SVM and Kernel Methods

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(these slides are available from www.kernel-machines.org)

Roadmap

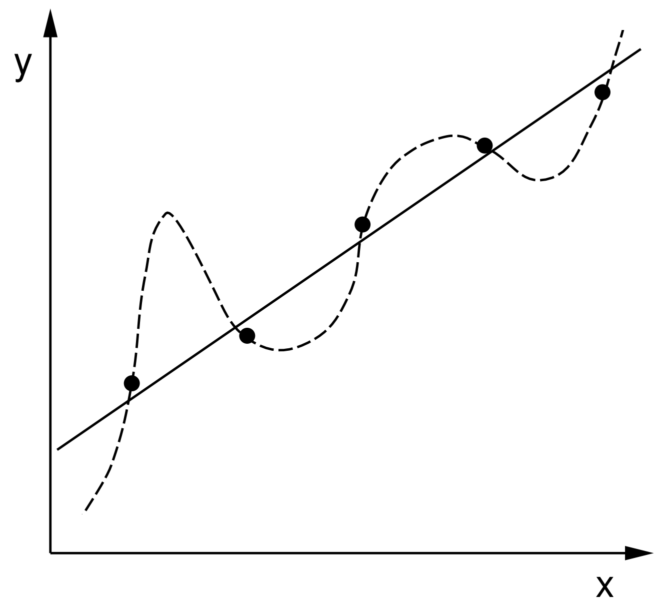
1. ideas of statistical learning theory
2. kernels and feature spaces
3. Support vector algorithms

Statistical Learning Theory

1. started by Vapnik and Chervonenkis in the Sixties
2. model: we observe data generated by an unknown stochastic regularity
3. *learning* = extraction of the regularity from the data
4. the analysis of the learning problem leads to notions of *capacity* of the function classes that a learning machine can implement.
5. *support vector machines* use a particular type of function class: classifiers with large “margins” in a feature space induced by a *kernel*.

[49, 50]

Example: Regression Estimation



- *Data:* input-output pairs $(x_i, y_i) \in \mathbb{R} \times \mathbb{R}$
- *Regularity:* $(x_1, y_1), \ldots (x_m, y_m)$ drawn from $\mathrm{P}(x, y)$
- *Learning:* choose a function $f : \mathbb{R} \to \mathbb{R}$ such that the error, averaged over P, is minimized.
- *Problem:* P is unknown, so the average cannot be computed — need an "*induction* principle"

Pattern Recognition

Learn $f : \mathcal{X} \to \{\pm 1\}$ from examples

$(x_1, y_1), \ldots, (x_m, y_m) \in \mathcal{X} \times \{\pm 1\}$, generated i.i.d. from $\mathrm{P}(x, y)$,

such that the expected misclassification error on a test set, also drawn from $\mathrm{P}(x, y)$,

$$R[f] = \int \frac{1}{2} |f(x) - y| \, d\mathrm{P}(x, y),$$

is minimal *(Risk Minimization (RM))*.

Problem: P is unknown. $\longrightarrow$ need an *induction principle*.

Empirical risk minimization (ERM): replace the average over $\mathrm{P}(x, y)$ by an average over the training sample, i.e. minimize the training error

$$R_{\mathrm{emp}}[f] = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} |f(x_i) - y_i|$$

- Regression estimation. RM: minimize

$$R[f] = \int (f(x) - y)^2 \, d\mathrm{P}(x, y)$$

— leads to the *regression* $y(x) = \int y \, d\mathrm{P}(y|x)$.

ERM gives least mean squares: minimize

$$\sum_i (f(x_i) - y_i)^2$$

- Density estimation. RM: minimize

$$R[f] = \int (-\log p(x)) \, d\mathrm{P}(x)$$

ERM gives maximum likelihood estimation: maximize

$$\sum_i \log p(x_i) = \log(\prod_i p(x_i))$$

Convergence of Means to Expectations

Law of large numbers:

$$R_{\mathrm{emp}}[f] \to R[f]$$

as $m \to \infty$.

Does this imply that for the function f^m minimizing R_{emp}, and the function f^{opt} minimizing R, we have

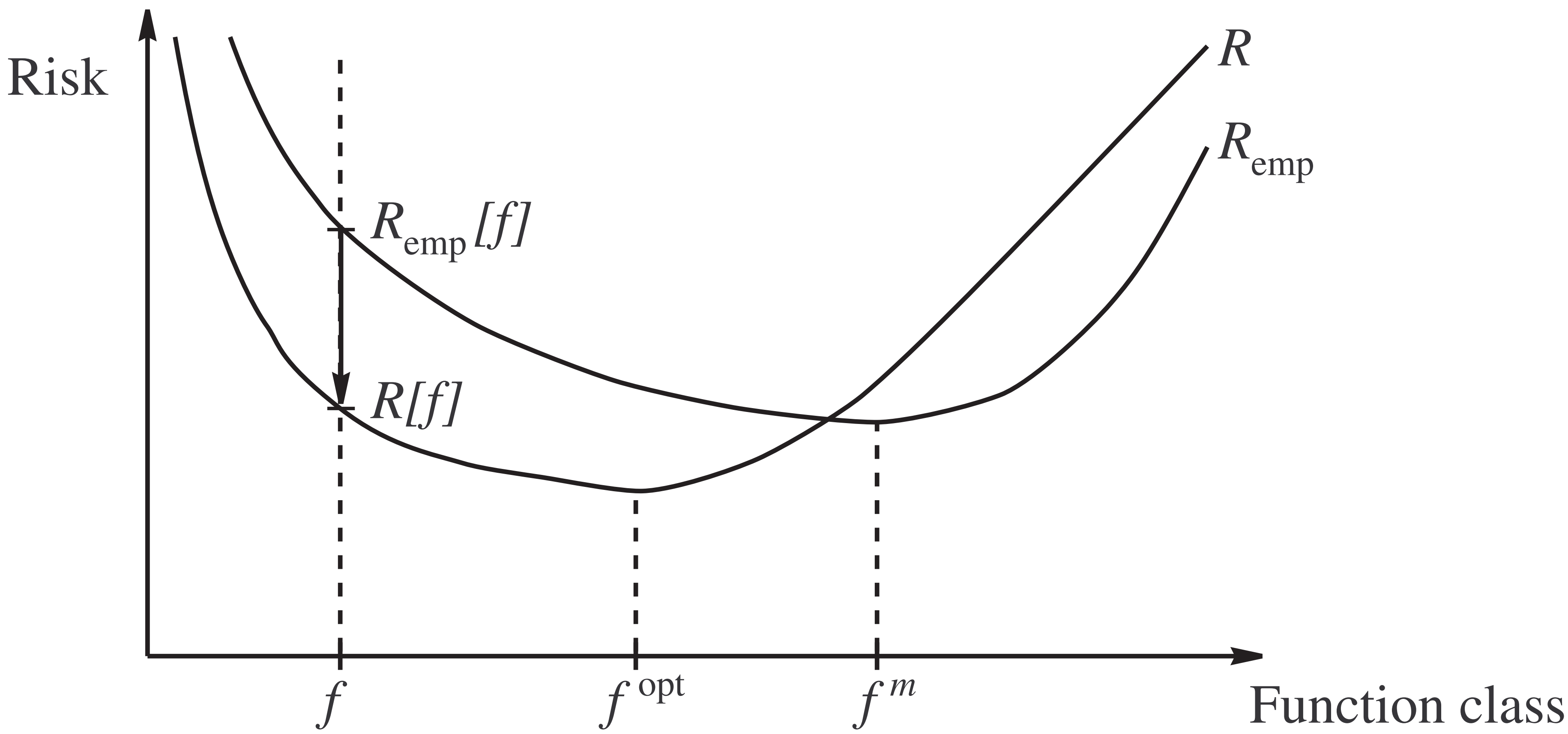
$$R_{\mathrm{emp}}[f^m] \to R[f^{\mathrm{opt}}], \quad R[f^m] \to R[f^{\mathrm{opt}}]$$

as $m \to \infty$ (*"consistency"* of empirical risk minimization)?

No.

Need a *uniform* version of the law of large numbers. Uniform over *all functions that the learning machine can implement.*

Consistency and Uniform Convergence



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.

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

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]

Conditions for Uniform Convergence

How to bound $\mathrm{P}\{\sup_{f\in\mathcal{F}}(R[f] - R_{\mathrm{emp}}[f]) > \epsilon\}$:

- if the function class $\mathcal{F}$ contains only one function, then *Chernoff's bound* suffices:

$$\mathrm{P}\{\sup_{f\in\mathcal{F}}(R[f] - R_{\mathrm{emp}}[f]) > \epsilon\} \leq 2\exp(-2m\epsilon^2)$$

- if there are finitely many functions, use the *union bound* to get a multiplicative constant on the RHS
- even if there are infinitely many, then *on any finite sample* there are effectively only finitely many (use *symmetrization*, [52])

- *VC entropy*: on an example (x, y), f causes a loss $Q(x, y, f)$. On a training set, different functions $f \in \mathcal{F}$ lead to $N^{\mathcal{F}}$ different loss vectors $q_f = (Q(x_1, y_1, f), \dots, Q(x_m, y_m, f))$. Define
$$H^{\mathcal{F}}(m) = \mathbf{E} \ln N^{\mathcal{F}}.$$
$H^{\mathcal{F}}(m)/m \to 0 \iff$ uniform convergence (hence consistency)
- exchange expectation and logarithm: *annealed entropy*.
$H^{\mathcal{F}}_{ann}(m)/m \to 0 \Longrightarrow$ exponential convergence
$$\mathrm{P}\{\sup_f (R[f] - R_{\mathrm{emp}}[f]) > \epsilon\} \leq 4 \cdot \exp(((H^{\mathcal{F}}_{ann}(2m)/m) - \epsilon^2) \cdot m).$$
- take 'max' instead of '$\mathbf{E}$': *growth function*.
$G^{\mathcal{F}}(m)/m \to 0 \iff$ exponential convergence for all underlying distributions

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 $1 - \eta$,

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

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.)

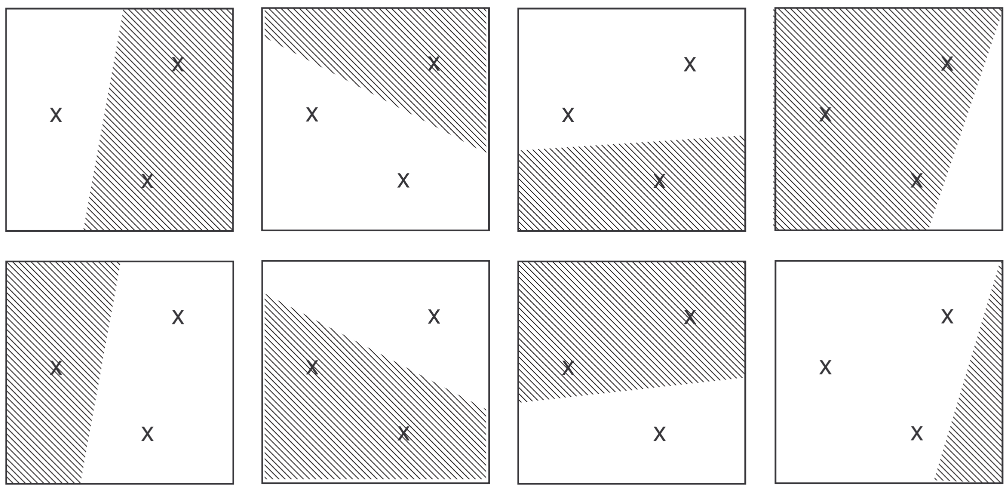
The study of the consistency of ERM has thus led to concepts and results which lets us formulate a better induction principle: minimize the RHS of the bound.

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

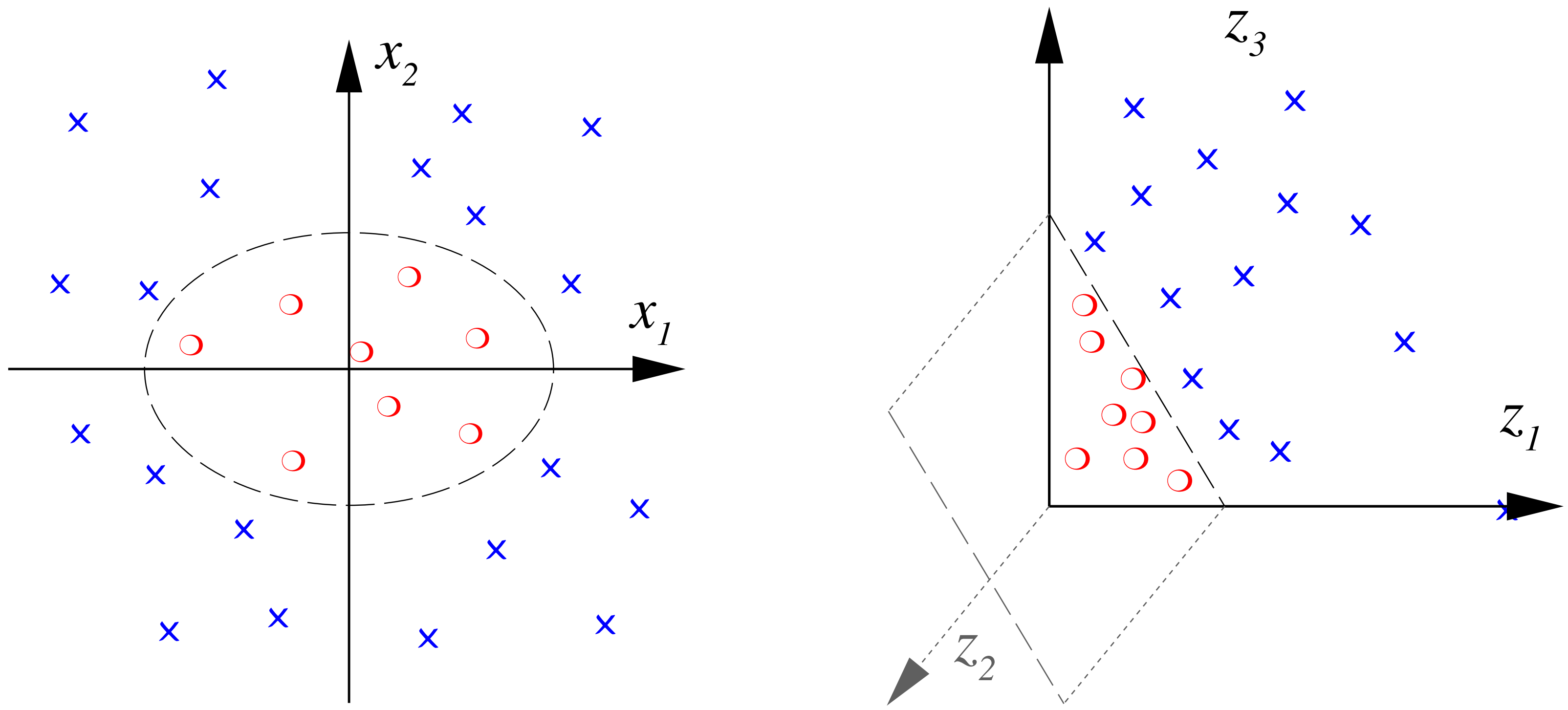
$$\begin{aligned} \Phi : \mathcal{X} &\to \mathcal{H} \\ x &\mapsto \Phi(x), \end{aligned}$$

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

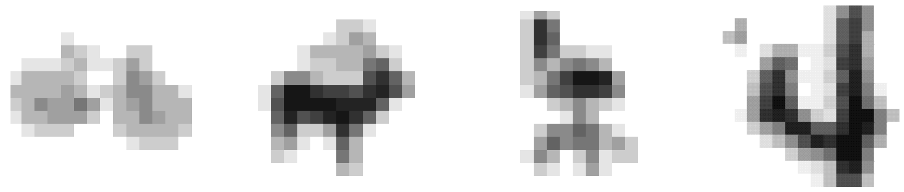
- usually, $\dim(\mathcal{X}) \ll \dim(\mathcal{H})$
- "Curse of Dimensionality"?
- crucial issue: *capacity*, not *dimensionality*

Example: All Degree 2 Monomials

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



General Product Feature Space



How about patterns $x \in \mathbb{R}^N$ and product features of order d?

Here, $\dim(\mathcal{H})$ grows like N^d.

E.g. $N = 16 \times 16$, and $d = 5 \longrightarrow$ dimension 10^{10}

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

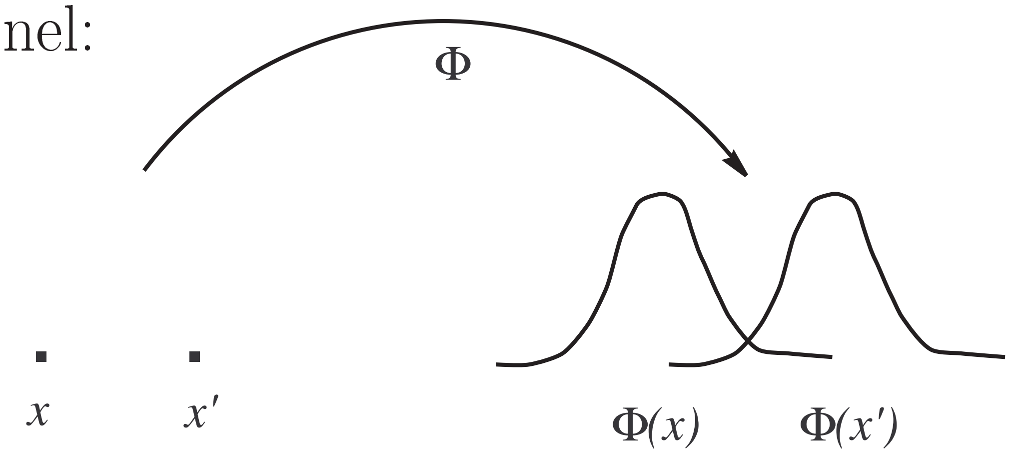
$$\sum_{i,j} a_i a_j K_{ij} \geq 0, \quad \text{where } K_{ij} := k(x_i, x_j).$$

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:

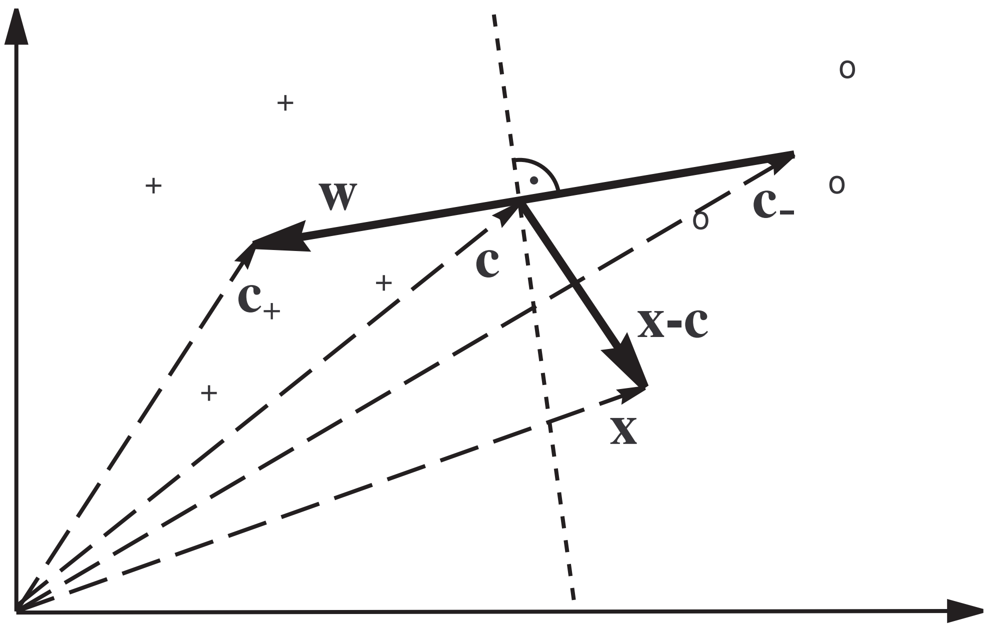
$$\begin{aligned} \text{Polynomial} \quad k(x, x') &= (\langle x, x' \rangle + c)^d \\ \text{Sigmoid} \quad k(x, x') &= \tanh(\kappa \langle x, x' \rangle + \Theta) \\ \text{Gaussian} \quad k(x, x') &= \exp(-\|x - x'\|^2 / (2\,\sigma^2)) \end{aligned}$$

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

An Example of a Kernel Algorithm

Idea: classify points $\mathbf{x} := \Phi(x)$ in feature space according to which of the two class means is closer.

$$\mathbf{c}_+ := \frac{1}{m_1} \sum_{y_i=1} \Phi(x_i), \quad \mathbf{c}_- := \frac{1}{m_2} \sum_{y_i=-1} \Phi(x_i)$$



Compute the sign of the dot product between $\mathbf{w} := \mathbf{c}_+ - \mathbf{c}_-$ and $\mathbf{x} - \mathbf{c}$.

An Example of a Kernel Algorithm, ctd.

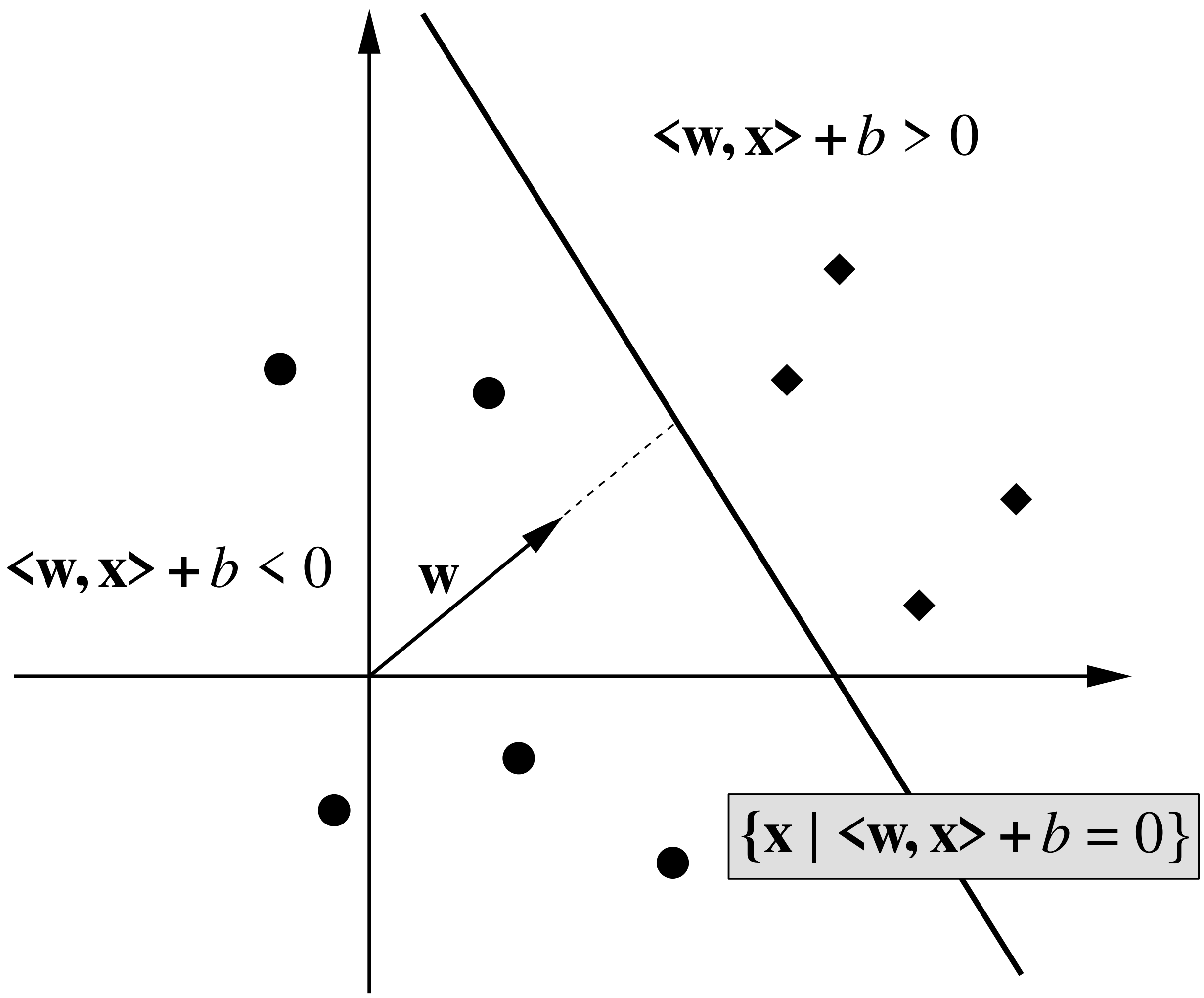
$$
\begin{aligned}
f(x) &= \operatorname{sgn}\left(\frac{1}{m_1}\sum_{\{i:y_i=+1\}}\langle\Phi(x),\Phi(x_i)\rangle-\frac{1}{m_2}\sum_{\{i:y_i=-1\}}\langle\Phi(x),\Phi(x_i)\rangle+b\right)\\
&= \operatorname{sgn}\left(\frac{1}{m_1}\sum_{\{i:y_i=+1\}}k(x,x_i)-\frac{1}{m_2}\sum_{\{i:y_i=-1\}}k(x,x_i)+b\right)
\end{aligned}
$$

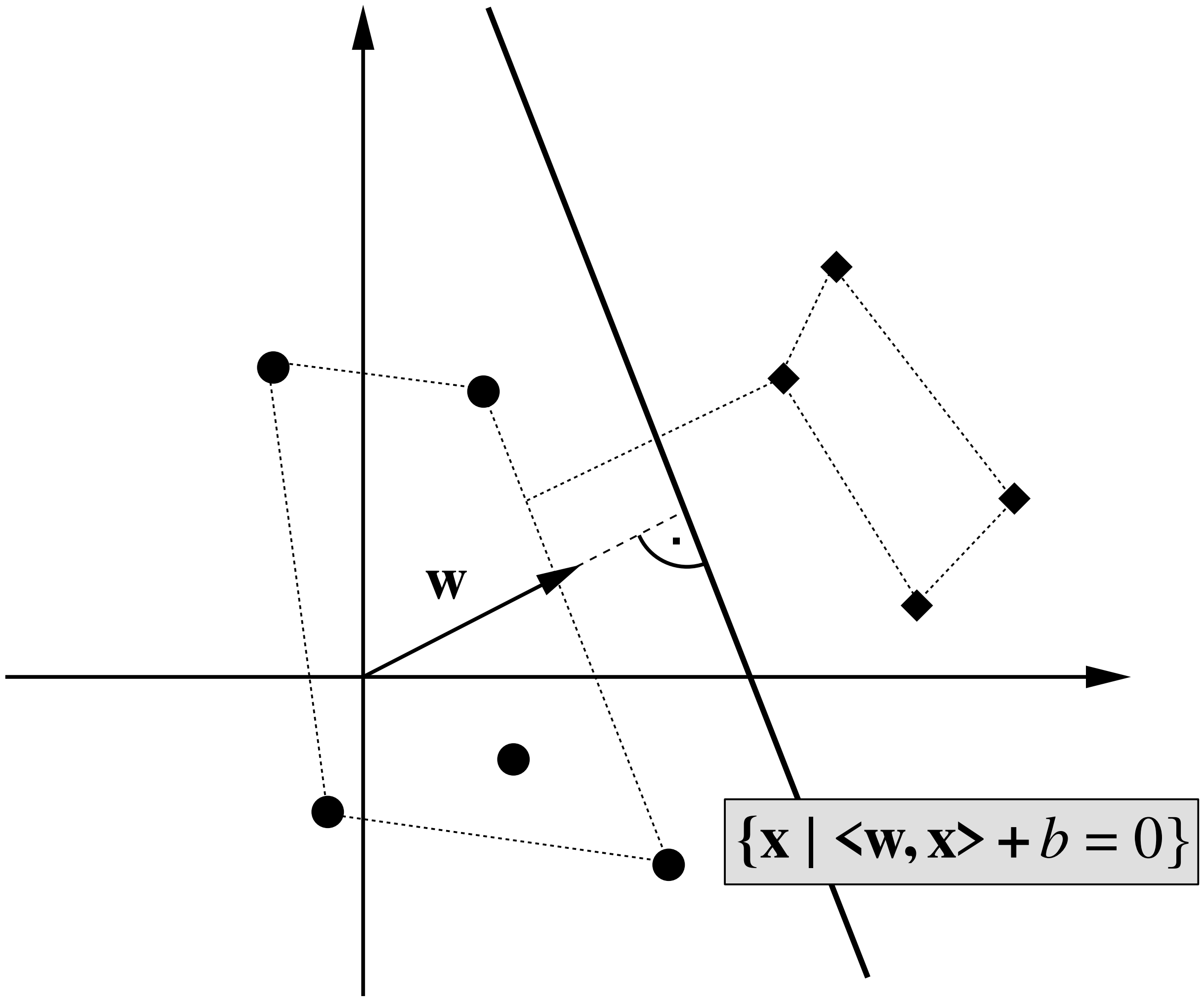
where

$$
b=\frac{1}{2}\left(\frac{1}{m_2^2}\sum_{\{(i,j):y_i=y_j=-1\}}k(x_i,x_j)-\frac{1}{m_1^2}\sum_{\{(i,j):y_i=y_j=+1\}}k(x_i,x_j)\right).
$$

- cf. Parzen windows
- the decision function is a hyperplane. Will it generalize well?

Separating Hyperplane




w
{x | <w, x> + b = 0}

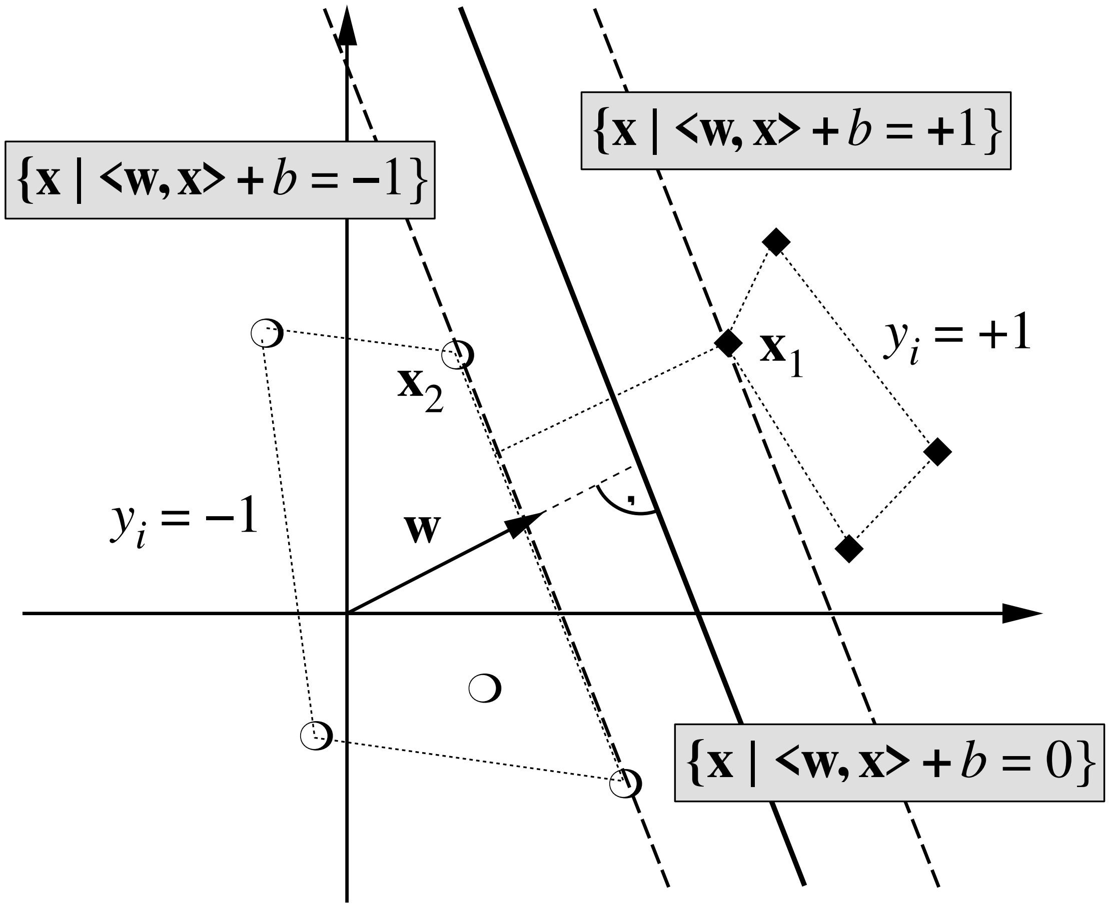
Note: if $c \neq 0$, then

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

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

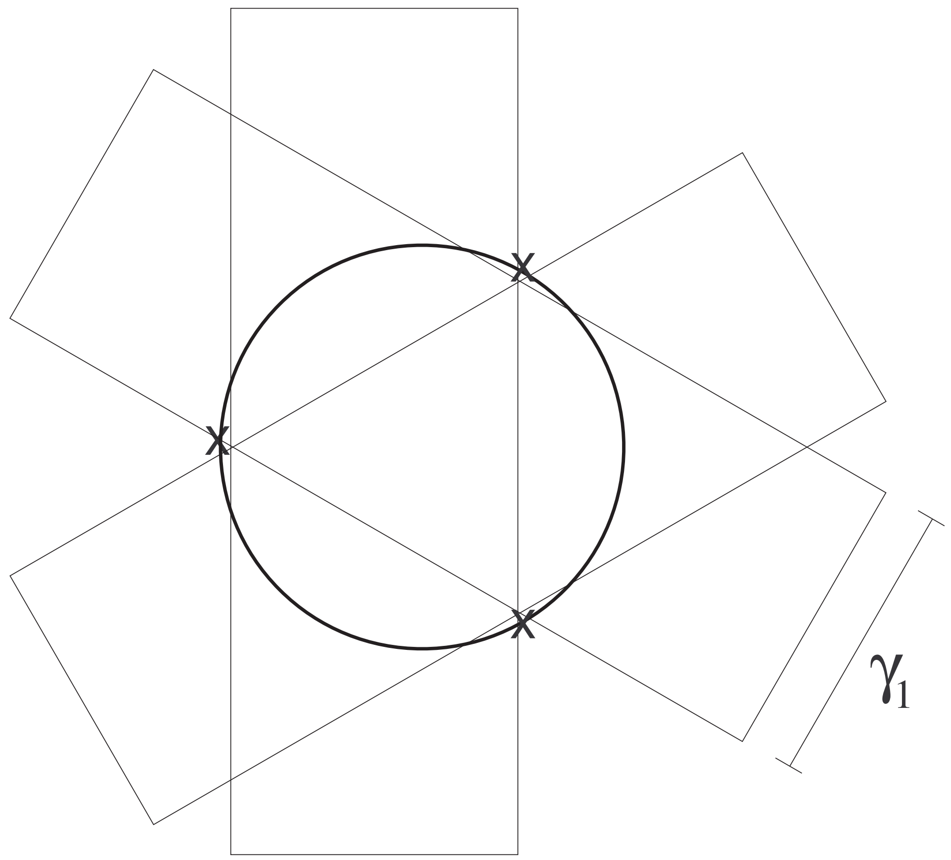
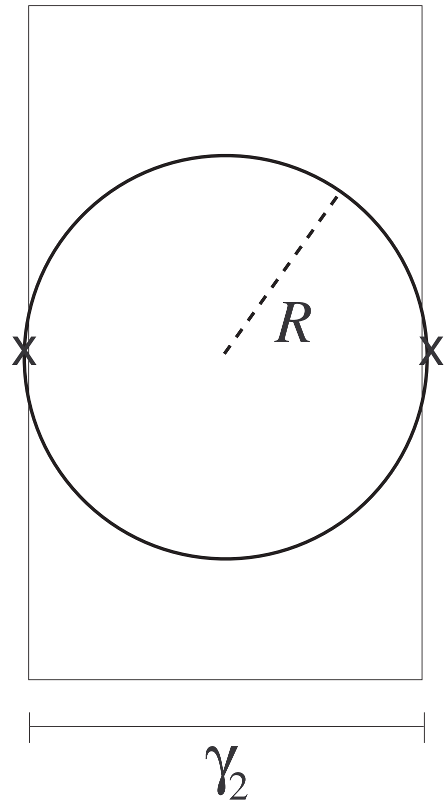
Theorem [48]. *Consider hyperplanes* $\langle \mathbf{w}, \mathbf{x} \rangle = 0$ *where* $\mathbf{w}$ *is normalized such that they are in canonical form w.r.t. a set of points* $X^* = \{\mathbf{x}_1, \ldots, \mathbf{x}_r\}$, *i.e.,*

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

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^**.*


γ1

R
γ2

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 $y_i \cdot (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) - 1 < 0 \longrightarrow$
  - · α_i will grow to increase L — how far?
  - · $\mathbf{w}$, 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

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

or

$y_i \cdot [\langle \mathbf{w}, \mathbf{x}_i \rangle + b] = 1$ (*on* the margin) $\longrightarrow \mathbf{x}_i$ "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].

Regularization Interpretation of Kernel Machines

The norm in $\mathcal{H}$ can be interpreted as a regularization term [21, 46, 19]: if P is a regularization operator such that k is Green's function of P^*P, then

$$\|\mathbf{w}\| = \|Pf\|,$$

where

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

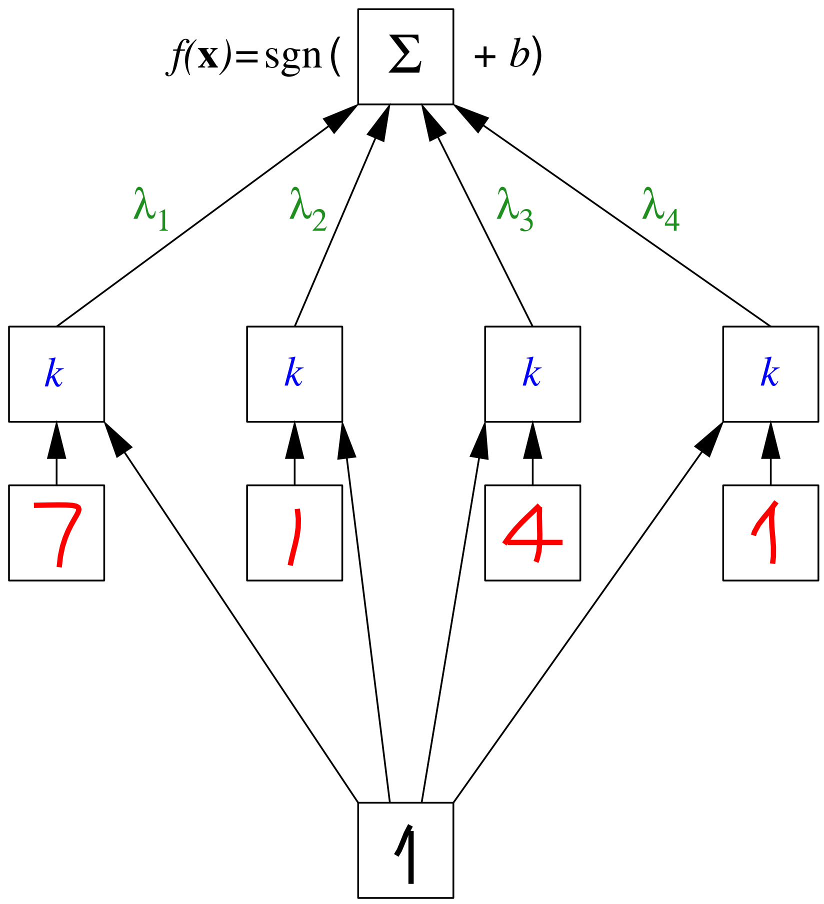
and

$$f(x) = \sum_i \alpha_i k(x_i, x).$$

Example: for Gaussian kernel, P is a linear combination of differential operators.

Corresponding MAP interpretation with prior $\exp\left(-\lambda \|Pf|^2\right)$ [29].

The SVM Architecture



classification

$f(\mathbf{x}) = \mathrm{sgn}\,(\Sigma\, \lambda_i \cdot k(\mathbf{x}, \mathbf{x}_i) + b)$

weights

comparison: $k(\mathbf{x}, \mathbf{x}_i)$, e.g.

$k(\mathbf{x}, \mathbf{x}_i) = (\mathbf{x} \cdot \mathbf{x}_i)^d$

$k(\mathbf{x}, \mathbf{x}_i) = \exp(-\|\mathbf{x} - \mathbf{x}_i\|^2 / c)$

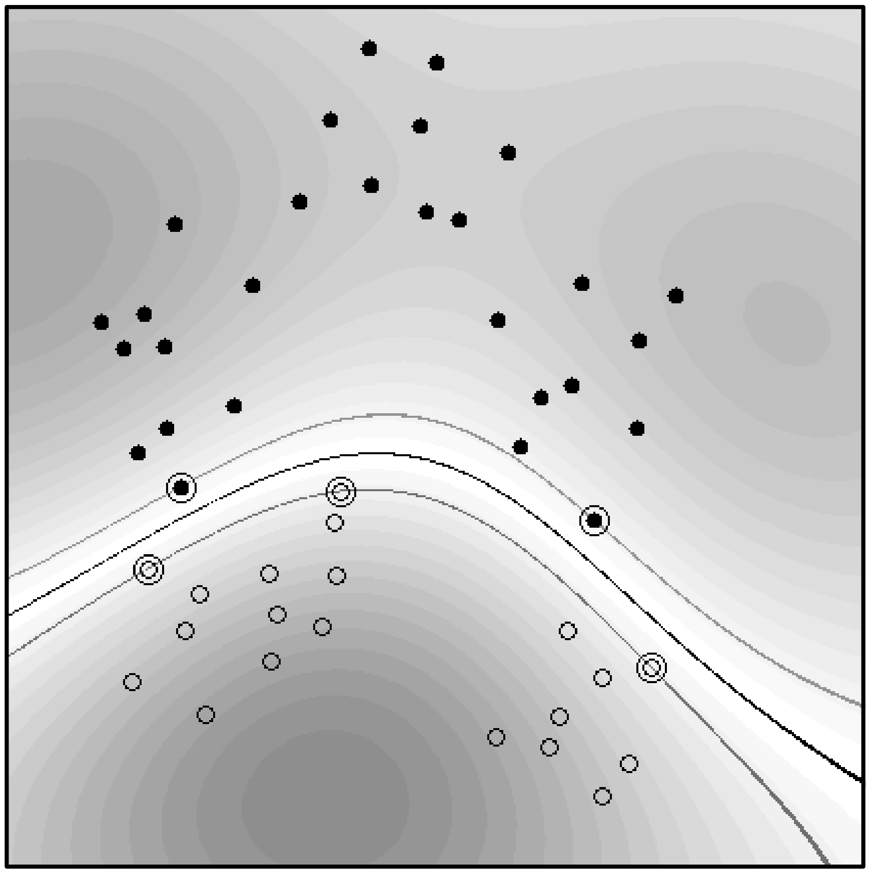
$k(\mathbf{x}, \mathbf{x}_i) = \tanh(\kappa(\mathbf{x} \cdot \mathbf{x}_i) + \theta)$

support vectors
$\mathbf{x}_1 \ldots \mathbf{x}_4$

input vector $\mathbf{x}$

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]

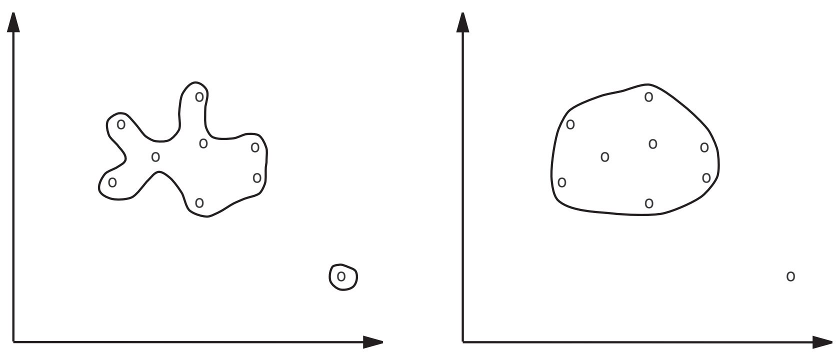
Unsupervised SVM Learning

$x_1, \ldots, x_m \in \mathcal{X}$ 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



Multi-Dimensional Quantiles

- $\mathcal{C}$ a class of measurable subsets of $\mathcal{X}$
- λ a real-valued function on $\mathcal{C}$
- *quantile function* with respect to $(\mathrm{P}, \lambda, \mathcal{C})$:

$$U(\alpha) = \inf\{\lambda(C) | \mathrm{P}(C) \geq \alpha, C \in \mathcal{C}\} \quad 0 < \alpha \leq 1.$$

- present case [41]: $\lambda(C) \propto \frac{1}{\mathrm{margin}^2}$, where

$$\mathcal{C} := \{\text{half-spaces in } \mathcal{H}, \text{ not containing the origin}\}$$

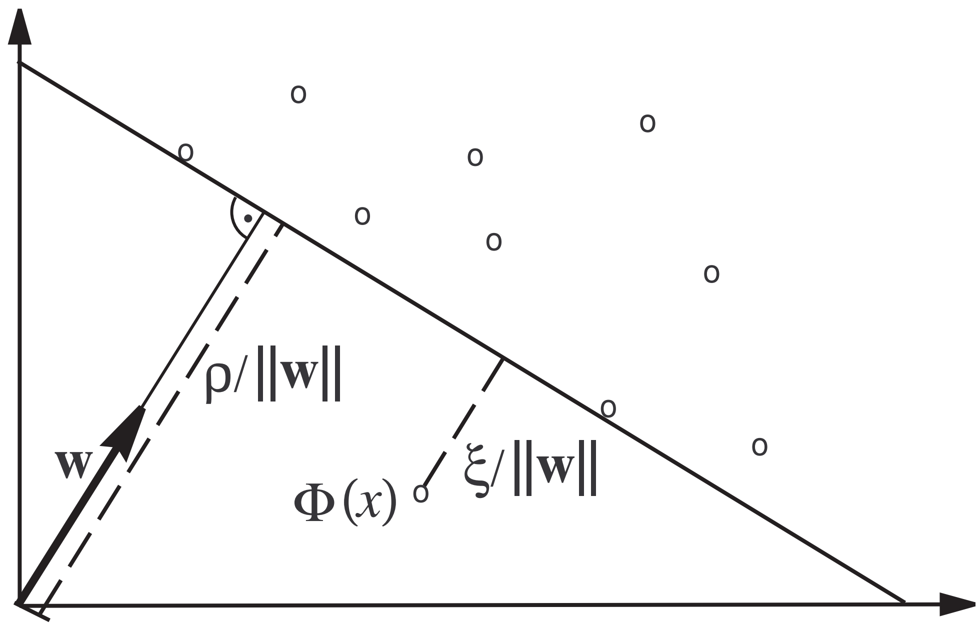
Separating Unlabelled Data from the Origin

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.

ν-Soft Margin Separation



For $\nu \in (0, 1]$, compute

$$\min_{\mathbf{w}\in\mathcal{H},\boldsymbol{\xi}\in\mathbb{R}^m,\rho\in\mathbb{R}} \quad \frac{1}{2}\|\mathbf{w}\|^2 + \frac{1}{m}\sum_i \xi_i - \nu\rho$$

$$\text{subject to} \quad \langle \mathbf{w}, \Phi(x_i)\rangle \geq \rho - \xi_i, \quad \xi_i \geq 0 \quad \text{for all } i.$$

Dual Problem

Derived using the Lagrange formalism:

$$\min_{\boldsymbol{\alpha}\in\mathbb{R}^m} \quad \tfrac{1}{2}\textstyle\sum_{ij}\alpha_i\alpha_j k(x_i,x_j)$$
$$\text{subject to } 0 \le \alpha_i \le \tfrac{1}{\nu m}, \quad \textstyle\sum_i \alpha_i = 1.$$

The decision function is

$$f(x) = \operatorname{sgn}\left(\sum_i \alpha_i k(x_i,x) - \rho\right).$$

— a thresholded sparsified Parzen windows estimator

Support Vectors and Outliers

$$SV := \{i | \alpha_i > 0\}; \quad OL := \{i | \xi_i > 0\}$$

The KKT-Conditions imply:

- $\xi_i > 0 \Longrightarrow \alpha_i = 1/(\nu m)$, hence $OL \subset SV$
- $SV \setminus OL \subset \{i | \sum_j \alpha_j k(x_j, x_i) - \rho = 0\}$

The Meaning of ν

Proposition.
(i)

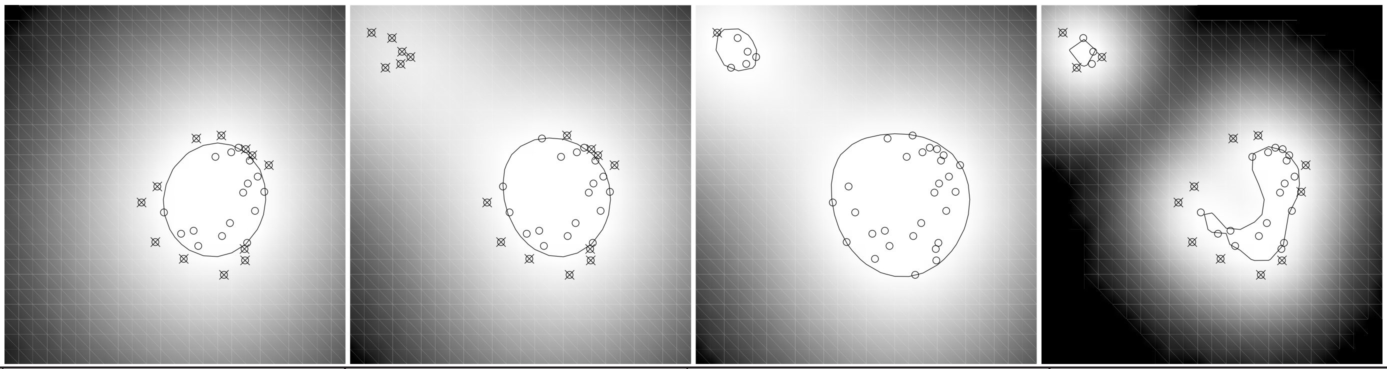
$$\frac{|OL|}{m} \leq \nu \leq \frac{|SV|}{m}$$

(ii) Suppose P *does not contain discrete components, and the kernel is analytic and non-constant. With probability 1, asymptotically,*

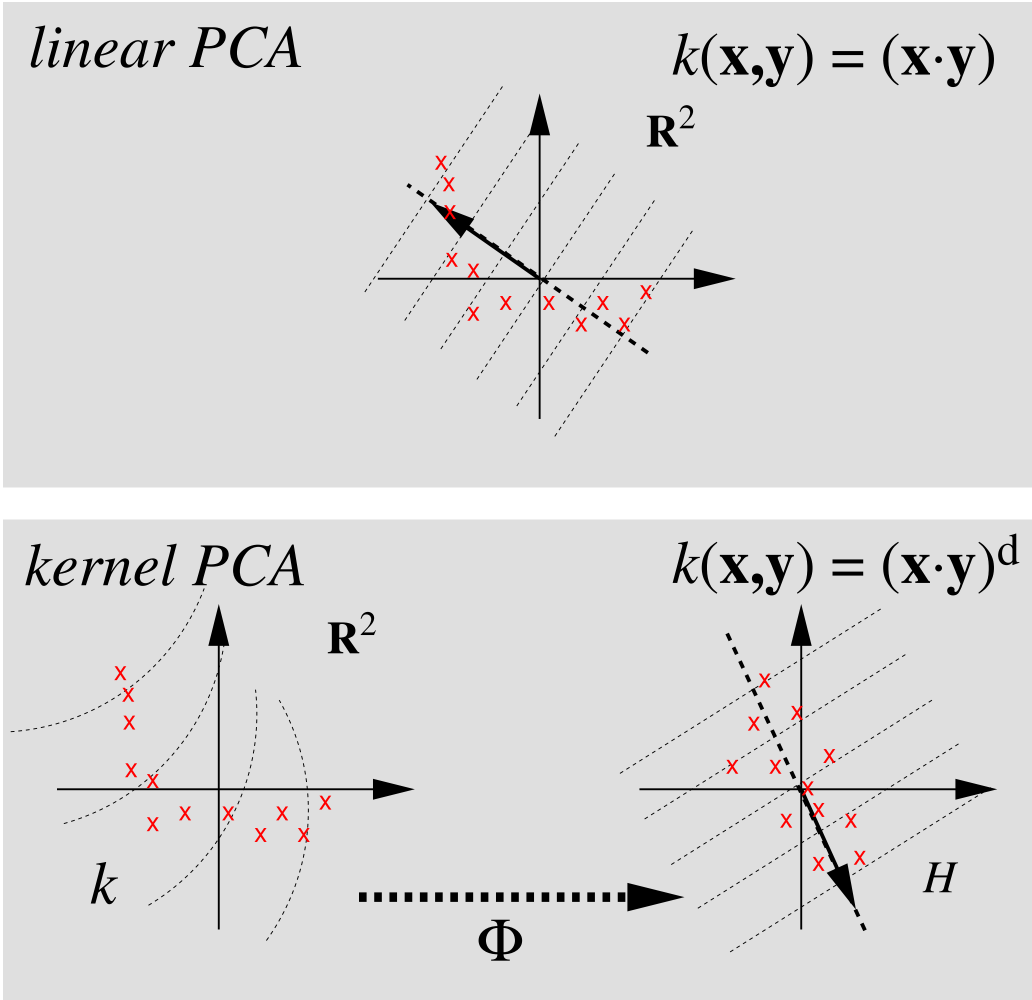
$$\frac{|OL|}{m} = \nu = \frac{|SV|}{m}.$$

There are also ν-versions of SV pattern recognition and SV regression.

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

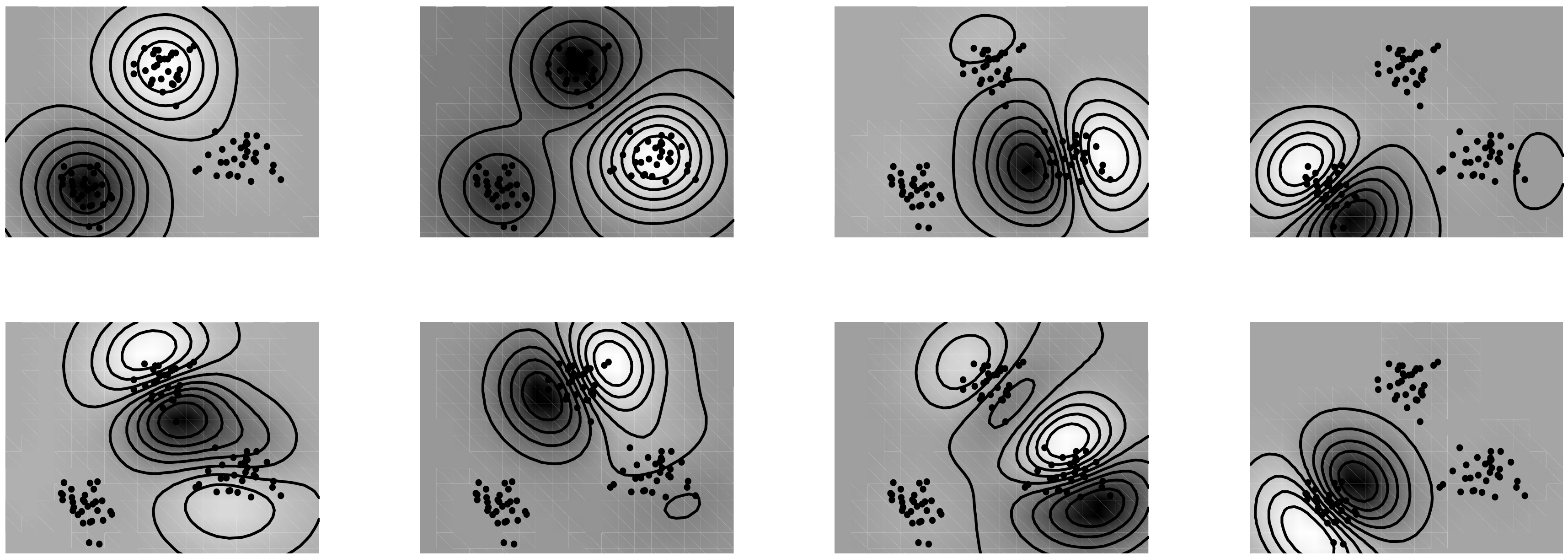


ν, width c	0.5, 0.5	0.5, 0.5	0.1, 0.5	0.5, 0.1
SVs/OLs	0.54, 0.43	0.59, 0.47	0.24, 0.03	0.65, 0.38


linear PCA
k(x,y) = (x·y)
R2
kernel PCA
k(x,y) = (x·y)d
R2
k
Φ
H

Toy Example with Gaussian Kernel

$$k(\mathbf{x}, \mathbf{y}) = \exp\left(-\|\mathbf{x} - \mathbf{y}\|^2\right)$$



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]

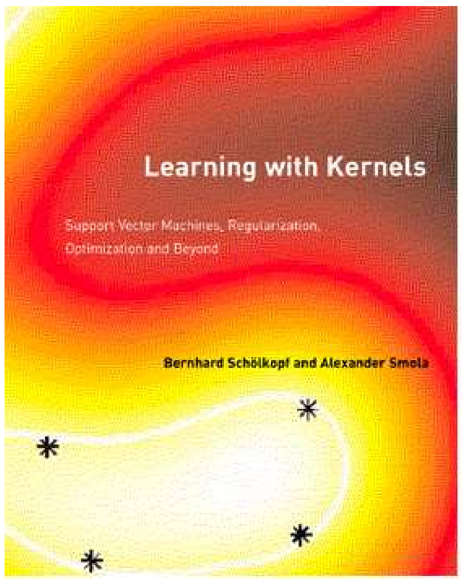
In general, the choice of a kernel corresponds to

- 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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