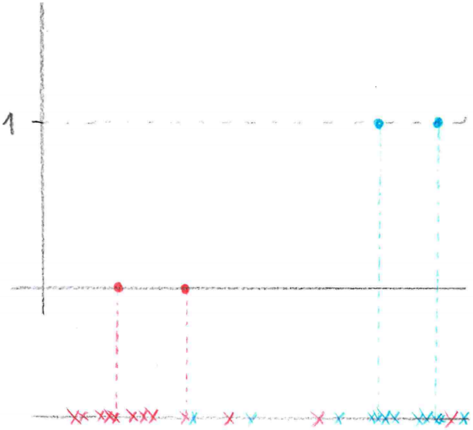
Logistic Regression & SVM

What about classification using regression?

Binary classification: Desired outputs 0 and 1
... we want to capture the probability distribution of the classes



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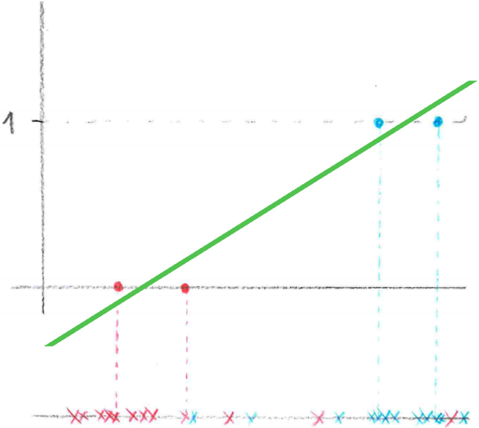

... does not capture the probability well (it is not a probability at all)

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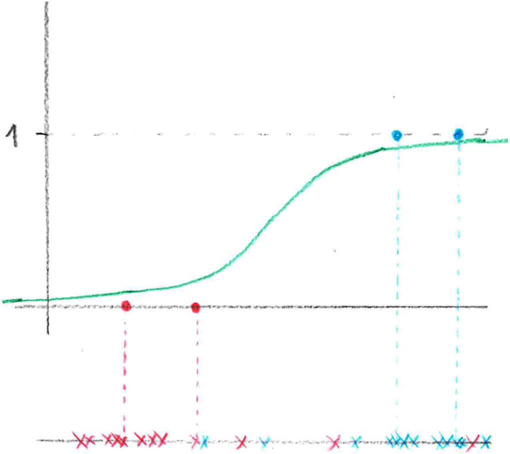

... logistic sigmoid $\frac{1}{1+e^{-(\vec{w}\cdot\tilde{\vec{x}})}}$ is much better!

Logistic Regression

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

Here

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

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 a probability using $1/(1+e^{-\vec{w}\cdot\tilde{\mathrm{x}}})$??

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

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

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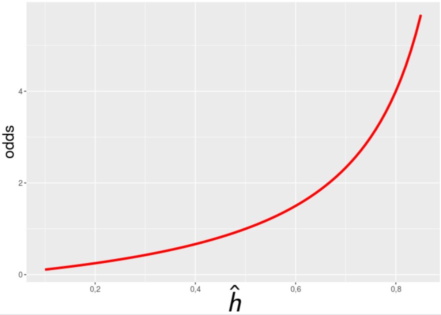
What about odds of the class 1?

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



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

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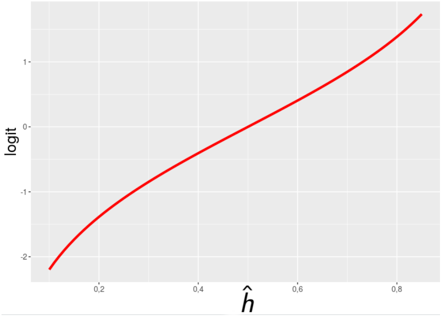
What about log odds (aka logit) of the class 1?

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



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

But what is the meaning of the sigmoid?

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

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and

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

That is, 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:

$$D = \{(\vec{x}_1, c(\vec{x}_1)), (\vec{x}_2, c(\vec{x}_2)), \ldots, (\vec{x}_p, c(\vec{x}_p))\}$$

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

In what follows we use c_k to denote $c(\vec{x}_k)$.

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

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

Fakt

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.

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

Logistic Regression – Learning

Gradient Descent:

- Weights $\vec{w}^{(0)}$ are initialized randomly close to $\vec{0}$.

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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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Tvrzení

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.

Logistic Regression - Using the Trained Model

Assume that we have already trained our logistic regression model, i.e., we have a vector of weights $\vec{w} = (w_0, w_1, \ldots, w_n)$.

The model is the function $h[\vec{w}]$ which for a given feature vector $\vec{x} = (x_1, \ldots, x_n)$ returns the probability

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

that $\vec{x}$ belongs to the class 1.

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 $h[\vec{w}](\vec{x}) \geq \xi$.

Maximum Likelihood vs Cross-entropy (Dim 1)

Fix a training set $D = \{(x_1, c_1), (x_2, c_2), \ldots, (x_p, c_p)\}$
Generate a sequence $c'_1, \ldots, c'_p \in \{0,1\}^p$ where each c'_k has been generated independently by the Bernoulli trial generating 1 with probability

$$h[w_0, w_1](x_k) = \frac{1}{1 + e^{-(\mathbf{w_0} + \mathbf{w_1} \cdot x_k)}}$$

and 0 otherwise.

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

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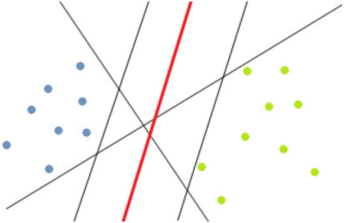
The following conditions are equivalent:

- 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.

SVM Idea – Which Linear Classifier is the Best?



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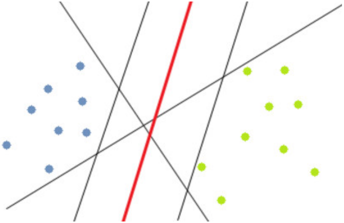

Benefits of maximum margin:

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

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Consider a linear classifier:

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

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The *signed distance* of $\vec{x}$ from the decision boundary determined by $\vec{w}$ is

$$d[\vec{w}](\vec{x}) = \frac{w_0 + \underline{\vec{w}} \cdot \vec{x}_k}{\|\underline{\vec{w}}\|}$$

Here $\|\underline{\vec{w}}\| = \sqrt{\sum_{i=1}^{n} w_i^2}$ is the Euclidean norm of $\underline{\vec{w}}$.

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$|d[\vec{w}](\vec{x})|$ is the distance of $\vec{x}$ from the decision boundary.
$d[\vec{w}](\vec{x})$ is positive for $\vec{x}$ on the side to which $\underline{\vec{w}}$ points and negative on the opposite side.

Support Vectors & Margin

- Given a training set

$$D = \{(\vec{x}_1, y(\vec{x}_1)), (\vec{x}_2, y(\vec{x}_2)), \ldots, (\vec{x}_p, y(\vec{x}_p))\}$$

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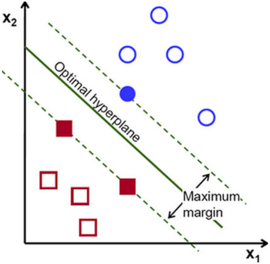
- Assume that D is linearly separable, let $\vec{w}$ *be consistent with* D.

- *Support vectors* are those $\vec{x}_k$ that minimize $|d[\vec{w}](\vec{x}_k)|$.

- *Margin* $\rho[\vec{w}]$ of $\vec{w}$ is twice the distance between support vectors and the decision boundary.



Our goal is to find $\vec{w}$ that maximizes the margin $\rho[\vec{w}]$.

Maximizing the Margin

For $\vec{w}$ consistent with D (such that no $\vec{x}_k$ lies on the decision boundary) we have

$$\rho[\vec{w}] = 2 \cdot \frac{|w_0 + \underline{\vec{w}} \cdot \vec{x}_k|}{\|\underline{\vec{w}}\|} = 2 \cdot \frac{y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k)}{\|\underline{\vec{w}}\|} > 0$$

where $\vec{x}_k$ is a support vector.

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We may safely consider only $\vec{w}$ such that $y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k) = 1$ for the support vectors.

Just adjust the length of $\vec{w}$ so that $y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k) = 1$, the denominator $\|\underline{\vec{w}}\|$ will compensate.

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Then maximizing $\rho[\vec{w}]$ is equivalent to maximizing $2/\|\underline{\vec{w}}\|$.

(In what follows we use a bit looser constraint:

$$y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k) \geq 1 \text{ for all } \vec{x}_k$$

However, the result is the same since even with this looser condition, the support vectors always satisfy $y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k) = 1$ whenever $2/\|\underline{w}\|$ is maximal.)

SVM – Optimization

Margin maximization can be formulated as a *quadratic optimization problem:*

Find $\vec{w} = (w_0, \ldots, w_n)$ such that

$$\rho = \frac{2}{\|\underline{\vec{w}}\|} \text{ is maximized}$$

and for all $(\vec{x}_k, y_k) \in D$ we have $y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k) \geq 1$.

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which can be reformulated as:

Find $\vec{w}$ such that

$$\Phi(\vec{w}) = \|\underline{\vec{w}}\|^2 = \underline{\vec{w}} \cdot \underline{\vec{w}} \text{ is minimized}$$

and for all $(\vec{x}_k, y_k) \in D$ we have $y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k) \geq 1$.

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But why the SVM have been so successful?

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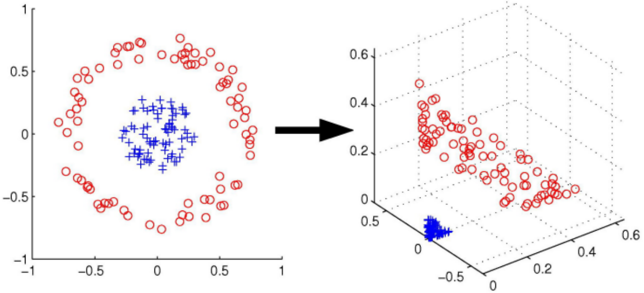
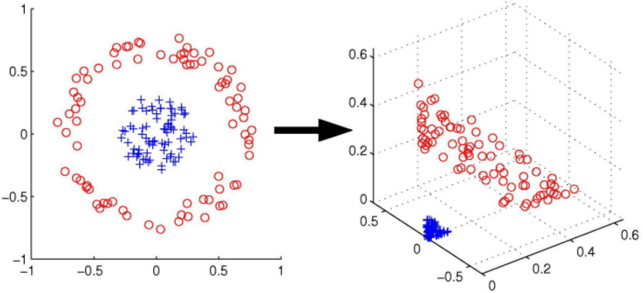
The answer lies in their ability to deal with non-linearly separable sets in an efficient way using so called *kernel trick*.

Non-linear Decision Boundary



Left: The original (x_1, x_2),

Non-linear Decision Boundary



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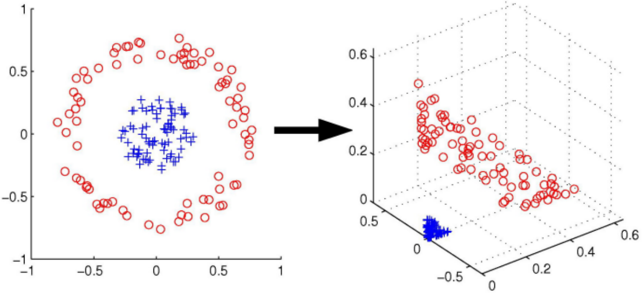

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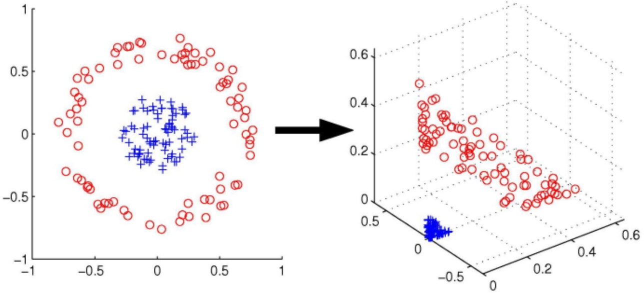

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Right: Linearly separable.

How to classify (in the original space): First, transform a given feature vector by squaring the features, then use the linear classifier.

Do We Need to Map Explicitly?

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But first we need to *dualize* our learning algorithm.

Dual SVM

The original SVM optimization:

Find $\vec{w}$ such that

$$\Phi(\vec{w}) = \|\underline{\vec{w}}\|^2 = \underline{\vec{w}} \cdot \underline{\vec{w}} \text{ is minimized}$$

and for all $(\vec{x}_k, y_k) \in D$ we have $y_k \cdot (w_0 + \underline{\vec{w}} \cdot \vec{x}_k) \geq 1$.

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The dual problem (here p is the number of training samples):

Find $\alpha = (\alpha_1, \ldots, \alpha_p)$ such that

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so that the following constraints are satisfied:

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The Optimization Problem Solution

- Given a solution $\alpha_1, \ldots, \alpha_n$ to the dual problem, solution $\vec{w} = (w_0, w_1, \ldots, w_n)$ to the original one is:

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- The classifier is then

$$\boxed{\begin{aligned} h(\vec{x}) &= sig(w_0 + \underline{\vec{w}} \cdot \vec{x}) \\ &= sig\left(y_k - \textstyle\sum_\ell \alpha_\ell \cdot y_\ell \cdot \vec{x}_\ell \cdot \vec{x}_k + \sum_\ell \alpha_\ell \cdot y_\ell \cdot \vec{x}_\ell \cdot \vec{x}\right) \end{aligned}}$$

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Kernel Dual SVM

Introduce a function $\kappa(\vec{u}, \vec{v}) = \varphi(\vec{u}) \cdot \varphi(\vec{v})$ which computes the scalar product in the space transformed by φ.

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... but now we no longer care what the φ is, right? We just need to know that it exists.

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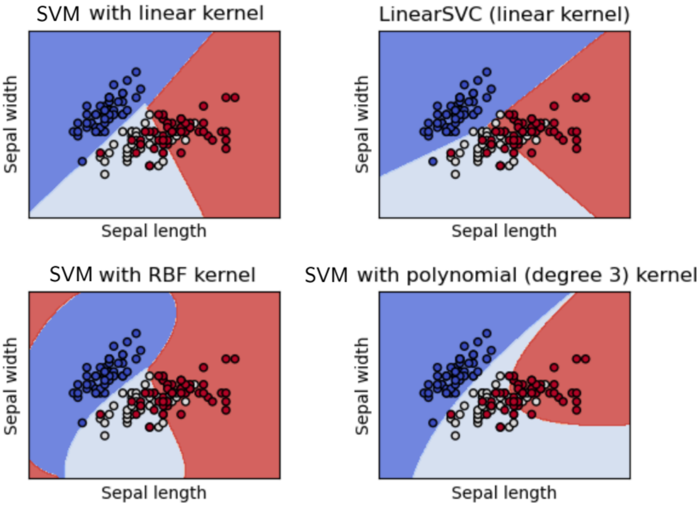
Choosing kernels remains to be black magic of kernel methods. They are usually chosen based on trial and error (of course, experience and additional insight into data helps).

Now let's go on to the main area where kernel methods are used: to enhance support vector machines.

Kernel SVM examples



SVM with linear kernel

LinearSVC (linear kernel)

SVM with RBF kernel

SVM with polynomial (degree 3) kernel

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- Most popular optimization algorithms for SVMs use decomposition to hillclimb over a subset of α_i's at a time, e.g. SMO [Platt '99] and [Joachims '99]
- Tuning SVMs remains a black art: selecting a specific kernel and parameters is usually done in a try-and-see manner.