

Learning with Kernels

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Learning Problem

Suppose we are given data

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

where $(x_i, y_i) \sim P(x, y)$.

We want to estimate a function $f \in \mathcal{F}$ such that

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

is minimized.

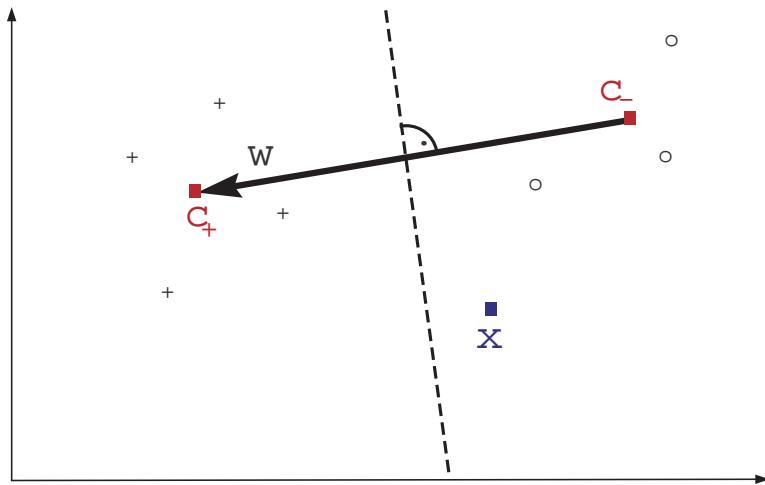
Here, $l(f(x), y)$ is the loss incurred when predicting $f(x)$ if the true output is y .

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

An Example of a Pattern Recognition Algorithm

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

$$c_+ := \frac{1}{m_1} \sum_{y_i=1} x_i, \quad c_- := \frac{1}{m_2} \sum_{y_i=-1} x_i$$



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

Kernel Feature Spaces

Preprocess the inputs with

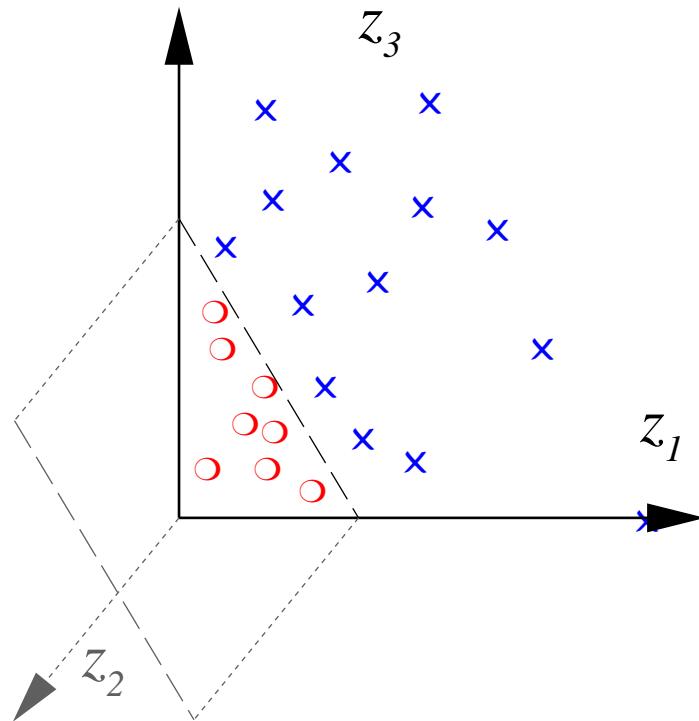
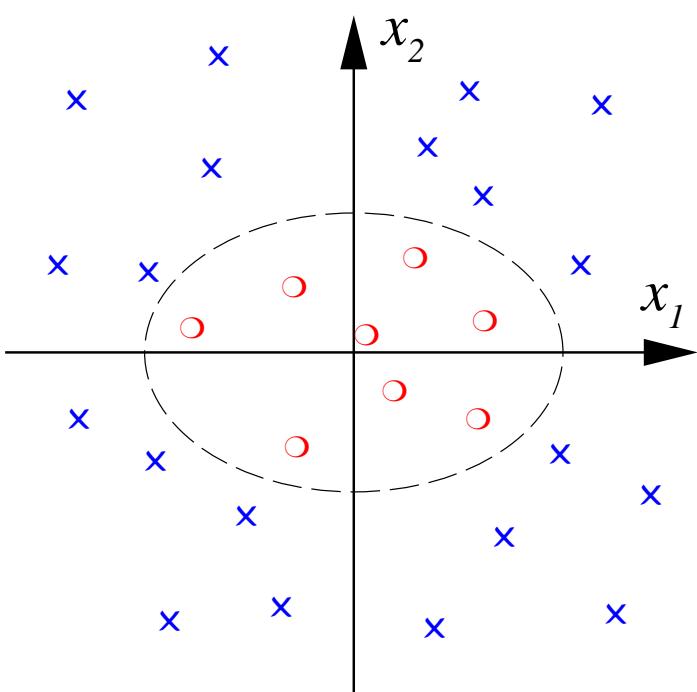
$$\begin{aligned}\Phi : \mathcal{X} &\rightarrow \mathcal{H} \\ x &\mapsto \Phi(x),\end{aligned}$$

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

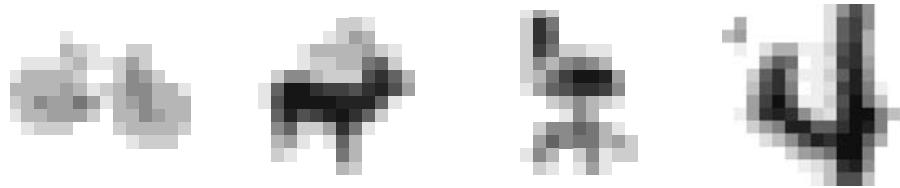
Example: All Degree 2 Monomials

$$\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$



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, $N = d = 2$

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

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

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

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

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

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 $x_1, \dots, x_m \in \mathcal{X}$ and
 - any $a_1, \dots, a_m \in \mathbb{R}$

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:

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

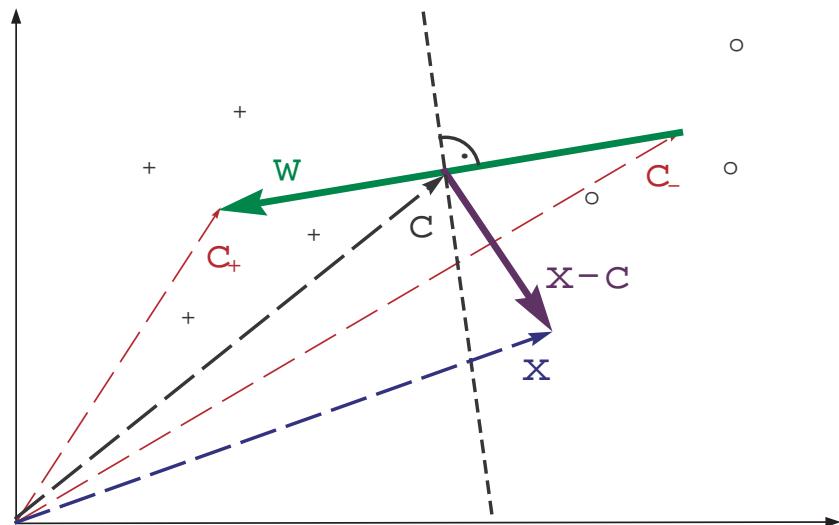
$$\text{Gaussian } k(x, x') = \exp(-\|x - x'\|^2 / (2 \sigma^2))$$

- 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.

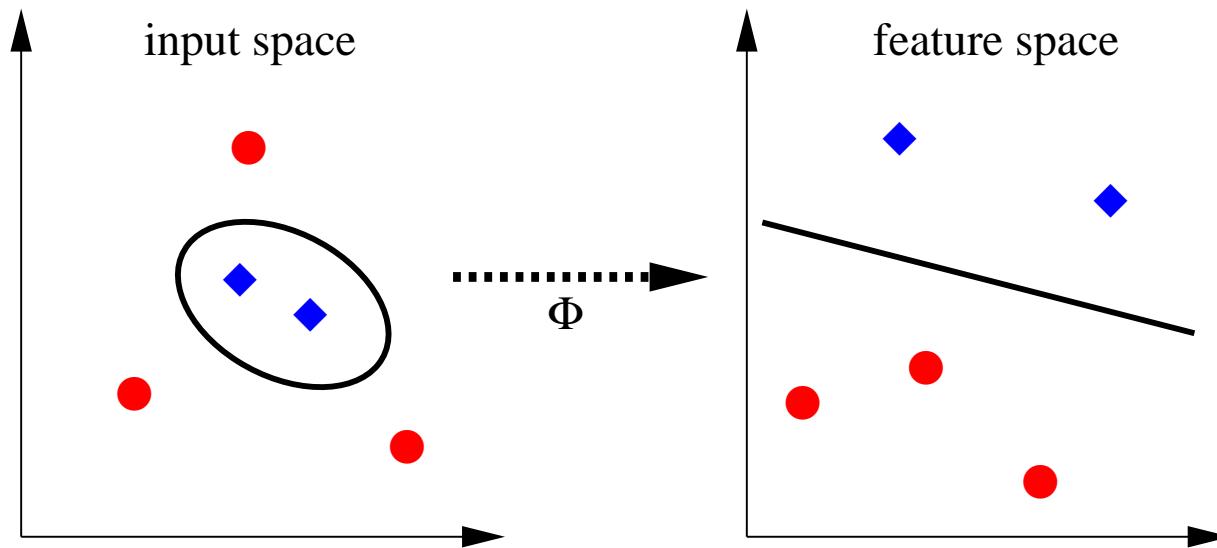
$$\begin{aligned} f(x) &= \operatorname{sgn} \left(\frac{1}{m_+} \sum_{\{i:y_i=1\}} \langle \Phi(x), \Phi(x_i) \rangle - \frac{1}{m_-} \sum_{\{i:y_i=-1\}} \langle \Phi(x), \Phi(x_i) \rangle + b \right) \\ &= \operatorname{sgn} \left(\frac{1}{m_+} \sum_{\{i:y_i=1\}} k(x, x_i) - \frac{1}{m_-} \sum_{\{i:y_i=-1\}}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

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
- Demo

Support Vector Classifiers

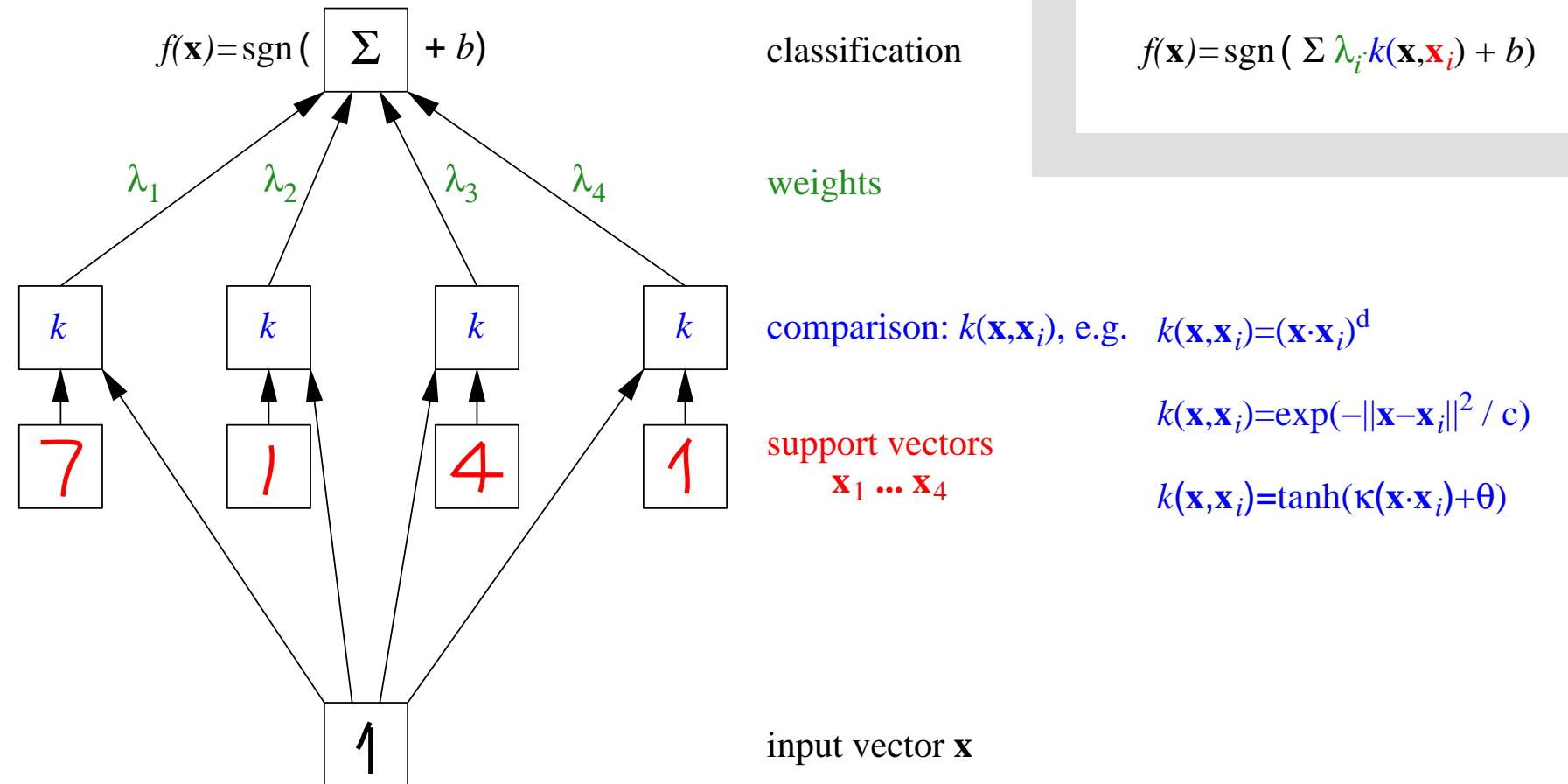


- large margin separation in \mathcal{H}
- sparse expansion of solution in terms of SVs:

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

- unique solution found by convex QP
- Demo

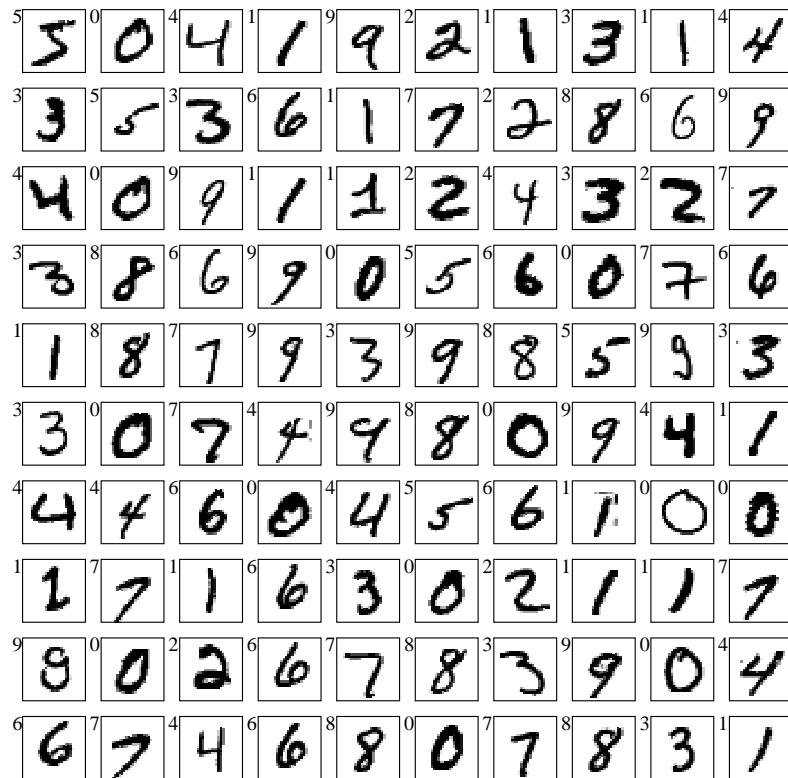
The SVM Architecture



○

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)

Some other successful applications: [bioinformatics](#) (*Jaakkola et al., 2000; Brown et al., 2000; Zien et al., 2000; Guyon et al., 2002; Furey et al., 2000; Pavlidis et al., 2001; Warmuth et al., 2002; Yeang et al., 2001*), [text](#) (*Joachims, 1998; Hearst et al., 1998; Tong and Koller, 2000; Drucker et al., 2001*), [computer vision](#) (*Blanz et al., 1996; Pontil and Verri, 1998; Chapelle et al., 1999*), [telephony](#) (*Chen and Harris, 2000*)

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

$(x_1, y_1), \dots, (x_m, y_m) \in \mathcal{X} \times \{\pm 1\}$, each pair generated from $P(x, y)$, such that the expected misclassification error on a test set, also drawn from $P(x, y)$,

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

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

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

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

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

Convergence of Means to Expectations

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

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

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)?

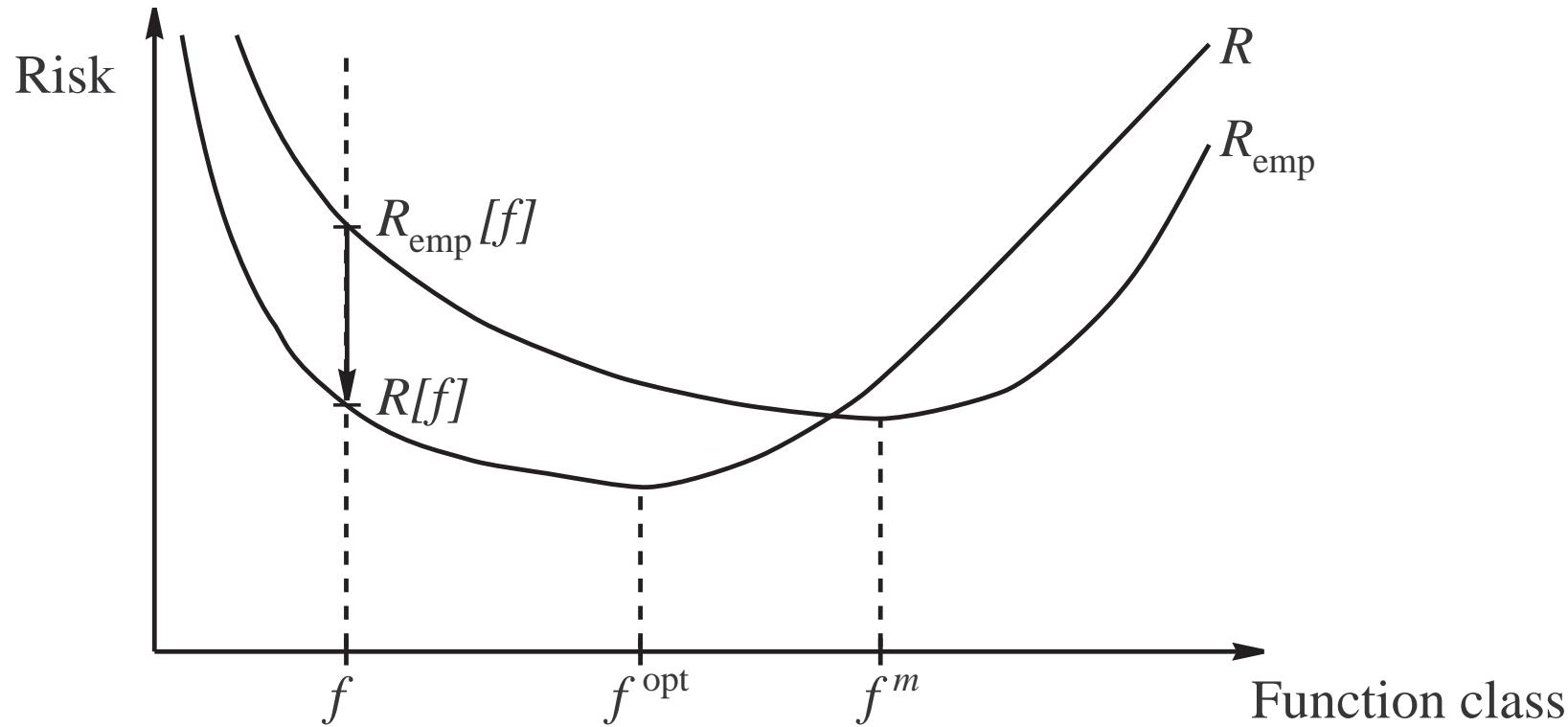
No.

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

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

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} .

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 (*Kolchinskii 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} .

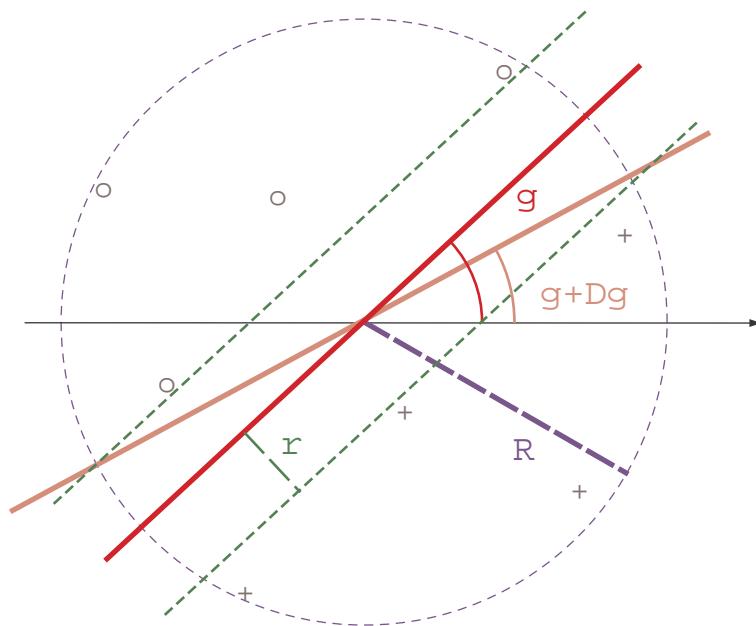
Sender		Receiver
x_1, \dots, x_m		x_1, \dots, x_m
y_1, \dots, y_m		
f	\longrightarrow	$f(x_1), \dots, f(x_m)$

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

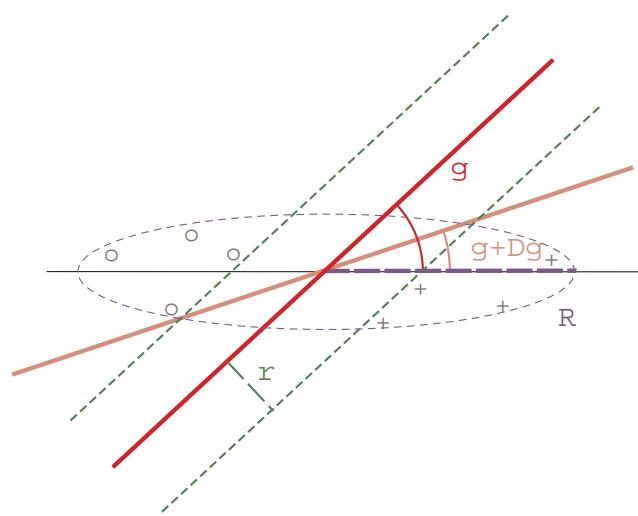
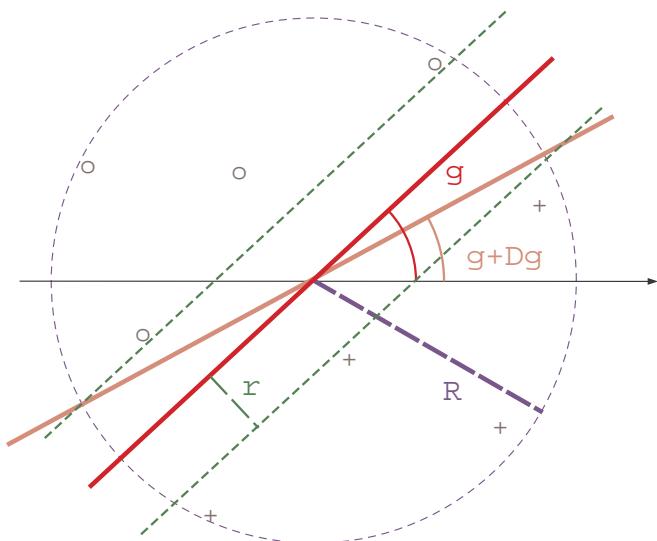


Can perturb γ by $\Delta\gamma$ with $|\Delta\gamma| < \arcsin \frac{\rho}{R}$ and still correctly separate the data.

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

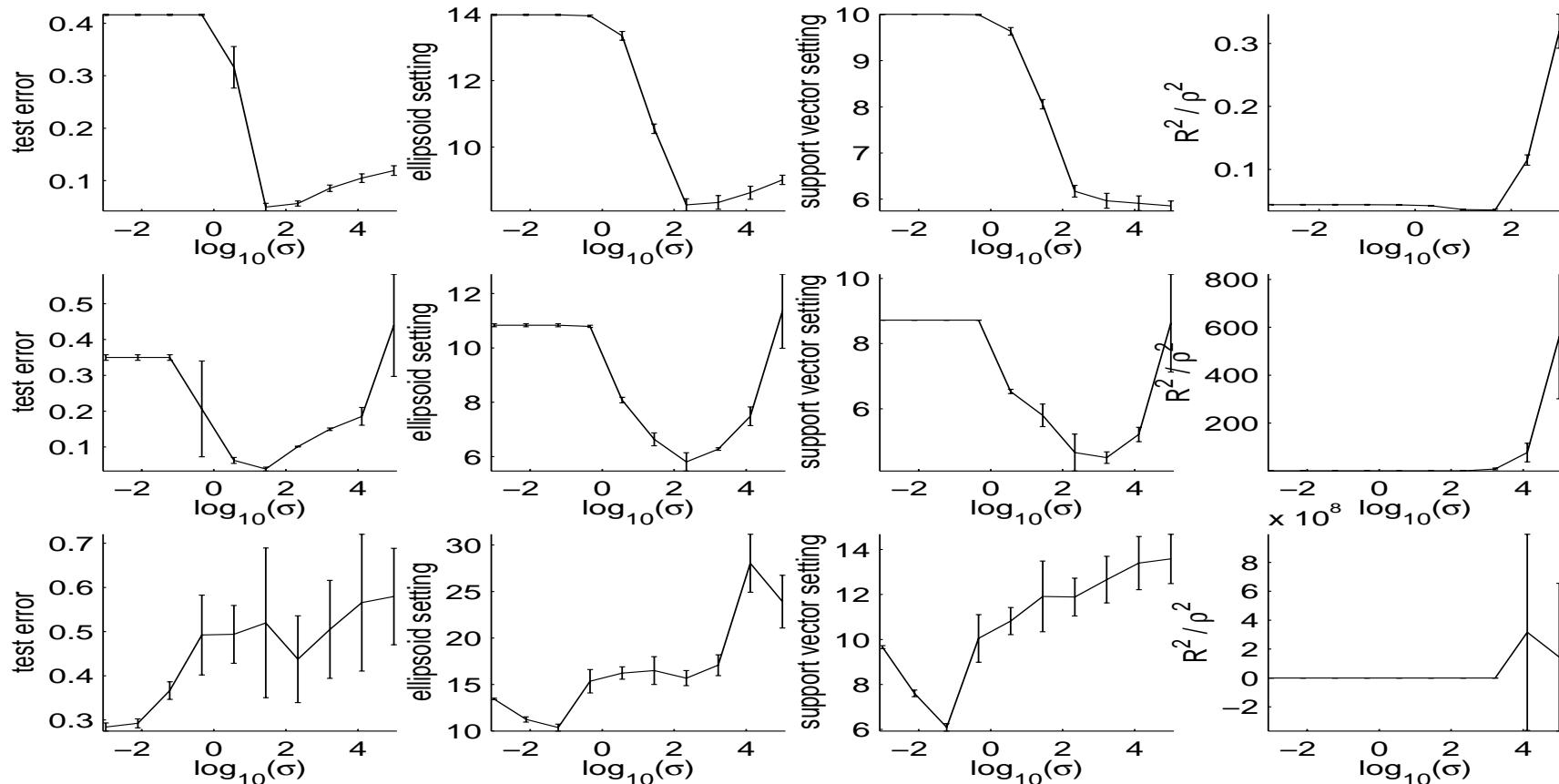
Can be done by computing a $\Delta\gamma$ -cover of $\mathcal{F} = \{\text{hyperplanes with } \|w\| = 1\}$

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”

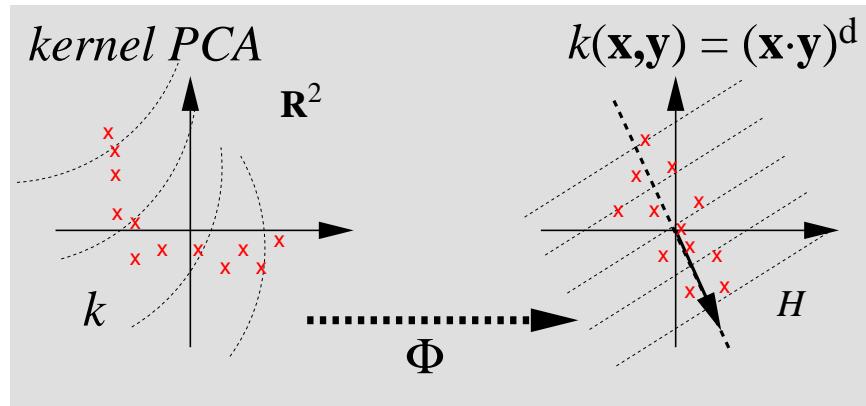
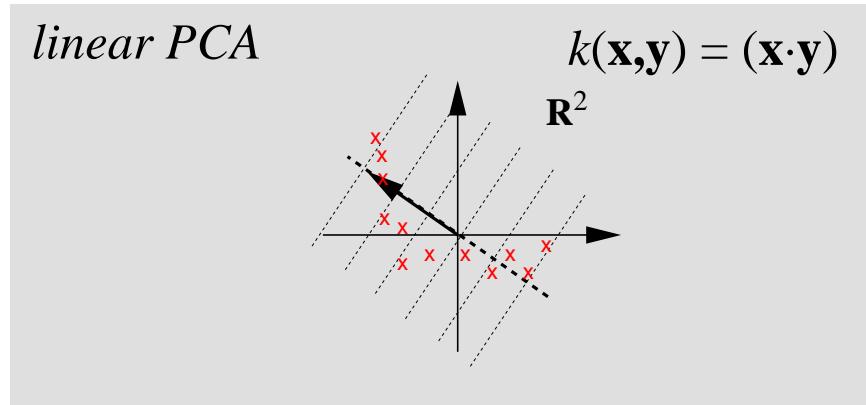
- similarity measure $k(x, x')$, where $x, x' \in \mathcal{X}$
- function class (“representer theorem,” $f(x) = \sum_i \alpha_i k(x, x_i)$)
- data representation
 - (in associated feature space where $k(x, x') = \langle \Phi(x), \Phi(x') \rangle$)
 - thus can construct geometric algorithms

2. “Learning module”

- classification
- quantile estimation / novelty detection
- feature extraction
- ...

Kernel PCA

(Schölkopf et al., 1998)



Demo



Denoising of USPS Digits

	Gaussian noise	'speckle' noise
orig.		
noisy		
$n = 1$		
P C A	$n = 4$ 	$n = 4$ 
	$n = 16$ 	$n = 16$ 
	$n = 64$ 	$n = 64$ 
	$n = 256$ 	$n = 256$ 
$n = 1$	$n = 1$ 	$n = 1$ 
K P C A	$n = 4$ 	$n = 4$ 
	$n = 16$ 	$n = 16$ 
	$n = 64$ 	$n = 64$ 
	$n = 256$ 	$n = 256$ 

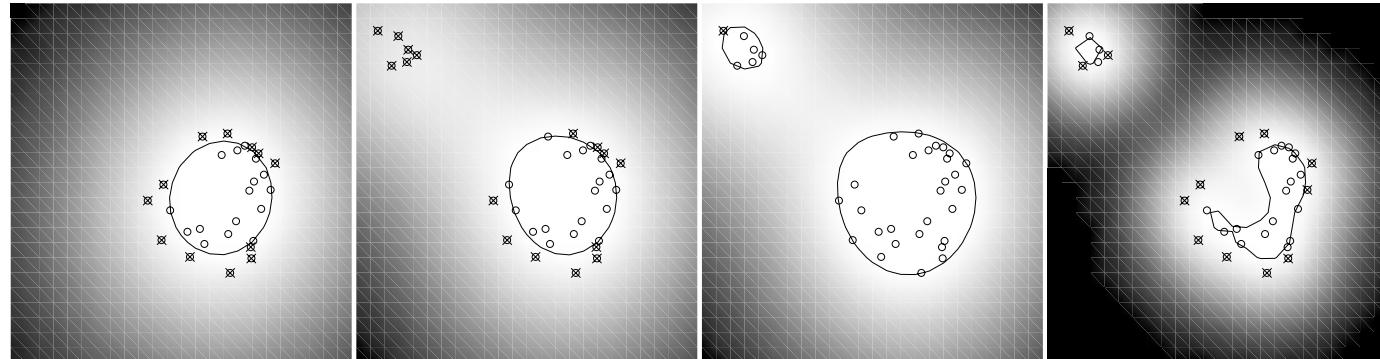
linear PCA
reconstruction

kernel PCA
reconstruction

(Mika *et al.*, 1999; Schölkopf *et al.*, 1999)

Another application: face modeling (Romdhani *et al.*, 1999).

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 $\mathbf{w} : \mathcal{H} \rightarrow \mathcal{H}'$

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

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

ORIG:	9 5 3 9 2 2 5 1 8 2 8 2 2 9 8 0 1 9 3 8 1 5 3 8 4
KDE:	9 5 3 9 2 2 5 2 9 2 8 2 3 8 9 0 1 9 3 8 1 5 3 9 5
k-NN:	8 5 3 8 2 2 5 1 8 7 9 2 2 9 8 1 7 8 7 5 8 7 9 3 4
	9 9 9 6 5 9 1 5 8 8 9 0 2 9 4 9 9 2 4 3 5 9 6 9 8 3 0
	9 9 8 6 5 8 8 5 8 8 9 0 3 9 4 9 9 2 4 3 5 9 6 9 8 3 0
	8 8 9 4 6 9 1 6 7 9 8 0 2 8 4 8 8 7 6 7 7 8 5 9 9 7 0
	2 3 3 0 5 3 5 3 0 2 4 9 4 6 2 5 8 3 8 1 7 7 7 3 9 2 5
	2 4 3 0 5 3 6 3 0 2 4 9 4 6 7 6 8 7 8 1 7 7 7 3 9 2 5
	3 3 8 9 5 3 5 6 9 2 8 8 1 5 2 5 9 3 7 3 2 3 7 8 8 3 5
	3 2 0 4 9 6 9 9 5 9 5 2 8 9 8 2 8 3 9 2 8 6 2 8 2 6 9
	3 3 6 1 9 6 9 9 5 9 5 4 8 9 8 2 9 3 9 4 8 6 3 8 7 8 2
	7 2 0 4 8 4 8 8 5 8 6 2 1 8 9 2 8 3 8 2 9 4 2 9 2 6 7

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

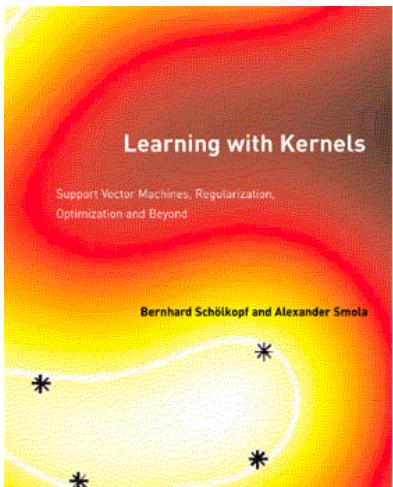
(from Weston et al. (2002))

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*)
 - 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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