Kernel methods

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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:

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

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 $v_i = \langle x, x_i \rangle$.

Motivation

- Model fitting becomes faster when $D > N$ (for complex feature transformation)
    - we can operate in multidimensional and even infinite dimensional feature spaces

Advantage of dual representation

No exact feature representation is needed - only the ability to calculate scalar products.

Kernel trick

Kernel trick

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

- $\langle x, x' \rangle$ has complexity $O(D)$. Complexity of $K(x, x')$ may be $O(1)$!
- In case of ridge regression and $O(1)$ complexity of $K(x, x')$:
  - training cost $O(N^2(D+N))$ becomes $O(N^3)$
  - prediction cost ND becomes N

Comments

Kernel trick applies not only to ridge regression:

- K-NN
- K-means, K-medoids
- nearest medoid
- PCA
- SVM
- many more

When vector feature representation x exist, we can define natural linear kernel:

$$K(x, x') = \langle x, x' \rangle = \sum_{d=1}^{D} x_d x'_d$$

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

Kernel definition

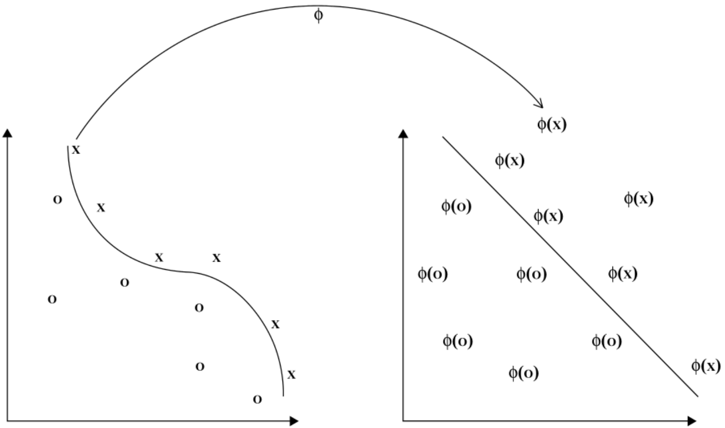
- x is replaced with $\phi(x)$
  - Example: $[x] \to [x,\ x^2,\ x^3]$

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 $\langle \phi(x), \phi(x') \rangle = K(x, x')$
- Specific types of kernels:
  - $K(x, x') = K(x - x')$ - stationary kernels (invariant to translations)
  - $K(x, x') = K(\|x - x'\|)$ - radial basis functions

Illustration



Polynomial kernel

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

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

- In general for $D \geq 1$ $(x^T z)^M$ yields all polynomials of degree M and $(1 + x^T z)^M$ yields all polynomials of degree less or equal to M.

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:
  - scalar product $\langle x, x' \rangle$
  - constant $K(x, x') \equiv 1$
  - $x^T A x$ for any $A \succcurlyeq 0$

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:

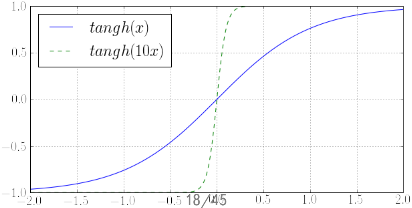
1. $K(x, x') = cK_1(x, x')$
2. $K(x, x') = K_1(x, x')K_2(x, x')$
3. $K(x, x') = K_1(x, x') + K_2(x, x')$
4. $K(x, x') = K_1(\varphi(x), \varphi(x'))$
5. $K(x, x') = h(x)K_1(x, x')h(x')$
6. $K(x, x') = e^{K_1(x, x')}$

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	$\exp(-\gamma \left\| x - x' \right\|^2)$
sigmoid	$\tanh(\gamma \langle x, y \rangle + r)$

- Comment: linear, polynomial and RBF are Mercer kernels and sigmoid - not.



Addition

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

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

- Scalar product of normalized vectors:

$$\langle \frac{\phi(x)}{\|\phi(x)\|}, \frac{\phi(x')}{\|\phi(x')\|}\rangle = \frac{\langle \phi(x), \phi(x')\rangle}{\sqrt{\langle \phi(x), \phi(x)\rangle}, \sqrt{\langle \phi(x'), \phi(x')\rangle}} = \frac{K(x,x')}{\sqrt{K(x,x)K(x',x')}}$$

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Linear SVM reminder

- Solution for weights:

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

Discriminant function

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

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

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.

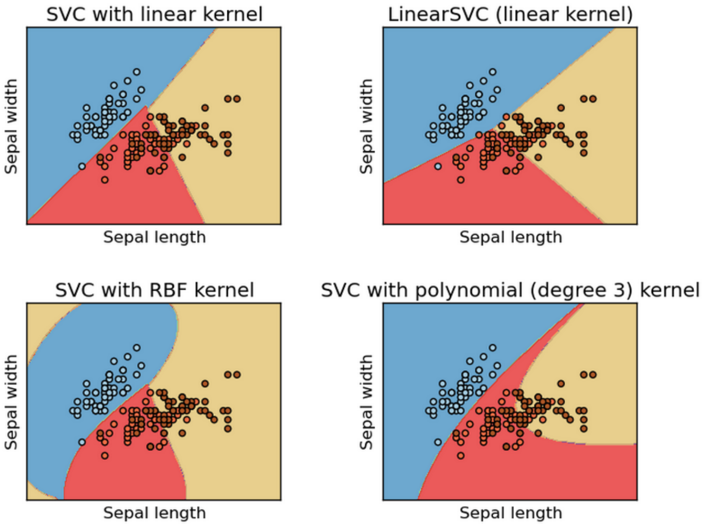
Kernel SVM

Discriminant function

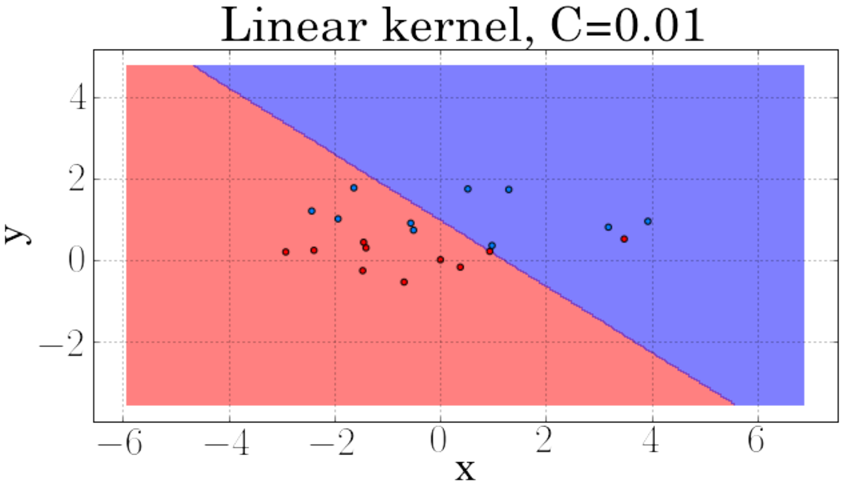
$$g(x) = \sum_{i \in \mathcal{SV}} \alpha_i y_i K(x_i, x) + w_0$$

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

Kernel results



Linear kernel - variable C



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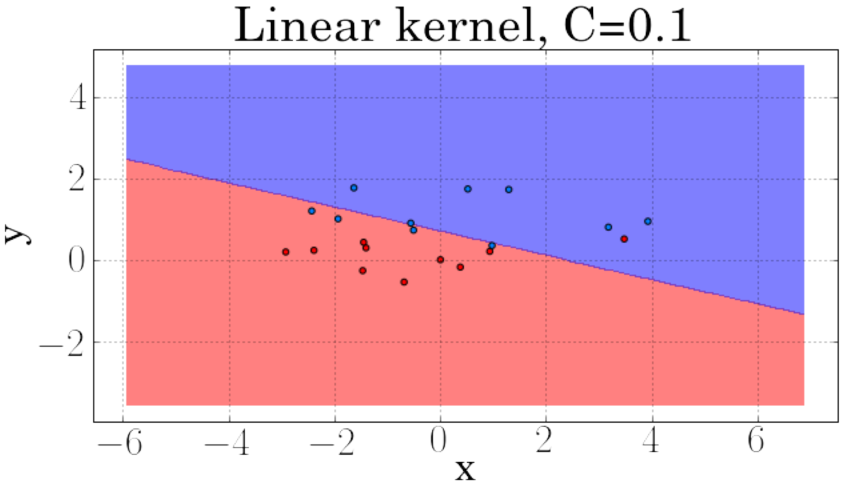

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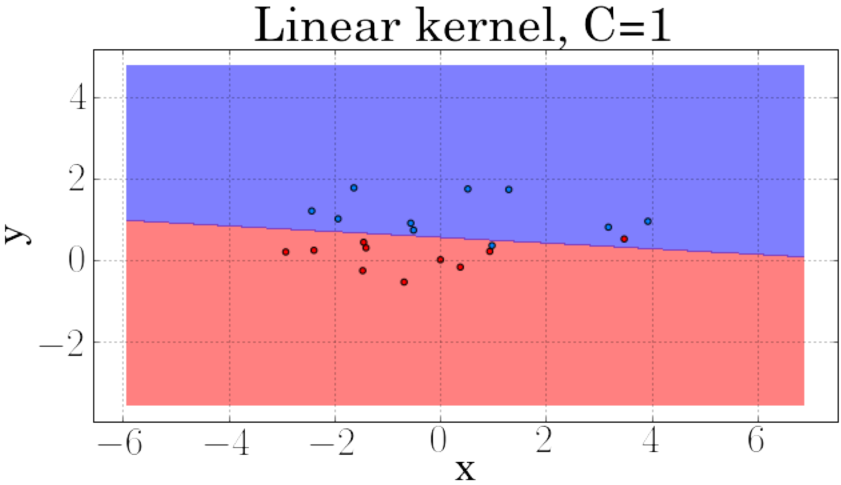

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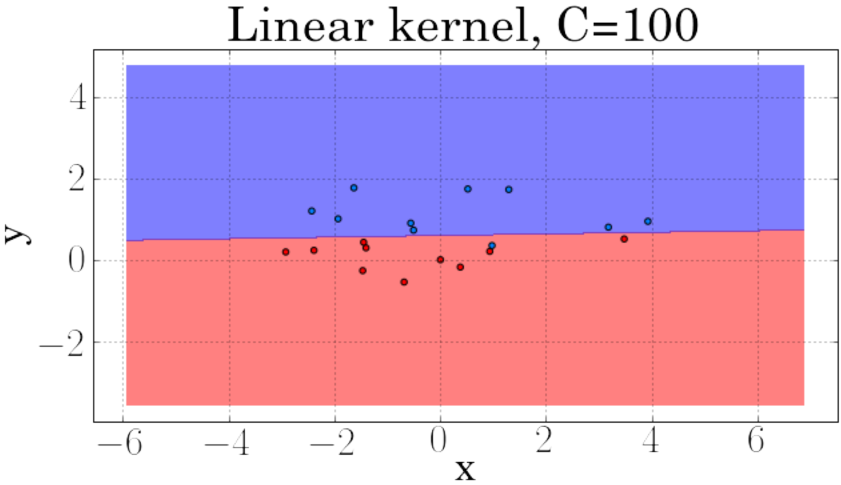
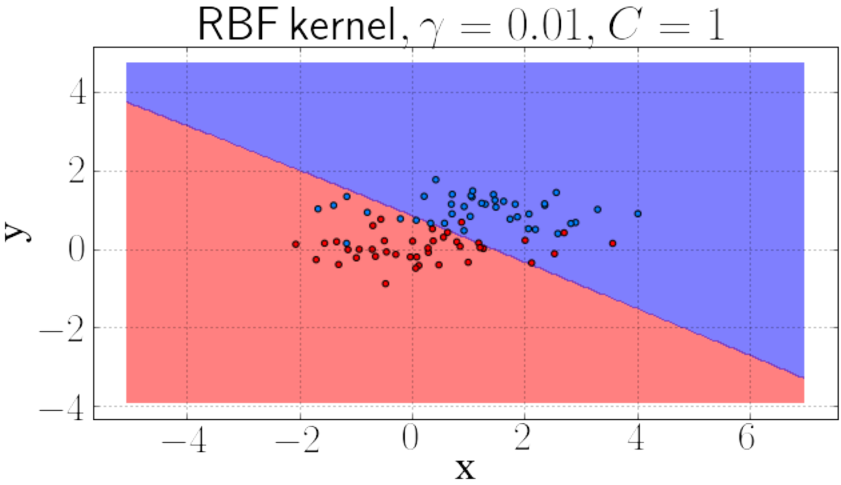


RBF kernel - variable γ



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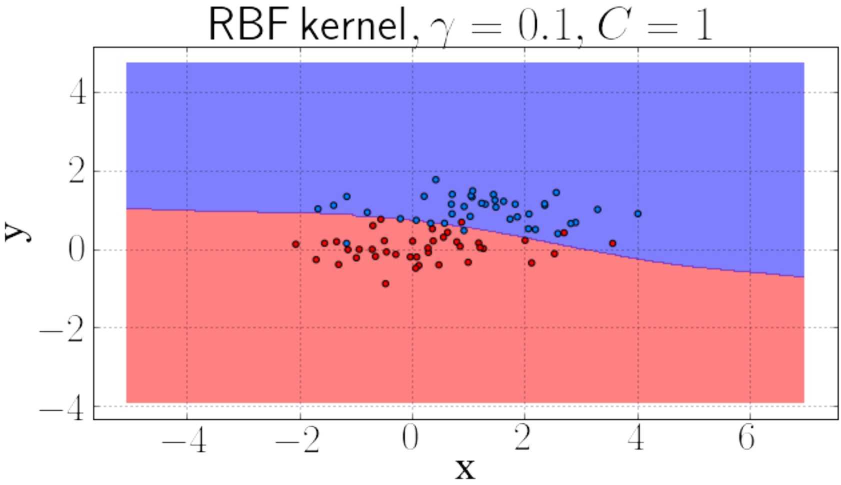

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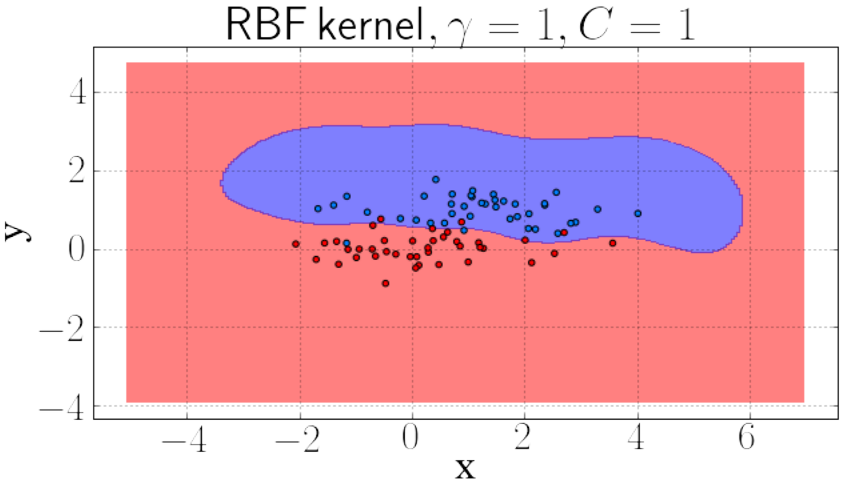

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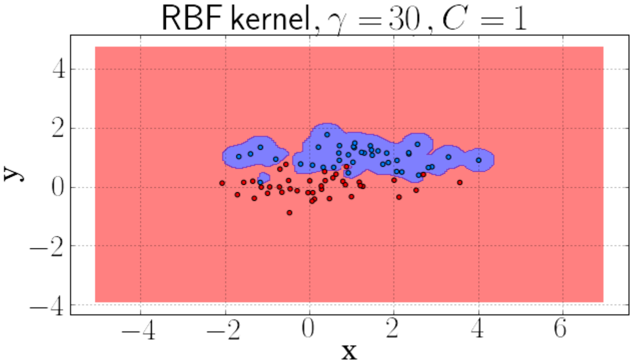

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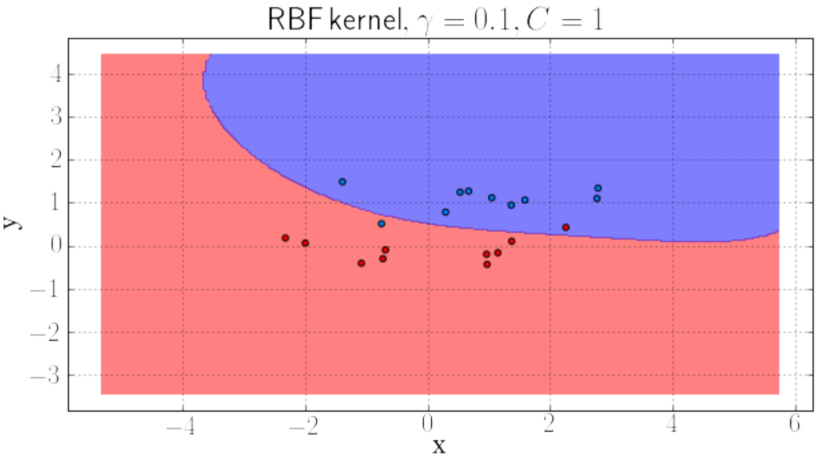

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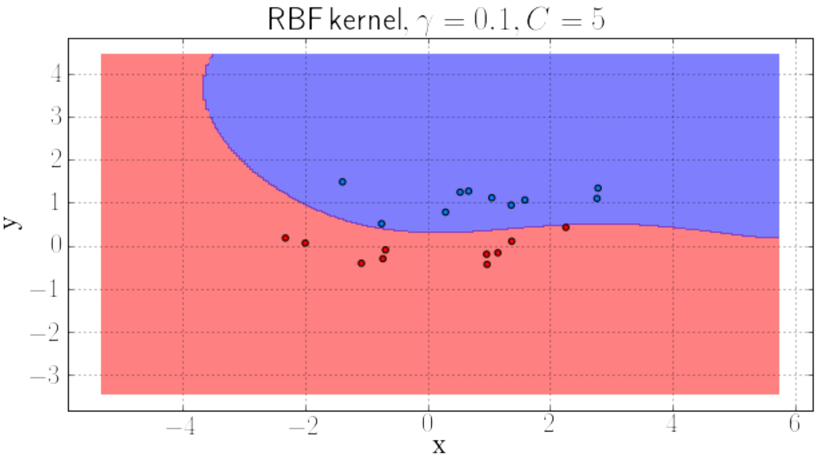

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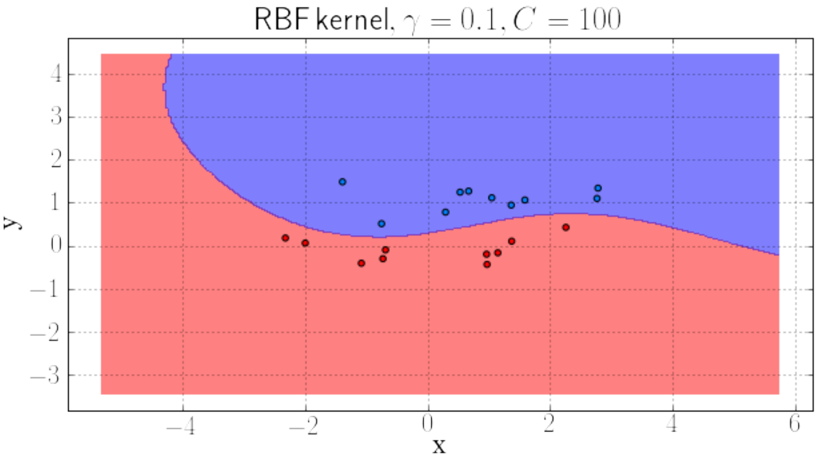
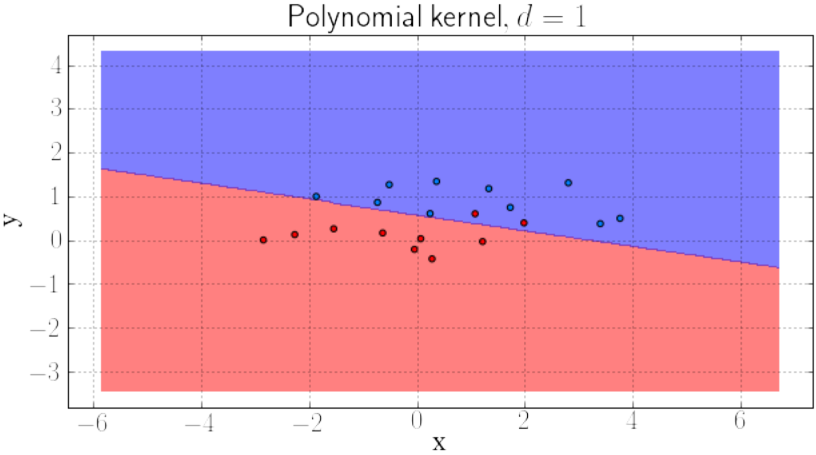


Polynomial kernel - variable d



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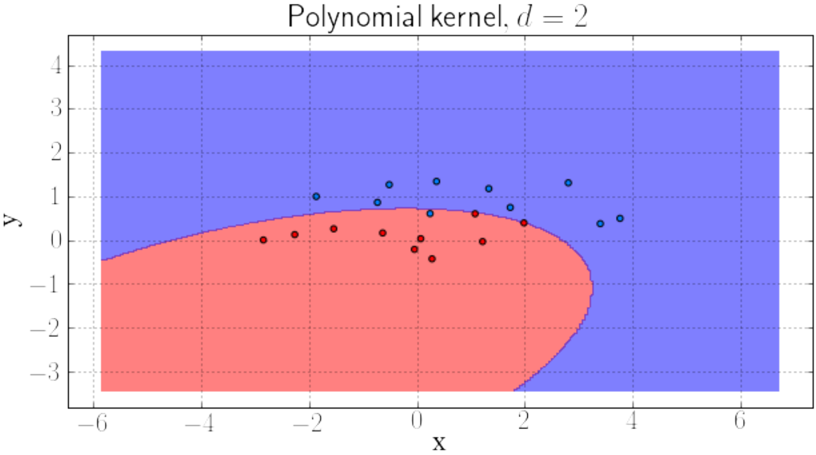

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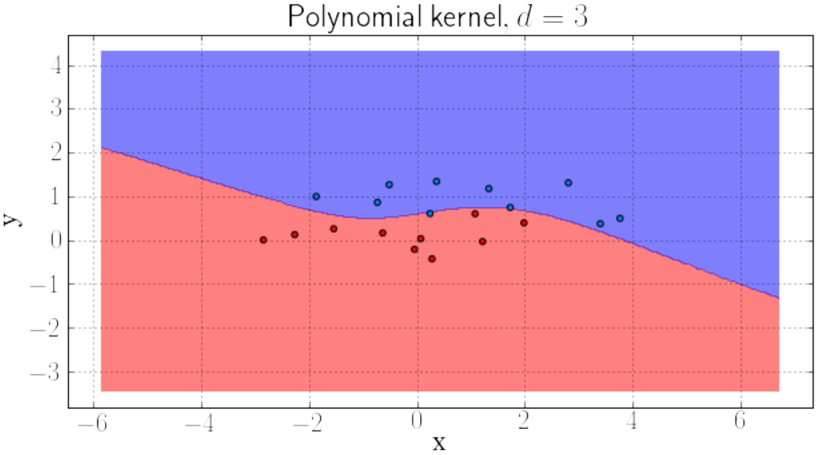

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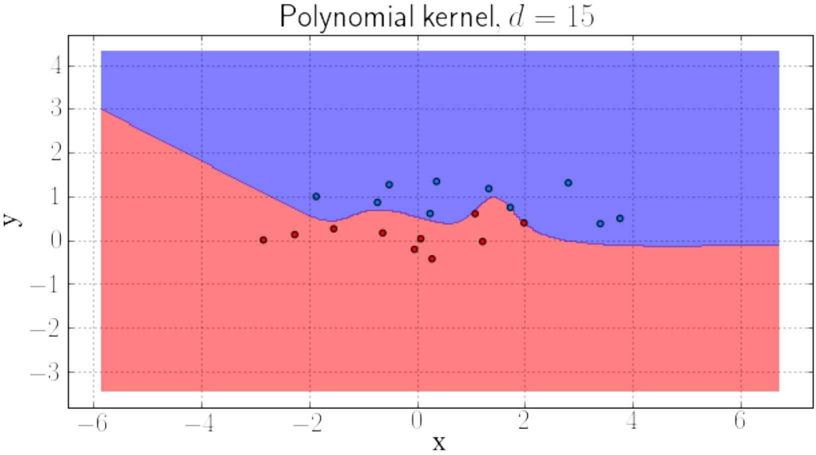
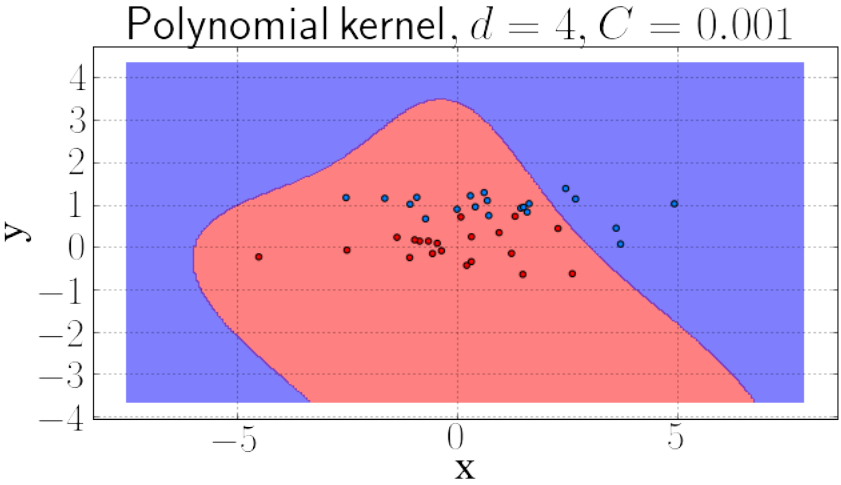


Polynomial kernel - variable C



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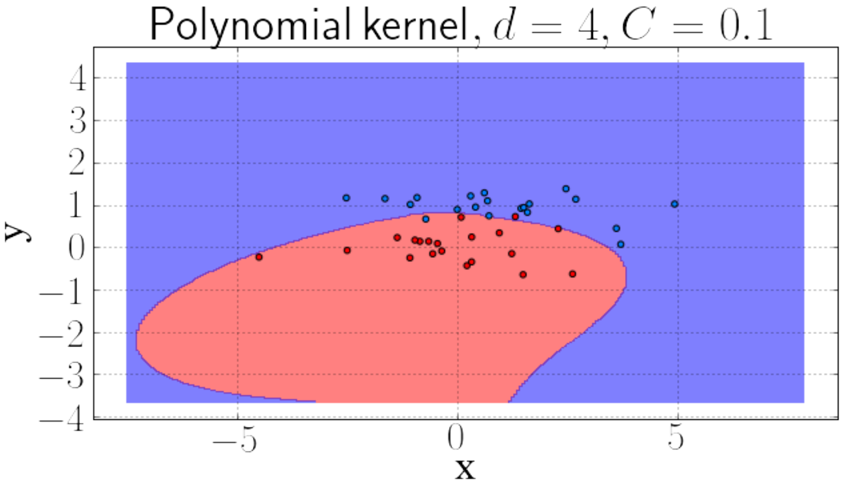

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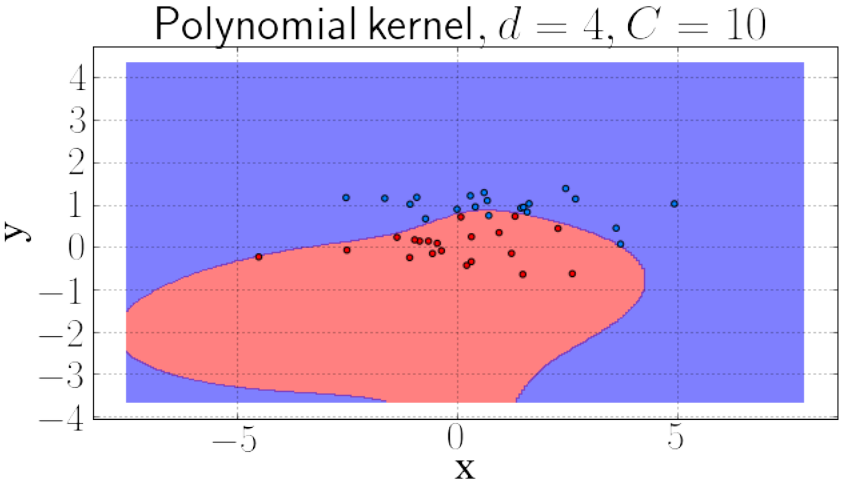
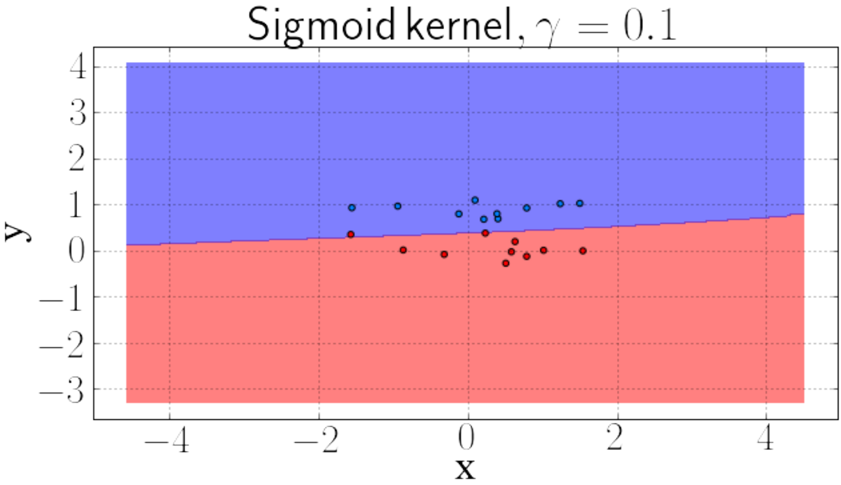


Sigmoid kernel - variable γ



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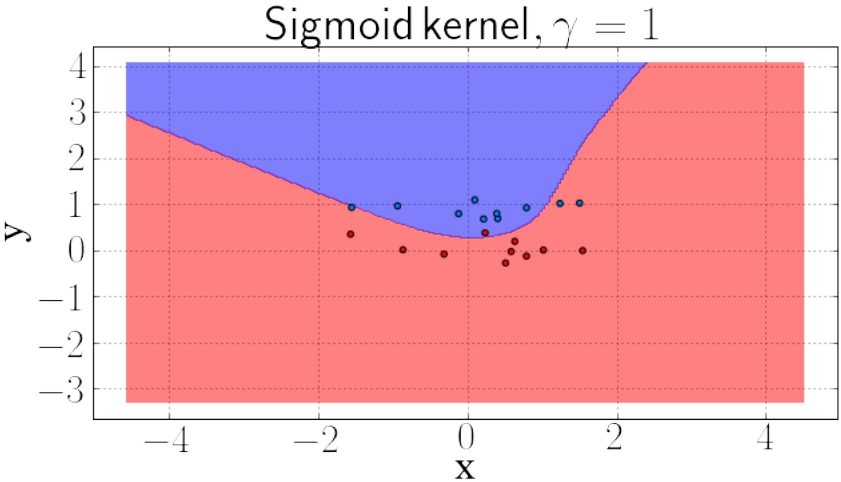

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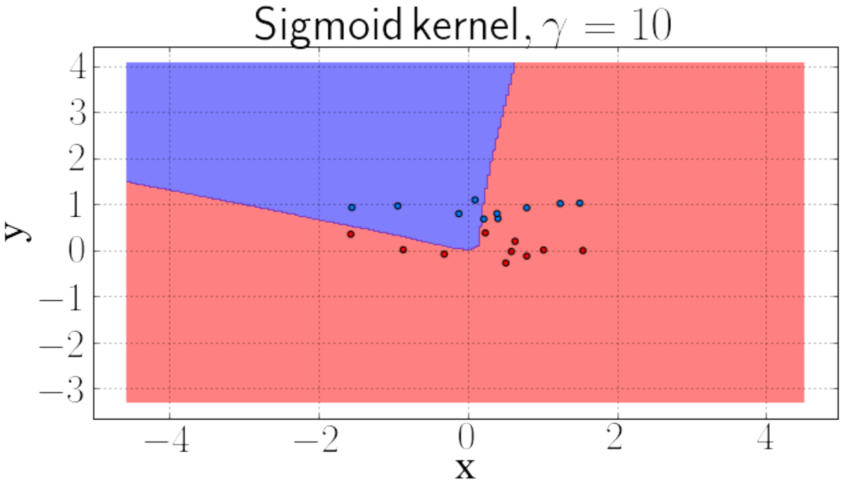

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