MLEA: Machine Learning

Kernels methods

Réda DEHAK
reda.dehak@epita.fr

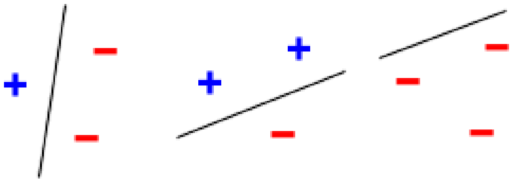
EPITA

January 22, 2020

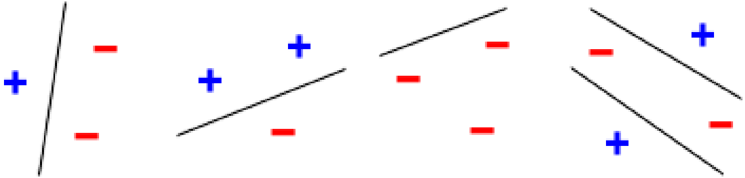
Vapnik-Chervonenkis dimension

- measure of the capacity of a statistical classification algorithm (how complicated it can be)
- cardinality of the largest set of points that the algorithm can shatter, for each possible combination of labels
- Core concept in Vapnik-Chervonenkis theory

Example



Example



VC dimension for a linear classifier handling data of dimension N: N + 1

VC dim-based model selection

Definition

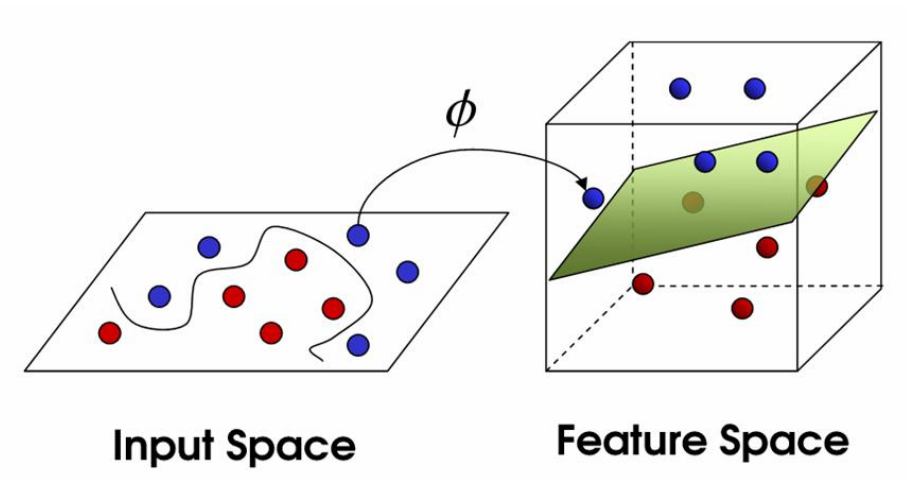
TestingSet Error $\leq$ TrainingSet Error $+ \sqrt{\frac{h(\log(2R/h)+1)-log(\mu/4)}{R}}$
With h the VC dimension of the classification model
R the size of the trainingset
True with probability $1-\mu$

Separability of patterns

Cover's Theorem (1965)

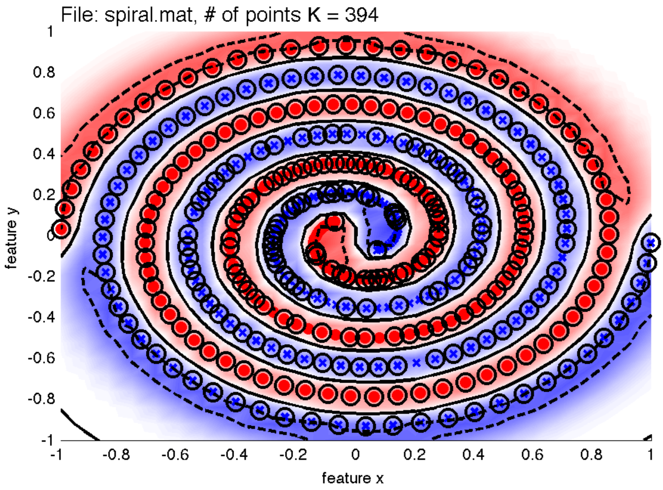
A complex pattern-classification problem cast in a high-dimensional space nonlinearly is more likely to be linearly separable than in low dimensional space

Feature Space projection



the two spirals

Separated by a hyperplane in feature space (gaussian kernels)



Feature and Feature Space

Definition

A function $\phi_i : \chi \to \mathbb{R}$ that maps each object $x \in \chi$ to a real value $\phi_i(x)$ is called a feature.
To be valid, $\forall x \in \chi, \phi_i(x)$ should be finite.

Feature and Feature Space

Definition

A function $\phi_i : \chi \to \mathbb{R}$ that maps each object $x \in \chi$ to a real value $\phi_i(x)$ is called a feature.
To be valid, $\forall x \in \chi, \phi_i(x)$ should be finite.
Combining n features $\phi_1 ... \phi_n$ results in a feature mapping $\phi : \chi \to \kappa \subseteq \mathbb{R}^n$ and the space κ is called a feature space.

Kernel

Definition

Suppose we are given a feature mapping $\phi : \chi \to \kappa \subseteq \mathbb{R}^n$
The corresponding kernel is the inner product function
$K : \chi \times \chi \to \mathbb{R}$ such as:

$$K(x_i, x_j) = < \phi(x_i), \phi(x_j) >$$

The kernel trick for SVM

- Replace dot product by kernel functions
- the dot product is done in the feature space

SVM reformulation

- Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$
  $\Rightarrow$

SVM reformulation

- Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$
  $\Rightarrow$Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j K(x_i, x_j)$
- Decision function: $f(x) = w^T x + b$

SVM reformulation

- Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$
  $\Rightarrow$Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j K(x_i, x_j)$
- Decision function: $f(x) = w^T x + b = \sum \alpha_i y_i \langle x_i, x \rangle + b$

SVM reformulation

- Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$
  $\Rightarrow$Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j K(x_i, x_j)$
- Decision function: $f(x) = w^T x + b = \sum \alpha_i y_i \langle x_i, x \rangle + b$
  $\Rightarrow$

SVM reformulation

- Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \langle x_i, \, x_j \rangle$
  $\Rightarrow$Maximize $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j K(x_i, x_j)$
- Decision function: $f(x) = w^T x + b = \sum \alpha_i y_i \langle x_i, \, x \rangle + b$
  $\Rightarrow f(x) = \sum \alpha_i y_i K(x_i, x) + b$

Example: XOR problem revisited

4 points dataset :

Data	**Class**
$(-1, -1)$	-1
$(-1, +1)$	$+1$
$(+1, -1)$	$+1$
$(+1, +1)$	-1

Find the Large margin SVM corresponding to the dataset using the polynomial Kernel $K(x, y) = (1 + x^t y)^2$.

Example: XOR problem revisited

4 points dataset :

Data	**Class**
$(-1,-1)$	-1
$(-1,+1)$	$+1$
$(+1,-1)$	$+1$
$(+1,+1)$	-1

Find the Large margin SVM corresponding to the dataset using the polynomial Kernel $K(x,y) = (1 + x^t y)^2$.
Consider $x = [x_1, x_2]^t$ and $y = [y_1, y_2]^t$.
The feature mapping is quite explicit:

$$K(x,y) = 1 + x_1^2 y_1^2 + 2x_1x_2y_1y_2 + x_2^2 y_2^2 + 2x_1y_1 + 2x_2y_2$$

The projection of x in the feature space is :

$$\phi(x) = [1, x_1^2, \sqrt{2}x_1x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2]^t$$

Common Kernels

- Linear : $K(x, y) = x^T y$
- Polynomial : $K(x, y) = (x^T y + 1)^d$
- Laplacian RBF : $exp\left(-\gamma\|x - y\|\right) = exp\left(-\frac{\|x-y\|}{\sigma^2}\right)$
- RBF : $K(x, y) = exp(-\gamma\|x - y\|^2) = exp(-\frac{\|x-y\|^2}{\sigma^2})$

Common Kernels

- Linear : $K(x, y) = x^T y$
- Polynomial : $K(x, y) = (x^T y + 1)^d$
- Laplacian RBF : $exp\left(-\gamma\|x - y\|\right) = exp\left(-\frac{\|x-y\|}{\sigma^2}\right)$
- RBF : $K(x, y) = exp(-\gamma\|x - y\|^2) = exp(-\frac{\|x-y\|^2}{\sigma^2})$
- RTFL...

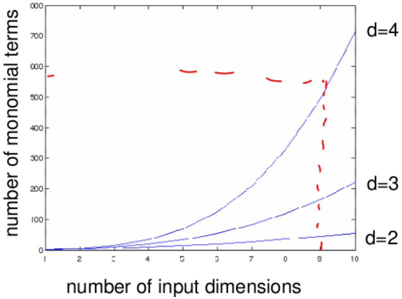
Exercise: Kernel VC Dimension

Give the VC dimension of a SVM using:

- Linear Kernel
- RBF Kernel
- Polynomial Kernel

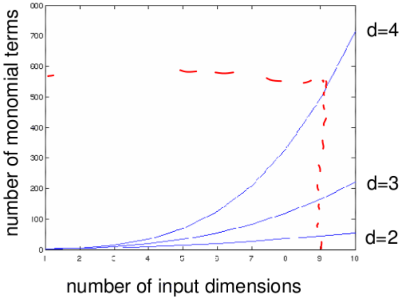
Polynomial Kernel Mapping

$$dim = \binom{d+m}{d} = \frac{(d+m)!}{d!m!}$$



Polynomial Kernel Mapping

$$dim = \binom{d+m}{d} = \frac{(d+m)!}{d!m!}$$



- implicit mapping not necessary
- allow to project the data to infinite feature space

Positive semi-definite Kernel Function

Definition

A kernel function K is said to be positive semi-definite if

$$\forall (x_1, .., x_n) \in \chi^n, \forall (c_1, .., c_n) \in \mathbb{R}^n \neq 0$$

$$\sum_{i,j} K(x_i, x_j) c_i c_j \geq 0$$

Gram matrix

Definition

Given a kernel K: $\chi \times \chi \rightarrow \mathbb{R}$ and a set $\mathbf{x} = (x_1, ..., x_m) \in \chi^m$ of m objects in χ, we call the $m \times m$ matrix $\mathbf{G}$ with:

$$\mathbf{G_{ij}} = K(x_i, x_j)$$

the Gram matrix of K at x.

Lemma

Definition

A $N \times N$ matrix $\mathcal{M}$ is said to be positive semi-definite if and only if:

$$\forall v \in \mathbb{R}^N, v^T \mathcal{M} v \geq 0$$

Lemma

Given a positive semi-definite kernel function K

$$\forall \mathbf{x} = (x_1, ..., x_m) \in \chi^m$$

the corresponding Gram Matrix $\mathbf{G}$ will be positive semi-definite.

Mercer Theorem

Theorem

If K is a positive semi-definite kernel then there exists a function ϕ such that:

$$K(x, y) = < \phi(x), \phi(y) >$$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$
- $K(x, y) = a\,K_1(x, y)$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$
- $K(x, y) = a\, K_1(x, y)$
- $K(x, y) = K_1(x, y) K_2(x, y)$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$
- $K(x, y) = a\,K_1(x, y)$
- $K(x, y) = K_1(x, y)K_2(x, y)$
- $K(x, y) = f(x)f(y)$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$
- $K(x, y) = a\, K_1(x, y)$
- $K(x, y) = K_1(x, y) K_2(x, y)$
- $K(x, y) = f(x) f(y)$
- $K(x, y) = K_3(\phi(x), \phi(y))$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$
- $K(x, y) = a\,K_1(x, y)$
- $K(x, y) = K_1(x, y)K_2(x, y)$
- $K(x, y) = f(x)f(y)$
- $K(x, y) = K_3(\phi(x), \phi(y))$
- $K(x, y) = x^t By$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$
- $K(x, y) = a\, K_1(x, y)$
- $K(x, y) = K_1(x, y)K_2(x, y)$
- $K(x, y) = f(x)f(y)$
- $K(x, y) = K_3(\phi(x), \phi(y))$
- $K(x, y) = x^t B y$
- $K(x, y) = \frac{K(x,y)}{\sqrt{K(x,x)K(y,y)}}$

Kernel Properties

Let K_1 and K_2 be kernels over χ, $a \geq 0$, B a symmetric positive semi-definite matrix, and K_3 a kernel over $\mathbb{R}^n$. Prove the following functions are kernels:

- $K(x, y) = K_1(x, y) + K_2(x, y)$
- $K(x, y) = a\,K_1(x, y)$
- $K(x, y) = K_1(x, y)K_2(x, y)$
- $K(x, y) = f(x)f(y)$
- $K(x, y) = K_3(\phi(x), \phi(y))$
- $K(x, y) = x^t By$
- $K(x, y) = \frac{K(x,y)}{\sqrt{K(x,x)K(y,y)}}$

Kernel Properties

Prove the following functions are kernels:

- $K(x, y) = p(K_1(x, y))$ with $p(x)$ a polynomial with positive coefficients

Kernel Properties

Prove the following functions are kernels:

- $K(x, y) = p(K_1(x, y))$ with $p(x)$ a polynomial with positive coefficients
- $K(x, y) = exp(K_1(x, y))$

Kernel Properties

Prove the following functions are kernels:

- $K(x, y) = p(K_1(x, y))$ with $p(x)$ a polynomial with positive coefficients
- $K(x, y) = exp(K_1(x, y))$
  Help: $exp(x) = \sum_{i=0}^{\infty} \frac{x^i}{i!}$

Kernel Properties

Prove the following functions are kernels:

- $K(x, y) = p(K_1(x, y))$ with $p(x)$ a polynomial with positive coefficients
- $K(x, y) = exp(K_1(x, y))$
  Help: $exp(x) = \sum_{i=0}^{\infty} \frac{x^i}{i!}$
- $K(x, y) = exp(-\frac{\|x-y\|^2}{2\sigma^2})$

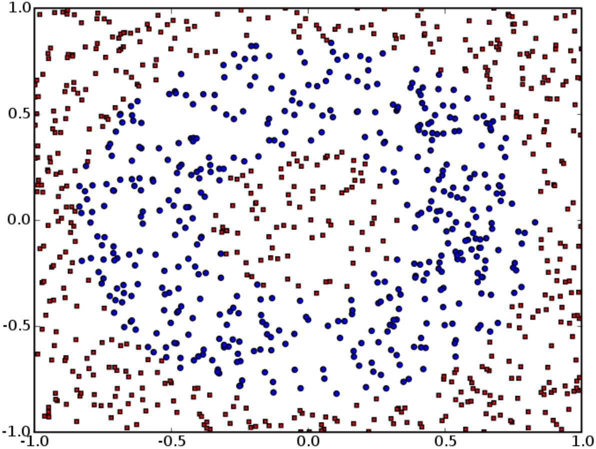
Kernels in practice

- Data should be centered and reduced
- if the number of feature is large, non linear mapping may not improve performances

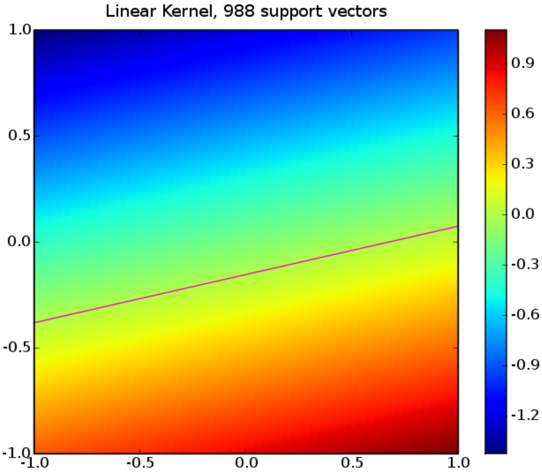
Kernels in practice

- Data should be centered and reduced
- if the number of feature is large, non linear mapping may not improve performances
- moreover it will be much slower!!
- Don't start with the RBF Kernel.

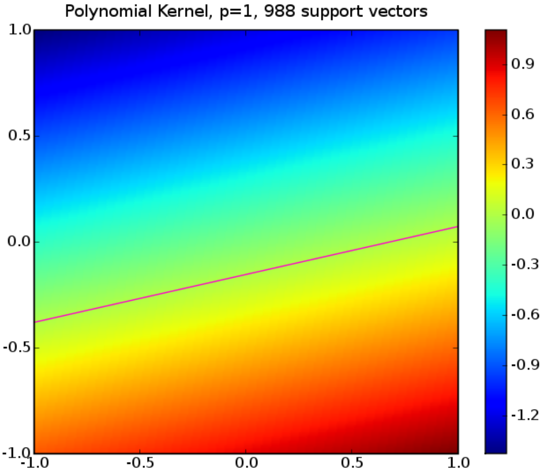
Donut...



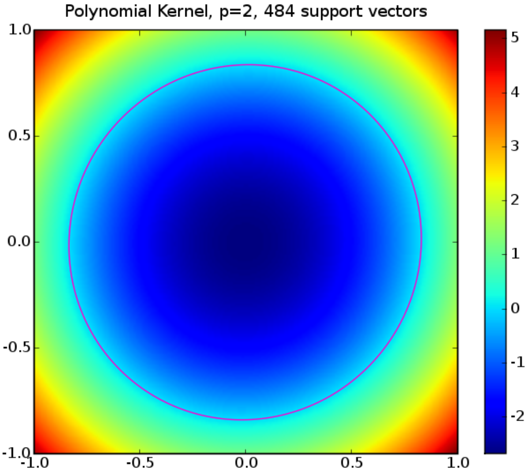
Linear Kernel



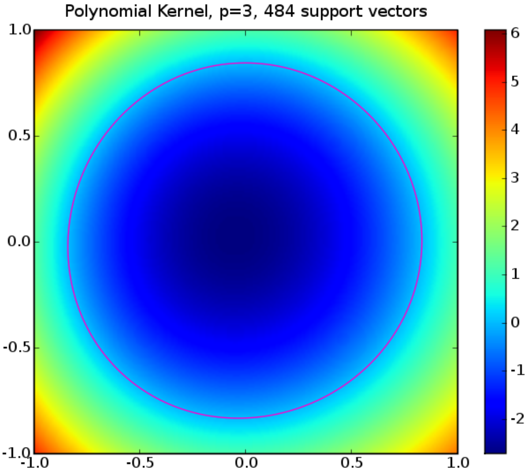
Polynomial Kernel



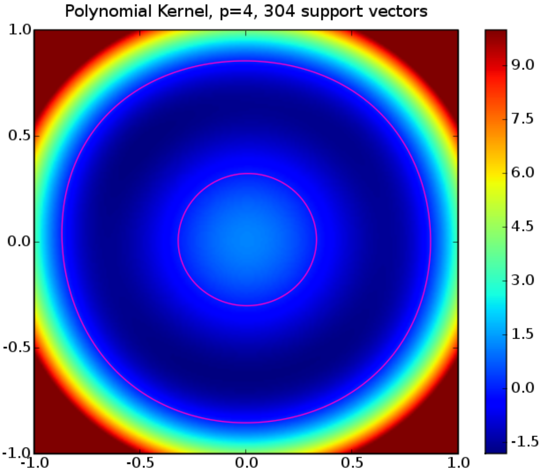
Polynomial Kernel



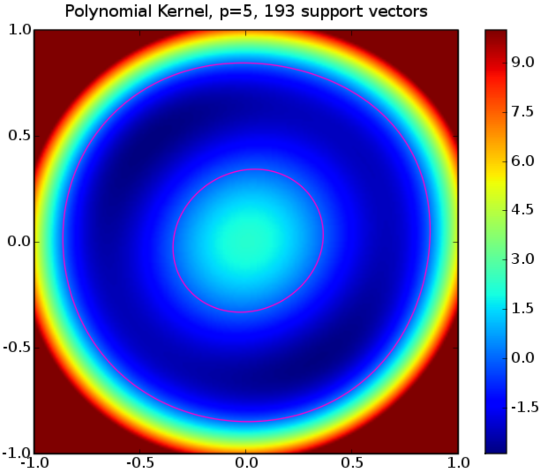
Polynomial Kernel



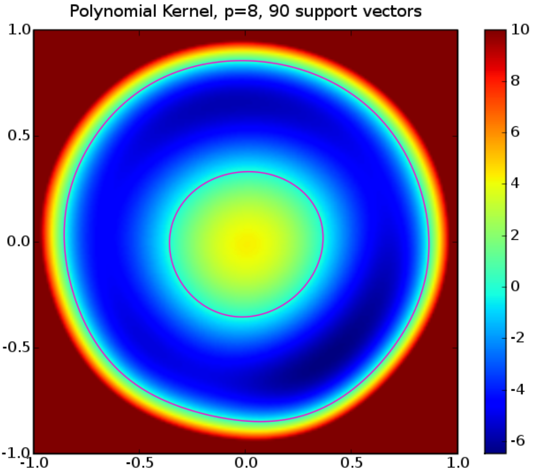
Polynomial Kernel



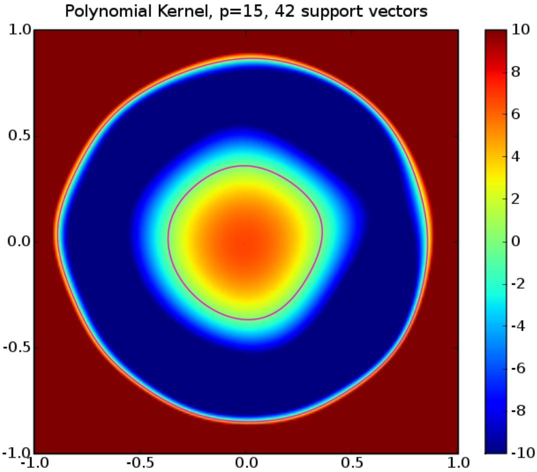
Polynomial Kernel



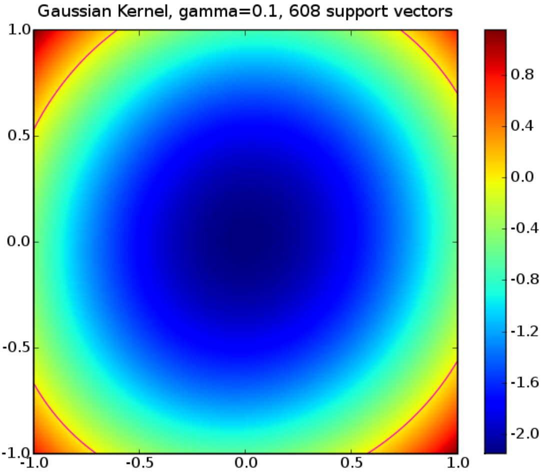
Polynomial Kernel



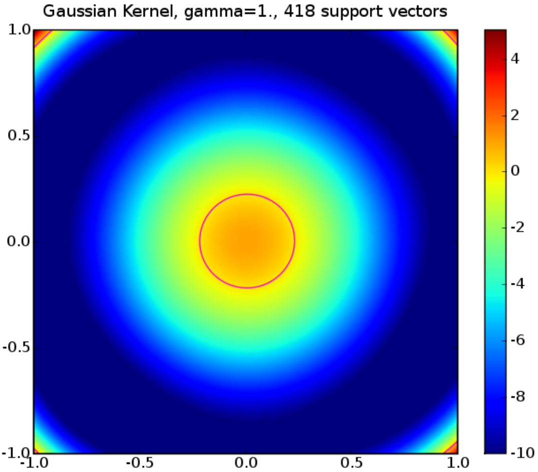
Polynomial Kernel



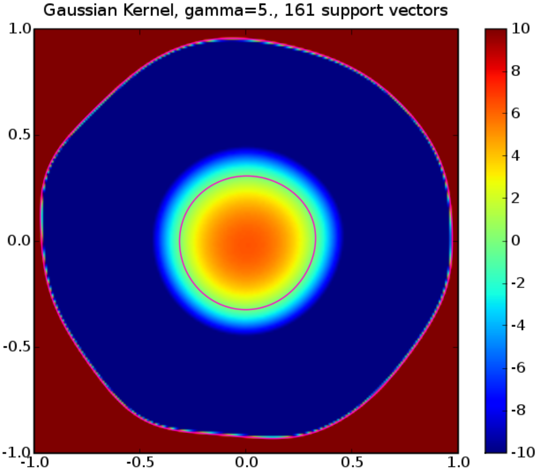
Gaussian Kernel



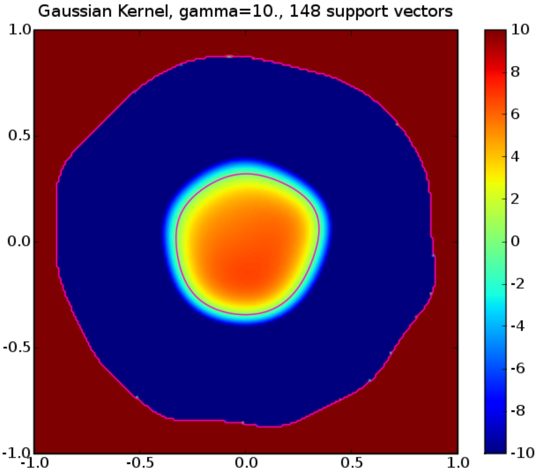
Gaussian Kernel



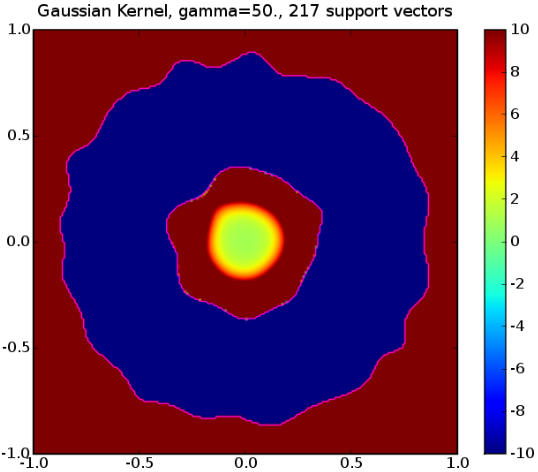
Gaussian Kernel



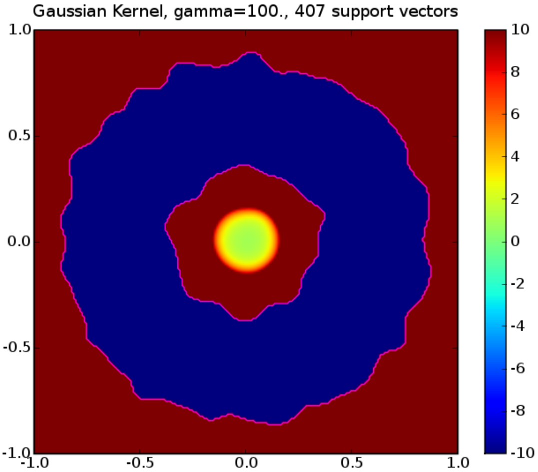
Gaussian Kernel



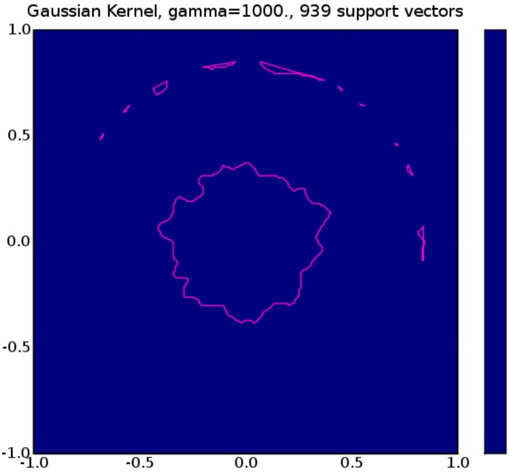
Gaussian Kernel



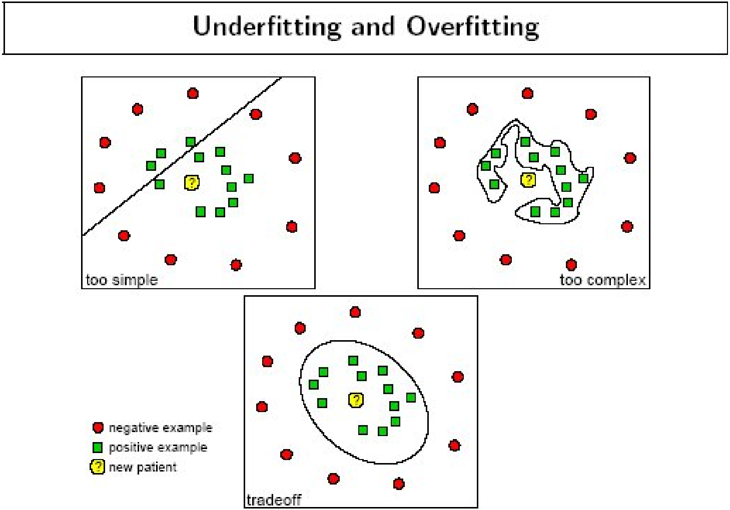
Gaussian Kernel



Gaussian Kernel



SVM parameters should be chosen wisely



Kernel trick

- Is there other algorithms such that we don't need to know ϕ?
- Compute L_2 distance in feature space

Kernel trick

- Is there other algorithms such that we don't need to know ϕ?
- Compute L_2 distance in feature space

$$
\begin{aligned}
\|\phi(x) - \phi(y)\|^2 &= (\phi(x) - \phi(y))^T(\phi(x) - \phi(y)) \\
&= \phi(x)^T\phi(x) + \phi(y)^T\phi(y) - 2\phi(x)^T\phi(y) \\
&= K(x,x) + K(y,y) - 2K(x,y)
\end{aligned}
$$

Kernel KMeans

Kernel KMeans

1. Compute Class center

$$\mu_c = \frac{1}{|C_c|} \sum_{x_i \in C_c} \phi(x_i)$$

Kernel KMeans

1. Compute Class center

$$\mu_c = \frac{1}{|C_c|} \sum_{x_i \in C_c} \phi(x_i)$$

2. Compute distance between example and Class center

$$\begin{aligned}
\|\phi(x) - \mu_c\|^2 &= (\phi(x) - \mu_c)^T(\phi(x) - \mu_c) \\
&= \phi(x)^T\phi(x) - 2\phi(x)^T\mu_c + \mu_c^T\mu_c \\
&= K(x,x) - \frac{2}{|C_c|} \sum_{x_i \in C_c} \phi(x)^T\phi(x_i) \\
&\quad + \frac{1}{|C_c|^2} \sum_{x_i \in C_c} \sum_{x_j \in C_c} \phi(x_i)^T\phi(x_j)
\end{aligned}$$

Kernel KMeans

1. Compute Class center

$$\mu_c = \frac{1}{|C_c|} \sum_{x_i \in C_c} \phi(x_i)$$

2. Compute distance between example and Class center

$$\|\phi(x) - \mu_c\|^2 = K(x,x) - \frac{2}{|C_c|} \sum_{x_i \in C_c} K(x, x_i) + \frac{1}{|C_c|^2} \sum_{x_i \in C_c} \sum_{x_j \in C_c} K(x_i, x_j)$$