Introduction to Kernel Methods

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Learning Problem

Suppose we are given data

$$(x_1, y_1), \ldots, (x_m, y_m) \in \mathcal{X} \times \mathcal{Y}$$

where $(x_i, y_i) \sim \mathrm{P}(x, y)$.
We want to estimate a function $f : \mathcal{X} \to \mathcal{Y}$ such that

$$R[f] = \int_{\mathcal{X}} l(f(x), y)\, d\mathrm{P}(x, y)$$

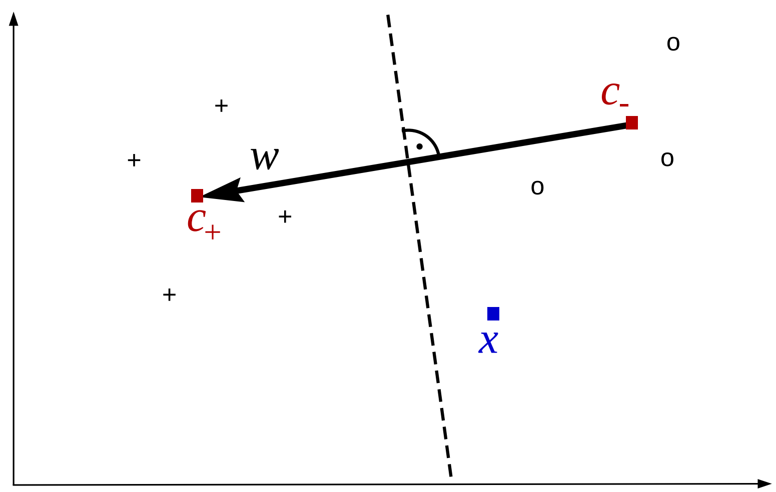
is minimized.
Here, $l(f(x), y)$ is the loss incurred when predicting $f(x)$ if the true output is y.

Special case: $\mathcal{Y} = \{\pm 1\}, l(f(x), z) = \frac{1}{2}|f(x) - y|$:
binary pattern recognition

An Example of a Pattern Recognition Algorithm

Idea: classify points x according to which of the two class means is closer.

$$c_+ := \frac{1}{m_+} \sum_{y_i=1} x_i, \quad c_- := \frac{1}{m_-} \sum_{y_i=-1} x_i$$



- Decision function: hyperplane with normal vector $w := c_+ - c_-$
- How about problems that are not linearly separable?

Kernel Feature Spaces

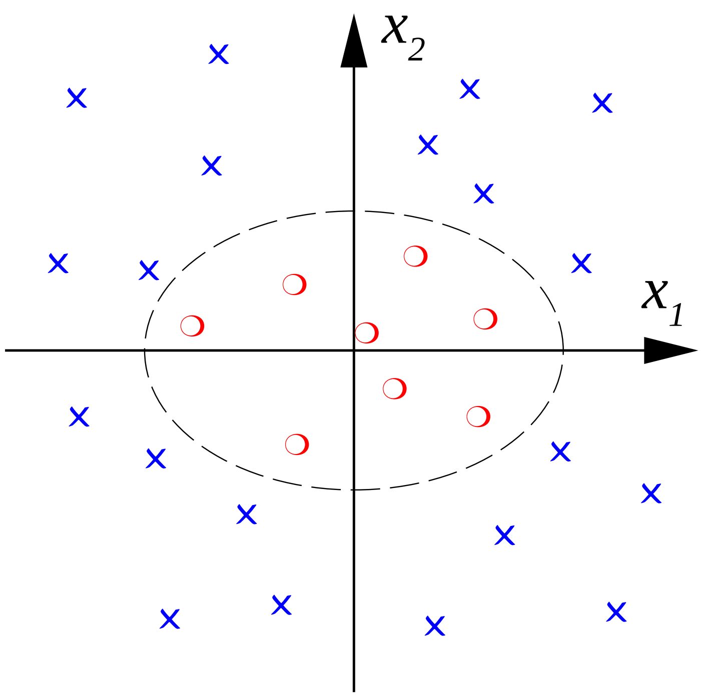
Preprocess the inputs with

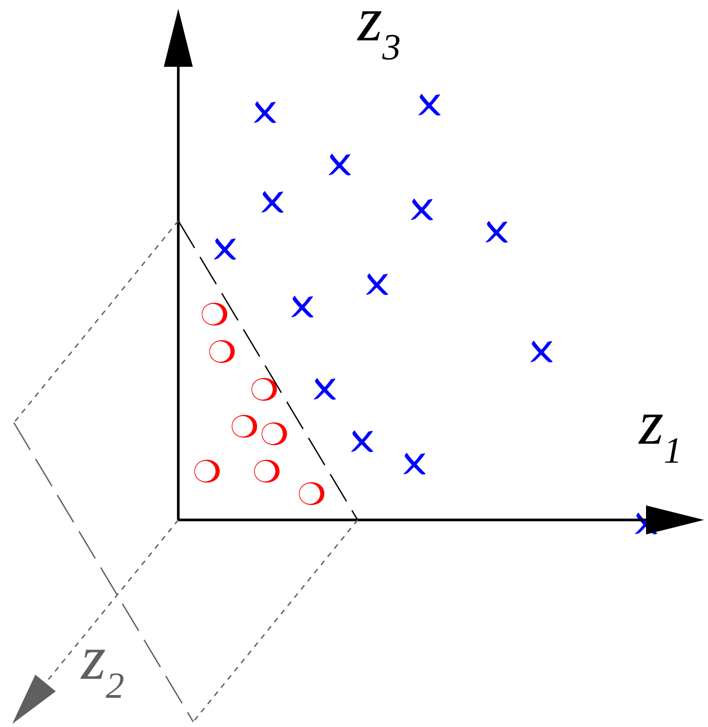
$$\begin{aligned}\Phi : \mathcal{X} &\to \mathcal{H} \\ x &\mapsto \Phi(x),\end{aligned}$$

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

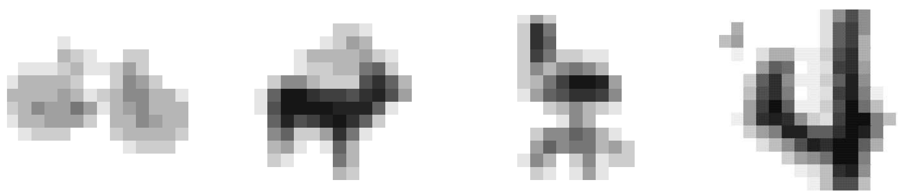
Example: All Degree 2 Monomials

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





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, $N = d = 2$

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

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

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

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

Positive Definite Kernels

Let $\mathcal{X}$ be a nonempty set. The following two are equivalent:

- k is *positive definite (pd)*, i.e., k is symmetric, and for
  - any set of training points $x_1, \ldots, x_m \in \mathcal{X}$ and
  - any $a_1, \ldots, a_m \in \mathbb{R}$

  we have

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

- there exists a map Φ into a dot product space $\mathcal{H}$ such that

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

$\mathcal{H}$ is a so-called *reproducing kernel Hilbert space.*

Special case of positive definite kernels: "Mercer kernels"

The Kernel Trick — Summary

- *any* algorithm that only depends on dot products can benefit from the kernel trick
- $\mathcal{X}$ need not be a vector space
- think of the kernel as a (nonlinear) *similarity measure*
- examples of common kernels:

$$\text{Polynomial} \quad k(x, x') = (\langle x, x' \rangle + c)^d$$

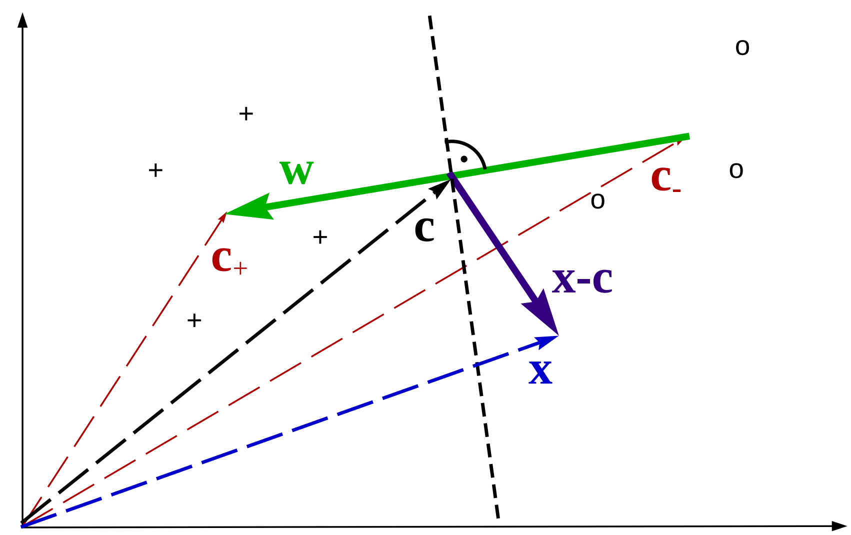
$$\text{Gaussian} \quad k(x, x') = \exp(-\|x - x'\|^2 / (2\,\sigma^2))$$

- Kernels are studied also in approximation theory *(Micchelli, 1986; Wahba, 1990; Berg et al., 1984)* and in the Gaussian Process prediction community (covariance functions) *(Weinert, 1982; Wahba, 1990; Williams, 1998; MacKay, 1998)*

An Example of a Kernel Algorithm

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

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



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.

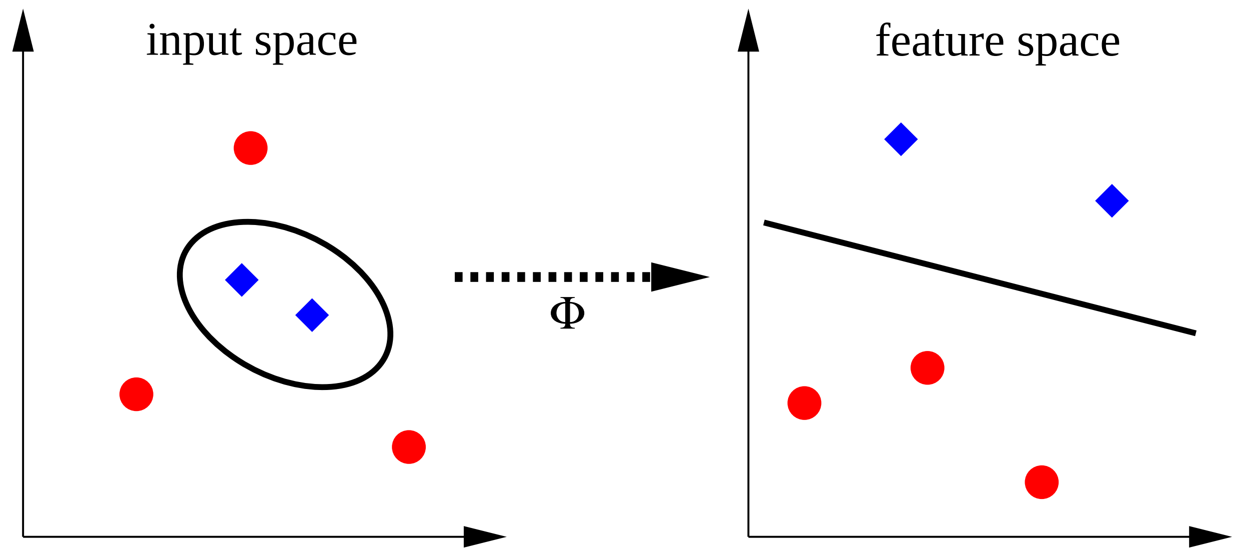
$$
\begin{aligned}
f(x) &= \operatorname{sgn}\left(\frac{1}{m_+}\sum_{\{i:y_i=1\}}\langle\Phi(x),\Phi(x_i)\rangle - \frac{1}{m_-}\sum_{\{i:y_i=-1\}}\langle\Phi(x),\Phi(x_i)\rangle + b\right)\\
&= \operatorname{sgn}\left(\frac{1}{m_+}\sum_{\{i:y_i=1\}} k(x,x_i) - \frac{1}{m_-}\sum_{\{i:y_i=-1\}} k(x,x_i)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

with the constant offset

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

- if k is a density: Parzen windows interpretation

Support Vector Classifiers



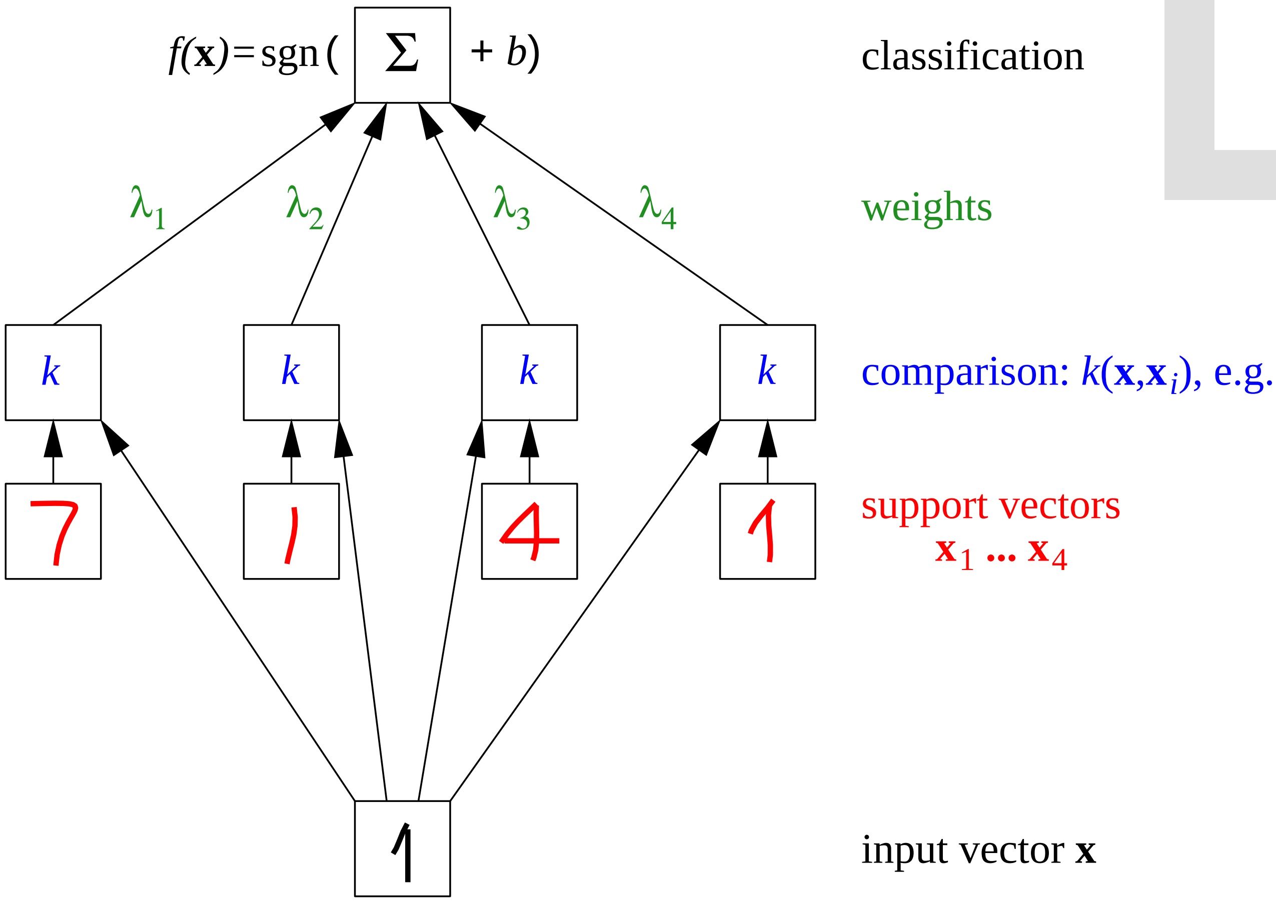
- large margin separation in $\mathcal{H}$
- sparse expansion of solution in terms of SVs:

$$f(x) = \mathrm{sgn}(\sum_i \lambda_i k(x_i, x) + b)$$

- unique solution found by convex QP
- Demo

Boser, Guyon, and Vapnik (1992)

The SVM Architecture



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

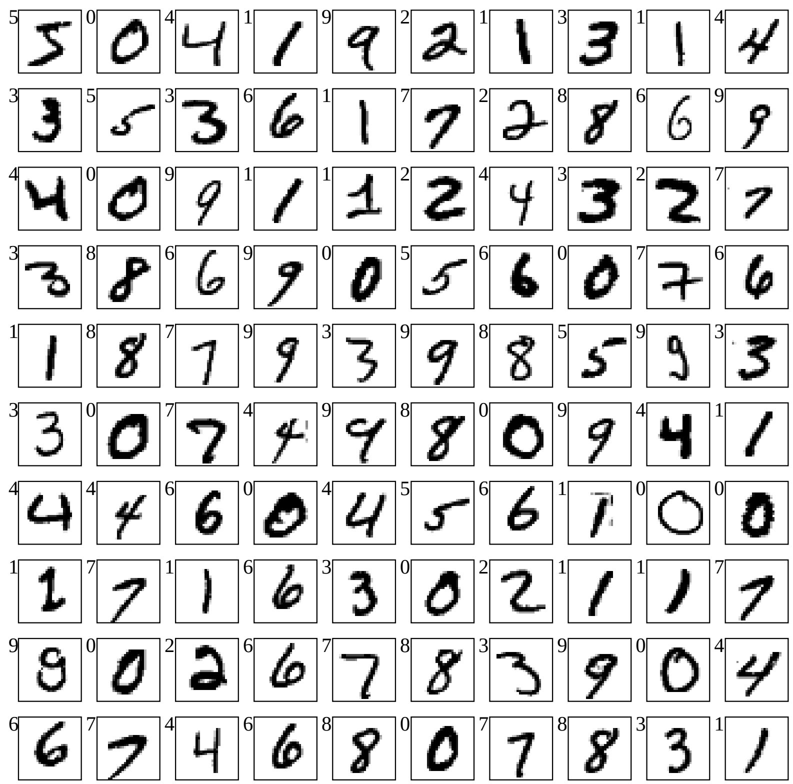
$k(\mathbf{x},\mathbf{x}_i) = (\mathbf{x} \cdot \mathbf{x}_i)^d$

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

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

MNIST Benchmark

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



MNIST Error Rates

Classifier	test error	reference
linear classifier	8.4%	*Bottou et al. (1994)*
3-nearest-neighbour	2.4%	*Bottou et al. (1994)*
SVM	1.4%	*Burges and Schölkopf (1997)*
Tangent distance	1.1%	*Simard et al. (1993)*
LeNet4	1.1%	*LeCun et al. (1998)*
Boosted LeNet4	0.7%	*LeCun et al. (1998)*
Translation invariant SVM	0.56%	*DeCoste and Schölkopf (2002)*

Dimensionality of the Feature Space

Note: the SVM system that holds the record on the MNIST set used a polynomial kernel of degree 9, corresponding to a feature space of dimensionality $\approx 3.2 \cdot 10^{20}$.

"Curse of Dimensionality"?

Statistical Learning Theory: there is a curse of *capacity*, not of *dimensionality*

Pattern Recognition

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

$(x_1, y_1), \ldots, (x_m, y_m) \in \mathcal{X} \times \{\pm 1\}$, each pair generated 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

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

Convergence of Means to Expectations

Law of large numbers: for every $f \in \mathcal{F}$,

$$\lim_{m \to \infty} \mathrm{P}\{|R[f] - R_{\mathrm{emp}}[f]| > \epsilon\} = 0$$

for all $\epsilon > 0$.

Does this imply that ERM will give us the optimal result in the limit of infinite sample size (*"consistency"* of empirical risk minimization)?

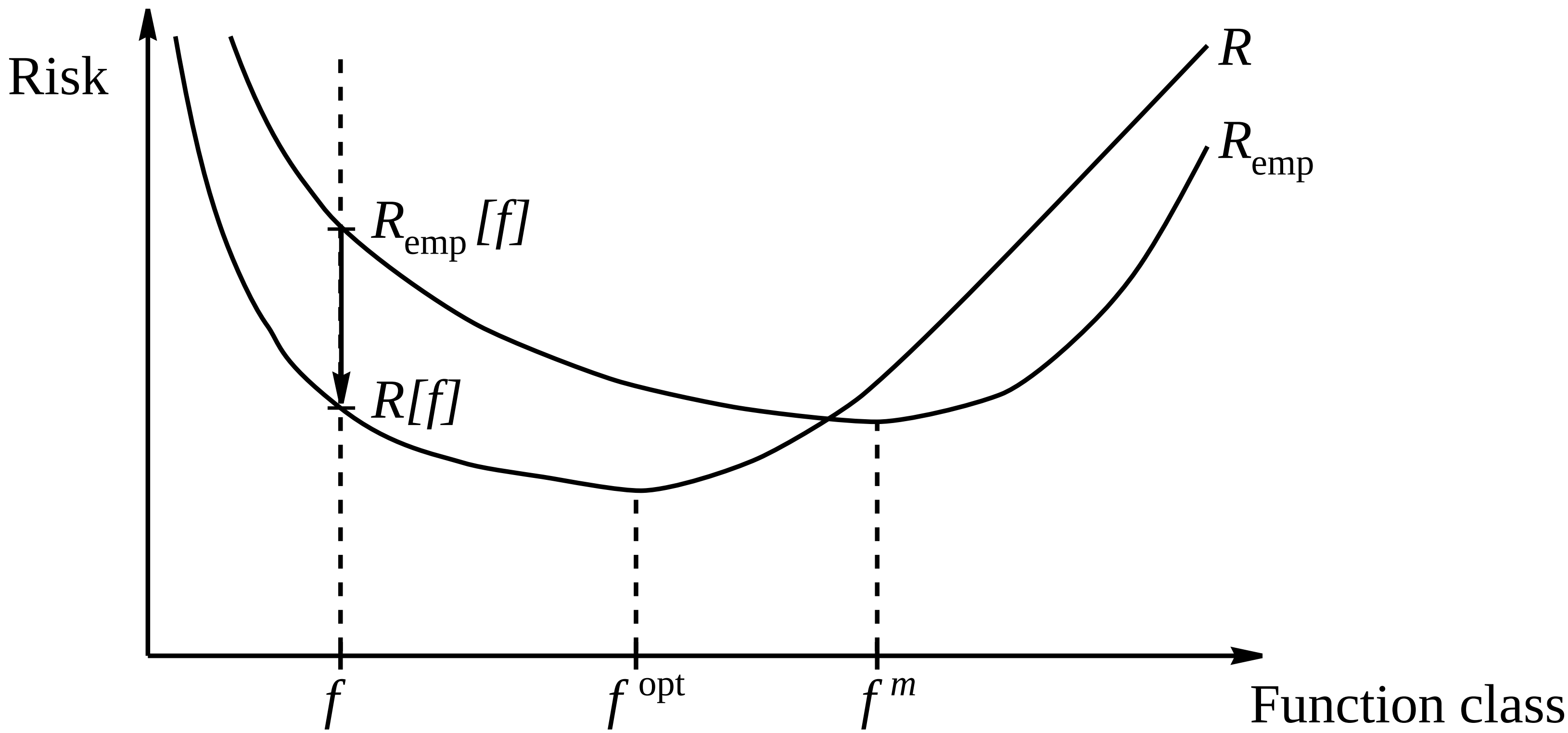
No.

Vapnik and Chervonenkis showed that ERM is (nontrivially) consistent if and only if the convergence is uniform:

$$\lim_{m \to \infty} \mathrm{P}\{\sup_{f \in \mathcal{F}} (R[f] - R_{\mathrm{emp}}[f]) > \epsilon\} = 0$$

for all $\epsilon > 0$.

Consistency and Uniform Convergence



How about taking $\mathcal{F} = \{\text{all functions mapping } \mathcal{X} \text{ to } \{\pm 1\}\}$?
Fix m. For every "good" function there exists a "bad" function with the same value of R_{emp}, and possibly rather different R.

Capacity

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

- the VC-entropy grows sublinearly with m
- the VC-dimension is finite
- the entropy numbers are well-behaved

(e.g. Vapnik and Chervonenkis, 1974; Vapnik, 1998; Shawe-Taylor et al., 1998; Williamson et al., 1998; Alon et al., 1997)

To have a low test error, we need a low training error and low capacity.

Justifications for Large Margins

- VC-dimension: $h \leq R^2/\rho^2$, where ρ is the margin and R is the radius of the smallest sphere containing the data *(Vapnik, 1979)*
- fat-shattering dimension and data dependent SRM *(Gurvits, 1997; Shawe-Taylor et al., 1998)*
- regularization theory *(Girosi, 1998; Smola and Schölkopf, 1998)* and Bayesian MAP estimation *(Kimeldorf and Wahba, 1970; Poggio and Girosi, 1990)*
- algorithmic stability *(Bousquet and Elisseeff, 2001)*
- Rademacher averages *(Kolchinskiĭ et al., 2001; Mendelson, 2001; Bousquet, 2002)*
- compression/MDL *(von Luxburg et al., 2002)*

Compression Bound

Given: a finite function class $\mathcal{F}$.

Denote by C the *compression coefficient* of the training labels given the training inputs, using functions from $\mathcal{F}$.

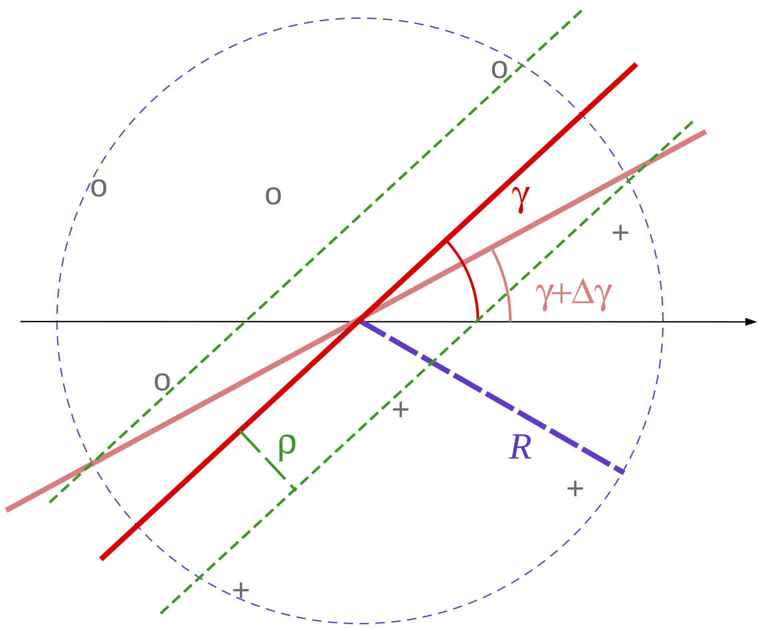
Sender		Receiver
$x_1, \ldots, x_m$		$x_1, \ldots, x_m$
$y_1, \ldots, y_m$		
f	$\longrightarrow$	$f(x_1), \ldots, f(x_m)$

Theorem. For all $f \in \mathcal{F}$, with probability $\geq 1 - \delta$,

$$R[f] \leq 2 \log(2) C - \frac{\ln(\delta)}{m}.$$

(Vapnik (1995), cf. also Littlestone and Warmuth (1986))

Maximum Margin vs. MDL — 2D Case

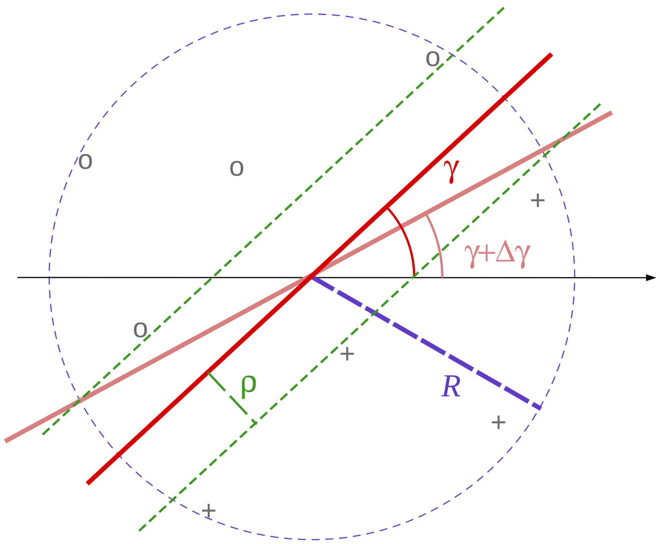


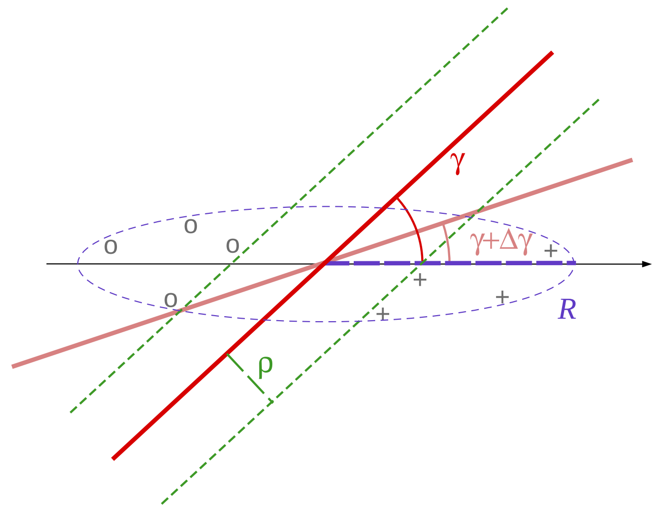
Can perturb γ by $\Delta\gamma$ with $|\Delta\gamma| < \arcsin\frac{\rho}{R}$ and still correctly separate the data.

Hence only need to transmit γ with accuracy $\Delta\gamma$ *(von Luxburg et al., 2002)*.

Can be done by computing a $\Delta\gamma$-cover of $\mathcal{F} = \{\text{hyperplanes with } \|w\| = 1\}$

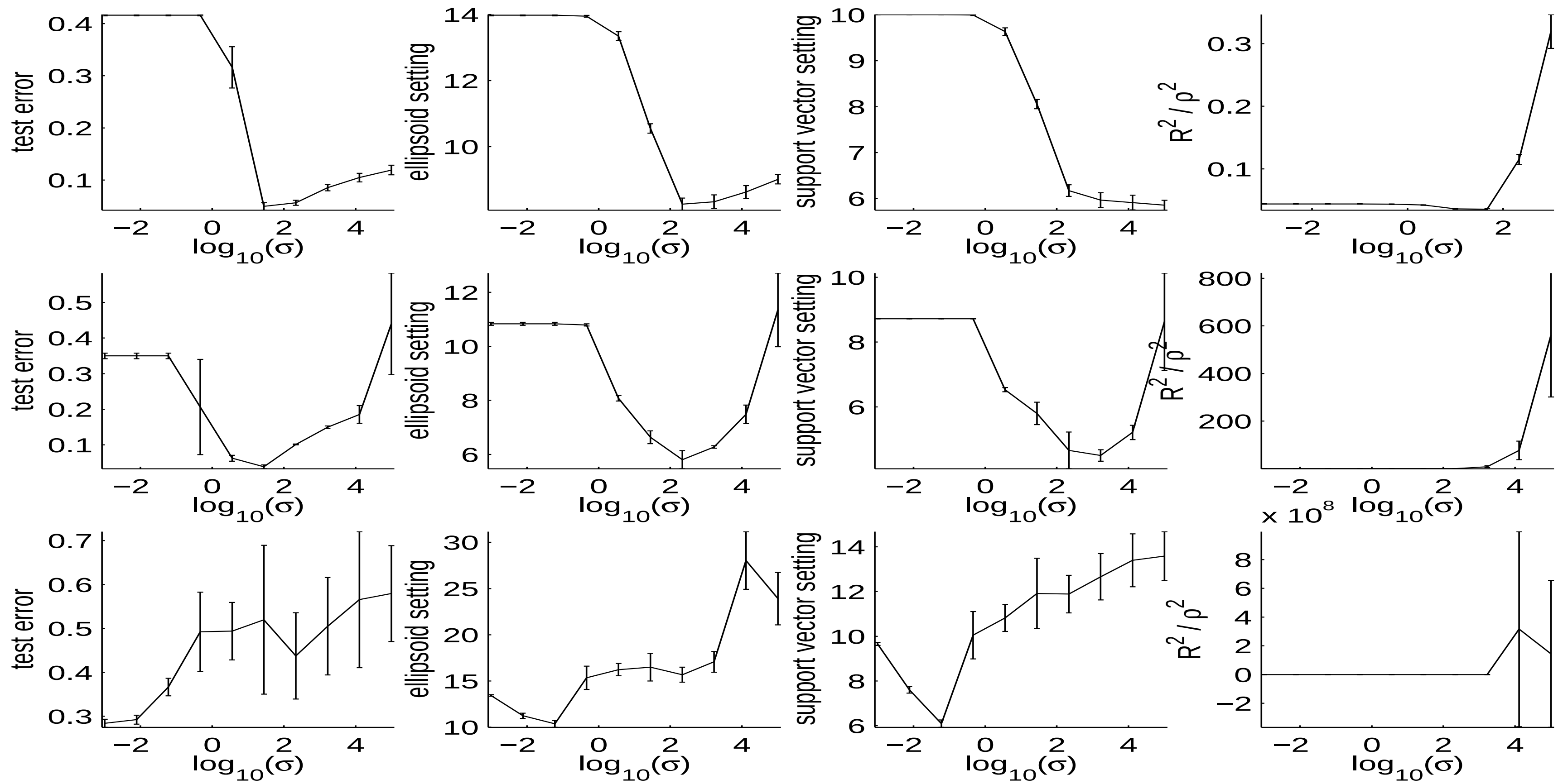
Ellipsoid Case





- ellipsoid setting: different directions imply different $\Delta\gamma$
- axes of ellipsoid can be computed from kernel eigenvalues

Experiments: Selecting σ in a Gaussian Kernel



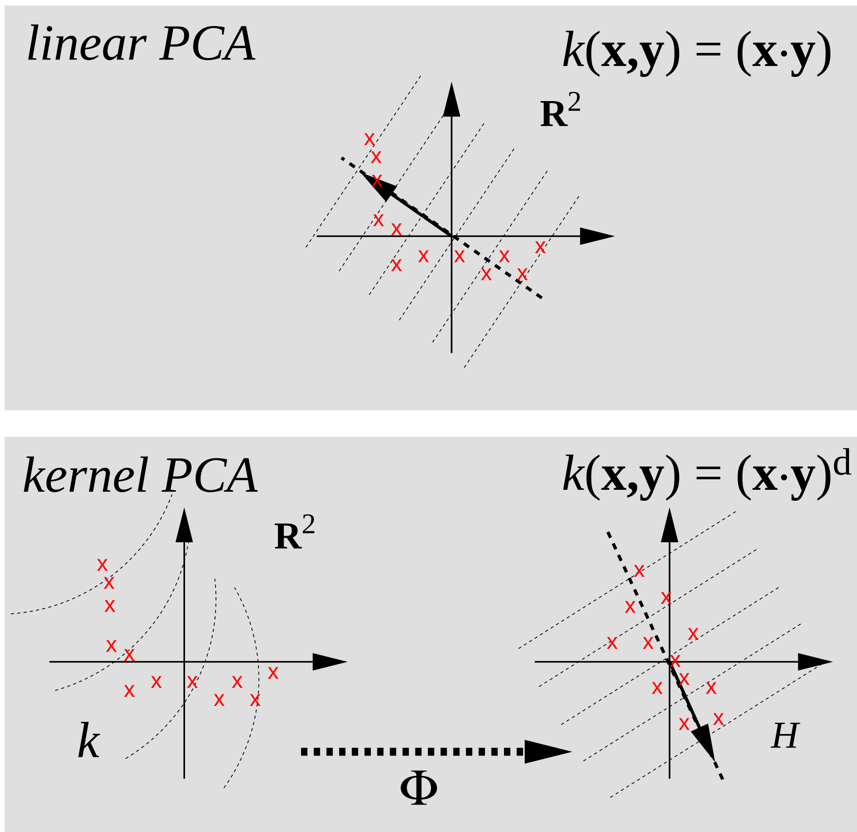
Datasets: USPS ($m = 500$)
Wisconsin breast cancer ($m = 200$)
Abalone ($m = 500$)

Further Kernel Algorithms — Design Principles

1. "Kernel module"
   - similarity measure $k(x, x')$, where $x, x' \in \mathcal{X}$
   - data representation
     (in associated feature space where $k(x, x') = \langle \Phi(x), \Phi(x') \rangle$)
     — thus can construct geometric algorithms
   - function class ("representer theorem," $f(x) = \sum_i \alpha_i k(x, x_i)$)
2. "Learning module"
   - classification
   - quantile estimation / novelty detection
   - feature extraction
   - ...

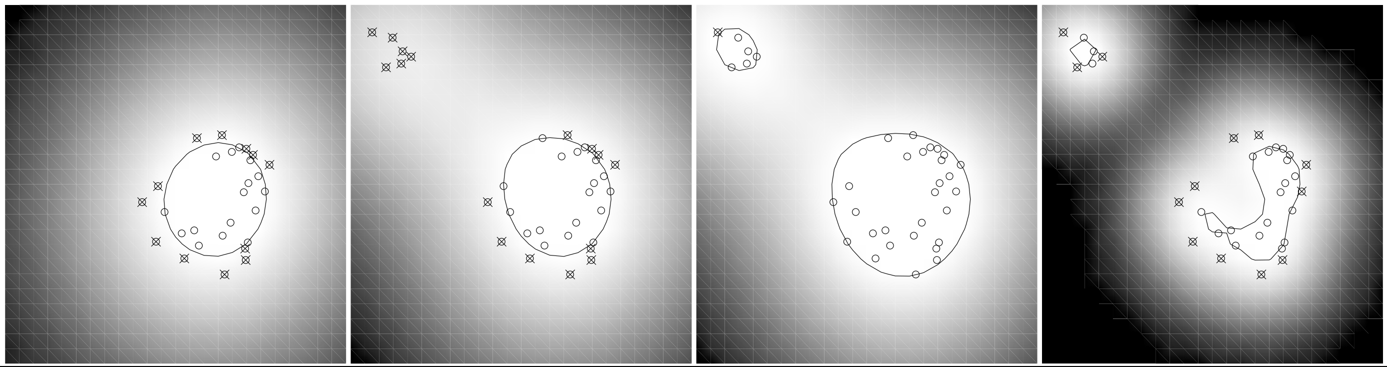
Kernel PCA

(Schölkopf et al., 1998)



Demo ○

One-Class SVMs



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

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

- Jet engine condition monitoring *(Hayton et al., 2001)*
- Network intrusion detection *(Wankadia et al., 2001)*
- Outlier detection *(Schölkopf et al., 2001)*
- Information retrieval

Kernel Dependency Estimation *(Weston et al., 2002)*

Given two sets $\mathcal{X}$ and $\mathcal{Y}$ with kernels k and k', and training data (x_i, y_i).

Estimate a dependency $\mathbf{w} : \mathcal{H} \to \mathcal{H}'$

$$\mathbf{w}(\cdot) = \sum_{ij} \alpha_{ij} \Phi'(y_j) \langle \Phi(x_i), \cdot \rangle \, .$$

This can be evaluated in various ways, e.g., given an x, we can compute the pre-image

$$y = \operatorname{argmin}_{\mathcal{Y}} \|\mathbf{w}(\Phi(x)) - \Phi'(y)\|.$$

A convenient way of learning the α_{ij} is to work in the kernel PCA basis.

Application to Image Completion

Shown are all digits where at least one of the two algorithms makes a mistake (73 mistakes for k-NN, 23 for KDE).

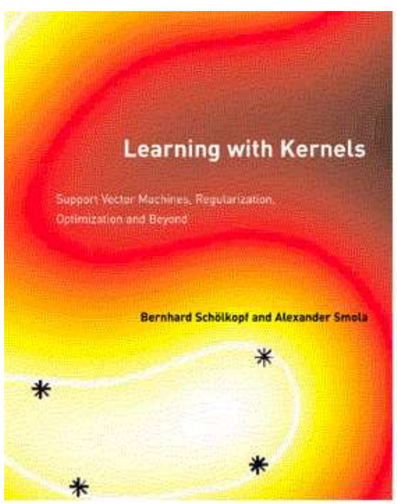
(from Weston et al. (2002))

Kernel Machines Research

- algorithms/tasks: KDE, feature selection *(Weston et al., 2002)*, multi-label-problems *(Elisseeff & Weston, 2001)*, unlabelled data *(Szummer & Jaakkola, 2002)*, ICA *(Harmeling et al., 2002)*, canonical correlations *(Bach & Jordan, 2002; Kuss, 2002)*
- optimization and implementation: QP, SDP *(Lanckriet et al., 2002)*, online versions, ...
- theory of empirical inference: sharper capacity measures and bounds *(Bartlett, Bousquet, & Mendelson, 2002)*, generalized evaluation spaces *(Mary & Canu, 2002)*, ...
- kernel design
  - transformation invariances *(Chapelle and Schölkopf, 2002)*
  - kernels for discrete objects *(Haussler, 1999; Watkins, 2000; Lodhi et al., 2000; Cristianini and Shawe-Taylor, 2000; Vert, 2002)*
  - kernels based on generative models *(Jaakkola and Haussler, 1999; Seeger, 1999; Tsuda et al., 2002)*
  - local kernels *(e.g., Zien et al., 2000)*
  - complex kernels from simple ones *(Haussler, 1999; Bartlett and Schölkopf, 2001)*, global kernels from local ones *(Kondor and Lafferty, 2002)*
  - functional calculus for kernel matrices *(Schölkopf et al., 2002)*
  - model selection, e.g., via alignment *(Cristianini et al., 2001)*

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,...) that work very well in practice
- kernels unify three aspects of empirical inference: similarity measures, function classes, and data representations. The choice of a kernel is crucial, and it is not a problem of statistics.



For further information, cf.
`http://www.kernel-machines.org`,
`http://www.learning-with-kernels.org`

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