Machine Learning

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Support Vector Machines

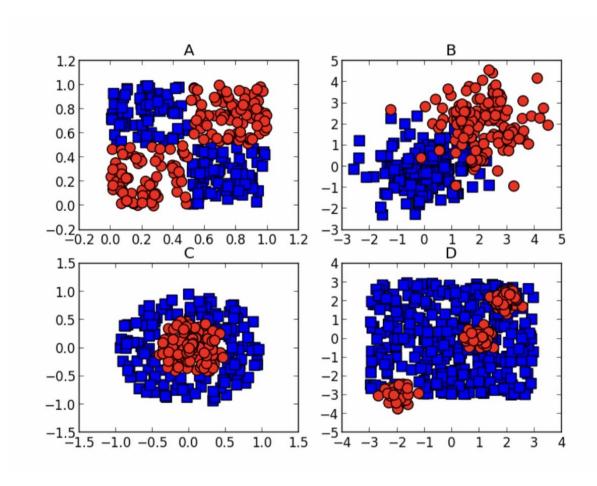
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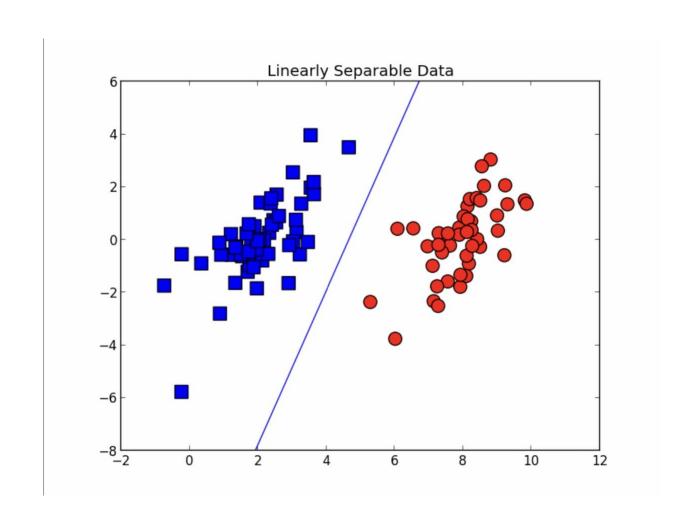
Introduction

- Support vector machines:
- One of the most popular machine learning algorithms!
- better separation of data than other machine learning methods (classification problems)
- It is relatively easy to use!
- Using the kernel trick:
- Classification, regression, estimation, distribution, single class classification and...

Linearly inseparable data

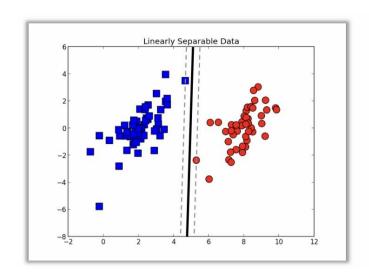


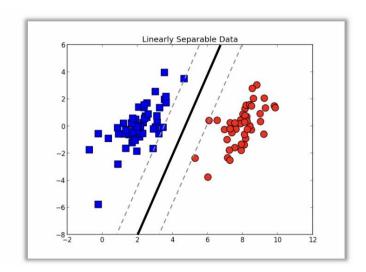
Linearly separable data



Optimum decision boundary

Question: which decision boundary is better?

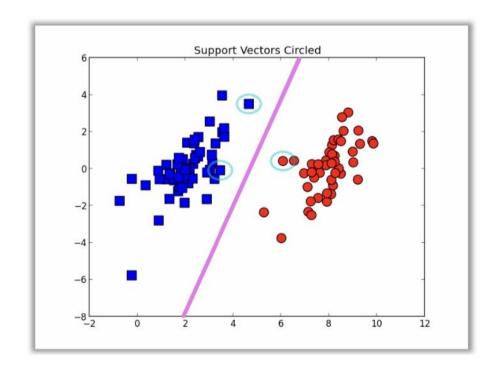




Maximum margin solution:
 Maximum stability against data destruction. (increasing generalizability)

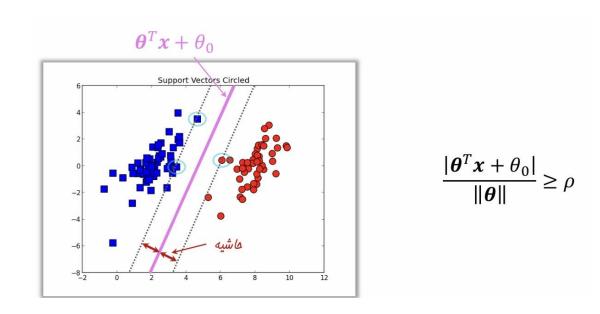
Support Vectors

- Support vector: the closest points to the decision boundary.
- Objective: to maximize the distance of the support vectors from the decision boundary.



Support Vector Machines: classifier with maximum margin

- Margin: the distance between support vectors and decision boundary.
- Goal: maximizing the distance between support vectors and decision boundary.



Optimum decision boundary: Symbols

Training samples

$$X = (x^t, y^t), y^t = \begin{cases} +1 & \text{if } x^t \in C_1 \\ -1 & \text{if } x^t \in C_2 \end{cases}$$

Goal: finding θ vector and θ_0 value so that:

$$\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0 \ge +1$$
 for $\boldsymbol{y}^t = +1$ $\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0 \le -1$ for $\boldsymbol{y}^t = -1$



$$y^t(\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) \ge +1$$

The objective function

- Objective: to maximize the distance of the support vectors from the decision boundary.
 - The distance between data x and decision boundary:

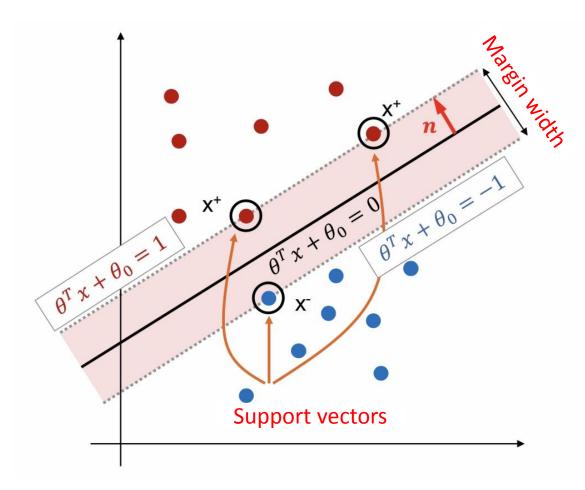
$$\frac{|\boldsymbol{\theta}^T \boldsymbol{x} + \boldsymbol{\theta}_0|}{\|\boldsymbol{\theta}\|} \ge \rho \quad \Rightarrow \quad |\boldsymbol{\theta}^T \boldsymbol{x} + \boldsymbol{\theta}_0| \ge \rho \|\boldsymbol{\theta}\|$$

• This equation has infinite answers. By considering $\rho \|\theta\| = 1$ we will have:

$$\rho \|\boldsymbol{\theta}\| = 1 \Rightarrow \rho = \frac{1}{\|\boldsymbol{\theta}\|}$$

- Goal: to maximize the margin, we can minimize the size of θ vector.
- Constraints: The decision boundary must correctly separate the data of two classes from each other.

The objective function



We know:

$$\theta^T x^+ + \theta_0 = +1$$

$$\theta^T x^+ + \theta_0 = +1$$
$$\theta^T x^- + \theta_0 = -1$$

So:

$$M = (x^{+} - x^{-}) \cdot n$$
$$= (x^{+} - x^{-}) \cdot \frac{\theta}{\|\theta\|} = \frac{2}{\|\theta\|}$$

s.t.

• Objective function:

$$\min \frac{1}{2} \|\boldsymbol{\theta}\|^2$$

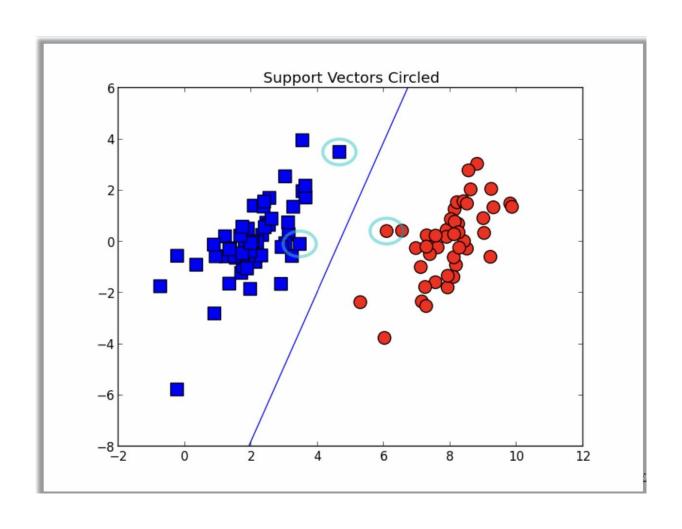
s.t. $(\boldsymbol{\theta}^T \boldsymbol{x}^t + \boldsymbol{\theta}_0) \ge +1$ if $y^t = +1$

 $(\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) \le -1$ if $y^t = -1$

• Simplification:

$$\min_{2}^{1} \|\boldsymbol{\theta}\|^{2}$$
$$y^{t}(\boldsymbol{\theta}^{T} \boldsymbol{x}^{t} + \boldsymbol{\theta}_{0}) \ge +1$$

Objective function

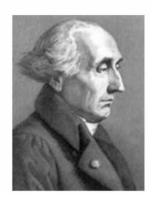


• Objective function:

$$\min \frac{1}{2} \|\boldsymbol{\theta}\|^2$$
 convex optimization s.t. $y^t(\boldsymbol{\theta}^T \boldsymbol{x}^t + \boldsymbol{\theta}_0) \ge +1$

Problem solving using lagrange factor:

$$\begin{split} L_p &= \frac{1}{2} \|\boldsymbol{\theta}\|^2 - \sum_{t=1}^m \alpha^t [y^t (\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) - 1] \\ &= \frac{1}{2} \|\boldsymbol{\theta}\|^2 - \sum_{t=1}^m \alpha^t y^t (\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) + \sum_{t=1}^m \alpha^t \end{split}$$



Joseph Louis Lagrange 1813-1736

$$L_p = \frac{1}{2} \|\boldsymbol{\theta}\|^2 - \sum_{t=1}^{m} \alpha^t [y^t (\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) - 1]$$

$$= \frac{1}{2} \|\boldsymbol{\theta}\|^2 - \sum_{t=1}^{m} \alpha^t y^t (\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) + \sum_{t=1}^{m} \alpha^t$$

Decision boundary of a linear combination of training data

$$\frac{\partial L_p}{\partial \boldsymbol{\theta}} = 0 \Rightarrow \boldsymbol{\theta} = \sum_{t=1}^m \alpha^t y^t \boldsymbol{x}^t$$

$$\frac{\partial L_p}{\partial \theta_0} = 0 \Rightarrow \sum_{t=1}^m \alpha^t y^t = 0$$

Minimal sequential optimization algorithm → Pellet (1999)

$$L_d = \frac{1}{2} (\boldsymbol{\theta}^T \boldsymbol{\theta}) - \boldsymbol{\theta}^T \sum_{t=1}^m \alpha^t y^t \boldsymbol{x}^t - \theta_0 \sum_{t=1}^m \alpha^t y^t + \sum_{t=1}^m \alpha^t$$

$$= -\frac{1}{2} (\boldsymbol{\theta}^T \boldsymbol{\theta}) + \sum_{t=1}^m \alpha^t$$

$$= -\frac{1}{2} \sum_{t=1}^m \sum_{s=1}^m \alpha^t \alpha^s y^t y^s (\boldsymbol{x}^t)^T \boldsymbol{x}^s + \sum_{t=1}^m \alpha^t$$

subject to $\sum_{t=1}^{m} \alpha^t y^t = 0$ and $\alpha^t \ge 0 \ \forall t$

- Most alphas are zero, and only a few are greater than zero.
- The x's for which the alpha value is greater than zero are the support vectors.

Objective Function: Simplified Format

Minimal sequential optimization algorithm —> Pellet (1999)

$$L_d = -\frac{1}{2} \sum_{t=1}^m \sum_{s=1}^m \alpha^t \alpha^s y^t y^s (\mathbf{x}^t)^T \mathbf{x}^s + \sum_{t=1}^m \alpha^t$$
$$= -\frac{1}{2} \alpha^T Q \alpha + e^T \alpha$$

$$Q_{ts} = y^t y^s (x^t)^T x^s,$$
 $e = \begin{bmatrix} 1 & 1 & \dots & 1 \end{bmatrix}^T \in \mathbb{R}^m$
subject to $\sum_{t=1}^m \alpha^t y^t = 0$ and $\alpha^t \ge 0 \ \forall t$

- Most alphas are zero, and only a few are greater than zero.
- The x's for which the alpha value is greater than zero are the support vectors.

Linearly inseparable data: soft margin

- Question: What if the data is not linearly separable?
- Soft Margin: Allowing a slight margin of error in separation
- Soft error:
- New objective function:

$$y^{t}(\boldsymbol{\theta}^{T}\boldsymbol{x}^{t} + \boldsymbol{\theta}_{0}) \geq 1 - \varepsilon^{t}$$

$$soft\ error = \sum_{t=1}^{m} \varepsilon^{t}$$

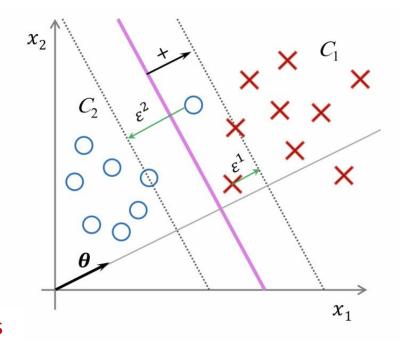
$$\min \frac{1}{2} \|\boldsymbol{\theta}\|^{2} + C \sum_{t=1}^{m} \varepsilon^{t}$$
s.t.
$$y^{t}(\boldsymbol{\theta}^{T}\boldsymbol{x}^{t} + \boldsymbol{\theta}_{0}) \geq 1 - \varepsilon^{t}$$

$$\varepsilon^{t} \geq 0$$

Linearly inseparable data: soft margin

$$\min \frac{1}{2} \|\boldsymbol{\theta}\|^2 + C \sum_{t=1}^m \varepsilon^t$$
s.t.
$$y^t (\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) \ge 1 - \varepsilon^t$$

$$\varepsilon^t \ge 0$$



Lagrange factors

$$L_p = \frac{1}{2} \|\boldsymbol{\theta}\|^2 + C \sum_{t=1}^m \varepsilon^t - \sum_{t=1}^m \alpha^t [y^t (\boldsymbol{\theta}^T \boldsymbol{x}^t + \theta_0) - 1 + \varepsilon^t] - \sum_{t=1}^m \mu^t \varepsilon^t$$

Linearly inseparable data: soft margin

$$L_p = \frac{1}{2} \|\boldsymbol{\theta}\|^2 + C \sum_{t=1}^m \varepsilon^t - \sum_{t=1}^m \alpha^t [y^t (\boldsymbol{\theta}^T \boldsymbol{x}^t + \boldsymbol{\theta}_0) - 1 + \varepsilon^t] - \sum_{t=1}^m \mu^t \varepsilon^t$$

$$\frac{\partial L_p}{\partial \boldsymbol{\theta}} = 0 \Rightarrow \boldsymbol{\theta} = \sum_{t=1}^m \alpha^t y^t \boldsymbol{x}^t$$

$$\frac{\partial L_p}{\partial \theta_0} = 0 \Rightarrow \sum_{t=1}^m \alpha^t y^t = 0$$

$$\frac{\partial L_p}{\partial \varepsilon^t} = 0 \Rightarrow C - \alpha^t - \mu^t = 0 \Rightarrow 0 \le \alpha^t \le C$$

Objective function: Dugan

$$L_d = -\frac{1}{2} \sum_{t=1}^m \sum_{s=1}^m \alpha^t \alpha^s y^t y^s (x^t)^T x^s + \sum_{t=1}^m \alpha^t$$

$$= -\frac{1}{2} \alpha^T Q \alpha + e^T \alpha$$
Subject to $\sum_{t=1}^m \alpha^t y^t = 0$ and $0 \le \alpha^t \le C \ \forall t$

Minimal sequential optimization algorithm Pellet (1999)

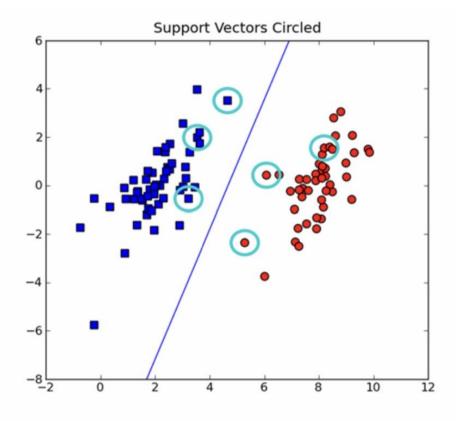
Error estimation based on the number of support vectors:

- Most alphas are zero, and only a few are greater than zero.
- The x's for which the alpha value is greater than zero are the support vectors.

$$E_m[P(error)] \le \frac{E_m[\#of \ support \ vectors]}{m}$$

Soft Margin Solution

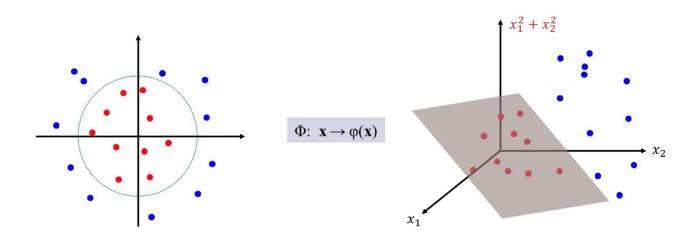
• Support Vectors:



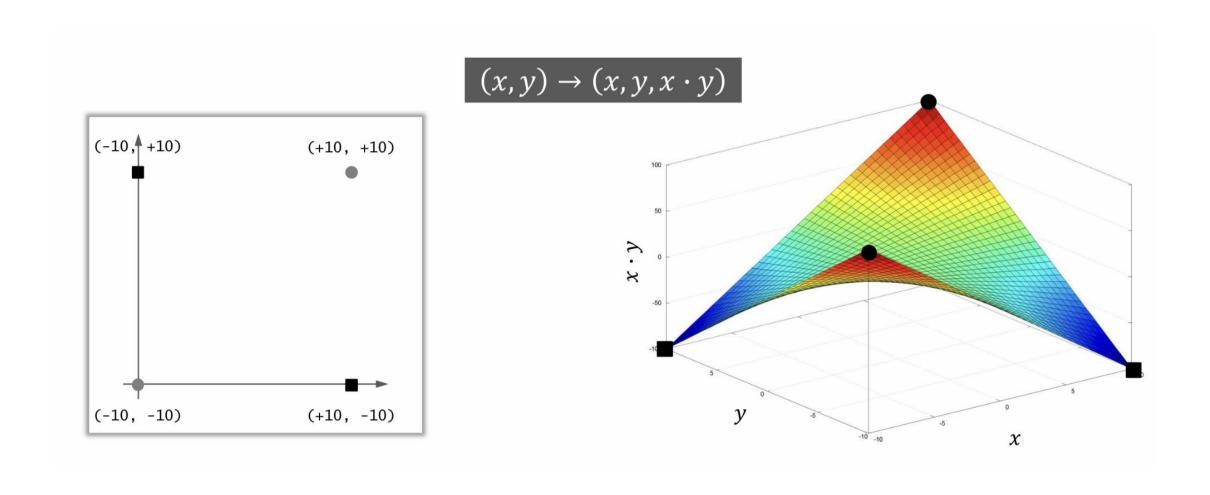
Kernel Trick

Kernel Function

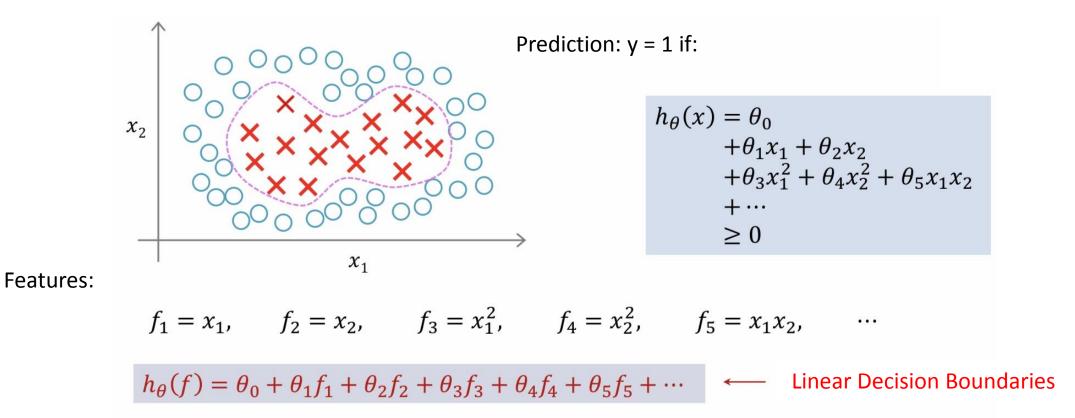
- Idea: Mapping the problem to a new feature space using non-linear transformations.
 - Using a linear model in the new space to classify data.
 - A linear model in the new space corresponds to a non-linear model in the original space.



Example: XOR problem



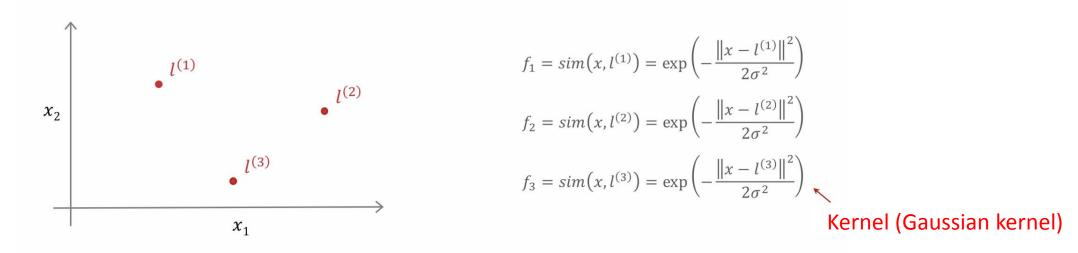
Non-linear Decision Boundaries



• Question: Is there a better way to select new features f₁, f₂, ...?

Kernel

• Idea: Given x, select a new set of features based on its similarity to guide points l_1 , l_2 , l_3 .



 Kernel function: a measure to calculate the similarity between x and y data

Kernel function:

$$f_i = sim(x, l^{(i)}) = \exp\left(-\frac{\|x - l^{(i)}\|^2}{2\sigma^2}\right)$$

The first situation: $x \approx I^{(i)}$

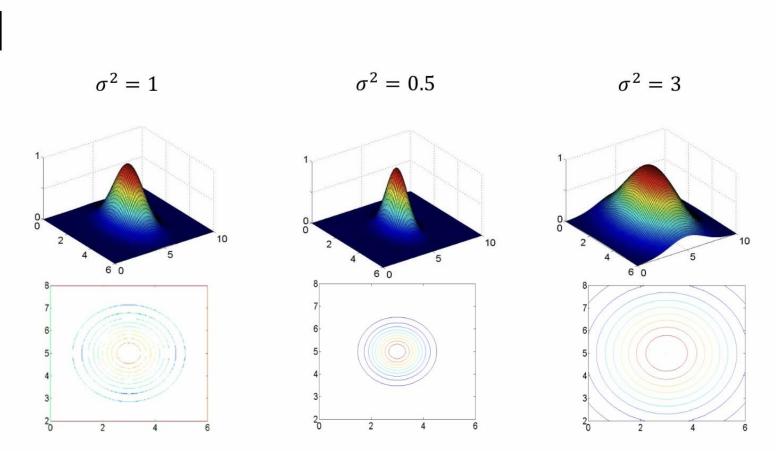
$$f_i \approx \exp\left(-\frac{0}{2\sigma^2}\right) = \exp(0) = 1$$

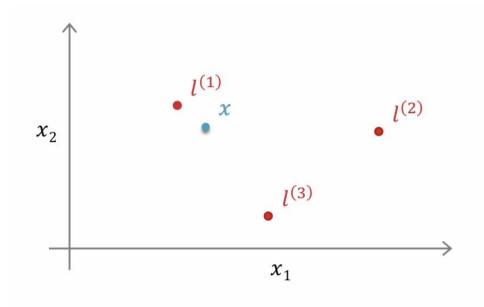
The second situation: x is too far from I (i)

$$f_i \approx \exp\left(-\frac{\infty}{2\sigma^2}\right) = \exp(-\infty) = 0$$

Example:

$$l^{(1)} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$$

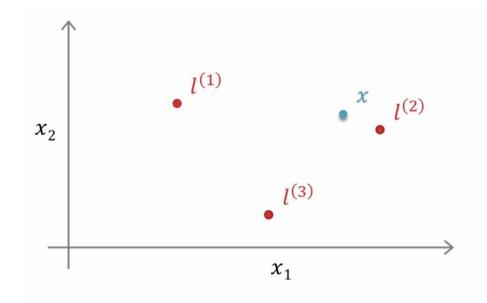




Prediction: y = 1 if:

$$f_1 \approx 1, f_2 \approx f_3 \approx 0$$

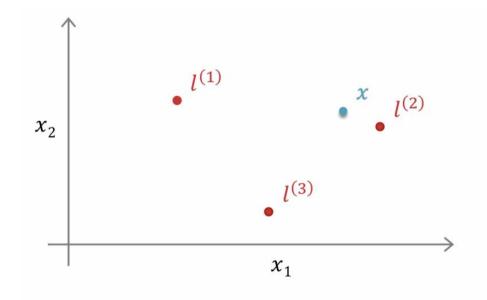
$$h_{\theta}(f) \approx -0.5 + (1.0)(1.0) + (1.0)(0.0) + (0.0)(0.0) = 0.5 \ge 0 \Rightarrow y = 1$$



Prediction: y = 1 if:

$$f_1 \approx f_3 \approx 0, f_2 \approx 1$$

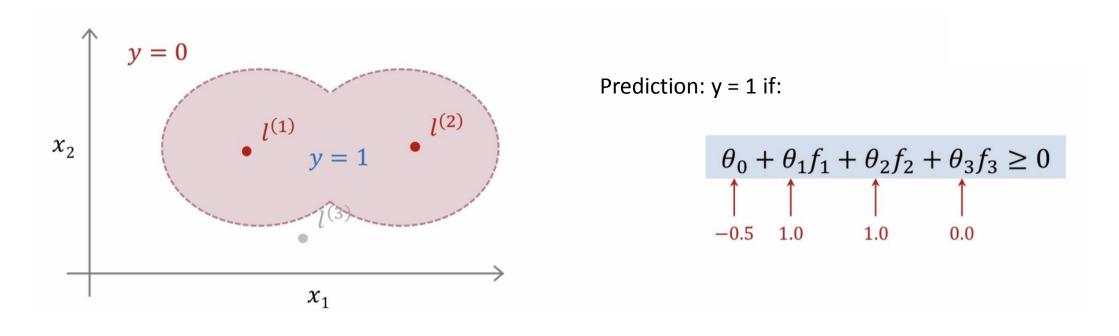
$$h_{\theta}(f) \approx -0.5 + (1.0)(0.0) + (1.0)(1.0) + (0.0)(0.0) = 0.5 \ge 0 \Rightarrow y = 1$$



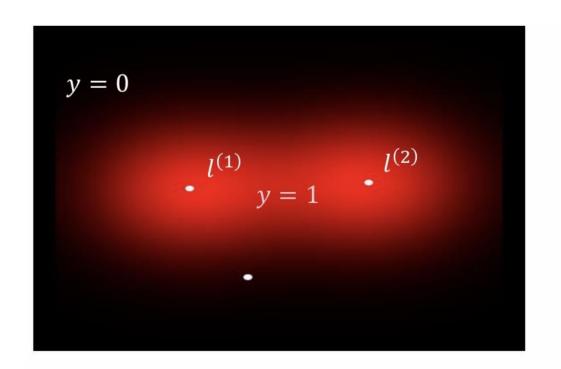
Prediction: y = 1 if:

$$f_1 \approx f_3 \approx 0, f_2 \approx 1$$

$$h_{\theta}(f) \approx -0.5 + (1.0)(0.0) + (1.0)(1.0) + (0.0)(0.0) = 0.5 \ge 0 \Rightarrow y = 1$$



• Decision boundary: it classifies points close to $I^{(1)}$ and $I^{(2)}$ in class 1 and other points in class zero.



Prediction: y = 1 if:

• Decision boundary: it classifies points close to $I^{(1)}$ and $I^{(2)}$ in class 1 and other points in class zero.

Remaining details:

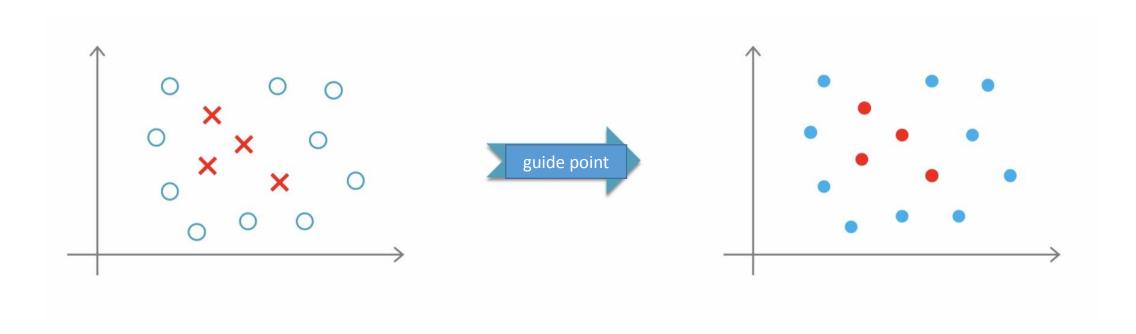
 Question: How does the learning algorithm automatically select guide points?

 Question: How are the appropriate values for kernel function parameters determined?

Question: Are there other types of kernels?

Selection of guide points

- Question: How does the learning algorithm automatically select guide points?
 - For each sample in the training set, a guide point equal to that sample is selected.



Mapping features

Training Set:

Guide Point:

Feature Area Mapping:

$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$$

$$l^{(1)} = x^{(1)}, l^{(2)} = x^{(2)}, \dots, l^{(m)} = x^{(m)}$$

$$x = \begin{bmatrix} x_0 = 1 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$
Feature
Area
Mapping
$$f = \begin{bmatrix} f_0 = 1 \\ f_1 = K(x, x^{(1)}) \\ f_2 = K(x, x^{(2)}) \\ \vdots \\ f_m = K(x, x^{(m)}) \end{bmatrix}$$

Kernel Trick

• Kernel function: preprocessing x data using kernel functions:

$$\mathbf{z} = \varphi(\mathbf{x})$$

$$= (\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x}), \dots, \varphi_k(\mathbf{x}))$$

$$g(\mathbf{z}) = \boldsymbol{\theta}^T \mathbf{z} + \theta_0$$
$$g(\mathbf{x}) = \boldsymbol{\theta}^T \varphi(\mathbf{x}) + \theta_0$$

It may be infinite!!

New data

classification:

$$\boldsymbol{\theta} = \sum_{t=1}^{m} \alpha^{t} y^{t} \mathbf{z}^{t} = \sum_{t=1}^{m} \alpha^{t} y^{t} \varphi(\mathbf{x}^{t})$$

$$g(\mathbf{x}) = \boldsymbol{\theta}^T \varphi(\mathbf{x}) + \theta_0 = \left(\sum_{t=1}^m \alpha^t y^t \varphi(\mathbf{x}^t)^T\right) \varphi(\mathbf{x}) + \theta_0 = \left(\sum_{t=1}^m \alpha^t y^t \varphi(\mathbf{x}^t)^T \varphi(\mathbf{x})\right) + \theta_0$$

$$g(\mathbf{x}) = \left(\sum_{t=1}^{m} \alpha^t y^t \mathbf{k}(\mathbf{x}^t, \mathbf{x})\right) + \theta_0$$

Decision Boundary

Kernel Functions

$$L_p = \frac{1}{2} \|\boldsymbol{\theta}\|^2 + C \sum_{t=1}^m \varepsilon^t$$

s.t.
$$y^t \boldsymbol{\theta}^T \varphi(\mathbf{x}^t) \ge 1 - \varepsilon^t$$

$$\varepsilon^t \geq 0$$

$$L_p = \frac{1}{2} \|\boldsymbol{\theta}\|^2 + C \sum_{t=1}^m \varepsilon^t - \sum_{t=1}^m \alpha^t [y^t \boldsymbol{\theta}^T \boldsymbol{\varphi}(\boldsymbol{x}^t) - 1 + \varepsilon^t] - \sum_{t=1}^m \mu^t \varepsilon^t$$

Lagrange factors

Lagrange factors

Kernel Functions: main issue

$$L_p = \frac{1}{2} \|\boldsymbol{\theta}\|^2 + C \sum_{t=1}^m \varepsilon^t - \sum_{t=1}^m \alpha^t [y^t \boldsymbol{\theta}^T \varphi(\boldsymbol{x}^t) - 1 + \varepsilon^t] - \sum_{t=1}^m \mu^t \varepsilon^t$$

$$\frac{\partial L_p}{\partial \boldsymbol{\theta}} = 0 \Rightarrow \boldsymbol{\theta} = \sum_{t=1}^m \alpha^t y^t \varphi(\boldsymbol{x}^t)$$

$$\frac{\partial L_p}{\partial s^t} = 0 \Rightarrow C - \alpha^t - \mu^t = 0 \Rightarrow 0 \le \alpha^t \le C$$

Kernel functions: Dugan's problem

$$L_{d} = -\frac{1}{2} \sum_{t=1}^{m} \sum_{s=1}^{m} \alpha^{t} \alpha^{s} y^{t} y^{s} \varphi(x^{t})^{T} \varphi(x^{s}) + \sum_{t=1}^{m} \alpha^{t}$$

subject to $\sum_{t=1}^{m} \alpha^t y^t = 0$ and $0 \le \alpha^t \le C \ \forall t$

The idea of kernel machines (kernel trick):

Replacing the inner product of basis functions with a kernel function in the form of $K(x^t, x^s)$

$$L_{d} = -\frac{1}{2} \sum_{t=1}^{m} \sum_{s=1}^{m} \alpha^{t} \alpha^{s} y^{t} y^{s} K(\mathbf{x}^{t}, \mathbf{x}^{s}) + \sum_{t=1}^{m} \alpha^{t}$$

Geram matrix: A symmetric and positive definite matrix (for linear separability)

Kernel functions: polynomial kernel

• Polynomial Kernel: A polynomial of degree q.

$$K(x^t, x) = (x^T x^t + 1)^q$$

• Example: [q = 2, d = 2]

3 multiplication, 2 sum

6 multiplication, 5 sum

$$K(x,y) = (x^{T}y + 1)^{2}$$

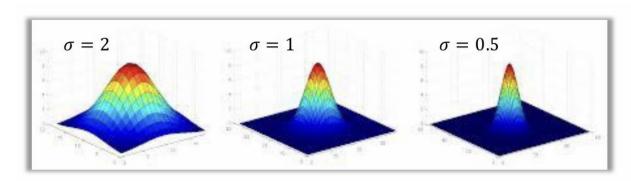
$$= (x_{1}y_{1} + x_{2}y_{2} + 1)^{2}$$

$$= 1 + 2x_{1}y_{1} + 2x_{2}y_{2} + 2x_{1}x_{2}y_{1}y_{2} + x_{1}^{2}y_{1}^{2} + x_{2}^{2}y_{2}^{2}$$

$$\varphi(x) = \left[1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2\right]^T$$

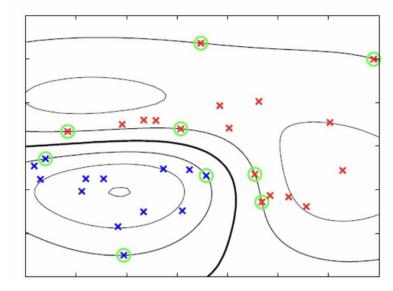
$$\varphi(y) = \left[1, \sqrt{2}y_1, \sqrt{2}y_2, \sqrt{2}y_1y_2, y_1^2, y_2^2\right]^T$$

Gaussian Kernel Function



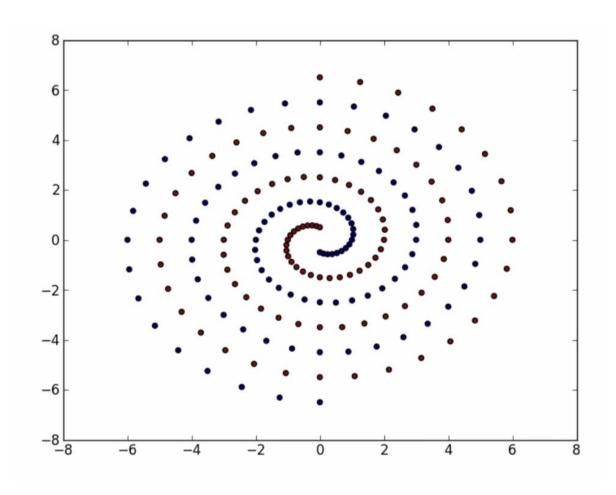
Gaussian Kernel Function:

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

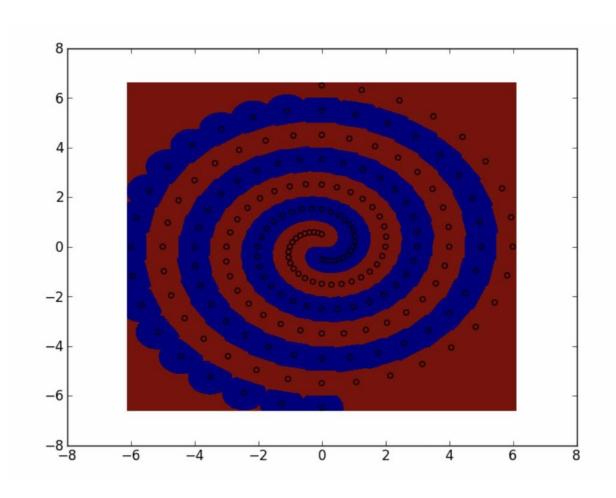


Finding a suitable value for sigma:
Using the validation set (model selection)
Larger values: smoother decision boundary

Example: Gaussian Kernel Function

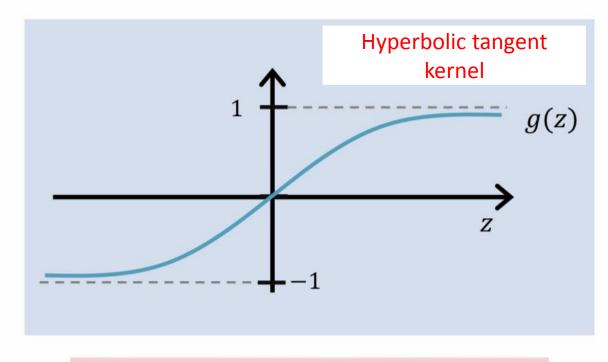


Example: Gaussian Kernel Function



Kernel Functions: Other Kinds

- Kernel function: a measure to calculate the similarity between x and y data.
- Other types:
- Hyperbolic tangent kernel
- Threaded kernel
- tree kernel
- Cornellography



$$K(x^t, x) = \tanh(2x^T x^t + 1)$$

SVM Parameters

- Question: How are the appropriate values for kernel function parameters determined?
- Parameter C:
- Smaller values: more bias, less variance
- Larger values: less bias, more variance
- Sigma parameter:
- Smaller values: less bias, more variance
- Larger values: more bias, less variance

Determining the values of both parameters:
Search networking

Multiclass classification

- First method: one against all (preferred method)
 - Training: training k support vector machines, one for each class
 - Experiment: Calculate $g_i(x)$ for $0 \le l \le k$ and choose the largest value

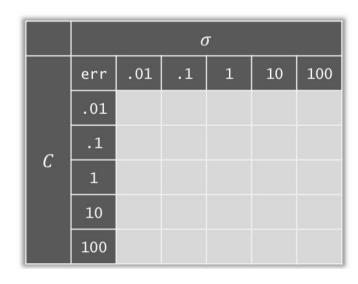
 $\arg\max_i g_i(x)$

- The second method: separating two by two
 - Training k(k-1)/2 support vector machine such that $g_{ij}(x)$ separates examples of two classes C_i and C_i .
 - Simpler and faster
- The third method: solving a multi-class optimization problem

$$\min \frac{1}{2} \sum_{i=1}^{k} ||\boldsymbol{\theta}_i||^2 + C \sum_{i} \sum_{t} \varepsilon_i^t$$
s.t.
$$\boldsymbol{\theta}_{z^t} \boldsymbol{x}^t + \boldsymbol{\theta}_{z^t 0} \ge \boldsymbol{\theta}_i \boldsymbol{x}^t + \boldsymbol{\theta}_{i0} + 2 - \varepsilon_i^t, \forall i \neq z^t$$

A guide to using SVM

- Implementation:
 - Using existing software packages such as LIBSVM and SVM light
- Determine the kernel function:
 - Linear kernel (not using kernel): when n is much larger than m.
 - Gaussian, polynomial, string and...
- Determining the value of parameters: grid search
 - Select a value for the C parameter
 - Value selection for kernel function parameters (such as sigma)



SVM, Logistic Regression or Neural Network?

- Case 1: (n much larger than m)
 - Example: Spam detection (1000 training examples, 50000 features)
 - Logistic regression or linear SVM
- Situation 2: (low number of features, high number of training samples)
 - SVM with Gaussian kernel
- Note: Neural networks can be used in all the above situations, but they may need more time for training.

More about Kernels

- Question: How do we know that the use of kernels helps us in separating data?
- In n-dimensional space, any set of n independent vectors are linearly separable.
- If the matrix K is a positive definite matrix, then the data are linearly separable.
- Theorem: The matrix K is a positive definite matrix, because $K = L^{T}L$
- column i in matrix L is equal to vector $\Phi(x^{(i)})$
- Proof: Consider a non-zero vector v. in this case:
- And since L and v are both opposite to zero,

vector W is also opposite to zero. that's mean:

$$v^T K v = v^T L^T L v = (Lv)^T (Lv) = w^T w = ||w||^2 \ge 0$$

 $||w||^2 > 0 \Rightarrow v^T K v > 0 \Rightarrow K$ is positive definite