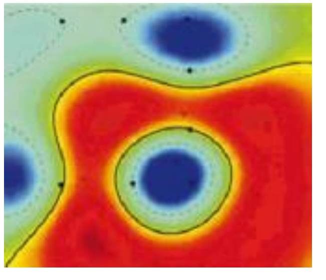
Kernel Methods

Introduction to SVMs, KPCA, RDE



Lecture by Klaus-Robert Müller, TUB 2024

Part II

Remember …

VC Theory applied to hyperplane classifiers

- Theorem (Vapnik 95): For hyperplanes in canonical form VC–dimension satisfying

$$d \leq \min\{[R^2\|\mathbf{w}\|^2] + 1, n + 1\}.$$

Here, R is the radius of the smallest sphere containing data.
Use d in SRM bound

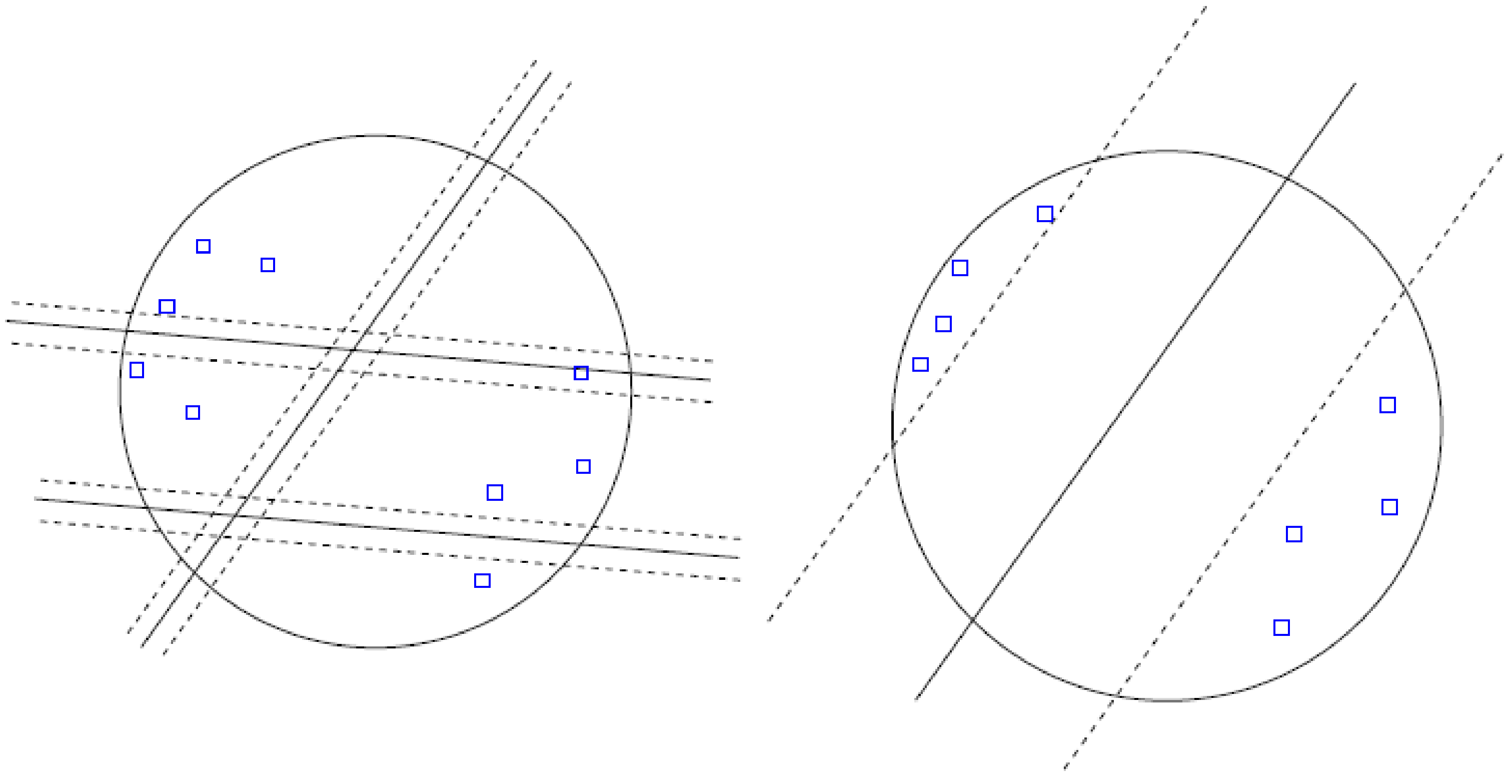
$$R[f] \leq R_{emp}[f] + \sqrt{\frac{d\left(\log\frac{2N}{d} + 1\right) - \log(\eta/4)}{N}}.$$

- maximal margin = minimum $\|\mathbf{w}\|^2 \rightarrow$ good generalization, i.e. low risk, i.e. optimize

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

- independent of the dimensionality of the space!

Margin Distributions – large margin hyperplanes



Hyperplane in $\mathcal{F}$ with slack variables: SVM

$$\min \quad \|\mathbf{w}\|^2 + C\sum_{i=1}^{N} {\xi_i}^p$$

$$\text{subject to} \quad y_i \cdot [(\mathbf{w} \cdot \Phi(\mathbf{x}_i)) + b] \geq 1 - \xi_i \text{ and } \xi_i \geq 0 \quad \text{for } i = 1 \ldots N$$

(introduce slack variables if training data not separated correctly)

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

obtain unique α_i by QP (no local minima!): dual problem

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

$$\text{i.e.} \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \quad \text{and} \quad \mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \Phi(\mathbf{x}_i).$$

Substitute both into L to get the *dual problem*

Dual Problem

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

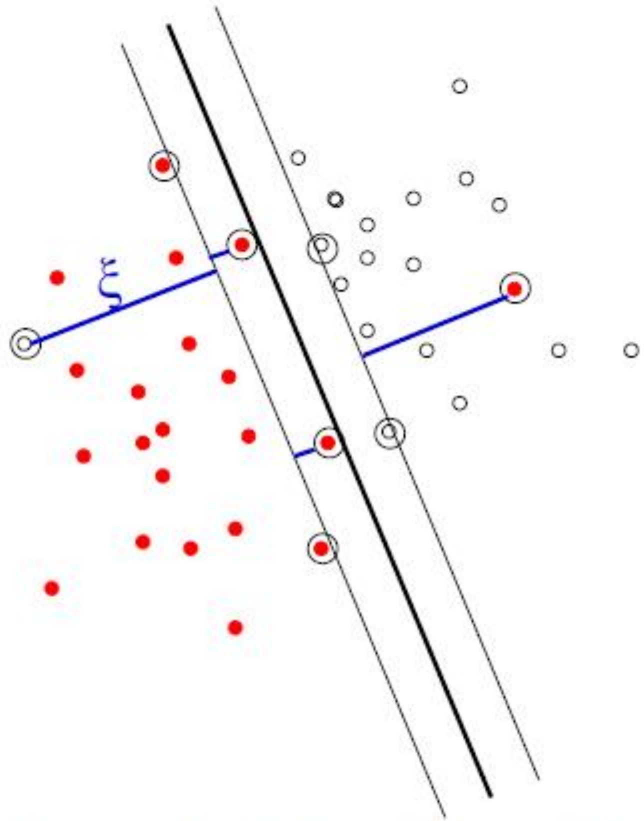
$$\text{subject to} \qquad C \geq \alpha_i \geq 0, \quad i = 1, \ldots, N, \quad \text{and} \quad \sum_{i=1}^{N} \alpha_i y_i = 0.$$

Note: solution determined by training examples (SVs) on /in the margin. Remark: duality gap.

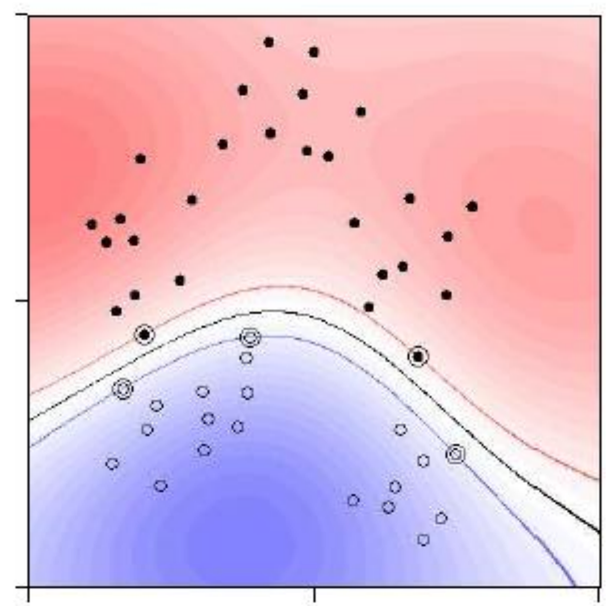
$$y_i \cdot [(\mathbf{w} \cdot \Phi(\mathbf{x}_i)) + b] > 1 \qquad \Longrightarrow \alpha_i = 0 \longrightarrow \quad \mathbf{x}_i \text{ irrelevant or}$$

$$y_i \cdot [(\mathbf{w} \cdot \Phi(\mathbf{x}_i)) + b] = 1 \quad (on\ /\text{in margin}) \longrightarrow \quad \mathbf{x}_i \text{ Support Vector}$$

A Toy Example: $k(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|^2)$



linear SV with slack variables



nonlinear SVM, Domain: $[-1, 1]^2$

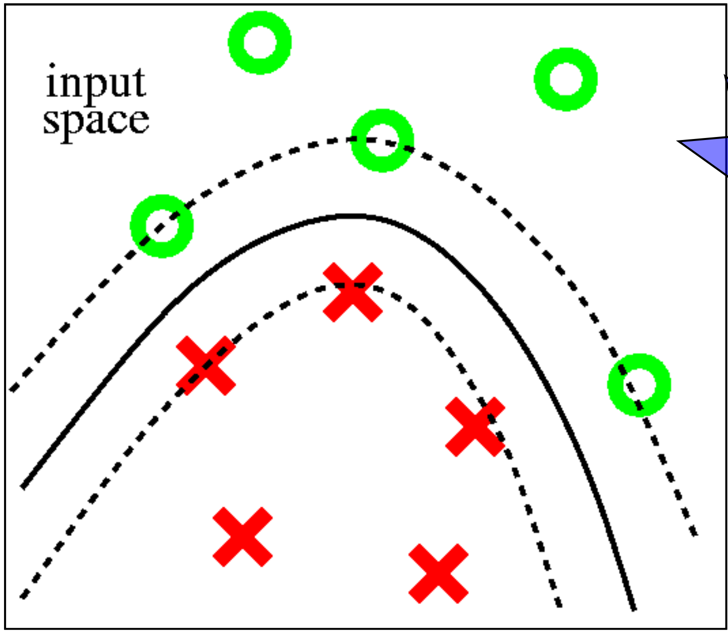
Kernel Trick

- Saddle Point: $\mathrm{w} = \sum_{i=1}^{N} \alpha_i y_i \Phi(\mathrm{x}_i)$.
- Hyperplane in $\mathcal{F}$: $y = \mathrm{sgn}\left(\mathrm{w} \cdot \Phi(x) + b\right)$
- putting things together "kernel trick"

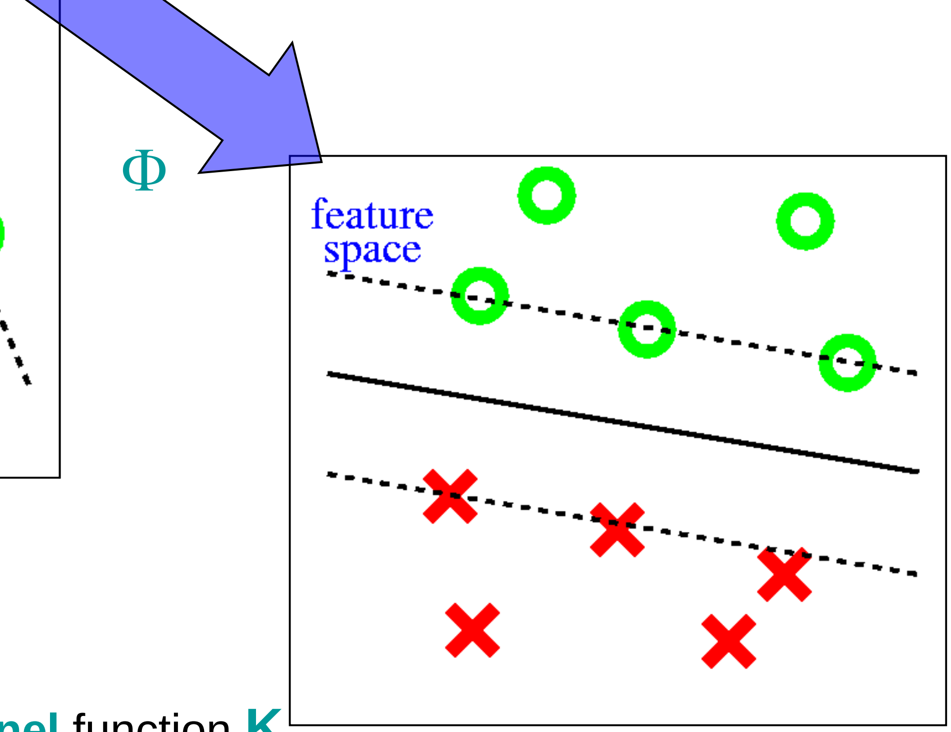
$$
\begin{aligned}
f(\mathrm{x}) &= \mathrm{sgn}\left(\mathrm{w} \cdot \Phi(\mathrm{x}) + b\right) \\
&= \mathrm{sgn}\left(\sum_{i=1}^{N} \alpha_i y_i \, \Phi(\mathrm{x}_i) \cdot \Phi(\mathrm{x}) + b\right) \\
&= \mathrm{sgn}\left(\sum_{i \in \#\mathrm{SVs}} \alpha_i y_i k(\mathrm{x}, \mathrm{x}_i) + b\right) \qquad \textbf{sparse!}
\end{aligned}
$$

- trick: $k(\mathrm{x}, \mathrm{y}) = \Phi(\mathrm{x}) \cdot \Phi(\mathrm{y})$, i.e. **never use Φ: only k!!!**

Support Vector Machines in a nutshell



Φ rsp. $K(x,y) = \Phi(x) \bullet \Phi(y)$



good theory
non-linear decision by
implicitely mapping the data
into feature space by SV **kernel** function **K**

Digestion

$$R[f] \leq R_{emp}[f] + \sqrt{\frac{d\left(\log\frac{2N}{d}+1\right)-\log(\eta/4)}{N}}$$

$$K(\mathbf{x},\mathbf{y}) = \Phi(\mathbf{x})\cdot\Phi(\mathbf{y})$$

SRM (VC theory)

feature spaces & RKHS

kernel trick

mathematical programs

SV classification & regression

feature extraction $\longrightarrow$ **kernelize it!**

kernel choice

Boosting
Large margins
Bounds, sparsity

APPLICATIONS

OCR, Bioinformatics **(DNA, drug discovery)**
categorization, biomedical data (BCI, EEG),
benchmarks, time-series analysis, power,
quarks, object recognition, textmining

Optimizing SVMs

Implementation Issues: working set methods

matrix notation: Let $\boldsymbol{\alpha} = (\alpha_1, \dots \alpha_M)^\top$, let $\mathbf{y} = (y_1, \dots, y_M)^\top$, let H be the matrix with the entries $H_{ij} = y_i y_j \, \mathrm{k}(\mathbf{x}_i, \mathbf{x}_j)$, and let $\mathbf{1}$ denote the vector of length M consisting of all 1s.

dual SVM Problem becomes:

$$
\begin{aligned}
\max_{\boldsymbol{\alpha}} \quad & \mathbf{1}^\top \boldsymbol{\alpha} - \frac{1}{2} \boldsymbol{\alpha}^\top H \boldsymbol{\alpha}, && (1)\\
\text{subject to} \quad & \mathbf{y}^\top \boldsymbol{\alpha} = 0, && (2)\\
& \boldsymbol{\alpha} - C\mathbf{1} \leq 0, && (3)\\
& \boldsymbol{\alpha} \geq 0. && (4)
\end{aligned}
$$

Implementation Issues: working set methods II

$\boldsymbol{\alpha}_B$ of the variables in the working set at a current iteration and $\boldsymbol{\alpha}_N$ remaining variables. H is thus partitioned as $H = \begin{bmatrix} H_{BB} & H_{BN} \\ H_{NB} & H_{NN} \end{bmatrix}$, at each iteration, is obtained:

$$\max_{\boldsymbol{\alpha}} \quad (\mathbf{1}_B^\top - \boldsymbol{\alpha}_N^\top H_{NB})\boldsymbol{\alpha}_B - \frac{1}{2}\boldsymbol{\alpha}_B^\top H_{BB}\boldsymbol{\alpha}_B, \tag{5}$$

$$\text{subject to} \quad \mathbf{y}_B^\top \boldsymbol{\alpha}_B = -\mathbf{y}_N \boldsymbol{\alpha}_N, \tag{6}$$

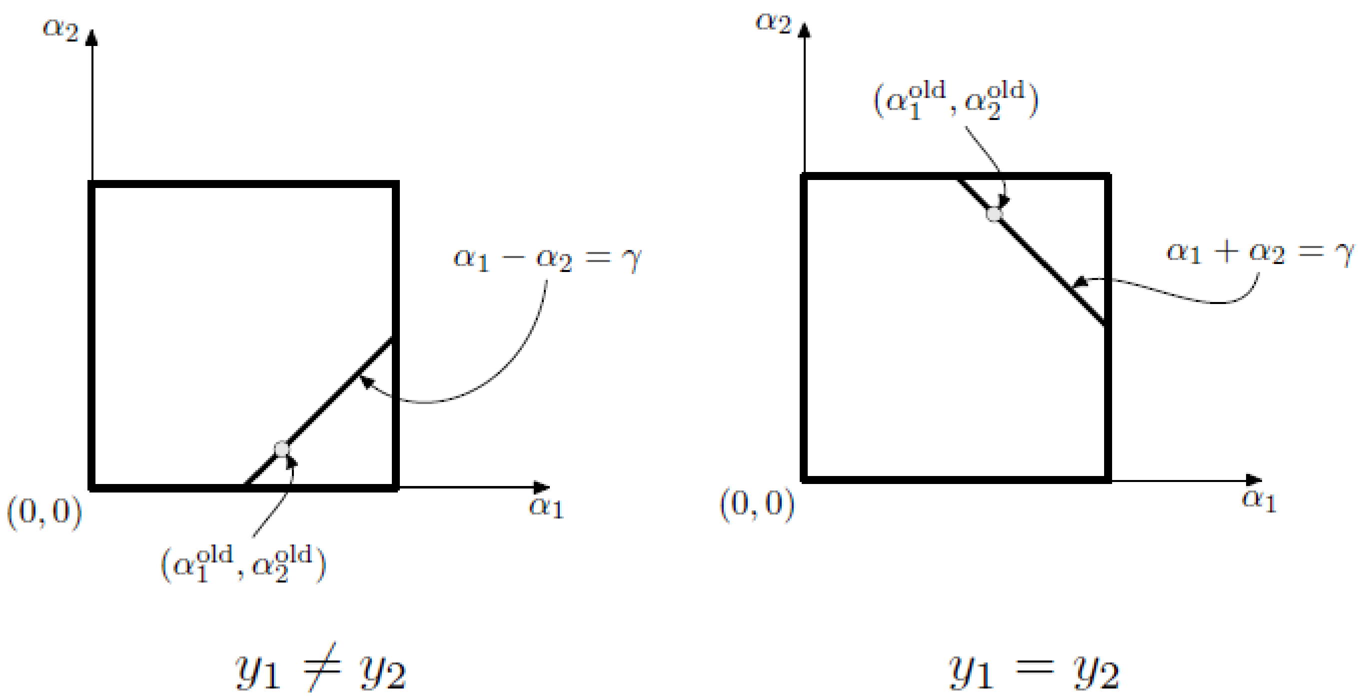
$$\boldsymbol{\alpha}_B - C\mathbf{1}_B \leq 0, \tag{7}$$

$$\boldsymbol{\alpha}_B \geq 0. \tag{8}$$

Usuall small working set, iteration is carried out until KKT conditions, are satisfied to the required precision ϵ. monitor gap.

John Platt‘s SMO

- extreme: use only two points in working set and compute optimal solution *analytically*



SMO continued

eliminating α_1 yields update rule for α_2:

$$\alpha_2^{\text{new}} = \alpha_2^{\text{old}} - \frac{y_2(E_1 - E_2)}{\eta}, \tag{9}$$

where

$$E_1 = \sum_{j=1}^{M} y_j \alpha_j \,\mathrm{k}(\mathbf{x}_1, \mathbf{x}_j) + b - y_1, \tag{10}$$

$$E_2 = \sum_{j=1}^{M} y_j \alpha_j \,\mathrm{k}(\mathbf{x}_2, \mathbf{x}_j) + b - y_2, \tag{11}$$

$$\eta = 2\,\mathrm{k}(\mathbf{x}_1, \mathbf{x}_2) - \mathrm{k}(\mathbf{x}_1, \mathbf{x}_1) - \mathrm{k}(\mathbf{x}_2, \mathbf{x}_2). \tag{12}$$

Next, the bound constraints should be taken care of. Depending on the geometry, one computes the following lower and upper bounds on the value of the variable α_2:

$$L = \begin{cases} \max\left(0, \alpha_2^{\text{old}} - \alpha_1^{\text{old}}\right), & \text{if } y_1 \neq y_2, \\ \max\left(0, \alpha_2^{\text{old}} + \alpha_1^{\text{old}} - C\right), & \text{if } y_1 = y_2, \end{cases}$$

$$H = \begin{cases} \min\left(C, C + \alpha_2^{\text{old}} - \alpha_1^{\text{old}}\right), & \text{if } y_1 \neq y_2, \\ \min\left(C, \alpha_2^{\text{old}} + \alpha_1^{\text{old}}\right), & \text{if } y_1 = y_2. \end{cases}$$

The constrained optimum is then found by clipping the unconstrained optimum to the ends of the line segment:

$$\alpha_2^{\text{new}} := \begin{cases} H, & \text{if } \alpha_2^{\text{new}} \geq H, \\ L, & \text{if } \alpha_2^{\text{new}} \leq L, \\ \alpha_2^{\text{new}}, & \text{otherwise.} \end{cases}$$

Finally, the value of α_1^{new} is computed:

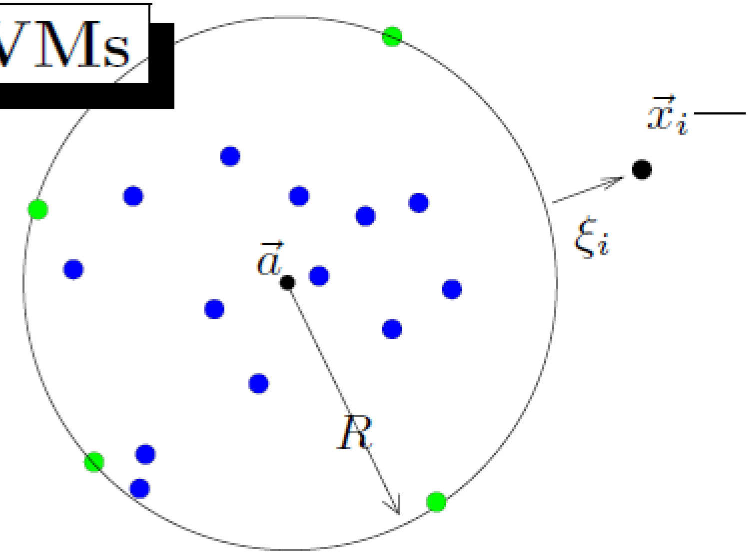
$$\alpha_1^{\text{new}} = \alpha_1^{\text{old}} + y_1 y_2 (\alpha_2^{\text{old}} - \alpha_2^{\text{new}}). \tag{13}$$

- Use heuristics to choose examples

Kernel-Based ML:

Beyond Classification

One-Class SVMs



Fitting a hypersphere around the data

$$\max_{\boldsymbol{\alpha}} \quad \sum_{i=1}^{M} \alpha_i \, \mathrm{k}(\mathbf{x}_i, \mathbf{x}_i) - \frac{1}{2} \sum_{i,j=1}^{M} \alpha_i \alpha_j \, \mathrm{k}(\mathbf{x}_i, \mathbf{x}_j), \tag{14}$$

$$\text{subject to} \quad 0 \leq \alpha_i \leq C, \; i = 1, \ldots, M,$$

$$\sum_{i=1}^{M} \alpha_i = 1.$$

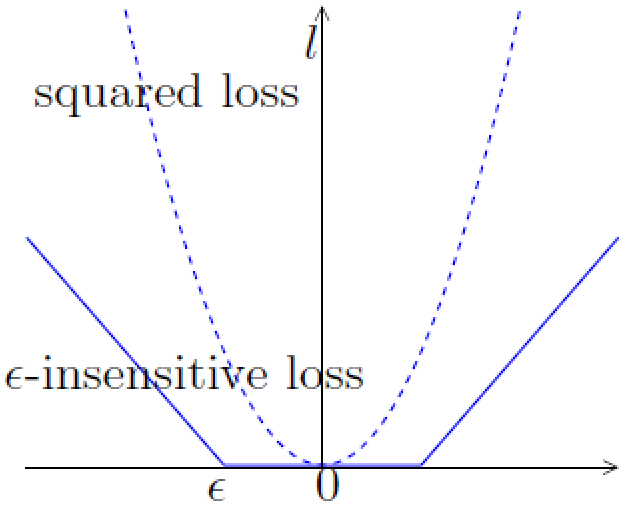
new object belongs to target class? (cf. Tax 01, Schölkopf et al. 01)

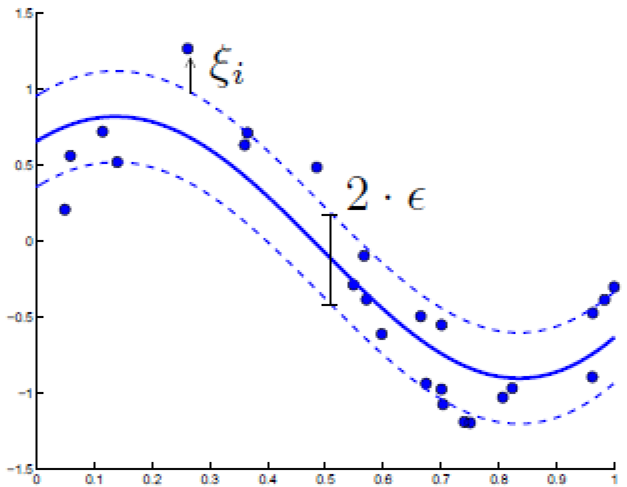
$$f(\mathbf{x}) = \mathrm{sign}(R^2 - \mathrm{k}(\mathbf{x}, \mathbf{x}) + 2 \sum_i \alpha_i \, \mathrm{k}(\mathbf{x}, \mathbf{x}_i) - \sum_{i,j} \alpha_i \alpha_j \, \mathrm{k}(\mathbf{x}_i, \mathbf{x}_j)). \tag{15}$$

SVMs for Regression

$$\ell(f(\mathbf{x}), y) = (f(\mathbf{x}) - y)^2,$$

$$\ell(f(\mathbf{x}), y) = \begin{cases} |f(\mathbf{x}) - y| - \epsilon, & \text{if } |f(\mathbf{x}) - y| > \epsilon, \\ 0, & \text{otherwise.} \end{cases}$$





(cf. Vapnik 95, Smola and Schölkopf 02)

SVMs for Regression II

The primal formulation for the SVR

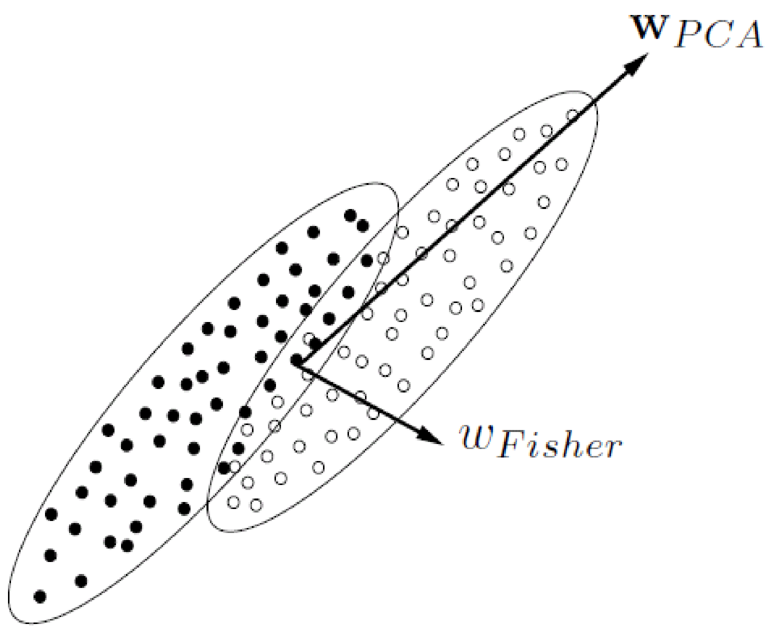
$$\min_{\mathbf{w},b,\boldsymbol{\xi}^{(*)}} \quad \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{M}(\xi_i + \xi_i^*),$$

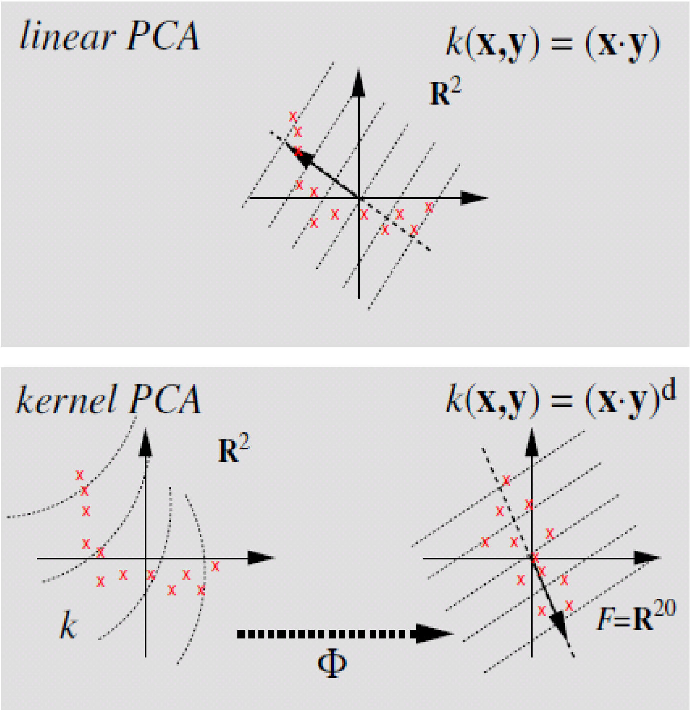
$$\text{subject to} \quad ((\mathbf{w}^\top \mathbf{x}_i) + b) - y_i \leq \epsilon + \xi_i,$$

$$y_i - ((\mathbf{w}^\top \mathbf{x}_i) + b) \leq \epsilon + \xi_i^*,$$

$$\xi_i^{(*)} \geq 0, \quad i = 1, \dots, M.$$

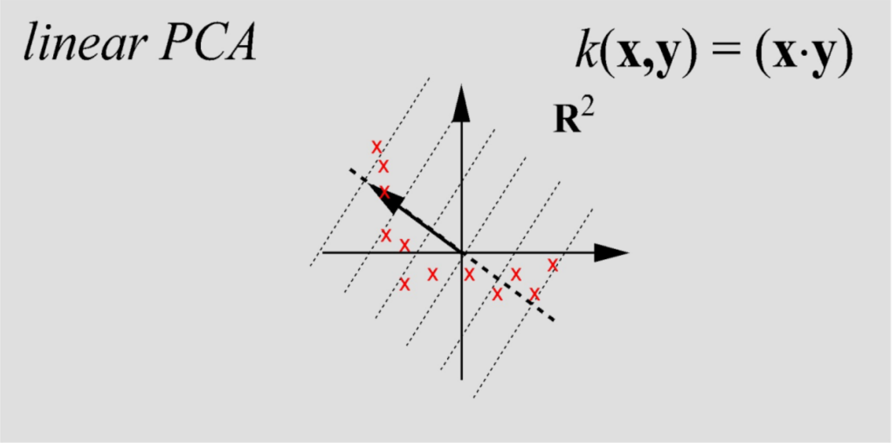
Remark: Kernelizing linear algorithms

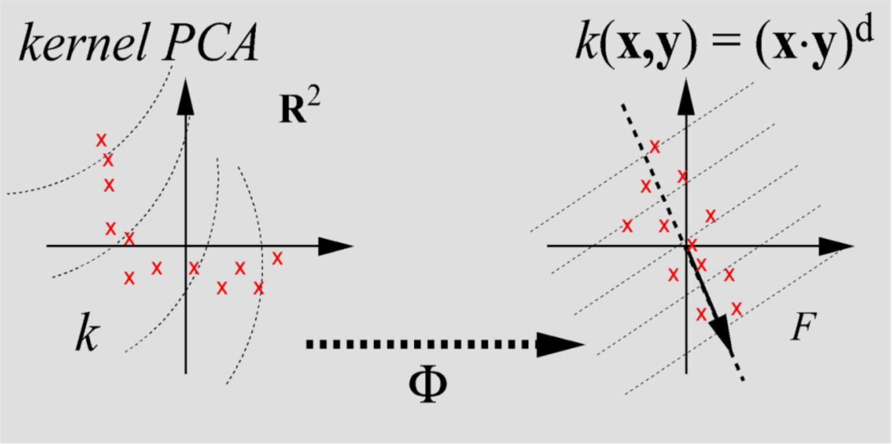




(cf. Schölkopf, Smola and Müller 1996, 1998, Schölkopf et al 1999, Mika et al, 1999, 2000, 2001, Müller et al 2001, Harmeling et al 2003, ...)

Kernel PCA





[cf. Schölkopf, Smola, Müller 98]

PCA in high dimensional feature spaces

$$\mathbf{x}_1, \ldots, \mathbf{x}_N, \qquad \Phi : \mathbb{R}^D \to F, \qquad C = \frac{1}{N}\sum_{j=1}^{N} \Phi(\mathbf{x}_j)\Phi(\mathbf{x}_j)^\top$$

Eigenvalue problem

$$\lambda \mathbf{V} = C\mathbf{V} = \frac{1}{N}\sum_{j=1}^{N}(\Phi(\mathbf{x}_j)\cdot \mathbf{V})\Phi(\mathbf{x}_j).$$

For $\lambda \neq 0$, $\mathbf{V} \in \text{span}\{\Phi(\mathbf{x}_1), \ldots, \Phi(\mathbf{x}_N)\}$, thus $\mathbf{V} = \sum_{i=1}^{N} \alpha_i \Phi(\mathbf{x}_i)$.

Multiplying with $\Phi(\mathbf{x}_k)$ from the left yields

$$\mathbf{N}\lambda(\Phi(\mathbf{x}_k)\cdot \mathbf{V}) = (\Phi(\mathbf{x}_k)\cdot C\mathbf{V}) \text{ for all } k = 1, \ldots, N$$

Nonlinear PCA as an Eigenvalue problem

Define an $N \times N$ matrix

$$K_{ij} := (\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)) = k(\mathbf{x}_i, \mathbf{x}_j)$$

to get

$$N\lambda K\boldsymbol{\alpha} = K^2\boldsymbol{\alpha}$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N)^\top$.

Solve

$$N\lambda\boldsymbol{\alpha} = K\boldsymbol{\alpha}$$

$$\longrightarrow (\lambda_k, \boldsymbol{\alpha}^k)$$

$$(\mathbf{V}^k \cdot \mathbf{V}^k) = 1 \Longleftrightarrow \mathbf{N}\lambda_k(\boldsymbol{\alpha}^k \cdot \boldsymbol{\alpha}^k) = 1$$

Feature Extraction

Compute projections on the Eigenvectors

$$\mathbf{V}^k = \sum_{i=1}^{M} \alpha_i^k \Phi(\mathbf{x}_i)$$

in F:

for a test point $\mathbf{x}$ with image $\Phi(\mathbf{x})$ in F we get the features ("kernel PCA components")

$$\begin{aligned} f_k(x) = (\mathbf{V}^k \cdot \Phi(\mathbf{x})) &= \sum_{i=1}^{M} \alpha_i^k (\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x})) \\ &= \sum_{i=1}^{M} \alpha_i^k k(\mathbf{x}_i, \mathbf{x}) \end{aligned}$$

Centering in Feature Space

Center the data in F:

$$\tilde{\Phi}(\mathbf{x}_i) := \Phi(\mathbf{x}_i) - \frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x}_i)$$

For $\tilde{\Phi}(\mathbf{x}_i)$, everything works fine.

Express $\tilde{K}$ in terms of K, using $(1_N)_{ij} := 1/N$:

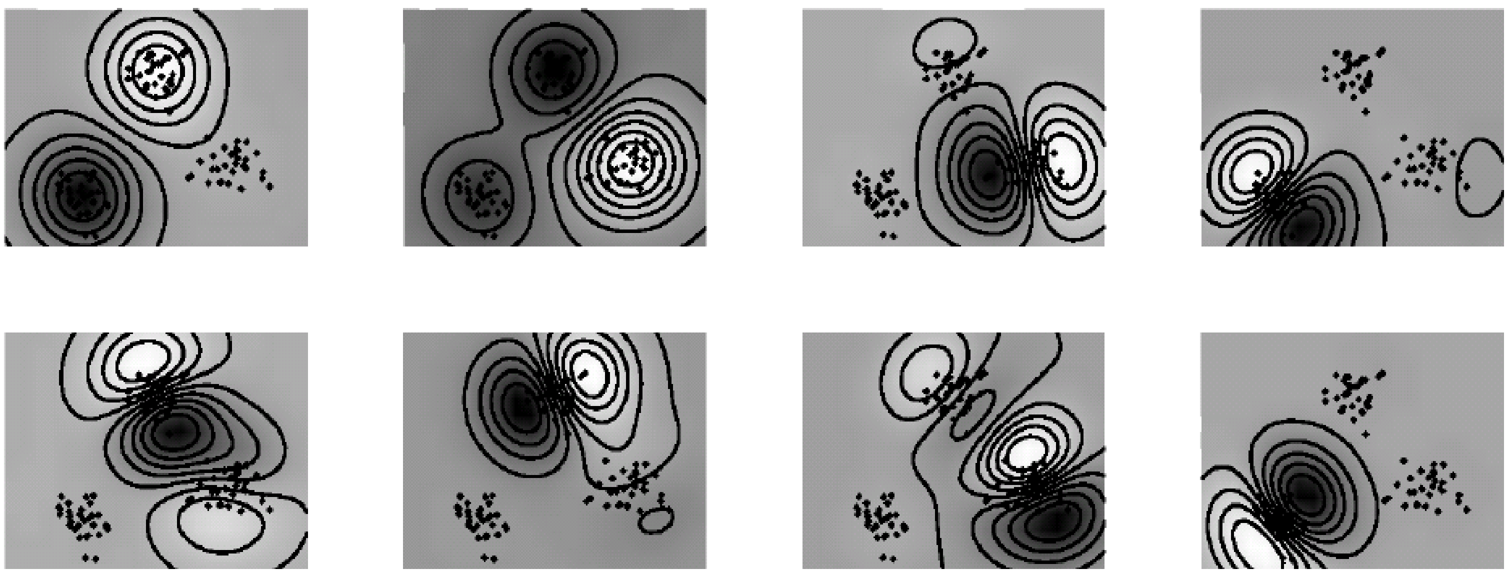
$$\tilde{K}_{ij} = K - 1_N K - K 1_N + 1_N K 1_N.$$

Compute $\tilde{K}$ and solve the Eigenvalue problem.

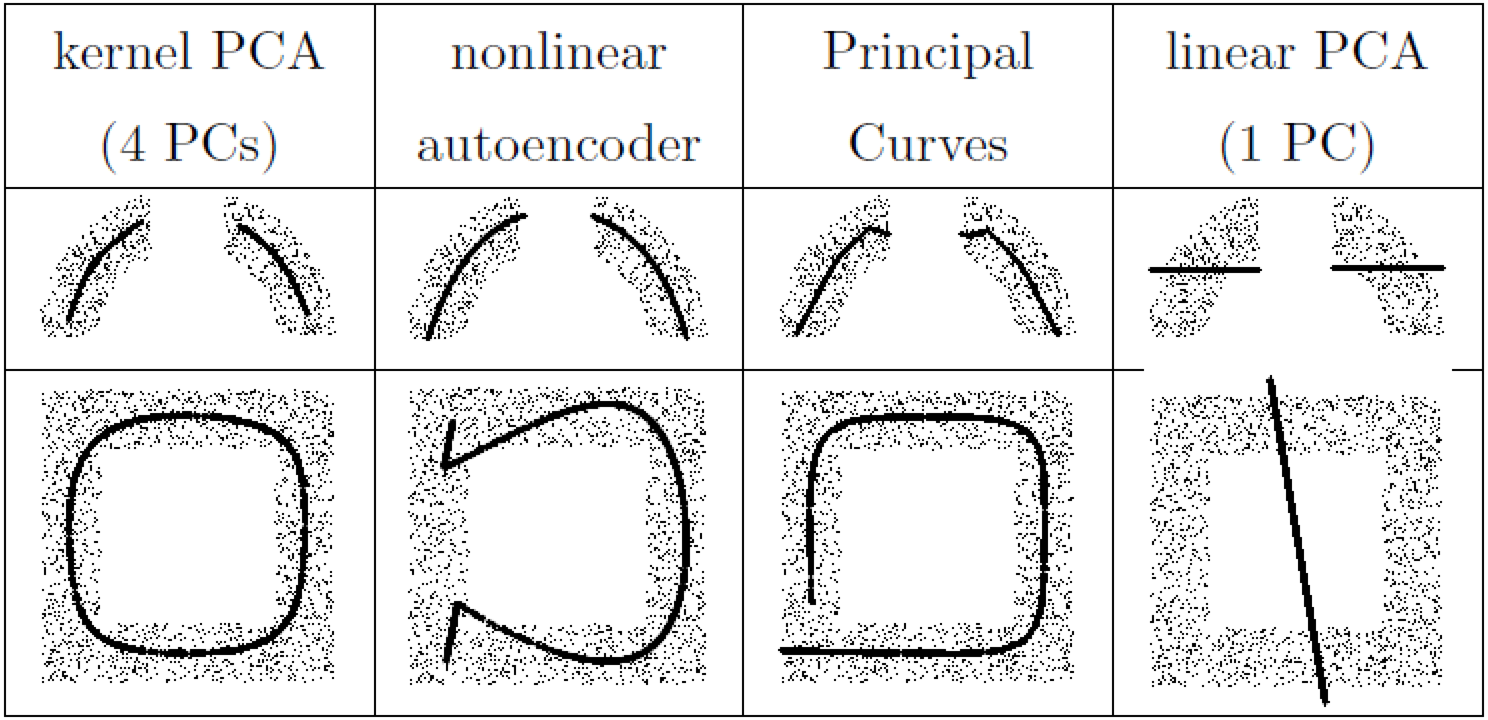
Similar for feature extraction.

Example: 8 kPCA components with RBF kernel

$$k(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{0.1}\right)$$



Denoising



Principal curves: Hastie & Stützle, 1989

Nonlinear autoencoder: e.g. Kramer, 1991

Denoising II