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Machine Learning

Session 18 - T

Support Vector Machines – Part 2

Ciência de Dados Aplicada

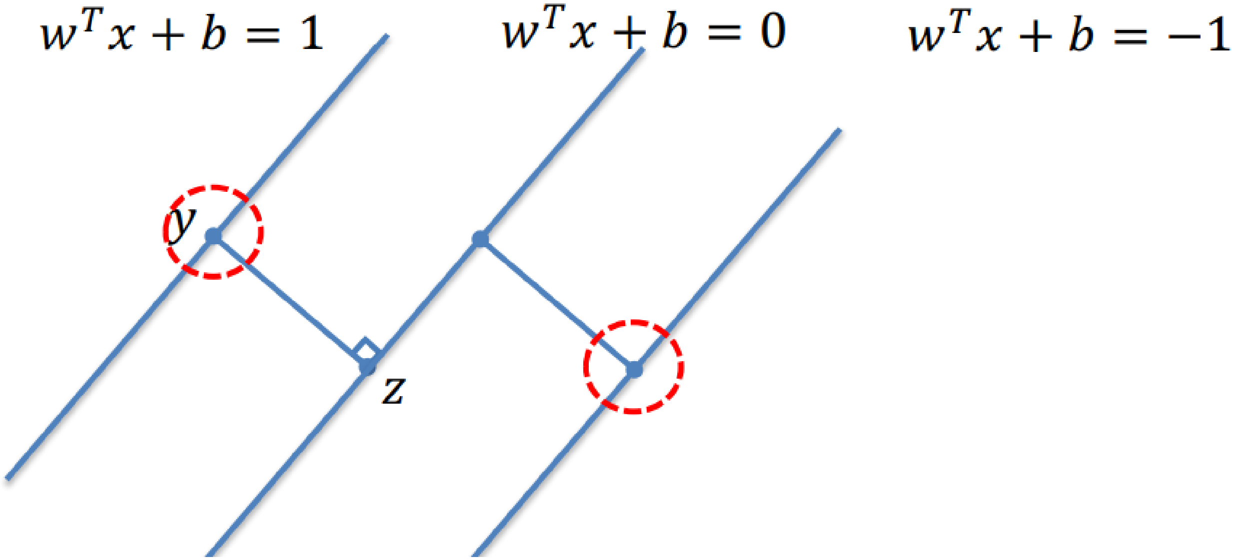
2023/2024

SVMs - Recap

$$\min_{w,b} ||w||^2$$

such that

$$y^{(i)}(w^T x^{(i)} + b) \geq 1, \text{for all } i$$

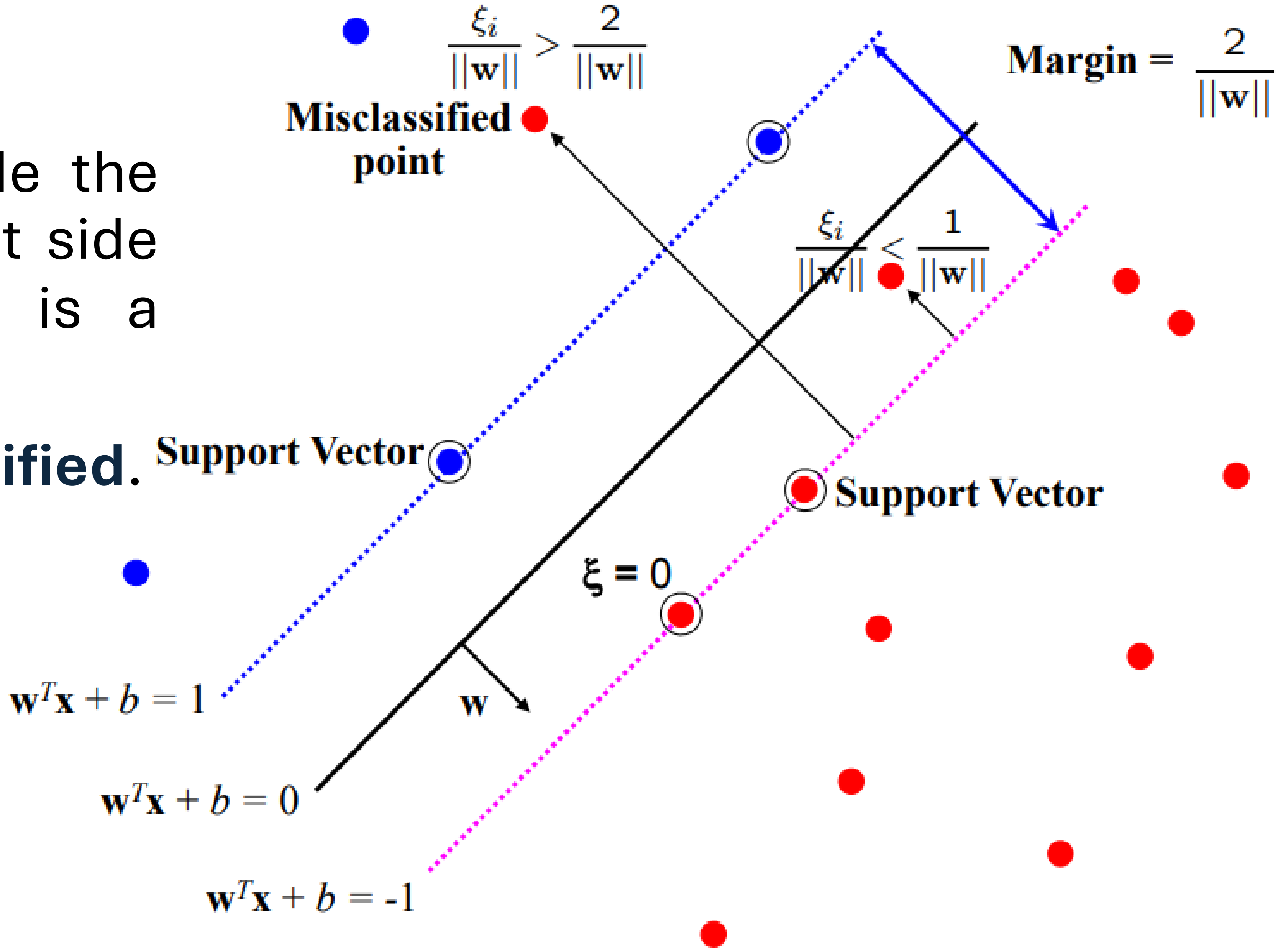


SVMs – Slack Variables

$$\xi_i \geq 0$$

- For $0 < \xi \leq 1$ point is inside the margin but on the correct side of the hyperplate. This is a **margin violation**;
- For $\xi > 1$ point is **misclassified**.

ξ allows margin violations or misclassified points, but with a **penalty**!



SVMs - Soft Margin Solution

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

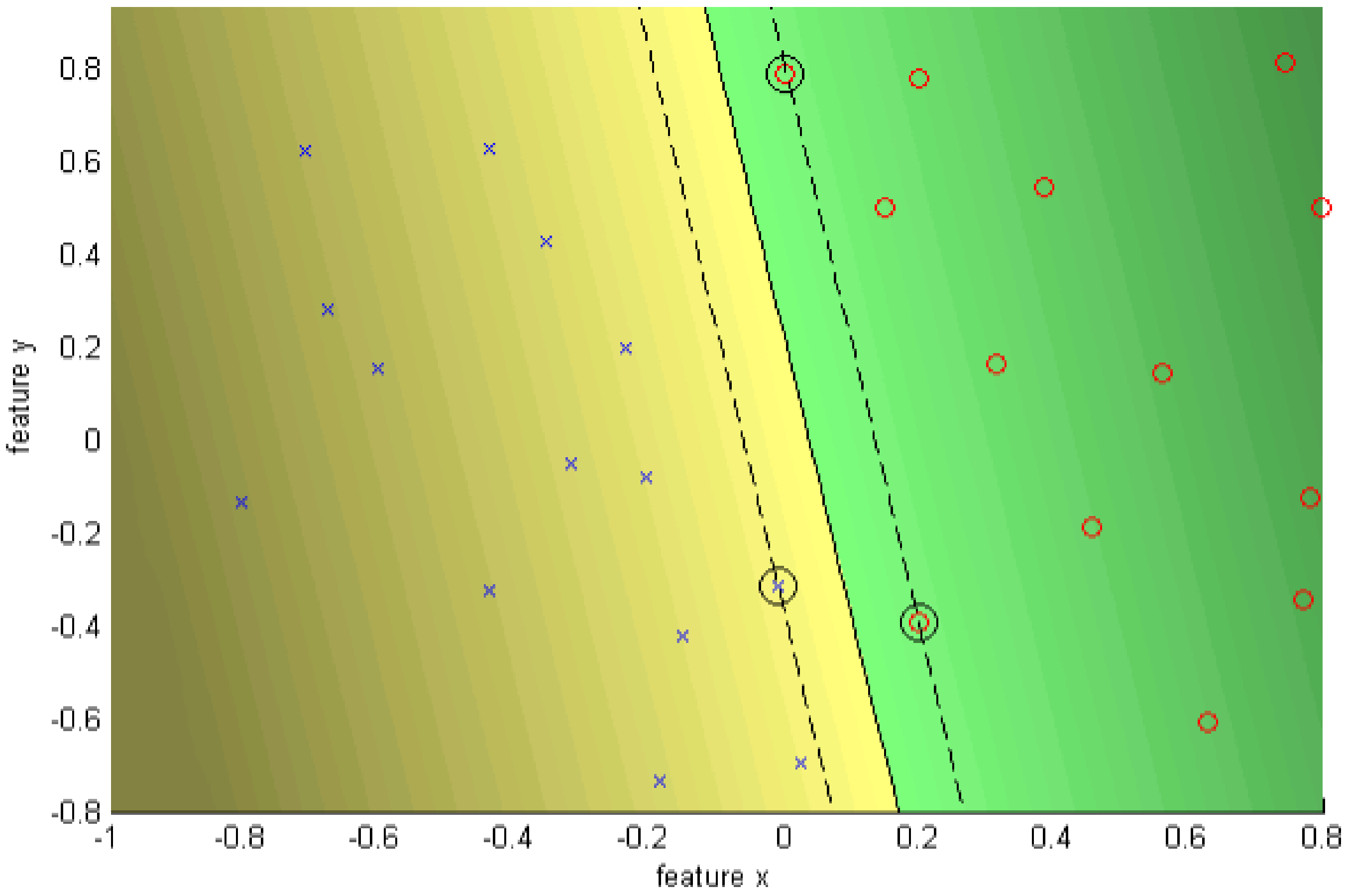
such that $y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1 \ldots N$

- Every constraint can be satisfied if ξ_i is sufficiently large.

- C is a regularization parameter:
  - **Small C** allows constraints to be easily ignores → **large margin**
  - **Large C** makes constraints hard to ignore → **narrow margin**
  - **C = ∞** enforces all constraints → **hard margin**

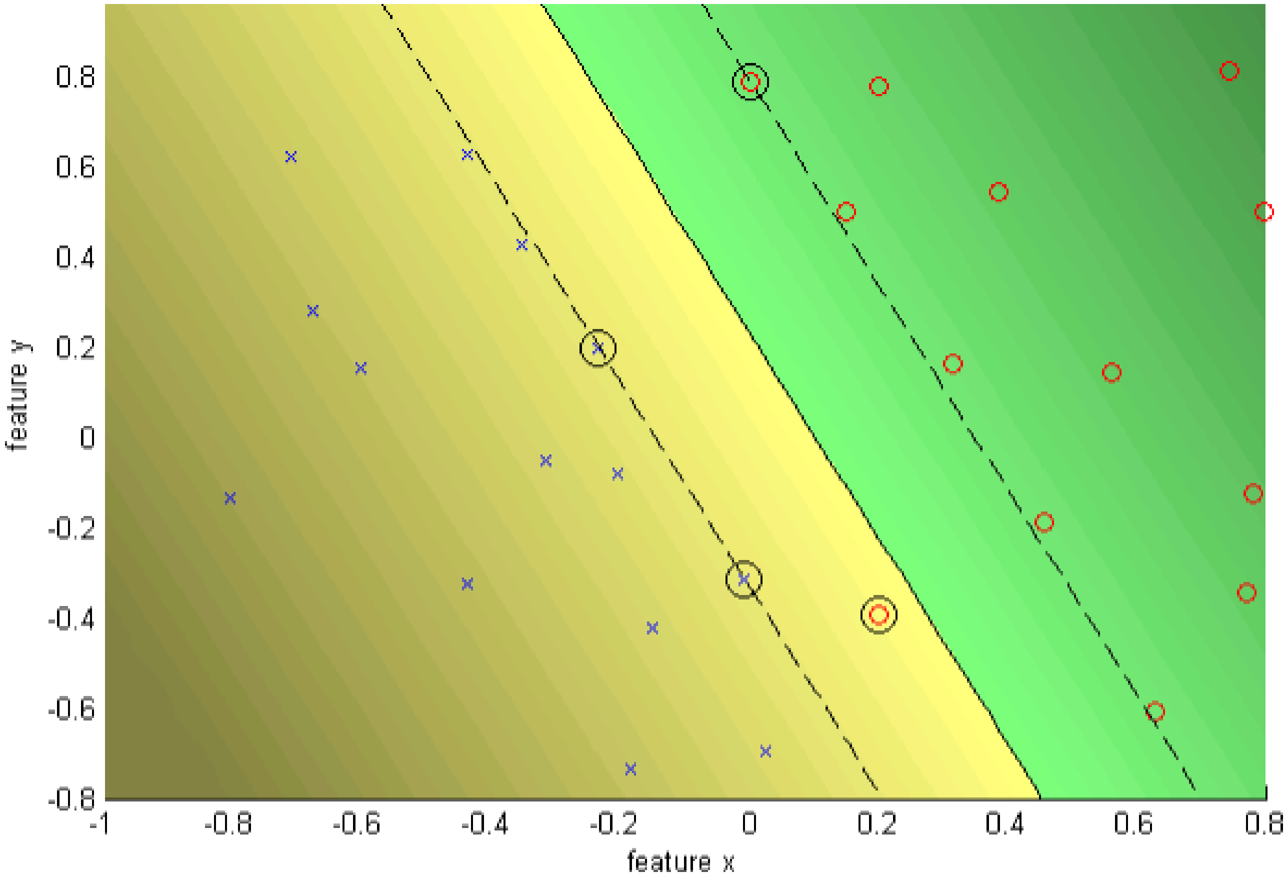
SVMs - C

C = Infinity   hard margin



SVMs - C

C = 10 soft margin



SVMs - Optimization

- Learning an SVM has been formulated as a **constrained** optimization problem over w and ξ

$$\min_{\mathbf{w}\in\mathbb{R}^d, \xi_i\in\mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i \text{ subject to } y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1\ldots N$$

- The constraint $y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i$, can be written more concisely as:

$$y_i f(\mathbf{x}_i) \geq 1 - \xi_i$$

which, together with $\xi_i \geq 0$, is equivalent to:

$$\xi_i = \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

SVMs - Optimization

- Hence, the learning problem is equivalent to the **unconstrained** optimization problem over w:

$$\min_{\mathbf{w}\in\mathbb{R}^d} \underbrace{||\mathbf{w}||^2}_{\text{regularization}} + C\sum_i^N \underbrace{\max\left(0, 1 - y_i f(\mathbf{x}_i)\right)}_{\text{loss function}}$$

- **If $y_i f(x_i) > 1$:**
  - Point is **outside the margin. No contribution to the loss.**

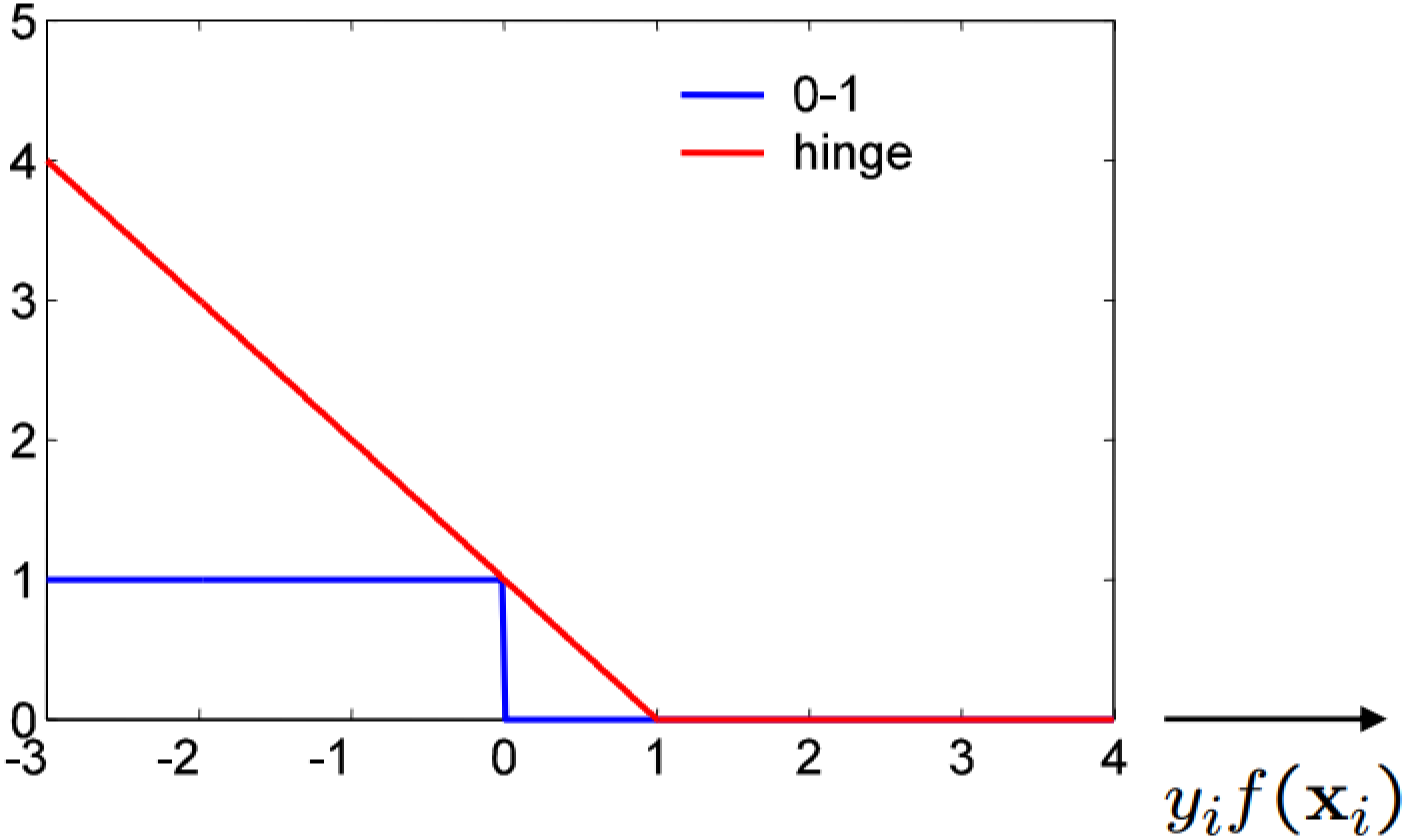
- **If $y_i f(x_i) = 1$:**
  - Point is **on the margin. No contribution to the loss.**

- **If yif(xi) < 1:**
  - Point **violates the margin** constraint. **Contributes to the loss.**

SVMs – Hinge Loss

- SVMs uses the **Hinge Loss** → $\max(0, 1 - y_i f(x_i))$

- Variation of the 0-1 loss.



SVMs – Dual Form

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- The previous 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 a n optimization problem over α_i.

- This is known as the **dual** problem!

SVMs – Dual Form

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- The Representer Theorem states that the solution w can always be written as a linear combination of the training data:

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

- If we substitute w in $f(x) = w^T x + b$

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

- And for w in the cost function $\min_w ||w||^2$ subject to $y_i(w^T x_i + b) \geq 1$

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

SVMs – Dual Form

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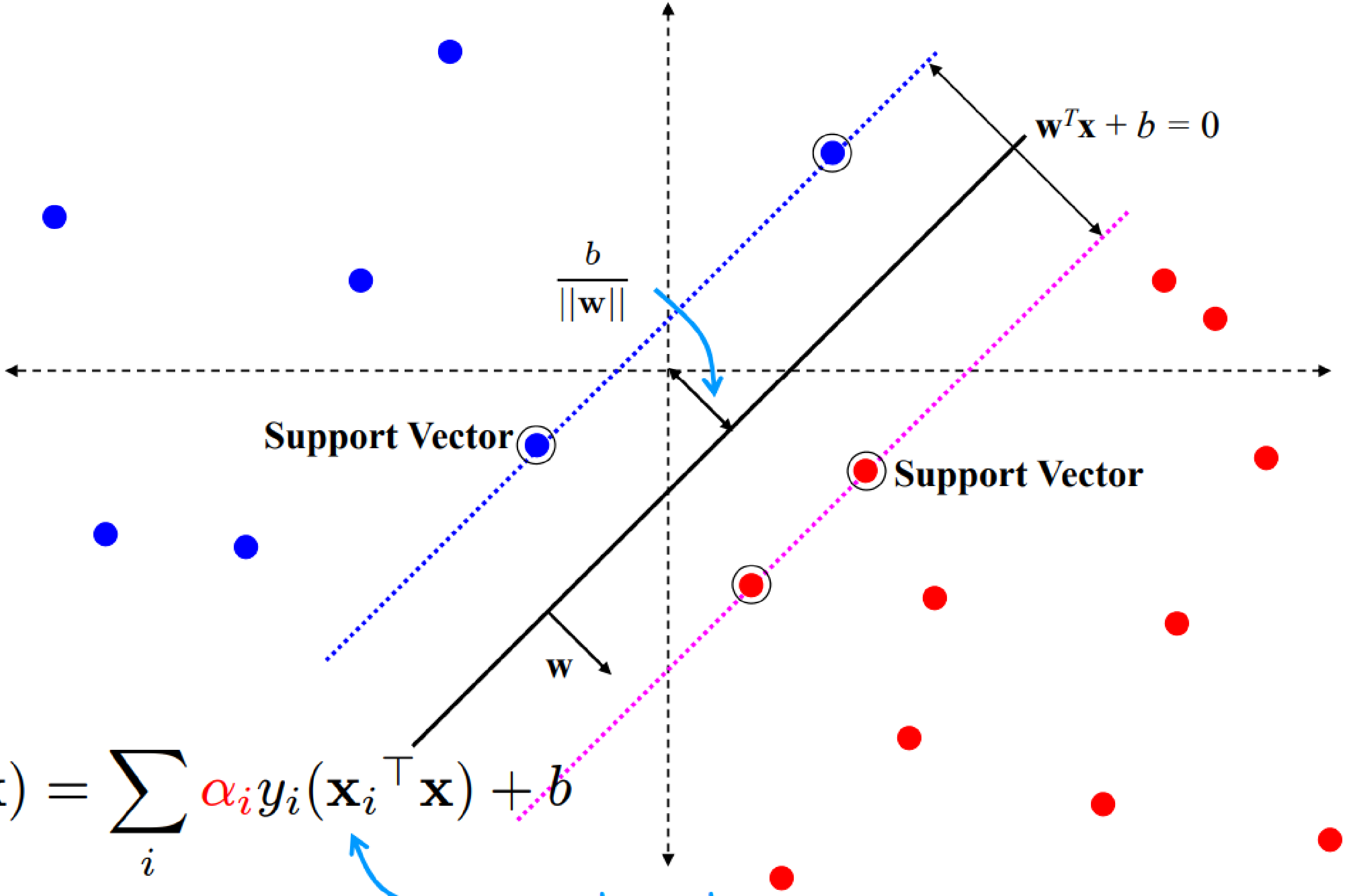
- Hence, a equivalent optimization problem over α_j

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

- Advantage of dual over primal form:
  - Dual form only involves $(x_j^T x_k)$ - which requires the training data points! However, many of α_i are 0 (the non support vectors).

SVMs – Dual Form

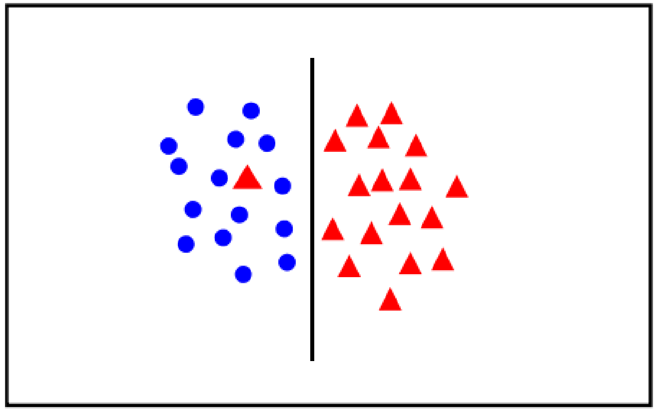


$$f(\mathbf{x}) = \sum_i \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

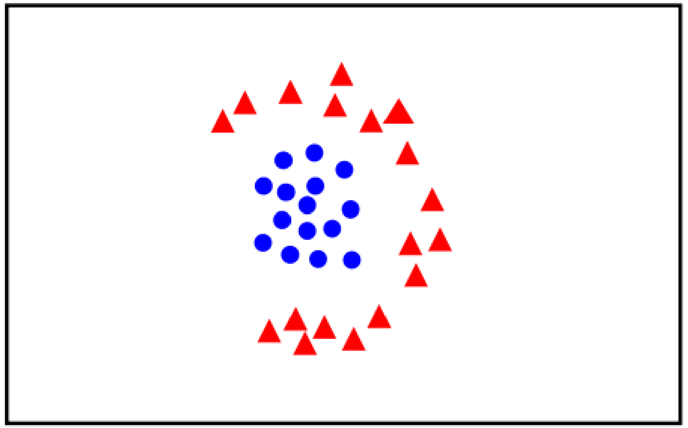
support vectors

SVMs – Handling non linear data

- Introduce slack variables

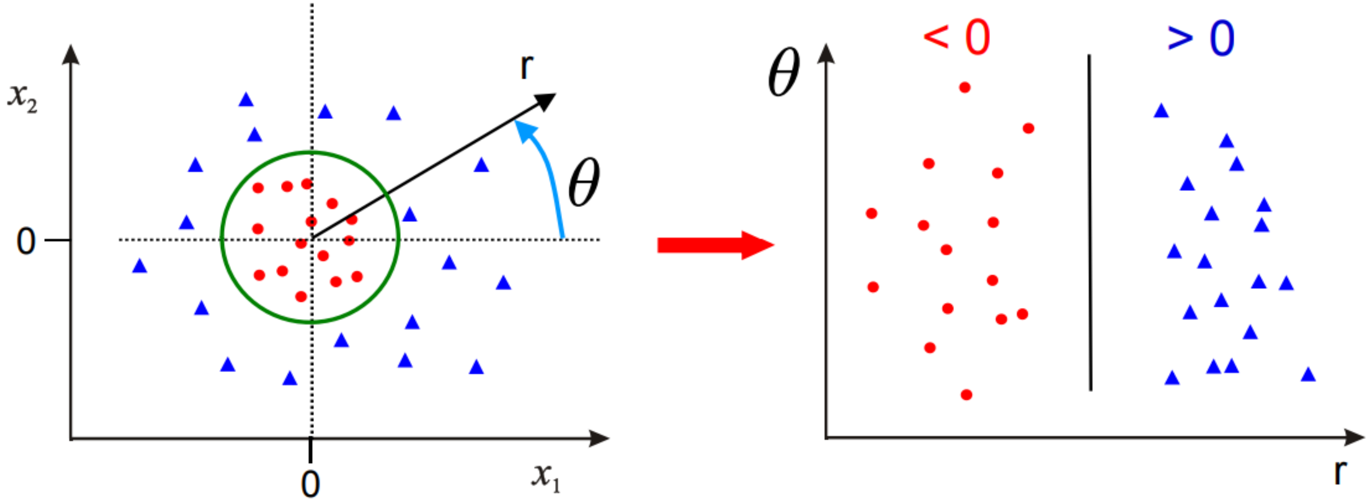


- Linear classifier not appropriate



SVMs – Solution 1

- Using polar coordinates



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

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

SVMs – Solution 2

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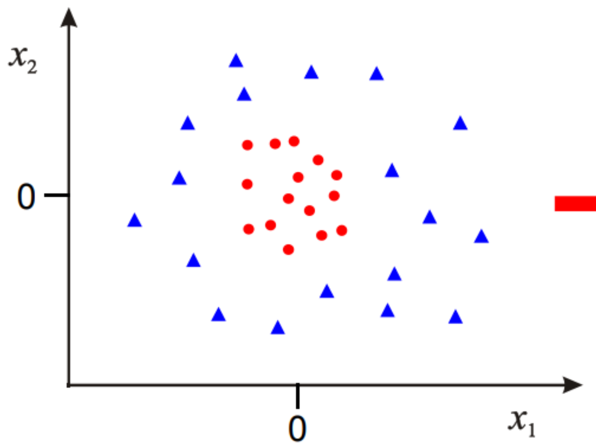
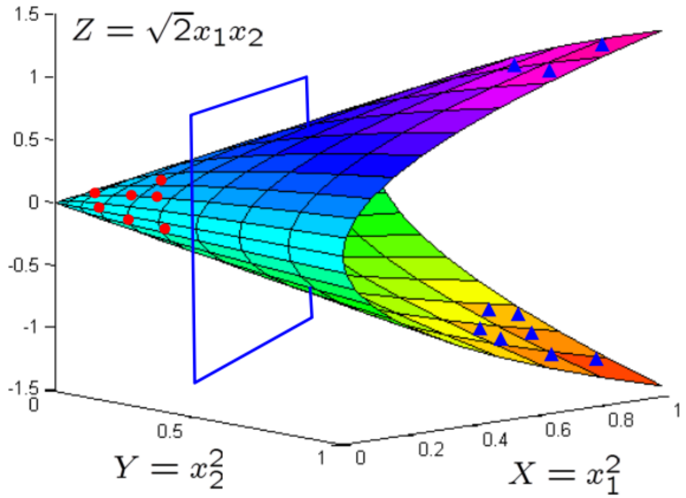
- Map data to a **higher dimension**

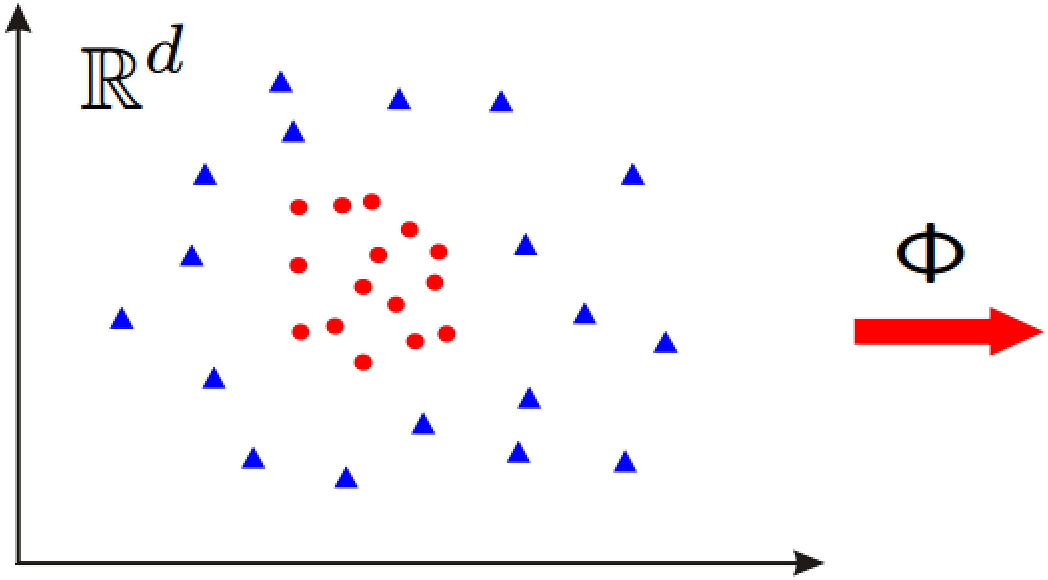
$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

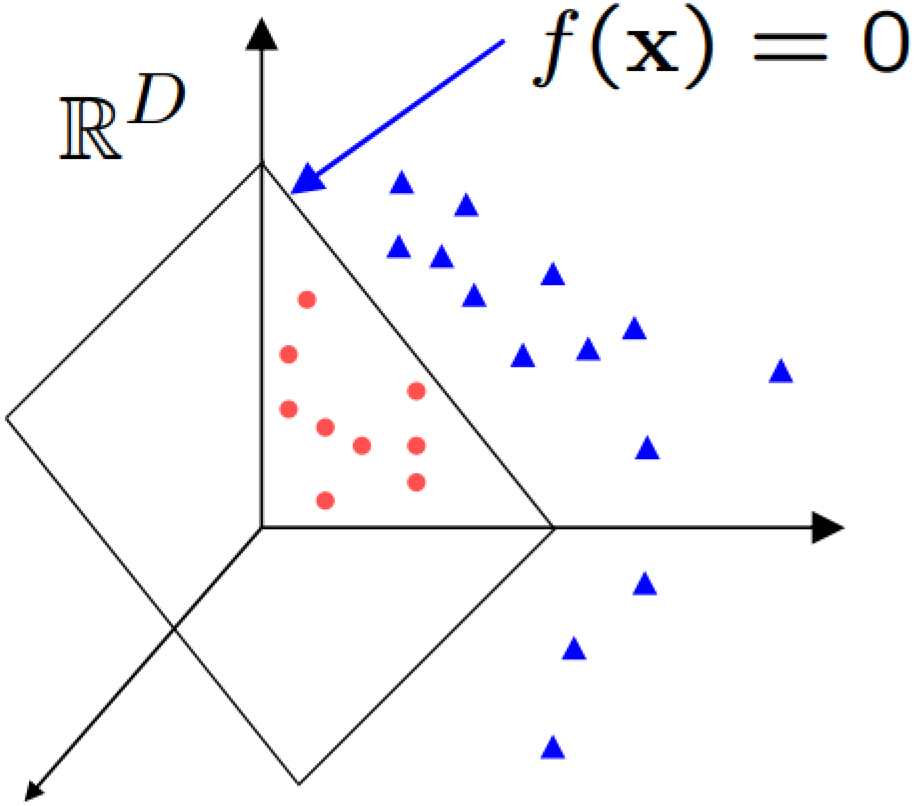




- Data is **linearly separable** in 3D.
- This means that the problem can still be solved by a **linear classifier**.

SVMs – Transformed Feature Space





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

- Learn a linear classifier in w for $\mathbb{R}^D$

$\Phi(\mathbf{x})$ is a **feature map**

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

Primal Classifier – Transformed Feature Space

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

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

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

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

- Map x to $\Phi(\mathbf{x})$ where data is linearly separable

- Solve for w in high dimensional space

Dual Classifier – Transformed Feature Space

- **Classifier:**

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

$$\rightarrow f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \, \Phi(\mathbf{x}_i)^\top \Phi(\mathbf{x}) + b$$

- **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 – 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, only the N dimensional vector $\boldsymbol{\alpha}$ needs to be learnt; 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 $$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

SVMs – Kernel Trick

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \quad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$\begin{aligned} \Phi(\mathbf{x})^\top \Phi(\mathbf{z}) &= \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \begin{pmatrix} z_1^2 \\ z_2^2 \\ \sqrt{2}z_1z_2 \end{pmatrix} \\ &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1x_2z_1z_2 \\ &= (x_1z_1 + x_2z_2)^2 \\ &= (\mathbf{x}^\top \mathbf{z})^2 \end{aligned}$$

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

SVMs – 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

SVM Classifer 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

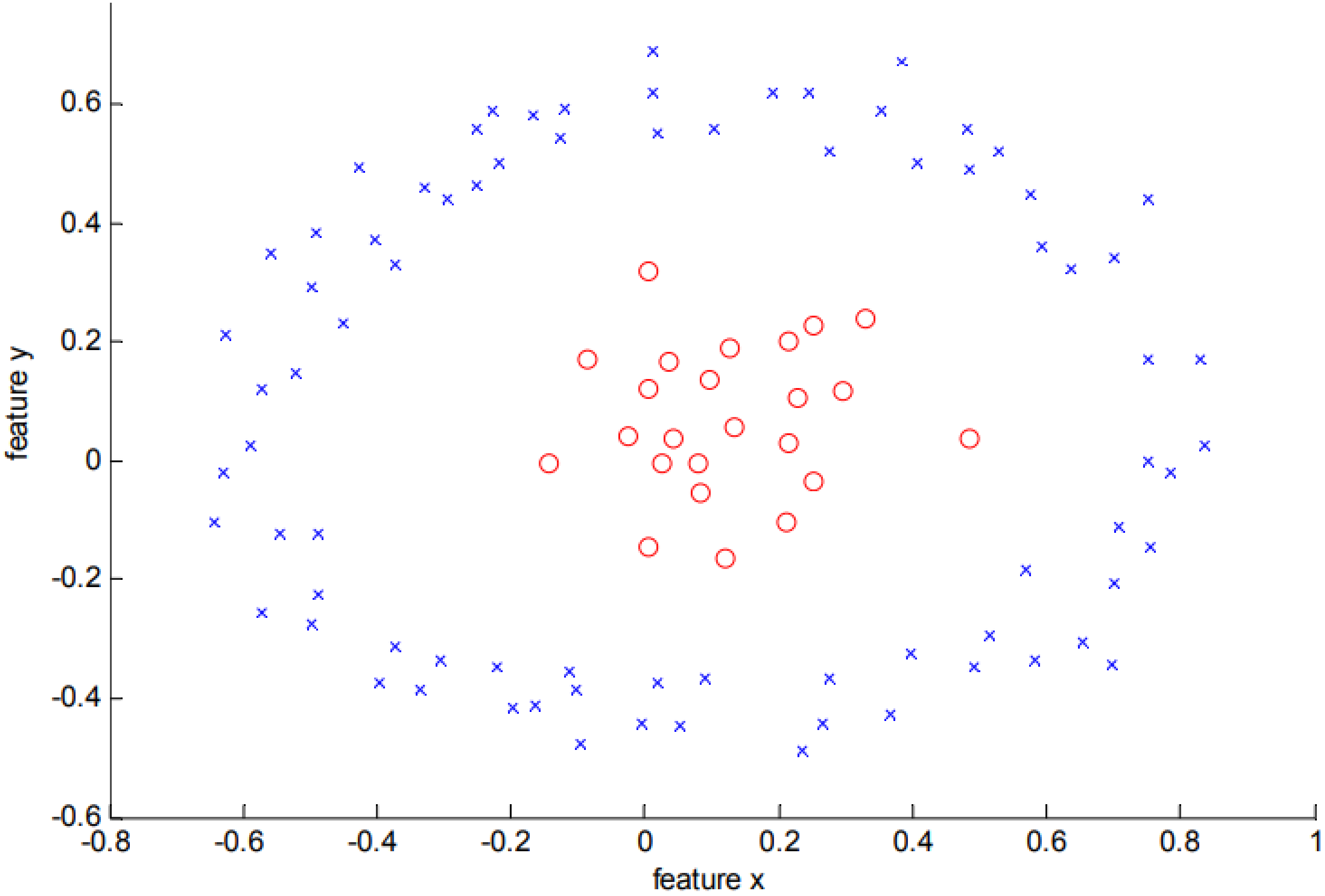
Gaussian kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2 / 2\sigma^2\right)$

Radial Basis Function (RBF) SVM

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

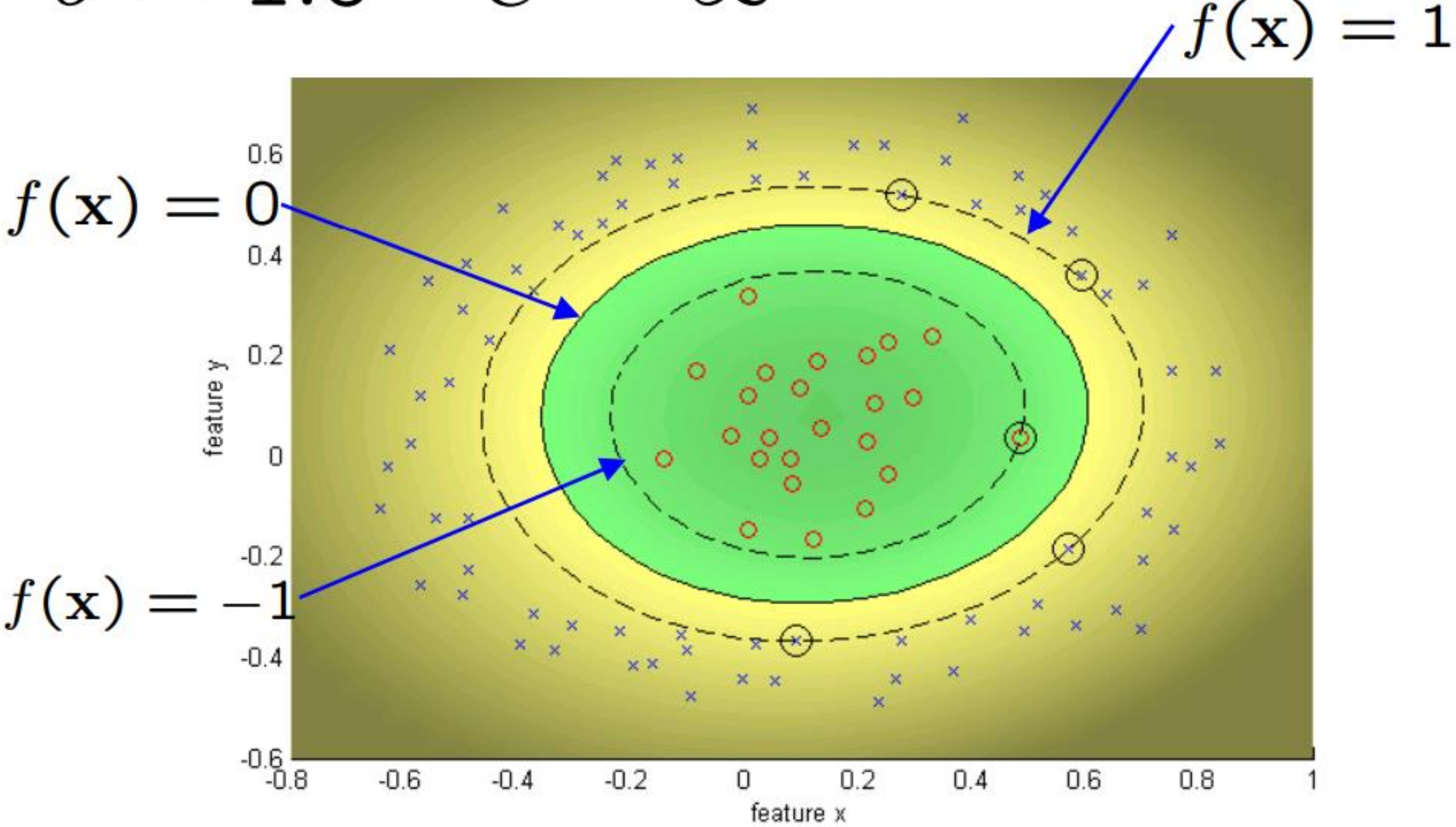
SVMs – RFB Kernel

- Data is not linearly separable in the original feature space



SVMs – RFB Kernel

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

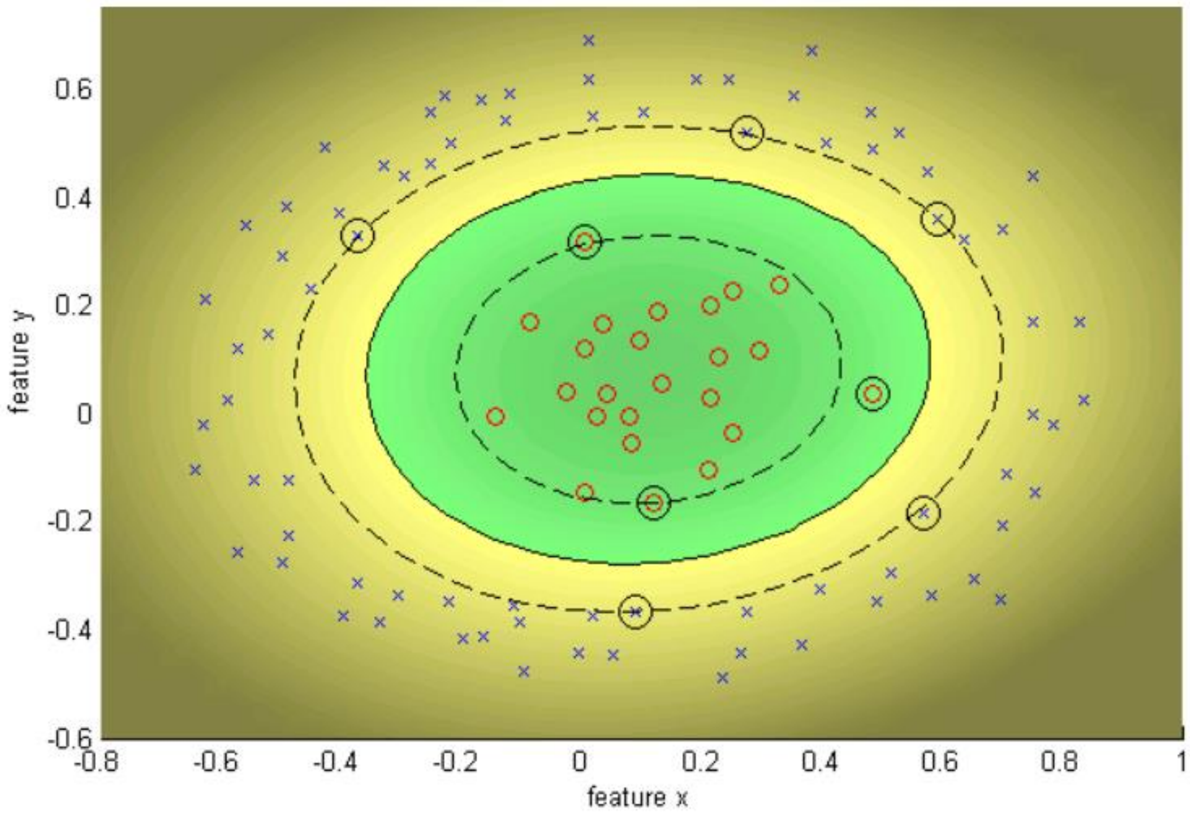


$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

SVMs – RFB Kernel

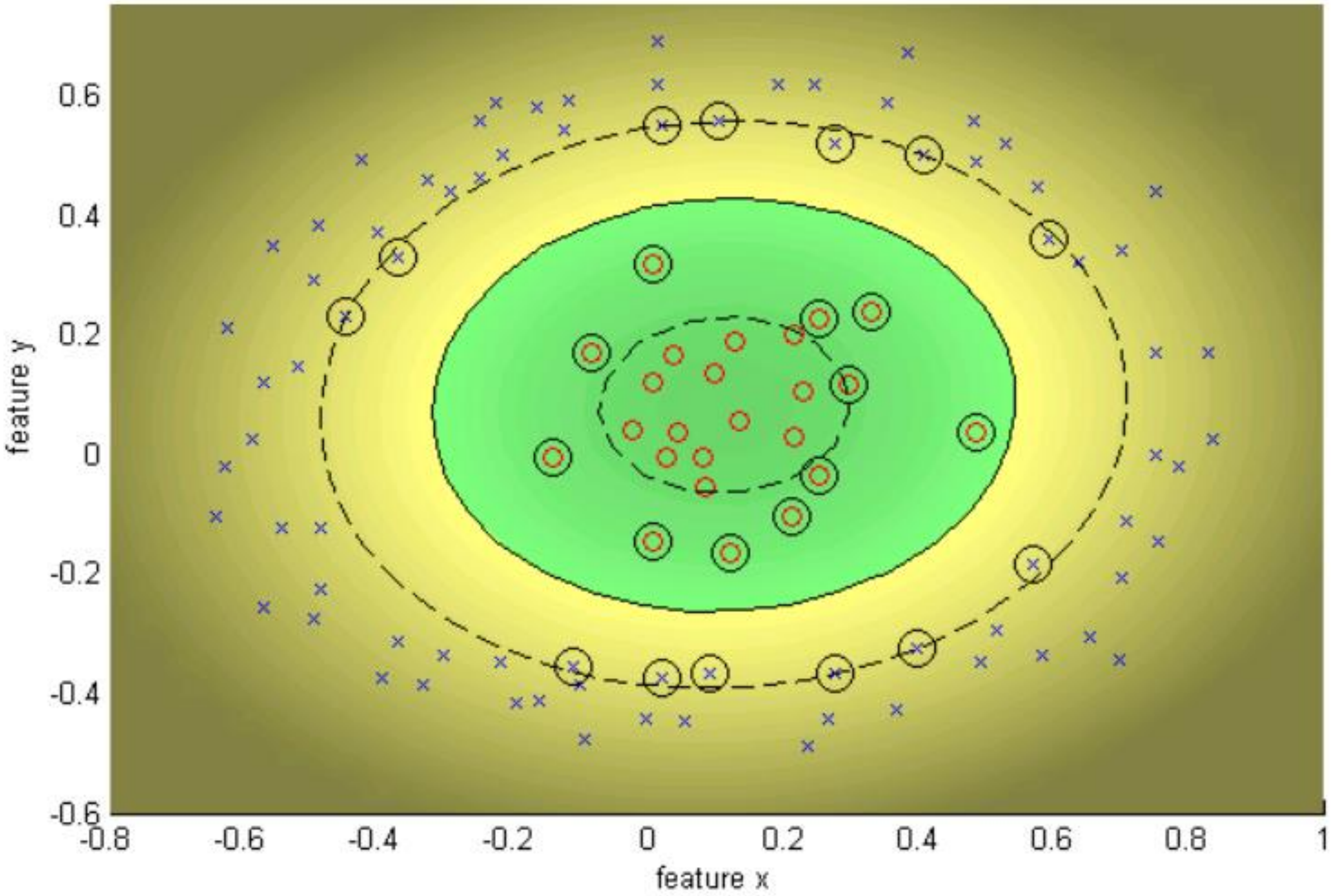
- Decrease C, gives wider (soft) margin.

$$\sigma = 1.0 \quad C = 100$$



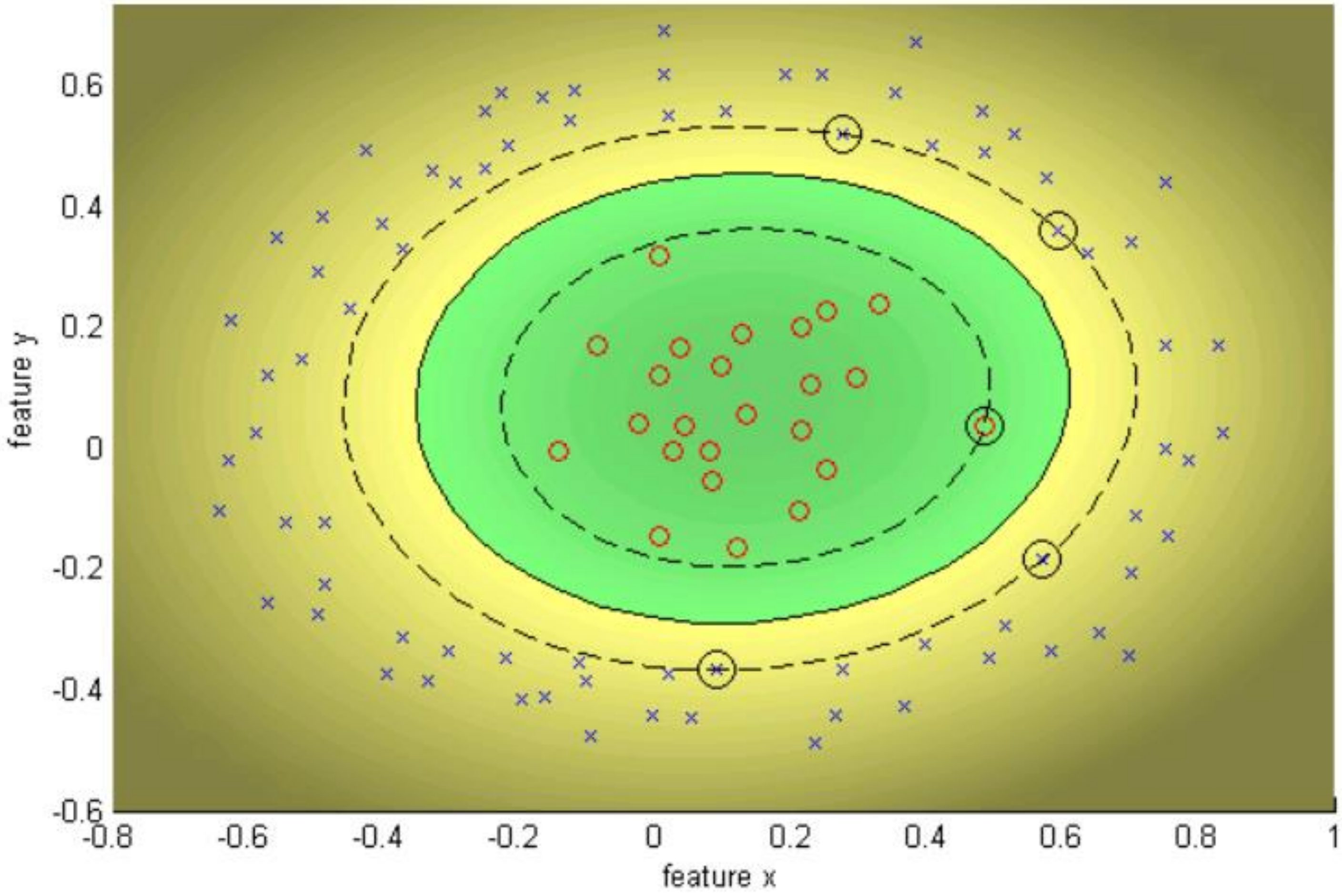
SVMs – RFB Kernel

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



SVMs – RFB Kernel

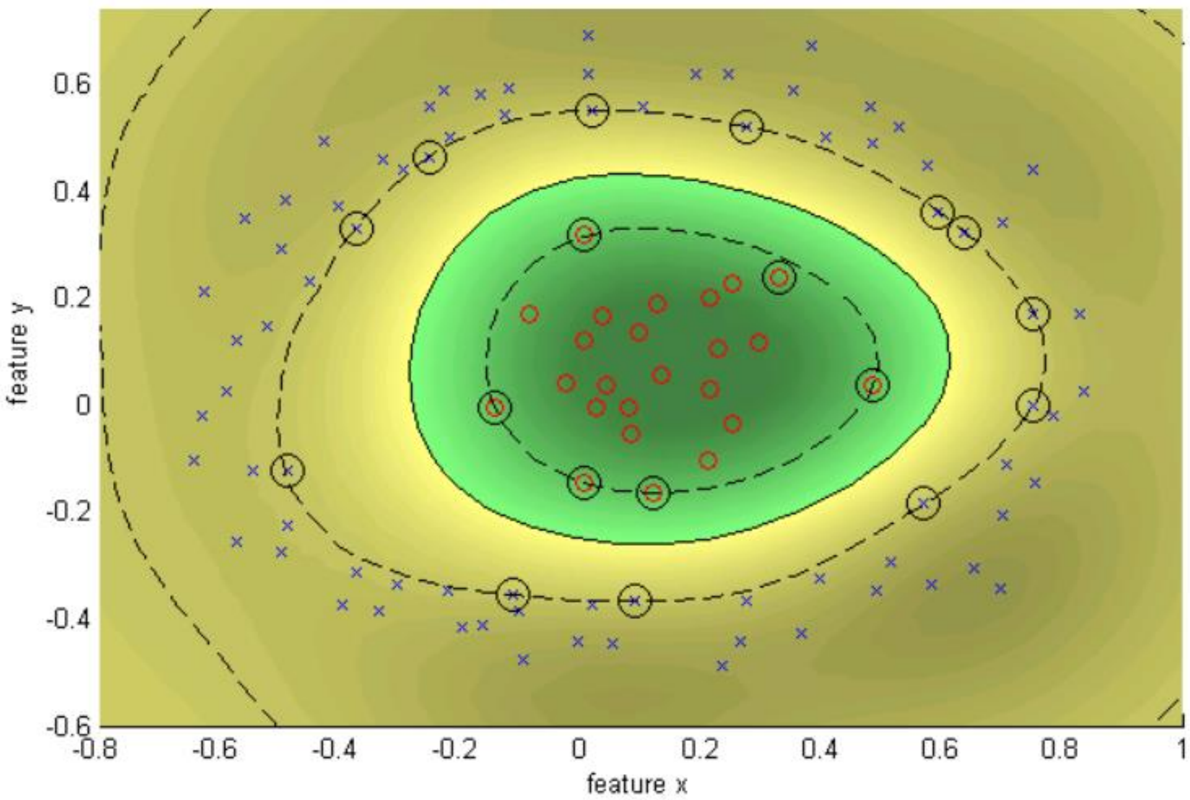
$$\sigma = 1.0 \quad C = \infty$$



SVMs – RFB Kernel

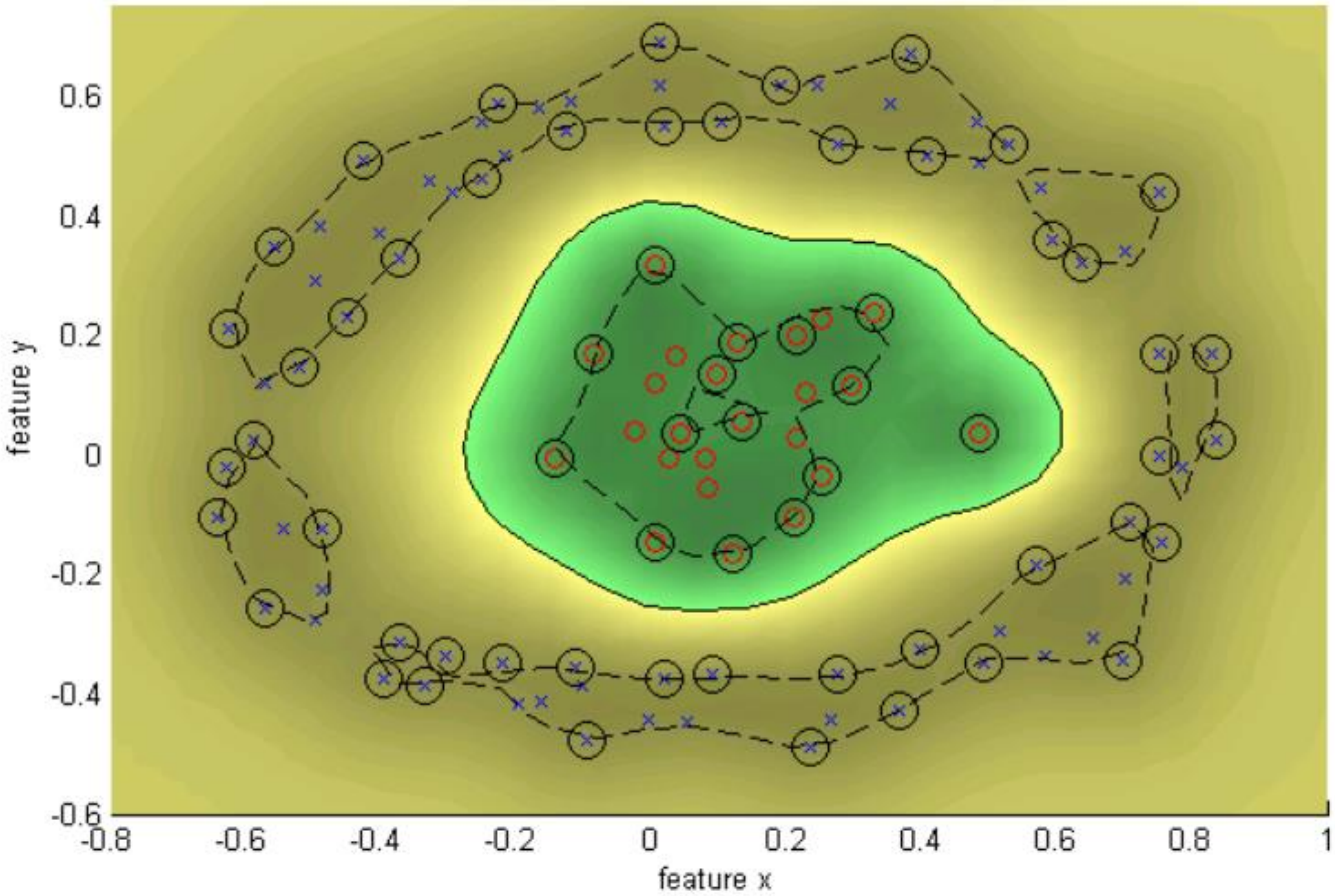
- Decrease sigma, moves towards nearest neighbour classifier

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



SVMs – RFB Kernel

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



Resources

- https://www.youtube.com/watch?v=efR1C6CvhmE

- https://www.youtube.com/watch?v=Toet3EiSFcM

- https://www.youtube.com/watch?v=Qc5IyLW_hns&t=1s