Introduction to Machine Learning CMU-10701

Support Vector Machines

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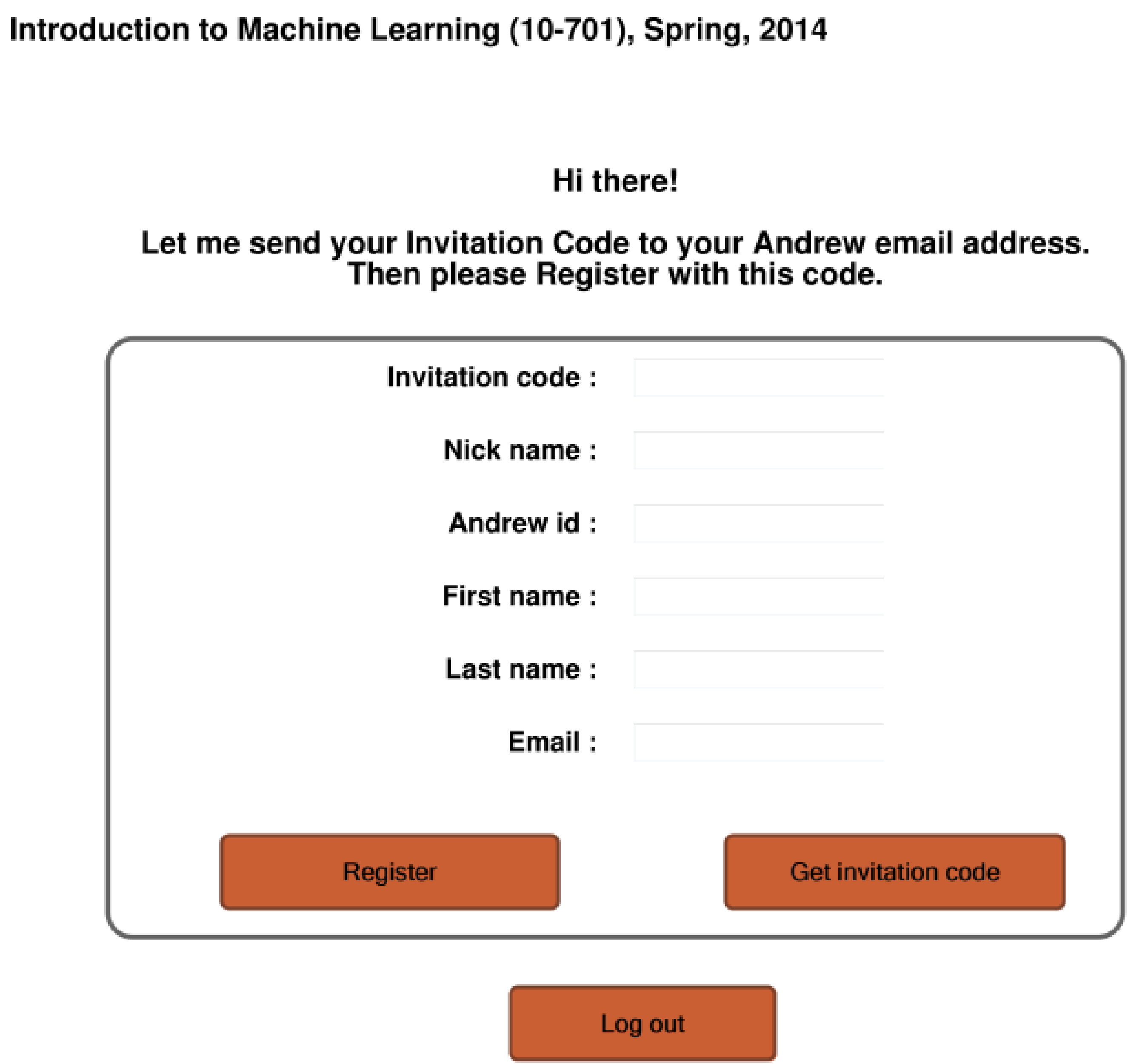
2014 Spring

http://barnabas-cmu-10701.appspot.com/



Introduction to Machine Learning (10-701), Spring, 2014

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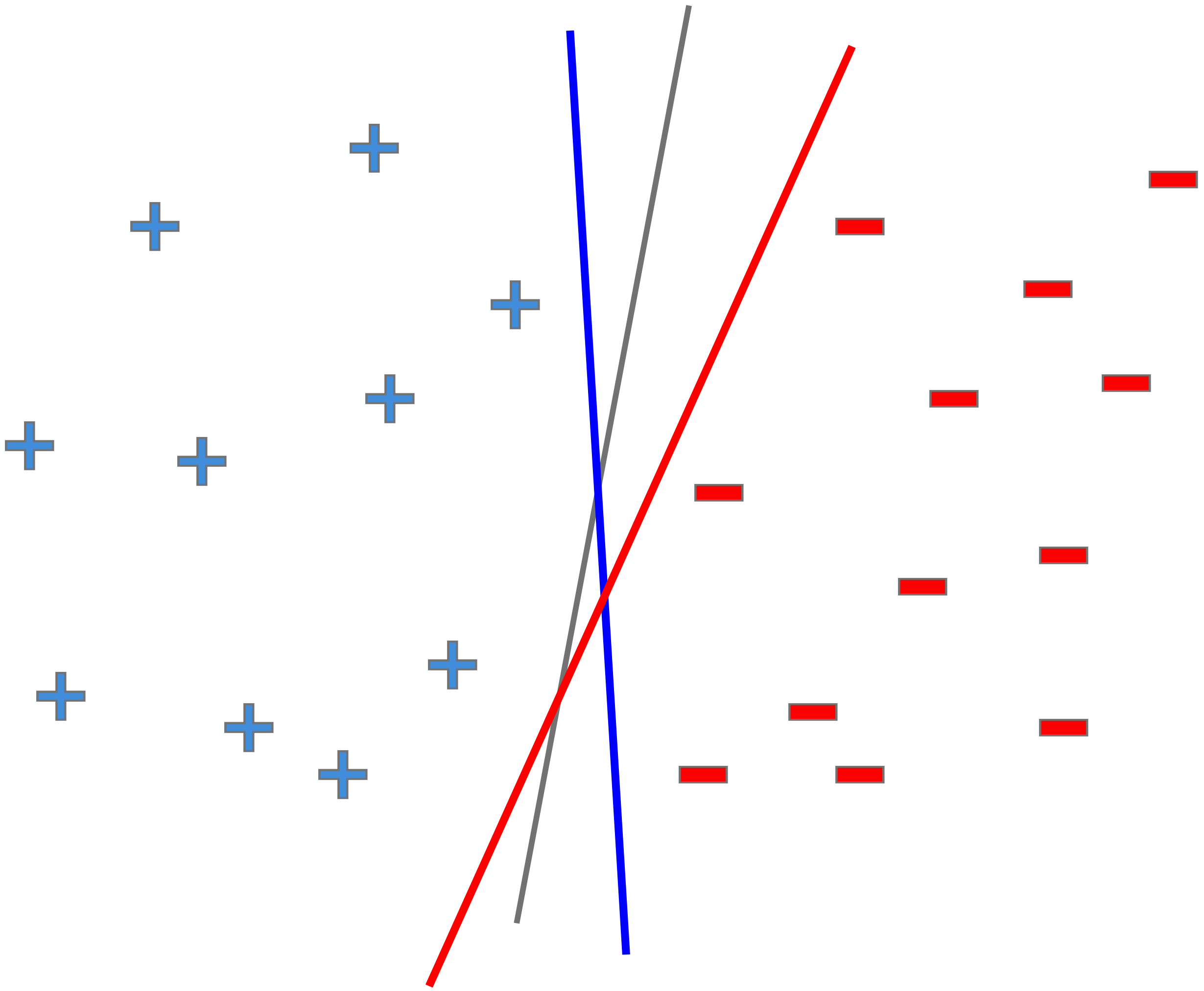
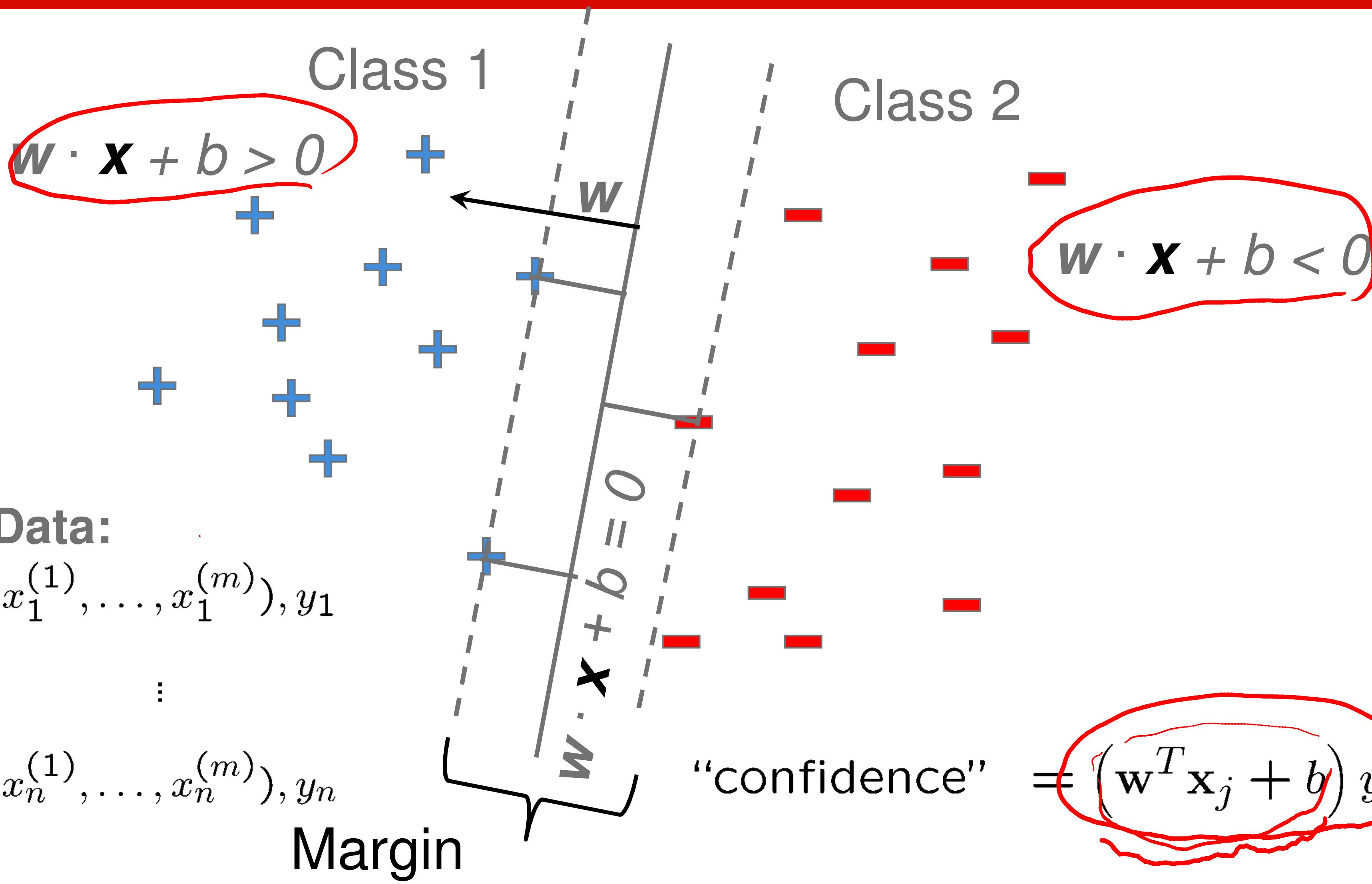
Linear classifiers
which line is better?



Which decision boundary is better?

Pick the one with the largest margin!



Data:

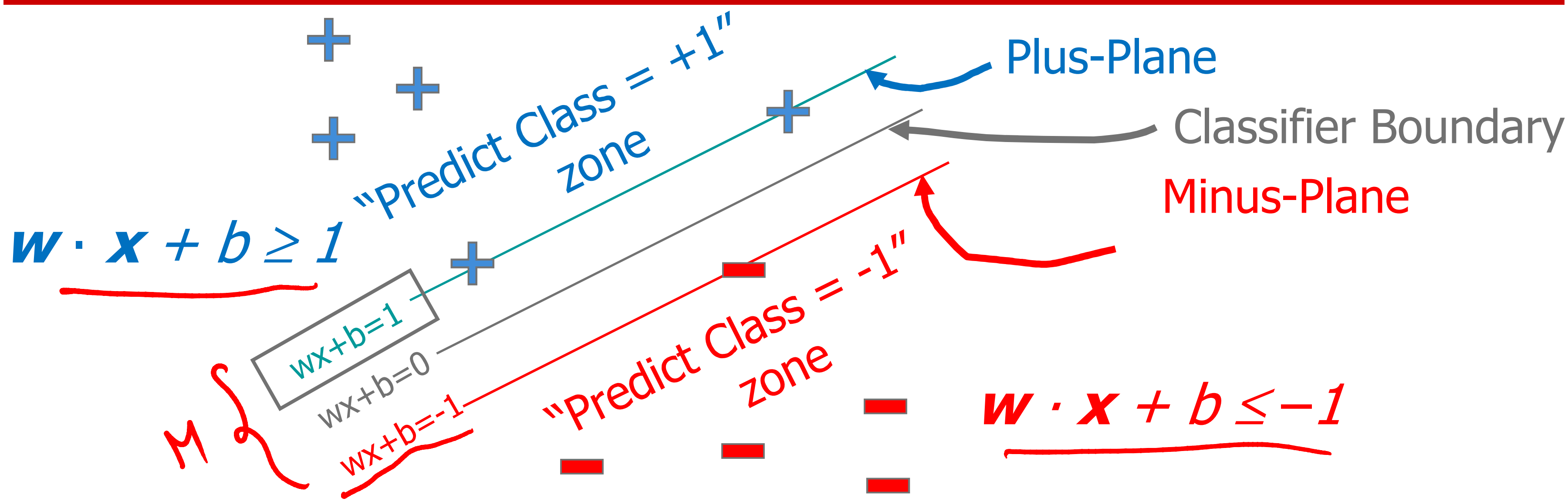
$$(x_1^{(1)}, \ldots, x_1^{(m)}), y_1$$

$$\vdots$$

$$(x_n^{(1)}, \ldots, x_n^{(m)}), y_n$$

"confidence" $= \left(\mathbf{w}^T \mathbf{x}_j + b\right) y_j$

Scaling



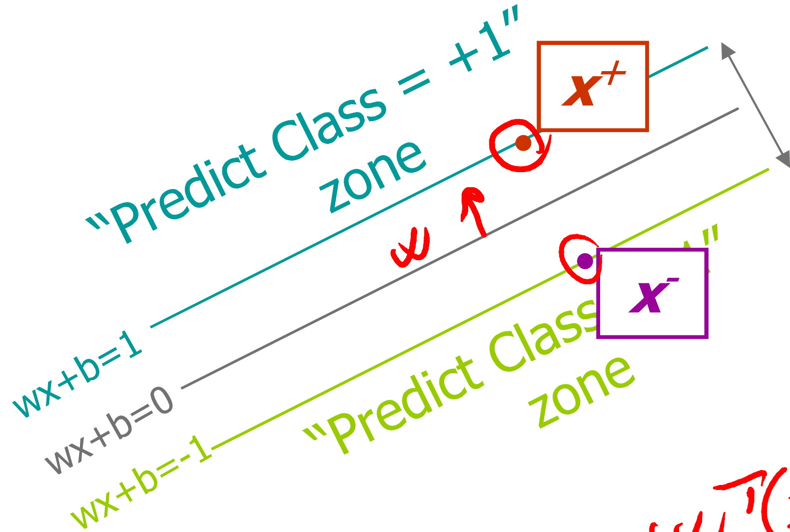
Classification rule:

Classify as..	+1	if	$\boldsymbol{w} \cdot \boldsymbol{x} + b \geq 1$
	−1	if	$\boldsymbol{w} \cdot \boldsymbol{x} + b \leq -1$
	Universe explodes	if	$-1 < \boldsymbol{w} \cdot \boldsymbol{x} + b < 1$

How large is the margin of this classifier?

Goal: Find the maximum margin classifier

Computing the margin width



M = Margin Width $= \dfrac{2}{\sqrt{\mathbf{w}\cdot\mathbf{w}}}$

$$w^T(\underbrace{x^+ - x^-}_{\lambda w}) = 2$$

$$\lambda \cdot w^T w = 2$$

$$\lambda = \frac{2}{w^T w}$$

$$M = |x^+ - x^-| = |\lambda w| = \left|\frac{2w}{w^T w}\right| = \frac{2}{\sqrt{w^T w}}$$

Let $\boldsymbol{x}^+$ and $\boldsymbol{x}^-$ be such that

- $\boldsymbol{w} \cdot \boldsymbol{x}^+ + b = +1$
- $\boldsymbol{w} \cdot \boldsymbol{x}^- + b = -1$
- $\boldsymbol{x}^+ = \boldsymbol{x}^- + \lambda\, \boldsymbol{w}$
- $|\boldsymbol{x}^+ - \boldsymbol{x}^-| = M$

Maximize M ≡ minimize **w·w !**

Observations

We can assume b=0

Classify as..	+1	if	$\boldsymbol{w} \cdot \boldsymbol{x} + b \geq 1$
	-1	if	$\boldsymbol{w} \cdot \boldsymbol{x} + b \leq -1$
	Universe explodes	if	$-1 < \boldsymbol{w} \cdot \boldsymbol{x} + b < 1$

This is the same as $y_i \langle \mathbf{x}_i, \mathbf{w} \rangle \geq 1, \ \forall i = 1, \ldots, n$

The Primal Hard SVM

- Given $D = \{(\mathbf{x}_i, y_i), i = 1, \ldots, n\}$ training data set.
- Assume that D is **linearly separable**.

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w} \in \mathbb{R}^m} \frac{1}{2} ||\mathbf{w}||^2$$

$$\text{subject to } y_i \langle \mathbf{x}_i, \mathbf{w} \rangle \geq 1, \ \forall i = 1, \ldots, n$$

Prediction: $f_{\hat{\mathbf{w}}}(\mathbf{x}) = \text{sign}(\langle \hat{\mathbf{w}}, \mathbf{x} \rangle)$

This is a QP problem (m-dimensional)
(Quadratic cost function, linear constraints)

Quadratic Programming

Find $\underset{w \in \mathbb{R}^n}{\mathrm{ARG\,MIN}}\; w^T H w + w^T q + e$

Subject to

$$A w \leq b$$

$$A \in \mathbb{R}^{n \times m} \quad w \in \mathbb{R}^m \quad b \in \mathbb{R}^n$$

and to $C w = d$

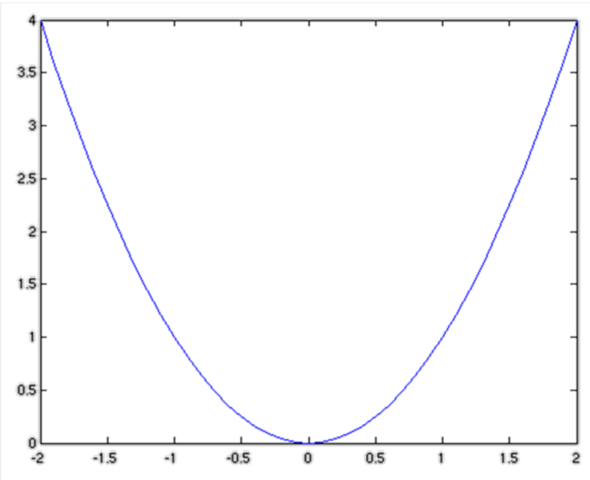
$$C \in \mathbb{R}^{s \times m} \quad d \in \mathbb{R}^s$$

Efficient Algorithms exist for QP.
They often solve the dual problem instead of the primal.

Constrained Optimization

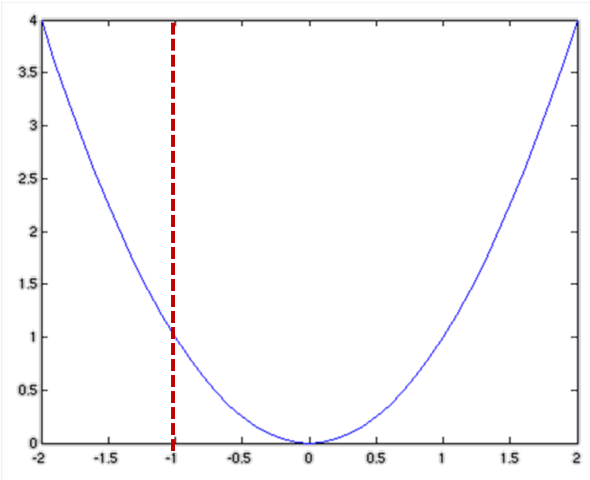
$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq b$$

$$\min_x \; x^2$$



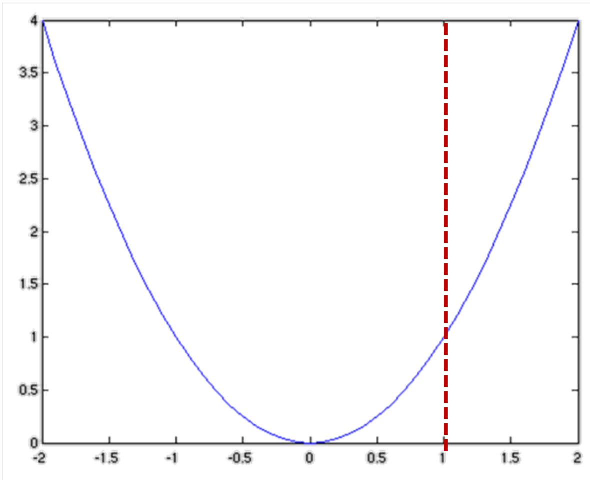
$$x^* = 0$$

$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq -1$$



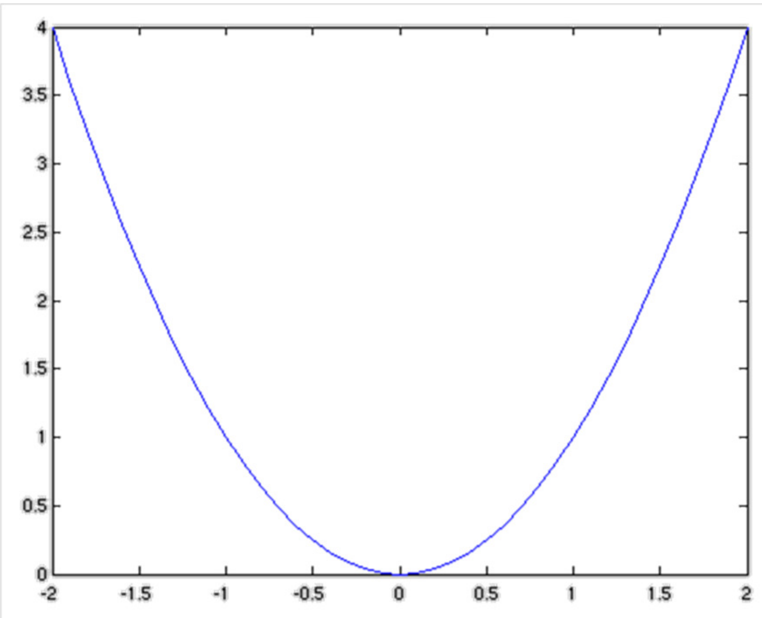
$$x^* = 0$$

$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq 1$$



$$x^* = 1$$

Lagrange Multiplier



$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq b$$

$x - b \geq 0$

Moving the constraint to objective function

Lagrangian:

$$L(x, \alpha) = x^2 - \alpha(x - b)$$
$$\text{s.t.} \quad \alpha \geq 0$$

Solve:

$$\min_x \max_\alpha \; L(x, \alpha)$$
$$\text{s.t.} \quad \alpha \geq 0$$

x^*, α^*

Constraint is active when α > 0

Lagrange Multiplier – Dual Variables

Solving:

$$\begin{cases} \min_x \max_\alpha \ \overbrace{x^2 - \alpha(x-b)}^{L(x,\alpha)} \\ \text{s.t.} \quad \alpha \geq 0 \end{cases}$$

$$\frac{\partial L}{\partial x} = 0 \ \Rightarrow x^* = \frac{\alpha}{2}$$

$$\frac{\partial L}{\partial \alpha} = 0 \ \Rightarrow \alpha^* = \max(2b, 0)$$

$$\frac{\partial L(x,\alpha)}{\partial x} = 2x - \alpha = 0$$

$$x^* = \boxed{\frac{\alpha}{2}}$$

$$L(x^*,\alpha) = \underbrace{\frac{\alpha^2}{4} - \alpha\left(\frac{\alpha}{2} - b\right)}_{-\frac{\alpha^2}{4} + \alpha b}$$

$$\frac{\partial L(x^*,\alpha)}{\partial \alpha} = -\frac{\alpha}{2} + b = 0 \Rightarrow \alpha^* = 2b$$

$$x^* = \mathrm{MAX}(b,0) \qquad \alpha^* = \mathrm{MAX}(2b,0)$$

When α > 0, constraint is tight

From Primal to Dual

Primal problem:

$$\hat{\mathbf{w}} = \text{arg} \min_{\mathbf{w} \in \mathbb{R}^m} \frac{1}{2} \|\mathbf{w}\|^2$$

$$\text{subject to } y_i \langle \mathbf{x}_i, \mathbf{w} \rangle \geq 1, \ \forall i = 1, \dots, n$$

Lagrange function:

$$\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)^T \geq 0 \text{ Lagrange multipliers}$$

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \big(y_i \langle \mathbf{x}_i, \mathbf{w} \rangle - 1 \big)$$

The Lagrange Problem

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \Big(y_i \langle \mathbf{x}_i, \mathbf{w} \rangle - 1 \Big)$$

The Lagrange problem:

$$(\hat{\mathbf{w}}, \hat{\boldsymbol{\alpha}}) = \arg \min_{\mathbf{w} \in \mathbb{R}^m} \max_{0 \leq \boldsymbol{\alpha} \in \mathbb{R}^n} L(\mathbf{w}, \boldsymbol{\alpha})$$

$$0 = \left. \frac{\partial L(\mathbf{w}, \boldsymbol{\alpha})}{\partial \mathbf{w}} \right|_{\mathbf{w} = \hat{\mathbf{w}}} = \hat{\mathbf{w}} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

$$\boxed{\Rightarrow \hat{\mathbf{w}} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i}$$

The Dual Problem

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \Big(y_i \langle \mathbf{x}_i, \mathbf{w} \rangle - 1 \Big)$$

$$\boxed{\Rightarrow \hat{\mathbf{w}} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i}$$

$$\Rightarrow L(\hat{\mathbf{w}}, \boldsymbol{\alpha}) = \frac{1}{2}\|\hat{\mathbf{w}}\|^2 - \sum_{i=1}^{n} \alpha_i \Big(y_i \langle \mathbf{x}_i, \hat{\mathbf{w}} \rangle - 1 \Big)$$

$$= \underbrace{\frac{1}{2} \| \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \|^2}_{\boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}} + \boldsymbol{\alpha}^T \mathbf{1}_n - \underbrace{\sum_{i=1}^{n} \alpha_i y_i \langle \mathbf{x}_i, \sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j \rangle}_{\boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}}$$

$$\boxed{= \boldsymbol{\alpha}^T \mathbf{1}_n - \frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}}$$

$$\boldsymbol{Y} \doteq diag(y_1, \ldots, y_n), \;\; y_i \in \{-1, 1\}^n$$

$\boldsymbol{G} \in \mathbb{R}^{n \times n} \doteq \{G_{ij}\}_{i,j}^{n,n}$, where $G_{ij} \doteq \langle \mathbf{x}_i, \mathbf{x}_j \rangle$ Gram matrix.

The Dual Hard SVM

$$\boldsymbol{Y} \doteq diag(y_1, \ldots, y_n), \; y_i \in \{-1, 1\}^n$$

$\boldsymbol{G} \in \mathbb{R}^{n \times n} \doteq \{G_{ij}\}_{i,j}^{n,n}$, where $G_{ij} \doteq \langle \mathbf{x}_i, \mathbf{x}_j \rangle$ Gram matrix.

$$\hat{\boldsymbol{\alpha}} = \underset{\boldsymbol{\alpha} \in \mathbb{R}^n}{\arg\max}\, \boldsymbol{\alpha}^T \mathbf{1}_n - \frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}$$

subject to $\alpha_i \geq 0, \; \forall i = 1, \ldots, n$

Quadratic Programming (n-dimensional)

Lemma $\hat{\mathrm{w}} = \sum_{i=1}^{n} \hat{\alpha}_i y_i \mathbf{x}_i$

Prediction: $f_{\hat{\mathrm{w}}}(x) = \mathrm{sign}(\langle \hat{\mathrm{w}}, \mathbf{x} \rangle) = \mathrm{sign}(\sum_{i=1}^{n} \hat{\alpha}_i y_i \underbrace{\langle \mathbf{x}_i, \mathbf{x} \rangle}_{k(\mathbf{x}_i, \mathbf{x})})$

The Problem with Hard SVM

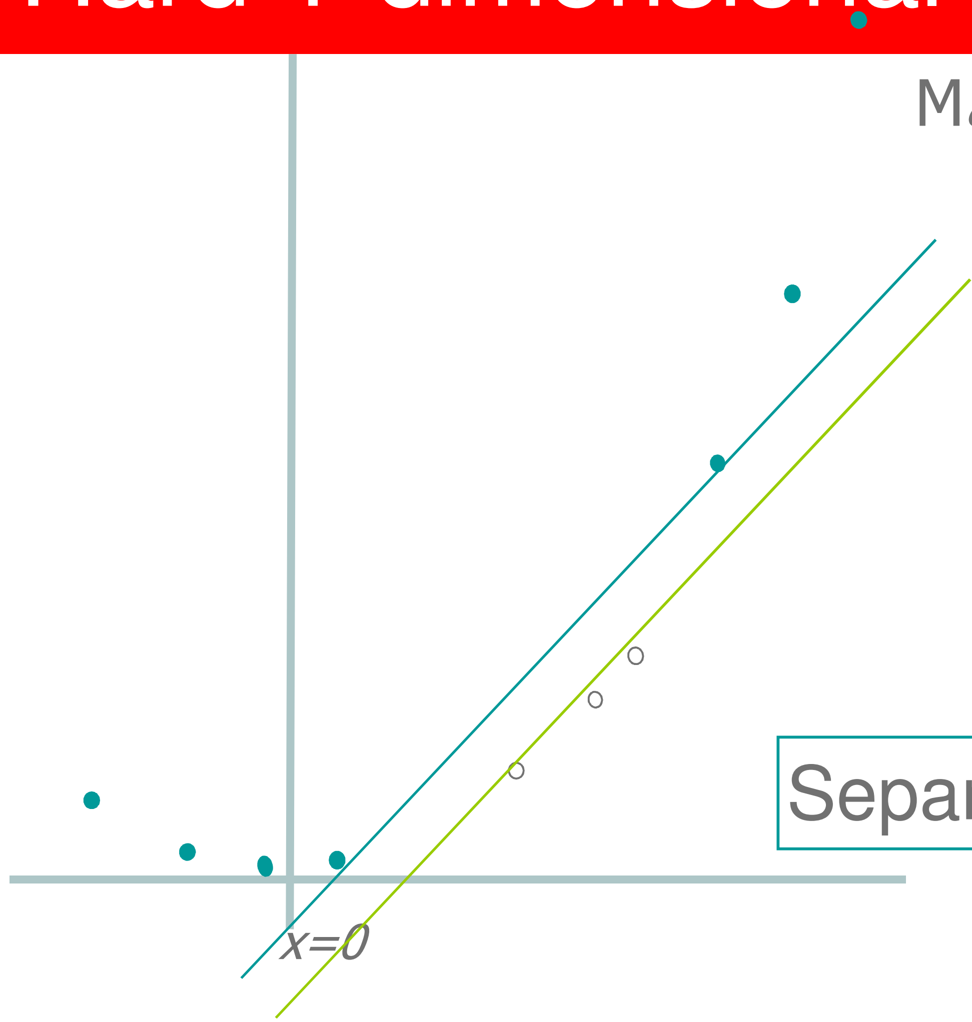
It assumes samples are linearly separable...

What can we do if data is not linearly separable???

Hard 1-dimensional Dataset

If the data set is **not** linearly separable, then adding new features (mapping the data to a larger feature space) the data might become linearly separable

Hard 1-dimensional Dataset



Make up a new feature!

Sort of…
… computed from original feature(s)

$$\mathbf{z}_k = (x_k, x_k^2)$$

Separable! MAGIC!

Now drop this "augmented" data into our linear SVM.

Feature mapping

- ❑ *n* general! points in an *n-1* dimensional space is always linearly separable by a hyperspace!
  $\Rightarrow$ it is good to map the data to high dimensional spaces

- ❑ Having *n* training data, is it always good enough to map the data into a feature space with dimension *n-1*?

  - *Nope... We have to think about the test data as well! Even if we don't know how many test data we have and what they are...*

- ❑ *We might want to map our data to a huge (∞) dimensional feature space*

- ❑ *Overfitting? Generalization error?... We don't care now...*

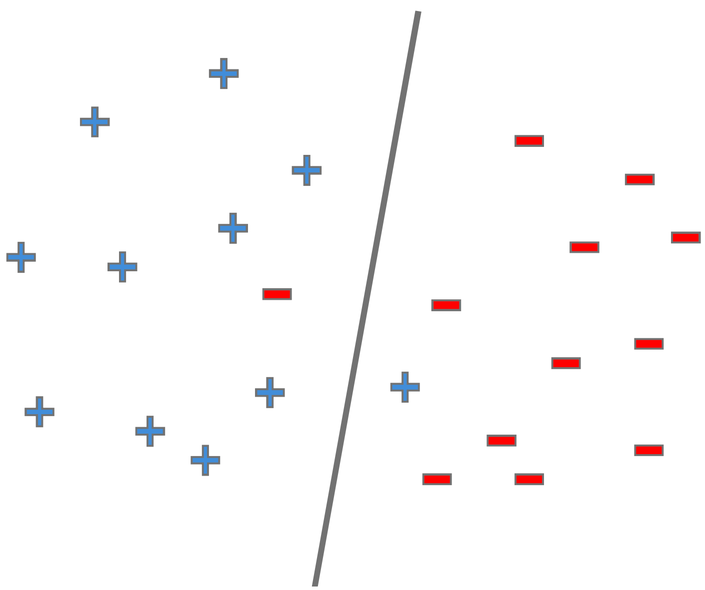
How to do feature mapping?

Let us have n training objects: $\vec{x}_i = [\vec{x}_{i,1}, \vec{x}_{i,2}] \in \mathbb{R}^2$, $i = 1, \ldots, n$

The possible test objects are denoted by $\vec{x} = [\vec{x}_1, \vec{x}_2] \in \mathbb{R}^2$

Use features of features of features of features….

$$\text{Let } \phi(\vec{x}) \doteq \underbrace{[sin(\vec{x}_2), \exp(\vec{x}_2 + \vec{x}_1), \vec{x}_1, \vec{x}_2^{\tan(\vec{x}_1)}, \ldots]}_{\infty}$$



The Problem with Hard SVM

It assumes samples are linearly separable...

Solutions:

1. Use feature transformation to a larger space

   $\Rightarrow$ each training samples are linearly separable in the feature space

   $\Rightarrow$ Hard SVM can be applied ☺

   $\Rightarrow$ overfitting... ☹

2. **Soft margin** SVM instead of Hard SVM

   - We will discuss this now

Hard SVM

The Hard SVM problem can be rewritten:

$$\hat{\mathbf{w}}_{hard} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to } y_i\langle\mathbf{x}_i, \mathbf{w}\rangle > 0, \; \forall i = 1, \ldots, n$$

$$\Downarrow$$

$$\boxed{\hat{\mathbf{w}}_{hard} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} l_{0-\infty}(\langle\mathbf{x}_i, \mathbf{w}\rangle, y_i) + \frac{\lambda}{2}\|\mathbf{w}\|^2}$$

where

$$l_{0-\infty}(a, b) \doteq \begin{cases} \infty : ab < 0 & \text{Misclassification} \\ 0 : ab > 0 & \text{Correct classification} \end{cases}$$

From Hard to Soft constraints

Instead of using hard constraints (points are linearly separable)

$$\hat{\mathbf{w}}_{hard} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} l_{0-\infty}(\langle \mathbf{x}_i, \mathbf{w}\rangle, y_i) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

We can try to solve the soft version of it:

Your loss is only 1 instead of ∞ if you misclassify an instance

$$\hat{\mathbf{w}}_{soft} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} l_{0-1}(\langle \mathbf{x}_i, \mathbf{w}\rangle, y_i) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

where

$$l_{0-1}(y, f(\mathbf{x})) = \begin{cases} 1 : y\underbrace{f(\mathbf{x})}_{x^T w} < 0 & \text{Misclassification} \\ 0 : yf(\mathbf{x}) > 0 & \text{Correct classification} \end{cases}$$

Problems with l_{0-1} loss

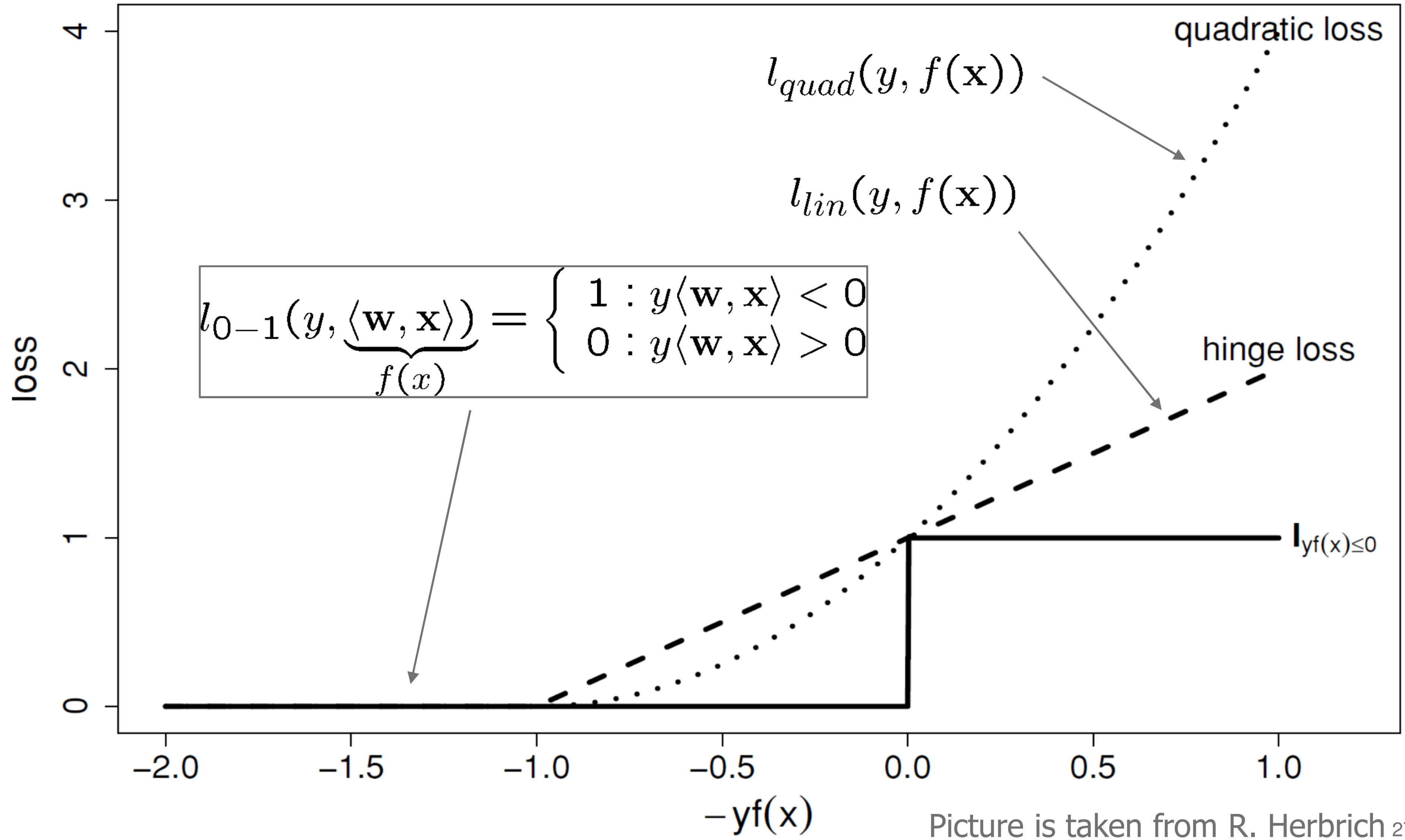
$$\hat{\mathbf{w}}_{soft} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} l_{0-1}(\langle \mathbf{x}_i, \mathbf{w}\rangle, y_i) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

$$l_{0-1}(y, f(\mathbf{x})) = \begin{cases} 1 : yf(\mathbf{x}) < 0 \\ 0 : yf(\mathbf{x}) > 0 \end{cases}$$

It is not convex in $yf(\mathbf{x})$ $\Rightarrow$ It is not convex in **w**, either...
... and we like only convex functions...

Let us approximate it with convex functions!

Approximation of the Heaviside step function



Picture is taken from R. Herbrich

Approximations of $l_{0\text{-}1}$ loss

- Piecewise linear approximations (hinge loss, l_{lin})

$$l_{lin}(f(\mathbf{x}), y) = \max\{1 - yf(\mathbf{x}), 0)\}$$

[We want $yf(\mathbf{x}) > 1$]

- Quadratic approximation (l_{quad})

$$l_{quad}(f(\mathbf{x}), y) = \max\{1 - yf(\mathbf{x}), 0)\}^2$$

The hinge loss approximation of $l_{0\text{-}1}$

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} \underbrace{l_{lin}(\langle \mathbf{x}_i, \mathbf{w}\rangle, y_i)}_{\xi_i \geq 0} + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

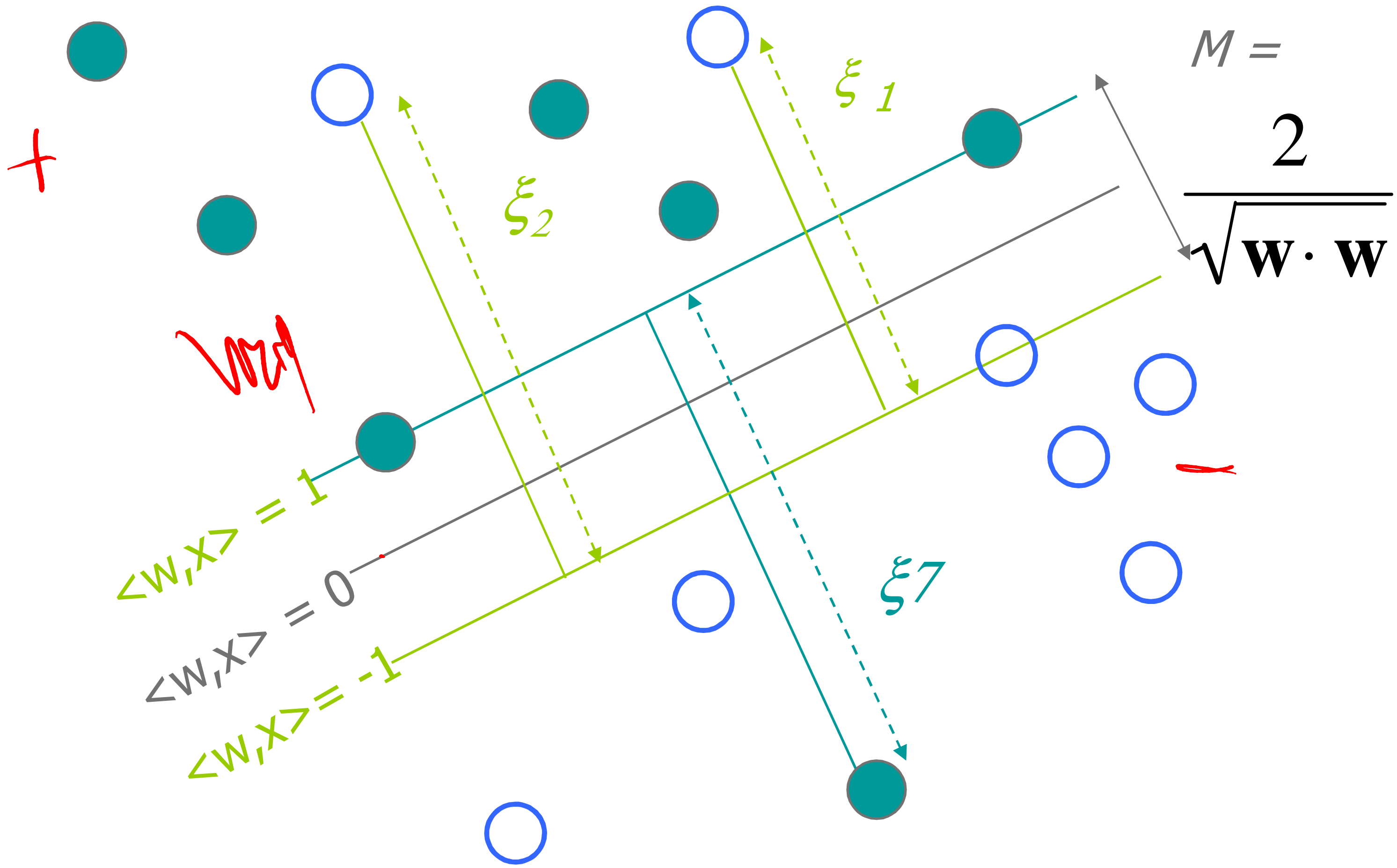
Where,

$$\xi_i \doteq l_{lin}(f(\mathbf{x}_i), y_i) = \max\{1 - y_i f(\mathbf{x}_i), 0)\}$$

$$\geq 1 - y_i \underbrace{\langle \mathbf{w}, \mathbf{x}_i \rangle}_{f(\mathbf{x}_i)} \geq l_{0-1}(y_i, f(\mathbf{x}_i))$$

The hinge loss upper bounds the 0-1 loss

Geometric interpretation: Slack Variables



$$\xi_i \doteq l_{lin}(f(\mathbf{x}_i), y_i) = \max\{1 - y_i f(\mathbf{x}_i), 0)\}$$
$$= \max\{1 - y_i(\mathbf{w}^T\mathbf{x}_i), 0\}$$

The Primal Soft SVM problem

$$\hat{\mathbf{w}}_{soft} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} \underbrace{l_{lin}(\langle \mathbf{x}_i, \mathbf{w}\rangle, y_i)}_{\xi_i \geq 0} + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

where

$$\xi_i \doteq l_{lin}(f(\mathbf{x}_i), y_i) = \max\{1 - y_i(\mathbf{w}^T\mathbf{x}_i), 0\}$$

Equivalently,

$$\hat{\mathbf{w}}_{soft} = \arg\min_{\mathbf{w}\in\mathbb{R}^m, \boldsymbol{\xi}\in\mathbb{R}^n} \sum_{i=1}^{n} \xi_i + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

$$\text{subject to } y_i\langle \mathbf{x}_i, \mathbf{w}\rangle \geq 1 - \xi_i,\ \forall i = 1, \ldots, n$$

$$\xi_i \geq 0,\ \forall i = 1, \ldots, n$$

ξ_i: Slack variables

The Primal Soft SVM problem

$$\hat{\mathbf{w}}_{soft} = \arg \min_{\mathbf{w}\in\mathbb{R}^m, \boldsymbol{\xi}\in\mathbb{R}^n} \sum_{i=1}^{n} \xi_i + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

$$\text{subject to } y_i\langle \mathbf{x}_i, \mathbf{w}\rangle \geq 1 - \xi_i, \ \forall i = 1, \ldots, n$$

$$\xi_i \geq 0, \ \forall i = 1, \ldots, n$$

Equivalently,

We can use this form, too.:

$$\hat{\mathbf{w}}_{soft} = \arg \min_{\mathbf{w}\in\mathbb{R}^m, \boldsymbol{\xi}\in\mathbb{R}^n} C \underbrace{\sum_{i=1}^{n} \xi_i}_{\boldsymbol{\xi}^T \mathbf{1}_n} + \frac{1}{2}\|\mathbf{w}\|^2$$

where $C = \frac{1}{\lambda}$

What is the dual form of primal soft SVM?

The Dual Soft SVM (using hinge loss)

$$\hat{\mathbf{w}}_{soft} = \arg \min_{\mathbf{w}\in\mathbb{R}^m, \boldsymbol{\xi}\in\mathbb{R}^n} C\sum_{i=1}^{n}\xi_i + \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to } y_i\langle \mathbf{x}_i, \mathbf{w}\rangle \geq 1 - \xi_i, \ \forall i = 1,\dots,n \qquad \alpha_i$$

$$\xi_i \geq 0, \ \forall i = 1,\dots,n \qquad \beta_i$$

- $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)^T \geq 0$ Largrange multipliers
- $\boldsymbol{\beta} = (\beta_1, \dots, \beta_n)^T \geq 0$ Largrange multipliers

$$(\hat{\mathbf{w}}, \hat{\boldsymbol{\xi}}, \hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}) = \arg \min_{\substack{\mathbf{w}\in\mathbb{R}^m \\ \boldsymbol{\xi}\in\mathbb{R}^n}} \max_{\substack{0\leq\boldsymbol{\alpha} \\ 0\leq\boldsymbol{\beta}}} L(\mathbf{w}, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

where

$$L(\mathbf{w}, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i\Big(y_i\langle \mathbf{x}_i, \mathbf{w}\rangle - 1 + \xi_i\Big) - \sum_{i=1}^{n}\beta_i\xi_i$$

The Dual Soft SVM (using hinge loss)

$$L(\mathbf{w},\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\boldsymbol{\xi}^T\mathbf{1}_n - \sum_{i=1}^{n}\alpha_i y_i\langle \mathbf{x}_i,\mathbf{w}\rangle + \boldsymbol{\alpha}^T\mathbf{1}_n - \boldsymbol{\xi}^T(\boldsymbol{\alpha}+\boldsymbol{\beta})$$

MIN MAX
w, ξ α, β ≥ 0

$$0 = \left.\frac{\partial L(\mathbf{w},\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\beta})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\hat{\mathbf{w}}} = \hat{\mathbf{w}} - \sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i \Rightarrow \boxed{\hat{\mathbf{w}} = \sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i}$$

$$0 = \left.\frac{\partial L(\mathbf{w},\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\beta})}{\partial \boldsymbol{\xi}}\right|_{\boldsymbol{\xi}=\hat{\boldsymbol{\xi}}} = C\mathbf{1}_n - \boldsymbol{\alpha} - \boldsymbol{\beta} \Rightarrow \boldsymbol{\beta} = C\mathbf{1}_n - \boldsymbol{\alpha} \geq 0$$

$$\boxed{\Rightarrow 0 \leq \boldsymbol{\alpha} \leq C}$$

$$\Rightarrow (\hat{\boldsymbol{\alpha}},\hat{\boldsymbol{\beta}}) = \arg \max_{\substack{0 \leq \boldsymbol{\alpha} \leq C \\ 0 \leq \boldsymbol{\beta}}} L(\hat{\mathbf{w}},\hat{\boldsymbol{\xi}},\boldsymbol{\alpha},\boldsymbol{\beta})$$

$$\boxed{\Rightarrow \hat{\boldsymbol{\alpha}} = \arg \max_{0 \leq \boldsymbol{\alpha} \leq C} \boldsymbol{\alpha}^T\mathbf{1}_m - \tfrac{1}{2}\boldsymbol{\alpha}^T \boldsymbol{YGY}\boldsymbol{\alpha}}$$

$$Y = \begin{pmatrix} y_1 & & 0 \\ & \ddots & \\ 0 & & y_n \end{pmatrix}$$

$$G_{ij} = \langle x_i, x_j \rangle$$

The Dual Soft SVM (using hinge loss)

$\boldsymbol{Y} \doteq diag(y_1, \ldots, y_n) \in \{-1, 1\}^n$ $\quad x_i \Rightarrow \phi(x_i) \quad \langle a, b \rangle = a^T b$

$\boldsymbol{G} \in \mathbb{R}^{n \times n} \doteq \{G_{ij}\}_{i,j}^{n,n}$, where $G_{ij} \doteq \overbrace{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}^{k(\mathbf{x}_i, \mathbf{x}_j)}$, Gram matrix.

$k_{ij} = \exp\left(-\frac{\|x_i - x_j\|^2}{\sigma^2}\right)$ $\quad \langle \phi(x_i), \phi(x_j) \rangle = k(x_i, x_j)$

$$\hat{\boldsymbol{\alpha}} = \arg\max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \boldsymbol{\alpha}^T \mathbf{1}_n - \frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}$$

subject to $0 \leq \alpha_i \leq C$

where $C = \frac{1}{\lambda}$

$\boxed{\text{If } \lambda \to \mathbf{0} \Rightarrow \text{soft-SVM} \to \text{hard-SVM}}$

This is the same as the dual hard-SVM problem, but now we have the additional $0 \leq \alpha_i \leq C$ constraints.

SVM classification in the dual space

Solve the dual problem

$$\hat{\boldsymbol{\alpha}} = \underset{\boldsymbol{\alpha}\in\mathbb{R}^n}{\text{arg max}}\ \boldsymbol{\alpha}^T \mathbf{1}_n - \frac{1}{2}\boldsymbol{\alpha}^T \boldsymbol{YGY}\boldsymbol{\alpha}$$

$$\text{subject to } 0 \leq \alpha_i \leq C \quad \forall i$$

where $C = \frac{1}{\lambda}$. Let $\hat{\mathbf{w}} = \sum_{i=1}^{n} \hat{\alpha}_i y_i \mathbf{x}_i$.

$k(x_i, x)$

$\langle \varphi(x_i), \varphi(x) \rangle$

On test data $\mathbf{x}$**:** $f_{\hat{\mathbf{w}}}(\mathbf{x}) = \langle \hat{\mathbf{w}}, \mathbf{x} \rangle = \sum_{i=1}^{n} \hat{\alpha}_i y_i \underbrace{\langle \mathbf{x}_i, \mathbf{x} \rangle}_{k(\mathbf{x}_i, \mathbf{x})}$

Why is it called Support Vector Machine?

$\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^T \geq 0$ Lagrange multipliers

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \underbrace{\left(y_i \langle \mathbf{x}_i, \mathbf{w} \rangle - 1\right)}_{0}$$

KKT conditions

COMPLEMENTARY SLACKNESS CONDITION

$\alpha_i > 0 \Rightarrow y_i \langle x_i, w \rangle = 1$

$\langle x_i, w \rangle = \begin{matrix} +1 \\ -1 \end{matrix}$

EITHER $\alpha_i = 0$ OR $\underbrace{(y_i \langle x_i, w \rangle - 1) = 0}$ AND $\alpha_i > 0$

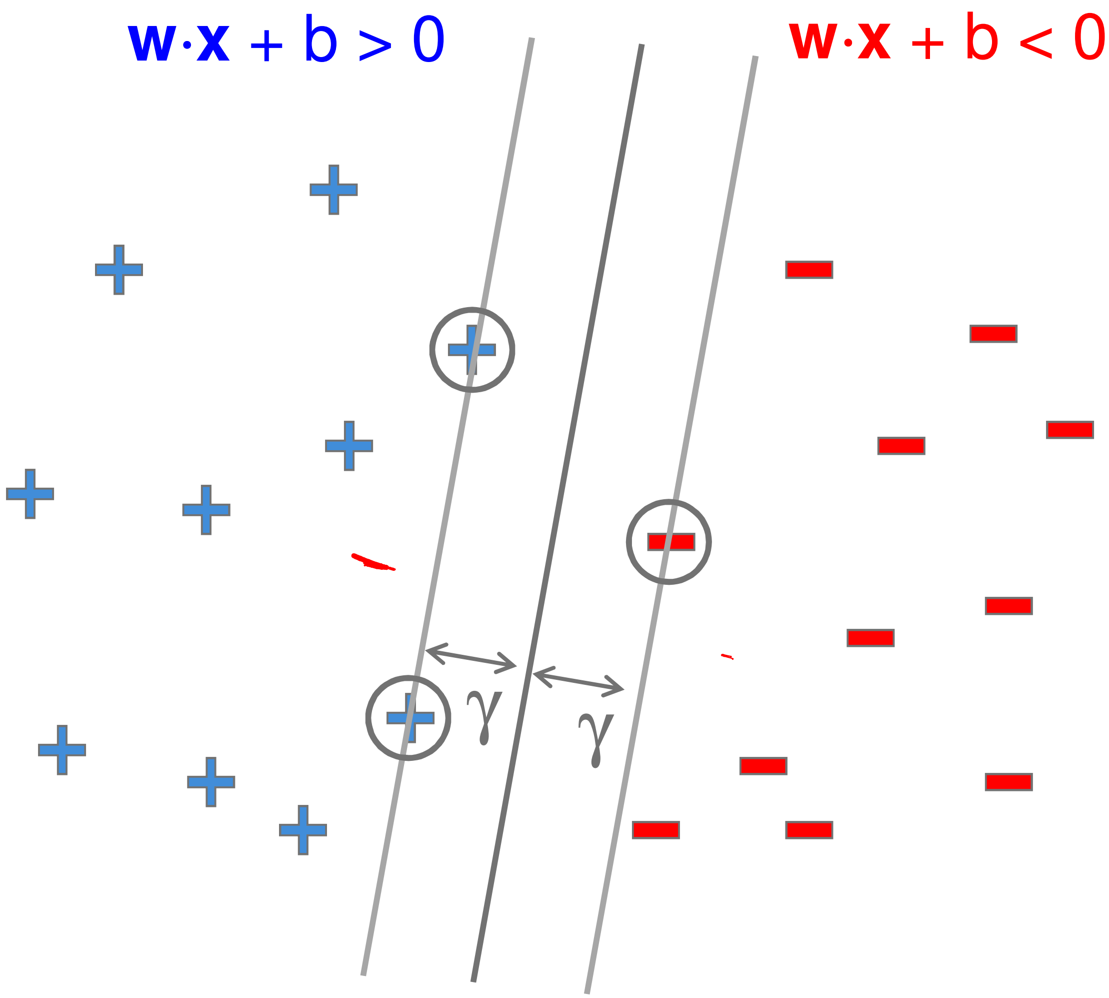
$(y_i \langle x_i, w \rangle - 1) \neq 0$

$\Downarrow$

x_i IS ON THE MARGIN LINES

SUPPORT VECTORS

Why is it called Support Vector Machine?



Hard SVM:

Linear hyperplane defined by "support vectors"

Moving other points a little doesn't effect the decision boundary

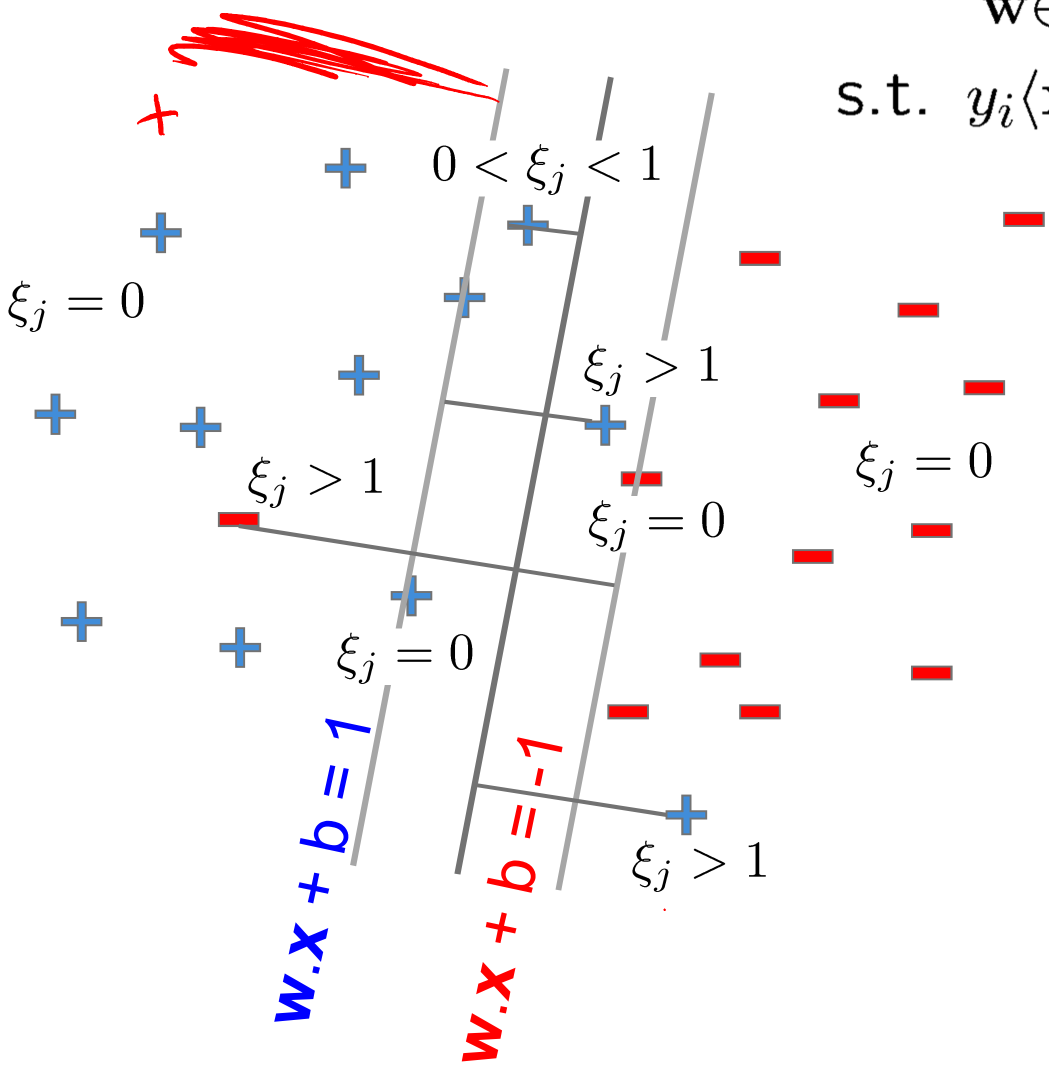
only need to store the support vectors to predict labels of new points

Support vectors in Soft SVM

$$\hat{\mathbf{w}}_{soft} = \arg \min_{\mathbf{w}\in\mathbb{R}^m, \boldsymbol{\xi}\in\mathbb{R}^n} C\sum_{i=1}^{n} \xi_i + \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{s.t. } y_i\langle \mathbf{x}_i, \mathbf{w}\rangle \geq 1 - \xi_i, \ \forall i = 1, \ldots, n$$

$$\xi_i \geq 0, \ \forall i = 1, \ldots, n$$



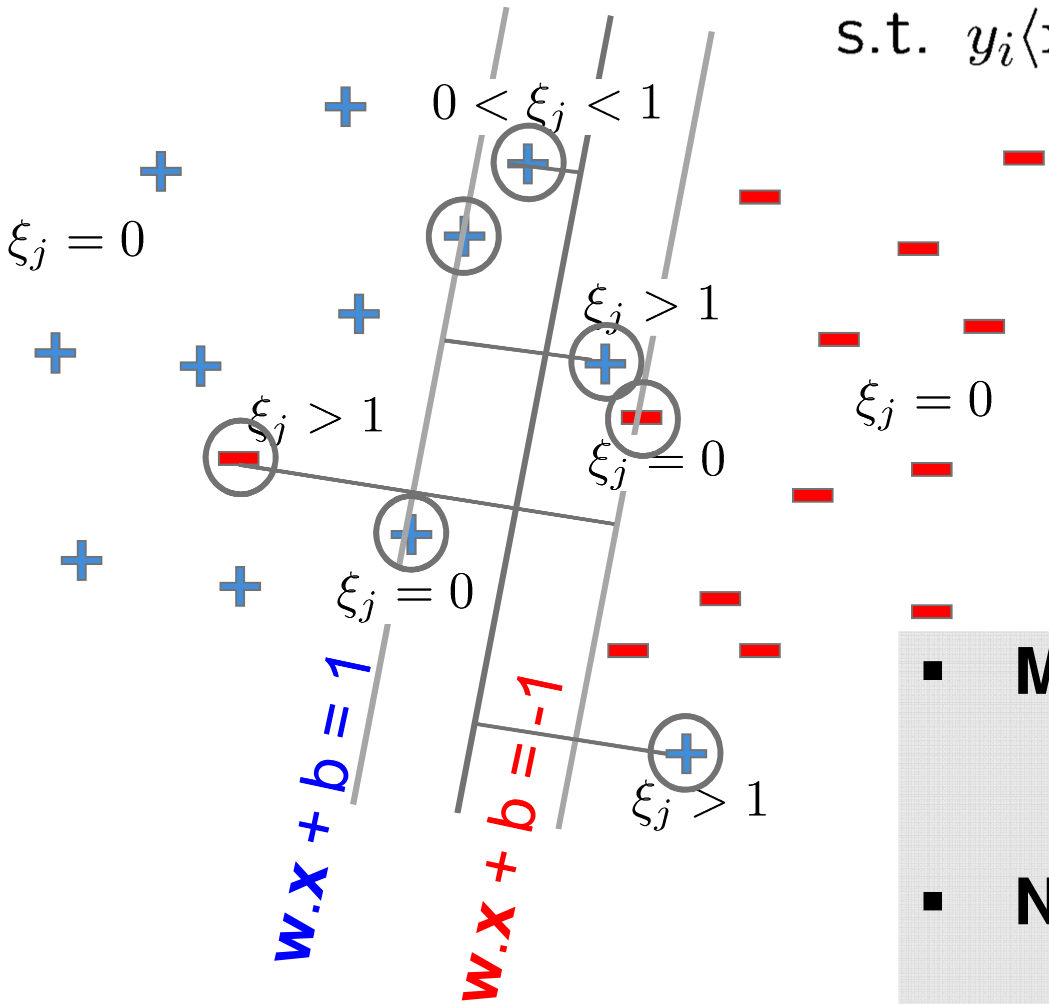
$\xi_j > 1$

Support vectors in Soft SVM

$$\widehat{\mathbf{w}}_{soft} = \arg\min_{\mathbf{w}\in\mathbb{R}^m, \boldsymbol{\xi}\in\mathbb{R}^n} C\sum_{i=1}^{n} \xi_i + \frac{1}{2}\|\mathbf{w}\|^2$$

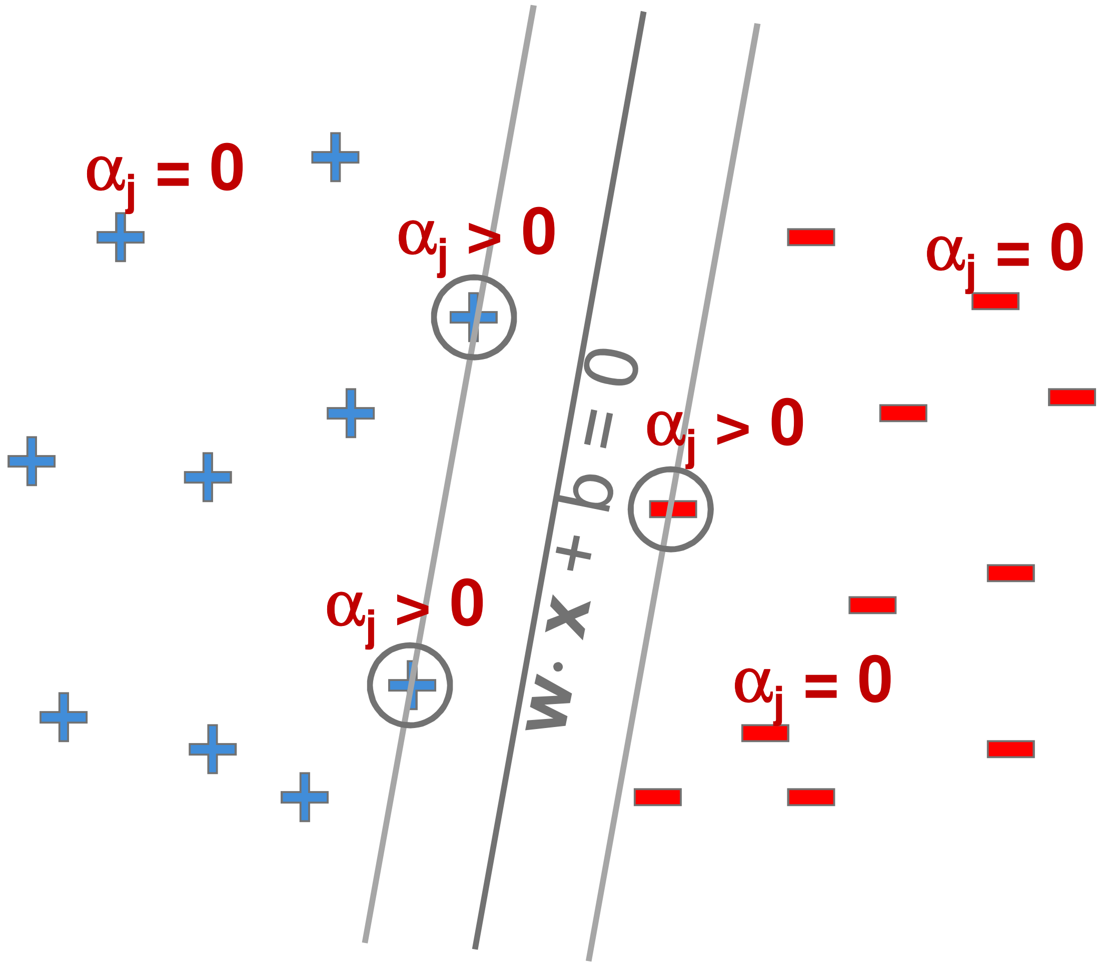
$$\text{s.t. } y_i\langle \mathbf{x}_i, \mathbf{w}\rangle \geq 1 - \xi_i, \ \forall i = 1,\ldots,n$$

$$\xi_i \geq 0, \ \forall i = 1,\ldots,n$$



- **Margin support vectors**
  $y_i\langle \mathbf{x}_i, \mathbf{w}\rangle = 1$
- **Nonmargin support vectors**
  $\xi_i > 0$

Dual SVM Interpretation: Sparsity

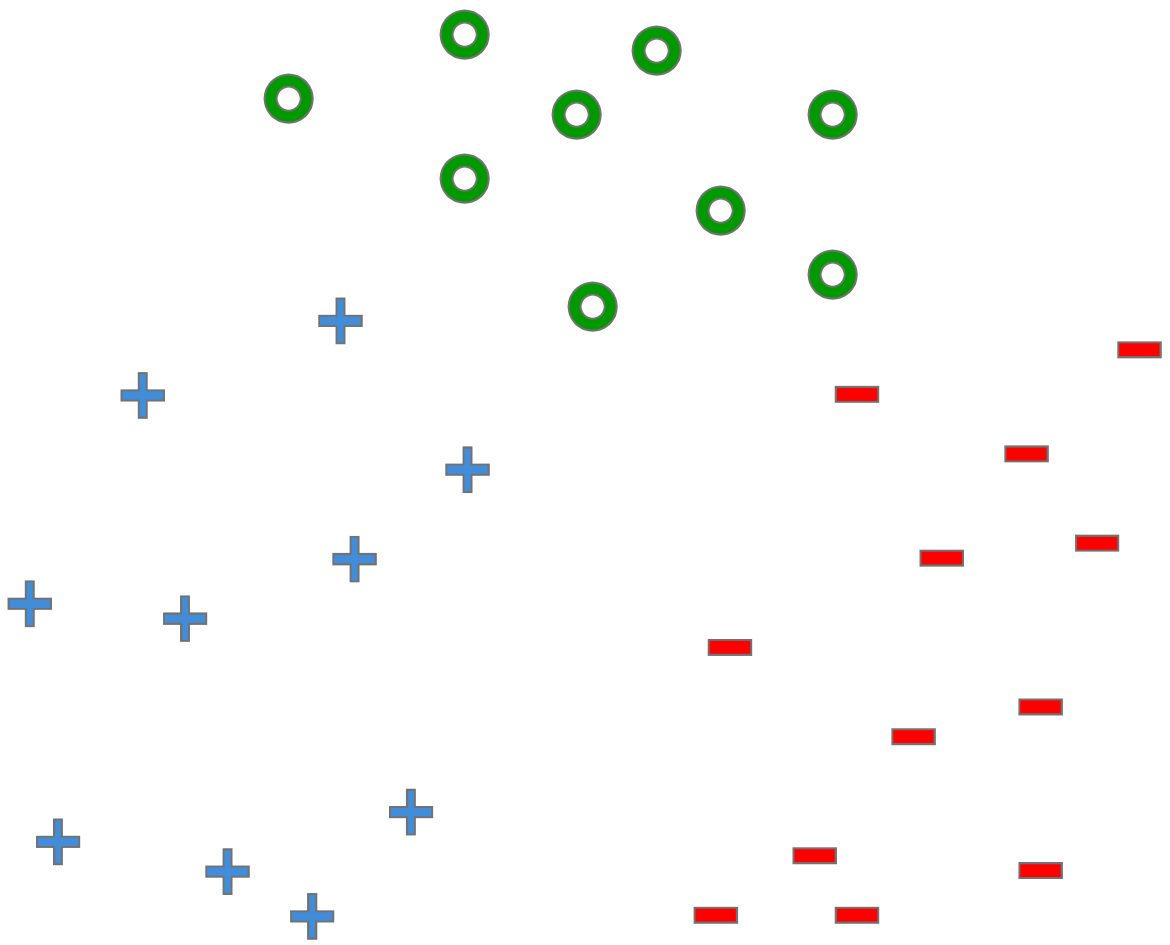


$$\mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j$$

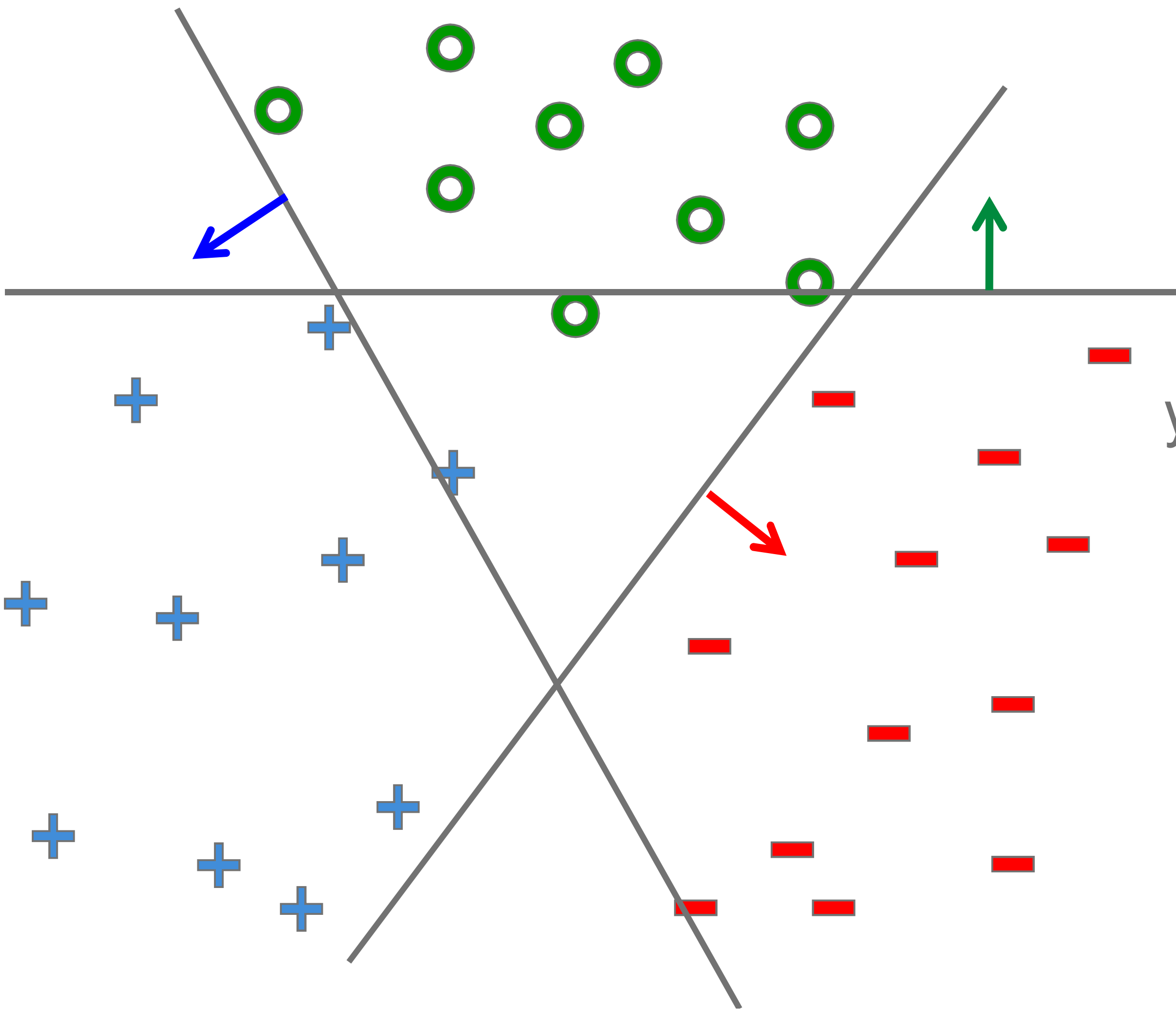
Only few α_js can be non-zero : where constraint is tight

$(<\mathbf{w},\mathbf{x}_j> + b)y_j = 1$

What about multiple classes?



One against all



Learn 3 classifiers separately:
Class k vs. rest
$(\mathbf{w}_k, b_k)_{k=1,2,3}$

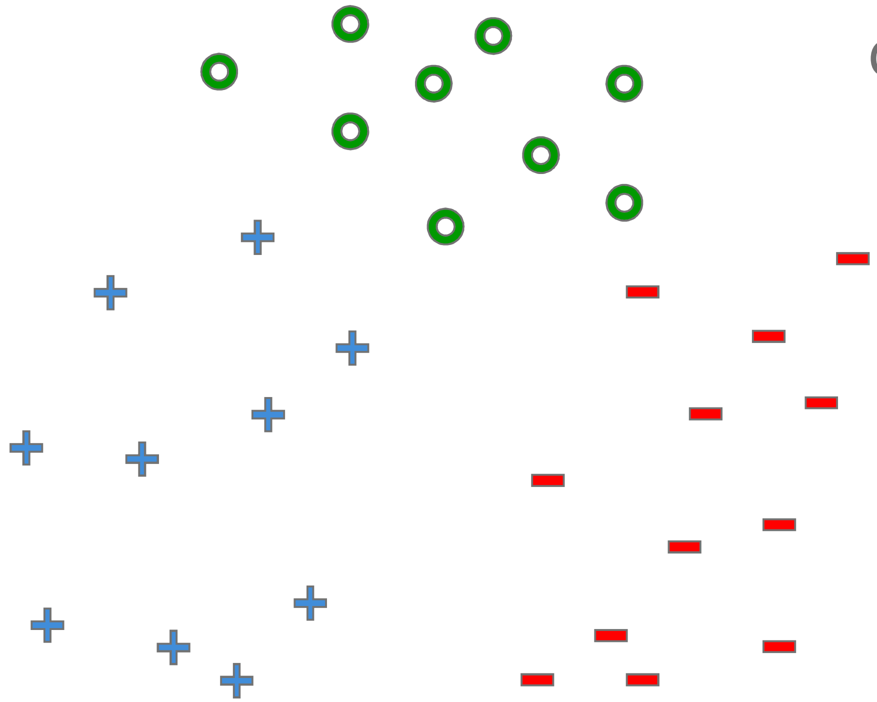
$$y = \arg\max_k \mathbf{w}_k \cdot x + b_k$$

But $\mathbf{w}_k$s may not be based on the same scale.
Note: $(a\mathbf{w}) \cdot x + (ab)$ is also a solution

Learn 1 classifier: Multi-class SVM

Simultaneously learn 3 sets of weights.
Constraints:

$$\mathbf{w}^{(y_j)} \cdot \mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y')} \cdot \mathbf{x}_j + b^{(y')} + 1, \ \forall y' \neq y_j, \ \forall j$$



Margin - gap between correct class and nearest other class

$y = \arg\max_k \mathbf{w}^{(k)} \cdot x + b^{(k)}$

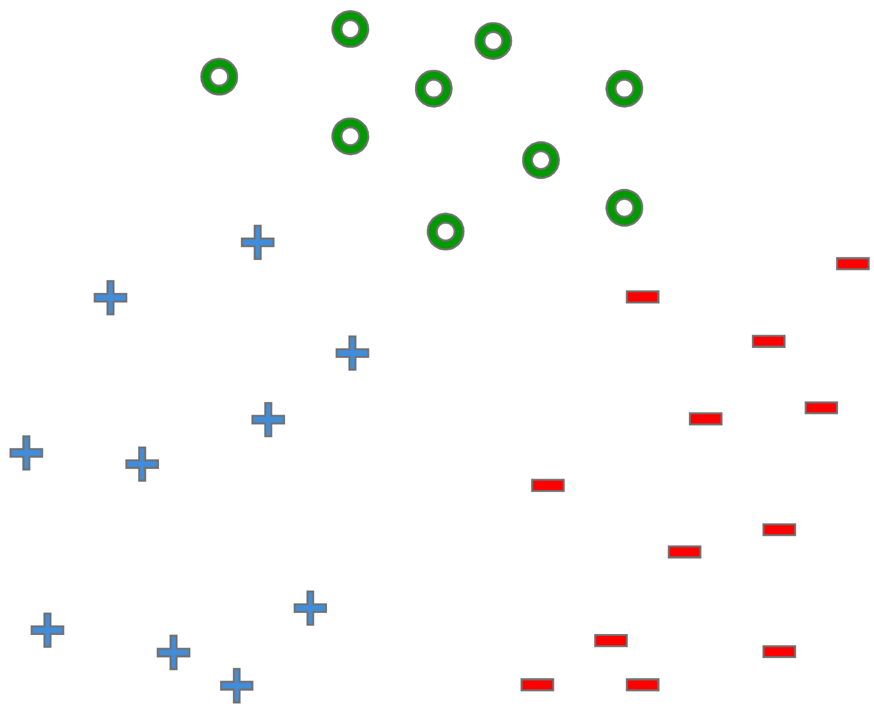
Learn 1 classifier: Multi-class SVM

Simultaneously learn 3 sets of weights

$$\text{minimize}_{\mathbf{w},b} \quad \sum_y \mathbf{w}^{(y)} \cdot \mathbf{w}^{(y)} + C \sum_j \sum_{y \neq y_j} \xi_j^{(y)}$$

$$\mathbf{w}^{(y_j)} \cdot \mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y)} \cdot \mathbf{x}_j + b^{(y)} + 1 - \xi_j^{(y)}, \ \forall y \neq y_j, \ \forall j$$

$$\xi_j^{(y)} \geq 0 \quad , \ \forall y \neq y_j, \ \forall j$$



$y = \arg\max_k \mathbf{w}^{(k)} \cdot x + b^{(k)}$

Joint optimization: $\mathbf{w}_k$s have the same scale.

What you need to know

- Maximizing margin
- Derivation of SVM formulation
- Slack variables and hinge loss
- Relationship between SVMs and logistic regression
  - 0/1 loss
  - Hinge loss
  - Log loss
- Tackling multiple class
  - One against All
  - Multiclass SVMs

SVM vs. Logistic Regression

SVM : **Hinge loss:** $\mathrm{loss}(f(\mathbf{x}_j), y_j) = (1 - (\mathbf{w} \cdot \mathbf{x}_j + b)y_j))_+$

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} \underbrace{\mathrm{loss}(\mathbf{x}_i \cdot \mathbf{w} + b, y_i)}_{\xi_i \geq 0} + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

Logistic Regression : **Log loss** (log conditional likelihood)

$$\mathrm{loss}(f(x_j), y_j) = -\log P(y_j \mid x_j, \mathbf{w}, b) = \log(1 + e^{-(\mathbf{w}\cdot x_j + b)y_j})$$

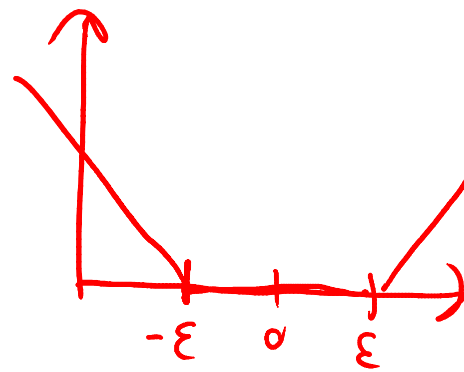
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}\in\mathbb{R}^m} \sum_{i=1}^{n} \mathrm{loss}(\mathbf{x}_i \cdot \mathbf{w} + b, y_i)$$

SVM for Regression

$$\text{LOSS}(y, w^T x) = (y - w^T x)^2$$

$$0 \text{ IF } |y - w^T x| \leq \varepsilon$$

$$|y - w^T x| \text{ OTHERWISE}$$



SVM classification in the dual space

"Without b"

$$\hat{\boldsymbol{\alpha}} = \text{arg} \max_{\boldsymbol{\alpha} \in \mathbb{R}^m} \boldsymbol{\alpha}^T \mathbf{1}_m - \frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}$$

subject to $0 \leq \alpha_i \leq C$

"With b" $$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \Big(y_i (\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \Big)$$

$$\hat{\boldsymbol{\alpha}} = \text{arg} \max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \boldsymbol{\alpha}^T \mathbf{1}_n - \frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}$$

subject to $0 \leq \alpha_i \leq C$

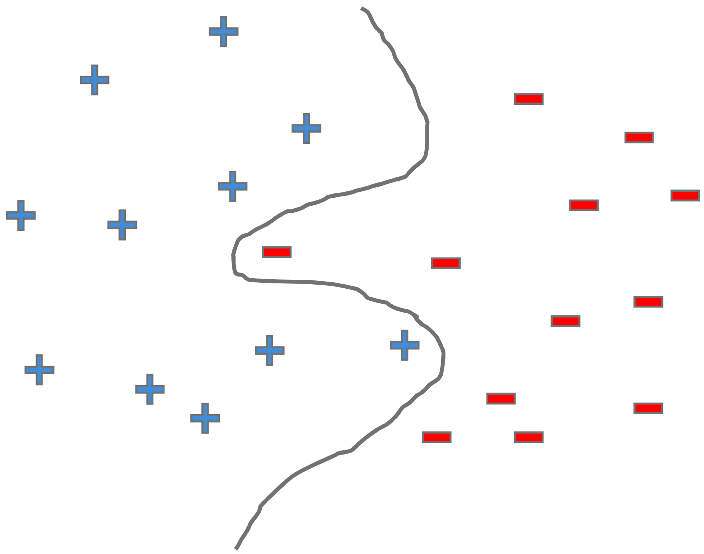
$$\sum_i \alpha_i y_i = 0$$

So why solve the dual SVM?

- There are some quadratic programming algorithms that can solve the dual faster than the primal, specially in high dimensions m>>n

- But, more importantly, the "**kernel trick**"!!!

What if data is not linearly separable?



Use features of features of features of features….

For example polynomials

$$\Phi(\mathbf{x}) = (x_1^3, x_2^3, x_3^3, x_1^2 x_2 x_3, \ldots.,)$$

Dot Product of Polynomials

$\Phi(\mathbf{x}) =$ polynomials of degree exactly d

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \mathbf{z} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

d=1 $\Phi(\mathbf{x}) \cdot \Phi(\mathbf{z}) = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \cdot \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = x_1 z_1 + x_2 z_2 = \mathbf{x} \cdot \mathbf{z}$

d=2

$$\begin{aligned} \Phi(\mathbf{x}) \cdot \Phi(\mathbf{z}) = \begin{bmatrix} x_1^2 \\ \sqrt{2} x_1 x_2 \\ x_2^2 \end{bmatrix} \cdot \begin{bmatrix} z_1^2 \\ \sqrt{2} z_1 z_2 \\ z_2^2 \end{bmatrix} &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2 \\ &= (x_1 z_1 + x_2 z_2)^2 \\ &= (\mathbf{x} \cdot \mathbf{z})^2 \end{aligned}$$

Dot Product of Polynomials

$d = 3$

$$\begin{pmatrix} x_1^3 \\ \sqrt{3}x_1^2 x_2 \\ \sqrt{3}x_1 x_2^2 \\ x_2^3 \end{pmatrix} \cdot \begin{pmatrix} z_1^3 \\ \sqrt{3}z_1^2 z_2 \\ \sqrt{3}z_1 z_2^2 \\ z_2^3 \end{pmatrix}$$

$$x_1^3 z_1^3 + 3x_1^2 x_2 z_1^2 z_2 + 3x_1 z_1 x_2^2 z_2^2 + x_2^3 z_2^3$$

$$= (x_1 z_1 + z_2 z_2)^3$$

d $\Phi(\mathbf{x}) \cdot \Phi(\mathbf{z}) = K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^d$

Higher Order Polynomials

Feature space becomes really large very quickly!

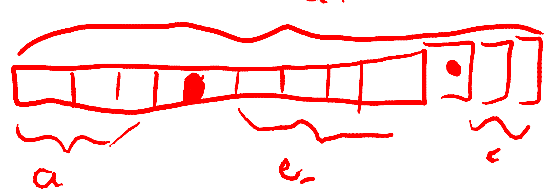
m – input features d – degree of polynomial

$$\text{num. terms} = \binom{d+m-1}{d} = \frac{(d+m-1)!}{d!(m-1)!} \sim m^d$$

grows fast: d = 6, m = 100, about 1.6 billion terms

$x_1^a \; x_2^b \; x_3^c$ $a+b+c=d$

$a+b+c+m-1 = d+m-1$



$\binom{d+m-1}{m-1}$

Dual formulation only depends on dot-products, not on w!

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \underbrace{\mathbf{x}_i \cdot \mathbf{x}_j}$$

$$C \geq \alpha_i \geq 0$$

$$\Downarrow$$

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \underbrace{K(\mathbf{x}_i, \mathbf{x}_j)}$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$$
$$C \geq \alpha_i \geq 0$$

$\Phi(\mathbf{x})$ – High-dimensional feature space, but never need it explicitly as long as we can compute the dot product fast using some Kernel K

Finally: The Kernel Trick!

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

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

$$\sum_i \alpha_i y_i = 0$$

$$C \geq \alpha_i \geq 0$$

$$\boxed{\begin{array}{c} \mathbf{w} = \sum_i \alpha_i y_i \Phi(\mathbf{x}_i) \\[1em] b = y_k - \mathbf{w} \cdot \Phi(\mathbf{x}_k) \\ \text{for any } k \text{ where } C > \alpha_k > 0 \end{array}}$$

- Never represent features explicitly
  - Compute dot products in closed form
- Constant-time high-dimensional dot-products for many classes of features

Common Kernels

- Polynomials of degree d $K(\mathbf{u},\mathbf{v}) = (\mathbf{u}\cdot\mathbf{v})^d$
- Polynomials of degree up to d $K(\mathbf{u},\mathbf{v}) = (\mathbf{u}\cdot\mathbf{v}+1)^d$
- Gaussian/Radial kernels (polynomials of all orders – recall series expansion)

$$K(\mathbf{u},\mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||^2}{2\sigma^2}\right)$$

- Sigmoid

$$K(\mathbf{u},\mathbf{v}) = \tanh(\eta\mathbf{u}\cdot\mathbf{v}+\nu)$$

Which functions can be used as kernels???
…and why are they called kernels???

Overfitting

- Huge feature space with kernels, what about overfitting???
  - Maximizing margin leads to sparse set of support vectors
  - Some interesting theory says that SVMs search for simple hypothesis with large margin
  - Often robust to overfitting

What about classification time?

$$\mathbf{w} = \sum_i \alpha_i y_i \Phi(\mathbf{x}_i)$$

$$b = y_k - \mathbf{w} \cdot \Phi(\mathbf{x}_k)$$

for any k where $C > \alpha_k > 0$

- For a new input **x**, if we need to represent Φ(**x**), we are in trouble!
- Recall classifier: sign(**w**·Φ(**x**)+b)
- Using kernels we are cool!

$$K(\mathbf{u}, \mathbf{v}) = \Phi(\mathbf{u}) \cdot \Phi(\mathbf{v})$$

Kernels in Logistic Regression

$$P(Y=1 \mid \mathbf{x}, \mathbf{w}) = \frac{1}{1+e^{-(\mathbf{w}\cdot\Phi(\mathbf{x})+b)}}$$

- Define weights in terms of features:

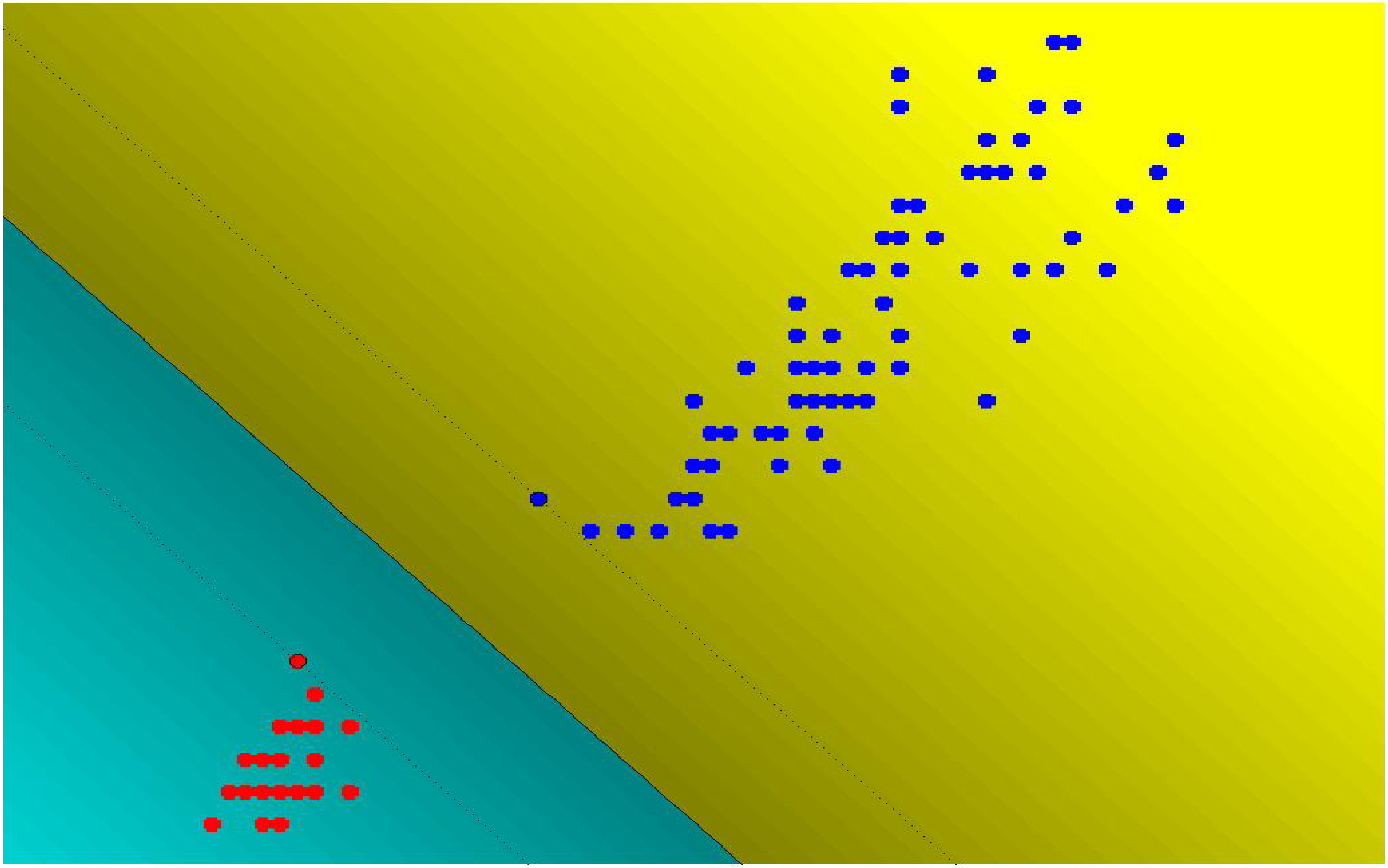
$$\mathbf{w} = \sum_i \alpha_i \Phi(\mathbf{x}_i)$$

$$\begin{aligned} P(Y=1 \mid \mathbf{x}, \mathbf{w}) &= \frac{1}{1+e^{-(\sum_i \alpha_i \Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x})+b)}} \\ &= \frac{1}{1+e^{-(\sum_i \alpha_i K(\mathbf{x},\mathbf{x}_i)+b)}} \end{aligned}$$

- Derive simple gradient descent rule on α_i

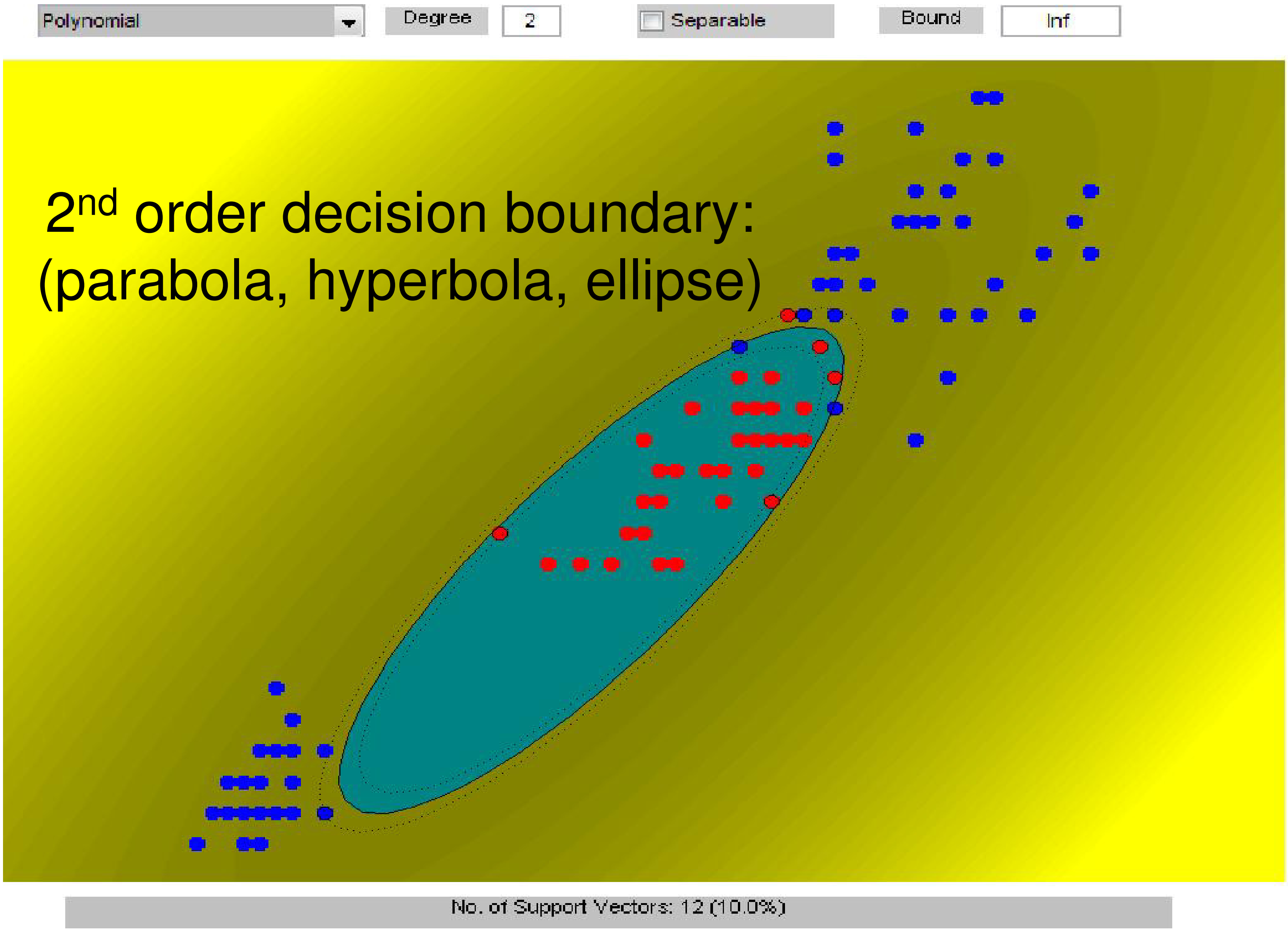
A few results

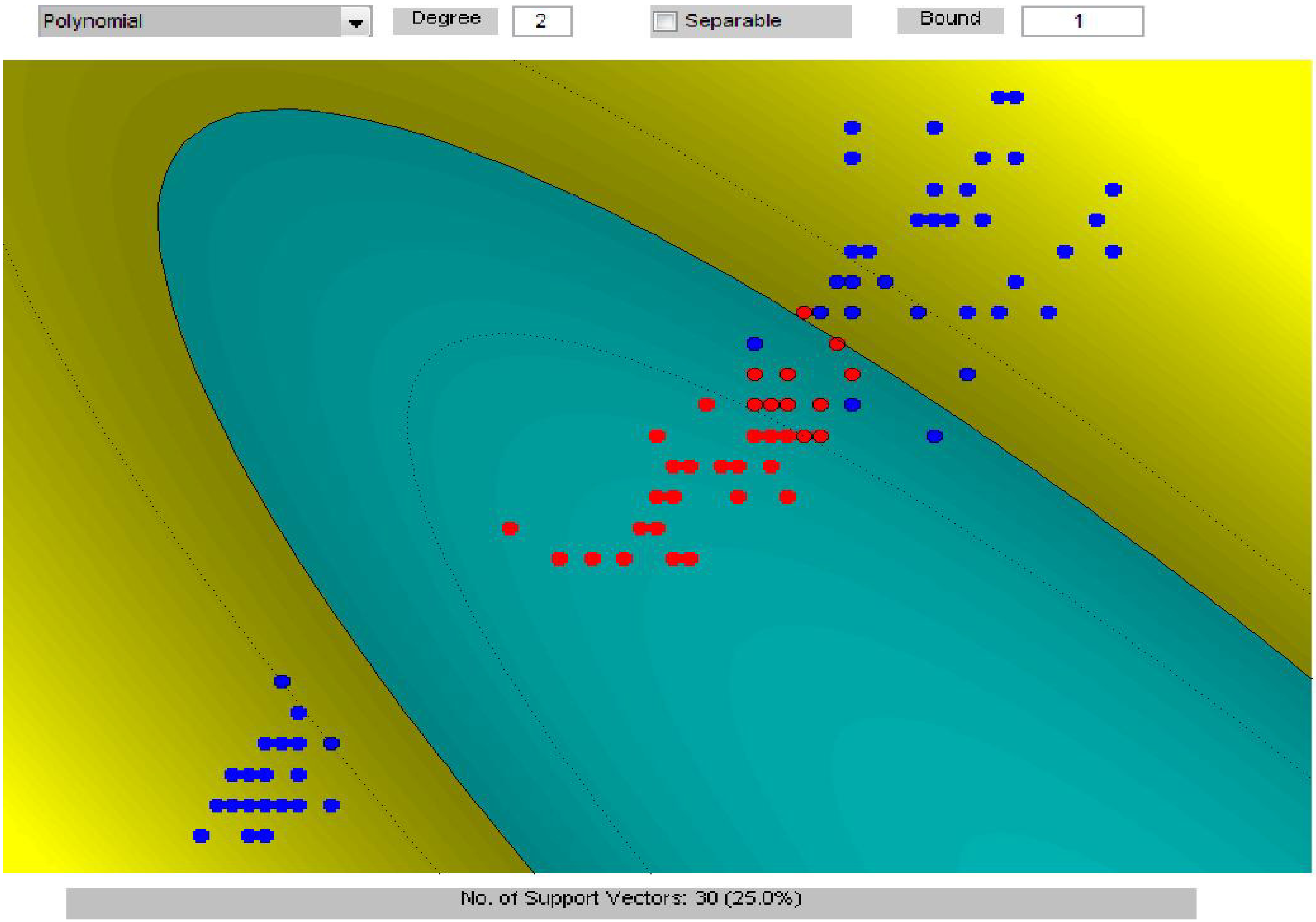
Steve Gunn's svm toolbox Results, Iris 2vs13, Linear kernel



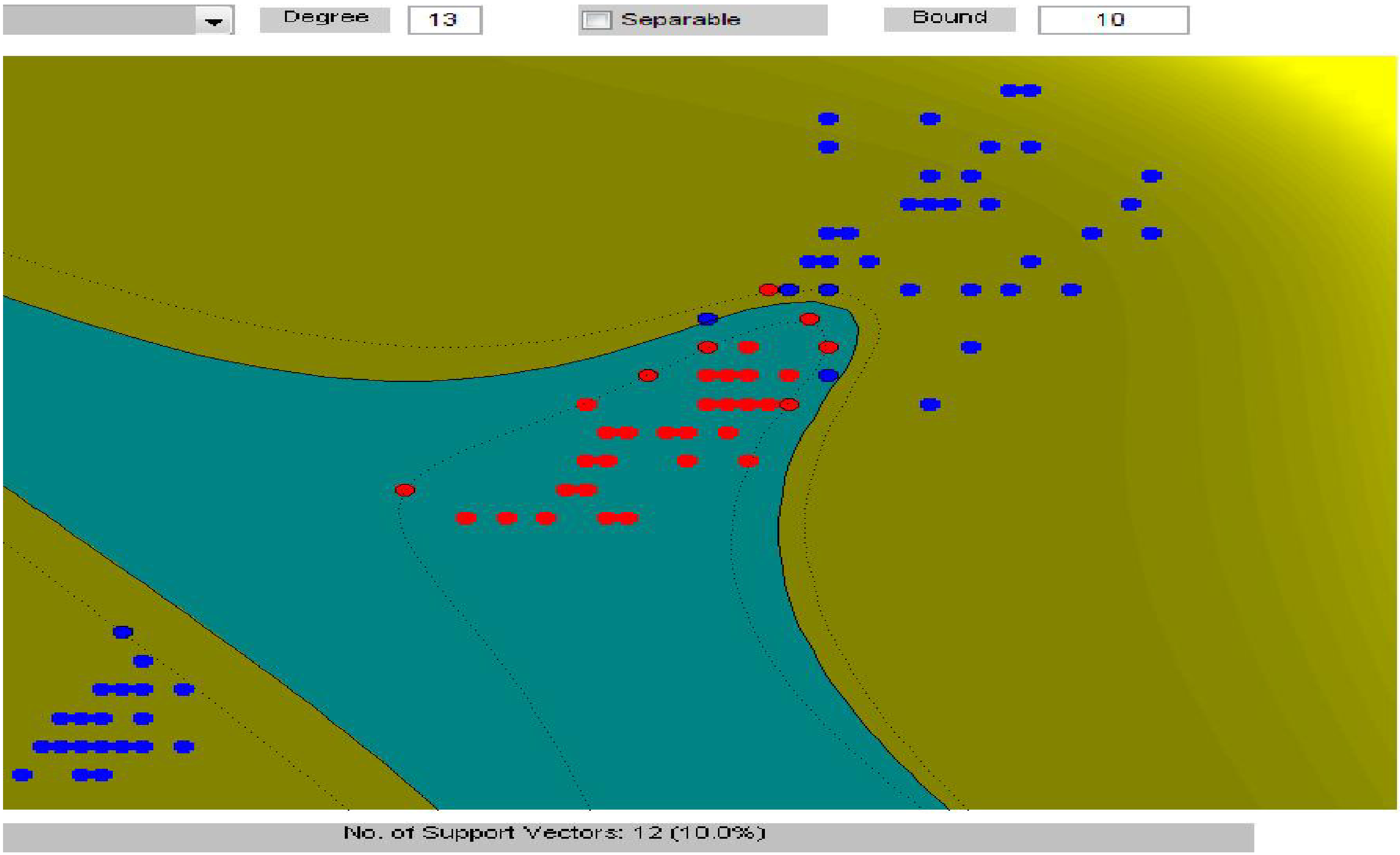
No. of Support Vectors: 2 (1.7%)

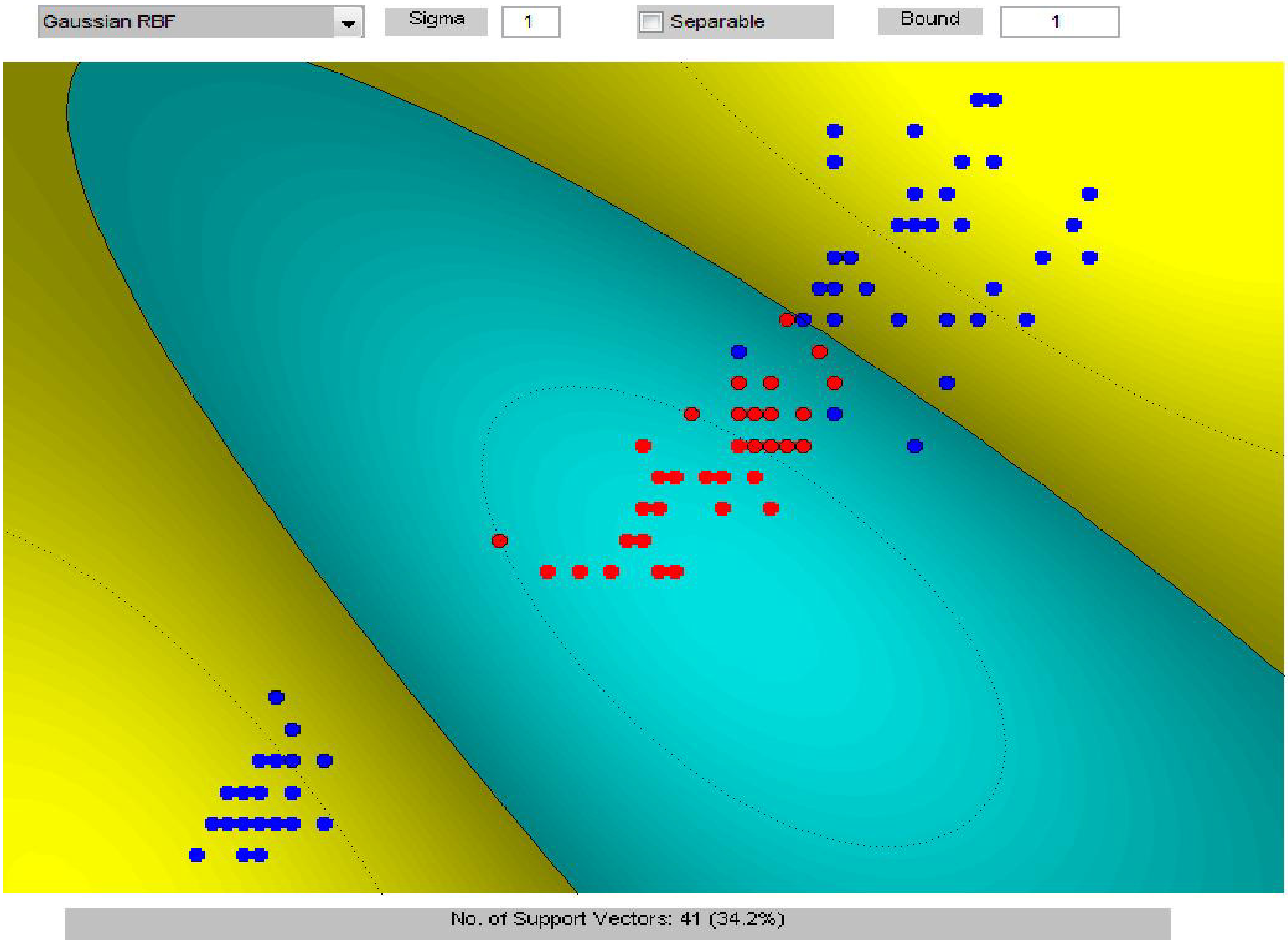
Results, Iris 1vs23, 2^{nd} order kernel




Polynomial
Degree
2
Separable
Bound
1
No. of Support Vectors: 30 (25.0%)

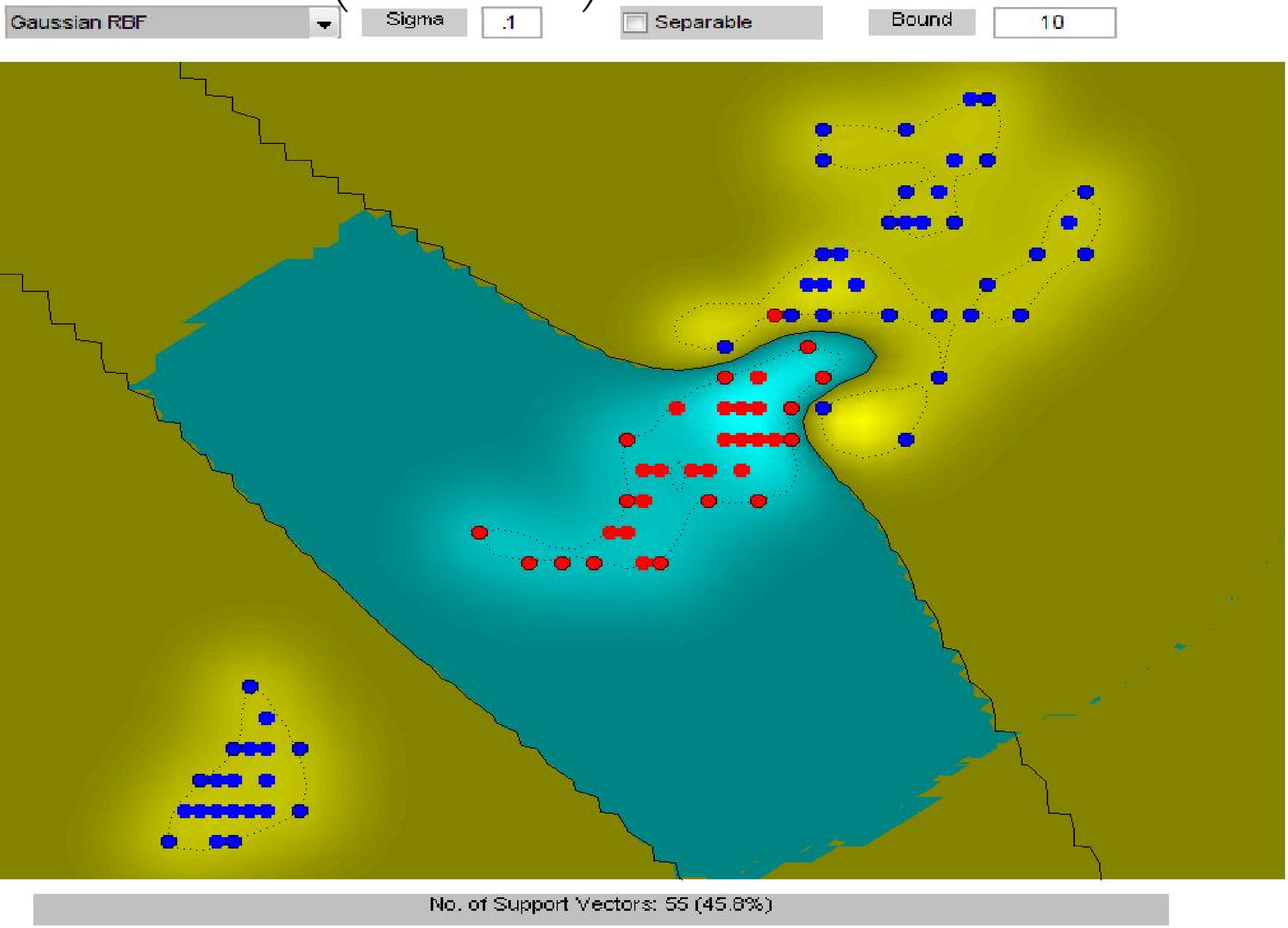
Results, Iris 1vs23, 13th order kernel



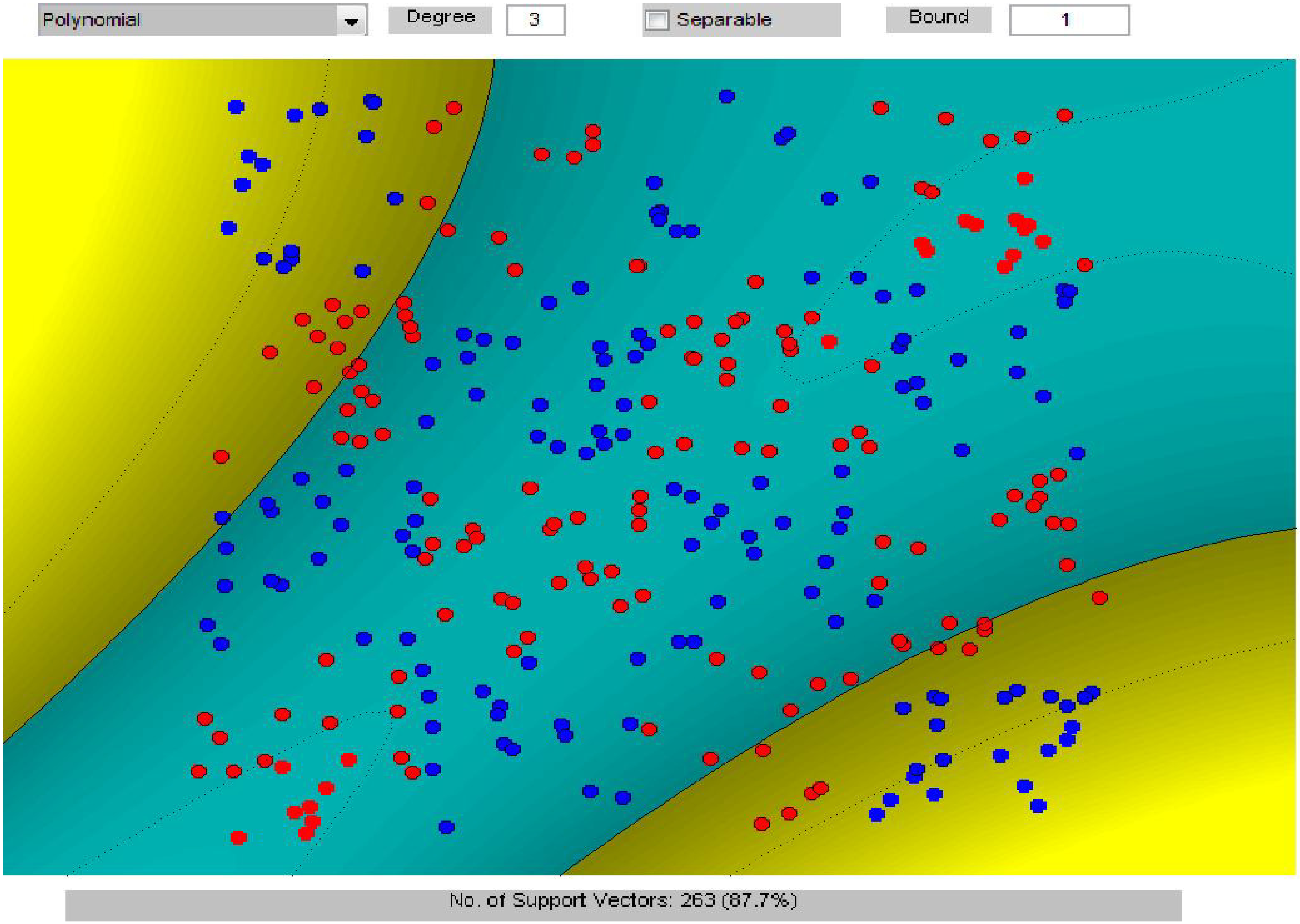

Gaussian RBF
Sigma
1
Separable
Bound
1
No. of Support Vectors: 41 (34.2%)

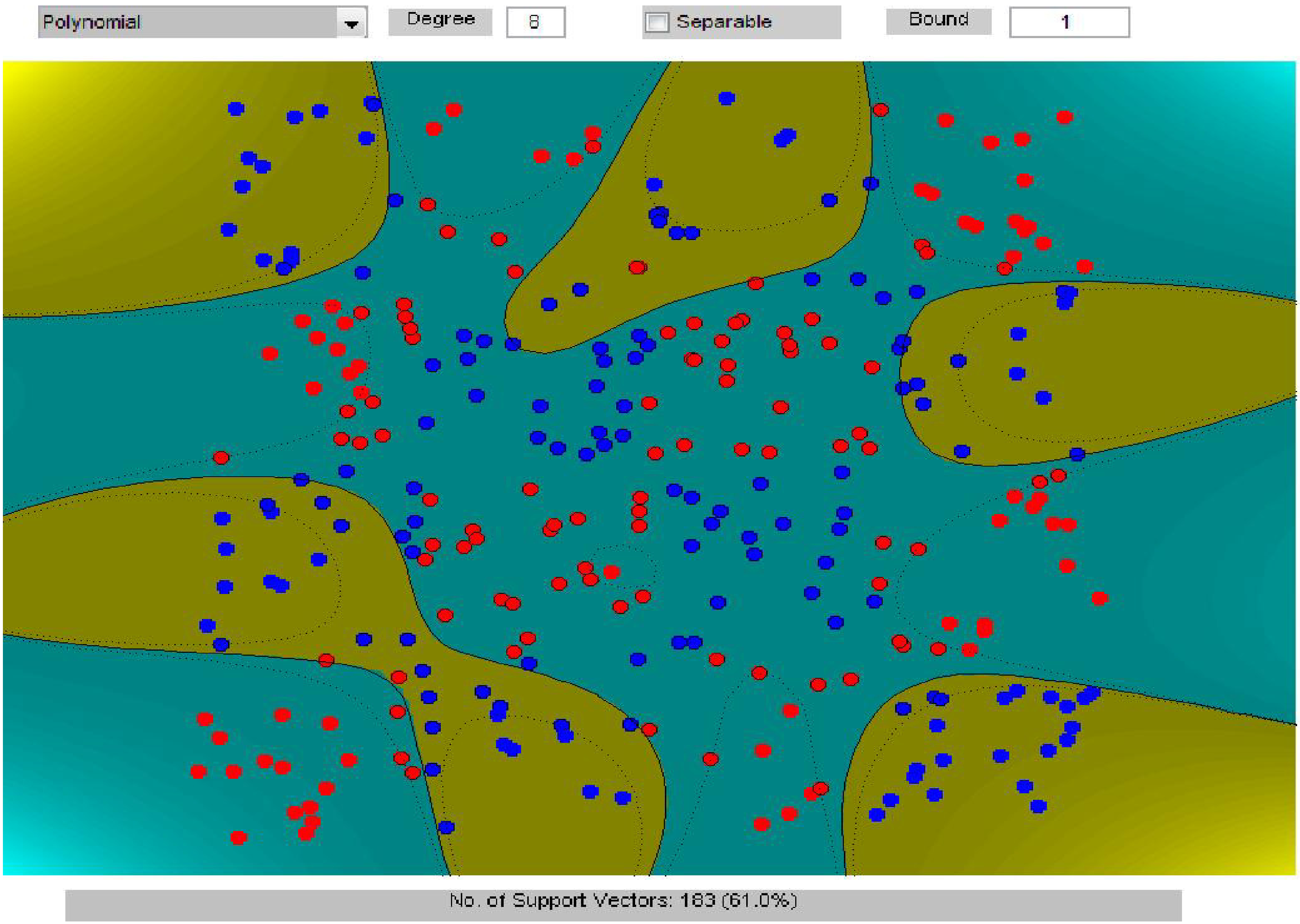
$$K(\mathbf{u},\mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||^2}{2\sigma^2}\right)$$

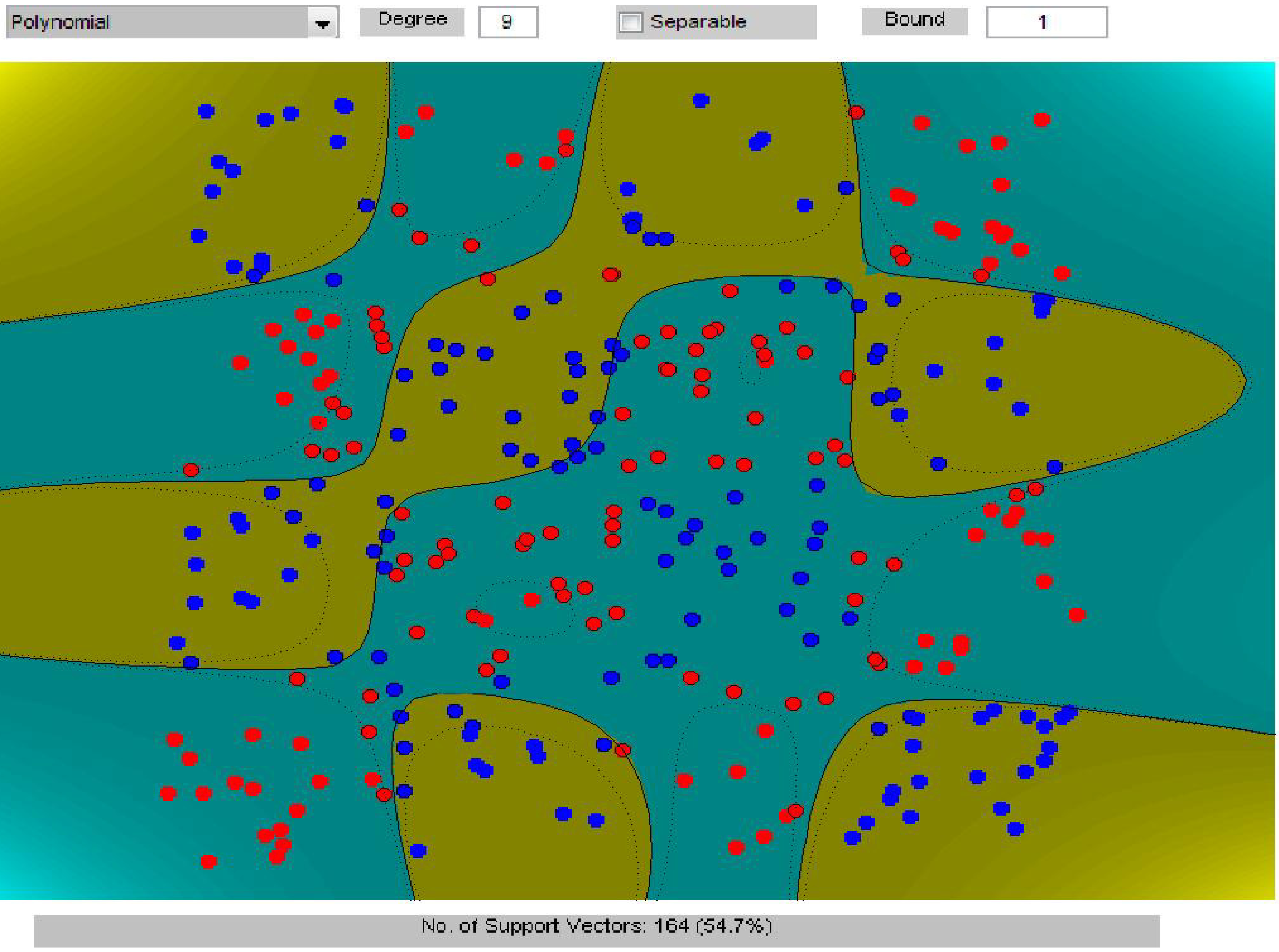
$\sigma \to 0 \Rightarrow$ MORE SUPPORT VECTORS

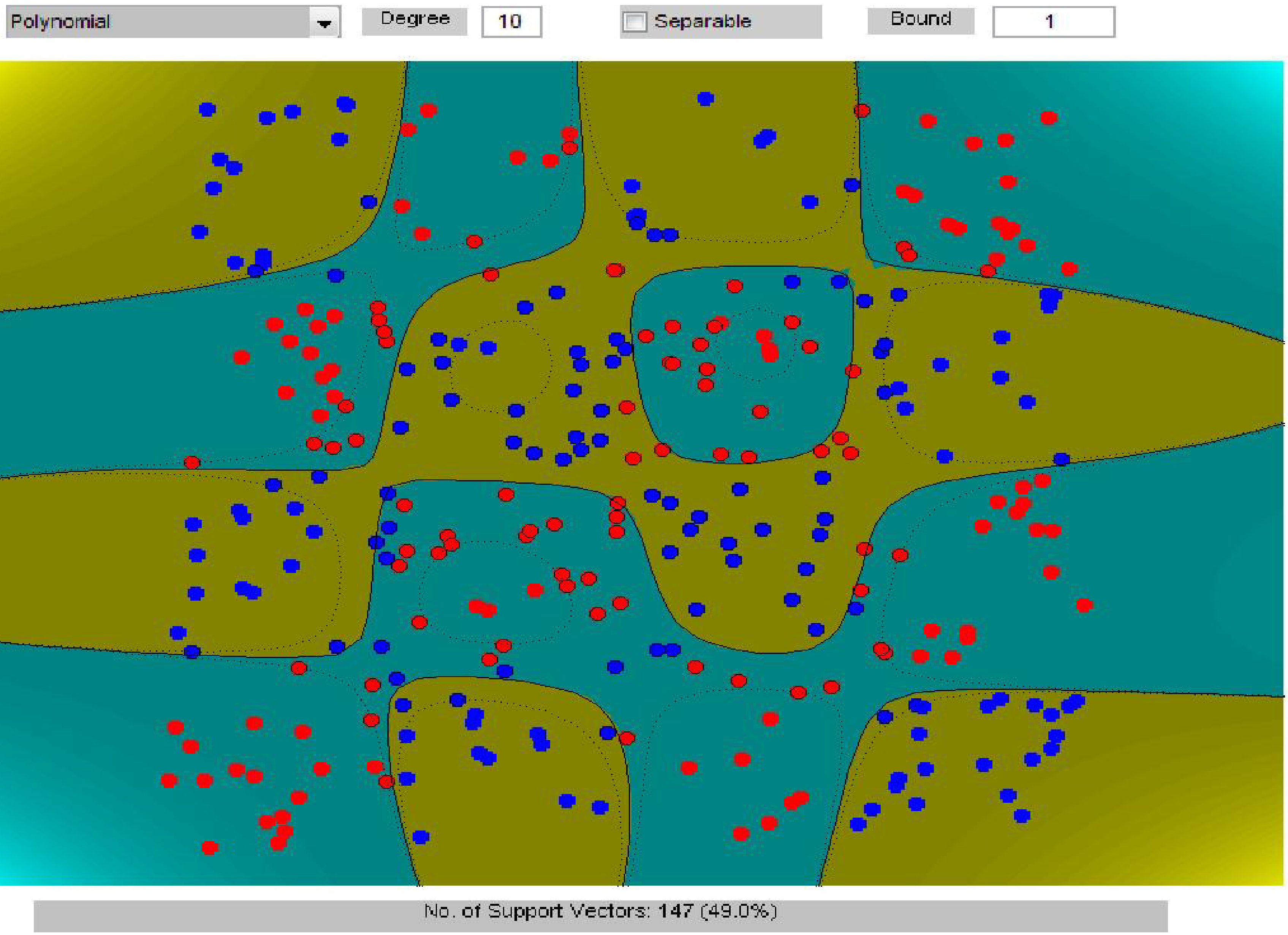


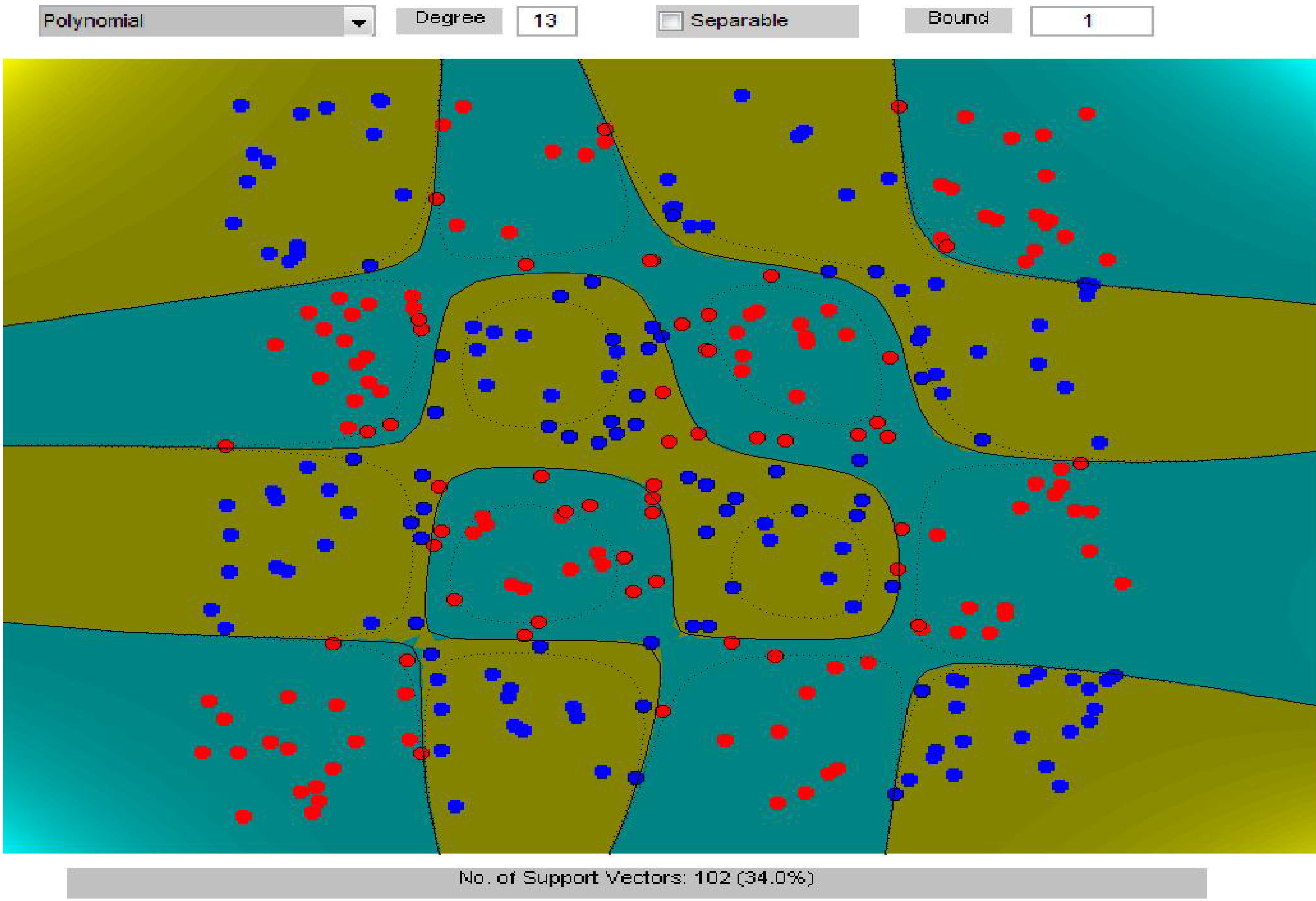
Chessboard dataset




Polynomial
Degree
8
Separable
Bound
1
No. of Support Vectors: 183 (61.0%)


Polynomial
Degree
9
Separable
Bound
1
No. of Support Vectors: 164 (54.7%)


Polynomial
Degree
10
Separable
Bound
1
No. of Support Vectors: 147 (49.0%)


Polynomial
Degree
13
Separable
Bound
1
No. of Support Vectors: 102 (34.0%)

Results, Chessboard, RBF kernel