Kernel methods

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Kernel trick

Perform feature transformation: $x \to \phi(x)$. Scalar product becomes $\langle x, x' \rangle \to \langle \phi(x), \phi(x') \rangle = K(x, x')$

Kernel trick

Define not the feature representation x but only scalar product function $K(x, x')$

- Comments:
  - required that the solution depends only on scalar products.Kernels can be constructed from other kernels, for example from:
    1. scalar product $\langle x, x' \rangle$
    2. constant $K(x, x') \equiv 1$
    3. $x^T A x$ for any $A \succcurlyeq 0$[1]
  - feature representation $\phi(x)$ not needed
  - $\langle x, x' \rangle$ has complexity $O(D)$. Complexity of $K(x, x')$ may be $O(1)$.
  - we can define natural linear kernel:

Kernelizable algorithms

- ridge regression:
- K-NN
- K-means
- PCA
- SVM
- many more...

Kernel trick use cases

- high-dimensional data
  - polynomial of order up to M
  - Gaussian kernel $K(x, x') = e^{-\frac{1}{2\sigma^2}\left\|x-x'\right\|^2}$ corresponds to infinite-dimensional feature space.
- hard to vectorize data
  - strings, sets, images, texts, graphs, 3D-structures, sequences, etc.
- natural scalar product exist
  - strings: number of co-occuring substrings
  - sets: size of intersection of sets
    - example: for sets S_1 and S_2: $K(S_1, S_2) = 2^{|S_1 \cap S_2|}$ is a possible kernel.
  - etc.
- scalar product can be computed efficiently

General motivation for kernel trick

- perform generalization of linear methods to non-linear case
    - as efficient as linear methods
    - local minimum is global minimum
    - no local optima=>less overfitting
- non-vectorial objects
    - hard to obtain vector representation

Kernel definition

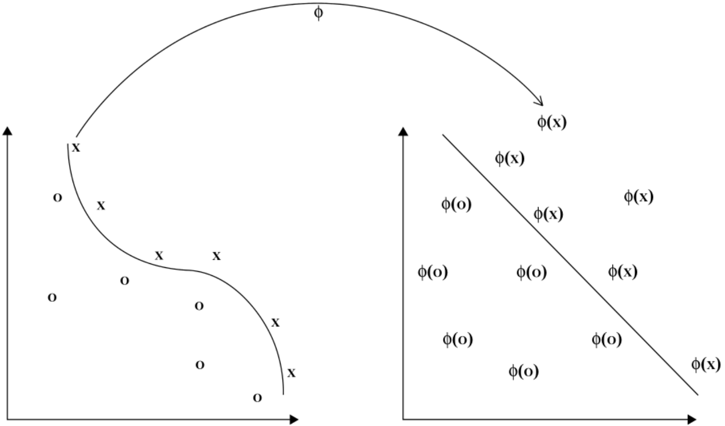
- x is replaced with $\phi(x)$
  - Example: $[x] \to [x,\, x^2,\, x^3]$

Kernel

Function $K(x,x'): X \times X \to \mathbb{R}$ is a kernel function if it may be represented as $K(x,x') = \langle \phi(x), \phi(x') \rangle$ for some mapping $\phi: X \to H$, with scalar product defined on H.

- $\langle x, x' \rangle$ is replaced by $\langle \phi(x), \phi(x') \rangle = K(x,x')$

Illustration



Specific types of kernels

- $K(x, x') = K(x - x')$ - stationary kernels (invariant to translations)
- $K(x, x') = K(\|x - x'\|)$ - radial basis functions

Polynomial kernel[2]

- Example 1: let $D=2$.

$$\begin{aligned}K(x,z) &= (x^T z)^2 = (x_1 z_1 + x_2 z_2)^2 = \\ &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 z_1 x_2 z_2 \\ &= \phi^T(x)\phi(z)\end{aligned}$$

for $\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1 x_2)$

[2] What kind of feature transformation will correspond to $K(x,z) = (x^T z)^M$ for arbitrary M and D?

Polynomial kernel[3]

- Example 2: let $D=2$.

$$\begin{aligned} K(x,z) &= (1+x^T z)^2 = (1+x_1 z_1 + x_2 z_2)^2 = \\ &= 1 + x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 z_1 + 2x_2 z_2 + 2x_1 z_1 x_2 z_2 \\ &= \phi^T(x)\phi(z) \end{aligned}$$

for $\phi(x) = (1,\, x_1^2,\, x_2^2,\, \sqrt{2}x_1,\, \sqrt{2}x_2,\, \sqrt{2}x_1 x_2)$

[3] What kind of feature transformation will correspond to $K(x,z) = (1+x^T z)^M$ kernels for arbitrary M and D?

Kernel properties

Theorem (Mercer): Function $K(x, x')$ is a kernel is and only if

- it is symmetric: $K(x, x') = K(x', x)$
- it is non-negative definite:
  - definition 1: for every function $g : X \to \mathbb{R}$

$$\int_X \int_X K(x, x') g(x) g(x') dx dx' \geq 0$$

  - definition 2 (equivalent): for every finite set $x_1, x_2, ...x_M$ Gramm matrix $\{K(x_i, x_j)\}_{i,j=1}^M \succeq 0$ (p.s.d.)

Kernel construction

- Kernel learning - separate field of study.
- Hard to prove non-negative definitness of kernel in general.
- Kernels can be constructed from other kernels, for example from:
  1. scalar product $\langle x, x' \rangle$
  2. constant $K(x, x') \equiv 1$
  3. $x^T A x$ for any $A \succcurlyeq 0$[4]

[4] Under what feature transformation will case 1 transform to cases 2 and 3? You may use Choletsky decomposition.

Constructing kernels from other kernels

If $K_1(x, x')$, $K_2(x, x')$ are arbitrary kernels, $c > 0$ is a constant, $q(\cdot)$ is a polynomial with non-negative coefficients, $h(x)$ and $\varphi(x)$ are arbitrary functions $\mathcal{X} \to \mathbb{R}$ and $\mathcal{X} \to \mathbb{R}^M$ respectively, then these are valid kernels[5]:

1. $K(x, x') = cK_1(x, x')$
2. $K(x, x') = K_1(x, x')K_2(x, x')$
3. $K(x, x') = K_1(x, x') + K_2(x, x')$
4. $K(x, x') = K_1(\varphi(x), \varphi(x'))$
5. $K(x, x') = h(x)K_1(x, x')h(x')$
6. $K(x, x') = e^{K_1(x, x')}$

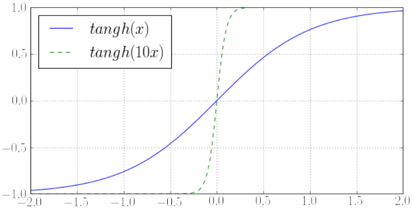
[5] prove some of these statements

Commonly used kernels

Let x and x' be two objects.

Kernel	Mathematical form
linear	$\langle x, x' \rangle$
polynomial	$(\gamma \langle x, x' \rangle + r)^d$
RBF	$\exp(-\gamma \left\| x - x' \right\|^2)$

- Standard transformation is also sigmoid=tangh$(\gamma \langle x, y \rangle + r)$ but its not a Mercer kernel.



Addition[6]

- Other kernelized algorithms: K-NN, K-means, K-medoids, nearest medoid, PCA, SVM, etc.
- Kernelization of distance:

[6] How can we calculate scalar product between normalized (unit norm) vectors $\phi(x)$ and $\phi(x')$?

Addition[6]

- Other kernelized algorithms: K-NN, K-means, K-medoids, nearest medoid, PCA, SVM, etc.
- Kernelization of distance:

$$
\begin{aligned}
\rho(x, x')^2 &= \langle \phi(x) - \phi(x'), \phi(x) - \phi(x') \rangle \\
&= \langle \phi(x), \phi(x) \rangle + \langle \phi(x'), \phi(x') \rangle - 2\langle \phi(x), \phi(x') \rangle \\
&= K(x, x) + K(x', x') - 2K(x, x')
\end{aligned}
$$

[6] How can we calculate scalar product between normalized (unit norm) vectors $\phi(x)$ and $\phi(x')$?

Table of Contents

Linear SVM reminder

- Solution for weights:

$$w = \sum_{i \in \mathcal{SV}} \alpha_i y_i x_i$$

Discriminant function

$$g(x) = \sum_{i \in \mathcal{SV}} \alpha_i y_i \langle x_i, x \rangle + w_0$$

$$w_0 = \frac{1}{n_{\widetilde{\mathcal{SV}}}} \left(\sum_{j \in \widetilde{\mathcal{SV}}} y_j - \sum_{j \in \widetilde{\mathcal{SV}}} \sum_{i \in \mathcal{SV}} \alpha_i y_i \langle x_i, x_j \rangle \right)$$

where $SV = \{i : y_i(x_i^T w + w_0) \le 1)\}$ are indexes of all support vectors and $\tilde{SV} = \{i : y_i(x_i^T w + w_0) = 1\}$ are boundary support vectors.

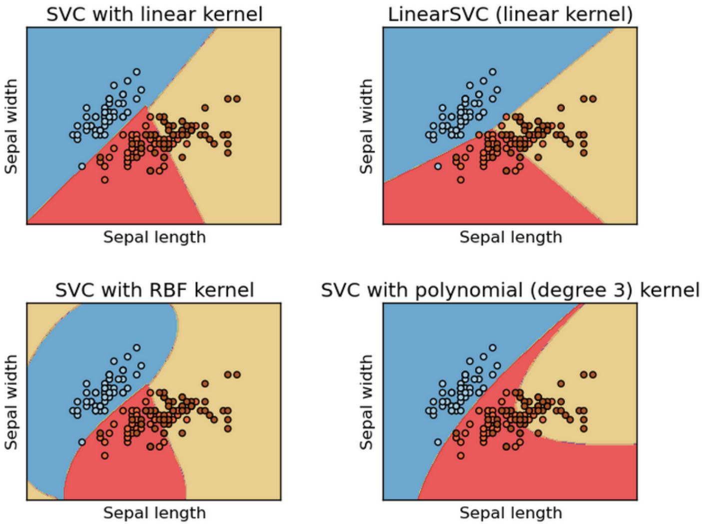
Kernel SVM

Discriminant function

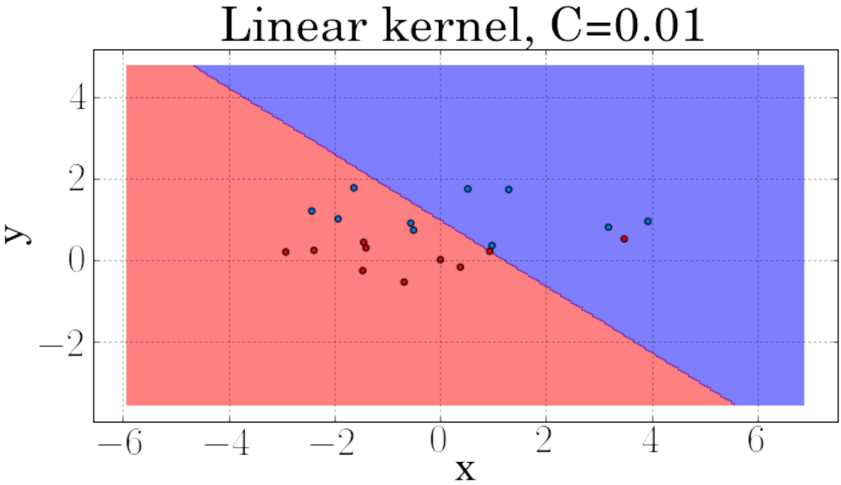
$$g(x) = \sum_{i \in \mathcal{SV}} \alpha_i y_i K(x_i, x) + w_0$$

$$w_0 = \frac{1}{n_{\widetilde{\mathcal{SV}}}} \left(\sum_{j \in \widetilde{\mathcal{SV}}} y_j - \sum_{j \in \widetilde{\mathcal{SV}}} \sum_{i \in \mathcal{SV}} \alpha_i y_i K(x_i, x_j) \right)$$

Kernel results



Linear kernel - variable C



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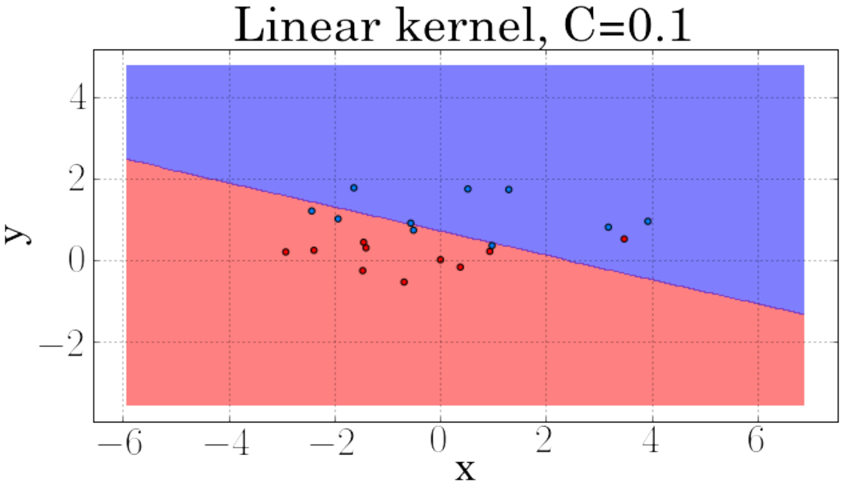

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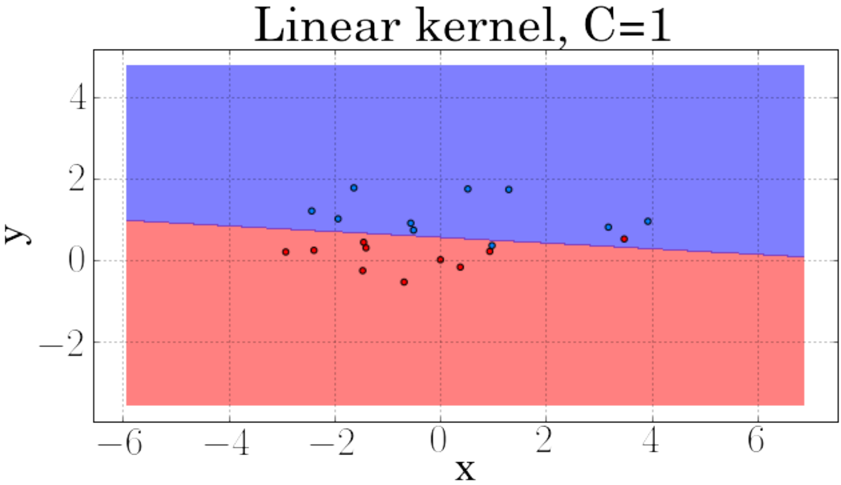

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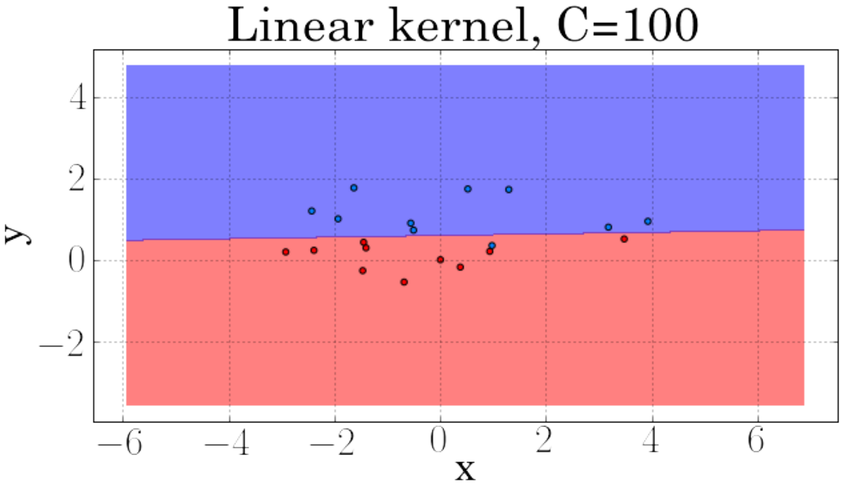
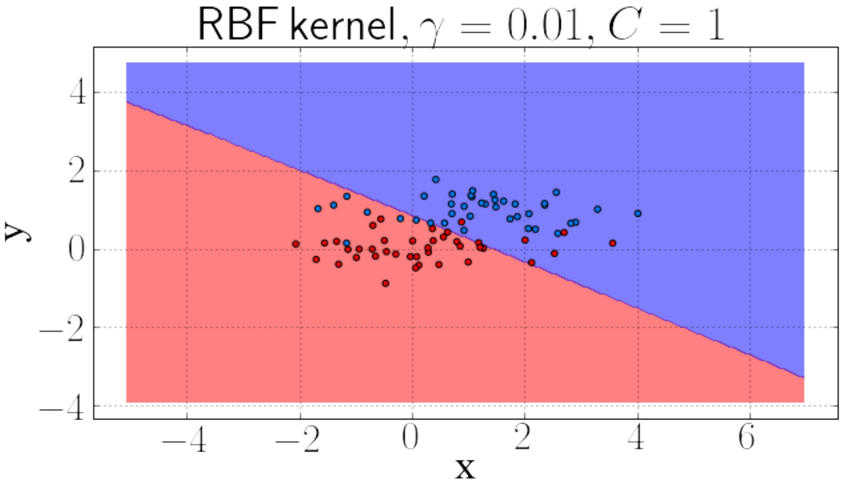


RBF kernel - variable γ



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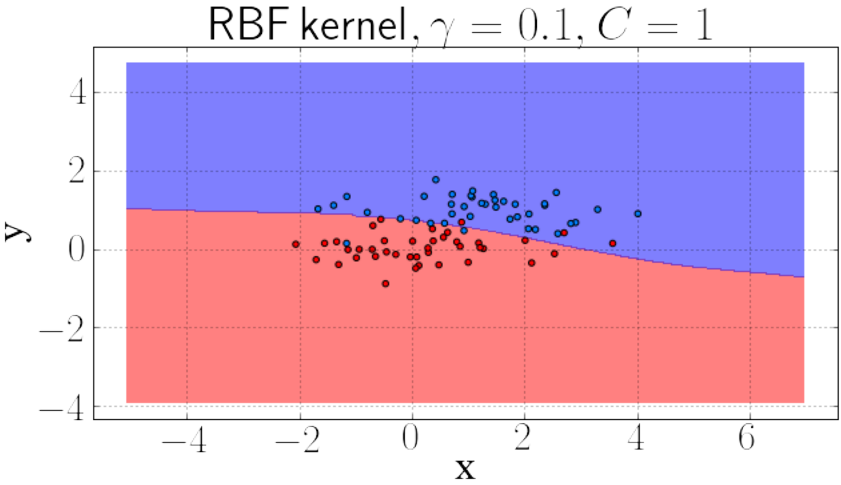

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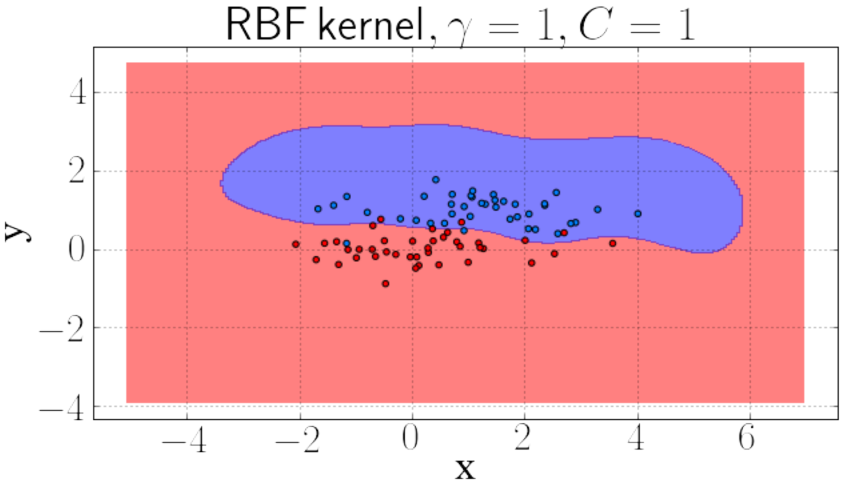

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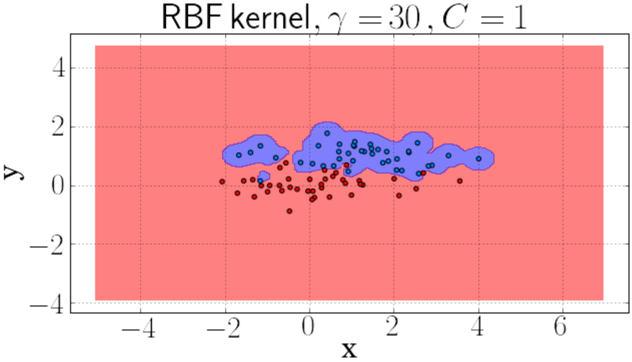

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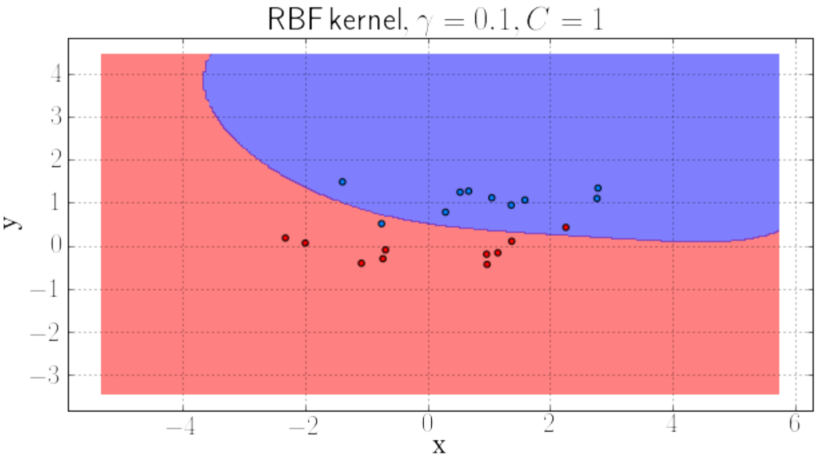

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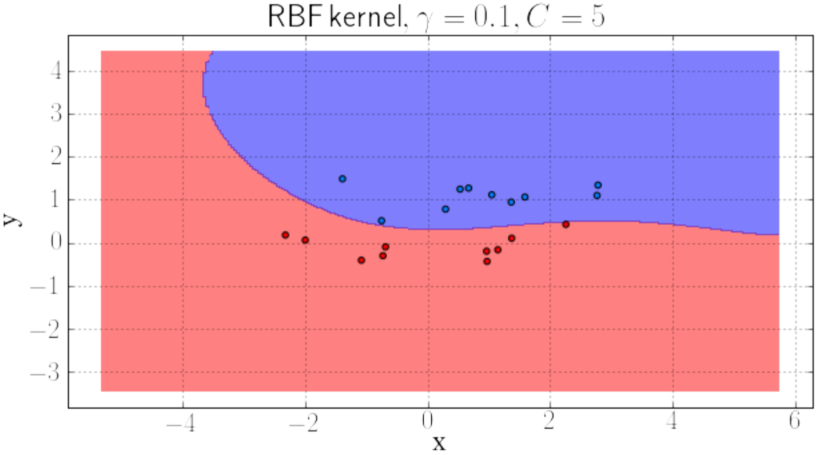

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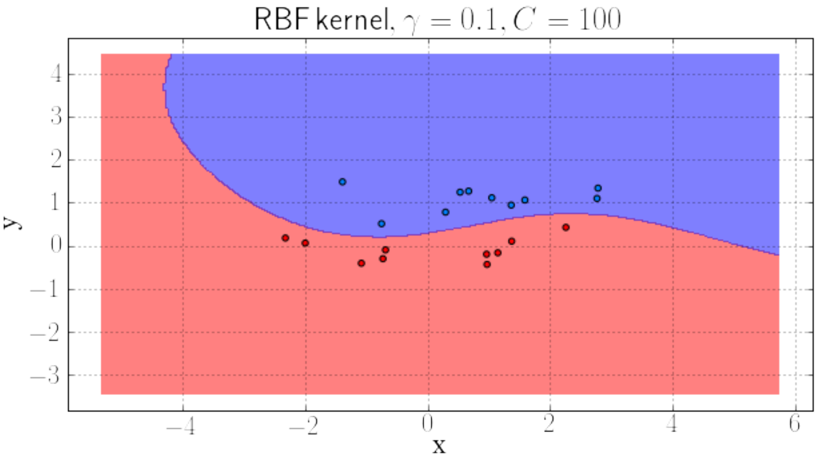
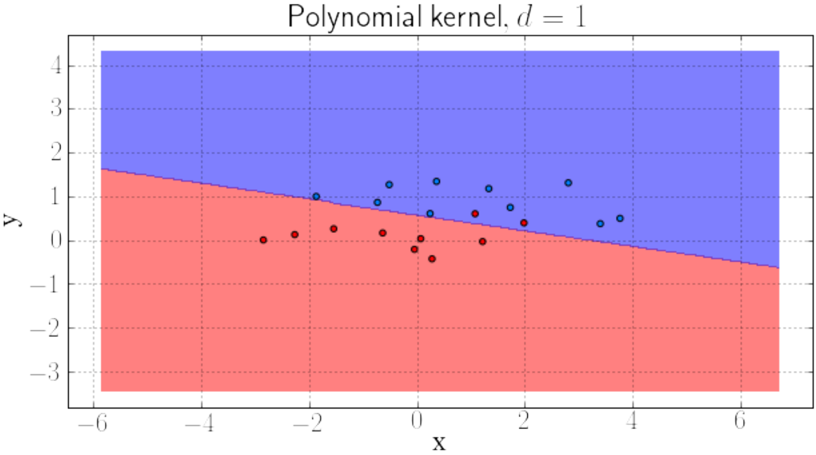


Polynomial kernel - variable d



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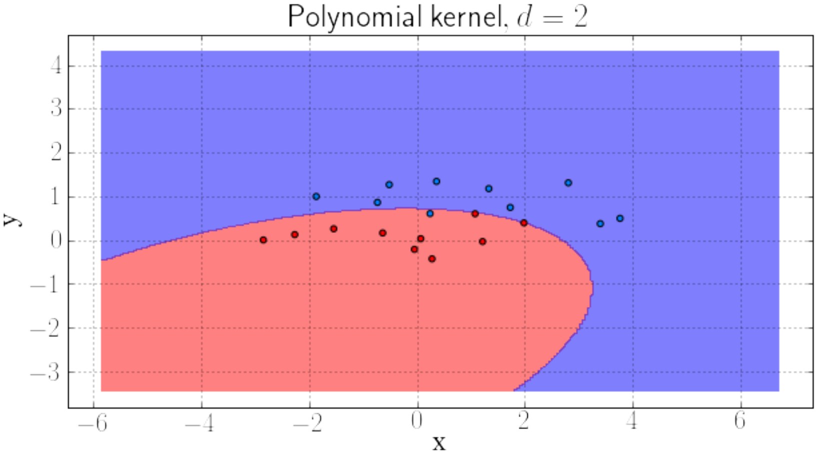

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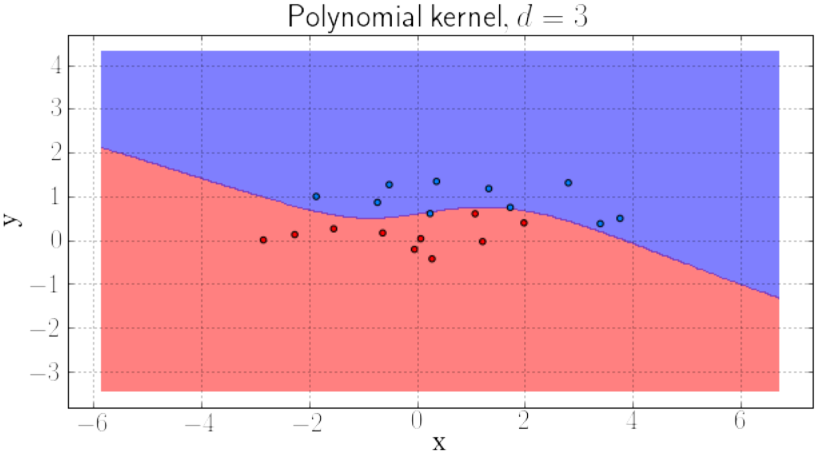

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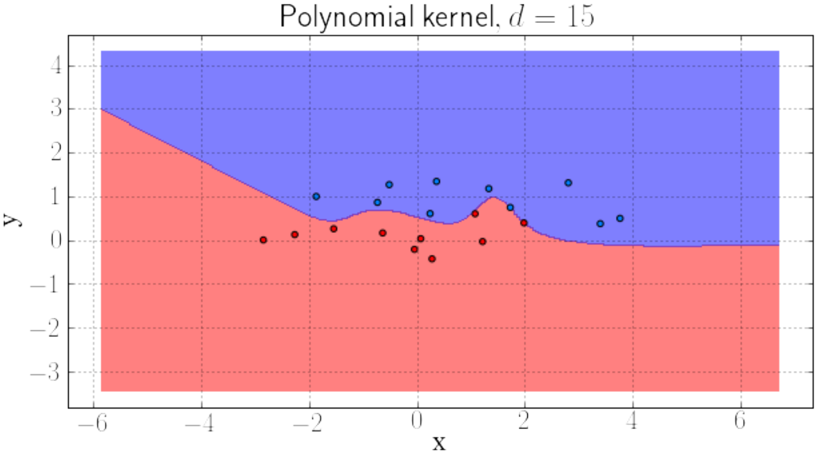
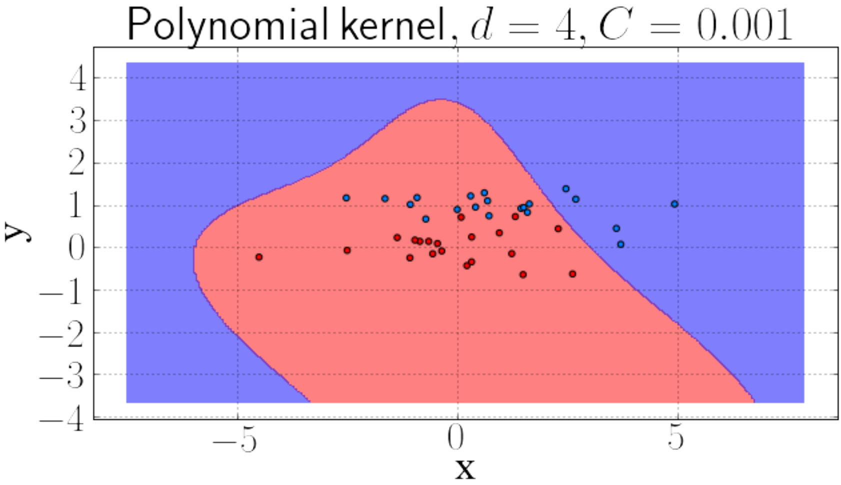


Polynomial kernel - variable C



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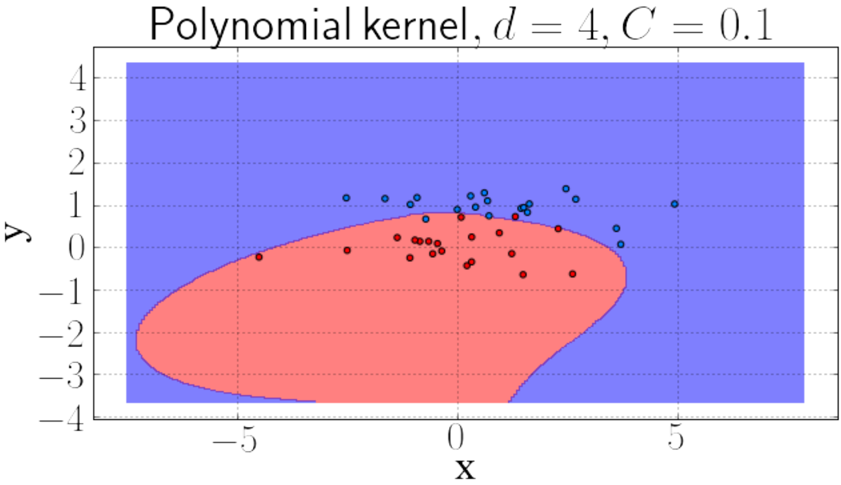
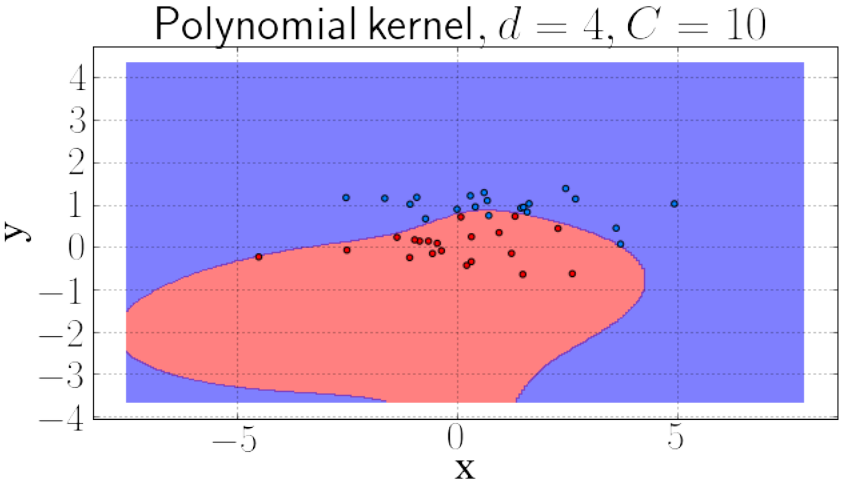
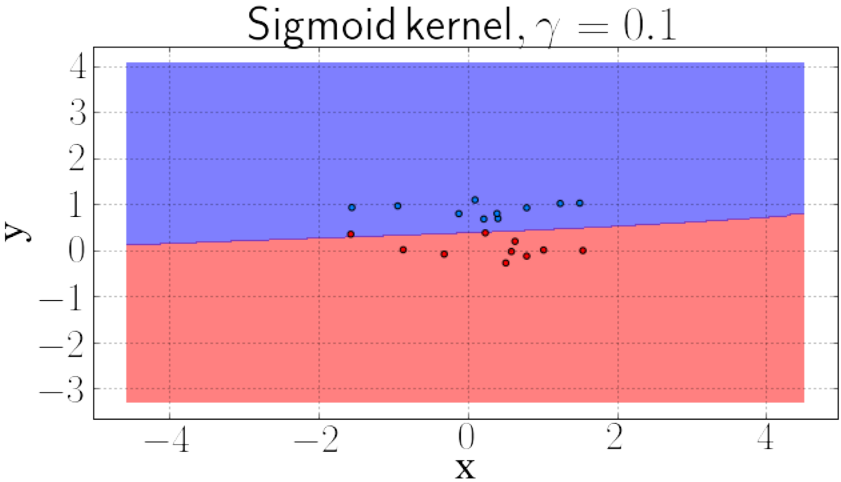


Polynomial kernel - variable C



Sigmoid kernel - variable γ



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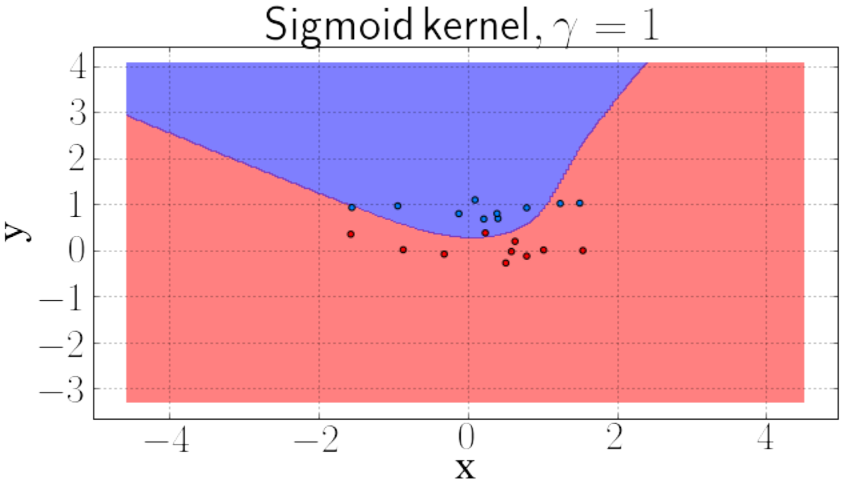

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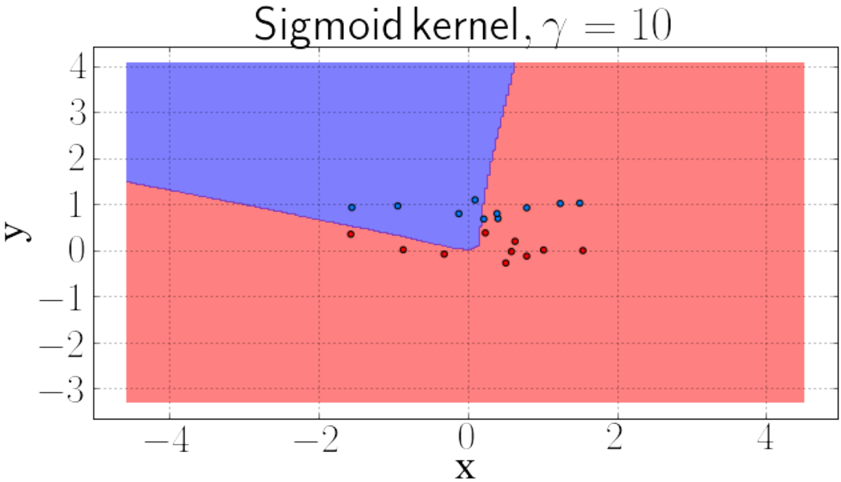

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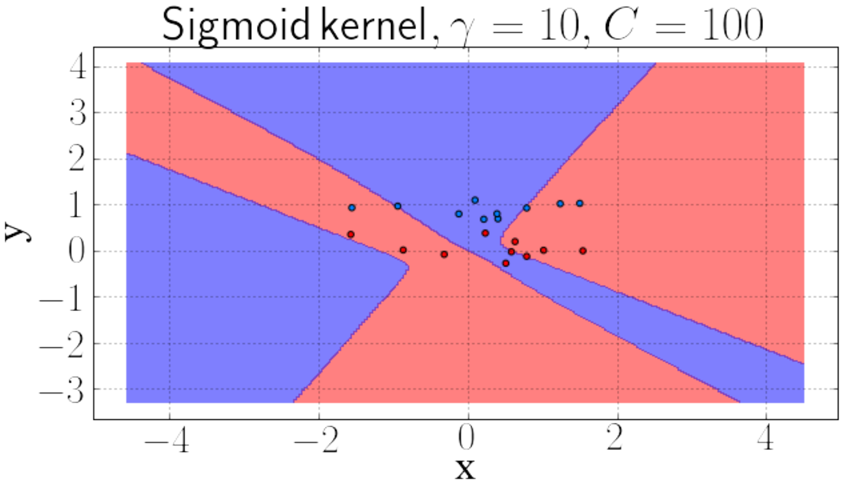

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Ridge regression

- Ridge regression criterion:

$$Q(\beta)=\sum_{n=1}^{N}\left(x_n^T\beta-y_n\right)^2+\lambda\sum_{d=1}^{D}\beta_d^2\to\min_{\beta}$$

- Stationarity condition:

$$\frac{dQ(\beta)}{d\beta}=2\sum_{n=1}^{N}\left(x_n^T\beta-y_n\right)x_n+2\lambda\beta=0$$

- In vector form:

$$X^T\left(X\beta-Y\right)+\lambda\beta=0$$

Ridge regression

- Primal solution:

$$X^T X + \lambda I \beta = X^T Y$$
$$\beta = (X^T X + \lambda I)^{-1} X^T Y$$

- Comment: $X^T X \succcurlyeq 0$ (positive semi-definite) and $X^T X + \lambda I \succ 0$ (positive definite), so ridge regression is always identifiable.
- Cost of estimation:
  - $X^T X + \lambda I$: $ND^2 + D$
  - $X^T Y$: DN
  - $(X^T X + \lambda I)^{-1}$: D^3
  - $(X^T X + \lambda I)^{-1} X^T Y$: D^2
  - Total training cost is $O(ND^2 + D^3) = O(D^2(N + D))$.
- Cost of prediction $\widehat{y}(x) = \langle x, \beta \rangle$ is D.

Dual solution

From vector stationarity condition:

$$X^T(X\beta - Y) + \lambda\beta = 0$$

follows the dual solution (a linear combination of training vectors):

$$\beta = \frac{1}{\lambda}X^T(Y - X\beta) = X^T\alpha \tag{1}$$

where

$$\alpha = \frac{1}{\lambda}(Y - X\beta) \tag{2}$$

is called a vector of *dual variables*.

Prediction:

$$\widehat{y}(x) = x^T\beta = x^TX^T\alpha = \sum_{i=1}^{N}\alpha_i\langle x, x_i\rangle$$

Dual solution

To find α we plug (1) into (2):

$$\alpha = \frac{1}{\lambda}(Y - X\beta) = \frac{1}{\lambda}(Y - XX^T\alpha)$$
$$\left(XX^T + \lambda I\right)\alpha = Y$$
$$\alpha = \left(XX^T + \lambda I\right)^{-1} Y$$

Cost of estimation:
$XX^T + \lambda I$: $N^2D + N$
$\left(XX^T + \lambda I\right)^{-1}$: N^3
$\left(XX^T + \lambda I\right)^{-1} Y$: N^2
Total training cost is $O(N^2D + N^3) = O(N^2(D + N))$.
Cost of prediction $\widehat{y}(x) = \langle x, \beta \rangle$ is ND.

Dual solution motivation

- Optimal α depends not on exact features but only on scalar products:

$$\alpha = \left(XX^T + \lambda I\right)^{-1} Y = (G + \lambda I)^{-1} Y$$

where $G \in \mathbb{R}^{NxN}$ and $\{G\}_{ij} = \langle x_i, x_j \rangle$ - G is called *Gram matrix*.

- Prediction also depends only on scalar products:

$$\widehat{y}(x) = \sum_{i=1}^{N} \alpha_i \langle x, x_i \rangle = \alpha^T v$$

where $v \in \mathbb{R}^N$ and $v_i = \langle x, x_i \rangle$.