Support Vector Machines (1/2)

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Content

Confident predictions

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- Consider a positive training example ($y = 1$), the larger the $\theta^\top \mathrm{x}$ is, the larger also is $h_\theta(\mathrm{x}) = p(y = 1|\mathrm{x}; w, b)$, and thus also the higher our degree of confidence that the label is 1.

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- Thus, informally we can think of our prediction as being a very confident one that $y = 1$ if $\theta^\top \mathrm{x} \gg 0$.

Confident predictions

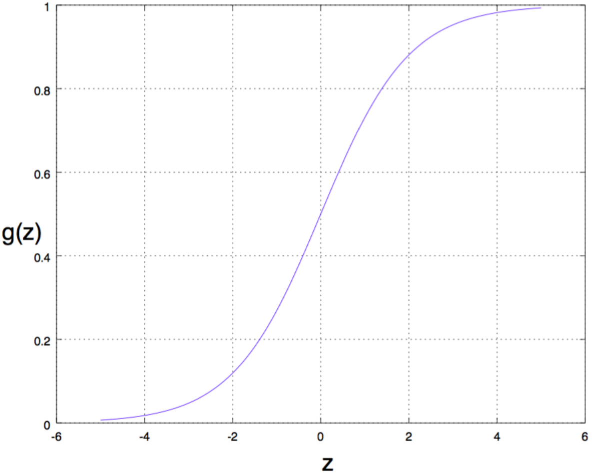

Figure: Sigmoid function (where $z = \theta^\top x$).

Confident predictions

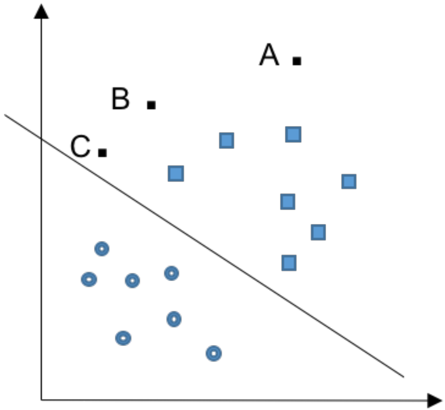

Figure: Separating hyperplane, this is the line given by the equation $\theta^\top x = 0$.

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- Similarly, we think of logistic regression as making a very confident prediction of $y = 0$, if $\theta^\top \mathrm{x} \ll 0$.
- Given a training set, again informally it seems that we'd have found a good fit to the training data if we can find θ so that:

  $\theta^\top \mathrm{x} \gg 0$ whenever $y^{(i)} = 1$

  and

  $\theta^\top \mathrm{x} \ll 0$ whenever $y^{(i)} = 0$

  since this would reflect a very confident (and correct) set of classifications for all the training examples.

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- So our classifier can be written as $h_{w,b}(\mathrm{x}) = g(w^\top \mathrm{x} + b)$.
- Here, $g(z) = 1$ if $z \geq 0$, and $g(z) = -1$ otherwise.

Functional Margin

- Given a training example $(x^{(i)}, y^{(i)})$, we define the functional margin of (w, b) with respect to that training example as

  $\hat{\gamma}^{(i)} = y^{(i)}(w^\top \mathrm{x}^{(i)} + b).$

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- Conversely, if $y^{(i)} = -1$, then for the functional margin to be large, then we need $w^\top \mathrm{x} + b$ to be a large negative number.
- Moreover, if $y^{(i)}(w^\top \mathrm{x} + b) > 0$, then our prediction on this example is correct. Hence, a large functional margin represents a confident and a correct prediction.

Functional Margin

- For a linear classifier with the choice of $h_{w,b}(\mathrm{x}) = g(w^\top \mathrm{x} + b)$, note that if we replace w with $2w$ and b with $2b$, then $g(w^\top x + b) = g(2w^\top x + 2b)$ and this would not change $h_{w,b}(\mathrm{x})$.

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- Hence $h_{w,b}(\mathrm{x})$ depends only on the sign and not on the magnitude of $w^\top \mathrm{x} + b$.
- However, replacing (w, b) with $(2w, 2b)$ also results in multiplying our functional margin by a factor of 2.
- Thus, it seems that by exploiting our freedom to scale w and b, we can make the functional margin arbitrarily large without really changing anything meaningful.

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- We might replace (w, b) with $(w/||w||_2, b/||w||_2)$ and instead consider the functional margin of $(w/||w||_2, b/||w||_2)$.

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- We might replace (w, b) with $(w/||w||_2, b/||w||_2)$ and instead consider the functional margin of $(w/||w||_2, b/||w||_2)$.
- Given a training set $S = \{(\mathrm{x}^{(i)}, y^{(i)}); i = 1, \ldots, m\}$, we define the functional margin of (w, b) with respect to S as the smallest of the functional margins of the individual training examples, denoted by $\hat{\gamma}$:

$$\hat{\gamma} = \min_{i=1,\ldots,m} \hat{\gamma}^{(i)}.$$

Geometric Margin

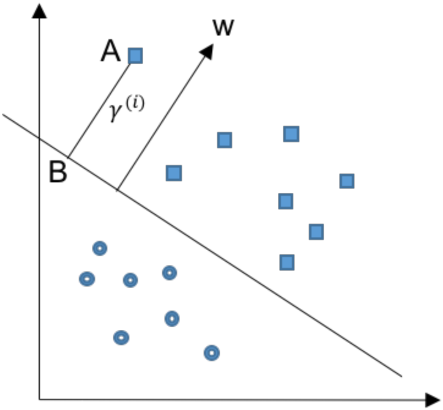
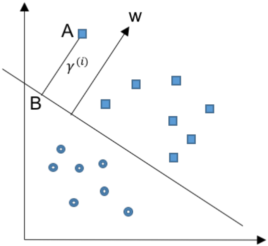


Figure: The decision boundary corresponding to (w, b) is shown, along with the vector w. Note that w is orthogonal (at 90°) to the separating hyperplane.

Geometric Margin

- How can we find $\gamma^{(i)}$?



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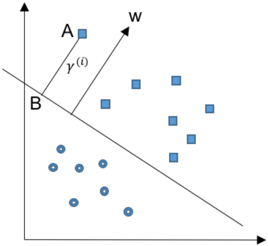

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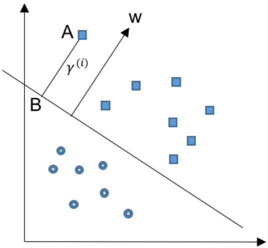

- Since A represents example $\mathrm{x}^{(i)}$, point B is given by $\mathrm{x}^{(i)} - \gamma^{(i)} \cdot \frac{w}{||w||}$.
- But this point lies on the decision boundary and satisfies $w^\top \mathrm{x} + b = 0$.

Geometric Margin

- Hence

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- Solving for $\gamma^{(i)}$

$$\gamma^{(i)} = \frac{w^\top \mathrm{x}^{(i)} + b}{||w||} = \left(\frac{w}{||w||} \right)^\top \mathrm{x}^{(i)} + \frac{b}{||w||}.$$

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- More generally we define the geometric margin for (w, b) with respect to a training example $(\mathrm{x}^{(i)}, y^{(i)})$ to be

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

Geometric Margin

- Given a training set $S = \{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$, we also define the geometric margin of (w, b) with respect to S to be the smallest of the geometric margins on the individual training examples:

$$\gamma = \min_{i=1,\ldots,m} \gamma^{(i)}.$$

Functional and Geometric Margins

- Functional margin

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- Note that if $||w|| = 1$, then the functional margin equals the geometric margin. This thus gives us a way of relating these two different notions of margin.

Optimal Margin Classifier

- Given a training set, it seems natural to try to find a decision boundary that maximizes the geometric margin, since this would reflect a very confident set of predictions on the training set and a good "fit" to the training data.

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- Specifically, this will result in a classifier that separates the positive and the negative training examples with a "gap" (geometric margin).

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- Given a training set, it seems natural to try to find a decision boundary that maximizes the geometric margin, since this would reflect a very confident set of predictions on the training set and a good "fit" to the training data.
- Specifically, this will result in a classifier that separates the positive and the negative training examples with a "gap" (geometric margin).
- We will assume that we are given a training set that is linearly separable; i.e., that it is possible to separate the positive and negative examples using some separating hyperplane. How can we find the one that achieves the maximum geometric margin?

Optimal Margin Classifier

- We can pose the following optimization problem:

$$\begin{aligned} \max_{\gamma,w,b} \quad & \gamma \\ \text{s.t.} \quad & y^{(i)}(w^\top x^{(i)} + b) \geq \gamma, i = 1, \ldots, m \\ & ||w|| = 1. \end{aligned}$$

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- We want to maximize γ, subject to each training example having functional margin at least γ.
- The $||w|| = 1$ constraint ensures that the functional margin equals to the geometric margin, so we are also guaranteed that all the geometric margins are at least γ.
- Thus, solving this problem will result in (w, b) with the largest possible geometric margin with respect to the training set.

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- We're going to maximize $\hat{\gamma}/||w||$, subject to the functional margins all being at least $\hat{\gamma}$. Since the geometric and functional margins are related by $\gamma = \hat{\gamma}/||w||$, this will give us the answer we want.
- Moreover, we've gotten rid of the constraint $||w|| = 1$ that we didn't like.

Optimal Margin Classifier

- Since maximizing $\hat{\gamma}/||w|| = 1/||w||$ is the same as minimizing $||w||^2$, we can solve the following optimization problem:

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- This optimization problem can be solved using commercial quadratic programming (QP) code.

Lagrange Multipliers

- Consider an optimization problem of the following form:

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- The β_i's called the Lagrange multipliers.

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- We would then find and set the $\mathcal{L}$'s partial derivatives to zero.

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0$$

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- Now, consider the following optimization problem:

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- The Lagrangian for this optimization problem can be defined as

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There must exist w^*, α^*, β^* so that w^* is the solution to the optimization problem, and w^*, α^*, β^* satisfy the Karush-Kuhn-Tucker (KKT) conditions, which are as follows:

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g_i(w^*) &\leq 0, i = 1, \ldots, k \\
\alpha^* &\geq 0, i = 1, \ldots, k
\end{aligned}
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Optimal Margin using Lagrange Method

Previously we posed the following optimization problem for finding the optimal margin classifier:

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

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We can write the constraints as

$$g_i(w) = -y^{(i)}(w^\top x^{(i)} + b) + 1 \leq 0.$$

Optimal Margin using Lagrange Method

From the KKT condition $\alpha_i g_i(w) = 0$ we have that $\alpha_i > 0$ only for the training examples that have a functional margin equal to one: the ones corresponding to constraints that hold with equality $g_i(w) = 0$.

Optimal Margin using Lagrange Method

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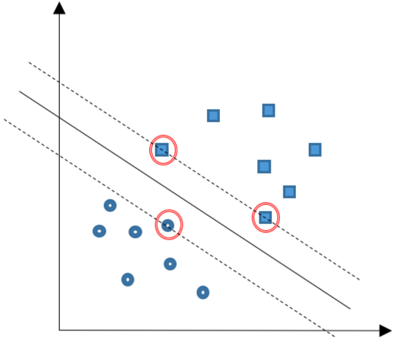

Optimal Margin using Lagrange Method

Then, we can construct the Lagrangian as:

$$\mathcal{L}(\mathrm{w}, b, \alpha) = \frac{1}{2}||\mathrm{w}||^2 - \sum_{i=1}^{m} \alpha_i \Big[y^{(i)}(\mathrm{w}^\top \mathrm{x}^{(i)} + b) - 1 \Big].$$

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To solve this Lagrangian first we set the derivatives of $\mathcal{L}$ with respect to w and b to zero:

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Optimal Margin using Lagrange Method

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with respect to b we obtain:

$$\frac{\partial}{\partial b} \mathcal{L}(\mathrm{w}, b, \alpha) = \sum_{i=1}^{m} \alpha_i y^{(i)} = 0.$$

Optimal Margin using Lagrange Method

Now, replacing

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

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and simplifying it, we get

$$\mathcal{L}(\mathrm{w}, b, \alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j (\mathrm{x}^{(i)})^\top \mathrm{x}^{(j)} - b \sum_{i=1}^{m} \alpha_i y^{(i)}.$$

Optimal Margin using Lagrange Method

And considering that

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Optimal Margin using Lagrange Method

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Optimal Margin using Lagrange Method

So, by minimizing $\mathcal{L}(\mathrm{w}, b, \alpha)$ with respect to w and b we have:

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which is now a just function of α:

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

Optimal Margin using Lagrange Method

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where

$$\left\langle \mathrm{x}^{(i)}, \mathrm{x}^{(j)} \right\rangle$$

is a dot product.

Optimal Margin using Lagrange Method

Now we need to maximize $\mathcal{W}(\alpha)$ subject to some constraints:

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

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \ldots, m$$

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

Optimal Margin using Lagrange Method

Once, we have found the optimal w, b, α values, we can predict a new input x to be 1 if

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$$\begin{aligned} \mathrm{w}^\top \mathrm{x} + b &= \left(\sum_{i=1}^{m} \alpha_i y^{(i)} \mathrm{x}^{(i)} \right)^\top \mathrm{x} + b \\ &= \sum_{i=1}^{m} \alpha_i y^{(i)} \langle \mathrm{x}^{(i)}, \mathrm{x} \rangle + b. \end{aligned}$$

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Thank You!

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