Learning From Data
Lecture 4: Support Vector Machines

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October 11, 2024

Previously on Learning from Data

Algorithms we learned so far are mostly **probabilistic linear models**:

Type	Examples
Discrimative probablistic model	linear regression, logistic regression, softmax
Generative probablistic model	GDA, naive Bayes

- Choice of model affects model performance; *may easily lead to model mismatch*
- Data are often sampled non-uniformly, forming a sparse distribution in high dimensional input space. *leading to ill-posed problems*

Possible solutions: regularization (more in later lectures), sparse kernel methods (today's lecture)

Today's Lecture

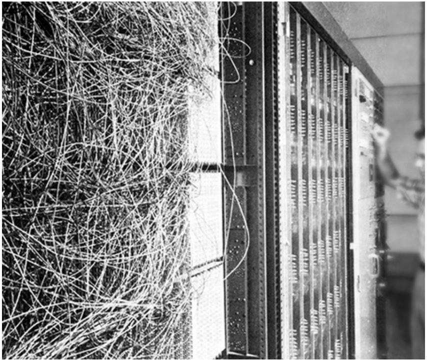
Supervised Learning (Part IV)

- Review: Perceptron Algorithm
- Support Vector Machines (SVM) $\leftarrow$ *another discriminative algorithm for learning linear classifiers*
- Kernel SVM $\leftarrow$ *non-linear extension of SVM*

Perceptron Learning Algorithm

The perceptron learning algorithm

- Invented in 1956 by Rosenblatt (Cornell University)
- One of the earliest learning algorithm, the first artificial neural network

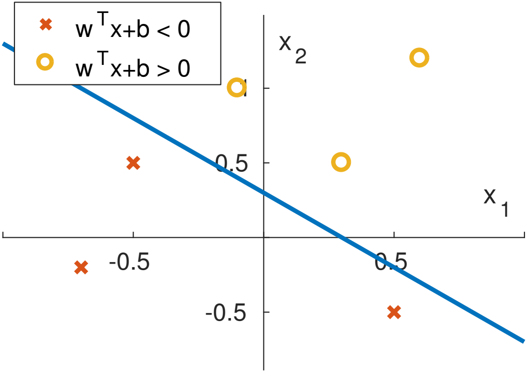


Hardware implementation: Mark I Perceptron

The perceptron learning algorithm

Given x, predict $y \in \{0, 1\}$

$$h_{w,b}(x) = \begin{cases} 1 & \text{if } w^T x + b \geq 0 \\ 0 & \text{otherwise} \end{cases}$$



The perceptron learning algorithm

Perceptron hypothesis function:

$$h_\theta(x) = \begin{cases} 1 & \text{if } \theta^T x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

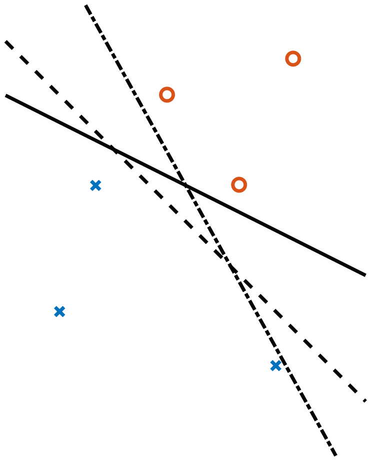
Parameter update rule:

$$\theta_j = \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)} \text{ for all } j = 0, \ldots, n$$

- When prediction is correct: $\theta_j = \theta_j$
- When prediction is incorrect:
  - predicted "1": $\theta_j = \theta_j - \alpha x_j$
  - predicted "0": $\theta_j = \theta_j + \alpha x_j$

Issues with linear hyperplane perceptron:

- Infinitely many solutions if data are separable
- Can not express "confidence" of the prediction

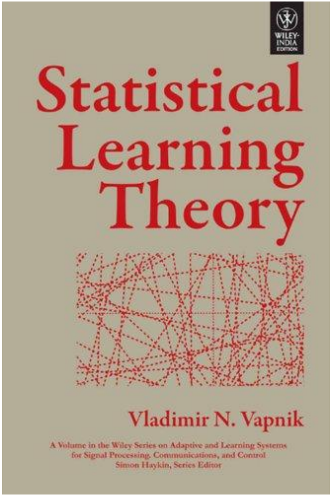


Support Vector Machines

Optimal margin classifier
Lagrange Duality
Soft margin SVM

Support Vector Machines in History

- Theoretical algorithm: developed from Statistical Learning Theory (Vapnik & Chervonenkis) since 60s
- Modern SVM was introduced in COLT 92 by Boser, Guyon & Vapnik



Support Vector Machines in History

- 1995 paper by Corte & Vapnik titled "Support-Vector Networks"
- Gained popularity in 90s for giving accuracy comparable to neural networks with elaborated features in a handwriting task

Machine Learning, 20, 273–297 (1995)

Support-Vector Networks

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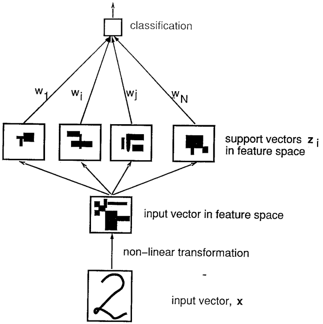
Editor: Lorenza Saitta

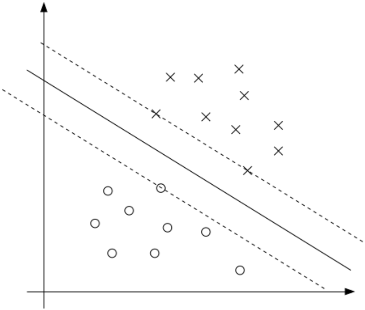
Abstract. The *support-vector network* is a new learning machine for two-group classification problems. The machine conceptually implements the following idea: input vectors are non-linearly mapped to a very high-dimension feature space. In this feature space a linear decision surface is constructed. Special properties of the decision surface ensures high generalization ability of the learning machine. The idea behind the support-vector network was previously implemented for the restricted case where the training data can be separated without errors. We here extend this result to non-separable training data.

High generalization ability of support-vector networks utilizing polynomial input transformations is demonstrated. We also compare the performance of the support-vector network to various classical learning algorithms that all took part in a benchmark study of Optical Character Recognition.

Keywords: pattern recognition, efficient learning algorithms, neural networks, radial basis function classifiers, polynomial classifiers.

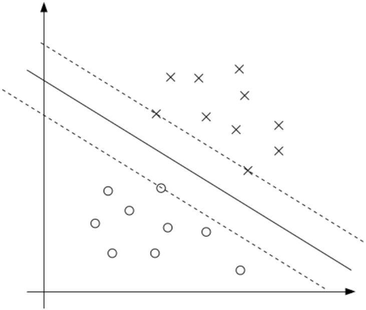


Support Vector Machine: Overview



Margin: smallest distance between the decision boundary to any samples *(Margin also represents classification confidence)*

Support Vector Machine: Overview



Margin: smallest distance between the decision boundary to any samples *(Margin also represents classification confidence)*

Linear SVM

Choose a linear classifier that maximizes the margin.

To be discussed:

- How to measure the margin? (functionally vs geometrically)
- How to find the decision boundary with optimal margin?
  + a detour on Lagrange Duality

Functional margins

Class labels: $y \in \{-1, 1\}$

$$h_{w,b}(x) = \begin{cases} 1 & \text{if } w^T x + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

Functional margins

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$$h_{w,b}(x) = \begin{cases} 1 & \text{if } w^T x + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

Functional Margin

Given training sample $(x^{(i)}, y^{(i)})$

$$\hat{\gamma}^{(i)} = y^{(i)} \left(w^T x^{(i)} + b \right)$$

$sign(\hat{\gamma}^{(i)})$: whether the hypothesis is correct

Functional margins

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- $\hat{\gamma}^{(i)} >> 0$: prediction is correct with high confidence

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Functional Margin

Given training sample $(x^{(i)}, y^{(i)})$

$$\hat{\gamma}^{(i)} = y^{(i)} \left(w^T x^{(i)} + b \right)$$

$sign(\hat{\gamma}^{(i)})$: whether the hypothesis is correct

- $\hat{\gamma}^{(i)} >> 0$: prediction is correct with high confidence
- $\hat{\gamma}^{(i)} << 0$: prediction is incorrect with high confidence

Function Margins

Functional margin of (w, b) with respect to training data S:

$$\hat{\gamma} = \min_{i=1,..,m} \hat{\gamma}^{(i)} = \min_{i=1,..,m} y^{(i)} \left(w^T x^{(i)} + b \right)$$

Function Margins

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$$\hat{\gamma} = \min_{i=1,..,m} \hat{\gamma}^{(i)} = \min_{i=1,..,m} y^{(i)} \left(w^T x^{(i)} + b \right)$$

Issue: $\hat{\gamma}$ depends on $||w||$ and b

e.g. Let $w' = 2w, b' = 2b$. The decision boundary parameterized by (w', b') and (w, b) are the same. However,

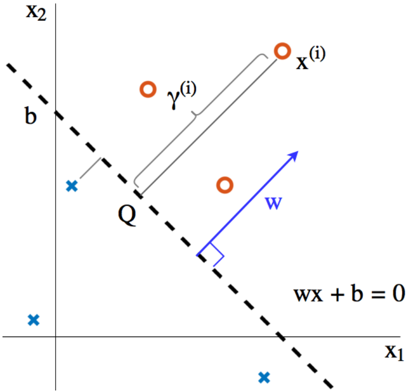
$$\hat{\gamma}'^{(i)} = y^{(i)} \left(2w^T x^{(i)} + 2b \right) = 2y^{(i)} (w^T x^{(i)} + b) = 2\hat{\gamma}^{(i)}$$

Can we express the margin so that it is invariant to $||w||$ and b?

Geometric Margins

The **geometric margin** $\gamma^{(i)}$ of a training example $(x^{(i)}, y^{(i)})$ is the distance from the hyperplane:

$$\gamma^{(i)} = y^{(i)} \left(\frac{w}{||w||}^{T} x^{(i)} + \frac{b}{||w||} \right)$$



- w is normal to hyperplane $w^T x + b = 0$
- We want $\gamma^{(i)} > 0$ when prediction is correct

Geometric Margins

The **geometric margin** of (w, b) with respect to training data S is the minimum distance from any point to the hyperplane:

$$\gamma = \min_{i=1,..,m} \gamma^{(i)} = \min_{i=1,..,m} y^{(i)} \left(\frac{w}{||w||}^T x^{(i)} + \frac{b}{||w||} \right)$$

Geometric Margins

The **geometric margin** of (w, b) with respect to training data S is the minimum distance from any point to the hyperplane:

$$
\begin{aligned}
\gamma = \min_{i=1,..,m} \gamma^{(i)} &= \min_{i=1,..,m} y^{(i)} \left(\frac{w}{||w||}^T x^{(i)} + \frac{b}{||w||} \right) \\
&= \frac{1}{||w||} \min_{i=1,..,m} y^{(i)} \left(w^T x^{(i)} + b \right) \\
&= \frac{1}{||w||} \hat{\gamma}
\end{aligned}
$$

Geometric Margins

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$$= \frac{1}{||w||} \min_{i=1,..,m} y^{(i)} \left(w^T x^{(i)} + b \right)$$

$$= \frac{1}{||w||} \hat{\gamma}$$

- $\hat{\gamma} = \gamma$ when $||w|| = 1$

Geometric Margins

The **geometric margin** of (w, b) with respect to training data S is the minimum distance from any point to the hyperplane:

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- $\hat{\gamma} = \gamma$ when $||w|| = 1$
- Geometric margins are invariant to parameter scaling

Optimal Margin Classifier

Assume data is linearly separable

Find (w, b) that maximize geometric margin $\gamma = \frac{\hat{\gamma}}{||w||}$ of the training data

$$\max_{\gamma, w, b} \frac{\hat{\gamma}}{||w||}$$
$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq \hat{\gamma}, \ i = 1, \ldots, m$$

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There exists some $\delta \in \mathbb{R}$ such that the functional margin of $(\delta w, \delta b)$ is $\hat{\gamma} = 1$

$$\max_{\gamma,w,b} \quad \frac{1}{||w||}$$
$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq 1 \ i = 1, \ldots, m$$

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$$\max_{\gamma,w,b} \quad \frac{1}{||w||}$$
$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq 1 \; i = 1, \ldots, m$$
$$\iff \min_{\gamma,w,b} \quad \frac{1}{2}||w||^2$$
$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq 1 \; i = 1, \ldots, m$$

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$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq 1\ i = 1, \dots, m$$

can be solved using QP software

Review: Lagrange Duality

The **primal** optimization problem:

$$
\begin{aligned}
\min_{w} \quad & f(w) \\
s.t. \quad & g_i(w) \leq 0, i, \ldots, k \\
& h_i(w) = 0, i = 1, \ldots, l
\end{aligned}
$$

Review: Lagrange Duality

The **primal** optimization problem:

$$\begin{aligned} \min_{w} \quad & f(w) \\ s.t. \quad & g_i(w) \leq 0, i, \dots, k \\ & h_i(w) = 0, i = 1, \dots, l \end{aligned}$$

Define the **generalized Lagrange function** :

$$L(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

α_i and β_i are called the **Lagrange multipliers**

For a given w,

$$\begin{aligned}\theta_P(w) &= \max_{\alpha,\beta:\alpha_i\geq 0} L(w,\alpha,\beta)\\ &= \max_{\alpha,\beta:\alpha_i\geq 0} f(w) + \sum_{i=1}^{k}\alpha_i g_i(w) + \sum_{i=1}^{l}\beta_i h_i(w)\end{aligned}$$

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Recall the primal constraints: $g_i(w) \leq 0$ and $h_i(w) = 0$:

- $\theta_P(w) = f(w)$ if w satisfies primal constraints

For a given w,

$$\theta_P(w) = \max_{\alpha,\beta:\alpha_i \geq 0} L(w,\alpha,\beta)$$

$$= \max_{\alpha,\beta:\alpha_i \geq 0} f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

Recall the primal constraints: $g_i(w) \leq 0$ and $h_i(w) = 0$:

- $\theta_P(w) = f(w)$ if w satisfies primal constraints
- $\theta_P(w) = \infty$ otherwise

The primal problem (alternative form)

$$\min_w \theta_P(w) = \min_w \max_{\alpha,\beta:\alpha_i \geq 0} L(w,\alpha,\beta)$$

The primal problem (P)

$$p^* = \min_{w} \theta_P(w) = \min_{w} \max_{\alpha,\beta:\alpha_i \geq 0} L(w, \alpha, \beta)$$

The dual problem (D)

$$d^* = \max_{\alpha,\beta:\alpha_i \geq 0} \theta_D(\alpha, \beta) = \max_{\alpha,\beta:\alpha_i \geq 0} \min_{w} L(w, \alpha, \beta)$$

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In general, $d^* \leq p^*$ (max-min inequality)

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The dual problem (D)

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In general, $d^* \leq p^*$ (max-min inequality)

Theorem (Lagrange Duality)

Suppose f and all g_i's are convex, all h_i's are affine, and there exists some w such that $g_i(w) < 0$ for all i (strictly feasible) *.*
There must exists w^*, α^*, β^* so that w^* is the solution to P and α^*,β^* are the solution to D, and

$$p^* = d^* = L(w^*, \alpha^*, \beta^*)$$

Karush-Kuhn-Tucker (KKT) conditions

Under previous conditions, w^*, α^*, β^* are solutions of P and D **if and only if** they statisty the following conditions:

$$\frac{\delta}{\delta w_i} L(w^*, \alpha^*, \beta^*) = 0, \;\; i = 1, \ldots n \quad (1)$$

$$\frac{\delta}{\delta \beta_i} L(w^*, \alpha^*, \beta^*) = 0, \;\; i = 1, \ldots l \quad (2)$$

$$\alpha_i^* g_i(w^*) = 0, \;\; i = 1, \ldots, k \quad (3)$$

$$g_i(w^*) \leq 0, \;\; i = 1, \ldots, k \quad (4)$$

$$\alpha^* \geq 0, \;\; i = 1, \ldots, k \quad (5)$$

Equation 3 is called the **complementary slackness condition**.

Optimal Margin Classifier

Optimal margin classifier

$$\min_{\gamma,w,b} \frac{1}{2}||w||^2$$
$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq 1 \ i = 1, \ldots, m$$

- $f(w) = \frac{1}{2}||w||^2$
- $g_i(w) = -\left(y^{(i)}(w^T x^{(i)} + b) - 1\right)$

Generalized Lagrangian function:

$$L(w, b, \alpha) = \frac{1}{2}||w||^2 - \sum_{i}^{m} \alpha_i \left[y^{(i)}(w^T x^{(i)} + b) - 1\right]$$

By the complementary slackness condition in KKT:

$$\alpha_i^* g_i(w^*) = 0,\ i = 1, \ldots, k$$
$$\alpha_i^* > 0 \iff g_i(w^*) = -y^{(i)}({w^*}^T x^{(i)} + b) + 1 = 0$$

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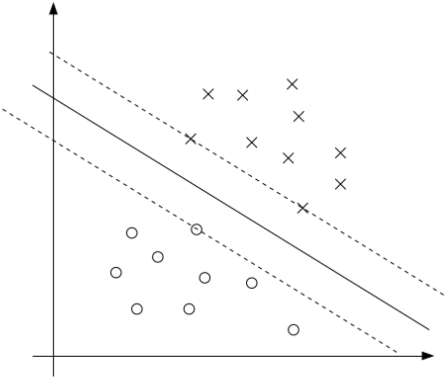
Training examples $(x^{(i)}, y^{(i)})$ such that $y^{(i)}({w^*}^T x^{(i)} + b) = 1$ are called **support vectors**



Support vectors lie on hyperplane ${w^*}^T x + b = 1$ when $y^{(i)} = 1$, or ${w^*}^T x + b = -1$ when $y^{(i)} = -1$

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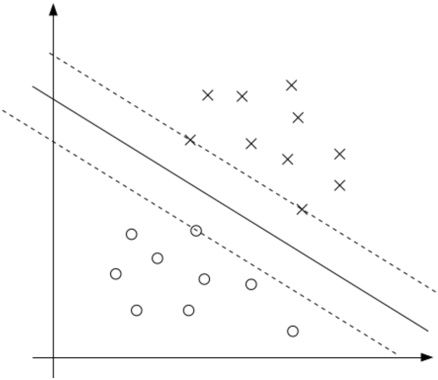
Training examples $(x^{(i)}, y^{(i)})$ such that $y^{(i)}({w^*}^T x^{(i)} + b) = 1$ are called **support vectors**



Support vectors lie on hyperplane ${w^*}^T x + b = 1$ when $y^{(i)} = 1$, or ${w^*}^T x + b = -1$ when $y^{(i)} = -1$

Constraints $g_i(w) \leq 0$ is only **active** on support vectors

Dual optimization problem: *(Check derivation)*

$$\max_{\alpha} \; W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle$$

$$s.t. \; \alpha_i \geq 0, i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$$

Dual optimization problem: *(Check derivation)*

$$\max_{\alpha} W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle$$

$$s.t.\ \alpha_i \geq 0, i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$$

Given optimal solutions of $\alpha_1, \ldots, \alpha_b$, how to find w^* and b^*?

Solution to the primal problem:

$$w^* = \sum_{i=1}^{m} \alpha_i^* y^{(i)} x^{(i)}$$

Solution to the primal problem:

$$w^* = \sum_{i=1}^{m} \alpha_i^* y^{(i)} x^{(i)}$$

$$b^* = -\frac{1}{2} \left(\max_{i:y^{(i)}=-1} {w^*}^T x^{(i)} + \min_{i:y^{(i)}=1} {w^*}^T x^{(i)} \right)$$

For a new sample z, the SVM prediction is sign $\left[{w^*}^T z + b \right]$

$w^T z + b = \sum_{i=1}^{m} \alpha_i y^{(i)} \langle x^{(i)}, z \rangle + b$

Linear SVM Summary

- Input:: m training samples $(x^{(i)}, y^{(i)}), y^i \in \{-1, 1\}$
- Output: optimal parameters w^*, b^*
- Step 1: solve the dual optimization problem

$$\alpha^* = \max_{\alpha} W(\alpha)$$

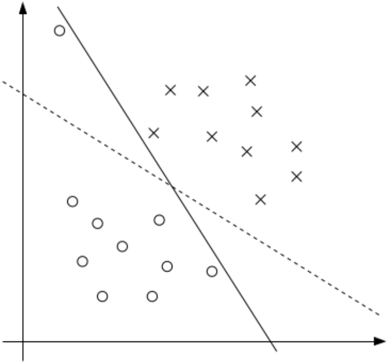
$$s.t.\ \alpha_i \geq 0, \sum_{i=1}^{m} \alpha_i y^{(i)} = 0, i = 1, \ldots, m$$

- Step 2: compute the optimal parameters w^*, b^*

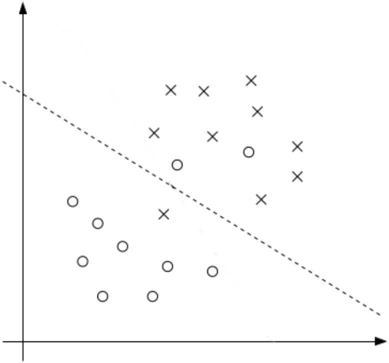
$$w^* = \sum_{i=1}^{m} \alpha_i^* y^{(i)} x^{(i)}$$

$$b^* = -\frac{1}{2}\left(\max_{i:y^{(i)}=-1} {w^*}^T x^{(i)} + \min_{i:y^{(i)}=1} {w^*}^T x^{(i)} \right)$$

Limitations of the basic SVM



Outliers



Non-linearly separable cases

Soft Margin SVM

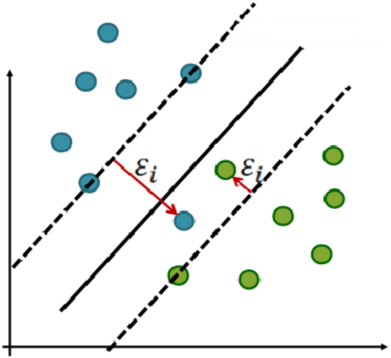
Functional margin $1 - \xi_i \leq 1$:

$$\min_{w,b,\xi} \frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi_i$$

$$s.t.\ y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0, i = 1, \ldots, m$$

- C: relative weight on the regularizer
- L_1 regularization let most $\xi_i = 0$, such that their functional margins $1 - \xi_i = 1$



Soft Margin SVM

The generalized Lagrangian function:

$$L(w, b, \xi, \alpha, r) = \frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi_i - \sum_{i}^{m}\alpha_i\left[y^{(i)}(w^T x^{(i)} + b) - 1 + \xi_i\right] - \sum_{i=1}^{m} r_i\xi_i$$

Soft Margin SVM

The generalized Lagrangian function:

$$L(w, b, \xi, \alpha, r) = \frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi_i - \sum_{i}^{m}\alpha_i\left[y^{(i)}(w^Tx^{(i)} + b) - 1 + \xi_i\right] - \sum_{i=1}^{m} r_i\xi_i$$

Dual problem:

Soft Margin SVM

The generalized Lagrangian function:

$$L(w, b, \xi, \alpha, r) = \frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi_i - \sum_{i}^{m}\alpha_i\left[y^{(i)}(w^Tx^{(i)} + b) - 1 + \xi_i\right] - \sum_{i=1}^{m}r_i\xi_i$$

Dual problem:

$$\max_{\alpha}\ W(\alpha) = \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{m}y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)}, x^{(j)}\rangle$$

$$s.t.\ 0 \leq \alpha_i \leq C, i = 1, \ldots, m$$

$$\sum_{i=1}^{m}\alpha_i y^{(i)} = 0$$

w^* is the same as the non-regularizing case, but b^* has changed.

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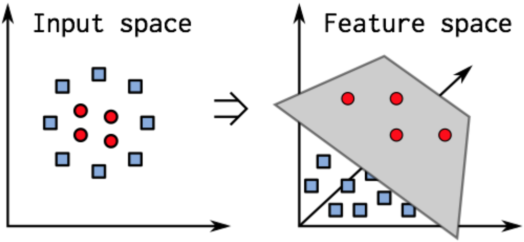
$\alpha_i = 0$	$\iff$	$y^{(i)}(w^T x^{(i)} + b) \geq 1$	correct side of margin
$\alpha_i = C$	$\iff$	$y^{(i)}(w^T x^{(i)} + b) \leq 1$	wrong side of margin
$0 < \alpha_i < C$	$\iff$	$y^{(i)}(w^T x^{(i)} + b) = 1$	at margin

Kernel SVM

Non-linear SVM

For non-separable data, we can use the **kernel trick**: Map input values $x \in \mathbb{R}^d$ to a higher dimension $\phi(x) \in \mathbb{R}^D$, such that the data becomes separable.



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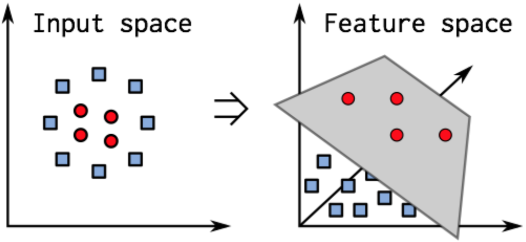

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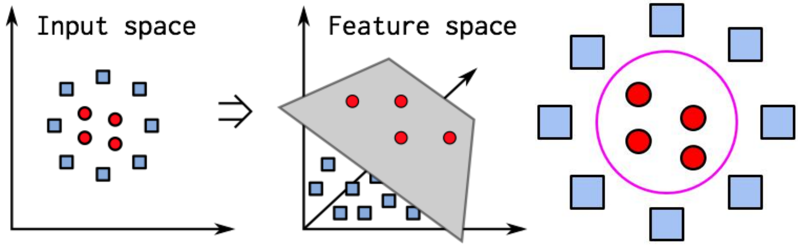

- ϕ is called a **feature mapping**.
- The classification function $w^T x + b$ becomes nonlinear: $w^T \phi(x) + b$

Kernel Function

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where $\phi(x) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ \vdots \\ x_n x_{n-1} \\ x_n x_n \end{bmatrix}$ takes $O(n^2)$ operations to compute, while $(x^T z)^2$ only takes $O(n)$

Kernel SVM

In the dual problem, replace $\langle x_i, y_j \rangle$ with $\langle \phi(x_i), \phi(y_i) \rangle = K(x_i, x_j)$

$$\max_{\alpha} W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j K(x_i, x_j)$$

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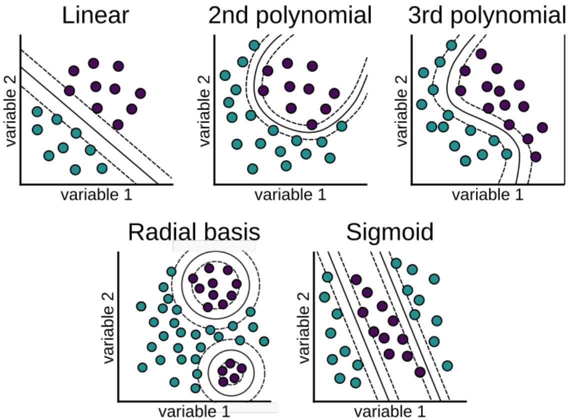
No need to compute $w^* = \sum_{i=1}^{m} \alpha_i^* y^{(i)} \phi(x^{(i)})$ explicitly since

$$\begin{aligned} f(x) = w^T \phi(x) + b &= \left(\sum_{i=1}^{m} \alpha_i y^{(i)} \phi(x^{(i)}) \right)^T \phi(x) + b \\ &= \sum_{i=1}^{m} \alpha_i y^{(i)} \langle \phi(x^{(i)}), \phi(x) \rangle + b \\ &= \sum_{i=1}^{m} \alpha_i y^{(i)} K(x^{(i)}, x) + b \end{aligned}$$

Kernel Matrix

kernel functions measure the similarity between samples x, z, e.g.

- Linear kernel: $K(x, z) = (x^T z)$
- Polynomial kernel: $K(x, z) = (x^T z + 1)^p$
- Gaussian / radial basis function (RBF) kernel: $K(x, z) = \exp\left(-\frac{||x-z||^2}{2\sigma^2}\right)$



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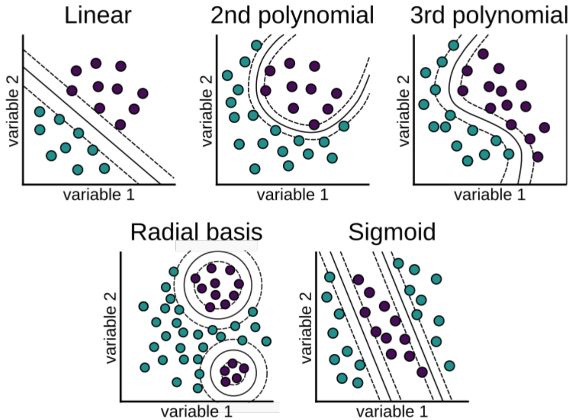

Can any function $K(x, y)$ be a kernel function?

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Represent kernel function as a matrix $K \in \mathbb{R}^{m \times m}$ where
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Theorem (Mercer)

Let $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ *Then* K *is a valid (Mercer) kernel if and only if for any finite training set* $\{x^{(i)}, \ldots, x^{(m)}\}$, K *is symmetric positive semi-definite.*

i.e. $K_{i,j} = K_{j,i}$ and $x^T K x \geq 0$ for all $x \in \mathbb{R}^n$

Kernel SVM Summary

- Input: m training samples $(x^{(i)}, y^{(i)}), y^i \in \{-1, 1\}$, kernel function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, constant $C > 0$
- Output: non-linear decision function $f(x)$
- Step 1: solve the dual optimization problem for α^*

$$\max_{\alpha} W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j K(x^{(i)}, x^{(j)})$$

$$s.t.\ 0 \le \alpha_i \le C, \sum_{i=1}^{m} \alpha_i y^{(i)} = 0, i = 1, \dots, m$$

- Step 2: compute the optimal decision function

$$b^* = y^{(j)} - \sum_{i=1}^{m} \alpha_i^* y^{(i)} K(x^{(i)}, x^{(j)}) \text{ for some } 0 < \alpha_j < C$$

$$f(x) = \sum_{i=1}^{m} \alpha_i y^{(i)} K(x^{(i)}, x) + b^*$$

In practice, it's more efficient to compute kernel matrix K in advance.

SVM in Practice

Sequential Minimal Optimization: a fast algorithm for training soft margin kernel SVM

- Break a large SVM problem into smaller chunks, update two α_i's at a time
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Other related algorithms

- Support Vector Regression (SVR)
- Multi-class SVM (Koby Crammer and Yoram Singer. 2002. *On the algorithmic implementation of multiclass kernel-based vector machines*. J. Mach. Learn. Res. 2 (March 2002), 265-292.)