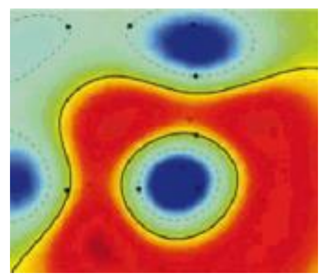
Kernel Methods

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

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

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

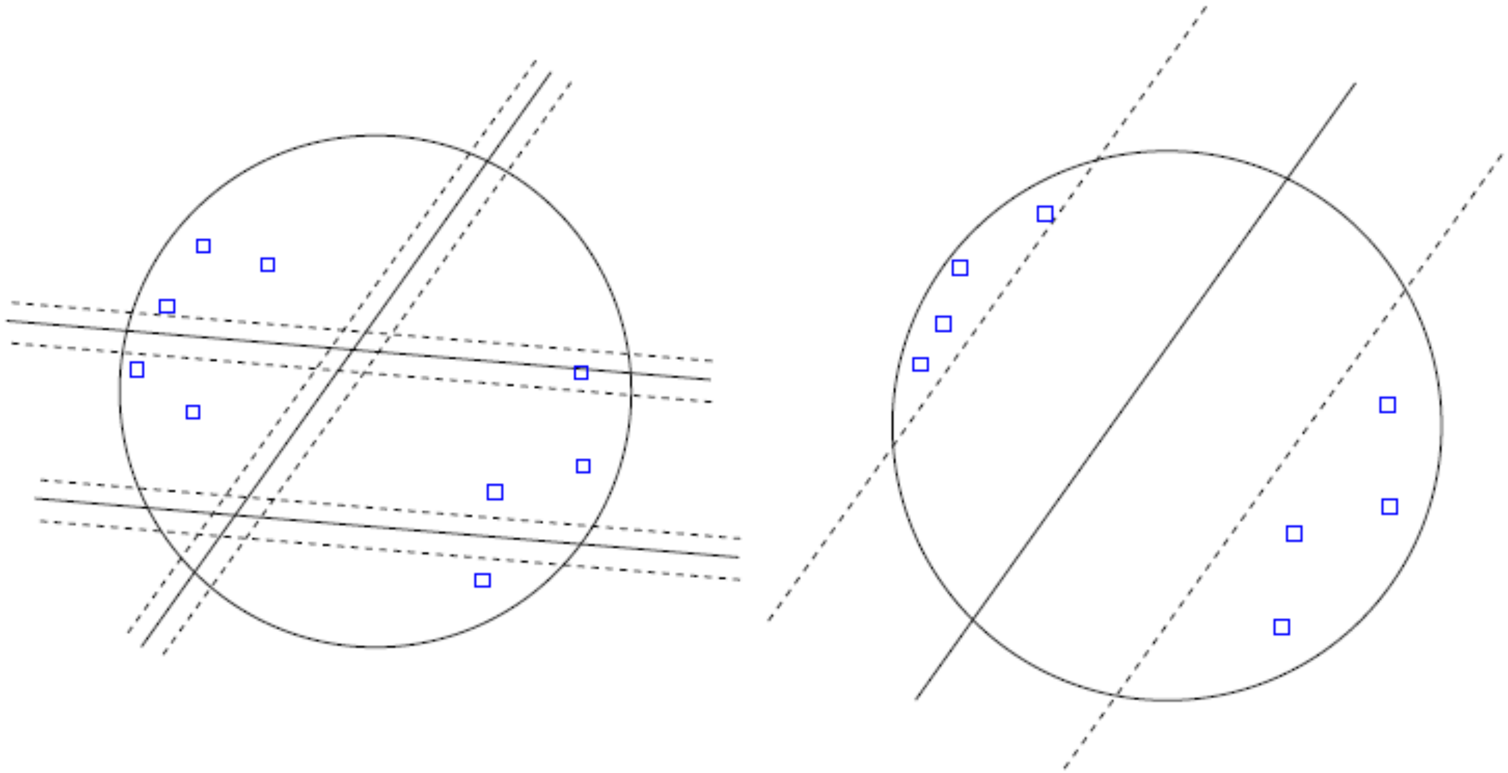
$$R[f] \leq R_{emp}[f] + \sqrt{\frac{d\left(\log \frac{2N}{d} + 1\right) - \log(\eta/4)}{N}}.$$

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

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

- independent of the dimensionality of the space!

Margin Distributions – large margin hyperplanes



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

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

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

(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

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

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

Substitute both into L to get the *dual problem*

Dual Problem

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

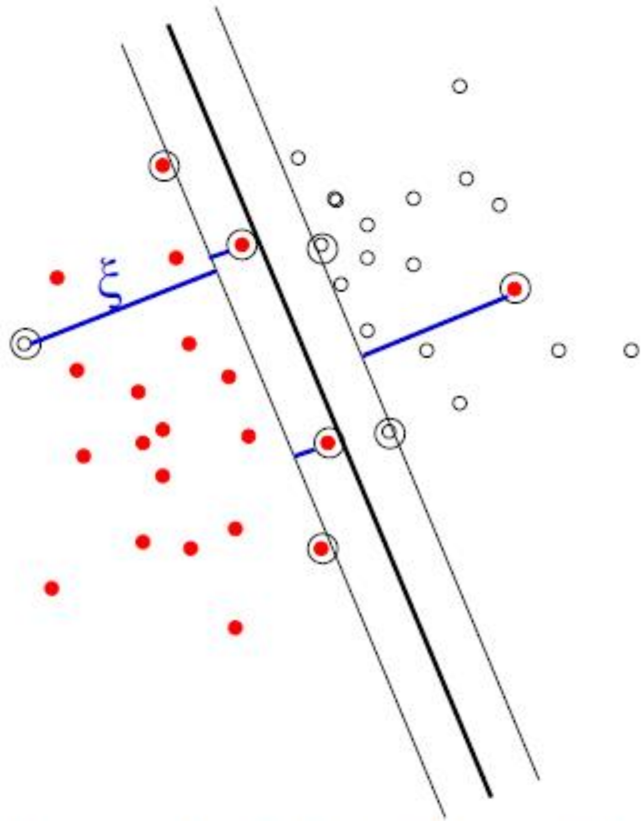
$$\text{subject to} \qquad C \geq \alpha_i \geq 0, \quad i = 1, \ldots, N, \quad \text{and} \quad \sum_{i=1}^{N} \alpha_i y_i = 0.$$

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

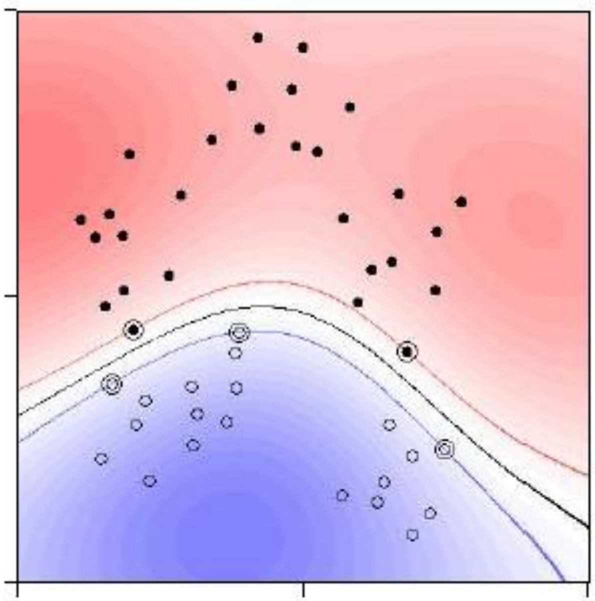
$$y_i \cdot [(\mathbf{w} \cdot \Phi(\mathbf{x}_i)) + b] > 1 \qquad \Longrightarrow \alpha_i = 0 \longrightarrow \quad \mathbf{x}_i \text{ irrelevant or}$$

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

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



linear SV with slack variables



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

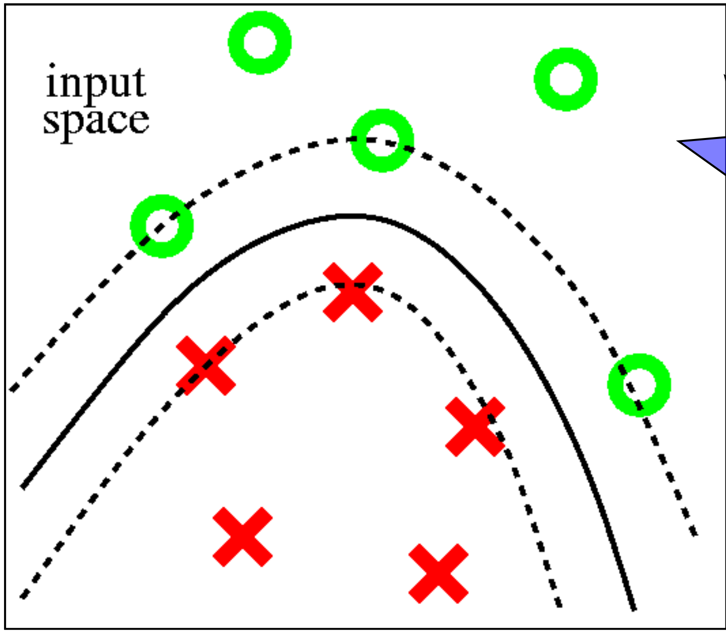
Kernel Trick

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

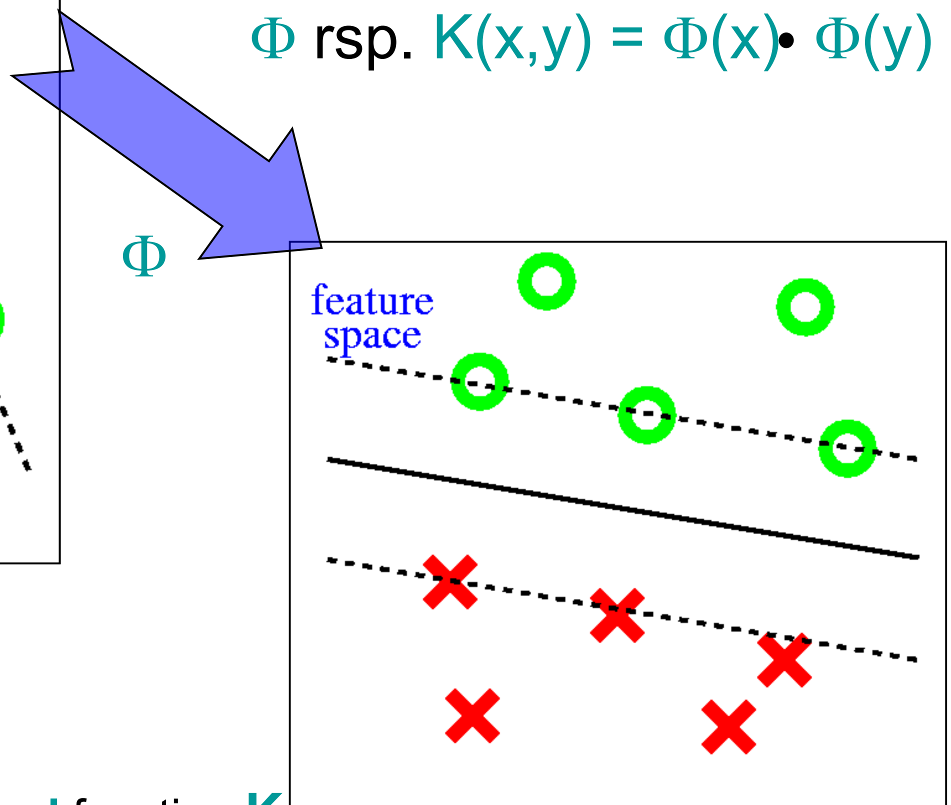
$$
\begin{aligned}
f(\mathbf{x}) &= \operatorname{sgn}(\mathbf{w} \cdot \Phi(\mathbf{x}) + b) \\
&= \operatorname{sgn}\left(\sum_{i=1}^{N} \alpha_i y_i \, \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}) + b\right) \\
&= \operatorname{sgn}\left(\sum_{i \in \#\mathrm{SVs}} \alpha_i y_i k(\mathbf{x}, \mathbf{x}_i)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

- trick: $k(\mathbf{x}, \mathbf{y}) = \Phi(\mathbf{x}) \cdot \Phi(\mathbf{y})$, 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 → **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 $\boldsymbol{\alpha} = (\alpha_1, \ldots \alpha_M)^\top$, let $\mathbf{y} = (y_1, \ldots, y_M)^\top$, 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:

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

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

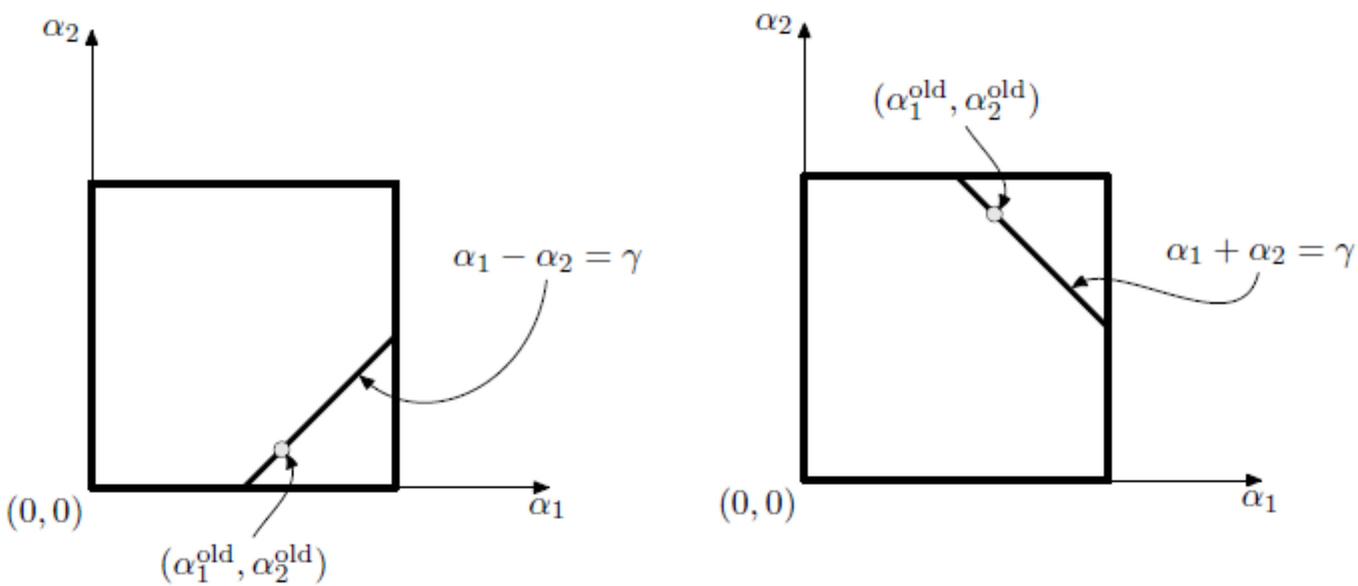
$$\boldsymbol{\alpha}_B - C\mathbf{1}_B \leq 0, \tag{7}$$

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

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*



$y_1 \neq y_2$ $\qquad$ $y_1 = y_2$

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:

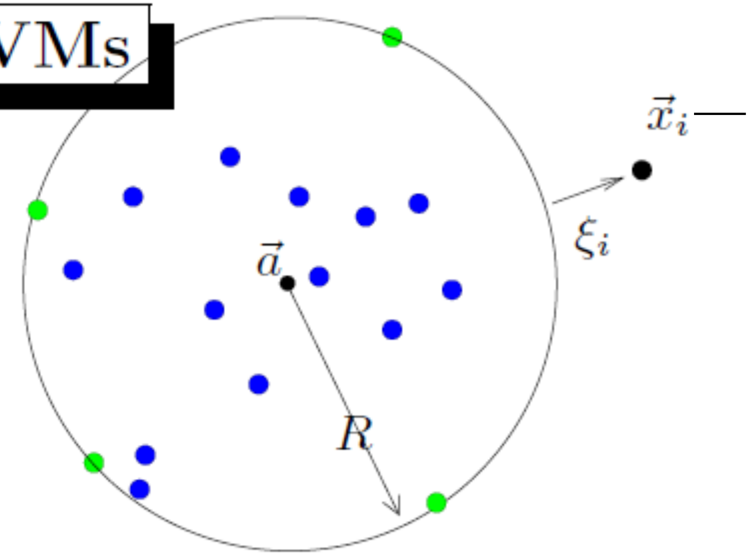
$$\alpha_1^{\text{new}} = \alpha_1^{\text{old}} + y_1 y_2 (\alpha_2^{\text{old}} - \alpha_2^{\text{new}}). \tag{13}$$

- Use heuristics to choose examples

Kernel-Based ML:

Beyond Classification

One-Class SVMs



Fitting a hypersphere around the data

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

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

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

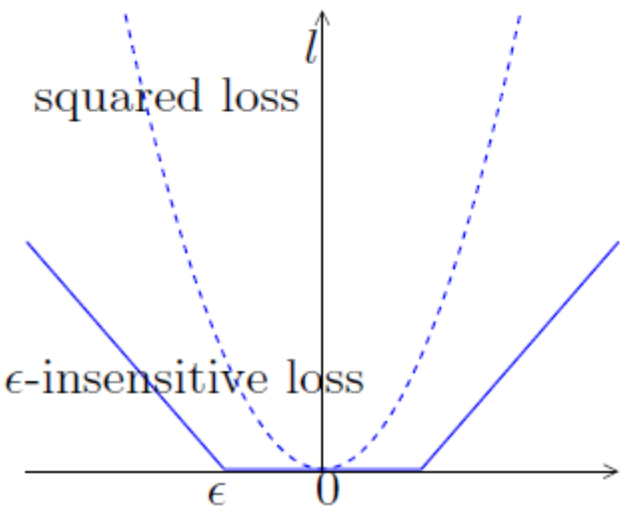
new object belongs to target class? (cf. Tax 01, Schölkopf et al. 01)

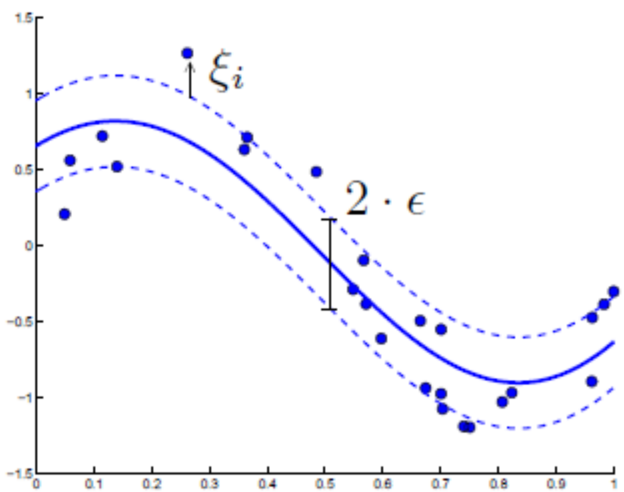
$$f(\mathbf{x}) = \mathrm{sign}(R^2 - \mathrm{k}(\mathbf{x}, \mathbf{x}) + 2 \sum_{i} \alpha_i \,\mathrm{k}(\mathbf{x}, \mathbf{x}_i) - \sum_{i,j} \alpha_i \alpha_j \,\mathrm{k}(\mathbf{x}_i, \mathbf{x}_j)). \tag{15}$$

SVMs for Regression

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

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





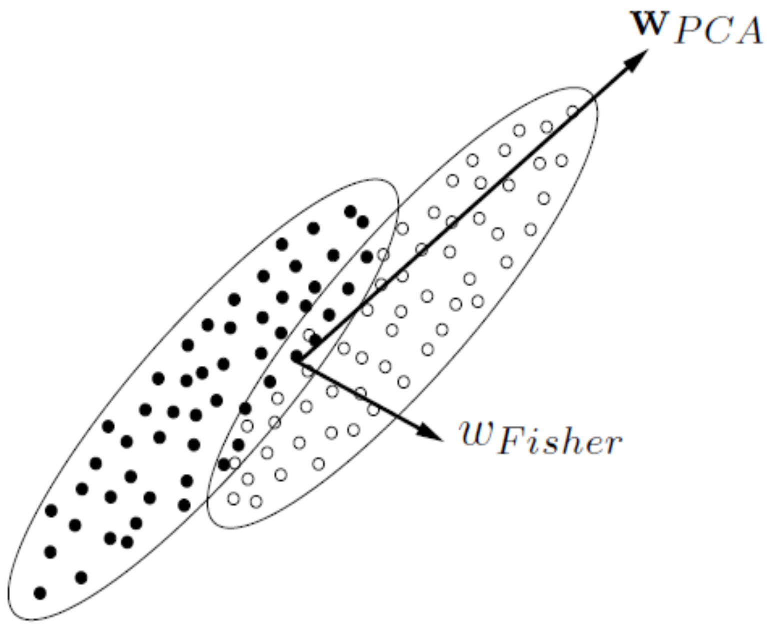
(cf. Vapnik 95, Smola and Schölkopf 02)

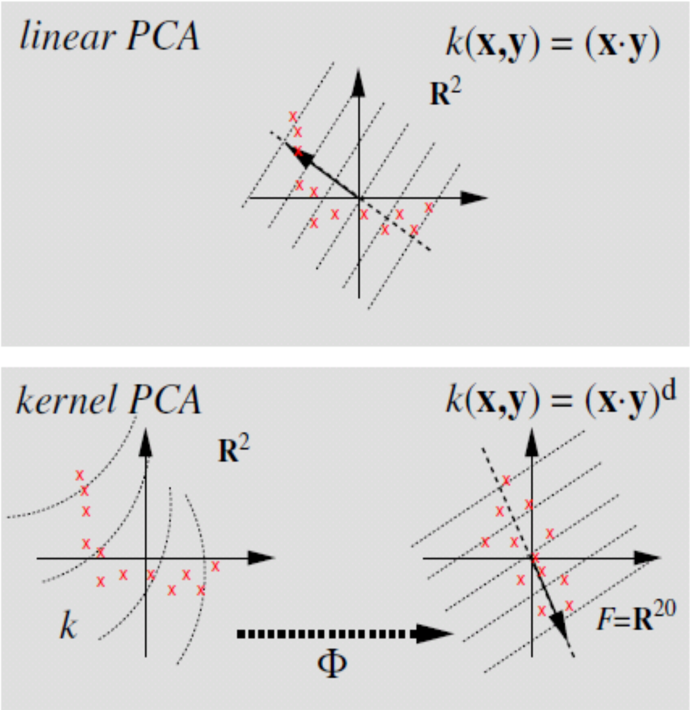
SVMs for Regression II

The primal formulation for the SVR

$$
\begin{aligned}
\min_{\mathbf{w},b,\boldsymbol{\xi}^{(*)}} \quad & \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{M}(\xi_i + \xi_i^*), \\
\text{subject to} \quad & ((\mathbf{w}^\top \mathbf{x}_i) + b) - y_i \leq \epsilon + \xi_i, \\
& y_i - ((\mathbf{w}^\top \mathbf{x}_i) + b) \leq \epsilon + \xi_i^*, \\
& \xi_i^{(*)} \geq 0, \quad i = 1, \ldots, M.
\end{aligned}
$$

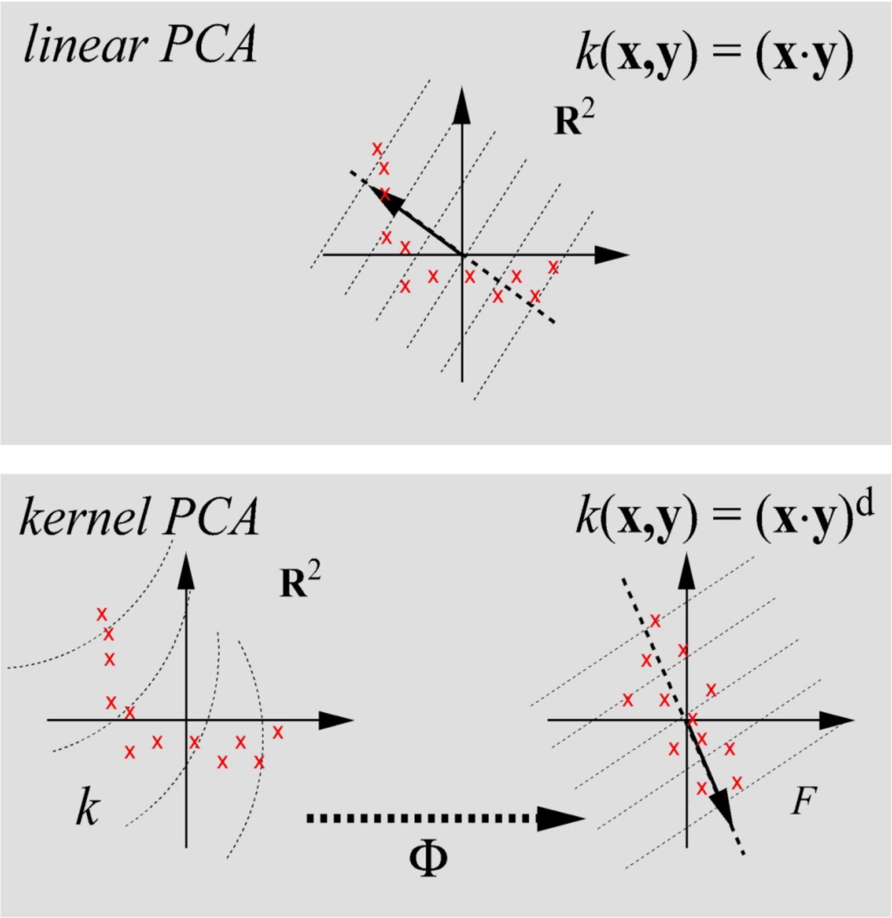
Remark: Kernelizing linear algorithms





(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 $\lambda \neq 0$, $\mathbf{V} \in \mathrm{span}\{\Phi(\mathbf{x}_1), \ldots, \Phi(\mathbf{x}_N)\}$, 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 $(1_N)_{ij} := 1/N$:

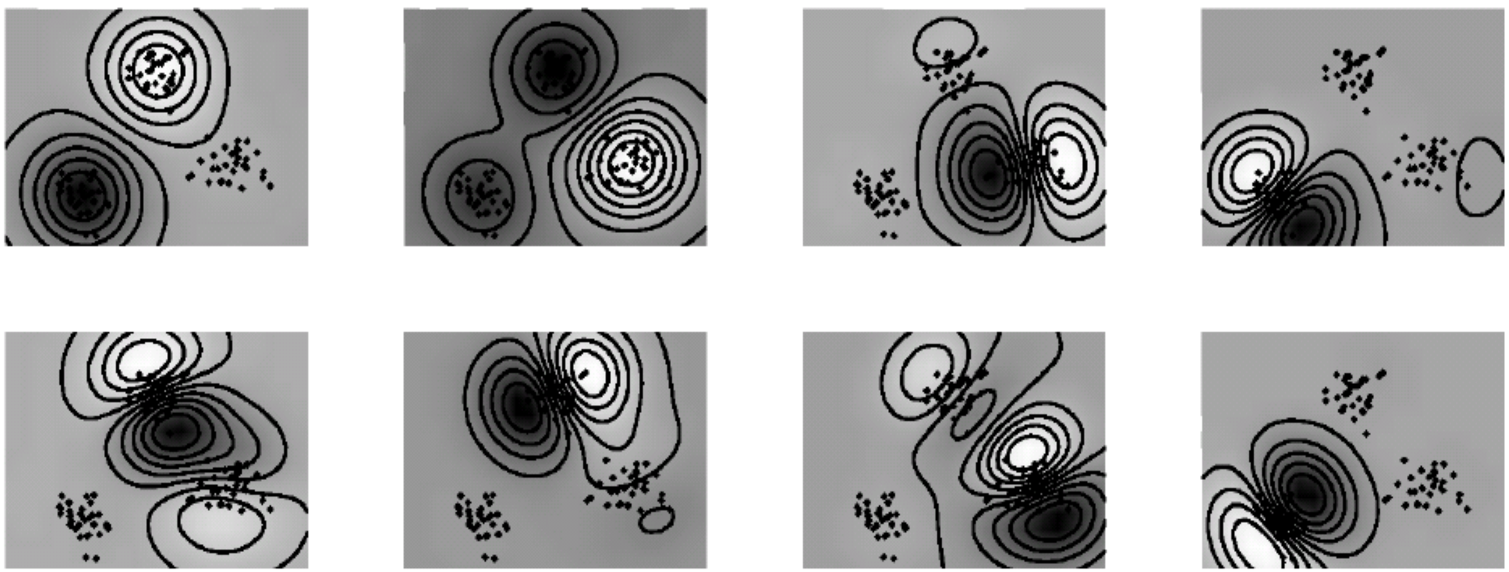
$$\tilde{K}_{ij} = K - 1_N K - K 1_N + 1_N K 1_N.$$

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

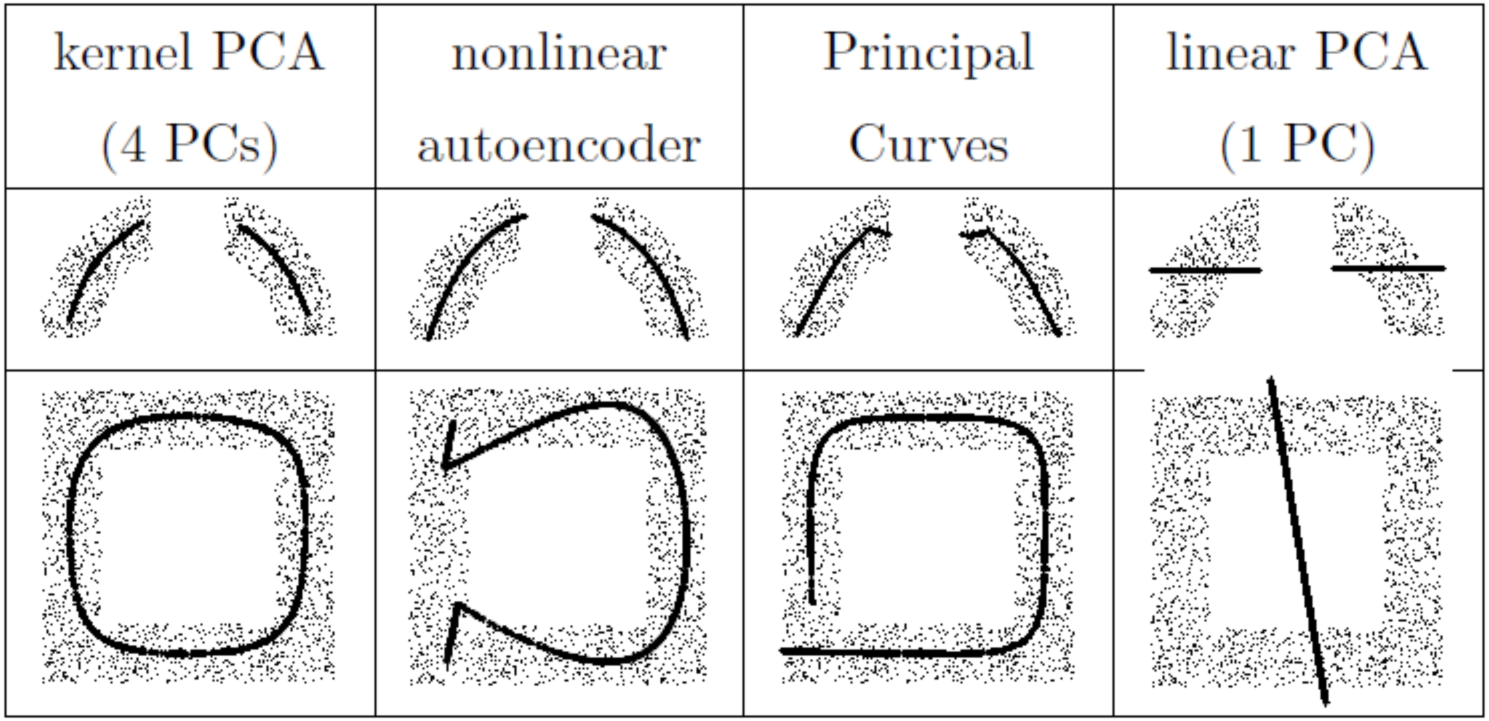
Similar for feature extraction.

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