\mathbf{x})$

Q: How would you prove that the "Gaussian kernel" is a valid kernel?

A: Expand the Euclidean norm as follows:

$$\exp\left(-\frac{||\vec{u}-\vec{v}||_2^2}{2\sigma^2}\right) = \exp\left(-\frac{||\vec{u}||_2^2}{2\sigma^2}\right)\exp\left(-\frac{||\vec{v}||_2^2}{2\sigma^2}\right)\exp\left(\frac{\vec{u}\cdot\vec{v}}{\sigma^2}\right)$$

Then, apply (e) from above

To see that this is a kernel, use the Taylor series expansion of the exponential, together with repeated application of (a), (b), and (c):

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

The feature mapping is infinite dimensional!

[Justin Domke]

Overfitting?

- Huge feature space with kernels: should we worry about overfitting?
  - SVM objective seeks a solution with large **margin**
    - Theory says that large margin leads to good generalization (we will see this in a couple of lectures)
  - But everything overfits sometimes!!!
  - Can control by:
    - Setting C
    - Choosing a better Kernel
    - Varying parameters of the Kernel (width of Gaussian, etc.)

Vapnik-Chervonenkis(VC)-Theory: Main Points

Necessary and sufficient conditions for consistency of empirical risk minimization: one-sided convergence, uniformly over all functions that can be implemented by the learning machine.

$$\lim_{m\to\infty} \mathrm{P}\{\sup_f (R[f] - R_{emp}[f]) > \epsilon\} = 0 \quad \text{for all } \epsilon > 0.$$

Vapnik, Chervonenkis and others give conditions for uniform convergence in terms of capacity concepts, e.g.

- the VC-entropy grows sublinearly with m
- the VC-dimension is finite
- the entropy numbers are well-behaved
- the classification "margin" is large

[e.g. 52, 50, 44, 61, 1]

Structure of the Growth Function

Either $G^{\mathcal{F}}(m) = m \cdot \ln(2)$ — this means that for any sample size m the points can be chosen such that by using functions of the learning machine, all 2^m possible loss vectors can be generated (i.e., they can be separated in all possible ways — *"shattered"*).

Or there exists some *maximal* m for which the above is possible. Call this number the *VC-dimension*, and denote it by h. Then one can prove that for $m > h$,

$$G^{\mathcal{F}}(m) \leq h\left(\ln\frac{m}{h} + 1\right).$$

Nothing "in between" linear growth and logarithmic growth is possible [51].

A VC Bound for Pattern Recognition

For any $f \in \mathcal{F}$ and $m > h$, with a probability of at least $1 - \eta$,

$$R[f] \leq R_{\mathrm{emp}}[f] + \phi\left(\frac{h}{m}, \frac{\log(\eta)}{m}\right)$$

holds, where ϕ is defined as

$$\phi\left(\frac{h}{m}, \frac{\log(\eta)}{m}\right) = \sqrt{\frac{h\left(\log\frac{2m}{h} + 1\right) - \log(\eta/4)}{m}}.$$

(Derivation: in uniform convergence bounds, set RHS $= \eta$, and solve for ϵ to get the confidence term.)

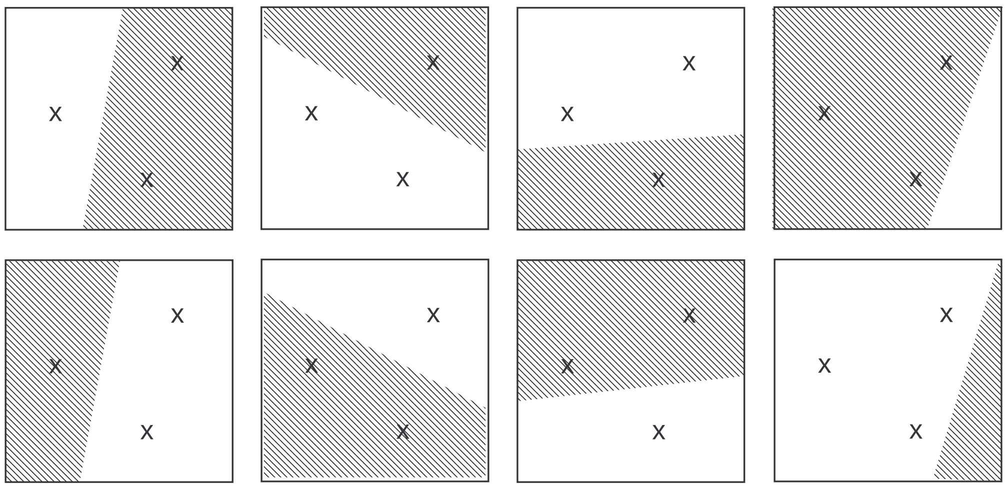
The study of the consistency of ERM has thus led to concepts and results which lets us formulate a better induction principle: minimize the RHS of the bound.

VC-Dimension: Example

Half-spaces in $\mathbb{R}^2$:

$$f(x, y) = \mathrm{sgn}(a + bx + cy), \quad \text{with parameters } a, b, c \in \mathbb{R}$$

- Clearly, we can shatter three non-collinear points.
- But we can never shatter four points.
- Hence the VC dimension is $h = 3$ (in this case, equal to the number of parameters)



VC-Dimension Example, ctd.

- more generally, separating hyperplanes in $\mathbb{R}^N$ have a VC dimension of $N + 1$.
- hence: separating hyperplanes in high-dimensional feature spaces have extremely large VC dimension, and may not generalize well
- however, *"margin"* hyperplanes can still have a small VC dimension (see below)

The Kernel Trick: Feature Spaces

Preprocess the data with

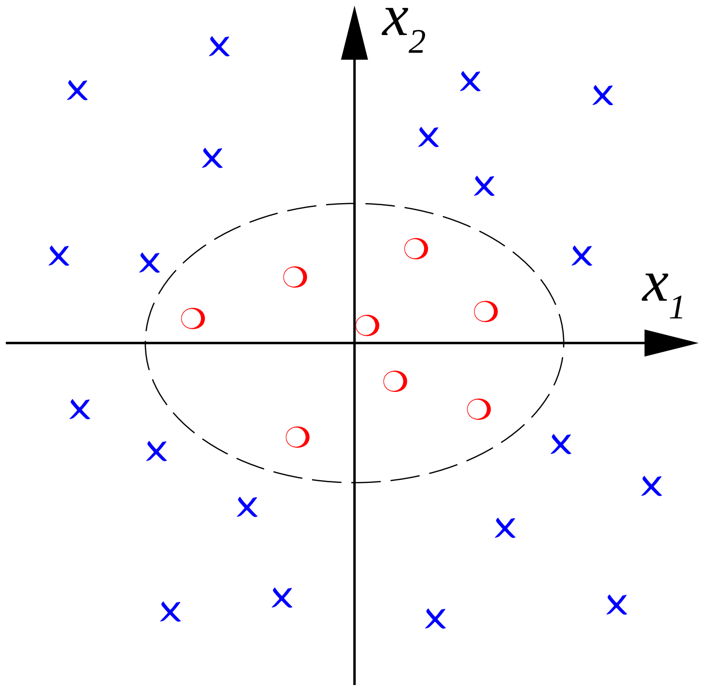
$$\begin{aligned} \Phi : \mathcal{X} &\to \mathcal{H} \\ x &\mapsto \Phi(x), \end{aligned}$$

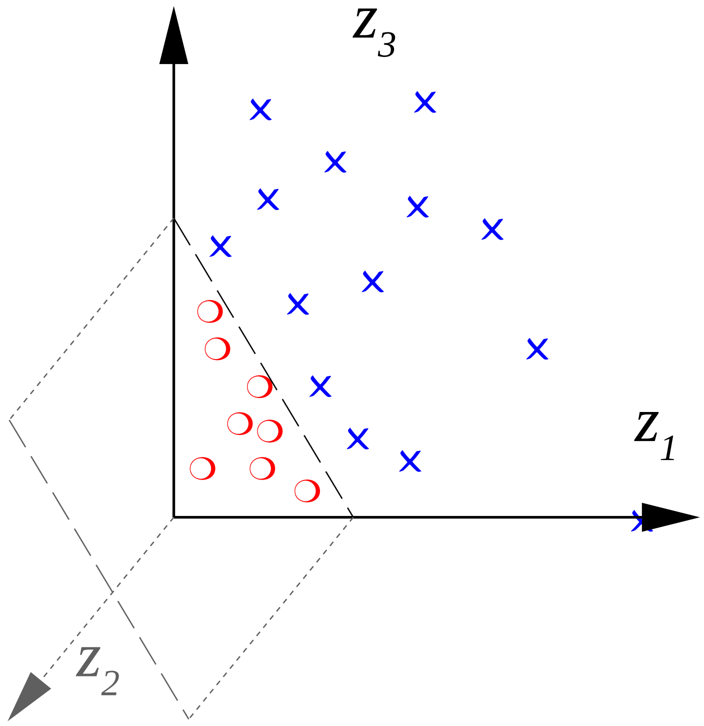
where $\mathcal{H}$ is a dot product space, and learn the mapping from $\Phi(x)$ to y.

- usually, $\dim(\mathcal{X}) \ll \dim(\mathcal{H})$
- "Curse of Dimensionality"?
- crucial issue: *capacity*, not *dimensionality*

Example: All Degree 2 Monomials

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





The Kernel Trick, $N = d = 2$

$$\begin{aligned}
\left\langle \Phi(x), \Phi(x') \right\rangle &= (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)({x'}_1^2, \sqrt{2}\, x'_1 x'_2, {x'}_2^2)^\top \\
&= \left\langle x, x' \right\rangle^2 \\
&= : k(x, x')
\end{aligned}$$

$\longrightarrow$ the dot product in $\mathcal{H}$ can be computed in $\mathbb{R}^2$

The Kernel Trick, II

More generally: $x, x' \in \mathbb{R}^N$, $d \in \mathbb{N}$:

$$\begin{aligned} \langle x, x' \rangle^d &= \left(\sum_{j=1}^{N} x_j \cdot x'_j \right)^d \\ &= \sum_{j_1, \ldots, j_d = 1}^{N} x_{j_1} \cdot \cdots \cdot x_{j_d} \cdot x'_{j_1} \cdot \cdots \cdot x'_{j_d} = \langle \Phi(x), \Phi(x') \rangle , \end{aligned}$$

where Φ maps into the space spanned by all ordered products of d input directions

Mercer's Theorem

If k is a continuous kernel of a positive definite integral operator on $L_2(\mathcal{X})$ (where $\mathcal{X}$ is some compact space),

$$\int_{\mathcal{X}} k(x, x')f(x)f(x')\, dx\, dx' \geq 0,$$

it can be expanded as

$$k(x, x') = \sum_{i=1}^{\infty} \lambda_i \psi_i(x) \psi_i(x')$$

using eigenfunctions ψ_i and eigenvalues $\lambda_i \geq 0$ [34].

In that case

$$\Phi(x) := \begin{pmatrix} \sqrt{\lambda_1}\psi_1(x) \\ \sqrt{\lambda_2}\psi_2(x) \\ \vdots \end{pmatrix}$$

satisfies $\langle \Phi(x), \Phi(x') \rangle = k(x, x')$.

Positive Definite Kernels

It can be shown that (modulo some details) the admissible class of kernels coincides with the one of positive definite (pd) kernels: kernels which are symmetric, and for

- any set of training points $x_1, \ldots, x_m \in \mathcal{X}$ and
- any $a_1, \ldots, a_m \in \mathbb{R}$

satisfy

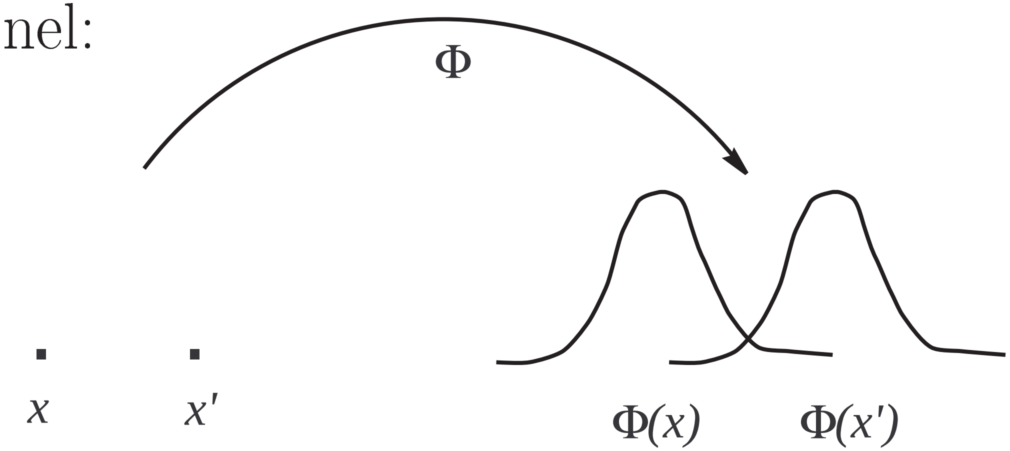
$$\sum_{i,j} a_i a_j K_{ij} \geq 0, \quad \text{where } K_{ij} := k(x_i, x_j).$$

The Feature Space for PD Kernels [5, 2, 38]

- define a feature map

$$\begin{aligned} \Phi : \mathcal{X} &\to \mathbb{R}^{\mathcal{X}} \\ x &\mapsto k(.,x). \end{aligned}$$

E.g., for the Gaussian kernel:



- turn $\Phi(\mathcal{X})$ into a linear space, $f(.) = \sum_{i=1}^{m} \alpha_i k(., x_i)$,
- endow it with a dot product satisfying $\left\langle k(.,x_i), k(.,x_j)\right\rangle = k(x_i, x_j)$
- complete the space to get a *reproducing kernel Hilbert space*

Some Properties of Kernels

If $k_1, k_2, \ldots$ are pd kernels, then so are

- αk_1, provided $\alpha \geq 0$
- $k_1 + k_2$
- $k_1 \cdot k_2$
- $k(x, x') := \lim_{n \to \infty} k_n(x, x')$, provided it exists

Further operations to construct kernels from kernels: tensor products, direct sums, convolutions [23].

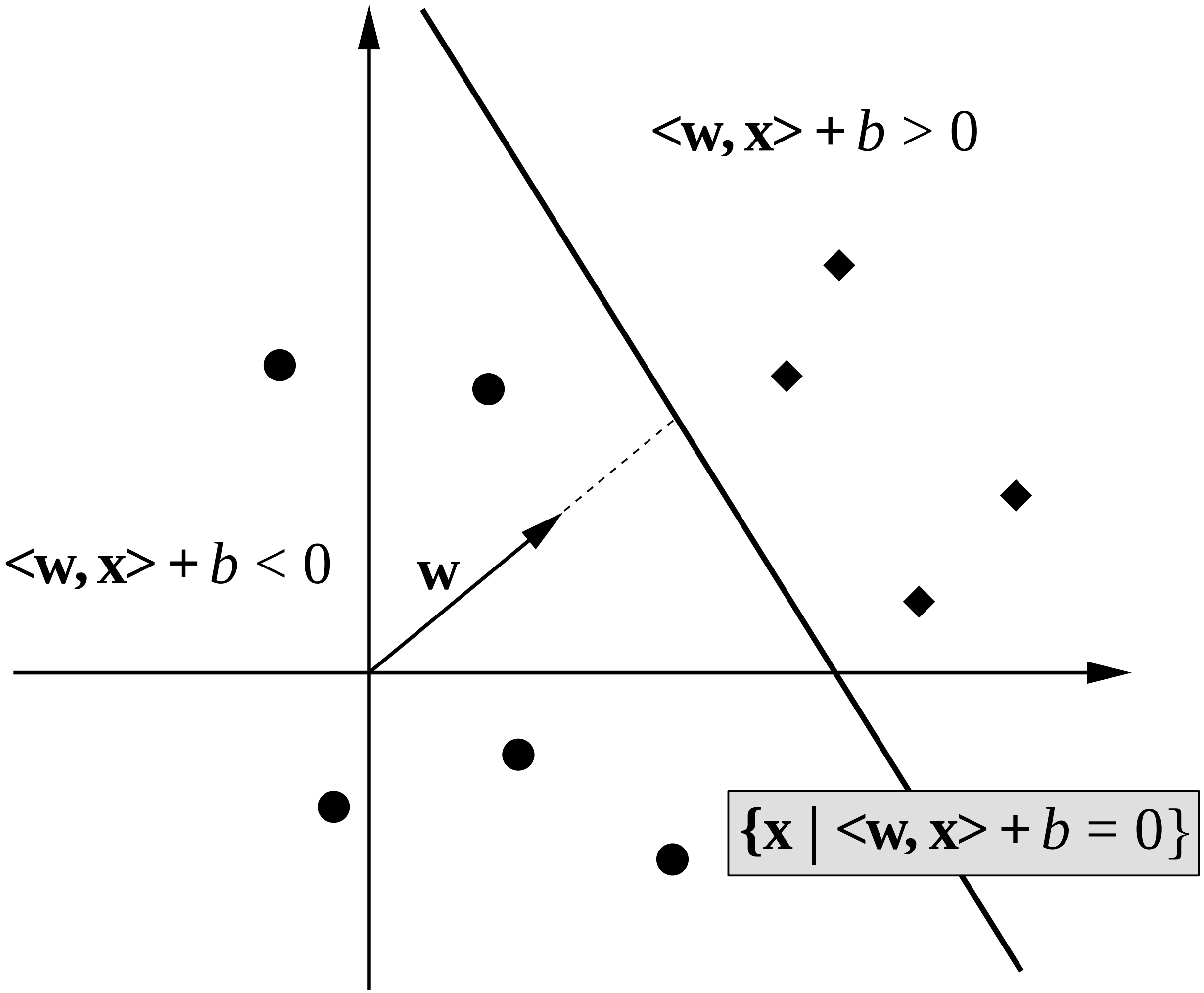
The Kernel Trick — Summary

- *any* algorithm that only depends on dot products can benefit from the kernel trick
- this way, we can apply linear methods to vectorial as well as *non-vectorial data*
- think of the kernel as a nonlinear *similarity measure*
- examples of common kernels:

$$\begin{aligned}
\text{Polynomial} \quad k(x, x') &= (\langle x, x' \rangle + c)^d \\
\text{Sigmoid} \quad k(x, x') &= \tanh(\kappa \langle x, x' \rangle + \Theta) \\
\text{Gaussian} \quad k(x, x') &= \exp(-\|x - x'\|^2 / (2\,\sigma^2))
\end{aligned}$$

- Kernel are studied also in the Gaussian Process prediction community (covariance functions) [57, 54, 58, 33]

Separating Hyperplane



Eliminating the Scaling Freedom

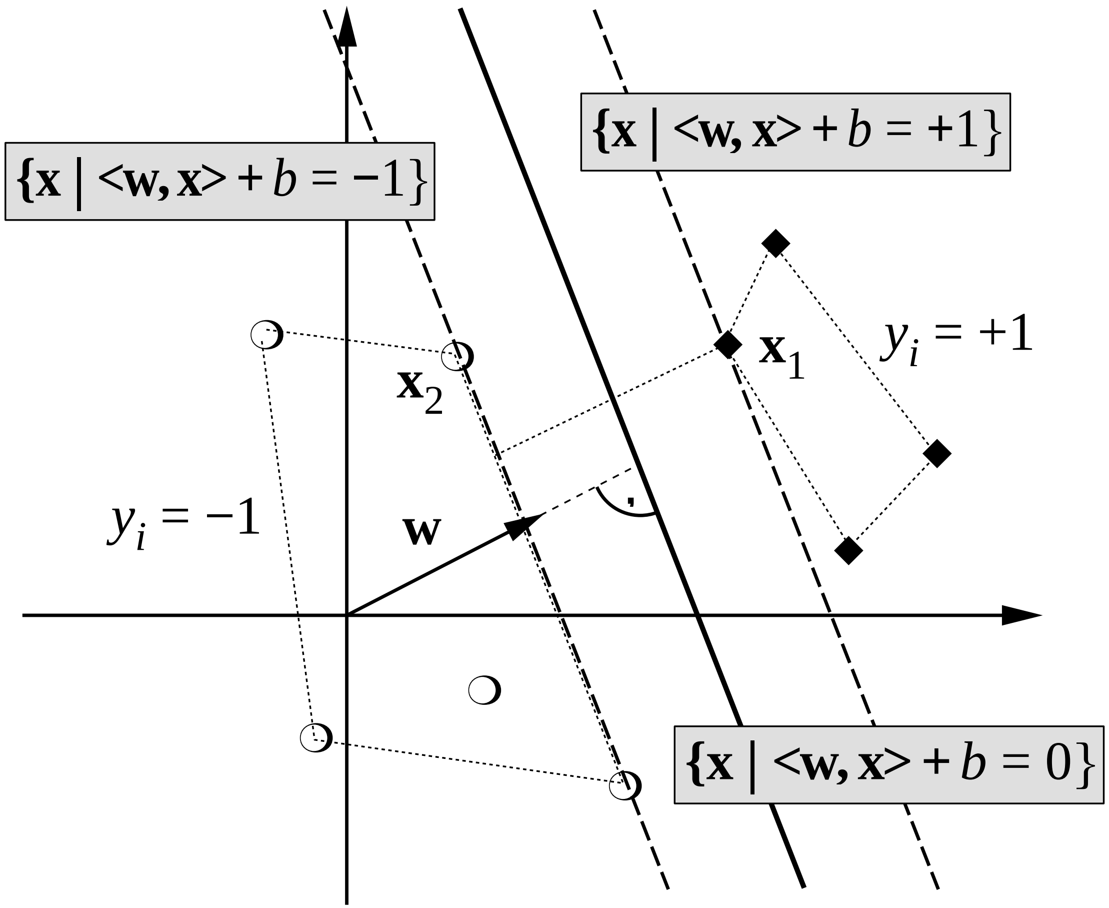
Note: if $c \neq 0$, then

$$\{\mathbf{x} | \langle \mathbf{w}, \mathbf{x} \rangle + b = 0\} = \{\mathbf{x} | \langle c\mathbf{w}, \mathbf{x} \rangle + cb = 0\}.$$

Hence $(c\mathbf{w}, cb)$ describes the same hyperplane as $(\mathbf{w}, b)$.

Definition: The hyperplane is in *canonical* form w.r.t. $X^* = \{\mathbf{x}_1, \ldots, \mathbf{x}_r\}$ if $\min_{\mathbf{x}_i \in X} |\langle \mathbf{w}, \mathbf{x}_i \rangle + b| = 1$.

Canonical Optimal Hyperplane



Note:

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

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

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

VC Dimension of Margin Hyperplanes

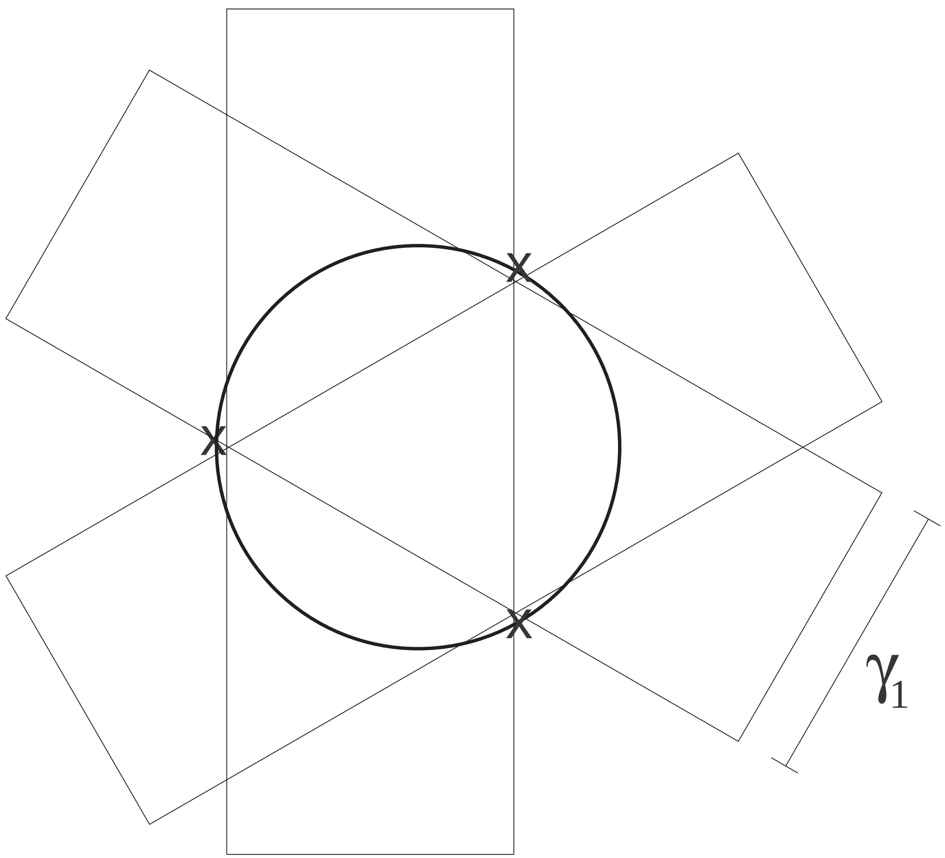
Theorem [48]. *Consider hyperplanes* $\langle \mathbf{w}, \mathbf{x} \rangle = 0$ *where* $\mathbf{w}$ *is normalized such that they are in canonical form w.r.t. a set of points* $X^* = \{\mathbf{x}_1, \ldots, \mathbf{x}_r\}$, *i.e.,*

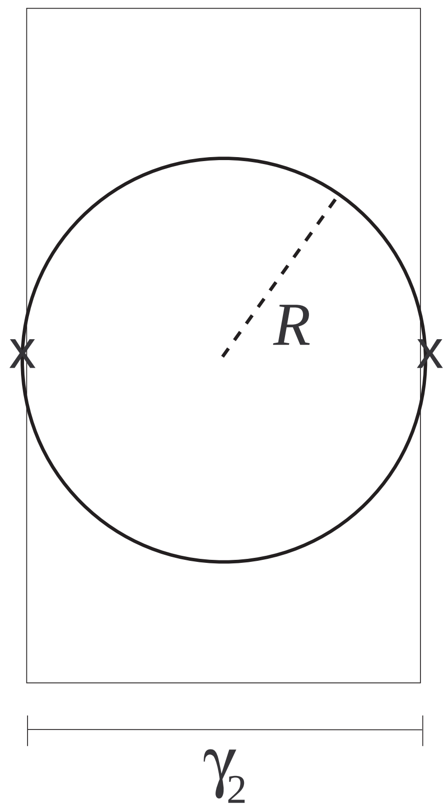
$$\min_{i=1,\ldots,r} |\langle \mathbf{w}, \mathbf{x}_i \rangle| = 1.$$

The set of decision functions $f_{\mathbf{w}}(\mathbf{x}) = sgn \langle \mathbf{x}, \mathbf{w} \rangle$ *defined on* X^* *and satisfying the constraint* $\|\mathbf{w}\| \leq \Lambda$ *has a VC dimension satisfying*

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

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


x
x
x
γ_1


R
x
x
γ_2

Formulation as an Optimization Problem

Hyperplane with maximum margin: minimize

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

(recall: margin $\sim 1/\|\mathbf{w}\|$) subject to

$$y_i \cdot [\langle \mathbf{w}, \mathbf{x}_i \rangle + b] \geq 1 \quad \text{for } i = 1 \ldots m$$

(i.e. the training data are separated correctly).

Lagrange Function (e.g., [6])

Introduce Lagrange multipliers $\alpha_i \geq 0$ and a Lagrangian

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{m} \alpha_i \left(y_i \cdot [\langle \mathbf{w}, \mathbf{x}_i \rangle + b] - 1 \right).$$

L has to minimized w.r.t. the *primal variables* $\mathbf{w}$ and b and maximized with respect to the *dual variables* α_i

- if a constraint is violated, then $y_i \cdot (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) - 1 < 0 \longrightarrow$
  - $\cdot$ α_i will grow to increase L — how far?
  - $\cdot$ $\mathbf{w}$, b want to decrease L; i.e. they have to change such that the constraint is satisfied. If the problem is separable, this ensures that $\alpha_i < \infty$.
- similarly: if $y_i \cdot (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) - 1 > 0$, then $\alpha_i = 0$: otherwise, L could be increased by decreasing α_i *(KKT conditions)*

Derivation of the Dual Problem

At the extremum, we have

$$\frac{\partial}{\partial b} L(\mathbf{w}, b, \boldsymbol{\alpha}) = 0, \quad \frac{\partial}{\partial \mathbf{w}} L(\mathbf{w}, b, \boldsymbol{\alpha}) = 0,$$

i.e.

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

and

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

Substitute both into L to get the *dual problem*

The Support Vector Expansion

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

where for all $i = 1, \ldots, m$ either

$$y_i \cdot [\langle \mathbf{w}, \mathbf{x}_i \rangle + b] > 1 \quad \Longrightarrow \alpha_i = 0 \longrightarrow \mathbf{x}_i \text{ irrelevant}$$

or

$$y_i \cdot [\langle \mathbf{w}, \mathbf{x}_i \rangle + b] = 1 \quad (\textit{on} \text{ the margin}) \longrightarrow \mathbf{x}_i \text{ ``Support Vector''}$$

The solution is determined by the examples on the margin.

Thus

$$\begin{aligned} f(\mathbf{x}) &= \operatorname{sgn}\left(\langle \mathbf{x}, \mathbf{w} \rangle + b\right) \\ &= \operatorname{sgn}\left(\sum_{i=1}^{m} \alpha_i y_i \langle \mathbf{x}, \mathbf{x}_i \rangle + b\right). \end{aligned}$$

Dual Problem

Dual: maximize

$$W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

subject to

$$\alpha_i \geq 0, \quad i = 1, \ldots, m, \quad \text{and} \quad \sum_{i=1}^{m} \alpha_i y_i = 0.$$

Both the final decision function and the function to be maximized are expressed in dot products $\longrightarrow$ can use a kernel to compute

$$\langle \mathbf{x}_i, \mathbf{x}_j \rangle = \langle \Phi(x_i), \Phi(x_j) \rangle = k(x_i, x_j).$$

The SV Expansion in Feature Space

- generally, the solution of kernel algorithms corresponds to a single vector in $\mathcal{H}$ ("Representer Theorem" [30, 39]),

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

  However, there is usually no $x \in \mathcal{X}$ such that

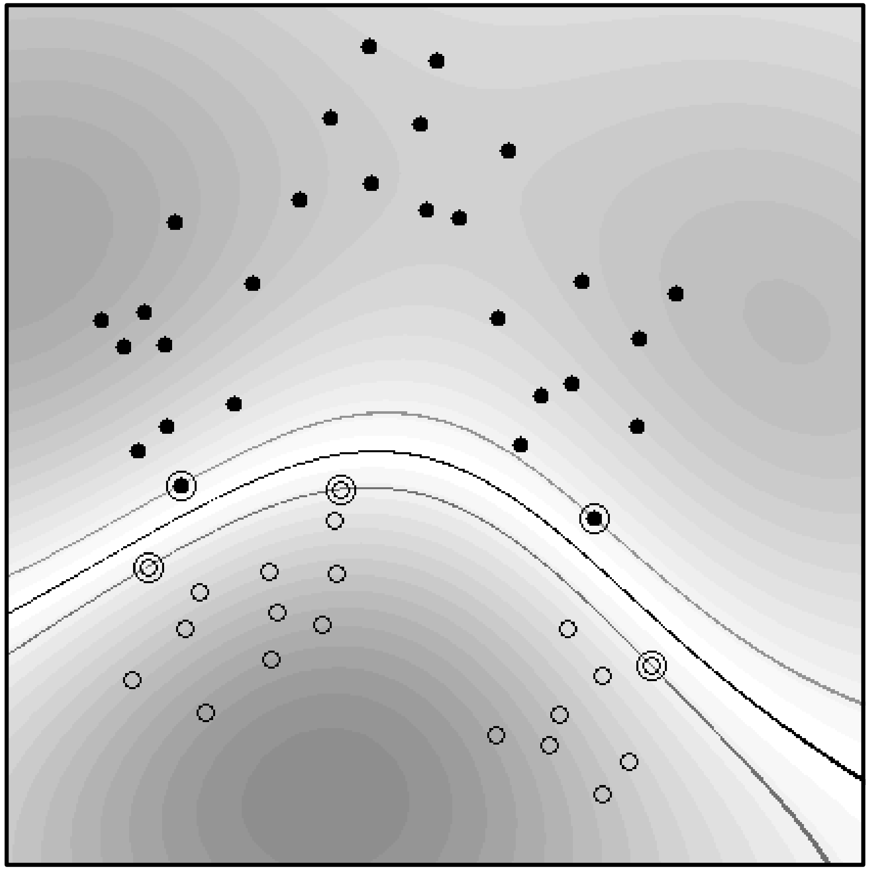
$$\Phi(x) = \mathbf{w},$$

  i.e., $\Phi(\mathcal{X})$ is not closed under linear combinations — it is a nonlinear manifold (cf. [10, 40]).

- $\Phi(\mathcal{X})$ is contained in a non-isotropic shape whose sidelengths scale like the square roots of the eigenvalues of k or K [cf. 61, 60, 13, 59].

Toy Example with Gaussian Kernel

$$k(x, x') = \exp\left(-\|x - x'\|^2\right)$$



Nonseparable Problems *[4, 15]*

If $y_i \cdot (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$ cannot be satisfied, then $\alpha_i \to \infty$.

Modify the constraint to

$$y_i \cdot (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i$$

with

$$\xi_i \geq 0$$

("*soft margin*") and add

$$C \cdot \sum_{i=1}^{m} \xi_i$$

in the objective function.

Same dual, with additional constraints $\alpha_i \leq C$.

SVM Training

- naive approach: the complexity of maximizing

$$W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j k(\mathbf{x}_i, \mathbf{x}_j)$$

  scales with the third power of the training set size m

- only SVs are relevant $\longrightarrow$ only compute $(k(\mathbf{x}_i, \mathbf{x}_j))_{ij}$ for SVs. Extract them iteratively by cycling through the training set in chunks [48].

- in fact, one can use chunks which do not even contain all SVs [35]. Maximize over these sub-problems, using your favorite optimizer.

- the extreme case: by making the sub-problems very small (just two points), one can solve them analytically [37].

- http://www.kernel-machines.org/software.html

MNIST Error Rates

handwritten character benchmark (60000 training & 10000 test examples, 28×28)

Classifier	test error	reference
linear classifier	8.4%	[7]
3-nearest-neighbour	2.4%	[7]
SVM	1.4%	[11]
Tangent distance	1.1%	[45]
LeNet4	1.1%	[31]
Boosted LeNet4	0.7%	[31]
Translation invariant SVM	0.56%	[17]

Note: the SVM used a polynomial kernel of degree 9, corresponding to a feature space of dimension $\approx 3.2 \cdot 10^{20}$.

Other successful applications: [28, 26, 24, 12, 47, 8, 63, 22, 20, 14, 18, 36, 55, 62]

Unsupervised SVM Learning

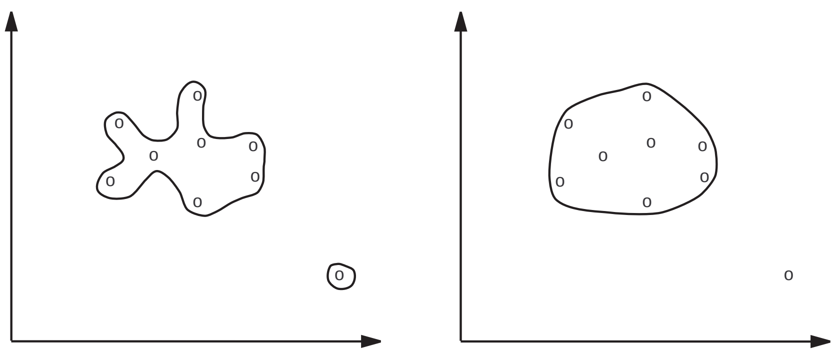
$x_1, \ldots, x_m \in \mathcal{X}$ i.i.d. sample from P

- extreme view: unsupervised learning = density estimation
- easier problem: for $\alpha \in (0, 1]$, compute a region R such that

$$\mathrm{P}(R) \approx \alpha,$$

  i.e., estimate *quantiles* of a distribution, not its density.

- becomes well-posed using a regularizer: find "smoothest" region that contains a certain fraction of the probability mass
- given only the training data, we will get a trade-off: try to enclose many training points (more than α) in a smooth region



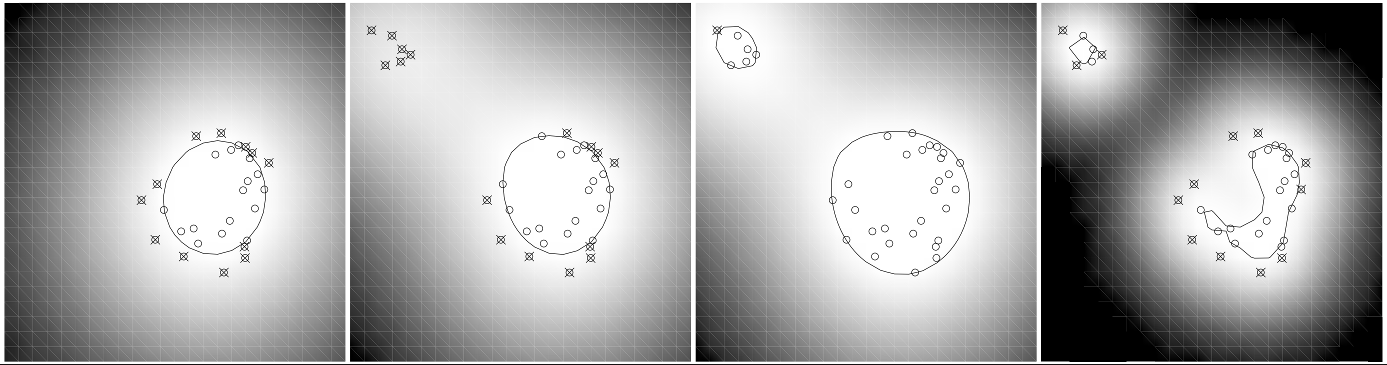
Separating Unlabelled Data from the Origin

One can show: if $\Phi(x_1), \ldots, \Phi(x_m)$ are separable from the origin in $\mathcal{H}$, then the solution of

$$\min_{\mathbf{w} \in \mathcal{H}} \frac{1}{2}\|\mathbf{w}\|^2 \qquad \text{subject to} \quad \langle \mathbf{w}, \Phi(x_i) \rangle \geq 1$$

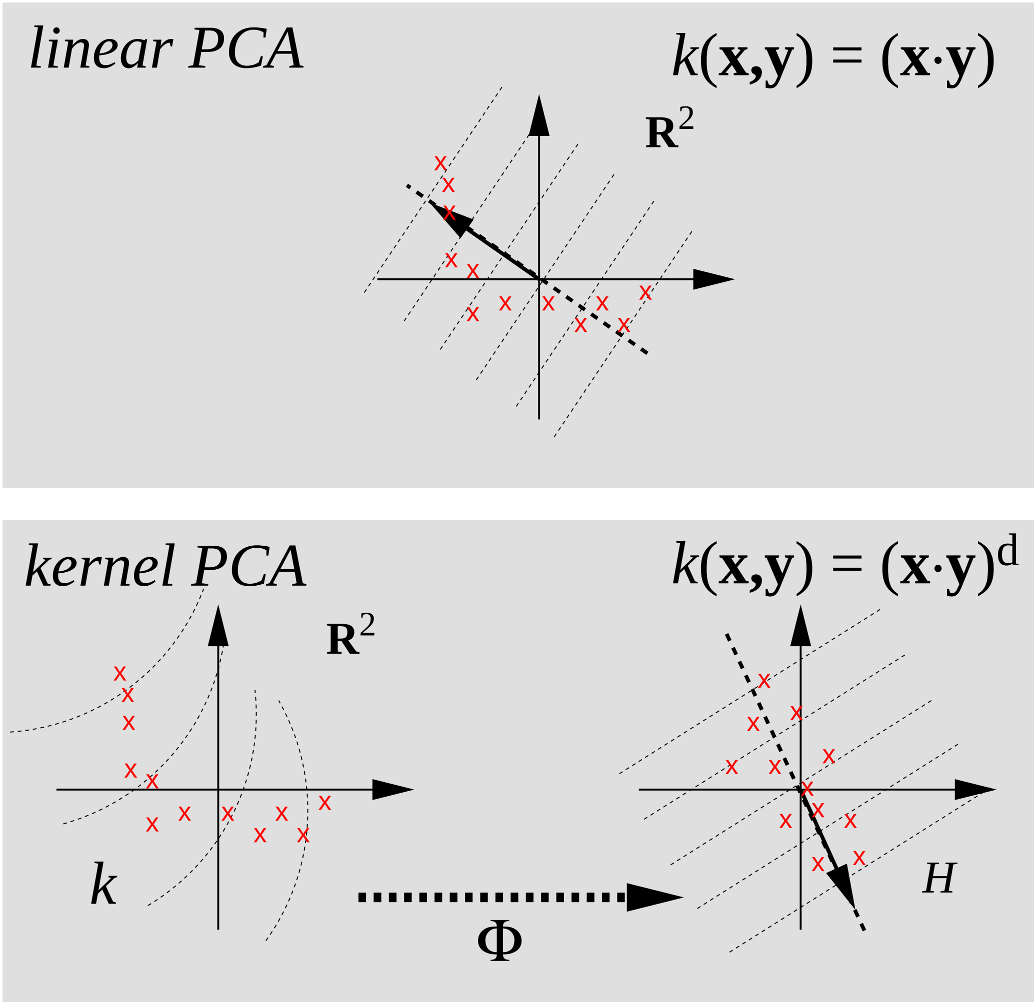
is the normal vector of the hyperplane separating the data from the origin with maximum margin.

Toy Examples using $k(x,y) = \exp(-\frac{\|x-y\|^2}{c})$



ν, width c	0.5, 0.5	0.5, 0.5	0.1, 0.5	0.5, 0.1
SVs/OLs	0.54, 0.43	0.59, 0.47	0.24, 0.03	0.65, 0.38

Kernel PCA



The Challenge: Designing Kernels

- transformation invariances (cf. poster of Olivier Chapelle)
- kernels for discrete objects [23, 56, 32, 3]
- kernels based on generative models: Fisher kernel [27]
- local kernels [e.g., 63]
- other sophisticated kernels: e.g., [5, 16, 42]

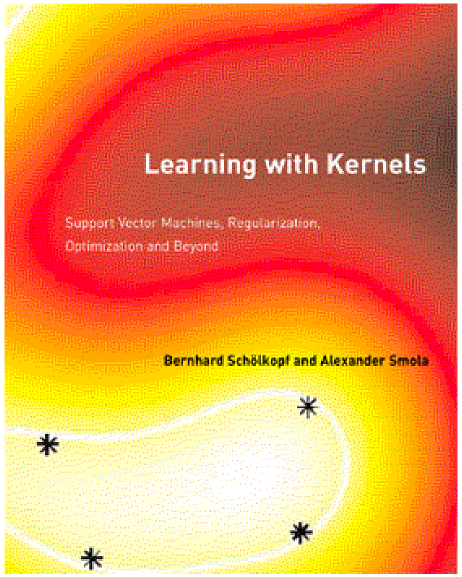
In general, the choice of a kernel corresponds to

- choosing a similarity measure for the data, or
- choosing a (linear) representation of the data, or
- choosing a hypothesis space for learning,

and should reflect prior knowledge about the problem at hand.
There is 'no free lunch' in kernel choice.

Conclusion

- crucial ingredients of SV algorithms: kernels that can be represented as dot products, and large margin regularizers
- kernels allow the formulation of a multitude of geometrical algorithms (Parzen windows, SV pattern recognition, SV quantile estimation, kernel PCA,...)
- not only do these algorithms lend themselves well to theoretical study — they also perform well in practice



For further information, cf. `http://www.kernel-machines.org`, `http://www.learning-with-kernels.org`, and [9, 16, 25, 42].

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