Support vector machines

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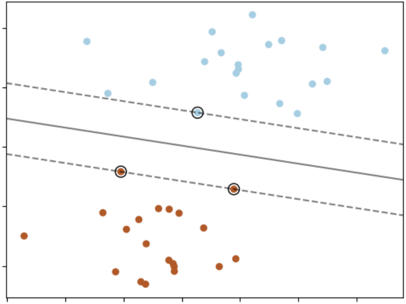

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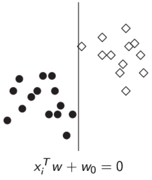
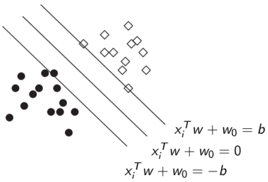
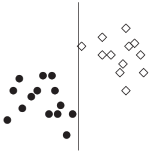
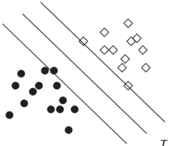




Support vector machines





Main idea

Select hyperplane maximizing the spread between classes.

Support vector machines

Objects x_i for $i = 1, 2, ...n$ lie at distance $b/|w|$ from discriminant hyperplane if

$$\begin{cases} x_i^T w + w_0 \geq b, & y_i = +1 \\ x_i^T w + w_0 \leq -b & y_i = -1 \end{cases} \quad i = 1, 2, ...N.$$

This can be rewritten as

$$y_i(x_i^T w + w_0) \geq b, \quad i = 1, 2, ...N.$$

The margin is equal to $2b/\|w\|$. Since w, w_0 and b are defined up to multiplication constant, we can set $b = 1$.

Problem statement

Problem statement:

$$\begin{cases} \frac{1}{2}w^T w \to \min\limits_{w, w_0} \\ y_i(x_i^T w + w_0) \ge 1, \quad i = 1, 2, ...N. \end{cases}$$

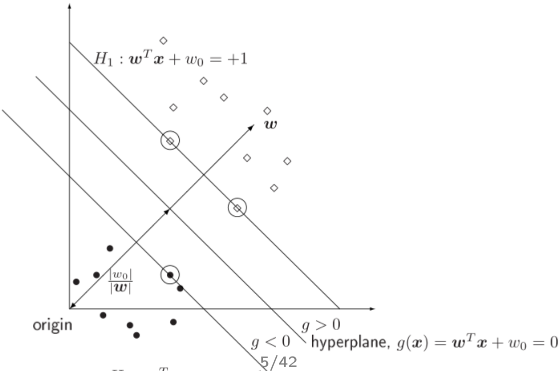
Support vectors

non-informative observations: $y_i(x_i^T w + w_0) > 1$

- do not affect the solution

support vectors: $y_i(x_i^T w + w_0) = 1$

- lie at distance $1/\|w\|$ to separating hyperplane
- affect the the solution.



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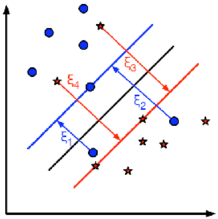
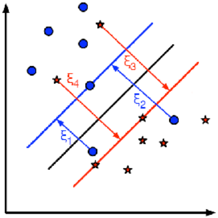
Linearly non-separable case

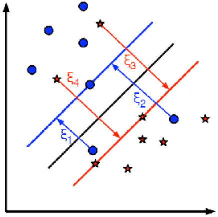


Linearly non-separable case



$$\begin{cases} \frac{1}{2} w^T w \to \min_{w, w_0} \\ y_i(x_i^T w + w_0) \geq 1, \quad i = 1, 2, ... N. \end{cases}$$

Linearly non-separable case



$$\begin{cases} \frac{1}{2}w^T w \to \min_{w,w_0} \\ y_i(x_i^T w + w_0) \geq 1, \quad i = 1, 2, \ldots N. \end{cases}$$

Problem

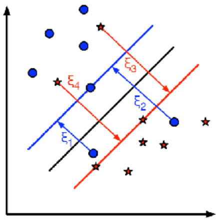
Constraints become incompatible and give empty set!

Linearly non-separable case

No separating hyperplane exists. Errors are permitted by including slack variables ξ_i:

$$\begin{cases} \frac{1}{2}w^T w + C\sum_{i=1}^N \xi_i \to \min_{w,\xi} \\ y_i(w^T x_i + w_0) \ge 1 - \xi_i,\ i = 1, 2, \dots N \\ \xi_i \ge 0,\ i = 1, 2, \dots N \end{cases}$$

- Parameter C is the cost for misclassification and controls the bias-variance trade-off.
- It is chosen on validation set.
- Other penalties are possible, e.g. $C\sum_i \xi_i^2$.



Classification of training objects

- **Non-informative objects**:
  - $y_i(w^T x_i + w_0) > 1$
- **Support vectors** SV**:**
  - $y_i(w^T x_i + w_0) \leq 1$
  - **boundary support vectors** $\widetilde{SV}$:
    - $y_i(w^T x_i + w_0) = 1$
  - **violating support vectors**:
    - $y_i(w^T x_i + w_0) > 0$: violating support vector is correctly classified.
    - $y_i(w^T x_i + w_0) < 0$: violating support vector is misclassified.

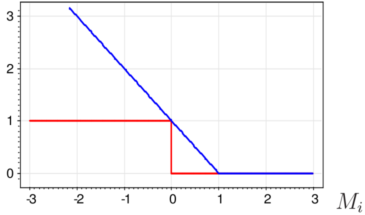
SVM with unconstrained optimization

Optimization problem:

$$\begin{cases} \frac{1}{2}w^T w + C\sum_{i=1}^N \xi_i \to \min_{w,w_0,\xi} \\ y_i(w^T x_i + w_0) = M_i(w, w_0) \geq 1 - \xi_i, \\ \xi_i \geq 0,\ i = 1, 2, ...N \end{cases}$$

can be rewritten as

$$\frac{1}{2C}\|w\|_2^2 + \sum_{i=1}^N [1 - M_i(w, w_0)]_+ \to \min_{w,w_0,\xi}$$



Thus SVM is linear discriminant function with cost approximated with $\mathcal{L}(M) = [1 - M]_+$ and L_2 regularization.

Sparsity of solution

- SVM solution depends only on support vectors
- This is also clear from loss function, satisfying $\mathcal{L}(M) = 0$ for $M \geq 1$.
    - objects with margin≥ 1 don't affect solution!
- Sparsity causes SVM to be less robust to outliers
    - because outliers are always support vectors

Multiclass SVM

C discriminant functions are built simultaneously:

$$g_c(x) = (\mathbf{w}^c)^T x + w_0^c, \qquad c = \overline{1, C}.$$

Linearly separable case:

$$\begin{cases} \sum_{c=1}^{C} (\mathbf{w}^c)^T \mathbf{w}^c \to \min_{\mathbf{w}} \\ (\mathbf{w}^{y_n})^T x_n + w_0^{y_n} - (\mathbf{w}^c)^T x - w_0^c \geq 1 \quad \forall c \neq y_n, \\ n = \overline{1, N}. \end{cases}$$

Linearly non-separable case:

$$\begin{cases} \sum_{c=1}^{C} (\mathbf{w}^c)^T \mathbf{w}^c + C \sum_{n=1}^{N} \xi_n \to \min_w \\ (\mathbf{w}^{y_n})^T x + w_0^{y_n} - (\mathbf{w}^c)^T x - w_0^c \geq 1 - \xi_n \quad \forall c \neq y_n, \\ \xi_n \geq 0, \quad n = \overline{1, N}. \end{cases}$$

Is slower, but shows similar accuracy to one-vs-all,one-vs-one SVM.

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Dual problem

Solving Karush-Kuhn-Takker conditions, get **dual optimization problem**:

$$\begin{cases} L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j \to \max_\alpha \\ \sum_{n=1}^{N} \alpha_n y_n = 0 \\ 0 \le \alpha_n \le C, \quad n = \overline{1, N} \end{cases} \tag{1}$$

It is standard quadratic programming task.

Comments on support vectors

- **non-informative vectors**: $y_i(w^T x_i + w_0) > 1$ have $\alpha_i = 0$
- **non-boundary support vectors** $SV \setminus \tilde{SV}$:
  $y_i(w^T x_i + w_0) < 1$ have $\alpha_i = C$.
- **boundary support vectors** $\widetilde{\mathcal{SV}}$: $y_i(w^T x_i + w_0) = 1$
  Typically $\alpha_i \in (0, C)$, though $\alpha_i = 0, C$ are possible as special cases.

Solution

1. Solve (1) to find optimal dual variables α_i^*
2. Find optimal w ($\alpha_i^* \neq 0$ only for support vectors):

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

3. w_0 can be found from any edge equality for boundary support vector:

$$y_i(x_i^T w + w_0) = 1, \forall i \in \widetilde{\mathcal{SV}} \tag{2}$$

Solution for w_0

By multiplyting (2) by y_i obtain

$$x_i^T w + w_0 = y_i \quad \forall i \in \widetilde{\mathcal{SV}} \tag{3}$$

Get more numerically stable from summing 3 over all $i \in \widetilde{\mathcal{SV}}$:

$$n_{\tilde{SV}} w_0 = \sum_{j \in \tilde{SV}} \left(y_j - x_j^T w \right) = \sum_{j \in \tilde{SV}} y_j - \sum_{j \in \tilde{SV}} x_j^T w, \quad n_{\tilde{SV}} = \left| \tilde{SV} \right|$$

$$w_0 = \frac{1}{n_{\tilde{SV}}} \left(\sum_{j \in \tilde{SV}} y_j - \sum_{j \in \tilde{SV}} \overbrace{\sum_{i \in \mathcal{SV}} \alpha_i^* y_i x_i^T}^{w^T} x_j \right)$$

If there exist no boundary support vectors (only violating SV), then find w_0 by grid search.

Making predictions

1. Solve dual task to find α_i^*, $i = 1, 2, ...N$

$$\begin{cases} \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \alpha_i\alpha_j y_i y_j \langle x_i, x_j \rangle \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \end{cases}$$

2. Find optimal w_0:

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

3. Make prediction for new x:

$$\widehat{y} = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i \in \mathcal{SV}} \alpha_i^* y_i \langle x_i, x \rangle + w_0]$$

Making predictions

1. Solve dual task to find α_i^*, $i = 1, 2, \dots N$

$$\begin{cases} L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \end{cases}$$

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

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$$\hat{y} = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i \in \mathcal{SV}} \alpha_i^* y_i \langle x_i, x \rangle + w_0]$$

- On all steps we don't need exact feature representations, only scalar products $\langle x, x' \rangle$!

Kernel trick generalization

1. Solve dual task to find α_i^*, $i = 1, 2, \dots N$

$$\begin{cases} L_D = \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j K(x_i, x_j) \to \max_\alpha \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C \end{cases}$$

2. Find optimal w_0:

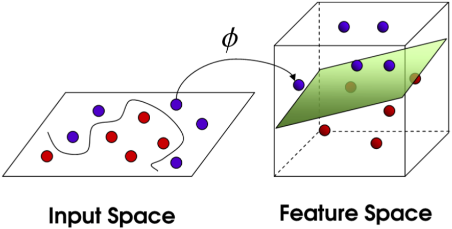
$$w_0 = \frac{1}{n_{\tilde{SV}}}\left(\sum_{j \in \tilde{SV}} y_j - \sum_{j \in \tilde{SV}} \sum_{i \in \mathcal{SV}} \alpha_i^* y_i K(x_i, x_j)\right)$$

3. Make prediction for new x:

$$\widehat{y} = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i \in \mathcal{SV}} \alpha_i^* y_i K(x_i, x) + w_0]$$

- We replaced $\langle x, x' \rangle \to K(x, x')$ for $K(x, x') = \langle \phi(x), \phi(x') \rangle$ for some feature transformation $\phi(\cdot)$.

Illustration



Consider 2-dimensional feature case: $x = (x_1, x_2)$, $z = (z_1, z_2)$

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

Kernel generalized prediction

Kernel generalized prediction for x:

$$\widehat{y}(x) = \text{sign}[w^T x + w_0] = \text{sign}[\sum_{i \in \mathcal{SV}} \alpha_i^* y_i K(x_i, x) + w_0]$$

$K(x,z) = \langle \phi(x), \phi(z) \rangle$ - kernel, corresponding to feature transformation $\phi(x)$

Kernel	$K(x,z)$
linear	$\langle x, z \rangle$
polynomial	$(a\langle x, z \rangle + b)^d, \ a > 0, \ b \geq 0, \ d = 1, 2, \dots$
RBF (Gaussian)	$e^{-\gamma \|x-z\|^2}, \ \gamma > 0$

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4. Visualization of kernel SVM
    - SVM - linear kernel
    - SVM - polynomial kernel
    - SVM - Gaussian kernel

Parameter C

Conditional optimization:

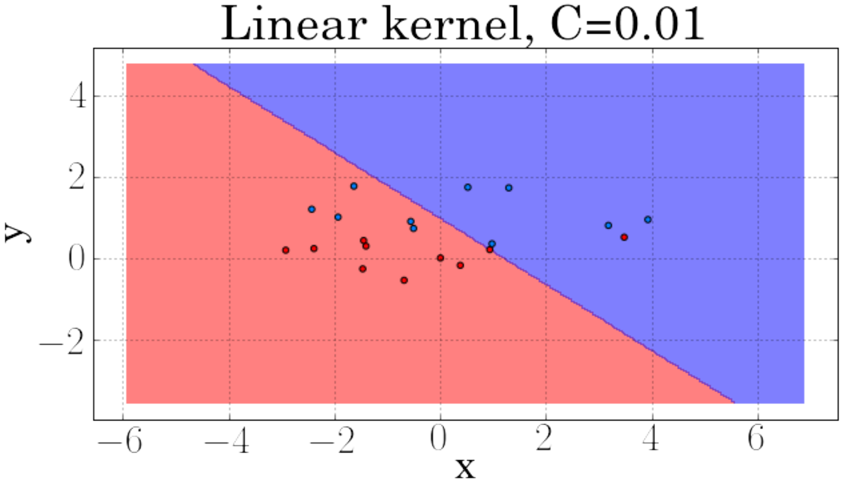
$$\begin{cases} \frac{1}{2} w^T w + C \sum_{i=1}^N \xi_i \to \min_{w, w_0, \xi} \\ y_i(w^T x_i + w_0) = M(x_i, y_i) \geq 1 - \xi_i, \; i = 1, 2, \ldots N \\ \xi_i \geq 0, \; i = 1, 2, \ldots N \end{cases}$$

Unconditional optimization:

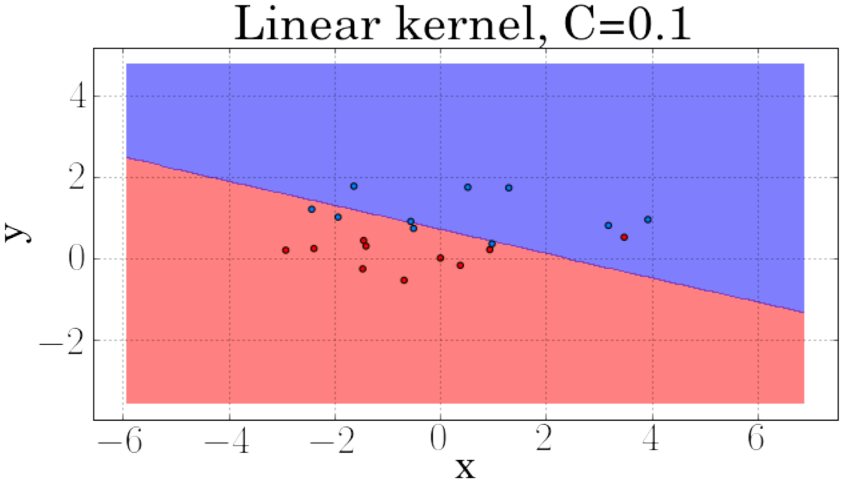
$$\frac{1}{2C} \|w\|_2^2 + \sum_{i=1}^N [1 - M_i(w, w_0)]_+ \to \min_{w, w_0}$$

Parameter C controls accuracy↔simplicity tradeoff.

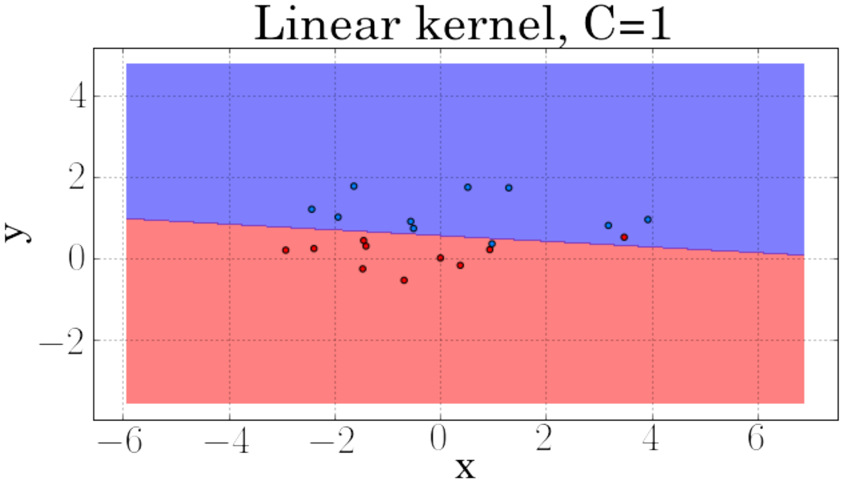
Linear kernel, influence of C



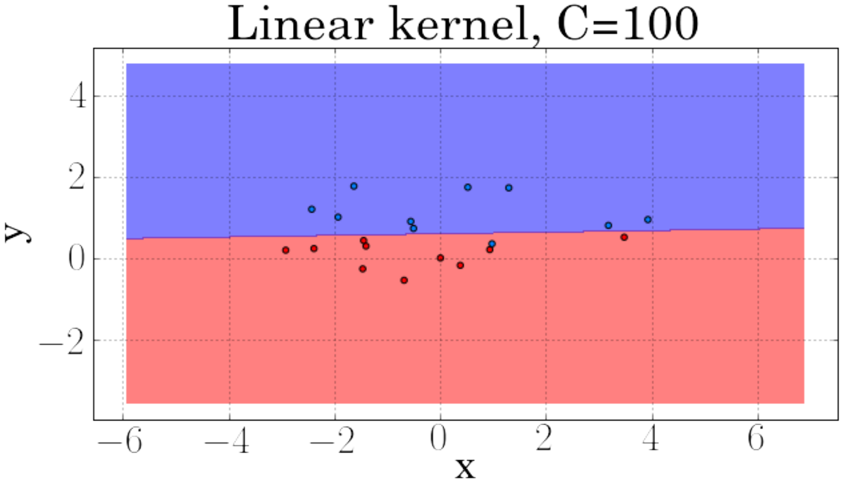
Linear kernel, influence of C



Linear kernel, influence of C



Linear kernel, influence of C



Polynomial kernel

Polynomial kernel:

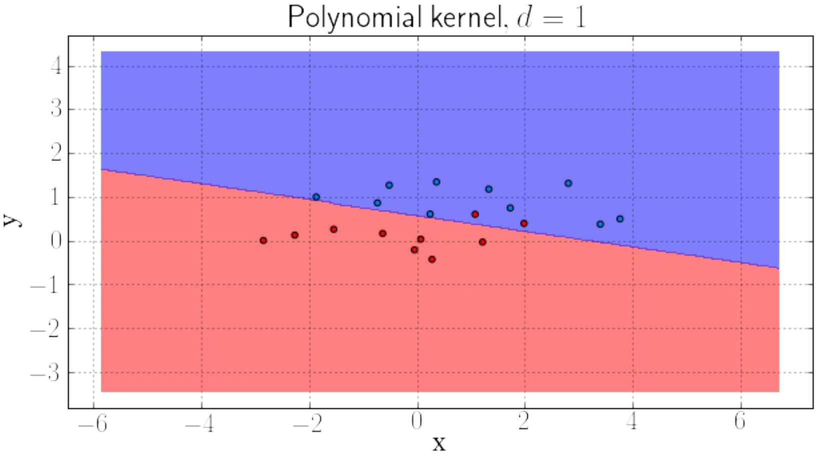
$$K(x,z) = (a\langle x,z\rangle + b)^{d}, \;\; a>0, \;\; b\geq 0, \;\; d=1,2,...$$

Prediction

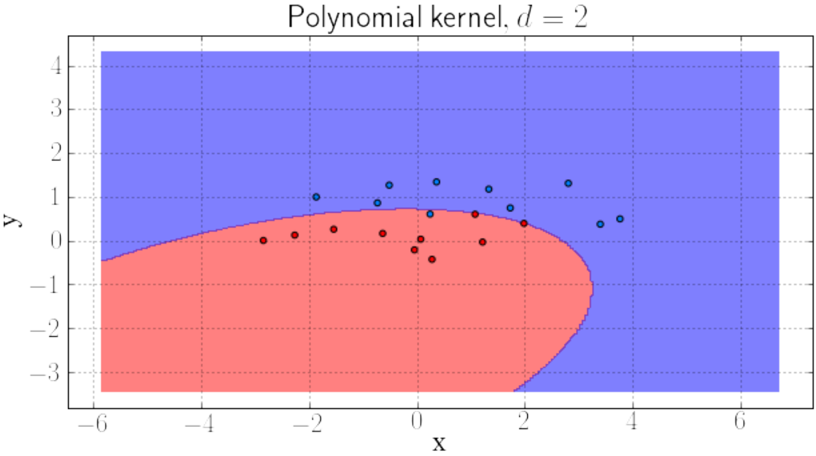
$$\begin{aligned}\widehat{y}(x) &= \text{sign}\left(\sum_{i\in\mathcal{SV}}\alpha_i^* y_i K(x_i,x) + w_0\right) = \\ &= \text{sign}\left(\sum_{i\in\mathcal{SV}}\alpha_i^* y_i \left(a\langle x,x_i\rangle + b\right)^{d} + w_0\right)\end{aligned}$$

The border between the classes - polynomial surface of order d.

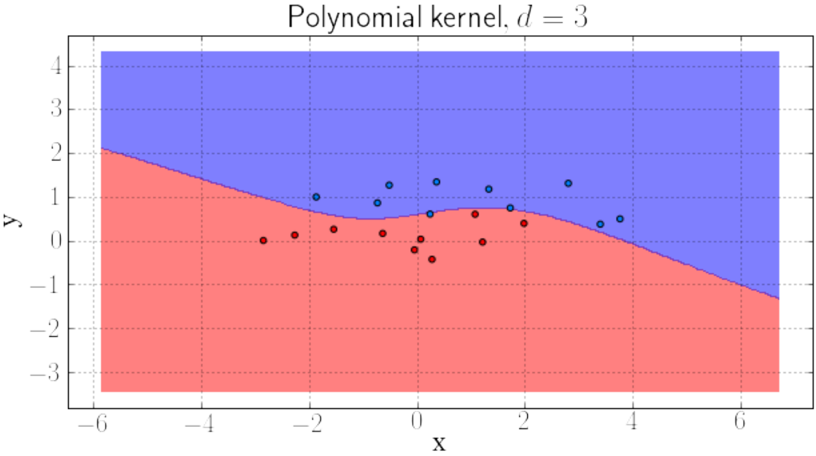
Polynomial kernel, influence of d



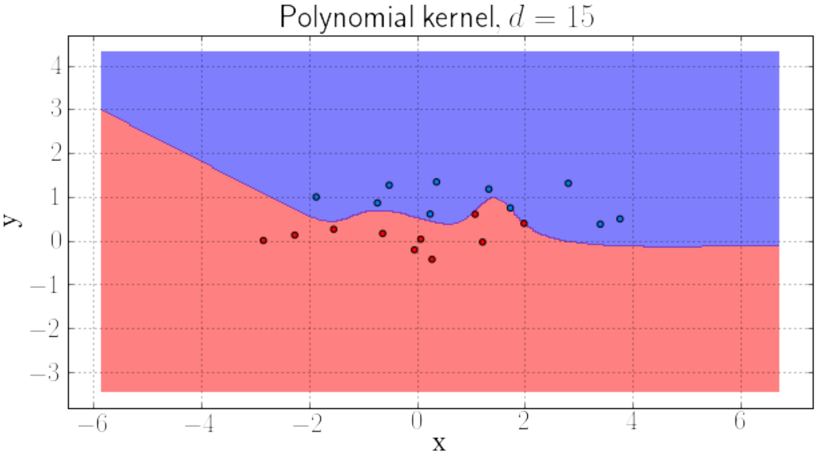
Polynomial kernel, influence of d



Polynomial kernel, influence of d



Polynomial kernel, influence of d



4. Visualization of kernel SVM
   - SVM - linear kernel
   - SVM - polynomial kernel
   - SVM - Gaussian kernel

Gaussian kernel

Gaussian kernel:

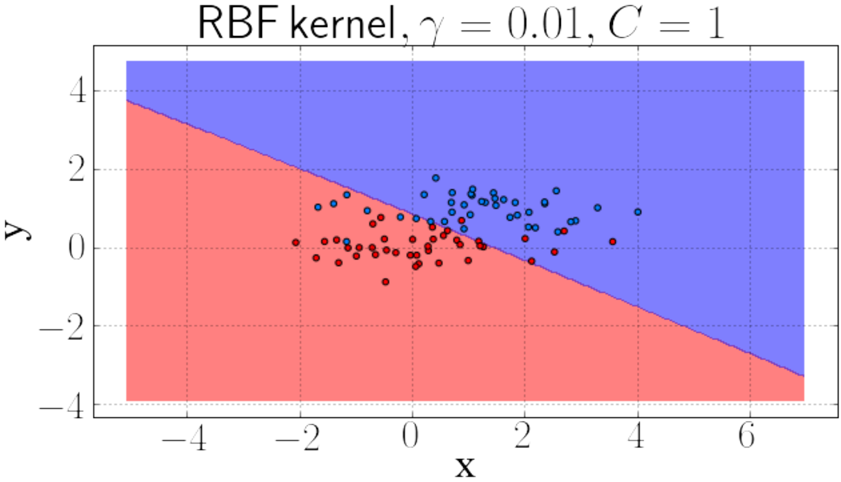
$$K(x,z) = e^{-\gamma \|x-z\|^2}, \ \gamma > 0$$

Prediction

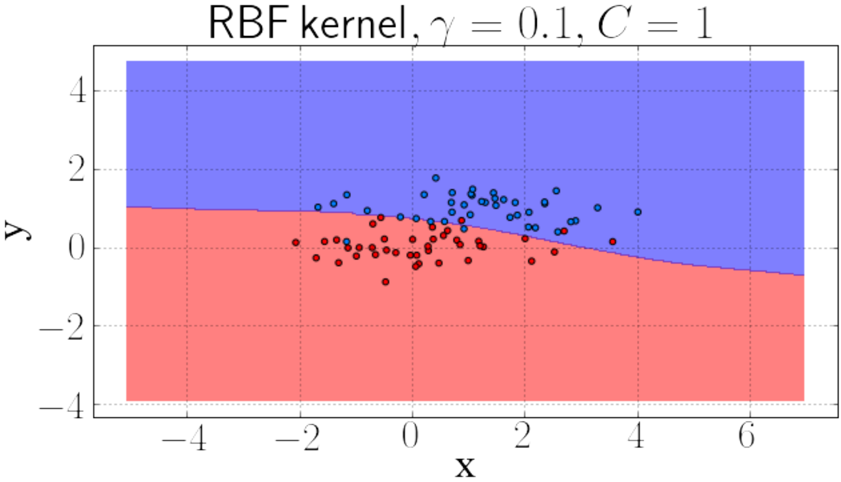
$$\begin{aligned}\widehat{y}(x) &= \text{sign}\left(\sum_{i\in\mathcal{SV}} \alpha_i^* y_i K(x_i, x) + w_0\right) \\ &= \text{sign}\left(\sum_{i\in\mathcal{SV}} \alpha_i^* y_i e^{-\gamma\|x-x_i\|^2} + w_0\right)\end{aligned}$$

Classification based on proximity of x to the support vectors weighted by α_i^*.

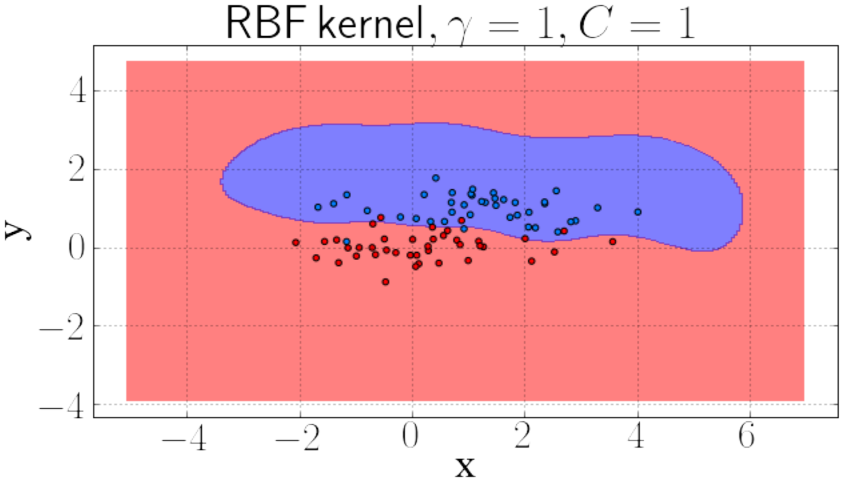
Gaussian kernel, influence of γ



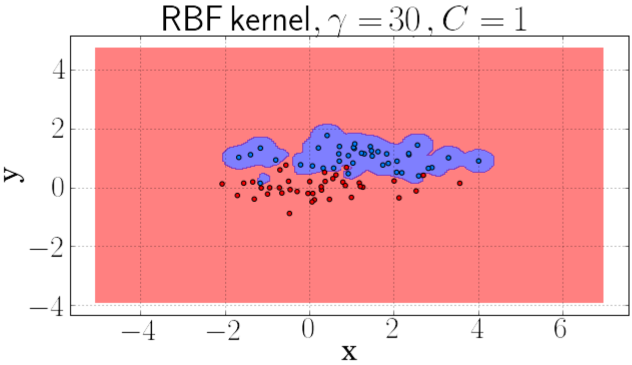
Gaussian kernel, influence of γ



Gaussian kernel, influence of γ



Gaussian kernel, influence of γ



Summary

- SVM - linear classifier with L_2 regularization and hinge loss.
- Geometrically SVM maximizes border between classes.
- Solution depends only on support vectors, having margin≤ 1.
- Solution depends on x only through $\langle x, x' \rangle$
    - "kernel trick" generalization
      $\langle x, x' \rangle \to K(x, x') = \langle \phi(x), \phi(x') \rangle$.
    - Gaussian kernel is the most popular
    - some other methods also allow kernel generalization:
        - e.g. kernel ridge regression, PCA, k-means.