Kernel Methods & SVM

Partially based on the ML lecture by Raymond J. Mooney
University of Texas at Austin

Back to Linear Classifier (Slightly Modified)

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Recall that given $\vec{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$, the *augmented feature vector* is

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

This makes the notation for the linear classifier more succinct:

$$h[\vec{w}](\vec{x}) = sig(\vec{w} \cdot \tilde{\mathbf{x}}) \text{ where } sig(y) = \begin{cases} 1 & y \geq 0 \\ -1 & y < 0 \end{cases}$$

Perceptron Learning Revisited

- Given a training set

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

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

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- A weight vector $\vec{w} \in \mathbb{R}^{n+1}$ is **consistent with** D if

  $$h[\vec{w}](\vec{x}_k) = sig(\vec{w} \cdot \tilde{\mathbf{x}}_k) = y_k \quad \text{for all } k = 1, \ldots, p$$

  D is **linearly separable** if there is a vector $\vec{w} \in \mathbb{R}^{n+1}$ which is consistent with D.

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  (This is a slight but harmless modification of the traditional algorithm.)
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  - If $sig(\vec{w} \cdot \tilde{\mathbf{x}}_k) \neq y_k$, then $\vec{w}^{(t+1)} = \vec{w}^{(t)} + y_k \cdot \tilde{\mathbf{x}}_k$.
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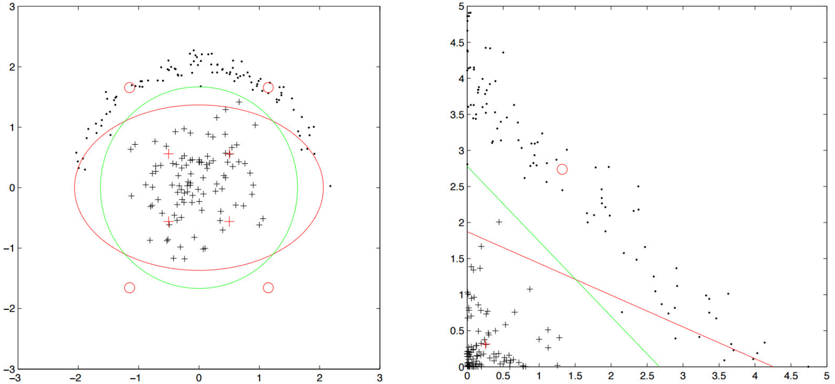
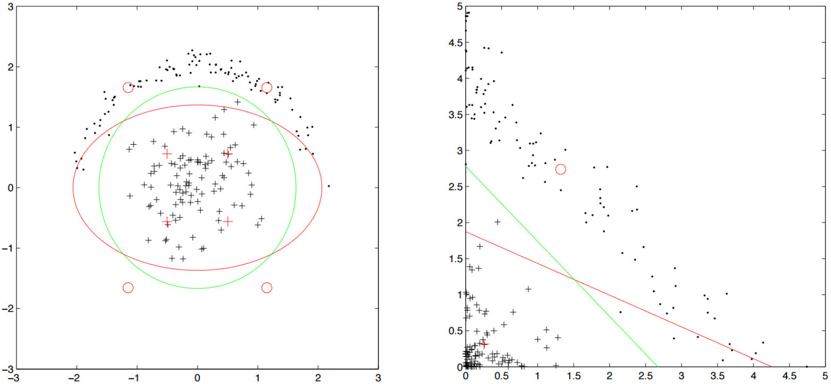
But what can we do if D is not linearly separable?

Quadratic Decision Boundary



Left: The original set,

Quadratic Decision Boundary



Left: The original set, Right: Transformed using the square of features.

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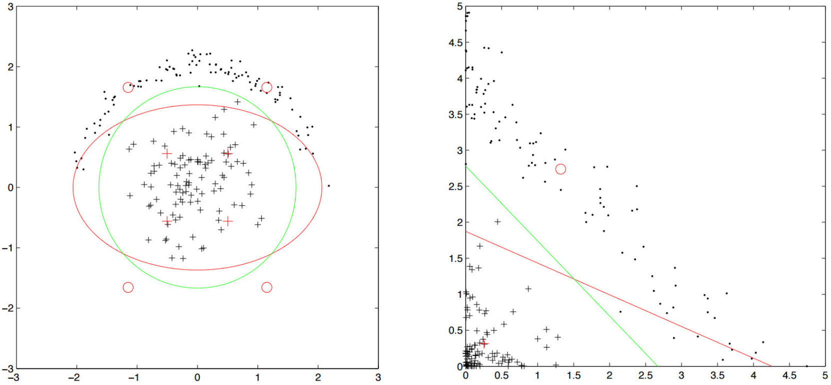

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Right: the green line is the decision boundary learned using the perceptron algorithm.

(The red boundary corresponds to another learning algorithm.)

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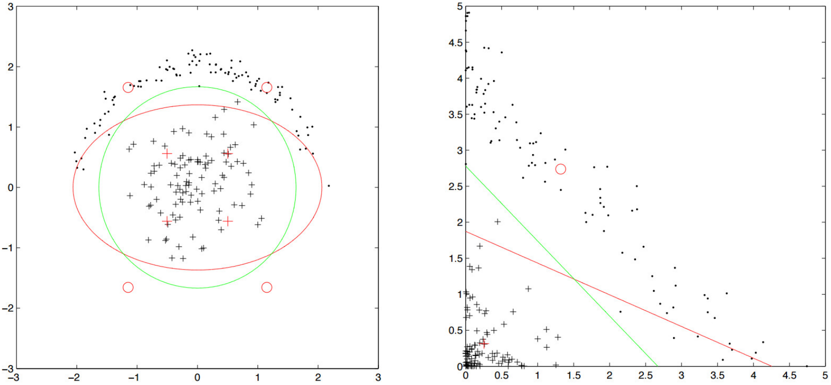

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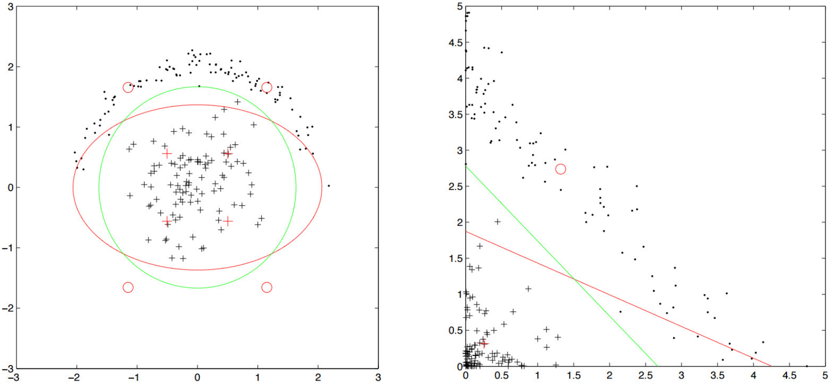

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How to classify (in the original space): First, transform a given feature vector by squaring the features, then use the linear classifier.

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

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Crucial observation:

Note that $\vec{w}^{(t)} = \sum_{\ell=1}^{p} n_\ell^{(t)} \cdot y_\ell \cdot \tilde{\mathbf{x}}_\ell$ for suitable $n_1^{(t)}, \ldots, n_p^{(t)} \in \mathbb{N}$.

Intuitively, $n_\ell^{(t)}$ counts how many times $\tilde{\mathbf{x}}_\ell$ was added to (if $y_\ell = 1$), or subtracted from (if $y_\ell = -1$) weights.

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If D is linearly separable, there exists t^* such that $\sum_{\ell=1}^{p} n_\ell^{(t^*)} \cdot y_\ell \cdot \tilde{\mathbf{x}}_\ell$ is consistent with D. The algorithm stops at such t^* and returns $(n_1^{(t^*)}, \ldots, n_p^{(t^*)})$ so that $\sum_{\ell=1}^{p} n_\ell^{(t^*)} \cdot y_\ell \cdot \tilde{\mathbf{x}}_\ell$ is consistent with D.

Example

Training set:

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$$\begin{aligned} \vec{x}_1 &= (2, -1) & \quad \tilde{\mathbf{x}}_1 &= (1, 2, -1) \\ \vec{x}_2 &= (2, 1) & \quad \tilde{\mathbf{x}}_2 &= (1, 2, 1) \\ \vec{x}_3 &= (1, 3) & \quad \tilde{\mathbf{x}}_3 &= (1, 1, 3) \end{aligned}$$

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

The initial values $n_1^{(0)} = n_2^{(0)} = n_3^{(0)} = 0$.

- $\sum_{\ell=1}^{3} n_\ell^{(0)} \cdot y_\ell \cdot \tilde{\mathbf{x}}_\ell \cdot \tilde{\mathbf{x}}_1 = 0$, thus $sig(\sum_{\ell=1}^{3} n_\ell^{(0)} \cdot y_\ell \cdot \tilde{\mathbf{x}}_\ell \cdot \tilde{\mathbf{x}}_1) = 1 = y_1$. Hence, $\vec{n}^{(1)} = (0, 0, 0)$.

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The result: $\tilde{\mathbf{x}}_2 - \tilde{\mathbf{x}}_3$.

Dual Perceptron Learning – Output

$\vec{w}$ =

Let $\sum_{\ell=1}^{p} n_\ell \cdot y_\ell \cdot \tilde{\mathbf{x}}_\ell$ result from the dual perceptron learning algorithm.

I.e., each $n_\ell = n_\ell^{(t^*)} \in \mathbb{N}$ for suitable t^* in which the algorithm found a consistent vector.

This vector of weights determines a linear classifier that for a given $\vec{x} \in \mathbb{R}^n$ gives

$$h[\vec{w}](\vec{x}) = sig\left(\sum_{\ell=1}^{p} n_\ell \cdot y_\ell \cdot \tilde{\mathbf{x}}_\ell \cdot \tilde{\mathbf{x}}\right)$$

(Here $\tilde{\mathbf{x}}$ is the augmented feature vector obtained from $\vec{x}$.)

Crucial observation: The (augmented) feature vectors $\tilde{\mathbf{x}}_\ell$ and $\tilde{\mathbf{x}}$ occur *only* in scalar products!

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For simplicity, assume bivariate data: $\tilde{\mathbf{x}}_k = (1, x_{k1}, x_{k2})$.

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But now consider a mapping ϕ to $\mathbb{R}^6$ defined by

$$\phi(\tilde{\mathbf{x}}_k) = (1, x_{k1}^2, x_{k2}^2, \sqrt{2}x_{k1}x_{k2}, \sqrt{2}x_{k1}, \sqrt{2}x_{k2})$$

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THE Idea: Define a *kernel* $\kappa(\tilde{\mathbf{x}}_k, \tilde{\mathbf{x}}_\ell) = (\tilde{\mathbf{x}}_k \cdot \tilde{\mathbf{x}}_\ell)^2$ and replace $\tilde{\mathbf{x}}_k \cdot \tilde{\mathbf{x}}_\ell$ in the dual perceptron algorithm with $\kappa(\tilde{\mathbf{x}}_k, \tilde{\mathbf{x}}_\ell)$.

Kernel Perceptron Learning

Kernel Perceptron learning algorithm :

Compute a sequence of vectors of numbers $\vec{n}^{(0)}, \vec{n}^{(1)}, \ldots$ where each $\vec{n}^{(t)} = (n_1^{(t)}, \ldots, n_p^{(t)}) \in \mathbb{N}^p$.

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- In $(t+1)$-th step, $(n_1^{(t+1)}, \ldots, n_p^{(t+1)})$ is computed as follows:
  - If $sig\left(\sum_{\ell=1}^{p} n_\ell^{(t)} \cdot y_\ell \cdot \kappa(\tilde{\mathbf{x}}_k, \tilde{\mathbf{x}}_\ell)\right) \neq y_k$, then $n_k^{(t+1)} := n_k^{(t)} + 1$,

    else, $n_k^{(t+1)} := n_k^{(t)}$.
  - $n_\ell^{(t+1)} := n_\ell^{(t)}$ for all $\ell \neq k$.

Here $k = (t \mod p) + 1$, the examples are considered cyclically.

$\tilde{x}_k \cdot \tilde{x}_\ell$

$\kappa(\bar{x}_k, \bar{x}_\ell) = (\bar{x}_k \cdot \bar{x}_\ell)^2$

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Intuition: The algorithm computes a linear classifier in $\mathbb{R}^6$ for training examples transformed using ϕ.
The trick is that the transformation ϕ itself *does not have to be explicitly computed!*

Dual Perceptron Learning

Let $\vec{n} = (n_1, \ldots, n_p)$ result from the kernel perceptron learning algorithm.
I.e., each $n_\ell = n_\ell^{(t^*)} \in \mathbb{N}$ for suitable t^* such that
$sig\left(\sum_{\ell=1}^{p} n_\ell^{(t^*)} \cdot y_\ell \cdot \kappa(\tilde{\mathbf{x}}_k, \tilde{\mathbf{x}}_\ell)\right) = y_k$ for all $k = 1, \ldots, p$.

We obtain a *non-linear classifier* that for a given $\vec{x} \in \mathbb{R}^n$ gives

$$h[\vec{w}](\vec{x}) = sig\left(\sum_{\ell=1}^{p} n_\ell \cdot y_\ell \cdot \kappa(\tilde{\mathbf{x}}, \tilde{\mathbf{x}}_\ell)\right)$$

(Here $\tilde{\mathbf{x}}$ is the augmented feature vector obtained from $\vec{x}$.)

Are there other kernels that correspond to the scalar product in higher dimensional spaces?

Kernels

Given a (potential) kernel $\kappa(\vec{x}_\ell, \vec{x}_k)$ we need to check whether $\kappa(\vec{x}_\ell, \vec{x}_k) = \phi(\vec{x}_\ell) \cdot \phi(\vec{x}_k)$ for a function ϕ. This might be very difficult.

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Kernels can be constructed from existing kernels by several operations

- linear combination (i.e. multiply by a constant, or sum),
- multiplication,
- exponentiation,
- multiply by a polynomial with non-negative coefficients,
- ...

(see e.g. "Pattern Recognition and Machine Learning" by Bishop)

Examples of Kernels

- Linear: $\kappa(\vec{x}_\ell, \vec{x}_k) = \vec{x}_\ell \cdot \vec{x}_k$
  The corresponding mapping $\phi(\vec{x}) = \vec{x}$ is identity (no transformation).

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- Polynomial of power m: $\kappa(\vec{x}_\ell, \vec{x}_k) = (1 + \vec{x}_\ell \cdot \vec{x}_k)^m$
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$\mathcal{K}(\vec{w}, \vec{x})$

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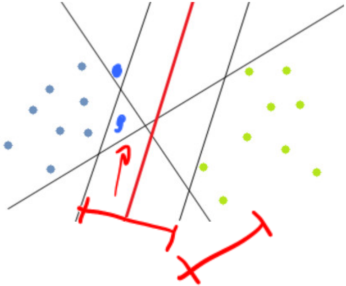
Choosing kernels remains to be black magic of kernel methods. They are usually chosen based on trial and error (of course, experience and additional insight into data helps).

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

SVM Idea – Which Linear Classifier is the Best?



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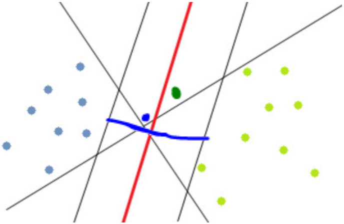

Benefits of maximum margin:

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

Support Vector Machines (SVM)

Notation:

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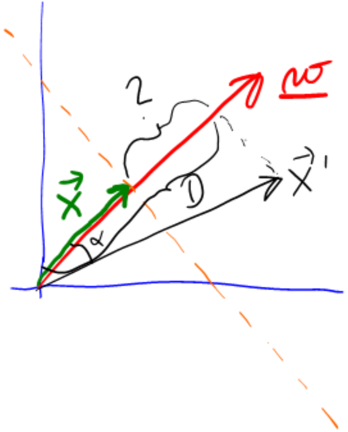
Consider a linear classifier:

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



$$\underline{w} \cdot \vec{x} = \|\underline{w}\| \cdot \|\vec{x}\|$$

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$$\|\vec{x}\| = \frac{-w_0}{\|\underline{w}\|}$$

$$\underline{w} \cdot \vec{x}\,' = \|\underline{w}\| \cdot \|\vec{x}\,'\| \cdot \cos\alpha = \|\underline{w}\| \cdot D$$

$$\iff D = \frac{\underline{w}\,\vec{x}\,'}{\|\underline{w}\|}$$

$$D - \|\vec{x}\| = \frac{\underline{w}\,\vec{x}\,'}{\|\underline{w}\|} - \left(\frac{-w_0}{\|\underline{w}\|}\right) = \frac{w_0 + \underline{w}\,\vec{x}\,'}{\|\underline{w}\|}$$

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

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

$\vec{x} \in \mathbb{R}^1 \quad : \quad w_0 + w_1 x$

$$w_0 + w_1 x_0 = 0 \iff x_0 = -\frac{w_0}{w_1}$$

$$x - x_0 = x - \left(-\frac{w_0}{w_1}\right) = \frac{w_0 + w_1 x}{w_1}$$

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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

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

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

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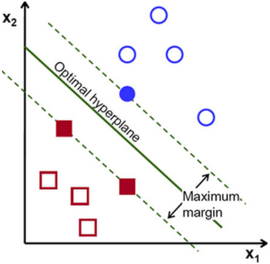

- *Support vectors* are those $\vec{x}_k$ that minimize $|d[\vec{w}](\vec{x}_k)|$.
- *Margin* ρ of $\vec{w}$ is twice the distance between support vectors and the decision boundary.

Our goal is to find a classifier that maximizes the margin.

Maximizing the Margin

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

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

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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 ϱ 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

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

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$\|\vec{w}\| = \sqrt{\vec{w} \cdot \vec{w}}$

$\Leftrightarrow \min \frac{\|\vec{w}\|}{2} \Leftrightarrow \min \frac{\|\vec{w}\|^2}{2} \Leftrightarrow \min \frac{\vec{w} \cdot \vec{w}}{2}$

which can be reformulated as:

Find $\vec{w}$ such that

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- The classifier is then

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

Note that both the dual optimization problem as well as the classifier contain training feature vectors only in the scalar product! We may apply the kernel trick!

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- Note that the optimization techniques remain the same as for the linear SVM without kernels!

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  - 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.

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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.