Support Vector Machine (SVM) and Kernel Methods

CE-717: Machine Learning
Sharif University of Technology
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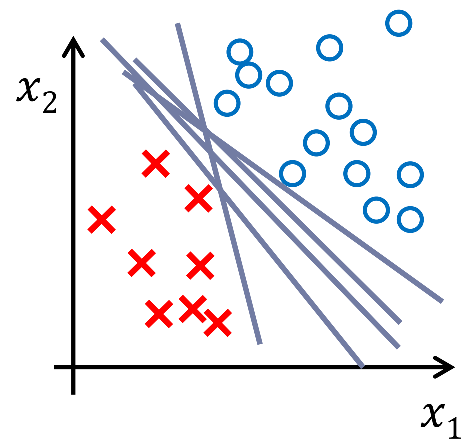
Outline

- Margin concept
- Hard-Margin SVM
- Soft-Margin SVM
- Dual Problems of Hard-Margin SVM and Soft-Margin SVM
- Nonlinear SVM
  - Kernel trick
- Kernel methods

Margin

- Which line is better to select as the boundary to provide more generalization capability?

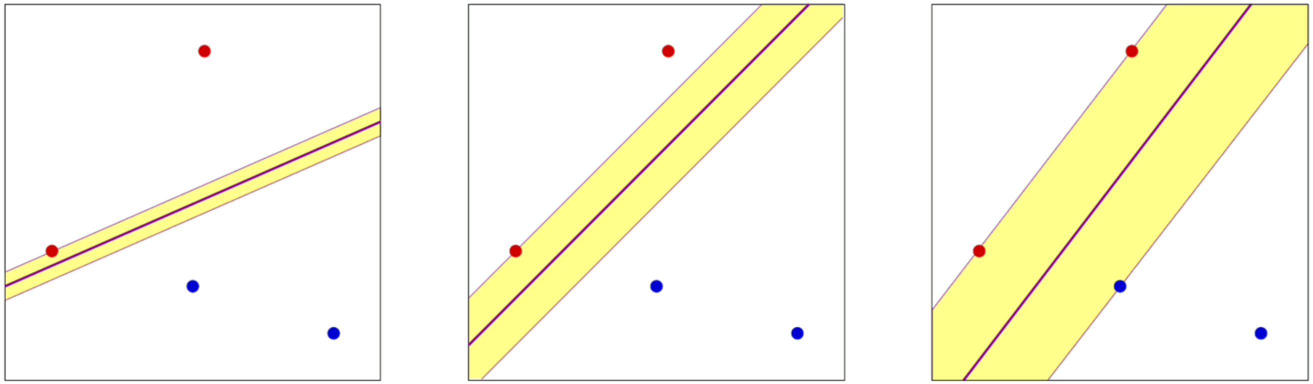
Larger margin provides better generalization to unseen data



- **Margin** for a hyperplane that separates samples of two linearly separable classes is:
  - The smallest distance between the decision boundary and any of the training samples

What is better linear separation

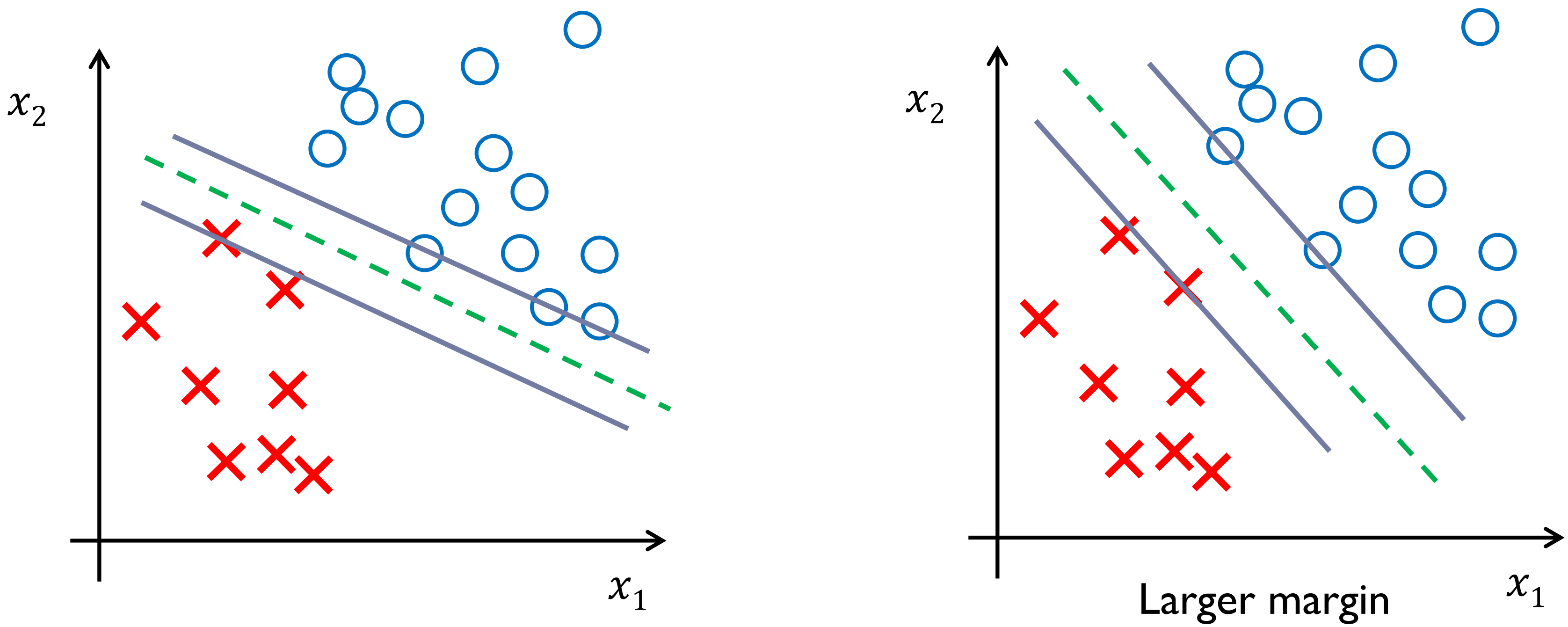
- Linearly separable data
- Which line is better?



- Why the bigger margin?

Maximum margin

- SVM finds the solution with maximum margin
  - Solution: a hyperplane that is farthest from all training samples



- The hyperplane with the largest margin has equal distances to the nearest sample of both classes

Finding $\boldsymbol{w}$ with large margin

- Two preliminaries:
  - Pull out w_0
  - $\boldsymbol{w}$ is $[w_1, \dots, w_d]$

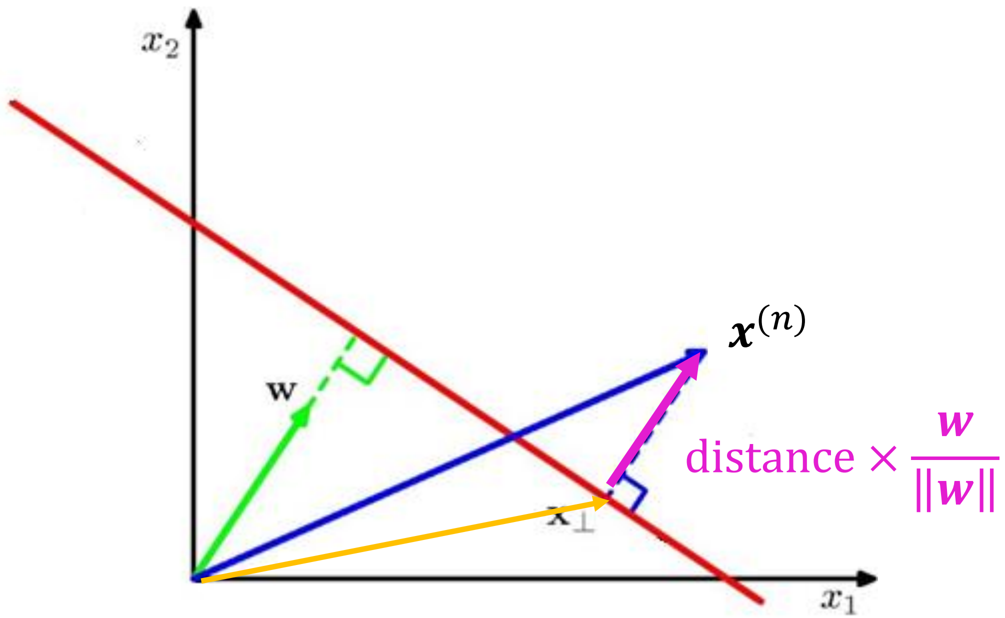
$$\boldsymbol{w}^T\boldsymbol{x} + w_0 = 0$$

We have no x_0

- Normalize $\boldsymbol{w}, w_0$
  - Let $\boldsymbol{x}^{(n)}$ be the nearest point to the plane
  - $\left|\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right| = 1$

Distance between an $\boldsymbol{x}^{(n)}$ and the plane

$$\text{distance} = \frac{\left|\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right|}{\|\boldsymbol{w}\|}$$



The optimization problem

$$\max_{\boldsymbol{w}, w_0} \frac{2}{\|\boldsymbol{w}\|}$$

$$\text{s.t.} \quad \min_{n=1,\dots,N} \left| \boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0 \right| = 1$$

From all the hyperplanes that correctly classify data

Notice: $\left| \boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0 \right| = y^{(n)} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0 \right)$

$$\min_{\boldsymbol{w}, w_0} \frac{1}{2} \|\boldsymbol{w}\|^2$$

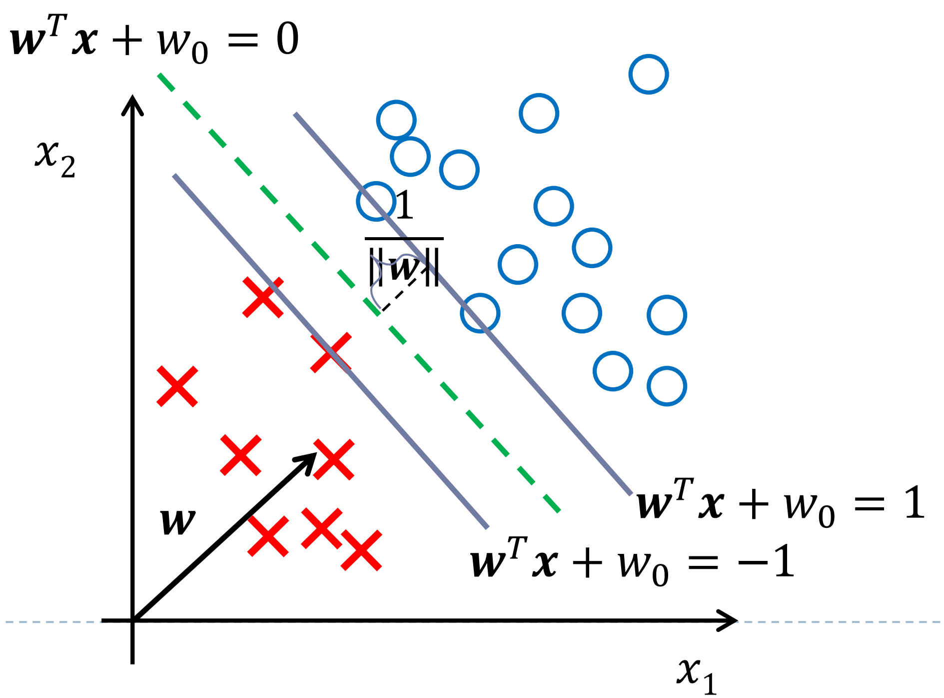
$$\text{s.t.} \quad y^{(n)} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0 \right) \geq 1 \quad n = 1, \dots, N$$

Hard-margin SVM: Optimization problem

$$\max_{\boldsymbol{w}, w_0} \frac{2}{\|\boldsymbol{w}\|}$$

$$\text{s.t. } \left|\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0\right| \geq 1 \;, n = 1, \dots, N$$

Margin: $\frac{2}{\|\boldsymbol{w}\|}$



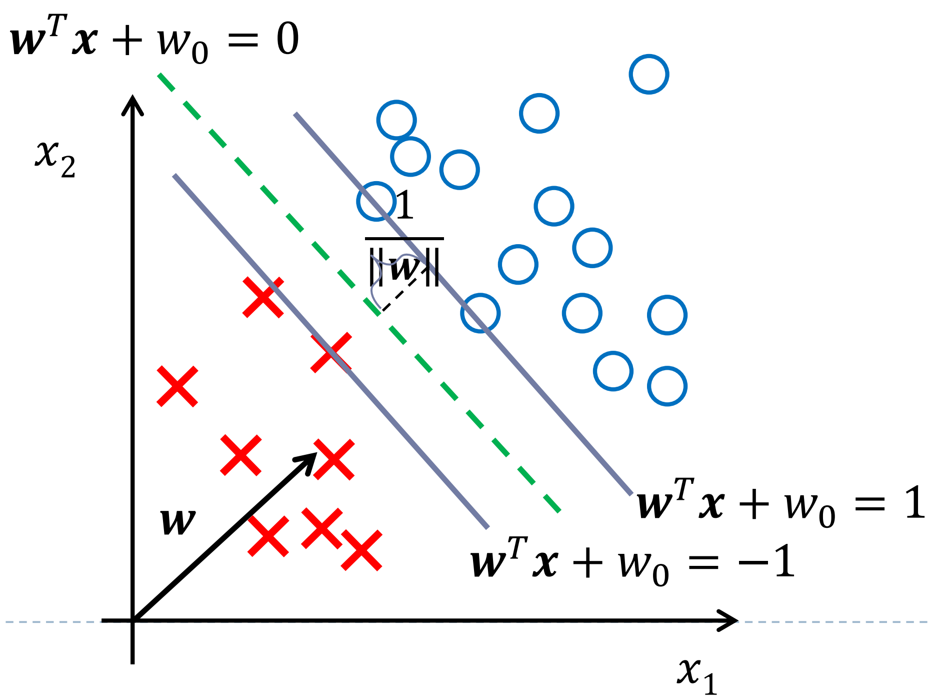
Hard-margin SVM: Optimization problem

$$\max_{\boldsymbol{w}, w_0} \frac{2}{\|\boldsymbol{w}\|}$$

$$\text{s.t.} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0\right) \geq 1 \quad \forall y^{(n)} = 1$$

$$\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0\right) \leq -1 \quad \forall y^{(n)} = -1$$

Margin: $\frac{2}{\|\boldsymbol{w}\|}$



Hard-margin SVM: Optimization problem

We can equivalently optimize:

$$\min_{\boldsymbol{w}, w_0} \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w}$$

$$\text{s.t.} \quad y^{(n)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0\right) \geq 1 \quad n = 1, \ldots, N$$

- It is a convex Quadratic Programming (QP) problem
  - There are computationally efficient packages to solve it.
  - It has a <u>global</u> minimum (if any).

Quadratic programming

$$
\begin{aligned}
\min_{\boldsymbol{x}} \ & \frac{1}{2}\boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x} + \boldsymbol{c}^T\boldsymbol{x} \\
\text{s.t.} \quad & \boldsymbol{A}\boldsymbol{x} \le \boldsymbol{b} \\
& \boldsymbol{E}\boldsymbol{x} = \boldsymbol{d}
\end{aligned}
$$

Dual formulation of the SVM

- We are going to introduce the *dual* SVM problem which is equivalent to the original *primal* problem. The dual problem:
  - is often easier
  - gives us further insights into the optimal hyperplane
  - enable us to exploit the kernel trick

Optimization: Lagrangian multipliers

$$p^* = \min_{\boldsymbol{x}} f(\boldsymbol{x})$$
$$\text{s.t. } g_i(\boldsymbol{x}) \le 0 \quad i = 1, \dots, m$$
$$h_i(\boldsymbol{x}) = 0 \quad i = 1, \dots, p$$

Lagrangian multipliers

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \sum_{i=1}^{m} \alpha_i g_i(\boldsymbol{x}) + \sum_{i=1}^{p} \lambda_i h_i(\boldsymbol{x})$$

$$\max_{\{\alpha_i \ge 0\},\{\lambda_i\}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\lambda}) = \begin{cases} \infty & \text{any } g_i(\boldsymbol{x}) > 0 \\ \infty & \text{any } h_i(\boldsymbol{x}) \ne 0 \\ f(\boldsymbol{x}) & \text{otherwise} \end{cases}$$

$$p^* = \min_{\boldsymbol{x}} \max_{\{\alpha_i \ge 0\},\{\lambda_i\}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\lambda})$$

$$\boldsymbol{\alpha} = [\alpha_1, \dots, \alpha_m]$$
$$\boldsymbol{\lambda} = [\lambda_1, \dots, \lambda_p]$$

Optimization: Dual problem

- In general, we have:

$$\max_x \min_y h(x, y) \le \min_y \max_x h(x, y)$$

- **Primal problem**: $p^* = \min_{\boldsymbol{x}} \max_{\{\alpha_i \ge 0\}, \{\lambda_i\}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\lambda})$

- **Dual problem**: $d^* = \max_{\{\alpha_i \ge 0\}, \{\lambda_i\}} \min_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\lambda})$
  - Obtained by swapping the order of min and max
  - $d^* \le p^*$

- When the original problem is convex (f and g are convex functions and h is affine), we have strong duality $d^* = p^*$

Hard-margin SVM: Dual problem

$$\min_{\boldsymbol{w},w_0} \frac{1}{2}\|\boldsymbol{w}\|^2$$
$$\text{s.t.} \quad y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + w_0\right) \geq 1 \quad i = 1,\dots,N$$

- By incorporating the constraints through lagrangian multipliers, we will have:

$$\min_{\boldsymbol{w},w_0} \max_{\{\alpha_n \geq 0\}} \left\{\frac{1}{2}\|\boldsymbol{w}\|^2 + \sum_{n=1}^{N} \alpha_n\left(1 - y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0)\right)\right\}$$

- Dual problem (changing the order of min and max in the above problem):

$$\max_{\{\alpha_n \geq 0\}} \min_{\boldsymbol{w},w_0} \left\{\frac{1}{2}\|\boldsymbol{w}\|^2 + \sum_{n=1}^{N} \alpha_n\left(1 - y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0)\right)\right\}$$

Hard-margin SVM: Dual problem

$$\max_{\{\alpha_n \geq 0\}} \min_{\boldsymbol{w}, w_0} \mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha})$$

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2}\|\boldsymbol{w}\|^2 + \sum_{n=1}^{N} \alpha_n \left(1 - y^{(n)}(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0)\right)$$

$$\nabla_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = 0 \Rightarrow \boldsymbol{w} - \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)} = \boldsymbol{0}$$

$$\Rightarrow \boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)}$$

$$\frac{\partial \mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha})}{\partial w_0} = 0 \Rightarrow \quad -\underbrace{\sum_{n=1}^{N} \alpha_n y^{(n)} = 0}$$

w_0 do not appear, instead, a "global" constraint on $\boldsymbol{\alpha}$ is created.

Substituting

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)} \qquad \sum_{n=1}^{N} \alpha_n y^{(n)} = 0$$

In the Largrangian

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \sum_{n=1}^{N} \alpha_n\left(1 - y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0)\right)$$

Substituting

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)} \qquad \sum_{n=1}^{N} \alpha_n y^{(n)} = 0$$

In the Largrangian

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \sum_{n=1}^{N} \alpha_n\left(-y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0)\right)$$

We get

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n$$

Substituting

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)} \qquad \sum_{n=1}^{N} \alpha_n y^{(n)} = 0$$

In the Largrangian

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \sum_{n=1}^{N} \alpha_n\left(\quad - y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} \qquad)\right)$$

We get

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n$$

Substituting

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)} \qquad \sum_{n=1}^{N} \alpha_n y^{(n)} = 0$$

In the Largrangian

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \sum\nolimits_{n=1}^{N} \alpha_n\Big(\quad - y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} \qquad)\Big)$$

We get

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum\nolimits_{n=1}^{N} \alpha_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n \alpha_m y^{(n)} y^{(m)} \boldsymbol{x}^{(n)T} \boldsymbol{x}^{(m)}$$

Maximize w.r.t. $\boldsymbol{\alpha}$ subject to $\alpha_n \geq 0$ for $n = 1, \dots, N$ and $\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$

Hard-margin SVM: Dual problem

$$\max_{\boldsymbol{\alpha}} \left\{ \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y^{(n)} y^{(m)} \boldsymbol{x}^{(n)^T} \boldsymbol{x}^{(m)} \right\}$$

Subject to $\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$

$$\alpha_n \geq 0 \quad n = 1, \dots, N$$

- It is a convex QP

Solution

- Quadratic programming:

$$\min_{\boldsymbol{\alpha}} \frac{1}{2}\boldsymbol{\alpha}^T \begin{bmatrix} y^{(1)}y^{(1)}\boldsymbol{x}^{(1)^T}\boldsymbol{x}^{(1)} & \cdots & y^{(1)}y^{(N)}\boldsymbol{x}^{(1)^T}\boldsymbol{x}^{(N)} \\ \vdots & \ddots & \vdots \\ y^{(N)}y^{(1)}\boldsymbol{x}^{(N)^T}\boldsymbol{x}^{(1)} & \cdots & y^{(N)}y^{(N)}\boldsymbol{x}^{(N)^T}\boldsymbol{x}^{(N)} \end{bmatrix} \boldsymbol{\alpha} + (-\mathbf{1})^T\boldsymbol{\alpha}$$

$$\text{s.t.} -\boldsymbol{\alpha} \leq \mathbf{0}$$
$$\boldsymbol{y}^T\boldsymbol{\alpha} = \mathbf{0}$$

Finding the hyperplane

- After finding $\boldsymbol{\alpha}$ by QP, we find $\boldsymbol{w}$:

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)}$$

- How to find w_0?
  - we discuss it after introducing support vectors

Karush-Kuhn-Tucker (KKT) conditions

- Necessary conditions for the solution $[\boldsymbol{w}^*, w_0^*, \boldsymbol{\alpha}^*]$:
  - $\nabla_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha})|_{\boldsymbol{w}^*, w_0^*, \boldsymbol{\alpha}^*} = 0$
  - $\frac{\partial \mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\alpha})}{\partial w_0}|_{\boldsymbol{w}^*, w_0^*, \boldsymbol{\alpha}^*} = 0$
  - $\alpha_n^* \geq 0 \quad n = 1, \dots, N$
  - $y^{(n)}\left(\boldsymbol{w}^{*T}\boldsymbol{x}^{(n)} + w_0^*\right) \geq 1 \quad n = 1, \dots, N$
  - $\alpha_i^* \left(1 - y^{(n)}\left(\boldsymbol{w}^{*T}\boldsymbol{x}^{(n)} + w_0^*\right)\right) = 0 \quad n = 1, \dots, N$

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$
$$\text{s.t. } g_i(\boldsymbol{x}) \leq 0 \quad i = 1, \dots, m$$

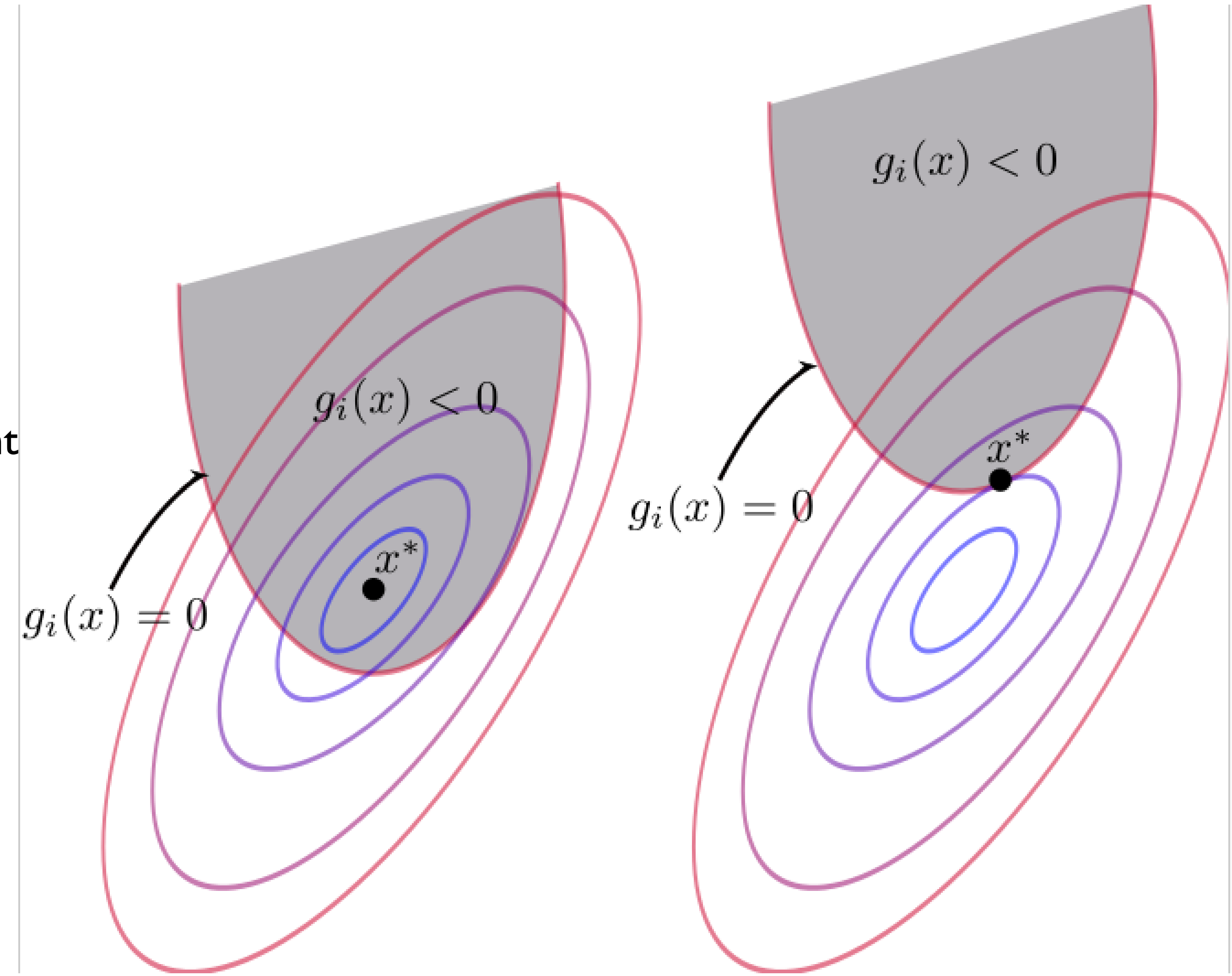
$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}) = f(\boldsymbol{x}) + \sum \alpha_i \, g_i(\boldsymbol{x})$$

In general, the optimal $\boldsymbol{x}^*, \boldsymbol{\alpha}^*$ satisfies KKT conditions:

$$\nabla_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha})\Big|_{\boldsymbol{x}^*, \boldsymbol{\alpha}^*} = 0$$
$$\alpha_i^* \geq 0 \quad i = 1, \dots, m$$
$$g_i(\boldsymbol{x}^*) \leq 0 \quad i = 1, \dots, m$$
$$\alpha_i^* g_i(\boldsymbol{x}^*) = 0 \quad i = 1, \dots, m$$

Karush-Kuhn-Tucker (KKT) conditions

Inactive constraint ($\alpha = 0$)

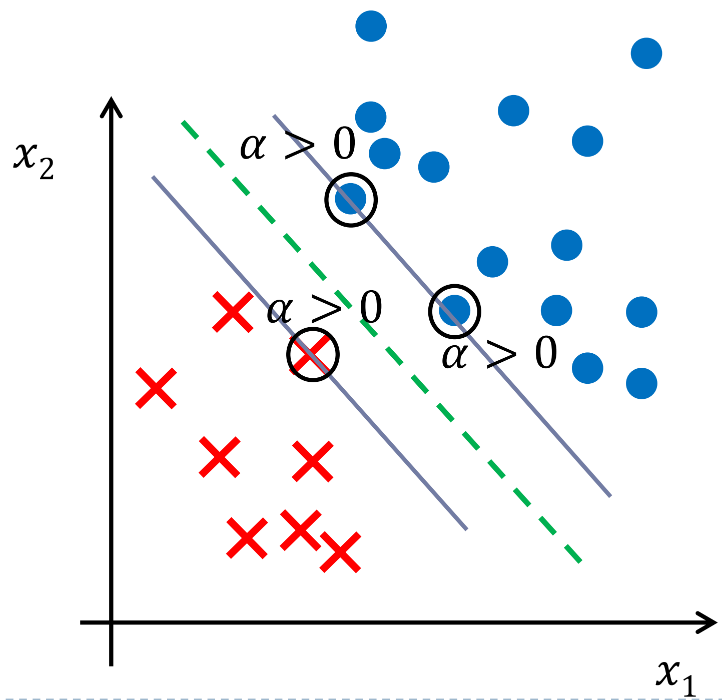


Active constraint

[wikipedia]

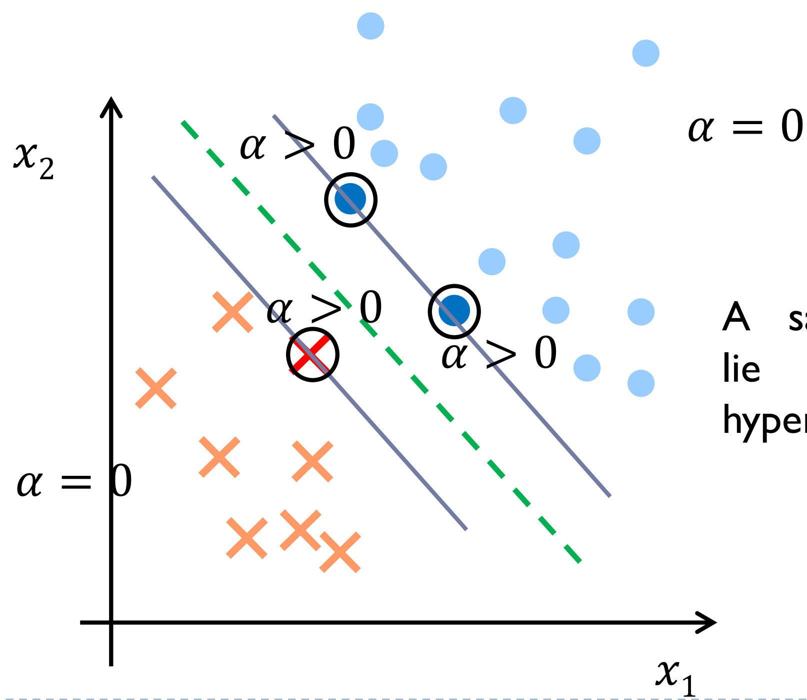
Hard-margin SVM: Support vectors

- **Inactive** constraint: $y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) > 1$
  - $\Rightarrow \alpha_n = 0$ and thus $\boldsymbol{x}^{(n)}$ is not a support vector.
- **Active** constraint: $y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) = 1$
  - $\Rightarrow \alpha_n$ can be greater than 0 and thus $\boldsymbol{x}^{(i)}$ can be a support vector.



Hard-margin SVM: Support vectors

- **Inactive** constraint: $y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) > 1$
  - $\Rightarrow \alpha_n = 0$ and thus $\boldsymbol{x}^{(n)}$ is not a support vector.
- **Active** constraint: $y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) = 1$

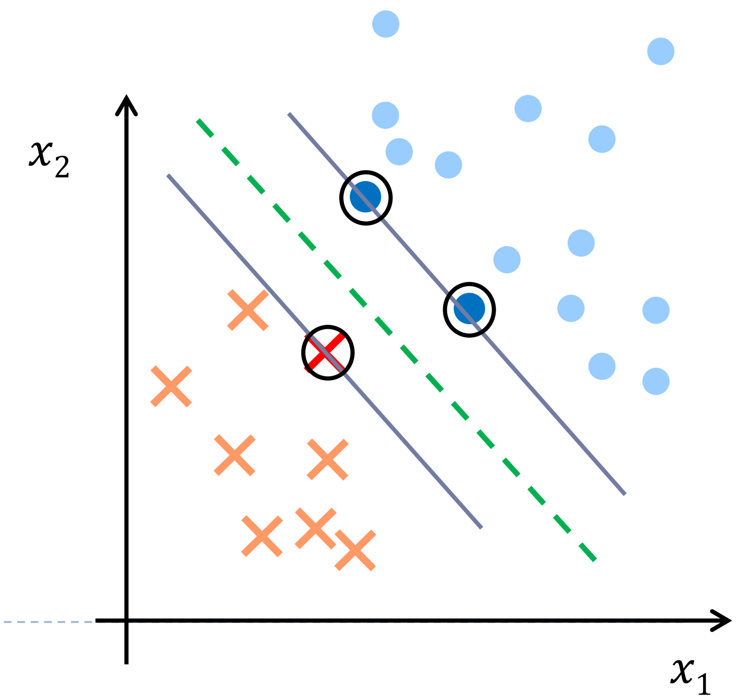


A sample with $\alpha_n = 0$ can also lie on one of the margin hyperplanes

Hard-margin SVM: Support vectors

- Support Vectors (SVs)= $\{\boldsymbol{x}^{(n)} | \alpha_n > 0\}$
- The **direction** of hyper-plane can be found only based on support vectors:

$$\boldsymbol{w} = \sum_{\alpha_n > 0} \alpha_n \, y^{(n)} \boldsymbol{x}^{(n)}$$



Finding the hyperplane

- After finding $\boldsymbol{\alpha}$ by QP, we find $\boldsymbol{w}$:

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} \boldsymbol{x}^{(n)}$$

- How to find w_0?
  - Each of the samples that has $\alpha_s > 0$ is on the margin, thus we solve for w_0 using any of SVs:

$$\left| \boldsymbol{w}^T \boldsymbol{x}^{(s)} + w_0 \right| = 1$$

$$y^{(s)} \left(\boldsymbol{w}^T \boldsymbol{x}^{(s)} + w_0 \right) = 1$$

$$\Rightarrow w_0 = y^{(s)} - \boldsymbol{w}^T \boldsymbol{x}^{(s)}$$

Hard-margin SVM: Dual problem Classifying new samples using only SVs

- Classification of a new sample $\boldsymbol{x}$:

$$\hat{y} = \text{sign}(w_0 + \boldsymbol{w}^T \boldsymbol{x})$$

$$\hat{y} = \text{sign}\left(w_0 + \left(\sum_{\alpha_n > 0} \alpha_n y^{(n)} \boldsymbol{x}^{(n)}\right)^T \boldsymbol{x}\right)$$

$$\hat{y} = \text{sign}(\underbrace{y^{(s)} - \sum_{\alpha_n > 0} \alpha_n y^{(n)} \boldsymbol{x}^{(n)^T} \boldsymbol{x}^{(s)}}_{w_0} + \sum_{\alpha_n > 0} \alpha_n y^{(n)} \boldsymbol{x}^{(n)^T} \boldsymbol{x})$$

Support vectors are sufficient to predict labels of new samples

- The classifier is based on the expansion in terms of dot products of $\boldsymbol{x}$ with support vectors.

Hard-margin SVM: Dual problem

$$\max_{\boldsymbol{\alpha}} \left\{ \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y^{(n)} y^{(m)} \boldsymbol{x}^{(n)^T} \boldsymbol{x}^{(m)} \right\}$$

Subject to $\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$

$$\alpha_n \geq 0 \quad n = 1, \dots, N$$

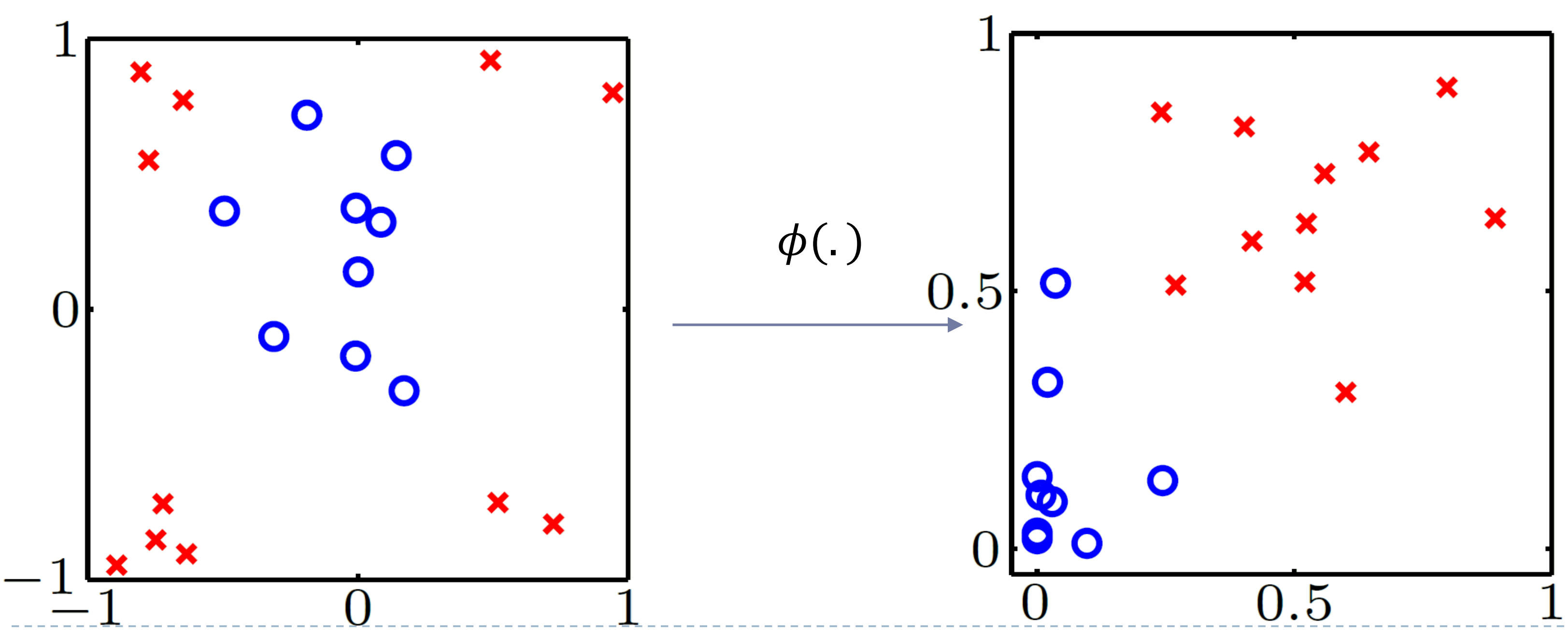
- Only the dot product of each pair of training data appears in the optimization problem
  - An important property that is helpful to extend to non-linear SVM

In the transformed space

$$\max_{\boldsymbol{\alpha}} \left\{ \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y^{(n)} y^{(m)} \phi\left(\boldsymbol{x}^{(n)}\right)^T \phi\left(\boldsymbol{x}^{(m)}\right) \right\}$$

Subject to $\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$

$\alpha_n \geq 0 \quad n = 1, \dots, N$



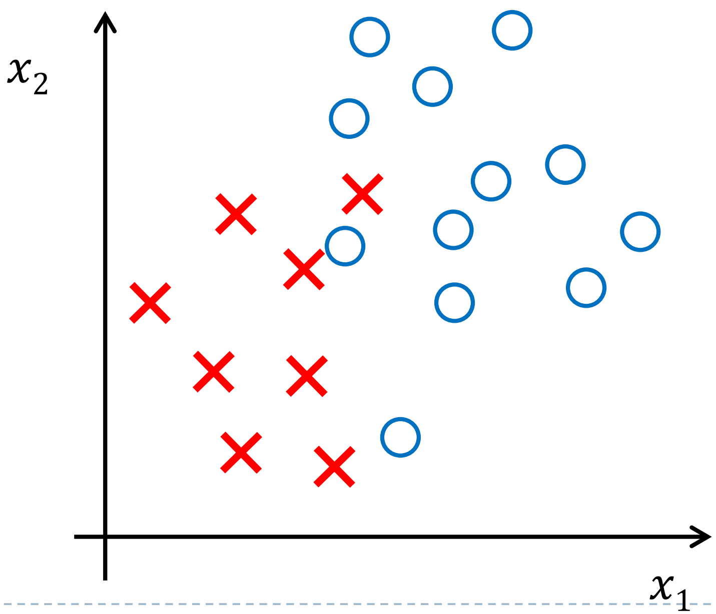
Beyond linear separability

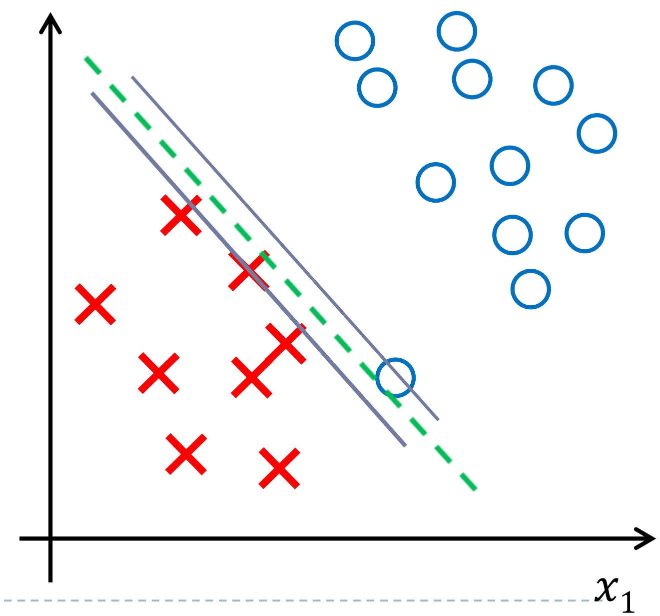
- When training samples are not linearly separable, it has no solution.

- How to extend it to find a solution even though the classes are not exactly linearly separable.

Beyond linear separability

- How to extend the hard-margin SVM to allow classification error
  - Overlapping classes that can be approximately separated by a linear boundary
  - Noise in the linearly separable classes





Beyond linear separability: Soft-margin SVM

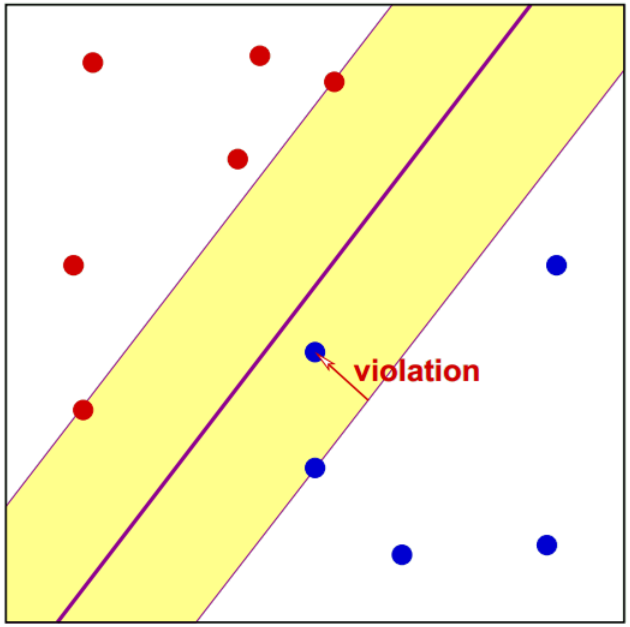
- Minimizing the number of misclassified points?!
  - NP-complete

- Soft margin:
  - Maximizing a margin while trying to minimize the *distance* between misclassified points and their correct margin plane

Error measure

- Margin violation amount ξ_n ($\xi_n \geq 0$):
  - $y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) \geq 1 - \xi_n$

- Total violation: $\sum_{n=1}^{N} \xi_n$



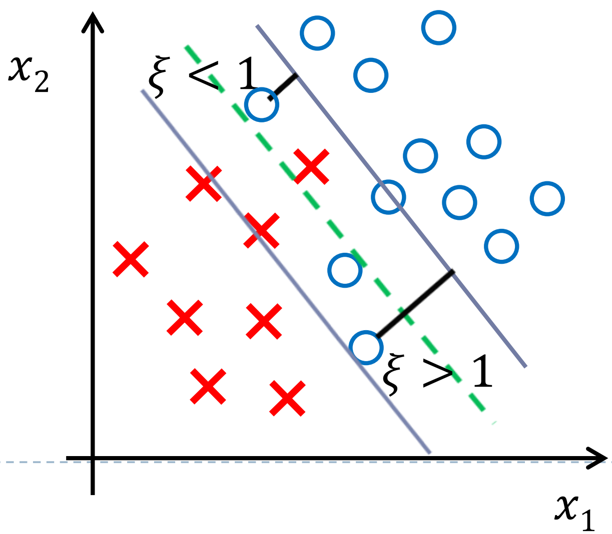
Soft-margin SVM: Optimization problem

- SVM with slack variables: allows samples to fall within the margin, but penalizes them

$$\min_{\boldsymbol{w}, w_0, \{\xi_n\}_{n=1}^{N}} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N} \xi_n$$

$$\text{s.t.} \quad y^{(n)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + w_0\right) \geq 1 - \xi_n \quad n = 1, \dots, N$$

$$\xi_n \geq 0$$



ξ_n: **slack** variables

$0 < \xi_n < 1$: if $\boldsymbol{x}^{(n)}$ is correctly classified but inside margin

$\xi_n > 1$: if $\boldsymbol{x}^{(n)}$ is misclassifed

Soft-margin SVM

- linear penalty (hinge loss) for a sample if it is misclassified or lied in the margin
  - tries to maintain ξ_n small while maximizing the margin.
  - always finds a solution (as opposed to hard-margin SVM)
  - more robust to the outliers
- Soft margin problem is still a convex QP

Soft-margin SVM: Parameter C

- C is a tradeoff parameter:
  - small C allows margin constraints to be easily ignored
    - large margin
  - large C makes constraints hard to ignore
    - narrow margin

- $C \to \infty$ enforces all constraints: hard margin

- C can be determined using a technique like cross-validation

Soft-margin SVM: Cost function

$$\min_{\boldsymbol{w},w_0,\{\xi_n\}_{n=1}^N} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

$$\text{s.t.} \quad y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) \geq 1 - \xi_n \quad n = 1, \dots, N$$

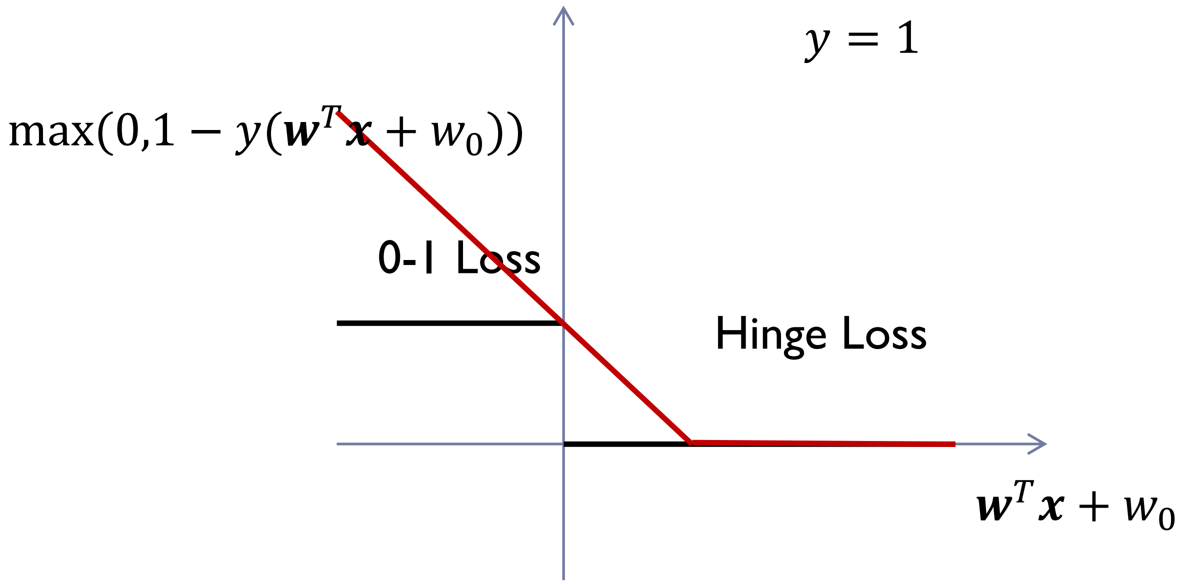
$$\xi_n \geq 0$$

- It is equivalent to the unconstrained optimization problem:

$$\min_{\boldsymbol{w},w_0} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\max(0,1 - y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0))$$

SVM loss function

- Hinge loss vs. 0-1 loss



Lagrange formulation

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$
$$= \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$
$$+ \sum_{n=1}^{N}\alpha_n\left(1 - \xi_n - y^{(n)}(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0)\right) - \sum_{n=1}^{N}\beta_n\xi_n$$

- Minimize w.r.t. $\boldsymbol{w}$, w_0, $\boldsymbol{\xi}$ and maximize w.r.t. $\alpha_n \geq 0$ and $\beta_n \geq 0$

$$\min_{\boldsymbol{w}, w_0, \{\xi_n\}_{n=1}^{N}} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$
$$\text{s.t.} \quad y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) \geq 1 - \xi_n \quad n = 1, \dots, N$$
$$\xi_n \geq 0$$

Lagrange formulation

$$\mathcal{L}(\boldsymbol{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N} \xi_n + \sum_{n=1}^{N} \alpha_n \big(1$$

Soft-margin SVM: Dual problem

$$\max_{\boldsymbol{\alpha}} \left\{ \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y^{(n)} y^{(m)} \boldsymbol{x}^{(n)^T} \boldsymbol{x}^{(m)} \right\}$$

Subject to $\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$

$$0 \leq \alpha_n \leq C \quad n = 1, \dots, N$$

- After solving the above quadratic problem, $\boldsymbol{w}$ is find as:

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n \, y^{(n)} \boldsymbol{x}^{(n)}$$

Soft-margin SVM: Support vectors

- Support Vectors: $\alpha_n > 0$
  - If $0 < \alpha_n < C$ (**margin** support vector)

    SVs on the margin

$$y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) = 1 \qquad (\xi_n = 0)$$

  - If $\alpha = C$ (**non-margin** support vector)

    SVs on or over the margin

$$y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + w_0\right) < 1 \qquad (\xi_n > 0)$$

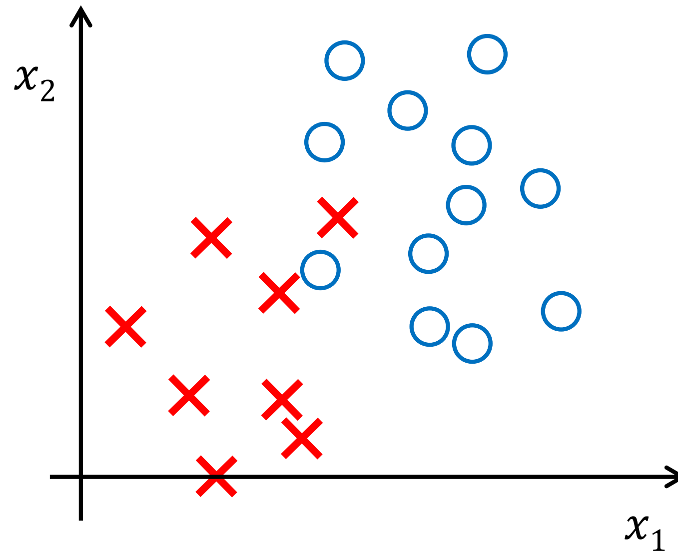
$$C - \alpha_n - \beta_n = 0$$

SVM: Summary

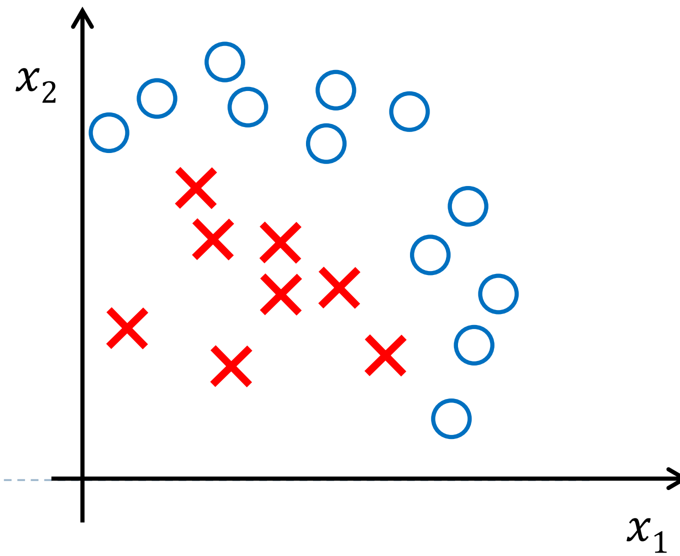
- Hard margin: maximizing margin
- Soft margin: handling noisy data and overlapping classes
  - Slack variables in the problem
- Dual problems of hard-margin and soft-margin SVM
  - Classifier decision in terms of *support vectors*
- Dual problems lead us to non-linear SVM method easily by kernel substitution

Not linearly separable data

- Noisy data or overlapping classes (we discussed about it: soft margin)
  - Near linearly separable



- Non-linear decision surface
  - Transform to a new feature space



Nonlinear SVM

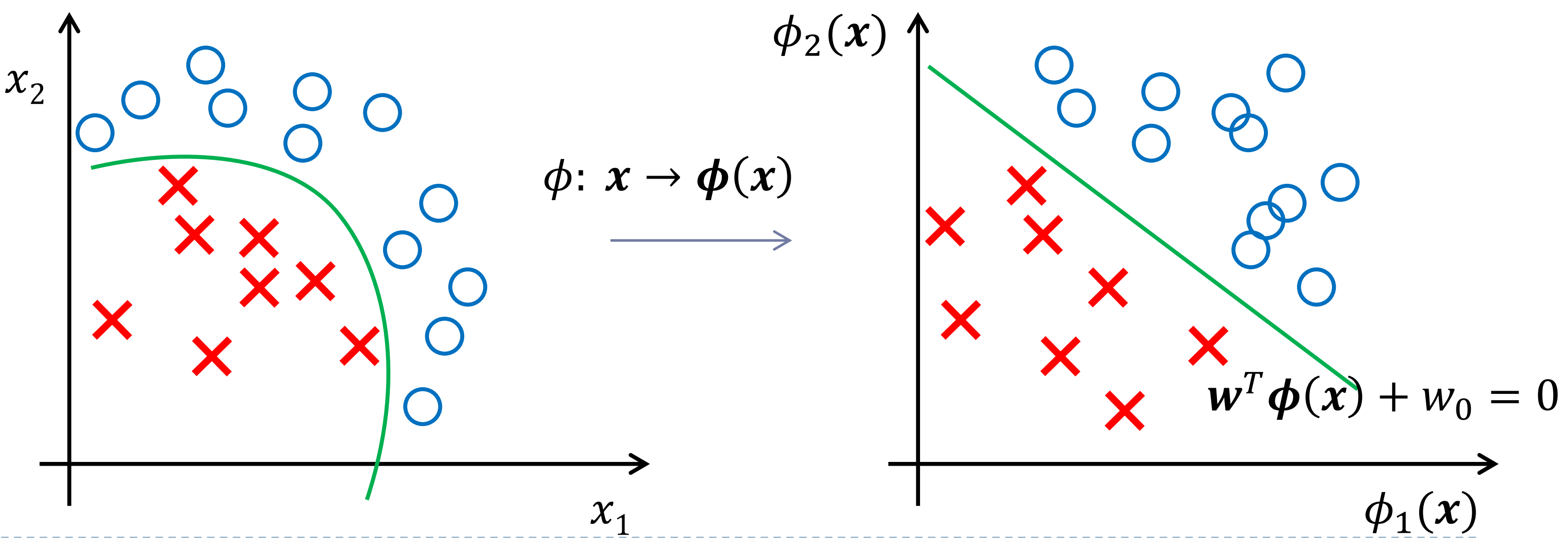
- Assume a transformation $\phi: \mathbb{R}^d \rightarrow \mathbb{R}^m$ on the feature space
  - $\boldsymbol{x} \rightarrow \boldsymbol{\phi}(\boldsymbol{x})$

$\boldsymbol{\phi}(\boldsymbol{x}) = [\phi_1(\boldsymbol{x}), \ldots, \phi_m(\boldsymbol{x})]$

$\{\phi_1(\boldsymbol{x}),\ldots,\phi_m(\boldsymbol{x})\}$: set of basis functions (or features)

$\phi_i(\boldsymbol{x}): \mathbb{R}^d \rightarrow \mathbb{R}$

- Find a hyper-plane in the transformed feature space:



Soft-margin SVM in a transformed space: Primal problem

- Primal problem:

$$\min_{\boldsymbol{w},w_0} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

$$\text{s.t.} \quad y^{(n)}\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}^{(n)}) + w_0\right) \geq 1 - \xi_n \quad n = 1, \dots, N$$

$$\xi_n \geq 0$$

  - $\boldsymbol{w} \in \mathbb{R}^m$: the weights that must be found
  - If $m \gg d$ (very high dimensional feature space) then there are many more parameters to learn

Soft-margin SVM in a transformed space: Dual problem

- Optimization problem:

$$\max_{\boldsymbol{\alpha}} \left\{ \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y^{(n)} y^{(m)} \boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right)^T \boldsymbol{\phi}\left(\boldsymbol{x}^{(m)}\right) \right\}$$

Subject to $\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$

$$0 \leq \alpha_n \leq C \quad n = 1, \dots, N$$

- If we have inner products $\boldsymbol{\phi}\left(\boldsymbol{x}^{(i)}\right)^T \boldsymbol{\phi}\left(\boldsymbol{x}^{(j)}\right)$, only $\boldsymbol{\alpha} = [\alpha_1, \dots, \alpha_N]$ needs to be learnt.
  - not necessary to learn m parameters as opposed to the primal problem

Classifying a new data

$$\hat{y} = sign\left(w_0 \ + \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})\right)$$

where $\boldsymbol{w} = \sum_{\alpha_n > 0} \alpha_n \, y^{(n)} \boldsymbol{\phi}(\boldsymbol{x}^{(n)})$

and $w_0 \ = y^{(s)} - \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}^{(s)})$

Kernel SVM

- Learns linear decision boundary in a high dimension space without explicitly working on the mapped data

- Let $\boldsymbol{\phi}(\boldsymbol{x})^T\boldsymbol{\phi}(\boldsymbol{x}') = K(\boldsymbol{x}, \boldsymbol{x}')$ (kernel)

- Example: $\boldsymbol{x} = [x_1, x_2]$ and second-order $\boldsymbol{\phi}$:

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

$$K(\boldsymbol{x}, \boldsymbol{x}') \\ = 1 + x_1x_1' + x_2x_2' + x_1^2x_1'^2 + x_2^2x_2'^2 + x_1x_1'x_2x_2'$$

Kernel trick

- Compute $K(\boldsymbol{x}, \boldsymbol{x}')$ without transforming $\boldsymbol{x}$ and $\boldsymbol{x}'$

- Example: Consider $K(\boldsymbol{x}, \boldsymbol{x}') = (1 + \boldsymbol{x}^T\boldsymbol{x}')^2$

$$= \left(1 + x_1x_1' + x_2x_2'\right)^2$$

$$= 1 + 2x_1x_1' + 2x_2x_2' + x_1^2x_1'^2 + x_2^2x_2'^2 + 2x_1x_1'x_2x_2'$$

This is an inner product in:

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

$$\boldsymbol{\phi}(\boldsymbol{x}') = \left[1, \sqrt{2}x_1', \sqrt{2}x_2', x'^2_1, x'^2_2, \sqrt{2}x_1'x_2'\right]$$

Polynomial kernel: Degree two

- We instead use $K(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^T\boldsymbol{x}' + 1)^2$ that corresponds to:

  d-dimensional feature space $\boldsymbol{x} = [x_1, \dots, x_d]^T$

$$\boldsymbol{\phi}(\boldsymbol{x}) = \left[1, \sqrt{2}x_1, \dots, \sqrt{2}x_d, x_1^2, \dots, x_d^2, \sqrt{2}x_1x_2, \dots, \sqrt{2}x_1x_d, \sqrt{2}x_2x_3, \dots, \sqrt{2}x_{d-1}x_d\right]^T$$

Polynomial kernel

- This can similarly be generalized to d-dimensioan $\boldsymbol{x}$ and ϕs are polynomials of order M:

$$K(\boldsymbol{x}, \boldsymbol{x}') = (1 + \boldsymbol{x}^T \boldsymbol{x}')^M$$
$$= \left(1 + x_1 x_1' + x_2 x_2' + \cdots + x_d x_d'\right)^M$$

- Example: SVM boundary for a polynomial kernel
  - $w_0 + \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}) = 0$

    $\Rightarrow w_0 + \sum_{\alpha_i > 0} \alpha_i y^{(i)} \boldsymbol{\phi}\left(\boldsymbol{x}^{(i)}\right)^T \boldsymbol{\phi}(\boldsymbol{x}) = 0$

    $\Rightarrow w_0 + \sum_{\alpha_i > 0} \alpha_i y^{(i)} k(\boldsymbol{x}^{(i)}, \boldsymbol{x}) = 0$

    $\Rightarrow w_0 + \sum_{\alpha_i > 0} \alpha_i y^{(i)} \left(1 + \boldsymbol{x}^{(i)T} \boldsymbol{x}\right)^M = 0$ $\Rightarrow$ Boundary is a polynomial of order M

Why kernel?

- kernel functions K can indeed be efficiently computed, with a cost proportional to d (the dimensionality of the input) instead of m.

- Example: consider the second-order polynomial transform:

$$\boldsymbol{\phi}(\boldsymbol{x}) = [1, x_1, \dots, x_d, x_1^2, x_1 x_2, \dots, x_d x_d]^T \qquad m = 1 + d + d^2$$

$$\boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}') = 1 + \sum_{i=1}^{d} x_i x_i' + \underbrace{\sum_{i=1}^{d} \sum_{j=1}^{d} x_i x_j x_i' x_j'}_{\sum_{i=1}^{d} x_i x_i' \times \sum_{j=1}^{d} x_j x_j'} \qquad O(m)$$

$$\boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}') = 1 + (x^T x') + (x^T x')^2 \qquad O(d)$$

Gaussian or RBF kernel

- If $K(\boldsymbol{x}, \boldsymbol{x}')$ is an inner product in some transformed space of x, it is good

- $K(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\frac{\|\boldsymbol{x}-\boldsymbol{x}'\|^2}{\gamma})$

- Take one dimensional case with $\gamma = 1$:

$$K(x, x') = \exp(-(x - x')^2)$$

$$= \exp(-x^2) \exp(-x'^2) \exp(2xx')$$

$$= \exp(-x^2) \exp(-x'^2) \sum_{k=1}^{\infty} \frac{2^k x^k x'^k}{k!}$$

Some common kernel functions

- Linear: $k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^T \boldsymbol{x}'$
- Polynomial: $k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^T \boldsymbol{x}' + 1)^M$
- Gaussian: $k(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\frac{\|\boldsymbol{x}-\boldsymbol{x}'\|^2}{\gamma})$
- Sigmoid: $k(\boldsymbol{x}, \boldsymbol{x}') = \tanh(a\boldsymbol{x}^T \boldsymbol{x}' + b)$

Kernel formulation of SVM

- Optimization problem:

$$\max_{\boldsymbol{\alpha}} \left\{ \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y^{(n)} y^{(m)} \quad k\left(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(m)}\right) \right\}$$

Subject to $\quad \sum_{n=1}^{N} \alpha_n y^{(n)} = 0$

$$0 \leq \alpha_n \leq C \quad n = 1, \dots, N$$

$$\boldsymbol{Q} = \begin{bmatrix} y^{(1)} y^{(1)} K\left(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(1)}\right) & \cdots & y^{(1)} y^{(N)} K\left(\boldsymbol{x}^{(N)}, \boldsymbol{x}^{(1)}\right) \\ \vdots & \ddots & \vdots \\ y^{(N)} y^{(1)} K\left(\boldsymbol{x}^{(N)}, \boldsymbol{x}^{(1)}\right) & \cdots & y^{(N)} y^{(N)} K\left(\boldsymbol{x}^{(N)}, \boldsymbol{x}^{(N)}\right) \end{bmatrix}$$

Classifying a new data

$$\hat{y} = sign\left(w_0 \ + \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})\right)$$

where $\boldsymbol{w} = \sum_{\alpha_n > 0} \alpha_n \, y^{(n)} \boldsymbol{\phi}(\boldsymbol{x}^{(n)})$

and $w_0 \ = y^{(s)} - \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}^{(s)})$

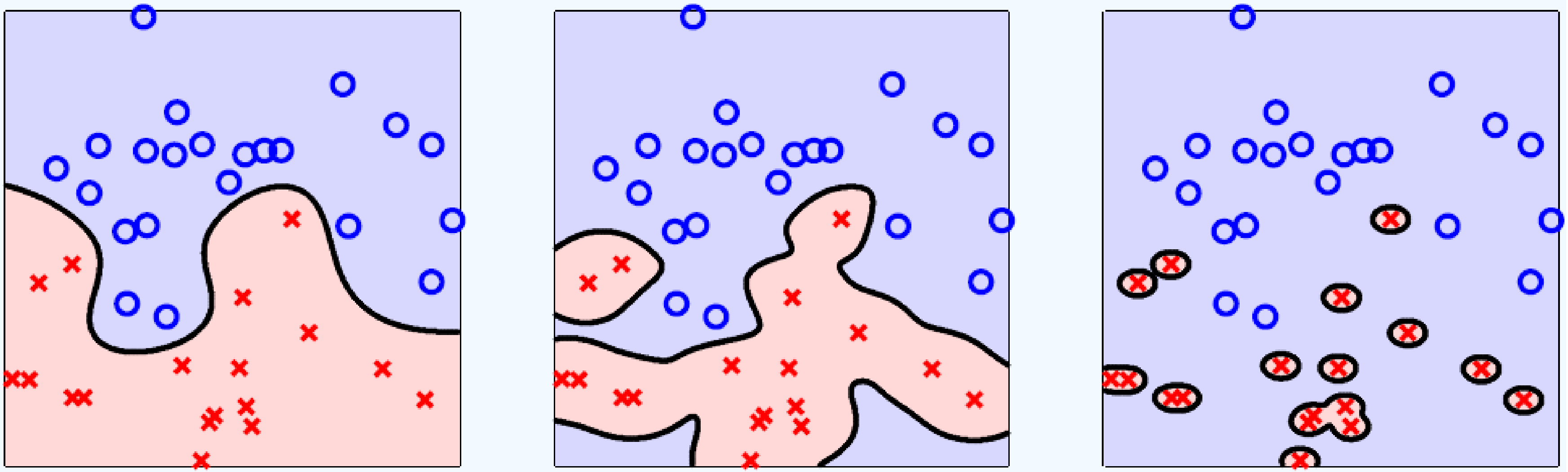
$$\hat{y} = sign\left(w_0 \ + \sum_{\alpha_n > 0} \alpha_n \, y^{(n)} \ \ k(\boldsymbol{x}^{(n)}, \boldsymbol{x}) \right)$$

$$w_0 \ = y^{(s)} - \sum_{\alpha_n > 0} \alpha_n \, y^{(n)} \ \ k(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(s)})$$

Gaussian kernel

- Example: SVM boundary for a gaussian kernel
  - Considers a Gaussian function around each data point.
  - $w_0 + \sum_{\alpha_i>0} \alpha_i y^{(i)} \exp(-\frac{\left\|\boldsymbol{x}-\boldsymbol{x}^{(i)}\right\|^2}{\sigma}) = 0$
  - SVM + Gaussian Kernel can classify any arbitrary training set
    - Training error is zero when $\sigma \to 0$
      - All samples become support vectors (likely overfiting)

Hard margin Example

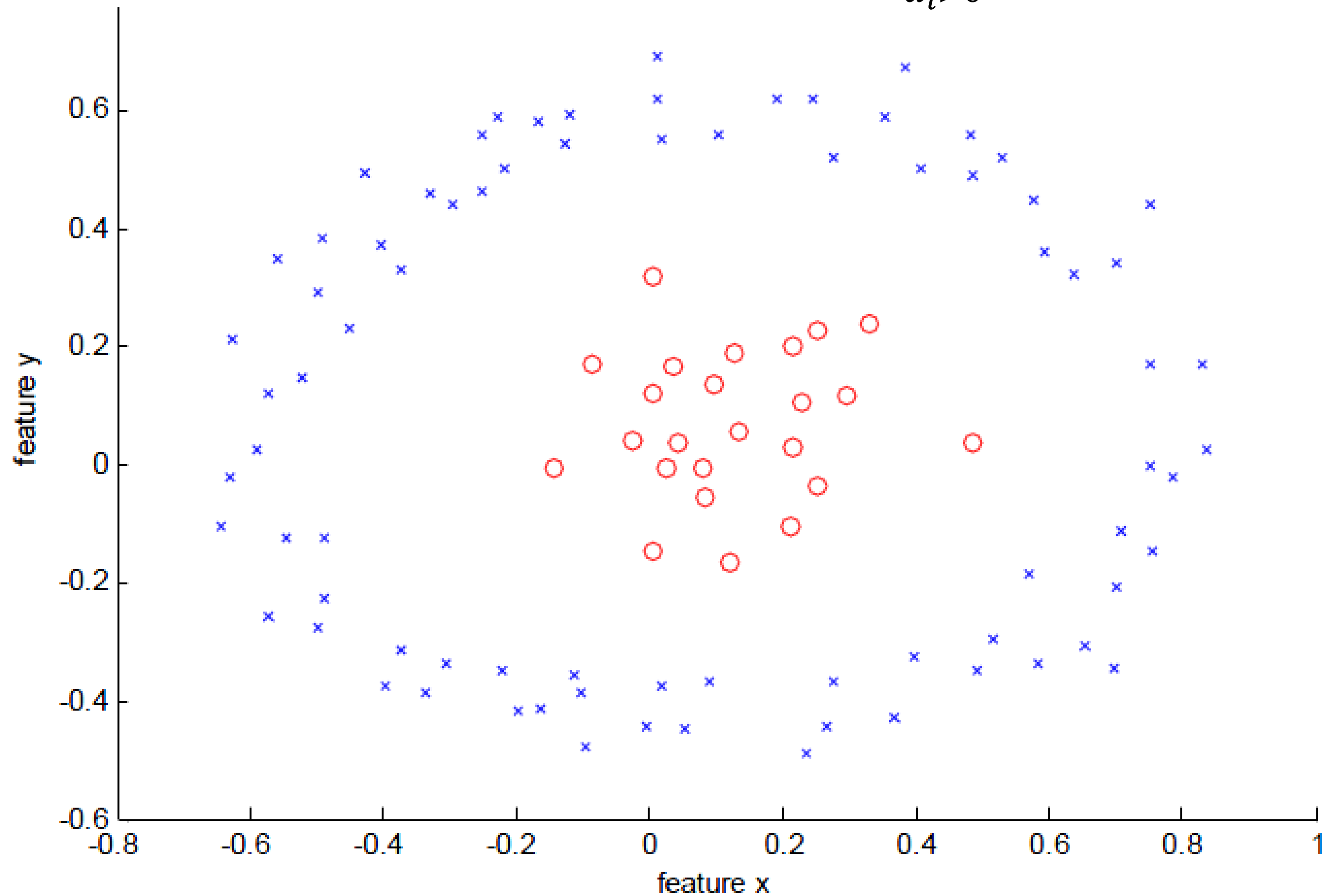


$\exp(-1\|\mathbf{x}-\mathbf{x}'\|^2)$ $\exp(-10\|\mathbf{x}-\mathbf{x}'\|^2)$ $\exp(-100\|\mathbf{x}-\mathbf{x}'\|^2)$

- For narrow Gaussian (large σ), even the protection of a large margin cannot suppress overfitting.

SVM Gaussian kernel: Example

$$f(\boldsymbol{x}) = w_0 + \sum_{\alpha_i > 0} \alpha_i y^{(i)} \exp\left(-\frac{\left\|\boldsymbol{x} - \boldsymbol{x}^{(i)}\right\|^2}{2\sigma^2}\right)$$



This example has been adopted from Zisserman's slides

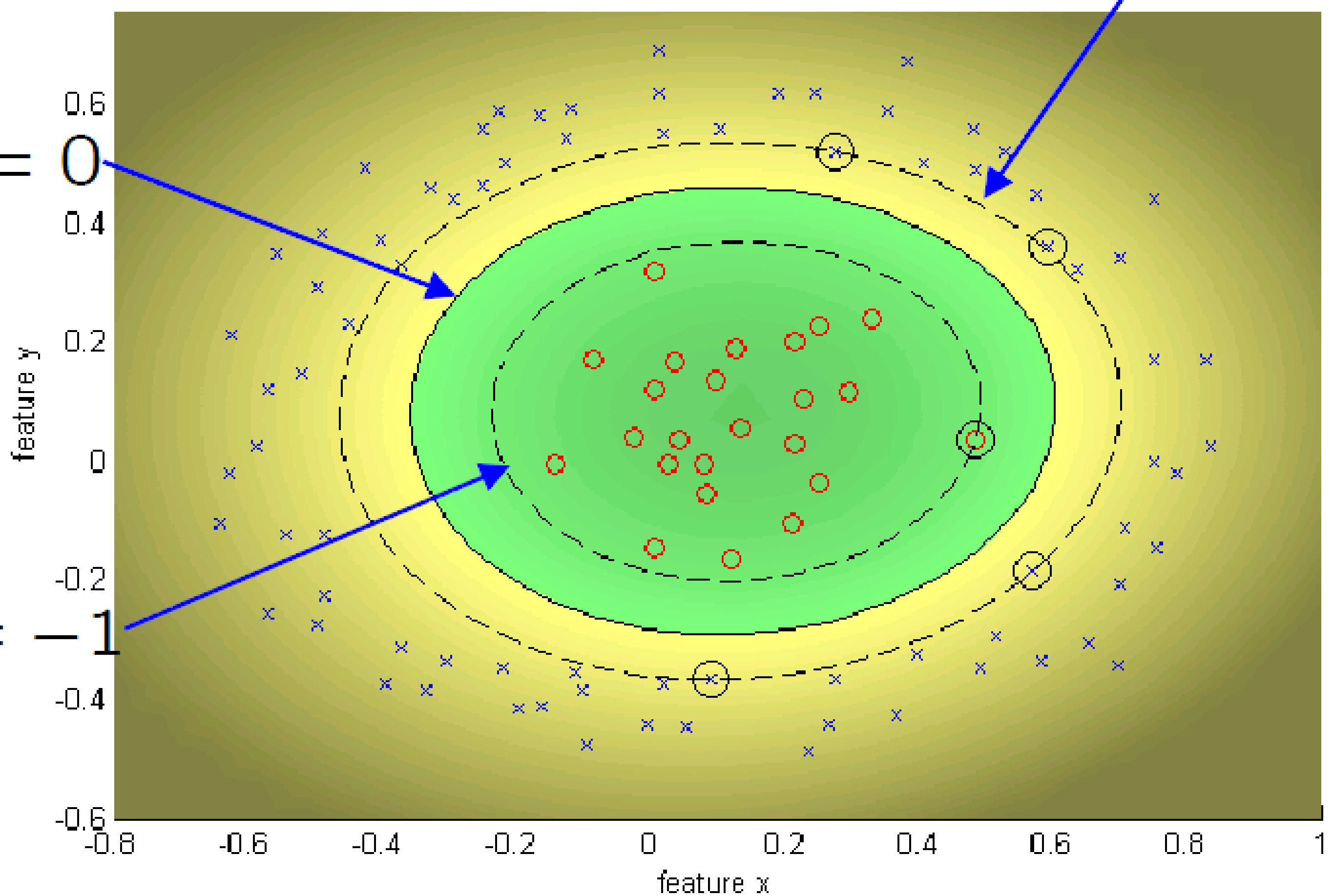
SVM Gaussian kernel: Example

$$\sigma = 1.0 \quad C = \infty$$

$$f(\mathbf{x}) = 1$$

$$f(\mathbf{x}) = 0$$

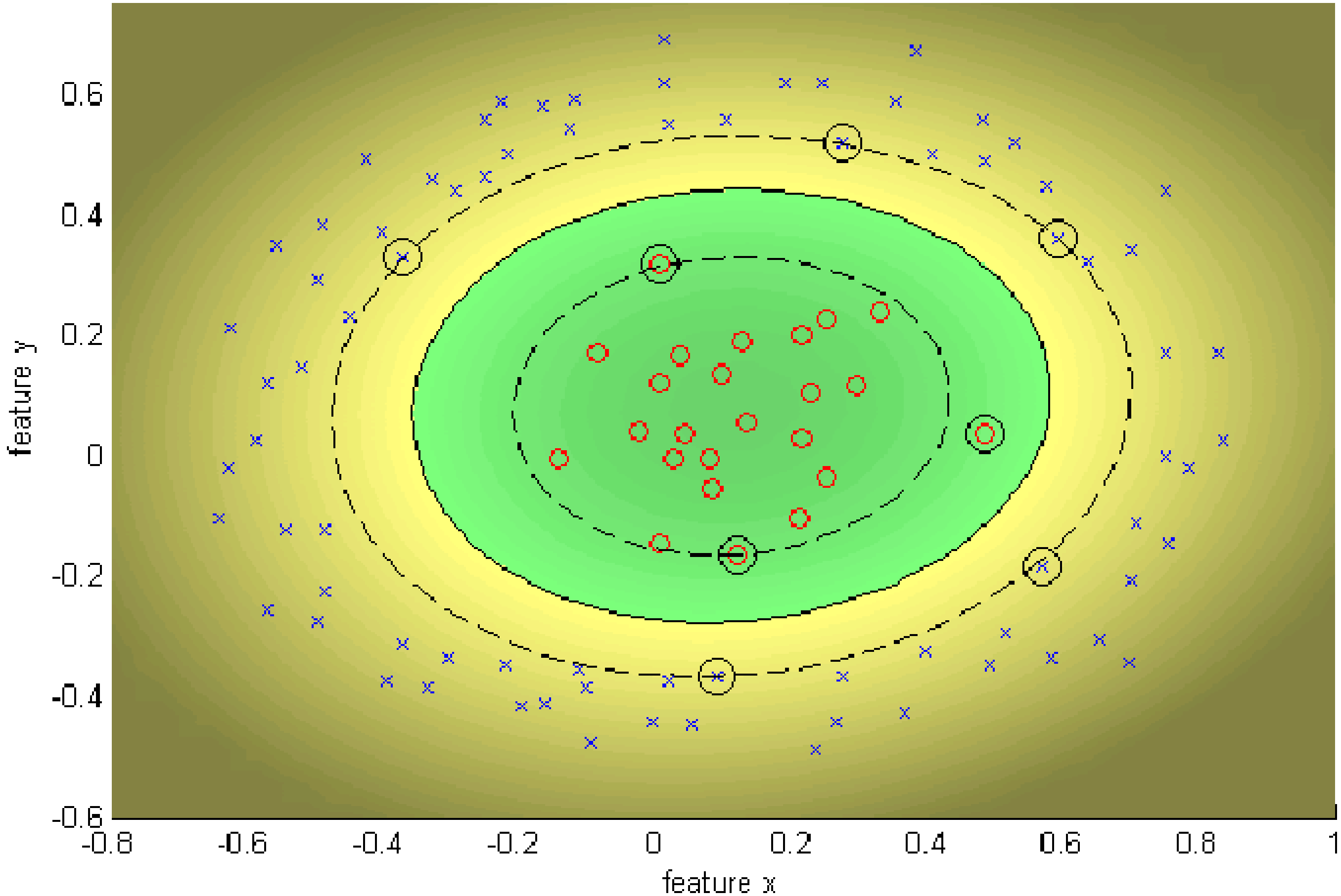
$$f(\mathbf{x}) = -1$$



This example has been adopted from Zisserman's slides

SVM Gaussian kernel: Example

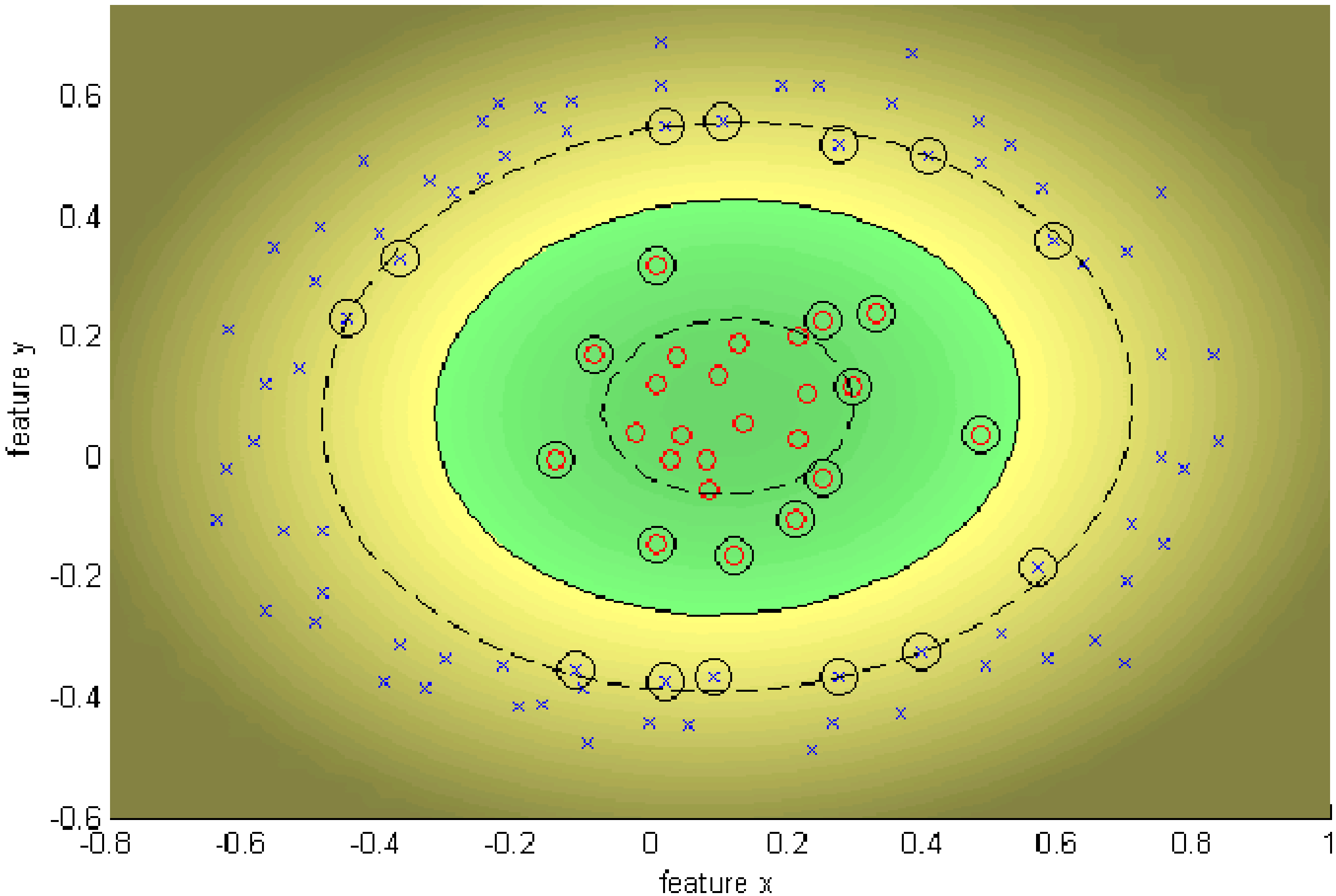
$\sigma = 1.0 \quad C = 100$



This example has been adopted from Zisserman's slides

SVM Gaussian kernel: Example

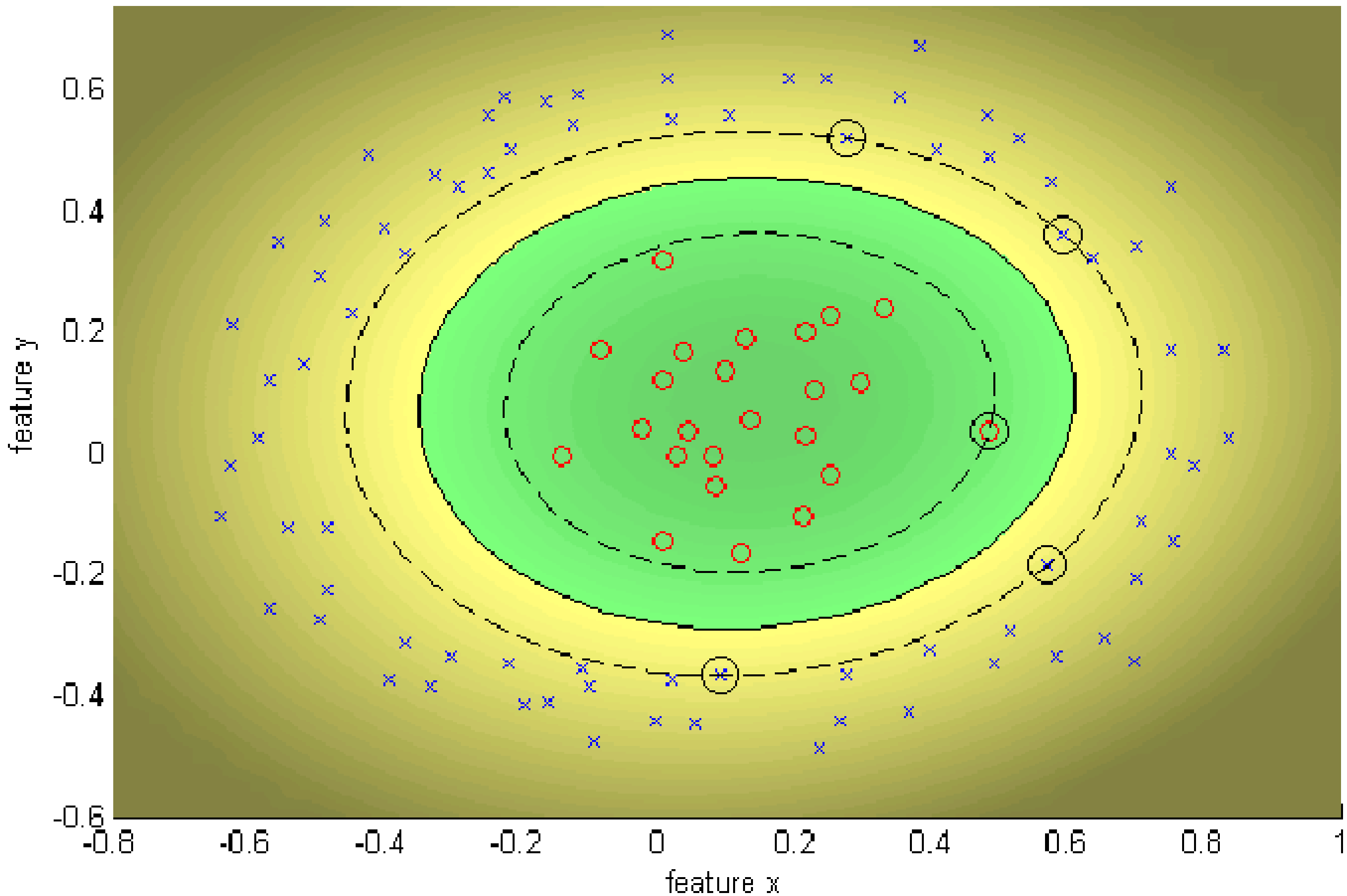
$$\sigma = 1.0 \quad C = 10$$



This example has been adopted from Zisserman's slides

SVM Gaussian kernel: Example

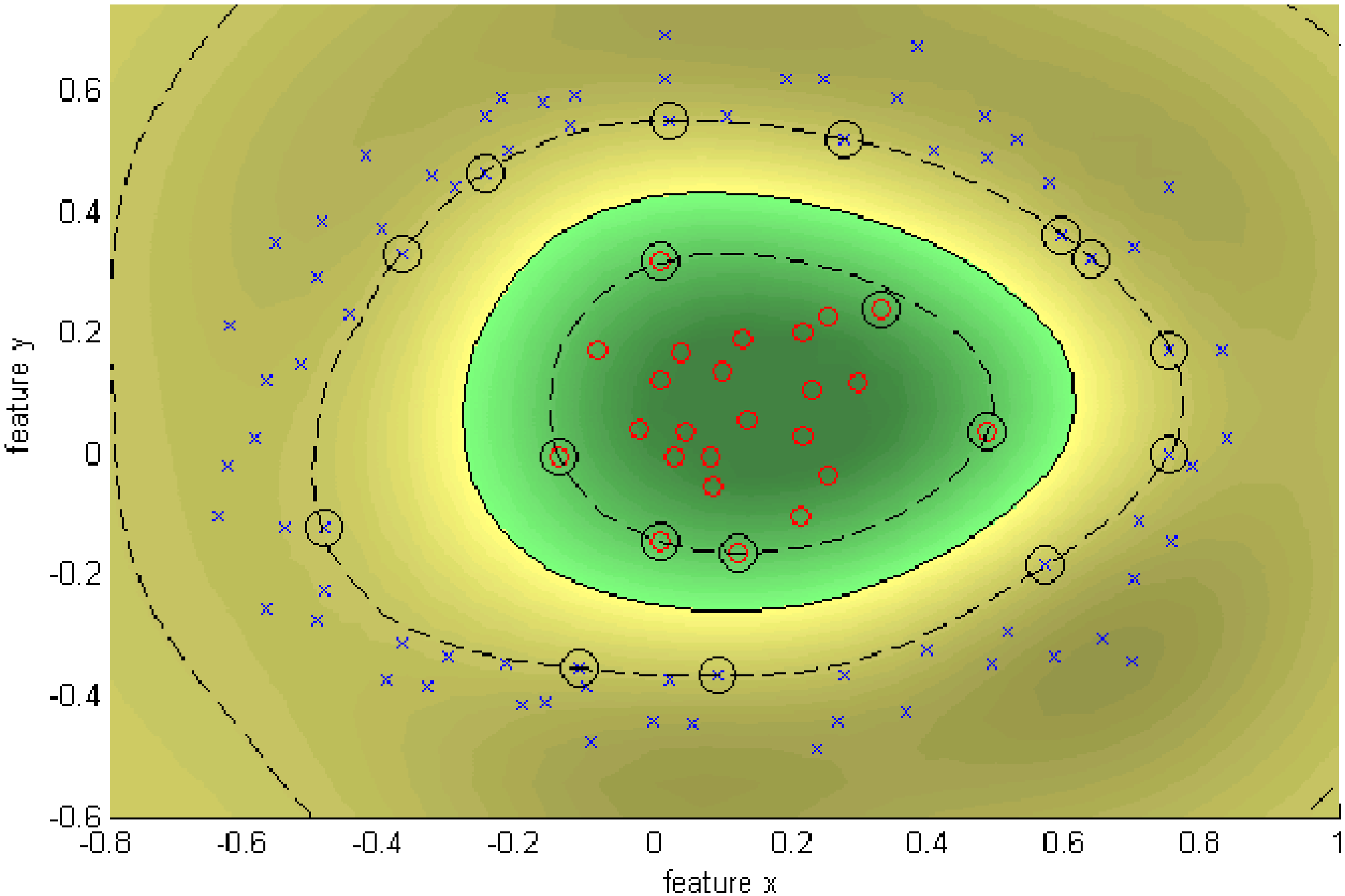
$$\sigma = 1.0 \quad C = \infty$$



This example has been adopted from Zisserman's slides

SVM Gaussian kernel: Example

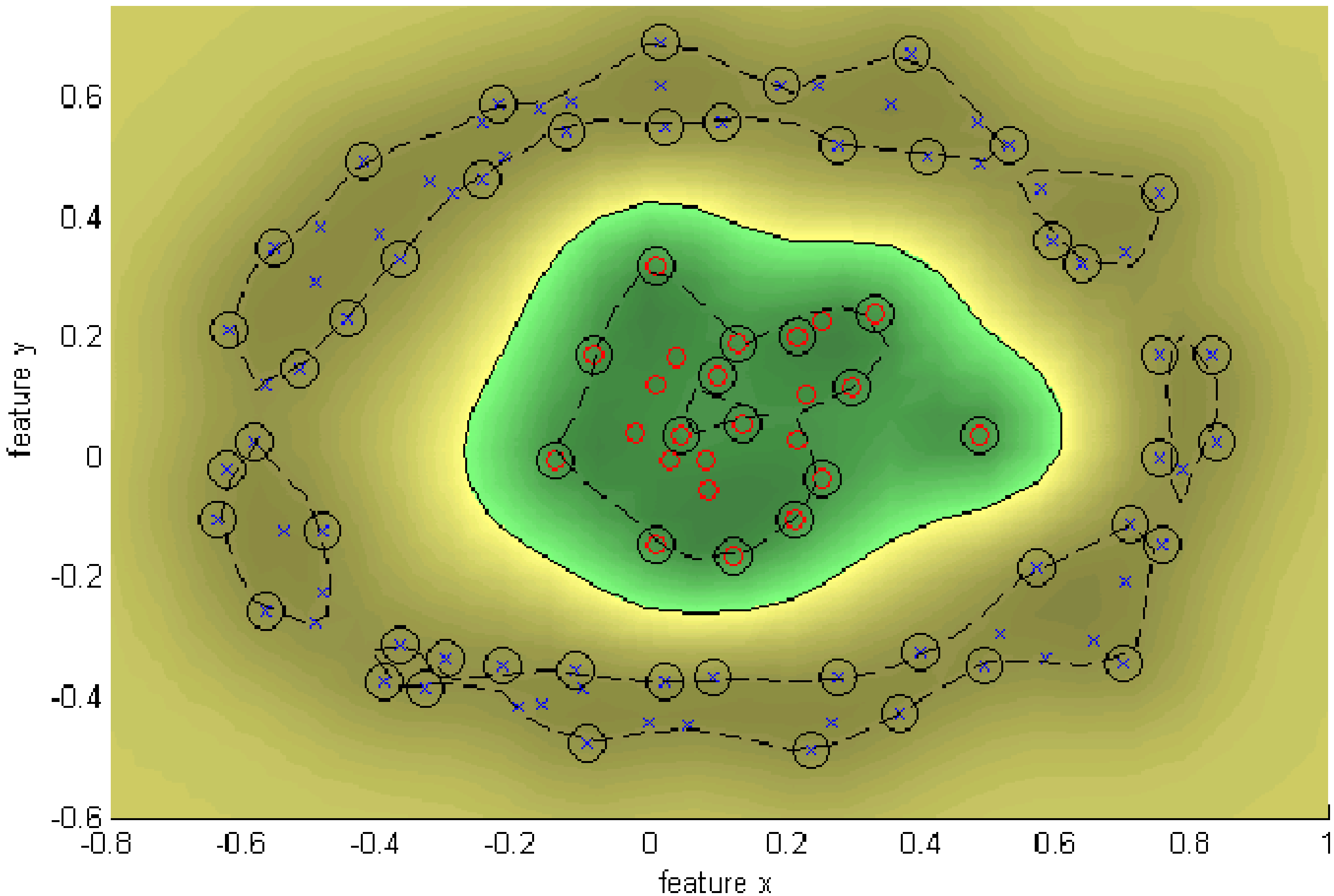
$$\sigma = 0.25 \quad C = \infty$$



This example has been adopted from Zisserman's slides

SVM Gaussian kernel: Example

$$\sigma = 0.1 \qquad C = \infty$$



This example has been adopted from Zisserman's slides

Kernel trick: Idea

- Kernel trick → Extension of many well-known algorithms to kernel-based ones
  - By substituting the dot product with the kernel function
    - $k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}')$
    - $k(\boldsymbol{x}, \boldsymbol{x}')$ shows the dot product of $\boldsymbol{x}$ and $\boldsymbol{x}'$ in the transformed space.

- Idea: when the input vectors appears only in the form of dot products, we can use kernel trick
  - Solving the problem without explicitly mapping the data
    - Explicit mapping is expensive if $\boldsymbol{\phi}(\boldsymbol{x})$ is very high dimensional

Kernel trick: Idea (Cont'd)

- Instead of using a mapping $\boldsymbol{\phi}: \mathcal{X} \leftarrow \mathcal{F}$ to represent $\boldsymbol{x} \in \mathcal{X}$ by $\boldsymbol{\phi}(\boldsymbol{x}) \in \mathcal{F}$, a similarity function $k: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is used.
  - We specify only an inner product function between points in the transformed space (not their coordinates)
  - In many cases, the inner product in the embedding space can be computed efficiently.

Constructing kernels

- Construct kernel functions directly
  - Ensure that it is a valid kernel
    - Corresponds to an inner product in some feature space.

- Example: $k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^T \boldsymbol{x}')^2$
  - Corresponding mapping: $\boldsymbol{\phi}(\boldsymbol{x}) = \left[x_1^2, \sqrt{2}x_1 x_2, x_2^2\right]^T$ for $\boldsymbol{x} = [x_1, x_2]^T$

- We need a way to test whether a kernel is valid without having to construct $\boldsymbol{\phi}(\boldsymbol{x})$

Valid kernel: Necessary & sufficient conditions

[Shawe-Taylor & Cristianini 2004]

- Gram matrix $\boldsymbol{K}_{N\times N}$: $K_{ij} = k(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)})$
  - Restricting the kernel function to a set of points $\{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(N)}\}$

$$K = \begin{bmatrix} k(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(1)}) & \cdots & k(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(N)}) \\ \vdots & \ddots & \vdots \\ k(\boldsymbol{x}^{(N)}, \boldsymbol{x}^{(1)}) & \cdots & k(\boldsymbol{x}^{(N)}, \boldsymbol{x}^{(N)}) \end{bmatrix}$$

- **Mercer** Theorem: The kernel matrix is **Symmetric Positive Semi-Definite** (for any choice of data points)
  - Any symmetric positive definite matrix can be regarded as a kernel matrix, that is as an inner product matrix in some space

Extending linear methods to kernelized ones

- Kernelized version of linear methods
  - Linear methods are famous
    - Unique optimal solutions, faster learning algorithms, and better analysis
  - However, we often require nonlinear methods in real-world problems and so we can use kernel-based version of these linear algorithms

- Replacing inner products with kernels in linear algorithms $\Rightarrow$ very flexible methods
  - We can operate in the mapped space without ever computing the coordinates of the data in that space

Example: kernelized minimum distance classifier

- If $\|\boldsymbol{x}-\boldsymbol{\mu}_1\| < \|\boldsymbol{x}-\boldsymbol{\mu}_2\|$ then assign $\boldsymbol{x}$ to $\mathcal{C}_1$

$$(\boldsymbol{x}-\boldsymbol{\mu}_1)^T(\boldsymbol{x}-\boldsymbol{\mu}_1) < (\boldsymbol{x}-\boldsymbol{\mu}_2)^T(\boldsymbol{x}-\boldsymbol{\mu}_2)$$

$$-2\boldsymbol{x}^T\boldsymbol{\mu}_1 + \boldsymbol{\mu}_1^T\boldsymbol{\mu}_1 < -2\boldsymbol{x}^T\boldsymbol{\mu}_2 + \boldsymbol{\mu}_2^T\boldsymbol{\mu}_2$$

$$-2\frac{\sum_{y^{(n)}=1}\boldsymbol{x}^T\boldsymbol{x}^{(n)}}{N_1} + \frac{\sum_{y^{(n)}=1}\sum_{y^{(m)}=1}\boldsymbol{x}^{(n)^T}\boldsymbol{x}^{(m)}}{N_1\times N_1} < -2\frac{\sum_{y^{(n)}=2}\boldsymbol{x}^T\boldsymbol{x}^{(n)}}{N_2} + \frac{\sum_{y^{(n)}=2}\sum_{y^{(m)}=2}\boldsymbol{x}^{(n)^T}\boldsymbol{x}^{(m)}}{N_2\times N_2}$$

$$-2\frac{\sum_{y^{(n)}=1}K\left(\boldsymbol{x},\boldsymbol{x}^{(n)}\right)}{N_1} + \frac{\sum_{y^{(n)}=1}\sum_{y^{(m)}=1}K\left(\boldsymbol{x}^{(n)},\boldsymbol{x}^{(m)}\right)}{N_1\times N_1} < -2\frac{\sum_{y^{(n)}=2}K\left(\boldsymbol{x},\boldsymbol{x}^{(n)}\right)}{N_2} + \frac{\sum_{y^{(n)}=2}\sum_{y^{(m)}=2}K\left(\boldsymbol{x}^{(n)},\boldsymbol{x}^{(m)}\right)}{N_2\times N_2}$$

Which information can be obtained from kernel?

- Example: we know all pairwise distances
  - $d\big(\boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z})\big)^2 = \|\boldsymbol{\phi}(\boldsymbol{x}) - \boldsymbol{\phi}(\boldsymbol{z})\|^2 = k(\boldsymbol{x}, \boldsymbol{x}) + k(\boldsymbol{z}, \boldsymbol{z}) - 2k(\boldsymbol{x}, \boldsymbol{z})$
  - Therefore, we also know distance of points from center of mass of a set

- Many dimensionality reduction, clustering, and classification methods can be described according to pairwise distances.
  - This allow us to introduce kernelized versions of them

Example: Kernel ridge regression

$$\min_{\boldsymbol{w}} \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)^2 + \lambda \boldsymbol{w}^T \boldsymbol{w}$$

$$\sum_{n=1}^{N} 2\boldsymbol{x}^{(n)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right) + 2\lambda \boldsymbol{w} \Rightarrow \boldsymbol{w} = \sum_{n=1}^{N} \alpha_n \boldsymbol{x}^{(n)}$$

$$\alpha_n = -\frac{1}{\lambda}\left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)$$

Example: Kernel ridge regression (Cont'd)

$$\min_{\boldsymbol{w}} \sum_{n=1}^{N} \left(\boldsymbol{w}^T \phi\left(\boldsymbol{x}^{(n)}\right) - y^{(n)}\right)^2 + \lambda \boldsymbol{w}^T \boldsymbol{w}$$

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n \phi\left(\boldsymbol{x}^{(n)}\right)$$

- Dual representation:

$$J(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^T \boldsymbol{\Phi}\boldsymbol{\Phi}^T \boldsymbol{\Phi}\boldsymbol{\Phi}^T \boldsymbol{\alpha} - 2\boldsymbol{\alpha}^T \boldsymbol{\Phi}\boldsymbol{\Phi}^T \boldsymbol{y} + \boldsymbol{y}^T \boldsymbol{y} + \lambda \boldsymbol{\alpha}^T \boldsymbol{\Phi}\boldsymbol{\Phi}^T \boldsymbol{\alpha}$$

$$J(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^T \boldsymbol{K}\boldsymbol{K}\boldsymbol{\alpha} - 2\boldsymbol{\alpha}^T \boldsymbol{K}\boldsymbol{y} + \boldsymbol{y}^T \boldsymbol{y} + \lambda \boldsymbol{\alpha}^T \boldsymbol{K}\boldsymbol{\alpha}$$

$$\nabla_{\boldsymbol{\alpha}} J(\boldsymbol{\alpha}) = \boldsymbol{0} \Rightarrow \boldsymbol{\alpha} = (\boldsymbol{K} + \lambda \boldsymbol{I}_N)^{-1} \boldsymbol{y}$$

Example: Kernel ridge regression (Cont'd)

- Prediction for new $\boldsymbol{x}$:

$$f(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x}) \qquad \boldsymbol{w} = \boldsymbol{\Phi}^T \boldsymbol{\alpha}$$

$$= \boldsymbol{\alpha}^T \boldsymbol{\Phi} \phi(\boldsymbol{x})$$

$$= \begin{bmatrix} K(\boldsymbol{x}^{(1)}, \boldsymbol{x}) \\ \vdots \\ K(\boldsymbol{x}^{(N)}, \boldsymbol{x}) \end{bmatrix}^T (\boldsymbol{K} + \lambda \boldsymbol{I}_N)^{-1} \boldsymbol{y}$$

Kernels for structured data

- Kernels also can be defined on general types of data
  - Kernel functions do not need to be defined over vectors
    - just we need a symmetric positive definite matrix
- Thus, many algorithms can work with general (non-vectorial) data
  - Kernels exist to embed strings, trees, graphs, …
- This may be more important than nonlinearity
  - kernel-based version of classical learning algorithms for recognition of structured data

Kernel function for objects

- Sets: Example of kernel function for sets:

$$k(A,B) = 2^{|A \cap B|}$$

- Strings: The inner product of the feature vectors for two strings can be defined as
  - e.g. sum over all common subsequences weighted according to their frequency of occurrence and lengths

A	E	G	A	T	E	A	G	G

E	G	T	E	A	G	A	E	G	A	T	G

Kernel trick advantages: summary

- Operating in the mapped space without ever computing the coordinates of the data in that space
- Besides vectors, we can introduce kernel functions for structured data (graphs, strings, etc.)
- Much of the geometry of the data in the embedding space is contained in all pairwise dot products
- In many cases, inner product in the embedding space can be computed efficiently.

Resources

- C. Bishop, “Pattern Recognition and Machine Learning”, Chapter 6.1-6.2, 7.1.
- Yaser S. Abu-Mostafa, et al., “Learning from Data”, Chapter 8.