Logistic Regression

What about classification using regression?

Binary classification: Desired outputs 0 and 1

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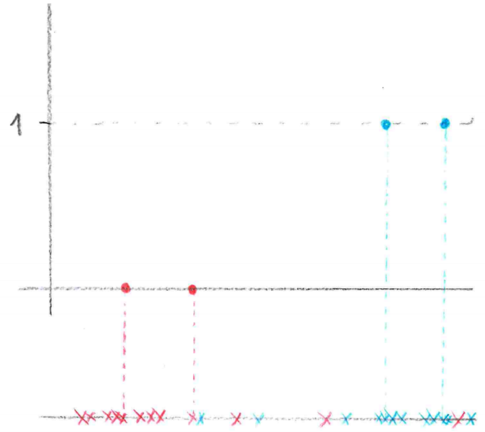

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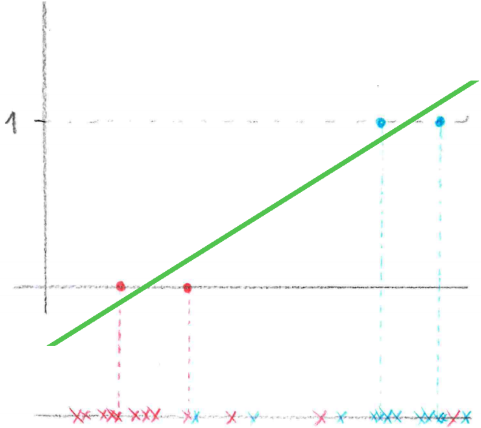

... does not capture the probability well (it is not probability at all)

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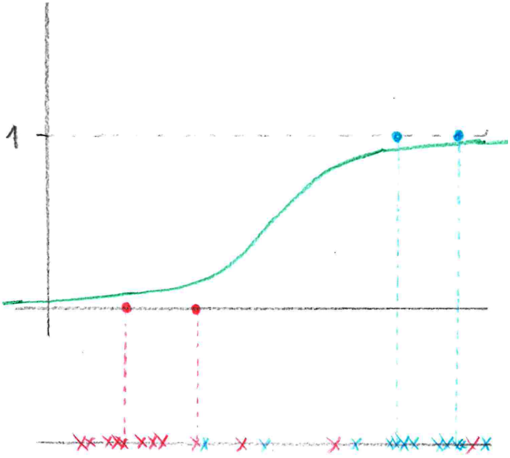

... logistic sigmoid $\frac{1}{1+e^{-(\vec{w}\cdot\tilde{\mathbf{x}})}}$ is much better!

Logistic Regression

Logistic regression model $h[\vec{w}]$ is determined by a vector of weights $\vec{w} = (w_0, w_1, \ldots, w_n) \in \mathbb{R}^{n+1}$ as follows:

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Given $\vec{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$,

$$h[\vec{w}](\vec{x}) := \frac{1}{1 + e^{-\left(w_0 + \sum_{k=1}^{n} w_k x_k\right)}} = \frac{1}{1 + e^{-\vec{w}\cdot\tilde{\mathbf{x}}}}$$

Here

$$\tilde{\mathbf{x}} = (x_0, x_1, \ldots, x_n) \quad \text{where } x_0 = 1$$

is the *augmented feature vector*.

But what is the meaning of the sigmoid?

The model gives probability $h[\vec{w}](\vec{x})$ of the class 1 given an input $\vec{x}$.
But why do we model such probability using $1/(1+e^{-\vec{w}\cdot\tilde{\mathbf{x}}})$??

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Denote by $\bar{h}$ the probability $P(Y = 1 \mid X = \vec{x})$, i.e., the "true" probability of the class 1 given features $\vec{x}$.

The probability $\bar{h}$ cannot be easily modeled using a linear function (the probabilities are between 0 and 1).

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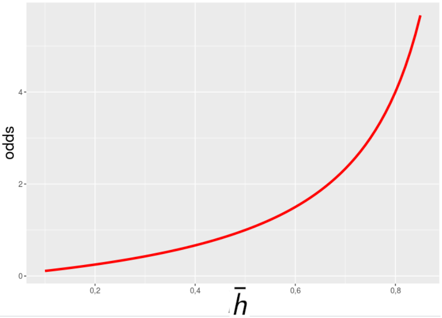
What about odds of the class 1?

$$odds(\bar{h}) = \bar{h}/(1-\bar{h})$$



Better, at least it is unbounded on one side ...

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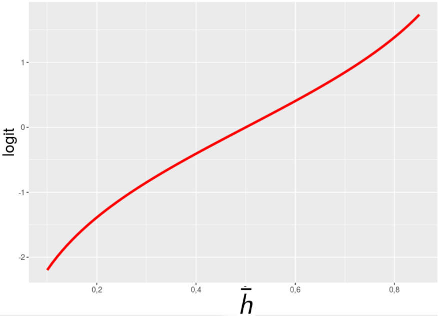
What about log odds (aka logit) of the class 1?

$$logit(\bar{h}) = \log(\bar{h}/(1 - \bar{h}))$$



Looks almost linear, at least for probabilities not too close to 0 or 1 ...

But what is the meaning of the sigmoid?

Assume that $\bar{h}$ is the actual probability of the class 1 for an "object" with features $\vec{x} \in \mathbb{R}^n$. Put

$$\log(\bar{h}/(1-\bar{h})) = \vec{w} \cdot \tilde{\mathbf{x}}$$

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and

$$\bar{h} = \frac{1}{1+e^{-\vec{w} \cdot \tilde{\mathbf{x}}}} = h[\vec{w}](\vec{x})$$

If we model log odds using a linear function, the probability is obtained by applying the logistic sigmoid on the result of the linear function.

Logistic Regression

- Given a set D of training samples:

$$D = \{(\vec{x}_1, c_1), (\vec{x}_2, c_2), \ldots, (\vec{x}_p, c_p)\}$$

Here $\vec{x}_k = (x_{k1} \ldots, x_{kn}) \in \mathbb{R}^n$ and $c_k \in \{0, 1\}$.

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Recall that $h[\vec{w}](\vec{x}_k) = 1 \,/\, \left(1 + e^{-\vec{w} \cdot \tilde{\mathbf{x}}_k}\right)$ where $\tilde{\mathbf{x}}_k = (x_{k0}, x_{k1} \ldots, x_{kn})$, here $x_{k0} = 1$

Our goal: Find $\vec{w}$ such that for every $k = 1, \ldots, p$ we have that $h[\vec{w}](\vec{x}_k) \approx c_k$

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- **Binary Cross-entropy:**

$$E(\vec{w}) = -\sum_{k=1}^{p} c_k \log(h[\vec{w}](\vec{x}_k)) + (1 - c_k)\log(1 - h[\vec{w}](\vec{x}_k))$$

Gradient of the Error Function

Consider the **gradient** of the error function:

$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \ldots, \frac{\partial E}{\partial w_n}(\vec{w})\right) = \sum_{k=1}^{p} \left(h[\vec{w}](\vec{x}_k) - c_k\right) \cdot \tilde{\mathbf{x}}_k$$

Fact 1

If $\nabla E(\vec{w}) = \vec{0} = (0, \ldots, 0)$*, then* $\vec{w}$ *is a global minimum of* E*.*

This follows from the fact that E is convex.

Using the squared error with the logistic sigmoid would lead to a non-convex error with several minima!

Logistic Regression – Learning

Gradient Descent:

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Here $0 < \varepsilon \leq 1$ is the learning rate.

Note that the algorithm is almost similar to the batch perceptron algorithm!

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Proposition

For sufficiently small $\varepsilon > 0$, the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (in a component-wise manner) to the global minimum of the error function E.

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$$h[\vec{w}](\vec{x}) = \frac{1}{1 + e^{-\left(w_0 + \sum_{k=1}^{n} w_k x_k\right)}}$$

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To decide whether a given $\vec{x}$ belongs to the class 1 we use $h[\vec{w}]$ as a Bayes classifier: Assign $\vec{x}$ to the class 1 iff $h[\vec{w}](\vec{x}) \geq 1/2$.

Other thresholds can also be used depending on the application and properties of the model. In such a case, given a threshold $\xi \in [0, 1]$, assign $\vec{x}$ to the class 1 iff $h[\vec{w}](\vec{x}) \geq \xi$.

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and 0 otherwise.

Here w_0, w_1 are **unknown weights**.

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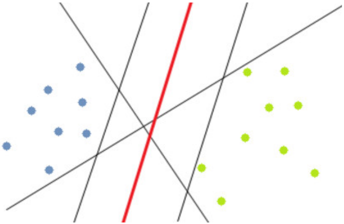
The following conditions are equivalent:

- w_0, w_1 minimize the binary cross-entropy E
- w_0, w_1 maximize the likelihood (i.e., the "probability") of generating the correct values $c_1, \ldots, c_p$ using the above described Bernoulli trials (i.e., that $c'_k = c_k$ for all $k = 1, \ldots, p$)

Note that the above equivalence is a property of the cross-entropy and is not dependent on the "implementation" of $h[w_0, w_1](x_k)$ using the logistic sigmoid.

Support Vector Machines (SVM)

SVM Idea – Which Linear Classifier is the Best?



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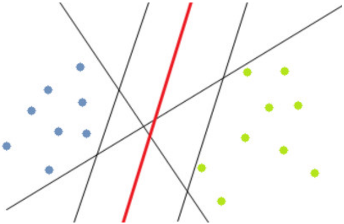

Benefits of maximum margin:

- Intuitively, the maximum margin is good w.r.t. generalization.
- Only the *support vectors* (those on the margin) matter; others can, in principle, be ignored.

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Consider a linear classifier:

$$h[\vec{w}](\vec{x}) := \begin{cases} 1 & w_0 + \sum_{i=1}^{n} w_i \cdot x_i = \vec{w} \cdot \tilde{\mathbf{x}} \geq 0 \\ -1 & w_0 + \sum_{i=1}^{n} w_i \cdot x_i = \vec{w} \cdot \tilde{\mathbf{x}} < 0 \end{cases}$$

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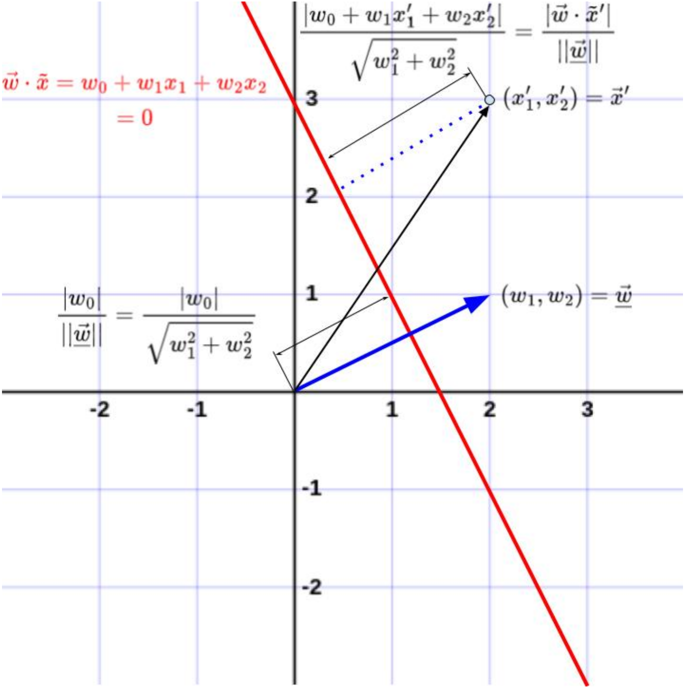
The *distance* of $\vec{x}$ from the separating hyperplane determined by $\vec{w}$ is

$$d[\vec{w}](\vec{x}) = \frac{|\vec{w} \cdot \tilde{\mathbf{x}}|}{\|\underline{\vec{w}}\|}$$

Recall that $\vec{w} \cdot \tilde{\mathbf{x}}$ is positive for $\vec{x}$ on the side to which $\underline{\vec{w}}$ points and negative on the opposite side.



$\frac{|w_0 + w_1 x'_1 + w_2 x'_2|}{\sqrt{w_1^2 + w_2^2}} = \frac{|\vec{w} \cdot \tilde{x}'|}{||\vec{w}||}$
$\vec{w} \cdot \tilde{x} = w_0 + w_1 x_1 + w_2 x_2$
$= 0$
$(x'_1, x'_2) = \tilde{x}'$
$(w_1, w_2) = \vec{w}$
$\frac{|w_0|}{||\vec{w}||} = \frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}$
-2
-1
1
2
3

Margin

- Given a training set

$$D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_p, y_p)\}$$

Here $\vec{x}_k = (x_{k1} \ldots, x_{kn}) \in X \subseteq \mathbb{R}^n$ and $y_k \in \{-1, 1\}$.

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Here $\vec{x}_k = (x_{k1} \dots, x_{kn}) \in X \subseteq \mathbb{R}^n$ and $y_k \in \{-1, 1\}$.

- Assume that D is linearly separable, let $\vec{w}$ *be consistent with* D*.*

Margin of $\vec{w}$ is twice the minimum distance between feature vectors $\vec{x}_k$ and the separating hyperplane determined by $\vec{w}$, i.e.,

$$2 \min_k d[\vec{w}](\vec{x}_k) = 2 \min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{\|\underline{\vec{w}}\|}$$

- Our goal is to find $\vec{w}$ consistent with D that maximizes the margin.

Note that to maximize the margin it suffices to maximize $\min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{\|\underline{\vec{w}}\|}$ over $\vec{w}$ consistent with D.

Finding the Maximum Margin Classifier

We want to maximize the minimum distance of the feature vectors $\vec{x}_k$ from the separating hyperplane determined by $\vec{w}$.

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Formally, we use the following:

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{||\underline{\vec{w}}||}$$

(= the distance of closest $\vec{x}_k$'s to the sep. hyperplane)

over the following constraints

$$\vec{w} \cdot \tilde{\mathbf{x}}_k > 0 \text{ for all } k \text{ satisfying } y_k = 1$$

$$\vec{w} \cdot \tilde{\mathbf{x}}_k < 0 \text{ for all } k \text{ satisfying } y_k = -1$$

(the contraints make sure that $\vec{w}$ is consistent with the training set D)

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{||\underline{\vec{w}}||}$$

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Can be made more succinct:

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{||\underline{\vec{w}}||} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) > 0$$

The reason is that $\vec{w}$ is consistent with D. That is, $\vec{w} \cdot \tilde{x}_k > 0$ for $y_k = 1$, and $\vec{w} \cdot \tilde{x}_k < 0$ for $y_k = -1$.

To maximize the margin, find $\vec{w}$ *maximizing*

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Proof: Just consider $\vec{w}' = \vec{w}/\xi$ where $\xi = \min_k(y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k)$. □

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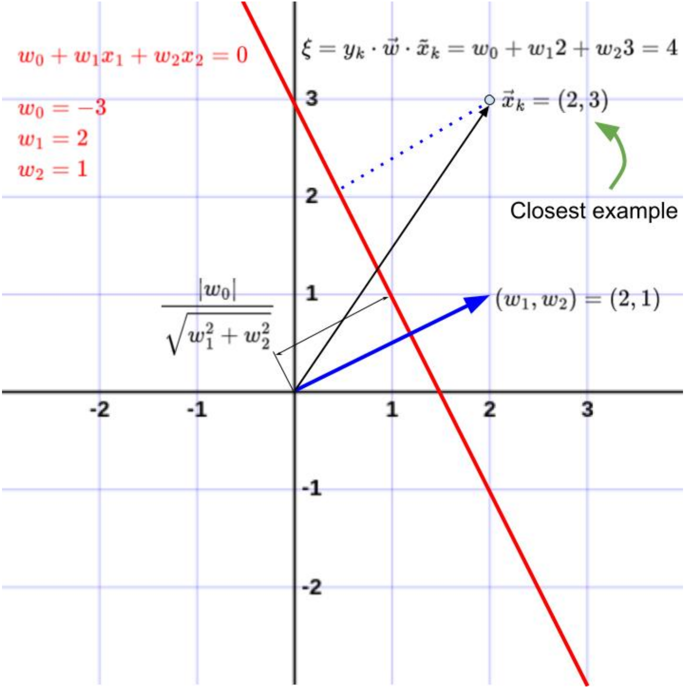
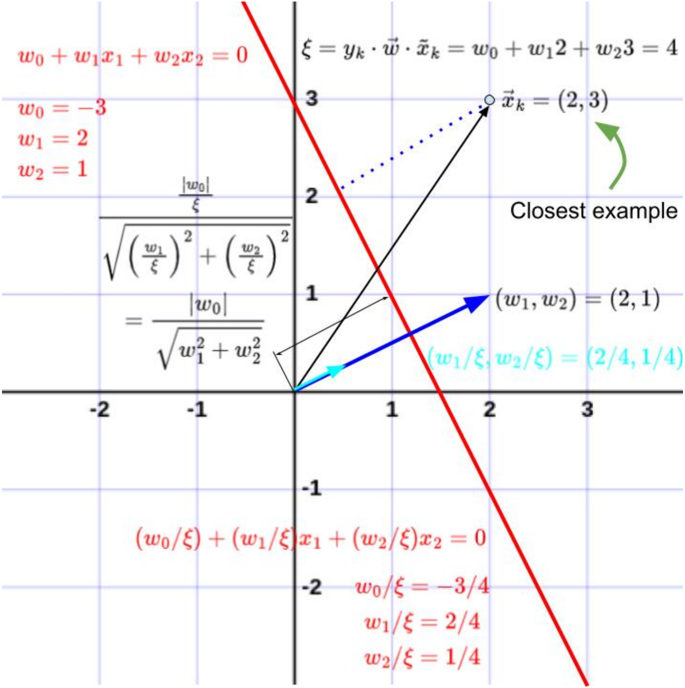
Proof: Just consider $\vec{w}' = \vec{w}/\xi$ where $\xi = \min_k(y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k)$. □

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$$


$w_0 + w_1 x_1 + w_2 x_2 = 0$
$w_0 = -3$
$w_1 = 2$
$w_2 = 1$
$\xi = y_k \cdot \vec{w} \cdot \tilde{x}_k = w_0 + w_1 2 + w_2 3 = 4$
$\vec{x}_k = (2, 3)$
Closest example
$(w_1, w_2) = (2, 1)$
$\frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}$
3
2
1
-1
-2
-2
-1
1
2
3



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$\frac{\frac{|w_0|}{\xi}}{\sqrt{\left(\frac{w_1}{\xi}\right)^2 + \left(\frac{w_2}{\xi}\right)^2}} = \frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}$
$(w_1, w_2) = (2, 1)$
$(w_1/\xi, w_2/\xi) = (2/4, 1/4)$
$(w_0/\xi) + (w_1/\xi)x_1 + (w_2/\xi)x_2 = 0$
$w_0/\xi = -3/4$
$w_1/\xi = 2/4$
$w_2/\xi = 1/4$

To maximize the margin, find $\vec{w}$ *maximizing*

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can be further simplified to

To maximize the margin, find $\vec{w}$ *maximizing*

$$\frac{1}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$$

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To maximize the margin, find $\vec{w}$ *maximizing*

$$\frac{1}{||\underline{\vec{w}}||} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$$

Can be adjusted by loosening the constraints:

To maximize the margin, find $\vec{w}$ *maximizing*

$$\frac{1}{||\underline{\vec{w}}||} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) \geq 1$$

If the latter is solved by $\vec{w}'$ with $\min_k (y_k \cdot \vec{w}' \cdot \tilde{\mathbf{x}}_k) > 1$, then

$$\min_k \frac{y_k \cdot \vec{w}' \cdot \tilde{\mathbf{x}}_k}{||\underline{\vec{w}'}||} > \frac{1}{||\underline{\vec{w}'}||} \geq \frac{1}{||\underline{\vec{w}}||} = \frac{\min_k y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{||\underline{\vec{w}}||}$$

For all $\vec{w}$ satisfying $\min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$, which contradicts the fact that the maximum margin is attained by such a $\vec{w}$.

To maximize the margin, find $\vec{w}$ *maximizing*

$$\frac{1}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1$$

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And, finally,

To maximize the margin, find $\vec{w}$ *minimizing*

$$\underline{\vec{w}} \cdot \underline{\vec{w}} \quad \text{over} \quad y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1 \text{ for all } k$$

Indeed, just note that $||\underline{\vec{w}}|| = \sqrt{\underline{\vec{w}} \cdot \underline{\vec{w}}}$.

SVM – Optimization

Assume a given training set

$$D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_p, y_p)\}$$

Here $\vec{x}_k = (x_{k1} \ldots, x_{kn}) \in X \subseteq \mathbb{R}^n$ and $y_k \in \{-1, 1\}$.
(recall $\tilde{x}_k = (x_{k0}, x_{k1}, \ldots, x_{kn})$ where $x_{k0} = 1$)

Margin maximization as a *quadratic optimization problem:*

Find $\vec{w}$ *minimizing*

$$\underline{\vec{w}} \cdot \underline{\vec{w}}$$

under the constraints

$$y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1 \text{ for all } k$$

Support vectors are vectors $\vec{x}_k$ closest to the *optimal* separating hyperplane, i.e., those satisfying $y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k = 1$ for a minimizing $\vec{w}$.

Example

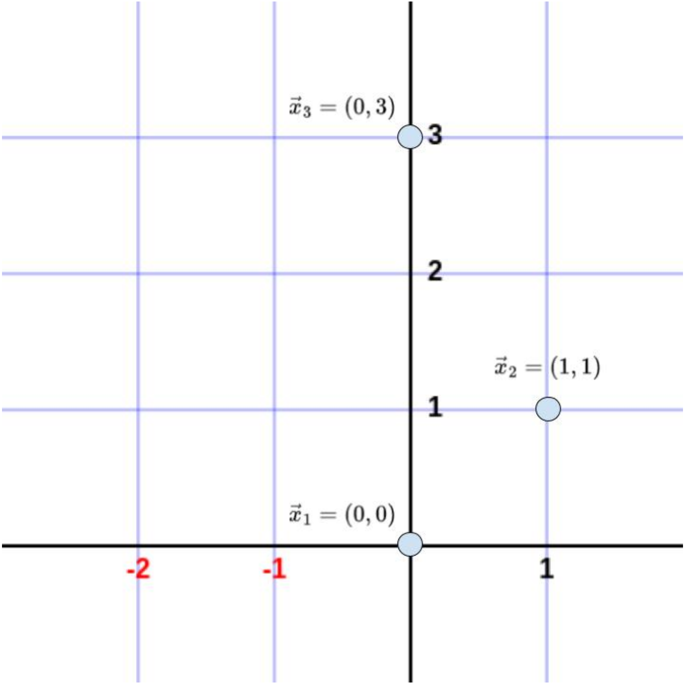
Training set:

$$D = \{((0,0),-1),((1,1),1),((0,3),1)\}$$

That is

$$\begin{aligned} \vec{x}_1 &= (0,0) \\ \vec{x}_2 &= (1,1) \\ \vec{x}_3 &= (0,3) \end{aligned} \qquad \begin{aligned} \tilde{\mathbf{x}}_1 &= (1,0,0) \\ \tilde{\mathbf{x}}_2 &= (1,1,1) \\ \tilde{\mathbf{x}}_3 &= (1,0,3) \end{aligned}$$

$$\begin{aligned} y_1 &= -1 \\ y_2 &= 1 \\ y_3 &= 1 \end{aligned}$$



$\vec{x}_3 = (0, 3)$
3
2
$\vec{x}_2 = (1, 1)$
1
$\vec{x}_1 = (0, 0)$
-2
-1
1

Find $\vec{w}$ minimizing $w_1^2 + w_2^2$ under the constraints

$$(-1) \cdot (1w_0 + 0w_1 + 0w_2) = -w_0 \geq 1$$
$$1 \cdot (1w_0 + 1w_1 + 1w_2) = w_0 + w_1 + w_2 \geq 1$$
$$1 \cdot (1w_0 + 0w_1 + 3w_2) = w_0 + 3w_2 \geq 1$$

It can be solved using a quadratic programming solver.

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To solve by hand, assume that we know that $\vec{x}_1$ and $\vec{x}_2$ are support vectors.

Find $\vec{w}$ minimizing $w_1^2 + w_2^2$ under the constraints

$$-w_0 = 1$$
$$w_0 + w_1 + w_2 = 1$$
$$w_0 + 3w_2 \geq 1$$

Note that the equality constraints correspond to our assumption that $\vec{x}_1$ and $\vec{x}_2$ are support vectors.

Find $\vec{w}$ minimizing $w_1^2 + w_2^2$ under the constraints

$$\begin{aligned} -w_0 &= 1 \\ w_0 + w_1 + w_2 &= 1 \\ w_0 + 3w_2 &\geq 1 \end{aligned}$$

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Can be transformed to

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Substituting $w_2 = 2 - w_1$ into the quadratic function we obtain

$$w_1^2 + (2 - w_1)^2 = w_1^2 + w_1^2 - 4w_1 + 4 = 2w_1^2 - 4w_1 + 4$$

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$$6 - 3w_1 \geq 2$$

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This reduces our problem to

Find $\vec{w}$ minimizing $2w_1^2 - 4w_1 + 4$ under the constraint $w_1 \leq \frac{4}{3}$

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From $-w_0 = 1$ we obtain

$$w_0 = -1$$

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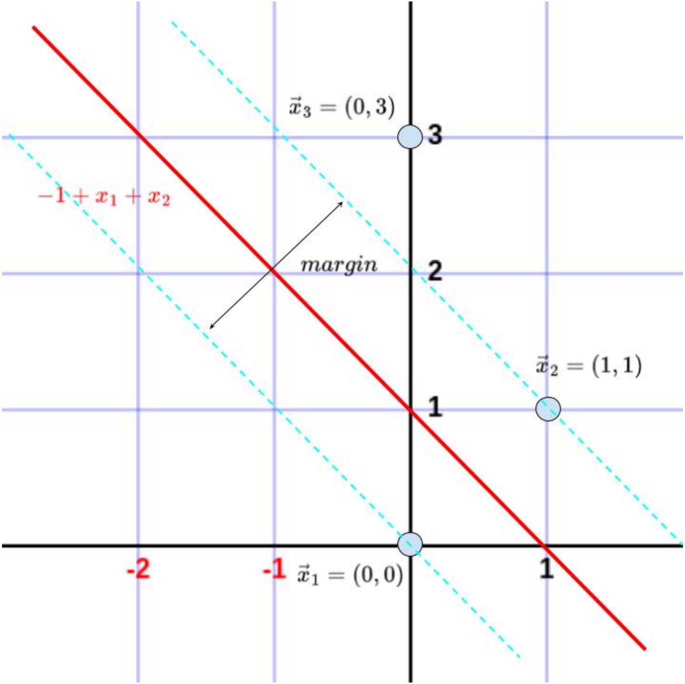
The final model is

$$h[\vec{w}](\vec{x}) = -1 + x_1 + x_2$$

The separating hyperplane is determined by

$$-1 + x_1 + x_2 = 0$$



$\vec{x}_3 = (0,3)$
3
$-1 + x_1 + x_2$
margin
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The answer lies in their ability to deal with non-linearly separable sets efficiently using the *kernel trick* (see a later lecture).

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    - Find an optimal solution using any solver.
    - Afterwards, only support vectors matter in the solution! Leave only them in the training set, and add new training examples.
    - This iterative procedure decreases the (general) cost function.

Soft-margin SVM

Trade-off few misclassifications with a wide margin for the rest.

Find $\vec{w}$ *minimizing*

$$\underline{\vec{w}} \cdot \underline{\vec{w}} + C \sum_k \zeta_k$$

C is a hyperparameter

under the constraints

$$y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1 - \zeta_k \text{ for all } k$$

$$\zeta_k \geq 0 \text{ for all } k$$

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under the constraints

$$y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1 - \zeta_k \text{ for all } k$$

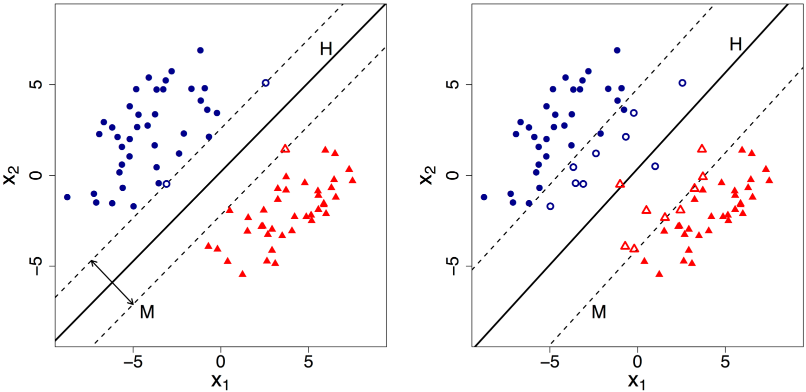
$$\zeta_k \geq 0 \text{ for all } k$$

Which is the same as the following *unconstrained* optimization:

Find $\vec{w}$ *minimizing* the *hinge loss*

$$\underline{\vec{w}} \cdot \underline{\vec{w}} + C \sum_k \max(0, 1 - y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k)$$

Hard vs Soft Margin SVM



Source: Dishaa Agarwal

https://www.analyticsvidhya.com/blog/2021/04/insight-into-svm-support-vector-machine-along-with-code/

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- SVMs can be applied to complex data types beyond feature vectors (e.g., graphs, sequences, relational data) by designing kernel functions for such data.
- SVM techniques have been extended to several tasks, such as regression [Vapnik et al. '97], principal component analysis [Schölkopf et al. '99], etc.