Lecture 3: Dual problems and Kernels

C4B Machine Learning — Hilary 2011 — A. Zisserman

- Primal and dual forms
- Linear separability revisted
- Feature mapping
- Kernels for SVMs
  - Kernel trick
  - requirements
  - radial basis functions

SVM – review

- We have seen that for an SVM learning a linear classifier

$$f(x) = \mathbf{w}^\top \mathbf{x} + b$$

is formulated as solving an optimization problem over $\mathbf{w}$:

$$\min_{\mathbf{w} \in \mathbb{R}^d} ||\mathbf{w}||^2 + C \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i))$$

- This quadratic optimization problem is known as the primal problem.

- Instead, the SVM can be formulated to learn a linear classifier

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

by solving an optimization problem over α_i.

- This is know as the dual problem, and we will look at the advantages of this formulation.

Sketch derivation of dual form

The Representer Theorem states that the solution $\mathbf{w}$ can always be written as a linear combination of the training data:

$$\mathbf{w} = \sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j$$

Proof: see example sheet .

Now, substitute for $\mathbf{w}$ in $f(x) = \mathbf{w}^\top \mathbf{x} + b$

$$f(x) = \left(\sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \right)^\top \mathbf{x} + b = \sum_{j=1}^{N} \alpha_j y_j \left(\mathbf{x}_j{}^\top \mathbf{x} \right) + b$$

and for $\mathbf{w}$ in the cost function $\min_{\mathbf{w}} ||\mathbf{w}||^2$ subject to $y_i \left(\mathbf{w}^\top \mathbf{x}_i + b \right) \geq 1, \forall i$

$$||\mathbf{w}||^2 = \left\{ \sum_j \alpha_j y_j \mathbf{x}_j \right\}^\top \left\{ \sum_k \alpha_k y_k \mathbf{x}_k \right\} = \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k)$$

Hence, an equivalent optimization problem is over α_j

$$\min_{\alpha_j} \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k) \quad \text{subject to } y_i \left(\sum_{j=1}^{N} \alpha_j y_j (\mathbf{x}_j{}^\top \mathbf{x}_i) + b \right) \geq 1, \forall i$$

and a few more steps are required to complete the derivation.

Primal and dual formulations

N is number of training points, and d is dimension of feature vector $\mathbf{x}$.

Primal problem: for $\mathbf{w} \in \mathbb{R}^d$

$$\min_{\mathbf{w} \in \mathbb{R}^d} ||\mathbf{w}||^2 + C \sum_{i}^{N} \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

Dual problem: for $\boldsymbol{\alpha} \in \mathbb{R}^N$ (stated without proof):

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k) \text{ subject to } 0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

- Complexity of solution is $O(d^3)$ for primal, and $O(N^3)$ for dual
- If $N << d$ then more efficient to solve for α than $\mathbf{w}$
- Dual form only involves $(\mathbf{x}_j{}^\top \mathbf{x}_i)$. We will return to why this is an advantage when we look at kernels.

Primal and dual formulations

Primal version of classifier:

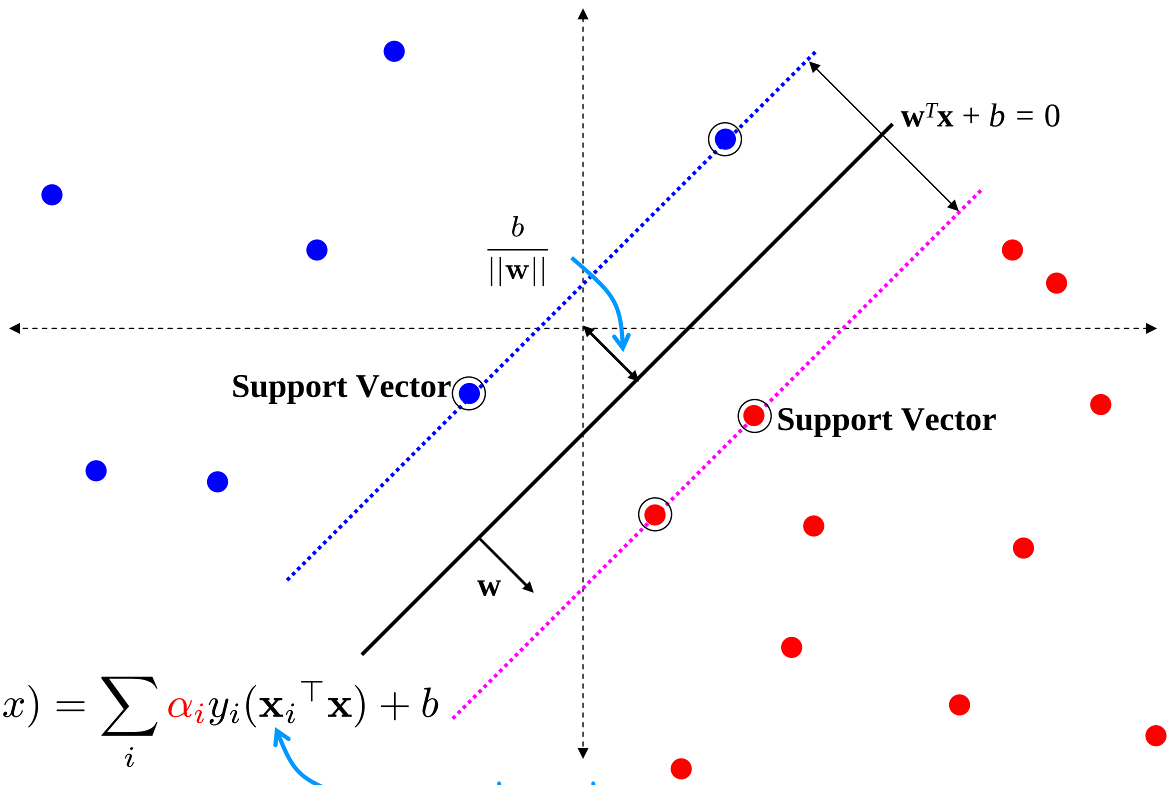
$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

Dual version of classifier:

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

At first sight the dual form appears to have the disadvantage of a K-NN classifier – it requires the training data points $\mathbf{x}_i$. However, many of the α_i's are zero. The ones that are non-zero define the support vectors $\mathbf{x}_i$.

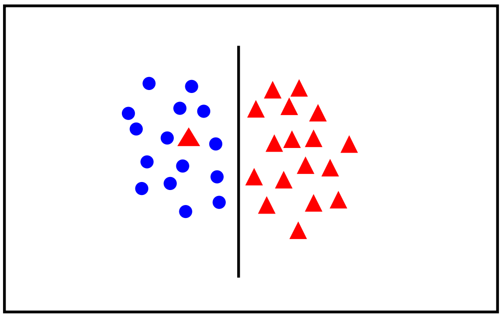
Support Vector Machine



$$f(x) = \sum_i \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

support vectors

Handling data that is not linearly separable

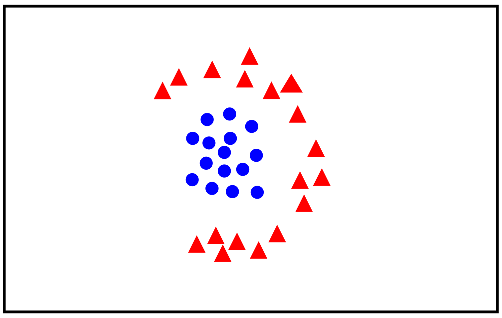


- introduce slack variables

$$\min_{\mathbf{w}\in\mathbb{R}^d, \xi_i \in \mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i$$

subject to

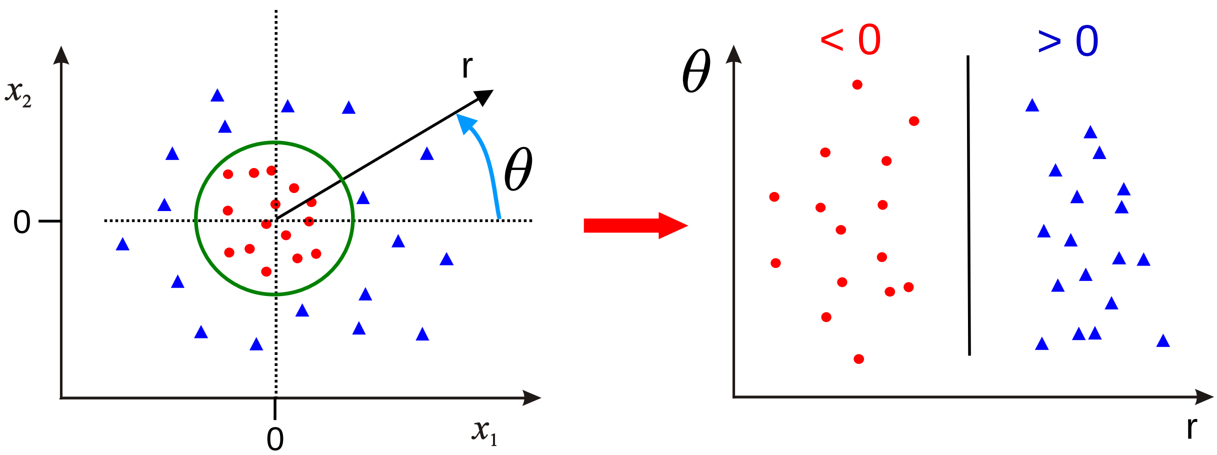
$$y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1 \dots N$$



- linear classifier not appropriate

??

Solution 1: use polar coordinates

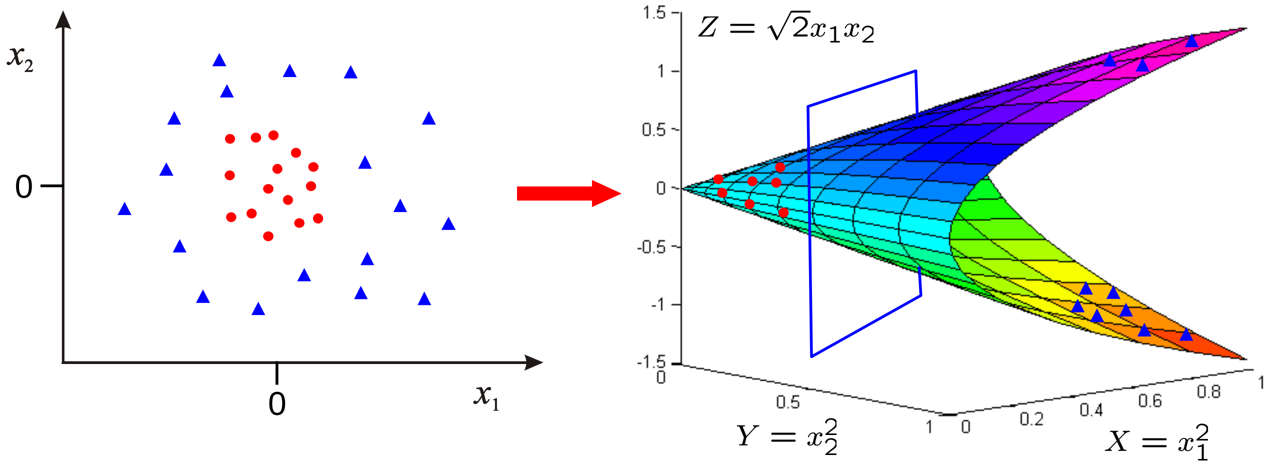


- Data is linearly separable in polar coordinates
- Acts non-linearly in original space

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} r \\ \theta \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^2$$

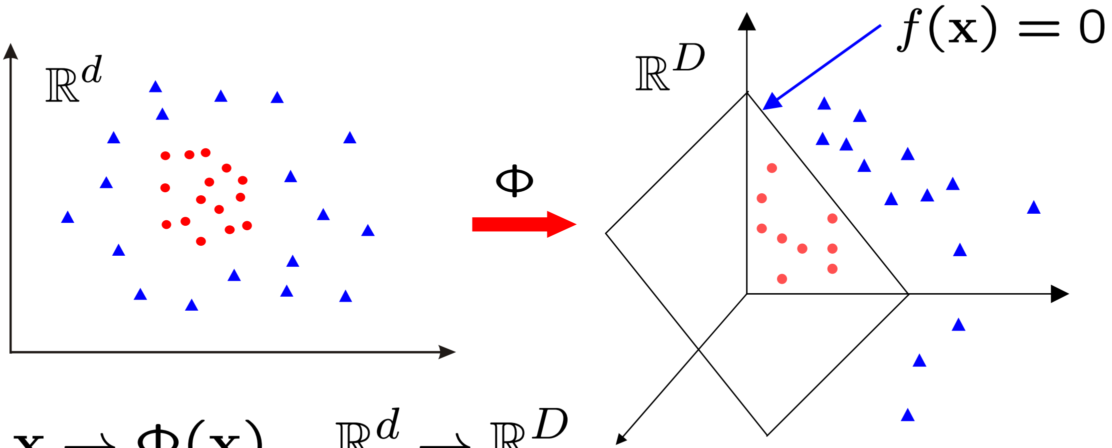
Solution 2: map data to higher dimension

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1 x_2 \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$



- Data is linearly separable in 3D
- This means that the problem can still be solved by a linear classifier

SVM classifiers in a transformed feature space



$$\Phi : \mathbf{x} \rightarrow \Phi(\mathbf{x}) \qquad \mathbb{R}^d \rightarrow \mathbb{R}^D$$

Learn classifier linear in $\mathbf{w}$ for $\mathbb{R}^D$:

$$f(\mathbf{x}) = \mathbf{w}^\top \Phi(\mathbf{x}) + b$$

Primal Classifier in transformed feature space

Classifier, with $\mathbf{w} \in \mathbb{R}^D$:

$$f(\mathbf{x}) = \mathbf{w}^\top \Phi(\mathbf{x}) + b$$

Learning, for $\mathbf{w} \in \mathbb{R}^D$

$$\min_{\mathbf{w} \in \mathbb{R}^D} ||\mathbf{w}||^2 + C \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i))$$

- Simply map $\mathbf{x}$ to $\Phi(\mathbf{x})$ where data is separable
- Solve for $\mathbf{w}$ in high dimensional space $\mathbb{R}^D$
- Complexity of solution is now $O(D^3)$ rather than $O(d^3)$

Dual Classifier in transformed feature space

Classifier:

$$\begin{aligned} f(\mathbf{x}) &= \sum_i^N \alpha_i y_i \mathbf{x}_i{}^\top \mathbf{x} + b \\ \rightarrow f(\mathbf{x}) &= \sum_i^N \alpha_i y_i \Phi(\mathbf{x}_i)^\top \Phi(\mathbf{x}) + b \end{aligned}$$

Learning:

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \mathbf{x}_j{}^\top \mathbf{x}_k$$

$$\rightarrow \quad \max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_k)$$

subject to

$$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

Dual Classifier in transformed feature space

- Note, that $\Phi(\mathbf{x})$ only occurs in pairs $\Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_i)$
- Once the scalar products are computed, complexity is again $O(N^3)$; it is not necessary to learn in the D dimensional space, as it is for the primal
- Write $k(\mathbf{x}_j, \mathbf{x}_i) = \Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_i)$. This is known as a Kernel

Classifier:

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \, k(\mathbf{x}_i, \mathbf{x}) + b$$

Learning:

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \, k(\mathbf{x}_j, \mathbf{x}_k)$$

subject to

$$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

Special transformations

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2} x_1 x_2 \end{pmatrix} \qquad \mathbb{R}^2 \to \mathbb{R}^3$$

$$\begin{aligned} \Phi(\mathbf{x})^\top \Phi(\mathbf{z}) &= \left(x_1^2, x_2^2, \sqrt{2} x_1 x_2\right) \begin{pmatrix} z_1^2 \\ z_2^2 \\ \sqrt{2} z_1 z_2 \end{pmatrix} \\ &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2 \\ &= (x_1 z_1 + x_2 z_2)^2 \\ &= (\mathbf{x}^\top \mathbf{z})^2 \end{aligned}$$

Kernel Trick

- Classifier can be learnt and applied without explicitly computing $\Phi(\mathbf{x})$
- All that is required is the kernel $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2$
- Complexity is still $O(N^3)$

Example kernels

- Linear kernels $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'$
- Polynomial kernels $k(\mathbf{x}, \mathbf{x}') = \left(1 + \mathbf{x}^\top \mathbf{x}'\right)^d$ for any $d > 0$
  - Contains all polynomials terms up to degree d
- Gaussian kernels $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2/2\sigma^2\right)$ for $\sigma > 0$
  - Infinite dimensional feature space

Valid kernels – when can the kernel trick be used?

- Given some arbitrary function $k(\mathbf{x}_i, \mathbf{x}_j)$, how do we know if it corresponds to a scalar product $\Phi(\mathbf{x}_i)^\top \Phi(\mathbf{x}_j)$ in some space?
- Mercer kernels: if $k(,)$ satisfies:
  - Symmetric $k(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_j, \mathbf{x}_i)$
  - Positive definite, $\boldsymbol{\alpha}^\top \mathtt{K} \boldsymbol{\alpha} \geq 0$ for all $\boldsymbol{\alpha} \in \mathbb{R}^N$, where $\mathtt{K}$ is the $N \times N$ Gram matrix with entries $\mathtt{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$.

  then $k(,)$ is a valid kernel.
- e.g. $k(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{z}$ is a valid kernel, $k(\mathbf{x}, \mathbf{z}) = \mathbf{x} - \mathbf{x}^\top \mathbf{z}$ is not.

SVM classifier with Gaussian kernel

N = size of training data

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b$$

weight (may be zero)

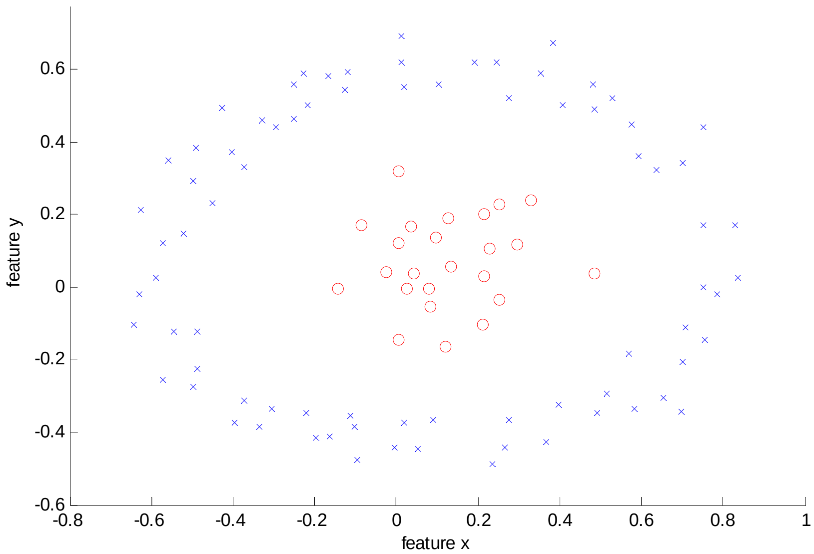
support vector

Gaussian kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2 / 2\sigma^2\right)$

Radial Basis Function (RBF) SVM

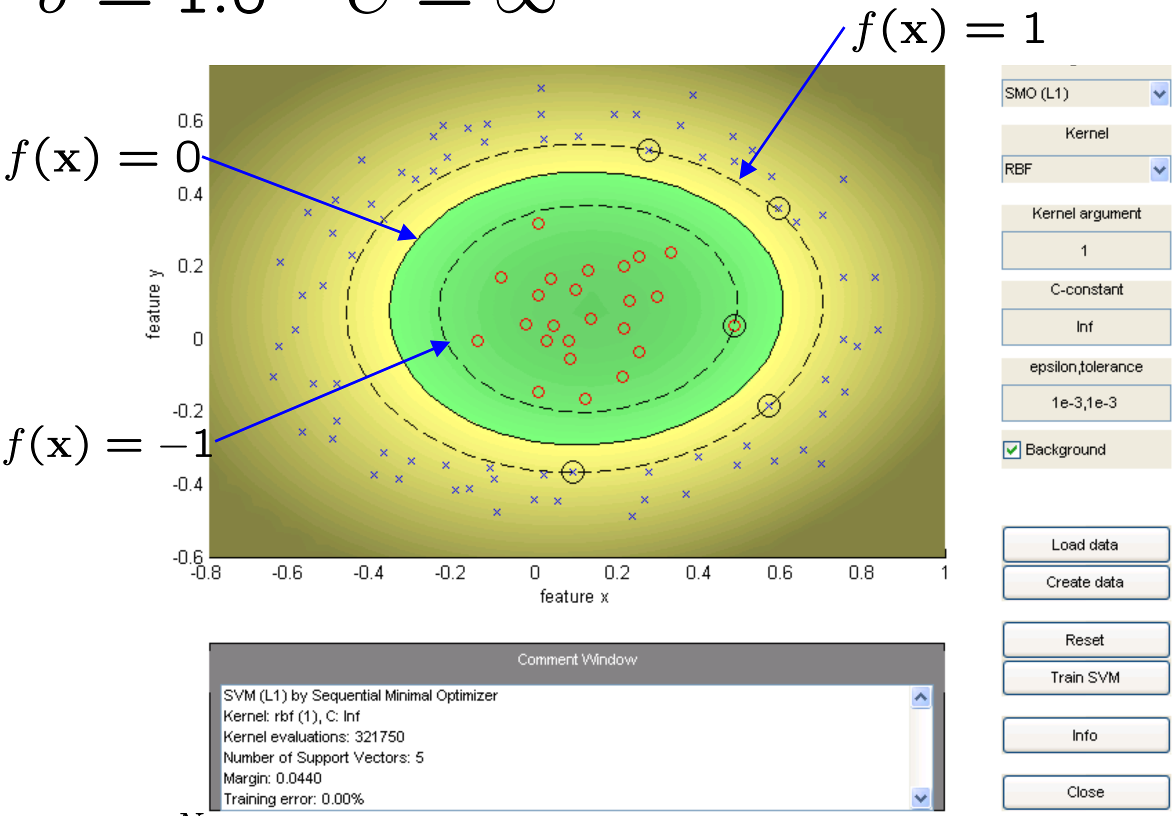
$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

RBF Kernel SVM Example



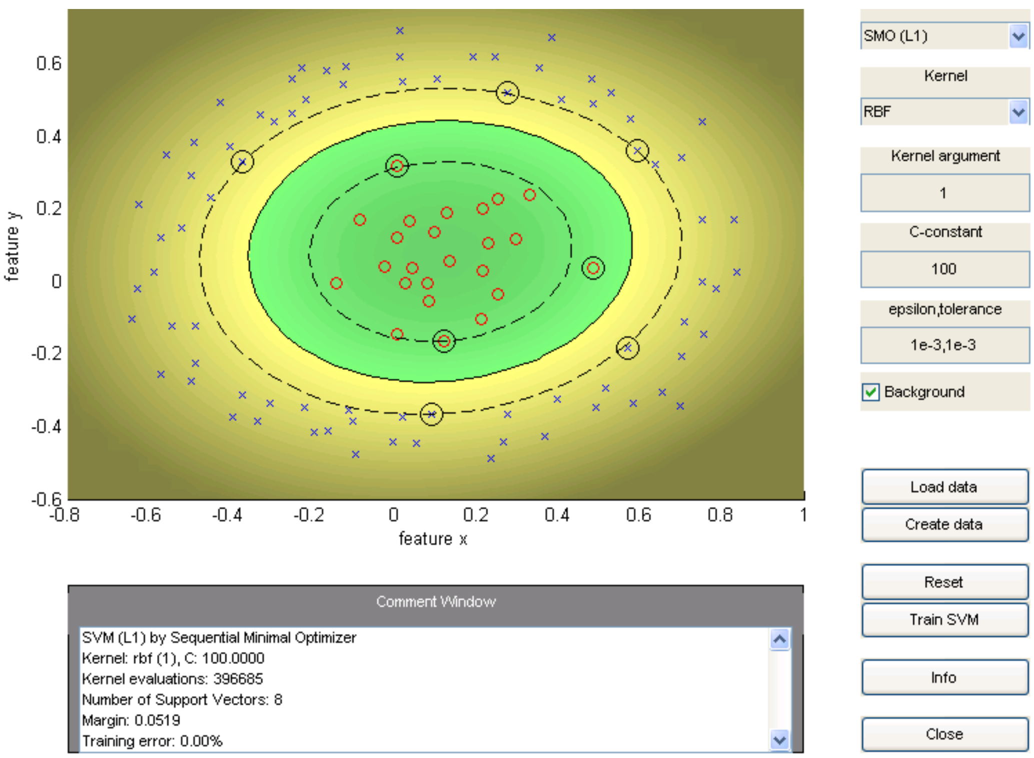
- data is not linearly separable in original feature space

$\sigma = 1.0 \quad C = \infty$



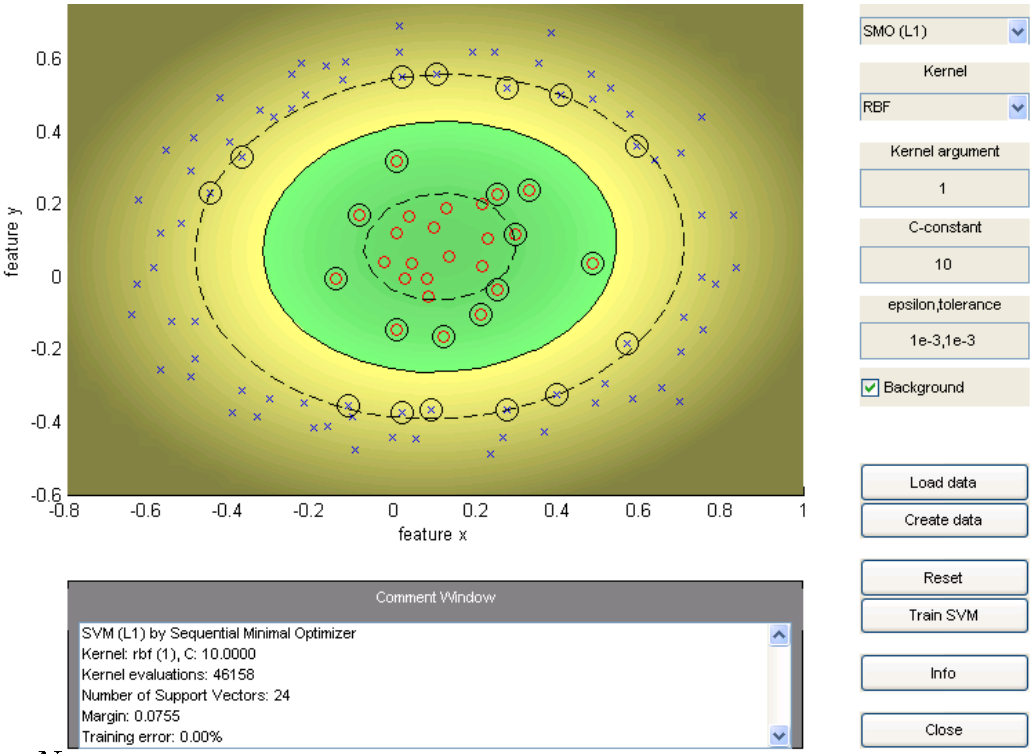
$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

$\sigma = 1.0 \quad C = 100$



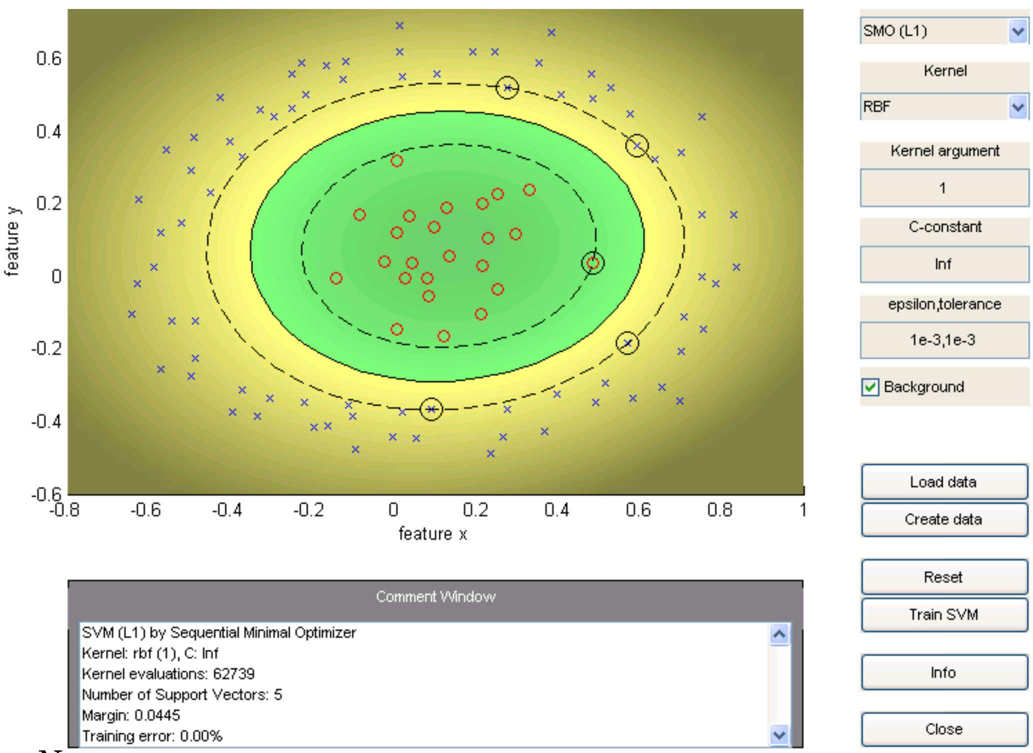
Decrease C, gives wider (soft) margin

$$\sigma = 1.0 \quad C = 10$$



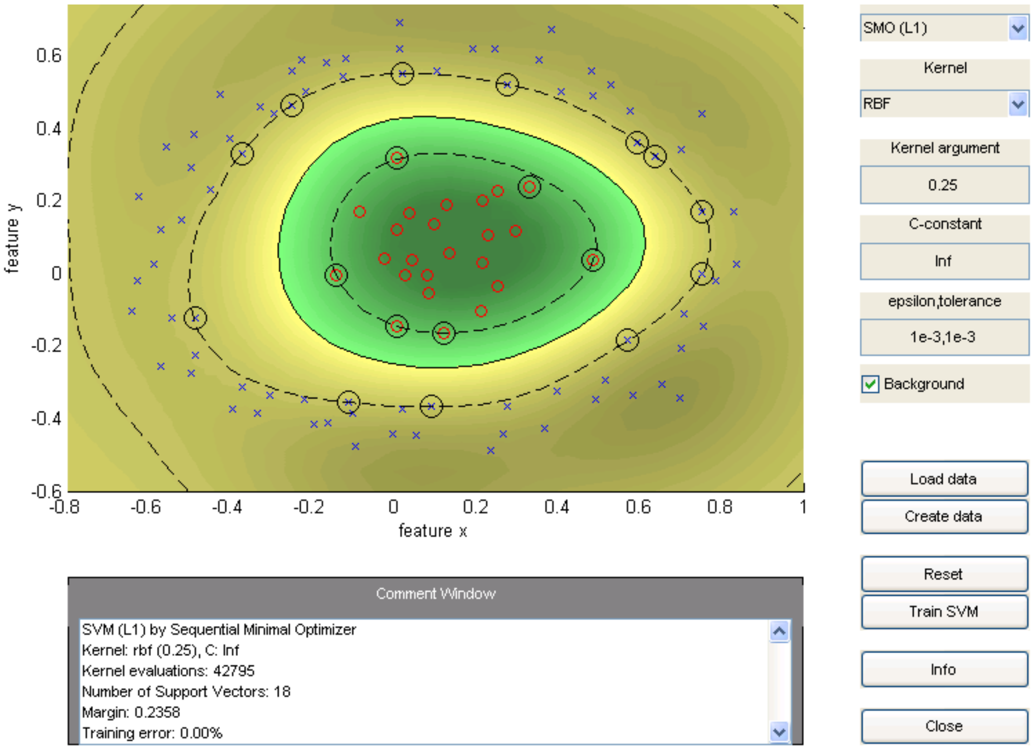
$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2/2\sigma^2\right) + b$$

$$\sigma = 1.0 \quad C = \infty$$



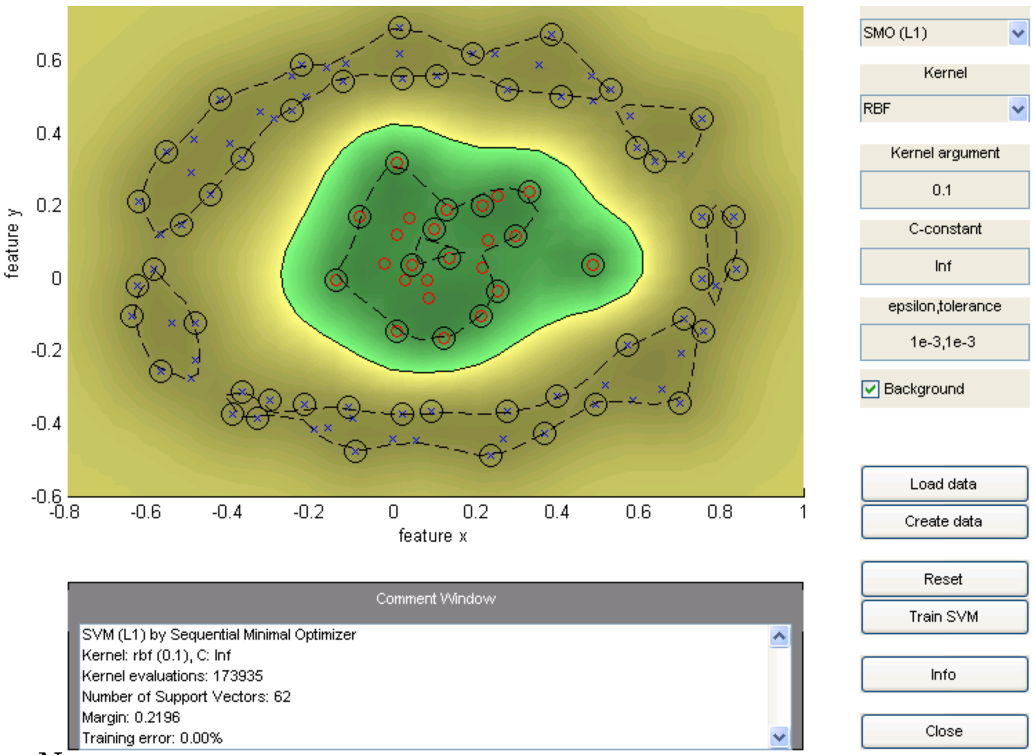
$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2/2\sigma^2\right) + b$$

$$\sigma = 0.25 \quad C = \infty$$



Decrease sigma, moves towards nearest neighbour classifier

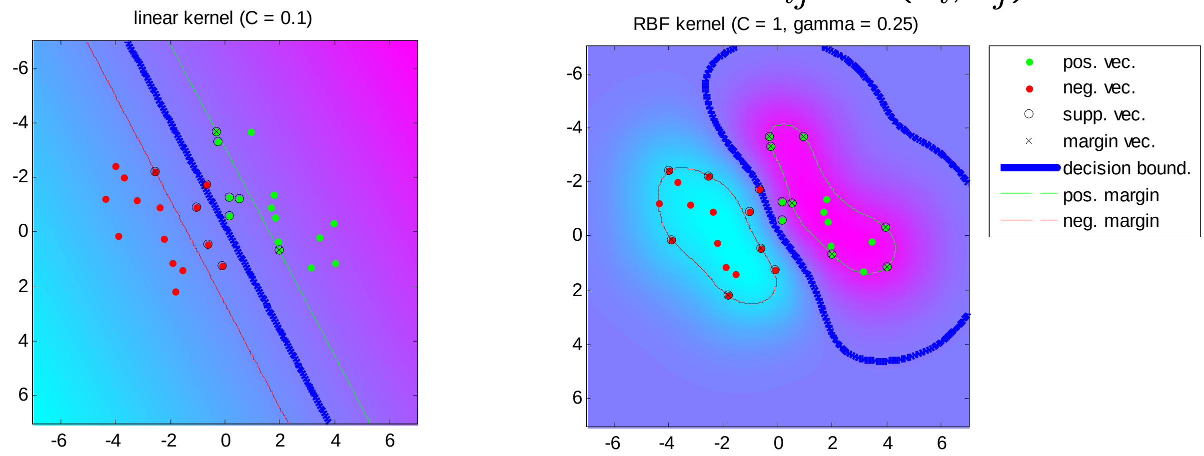
$$\sigma = 0.1 \quad C = \infty$$

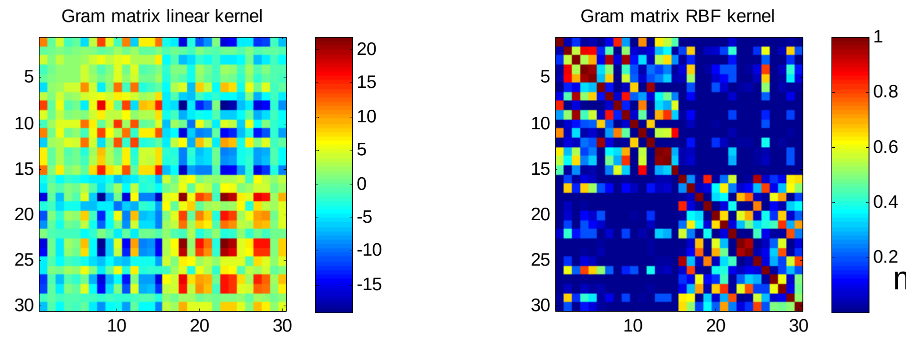


$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

Kernel block structure

$N \times N$ Gram matrix with entries $\mathrm{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$





The kernel measures similarity between the points

Kernel Trick - Summary

- Classifiers can be learnt for high dimensional features spaces, without actually having to map the points into the high dimensional space

- Data may be linearly separable in the high dimensional space, but not linearly separable in the original feature space

- Kernels can be used for an SVM because of the scalar product in the dual form, but can also be used elsewhere – they are not tied to the SVM formalism

- Kernels apply also to objects that are not vectors, e.g.

$$k(h, h') = \sum_k \min(h_k, h'_k) \text{ for histograms with bins } h_k, h'_k$$

- We will see other examples of kernels later in regression and unsupervised learning

Background reading

- Bishop, chapters 6.2 and 7
- Hastie et al, chapter 12
- More on web page:
  http://www.robots.ox.ac.uk/~az/lectures/ml