Support Vector Machines
Nonlinear SVM: Kernels

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Most slides from UT Austin Machine Learning Group

Linear SVMs: Overview

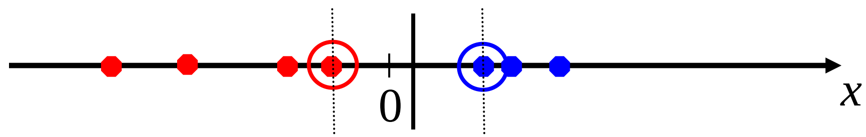
- The classifier is a *separating hyperplane.*
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation of the problem and in the solution training points appear only inside inner products:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \boxed{\mathbf{x}_i^T\mathbf{x}_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

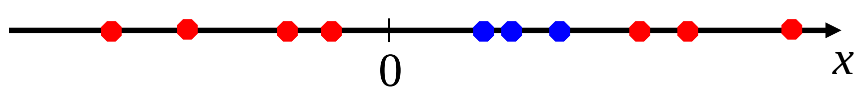
$$f(\mathbf{x}) = \Sigma\alpha_i y_i \boxed{\mathbf{x}_i^T\mathbf{x}} + b$$

Non-linear SVMs

- Datasets that are linearly separable with some noise work out great:

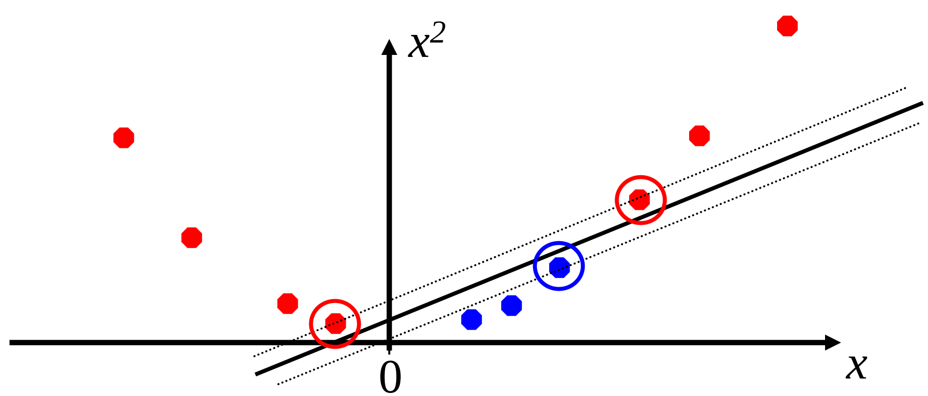


- But what are we going to do if the dataset is just too hard?



Invented 1995

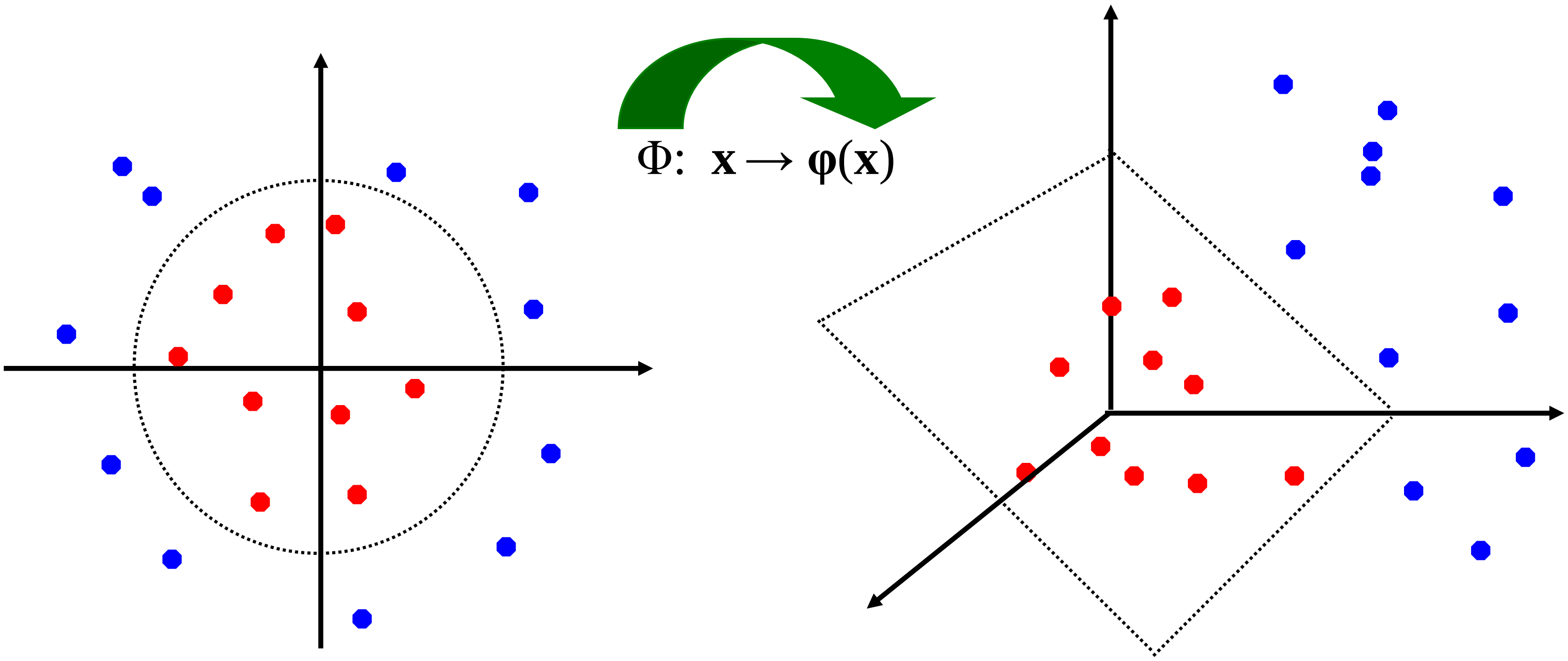
- How about… mapping data to a higher-dimensional space:



$z=(x, x^2)$

Non-linear SVMs: Feature spaces

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



Kernel trick

- Example: polynomial kernel

Transform 2D input space to 3D feature space

$$x = (x_1, x_2) \qquad \phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$
$$z = (z_1, z_2) \qquad \phi(z) = (z_1^2, z_2^2, \sqrt{2}z_1z_2)$$

$$\phi(x) \cdot \phi(z) = (x_1^2, x_2^2, \sqrt{2}x_1x_2) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2)$$
$$= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1z_1x_2z_2 = (x_1z_1 + x_2z_2)^2$$
$$= (x \cdot z)^2 = K(x, z)$$

Kernel trick + QP

- Max margin classifier can be found by solving

$$\arg\max_{\alpha}\left(\sum_j \alpha_j - \frac{1}{2}\sum_{j,k}\alpha_j\alpha_k y_j y_k (\phi(\mathbf{x}_j)\cdot\phi(\mathbf{x}_k))\right)$$
$$= \arg\max_{\alpha}\left(\sum_j \alpha_j - \frac{1}{2}\sum_{j,k}\alpha_j\alpha_k y_j y_k (K(\mathbf{x}_j,\mathbf{x}_k))\right)$$

- the weight matrix (no need to compute and store)

$$w = \sum_j \alpha_j y_j \phi(\mathbf{x}_j)$$

- the decision function is

$$h(\mathbf{x}) = \mathrm{sign}\left(\sum_j \alpha_j y_j (\phi(\mathbf{x})\cdot\phi(\mathbf{x}_j)) + b\right) = \mathrm{sign}\left(\sum_j \alpha_j y_j K(\mathbf{x},\mathbf{x}_j) + b\right)$$

SVM Kernel Functions

- Use kernel functions which compute

$$(z_i \cdot z_j) = (\phi(x_i) \cdot \phi(x_j)) = K(x_i, x_j)$$

- $K(\mathbf{a}, \mathbf{b}) = (\mathbf{a} \cdot \mathbf{b} + 1)^d$ is an example of an SVM polynomial Kernel Function
- Beyond polynomials there are other very high dimensional basis functions that can be made practical by finding the right Kernel Function
- Radial-Basis-style Kernel Function:

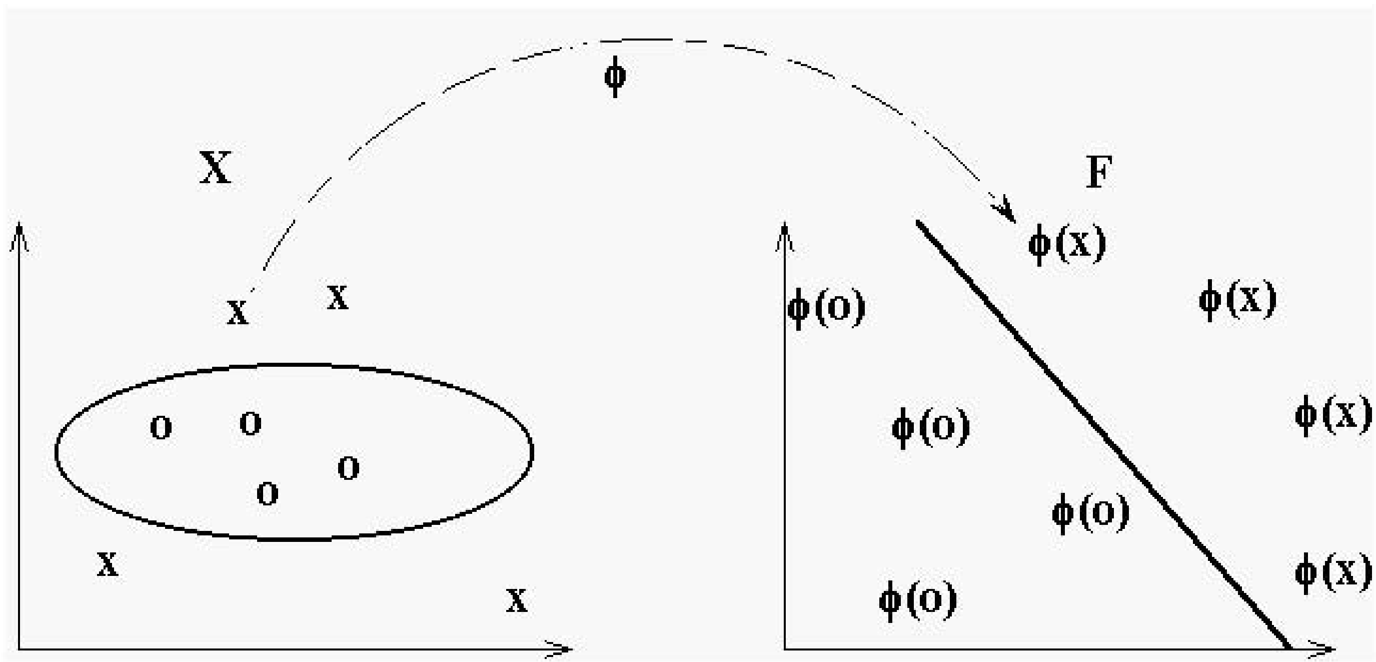
$$K(\mathbf{a},\mathbf{b}) = \exp\left(-\frac{(\mathbf{a}-\mathbf{b})^2}{2\sigma^2}\right)$$

- Neural-net-style Kernel Function:

$$K(\mathbf{a},\mathbf{b}) = \tanh(\kappa \mathbf{a}.\mathbf{b} - \delta)$$

σ, κ and δ are model parameters chosen by CV

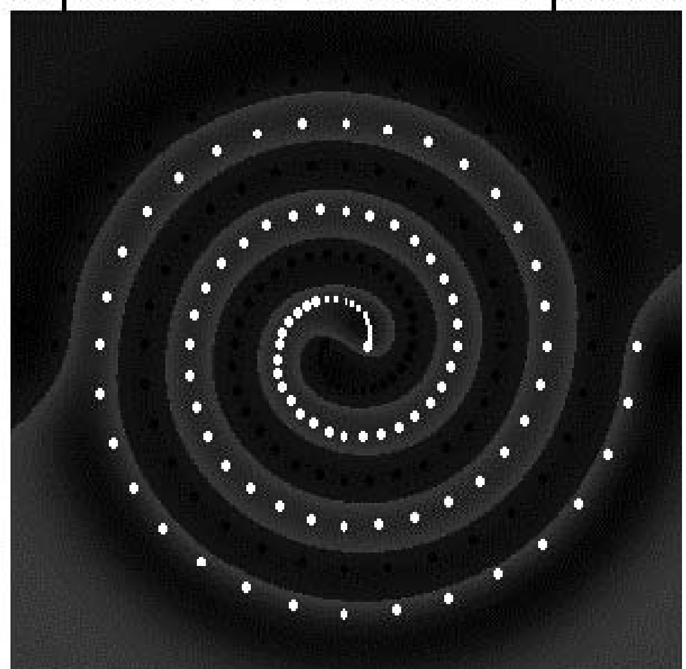
Example: Polynomial Kernels



www.support-vector.net

Example: the two spirals

- Separated by a hyperplane in feature space (gaussian kernels)



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The "Kernel Trick"

- The linear classifier relies on inner product between vectors $K(\mathbf{x}_i,\mathbf{x}_j)=\mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$
- If every datapoint is mapped into high-dimensional space via some transformation Φ: $\mathbf{x} \rightarrow \varphi(\mathbf{x})$, the inner product becomes:

$$K(\mathbf{x}_i,\mathbf{x}_j)= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$$

- A *kernel function* is a function that is eqiuvalent to an inner product in some feature space.
- Example:

  2-dimensional vectors $\mathbf{x}=[x_1 \ \ x_2]$; let $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^2$,

  Need to show that $K(\mathbf{x}_i,\mathbf{x}_j)= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$:

$$K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^2_{,}= 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2}=$$
$$= [1 \ \ x_{i1}^2 \ \ \sqrt{2}\, x_{i1}x_{i2} \ \ x_{i2}^2 \ \ \sqrt{2}x_{i1} \ \ \sqrt{2}x_{i2}]^{\mathbf{T}} [1 \ \ x_{j1}^2 \ \ \sqrt{2}\, x_{j1}x_{j2} \ \ x_{j2}^2 \ \ \sqrt{2}x_{j1} \ \ \sqrt{2}x_{j2}] =$$
$$= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j), \quad \text{where } \boldsymbol{\varphi}(\mathbf{x}) = [1 \ \ x_1^2 \ \ \sqrt{2}\, x_1x_2 \ \ x_2^2 \ \ \sqrt{2}x_1 \ \ \sqrt{2}x_2]$$

- Thus, a kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\boldsymbol{\varphi}(\mathbf{x})$ explicitly).

What Functions are Kernels?

- For some functions $K(\mathbf{x}_i,\mathbf{x}_j)$ checking that $K(\mathbf{x}_i,\mathbf{x}_j)= \varphi(\mathbf{x}_i)^{\mathbf{T}}\varphi(\mathbf{x}_j)$ can be cumbersome.
- Mercer's theorem:

Every semi-positive definite symmetric function is a kernel

- Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

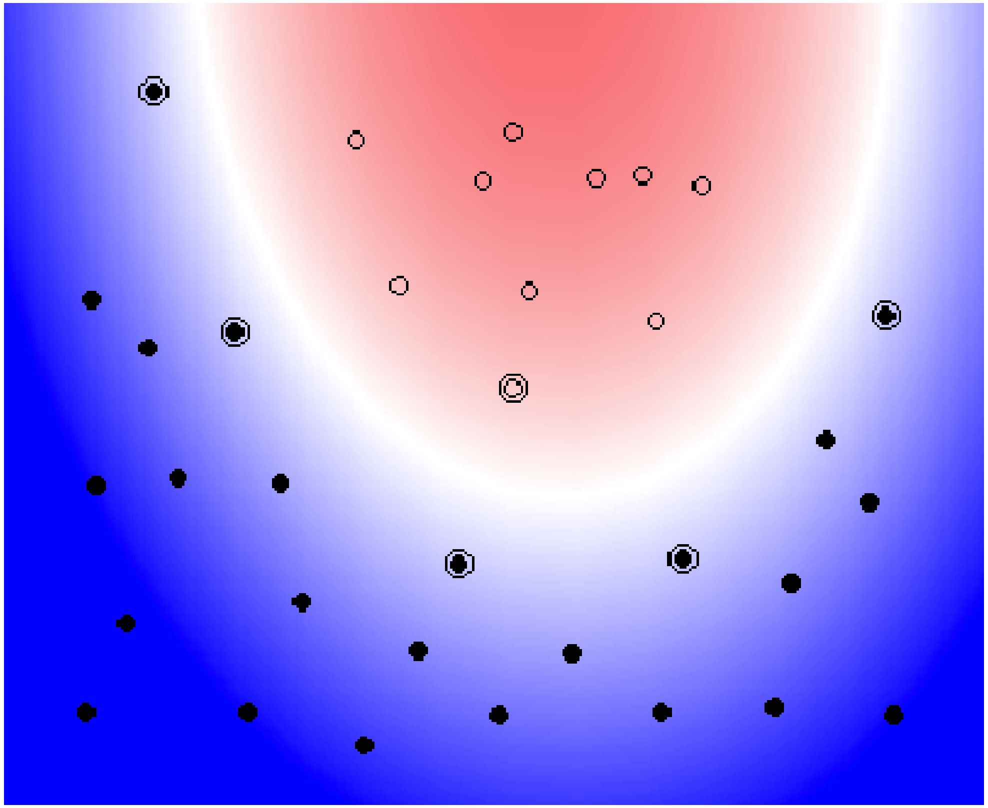
K=

$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x}_1,\mathbf{x}_2)$	$K(\mathbf{x}_1,\mathbf{x}_3)$	…	$K(\mathbf{x}_1,\mathbf{x}_n)$
$K(\mathbf{x}_2,\mathbf{x}_1)$	$K(\mathbf{x}_2,\mathbf{x}_2)$	$K(\mathbf{x}_2,\mathbf{x}_3)$		$K(\mathbf{x}_2,\mathbf{x}_n)$
…	…	…	…	…
$K(\mathbf{x}_n,\mathbf{x}_1)$	$K(\mathbf{x}_n,\mathbf{x}_2)$	$K(\mathbf{x}_n,\mathbf{x}_3)$	…	$K(\mathbf{x}_n,\mathbf{x}_n)$

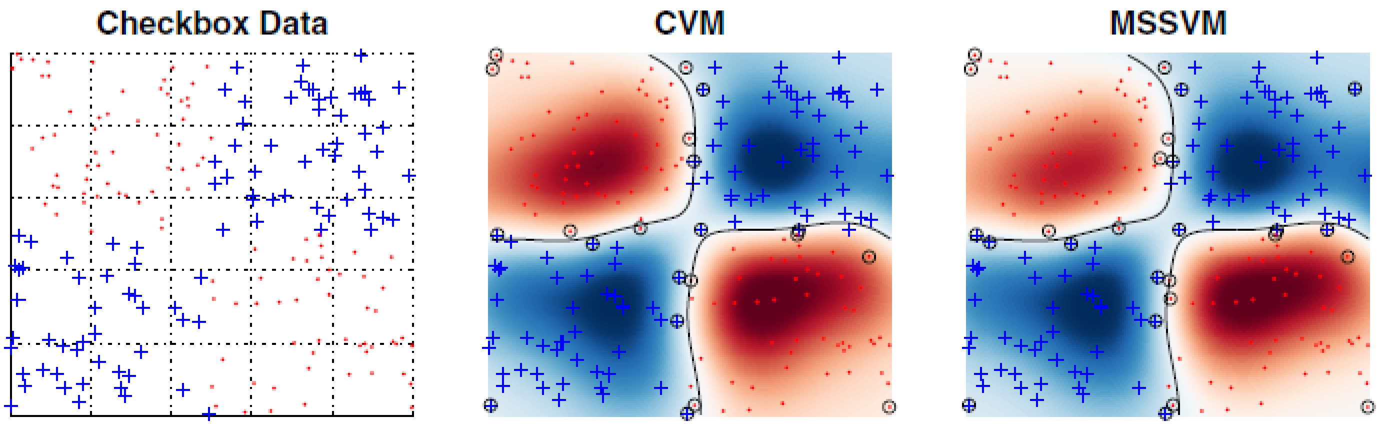
Example: SVM with Polynomial of Degree 2

Kernel: $K(\vec{x}_i, \vec{x}_j) = [\vec{x}_i \cdot \vec{x}_j + 1]^2$

plot by Bell SVM applet



Checkerboard data: Standard Linear Classifier cannot separate the two classes

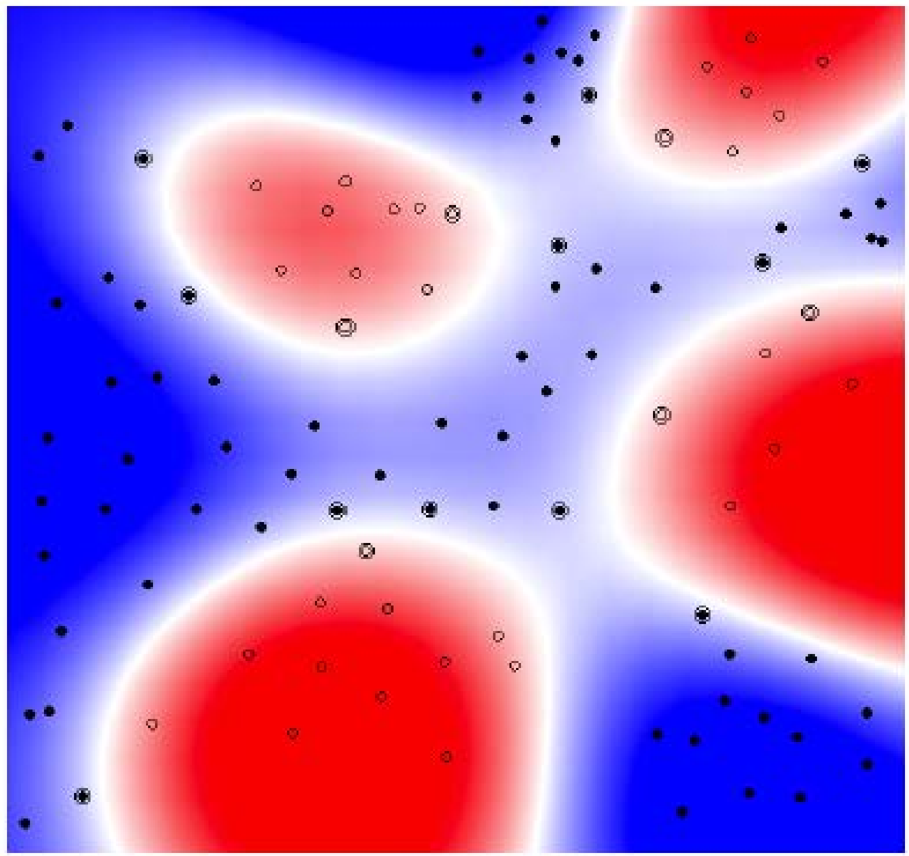


Nonlinear Kernel (II)

Example: SVM with RBF-Kernel

Kernel: $K(\vec{x}_i, \vec{x}_j) = \exp(-|\vec{x}_i - \vec{x}_j|^2 / \sigma^2)$

plot by Bell SVM applet



Examples of Kernel Functions

- Linear: $K(\mathbf{x}_i,\mathbf{x}_j)= \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ is $\mathbf{x}$ itself

- Polynomial of power p: $K(\mathbf{x}_i,\mathbf{x}_j)= (1+ \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^p$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ has $\binom{d+p}{p}$ dimensions

- Gaussian (radial-basis function): $K(\mathbf{x}_i,\mathbf{x}_j) = e^{-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}}$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ is *infinite-dimensional*: every point is mapped to *a function* (a Gaussian); combination of functions for support vectors is the separator.

- Higher-dimensional space still has *intrinsic* dimensionality d (the mapping is not *onto*), but linear separators in it correspond to *non-linear* separators in original space.

Non-linear SVMs Mathematically

- Dual problem formulation:

Find $\alpha_1 \ldots \alpha_n$ such that

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$ is maximized and

(1) $\Sigma\alpha_i y_i = 0$

(2) $\alpha_i \geq 0$ for all α_i

- The solution is:

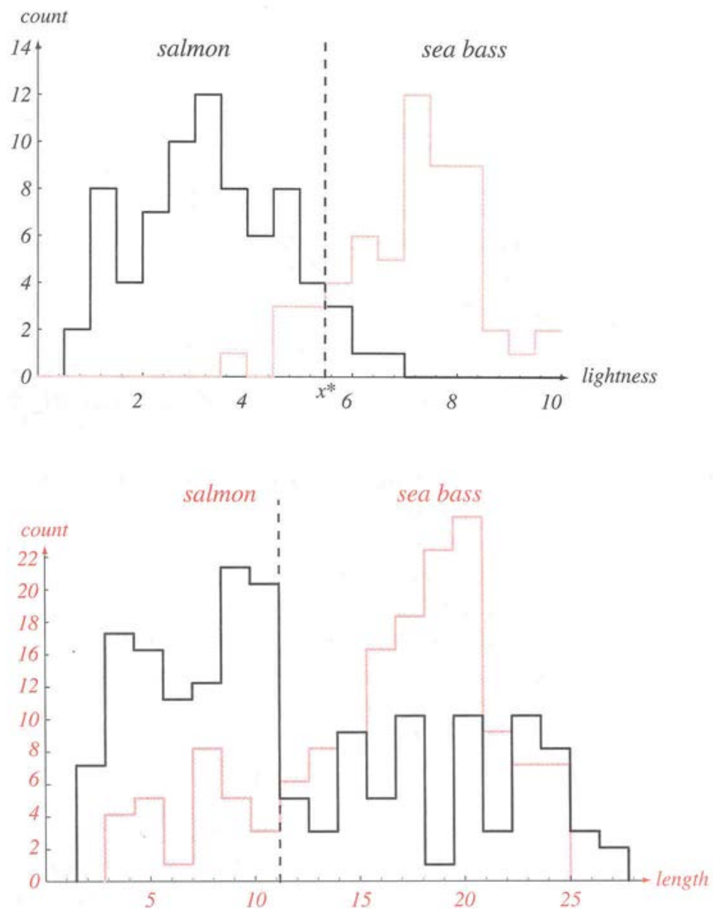
$$f(\mathbf{x}) = \Sigma\alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_j) + b$$

- Optimization techniques for finding α_i's remain the same!

SVM applications

- SVMs were originally proposed by Boser, Guyon and Vapnik in 1992 and gained increasing popularity in late 1990s.
- SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
- SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
- SVM techniques have been extended to a number of tasks such as regression [Vapnik *et al.* '97], principal component analysis [Schölkopf *et al.* '99], etc.
- Most popular optimization algorithms for SVMs use *decomposition* to hill-climb over a subset of α_i's at a time, e.g. SMO [Platt '99] and [Joachims '99]
- Tuning SVMs remains a black art: selecting a specific kernel and parameters is usually done in a try-and-see manner
- Most popular SVM software is LIBSVM from C.J.Lin

An example of fish classification



Bayes' classification