The Support Vector Machine

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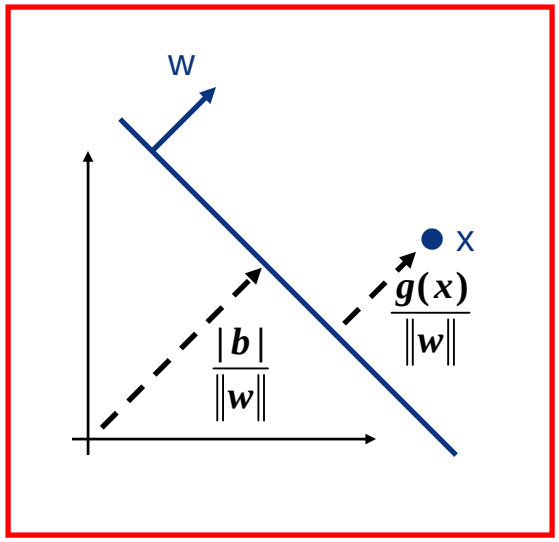
Geometric Interpretation

- Summarizing, the linear discriminant decision rule

$$h^*(x) = \begin{cases} 0 & \text{if } g(x) > 0 \\ 1 & \text{if } g(x) < 0 \end{cases} \quad \text{with} \quad g(x) = w^T x + b$$

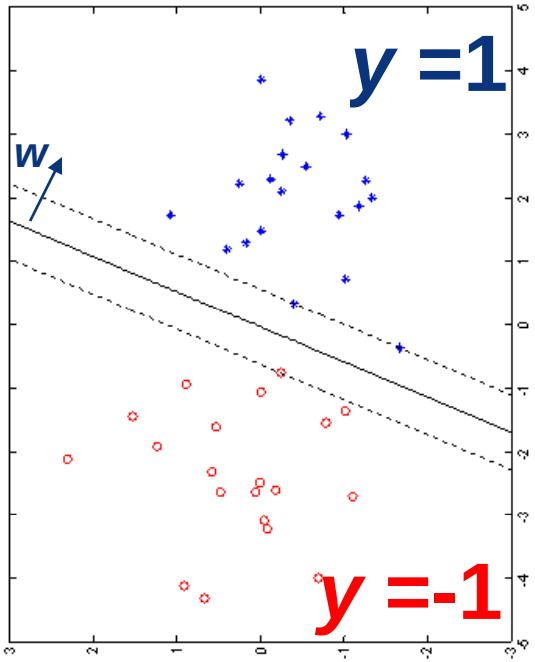
has the following properties

- It divides $\mathcal{X}$ into two "half-spaces"
- The boundary is the hyperplane with:
  - normal *w*
  - distance to the origin *b*/||*w*||
- g(*x*)/||*w*|| gives the signed distance from point *x* to the boundary
  - g(x) = 0 for points on the plane
  - g(x) > 0 for points on the side *w* points to ("positive side")
  - g(x) < 0 for points on the "negative side"



Linear Discriminants

- For now, our goal is to explore the simplicity of the linear discriminant
- let's assume linear separability of the training data
- One handy trick is to use class labels $y \in \{-1,1\}$ instead of $y \in \{0,1\}$, *where*
  - y = 1 for points on the positive side
  - y = -1 for points on the negative side
- The decision function then becomes



$$h^*(x) = \begin{cases} 1 & \text{if } g(x) > 0 \\ -1 & \text{if } g(x) < 0 \end{cases} \Leftrightarrow \boxed{h^*(x) = \text{sgn}\left[g(x)\right]}$$

Linear Discriminants & Separable Data

- We have a classification error if
  - $y = 1$ and $g(x) < 0$ or $y = -1$ and $g(x) > 0$
  - i.e., if $y\,g(x) < 0$
- We have a correct classification if
  - $y = 1$ and $g(x) > 0$ or $y = -1$ and $g(x) < 0$
  - i.e., if $y\,g(x) > 0$
- Note that, if the data is linearly separable, given a training set

$$D = \{(x_1, y_1), \cdots, (x_n, y_n)\}$$

  we can have zero training error.

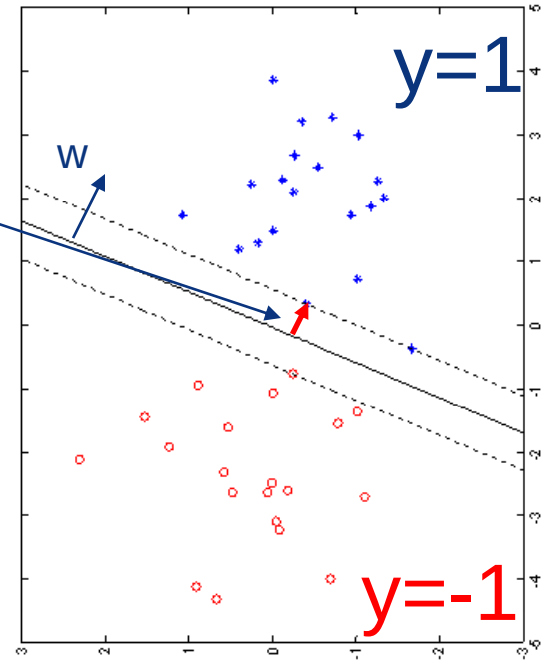
- The necessary & sufficient condition for this is that

$$\boxed{y_i \left(\boldsymbol{w}^T \boldsymbol{x}_i + \boldsymbol{b} \right) > 0, \quad \forall \boldsymbol{i} = \boldsymbol{1}, \cdots, \boldsymbol{n}}$$

The Margin

- The margin is the distance from the boundary to the closest point

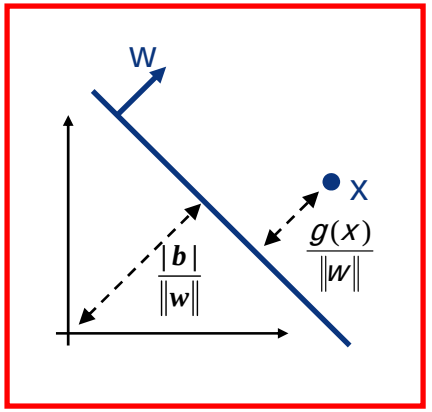
$$\gamma = \min_i \frac{\left| w^T x_i + b \right|}{\|w\|}$$



- There will be no error on the training set if it is strictly greater than zero:

$$y_i \left(w^T x_i + b \right) > 0, \quad \forall i \quad \Leftrightarrow \quad \boxed{\gamma > 0}$$

- Note that this is ill-defined in the sense that γ does not change if both w and b are scaled by a common scalar λ
- We need a normalization



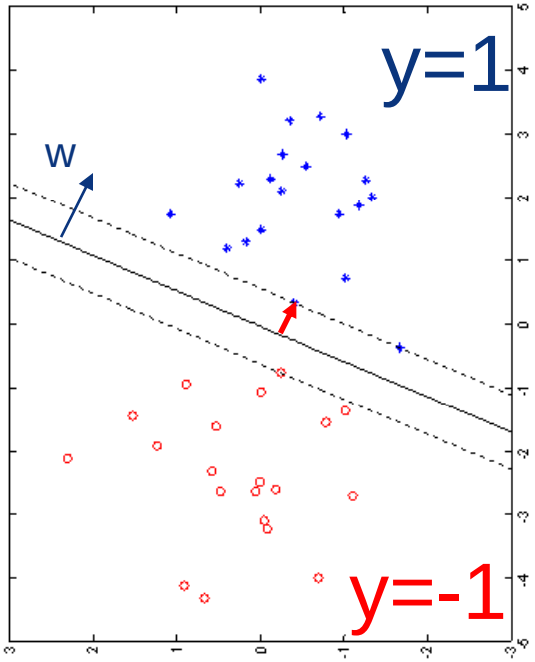
Support Vector Machine (SVM)

- A convenient normalization is to make $|g(x)| = 1$ for the closest point, i.e.

$$\min_i \left| w^T x_i + b \right| \equiv 1$$

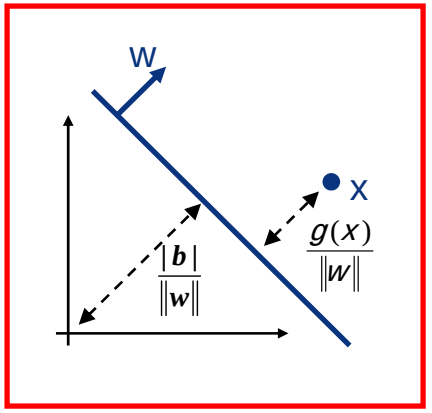
under which

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



- The Support Vector Machine (SVM) is the linear discriminant classifier that maximizes the margin subject to these constraints:

$$\min_{w,b} \|w\|^2 \quad \text{subject to} \quad y_i \left(w^T x_i + b \right) \geq 1 \quad \forall i$$



Duality

- We must solve an optimization problem with constraints
- There is a rich theory on how to solve such problems
  - We will not get into it here (take 271B if interested)
  - The main result is that we can often formulate a dual problem which is easier to solve
  - In the dual formulation we introduce a vector of Lagrange multipliers $\alpha_i > 0$, one for each constraint, and solve

$$\max_{\alpha \geq 0} q(\alpha) = \max_{\alpha \geq 0} \left\{ \min_{w} L(w, b, \alpha) \right\}$$

  - where

$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_i \alpha_i \left[y_i \left(w^T x_i + b \right) - 1 \right]$$

    is the Lagrangian

The Dual Optimization Problem

- For the SVM, the dual problem can be simplified into

$$\max_{\alpha \geq 0} \left\{ -\frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_{\mathbf{i}} \alpha_i \right\}$$

$$\textbf{subject to} \ \sum_{\mathbf{i}} y_i \alpha_i = 0$$

- Once this is solved, the vector

$$w^* = \sum_i \alpha_i y_i x_i$$

  is the normal to the maximum margin hyperplane

- Note: the dual solution does not determine the optimal *b**, since *b* drops out when we solve

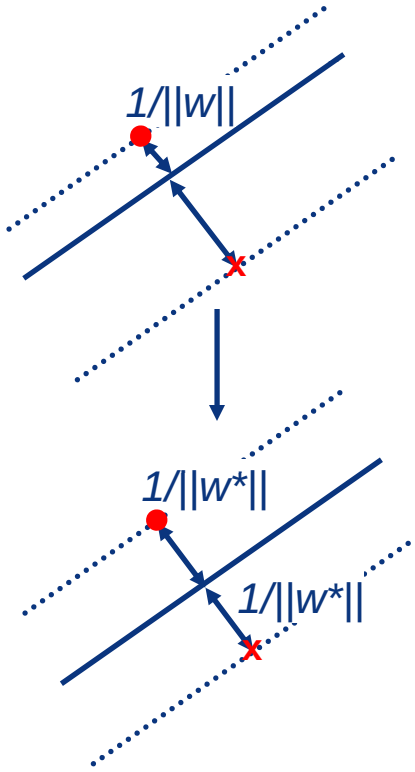
$$\min_{\mathbf{w}} L(w, b, \alpha)$$

The Dual Problem

- There are various possibilities for determining b^*.
  For example:
  - Pick one point x^+ on the margin on the $y = 1$ side and one point x^- on margin on the $y = -1$ side
  - Then use the margin constraint

$$\left.\begin{aligned} \boldsymbol{w}^T \boldsymbol{x}^+ + \boldsymbol{b} &= 1 \\ \boldsymbol{w}^T \boldsymbol{x}^- + \boldsymbol{b} &= -1 \end{aligned}\right\} \Leftrightarrow \boxed{\boldsymbol{b}^* = -\frac{\boldsymbol{w}^T (\boldsymbol{x}^+ + \boldsymbol{x}^-)}{2}}$$

- Note:
  - The maximum margin solution guarantees that there is always at least one point "on the margin" on each side
  - If not, we could move the hyperplane and get an even larger margin (see figure on the right)



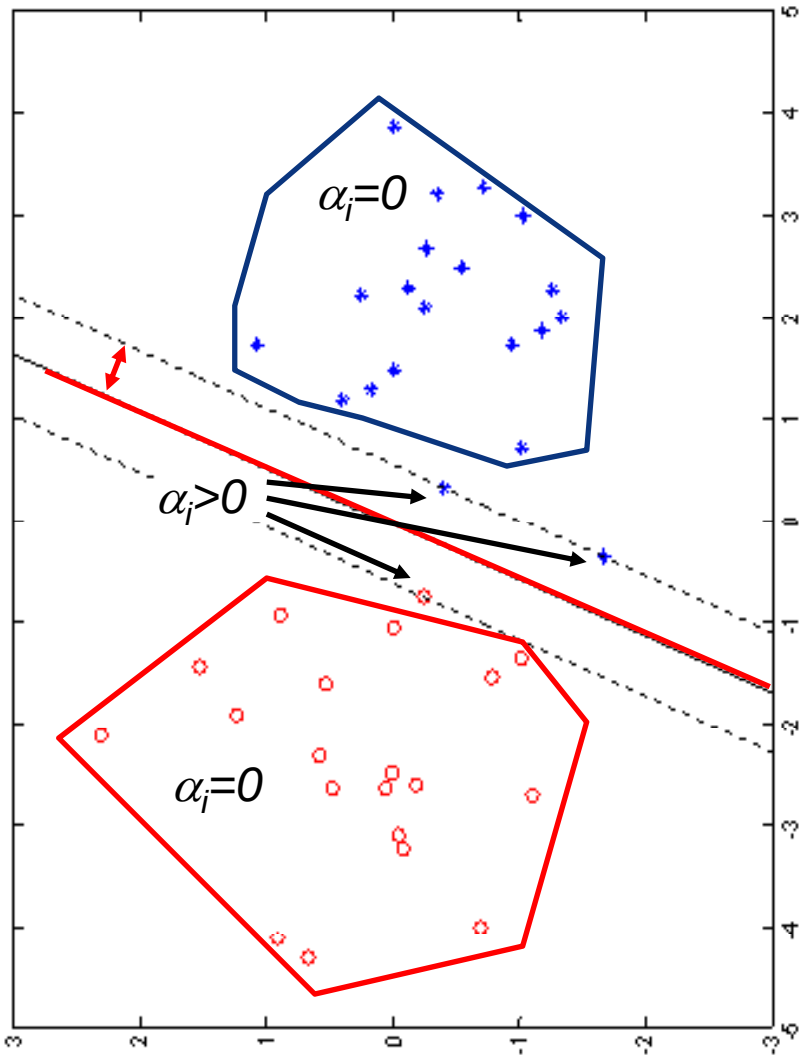
Support Vectors

It turns out that:

- An inactive constraint always has zero Lagrange multiplier α_i
- That is,
  - i) $\alpha_i > 0$ and $y_i(w^{*T}x_i + b^*) = 1$ or
  - ii) $\alpha_i = 0$ and $y_i(w^{*T}x_i + b^*) > 1$
- Hence $\alpha_i > 0$ only for points

$$|w^{*T}x_i + b^*| = 1$$

which are those that lie at a distance equal to the margin (i.e., those that are "on the margin"). These points are the "Support Vectors"



Support Vectors

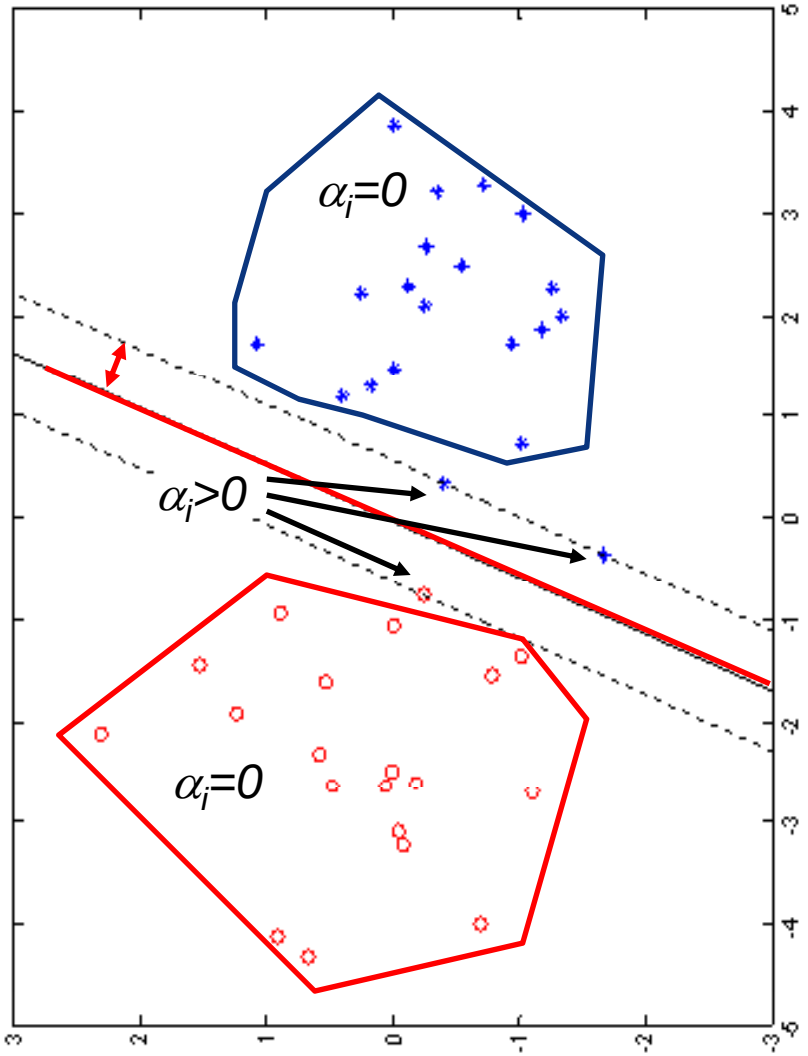
- The points with $\alpha_i > 0$ "support" the optimal hyperplane (w^*,b^*).
- This why they are called "Support Vectors"
- Note that the decision rule is

$$f(x) = \text{sgn}\left[w^{*T} x + b^* \right]$$

$$= \text{sgn}\left[\sum_i y_i \alpha_i^* x_i^T \left(x - \frac{x^+ + x^-}{2} \right) \right]$$

$$= \text{sgn}\left[\sum_{i \in SV} y_i \alpha_i^* x_i^T \left(x - \frac{x^+ + x^-}{2} \right) \right]$$

where SV = $\{i \mid \alpha^*_i > 0\}$ indexes the set of support vectors



Support Vectors and the SVM

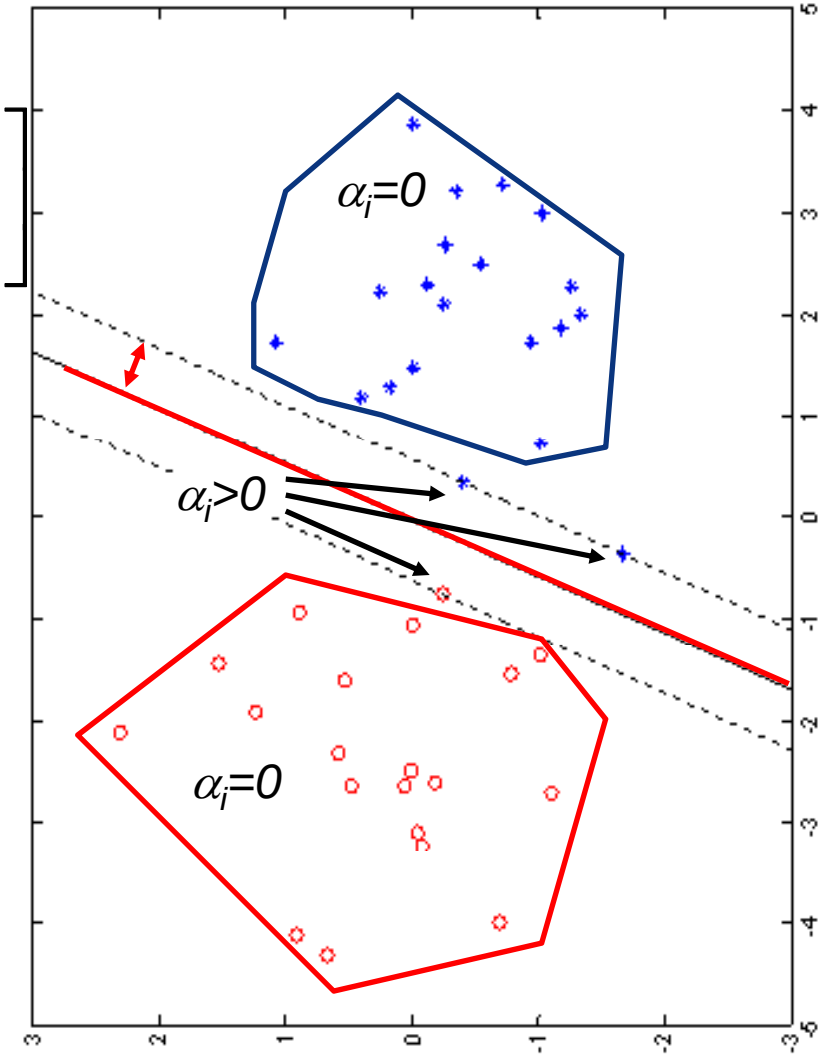
- Since the decision rule is

$$f(x) = \text{sgn}\left[\sum_{i \in \text{SV}} y_i \alpha_i^* x_i^T \left(x - \frac{x^+ + x^-}{2} \right) \right]$$

  where x^+ and x^- are support vectors, we see that we only need the support vectors to completely define the classifier!

- We can literally throw away all other points!!

- The Lagrange multipliers can also be seen as a measure of importance of each point



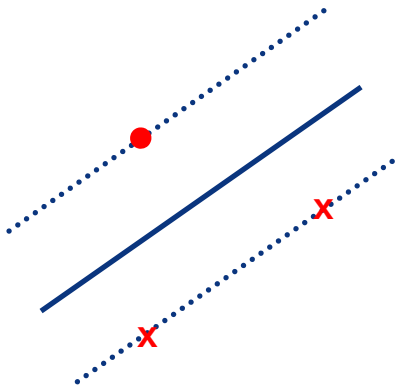
- Points with $\alpha_i = 0$ have no influence—a small perturbation does not change the solution

The Robustness of SVMs

- We talked a lot about the "curse of dimensionality"
  - In general, the number of examples required to achieve certain precision of pdf estimation, and pdf-based classification, is exponential in the number of dimensions
- It turns out that SVMs are remarkably robust to the dimensionality of the feature space
  - Not uncommon to see successful applications on 1,000D+ spaces
- Two main reasons for this:
  - 1) All that the SVM has to do is to learn a hyperplane.

    Although the number of dimensions may be large, the number of parameters is relatively small and there is not much room for overfitting

    In fact, *d+1* points are enough to specify the decision rule in R^d !!



Robustness: SVMs as Feature Selectors

- The second reason for robustness is that the data/feature space *effectively* is not *really* that large
  - 2) This is because the SVM is a feature selector

To see this let's look at the decision function

$$f(x) = \mathrm{sgn}\left[\sum_{i \in SV} y_i \alpha_i^* x_i^T x + b^*\right]$$

This is a thresholding of the quantity

$$\sum_{i \in SV} y_i \alpha_i^* x_i^T x$$

Note that each of the terms $x_i^T x$ is the projection (actually, inner product) of the vector which we wish to classify, x, onto the training (support) vector x_i

SVMs as Feature Selectors

- Define *z* to be the vector of the projection of *x* onto all of the support vectors

$$z(x) = \left(x^T x_{i_1}, \cdots, x^T x_{i_k} \right)^T$$

- The decision function is a hyperplane in the *z*-space

$$f(x) = \mathrm{sgn}\left[\sum_{i \in \mathrm{SV}} y_i \alpha_i^* x_i^T x + b^* \right] = \mathrm{sgn}\left[\sum_k w_k^* z_k(x) + b^* \right]$$

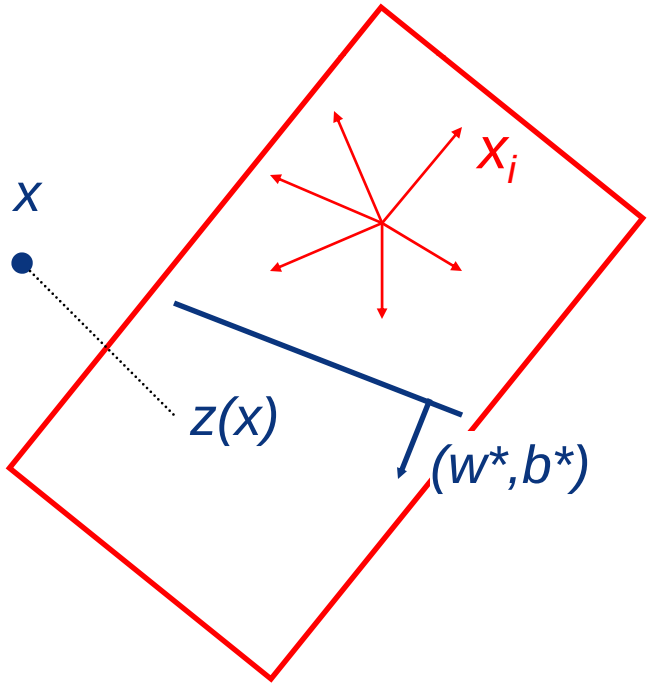
with

$$w^* = \left(\alpha_{i_1}^* y_{i_1}, \cdots, \alpha_{i_k}^* y_{i_k} \right)^T$$

- This means that
  - The classifier operates only on the span of the support vectors!
  - The SVM performs feature selection automatically.

SVMs as Feature Selectors

- Geometrically, we have:
  - 1) Projection of new data point x on the span of the support vectors
  - 2) Classification on this (sub)space



$$\boldsymbol{w^*} = \left(\alpha_{i_1}^* y_{i_1}, \cdots, \alpha_{i_k}^* y_{i_k} \right)^T$$

- The effective dimension is |SV| and, typically, |SV| << n !!

Summary of the SVM

- SVM training:
  - 1) Solve the optimization problem:

$$\max_{\alpha \geq 0} \left\{ -\frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_i \alpha_i \right\}$$

$$\text{subject to} \quad \sum_i y_i \alpha_i = 0$$

  - 2) Then compute the parameters of the "large margin" linear discriminant function:

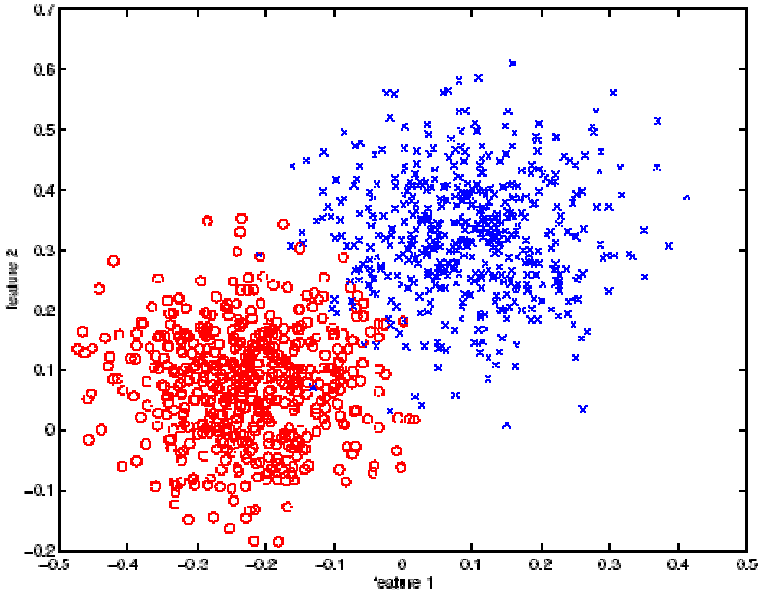
$$w^* = \sum_{i \in \text{SV}} \alpha_i^* y_i x_i \qquad b^* = -\frac{1}{2} \sum_{i \in SV} y_i \alpha_i^* \left(x_i^T x^+ + x_i^T x^- \right)$$

- SVM Linear Discriminant Decision Function:

$$f(x) = \text{sgn}\left[\sum_{i \in \text{SV}} y_i \alpha_i^* x_i^T x + b^* \right]$$

Non-Separable Problems

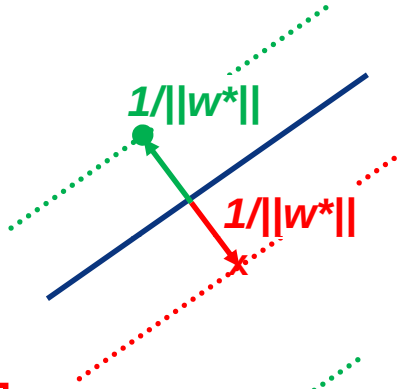
- So far we have assumed linearly separable classes
- This is rarely the case in practice
- A separable problem is “easy” most classifiers will do well
- We need to be able to extend the SVM to the non-separable case
- Basic idea:
  - With class overlap we cannot enforce a (“hard”) margin.
  - But we can enforce a “soft margin”
  - For most points there *is* a margin. But there are a few outliers that cross-over, or are closer to the boundary than the margin. So how do we handle the latter set of points?



Soft Margin Optimization

- Mathematically this is done by introducing slack variables
- Rather than solving the "hard margin" problem

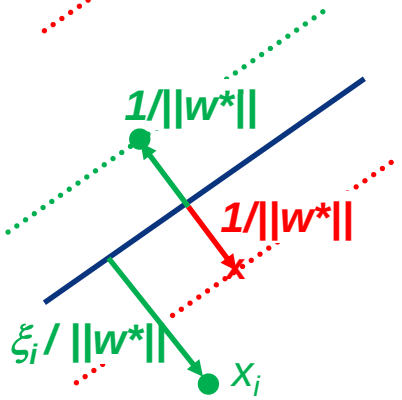
$$\min_{w,b} \|w\|^2 \quad \text{subject to } y_i\left(w^T x_i + b\right) \geq 1 \quad \forall i$$



instead we solve the "soft margin" problem

$$\min_{w,\xi,b} \|w\|^2 \quad \text{subject to } y_i\left(w^T x_i + b\right) \geq 1 - \xi_i \quad \forall i$$

$$\xi_i \geq 0, \forall i$$



- The ξ_i are called slack variables
- Basically, the same optimization as before but points with $\xi_i > 0$ are allowed to violate the margin

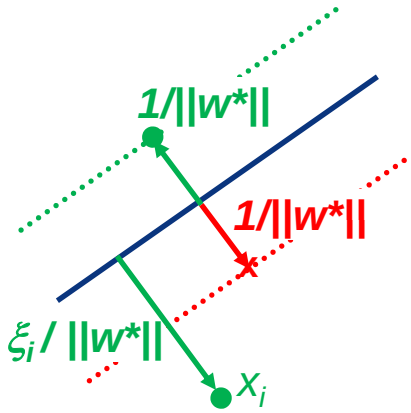
Soft Margin Optimization

- Note that, as it stands, the problem is not well defined
- By making ξ_i arbitrarily large, $w \approx 0$ is a solution!
- Therefore, we need to penalize large values of ξ_i
- Thus, instead we solve the penalized, or regularized, optimization problem:

$$\min_{w,\xi,b} \ \|w\|^2 + C\sum_i \xi_i$$

$$\text{subject to} \quad y_i\left(w^T x_i + b\right) \geq 1 - \xi_i \quad \forall i$$

$$\xi_i \geq 0, \forall i$$



- The quantity $C\sum_i \xi_i$ is the penalty, or regularization, term. The positive parameter C controls how harsh it is.

The Soft Margin Dual Problem

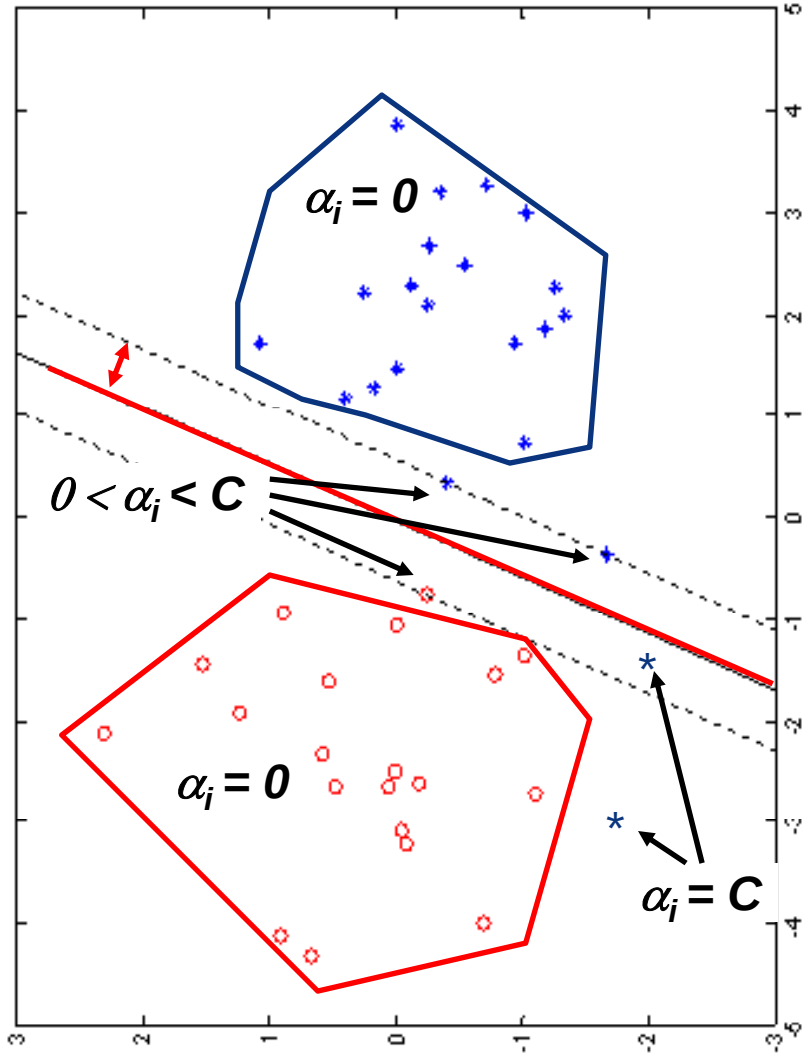
- The dual optimization problem:

$$\max_{\alpha \geq 0} \left\{ -\frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_i \alpha_i \right\}$$

$$\text{subject to} \quad \sum_i y_i \alpha_i = 0,$$

$$0 \leq \alpha_i \leq C$$

- The only difference with respect to the hard margin case is the "box constraint" on the Lagrange multipliers α_i
- Geometrically we have this



Support Vectors

- They are the points with $\alpha_i > 0$
- As before, the decision rule is

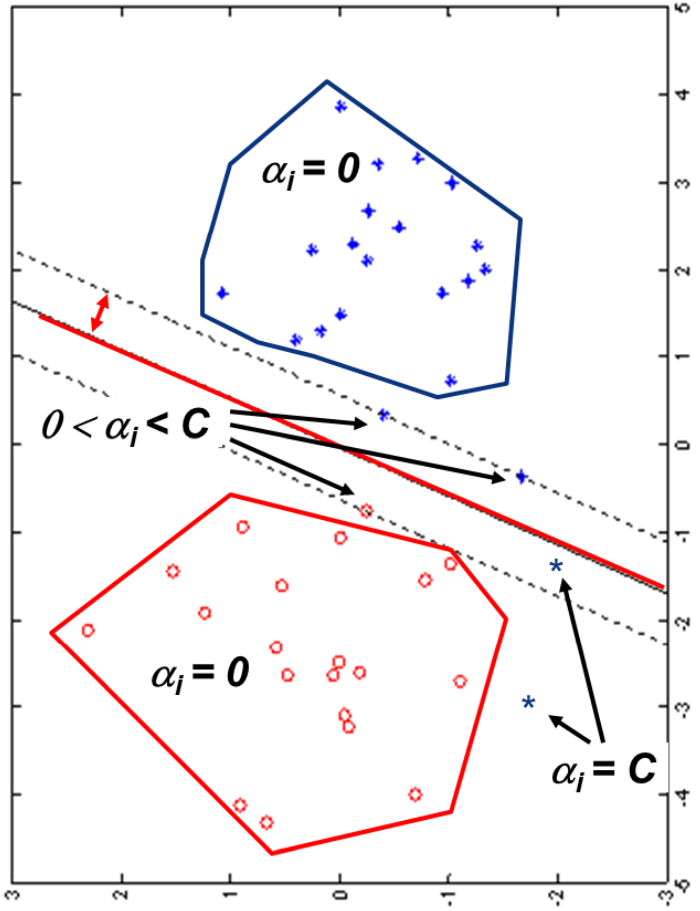
$$f(x) = \text{sgn}\left[\sum_{i \in SV} y_i \alpha_i^* x_i^T x + b^*\right]$$

where $SV = \{i \mid \alpha^*_i > 0\}$

and b^* is chosen s.t.

  - $y_i g(x_i) = 1$, for all x_i s.t. $0 < \alpha_i < C$

- The box constraint on the Lagrange multipliers:
  - makes intuitive sense as it prevents any single support vector outlier from having an unduly large impact in the decision rule.



Summary of the soft-margin SVM

- SVM training:
  - 1) Solve the optimization problem:

$$\max_{\alpha \geq 0} \left\{ -\frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_i \alpha_i \right\}$$

$$\text{subject to} \quad \sum_i y_i \alpha_i = 0,$$

$$0 \leq \alpha_i \leq C$$

  - 2) Then compute the parameters of the "large margin" linear discriminant function:

$$w^* = \sum_{i \in \text{SV}} \alpha_i^* y_i x_i \qquad b^* = -\frac{1}{2} \sum_{i \in SV} y_i \alpha_i^* \left(x_i^T x^+ + x_i^T x^- \right)$$

- SVM Linear Discriminant Decision Function:

$$f(x) = \text{sgn}\left[\sum_{i \in \text{SV}} y_i \alpha_i^* x_i^T x + b^* \right]$$

“The Kernel Trick”

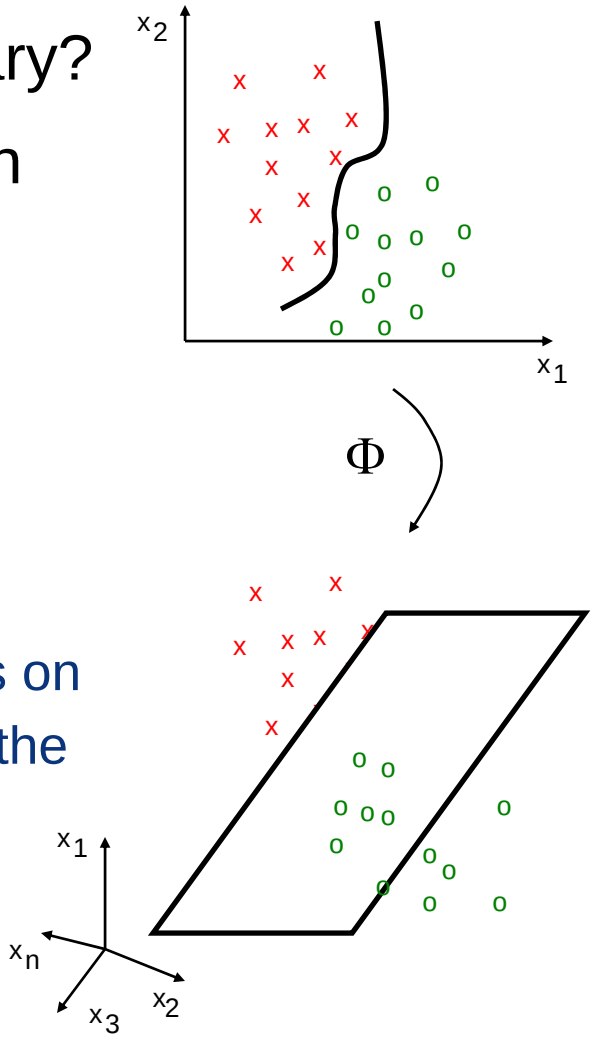
- What if we want a non-linear boundary?
- Consider the following transformation of the feature space:
  - Introduce a mapping to a “better” (i.e., linearly separable) feature space

$$\phi: \mathcal{X} \rightarrow \mathcal{Z}$$

where, generally, **dim($\mathcal{Z}$) > dim($\mathcal{X}$)**.

  - If a classification algorithm only depends on the data through inner products then, in the transformed space, it depends on

$$\langle \phi(x_i), \phi(x_j) \rangle = \phi^T(x_i)\phi(x_j)$$



The Inner Product Implementation

- In the transformed space, the learning algorithms only requires inner products

$$\langle \phi(x_i), \phi(x_j) \rangle = \phi(x_j)^T \phi(x_i)$$

- Note that we do not need to store the $\phi(x_j)$, but only the n^2 (scalar) component values of the inner product matrix
- Interestingly, this holds even if $\phi(x)$ takes its value in an infinite dimensional space.
  - We get a reduction from infinity to n^2!
  - There is, however, still one problem:
    - When $\phi(x_j)$ is infinite dimensional the computation of the inner product $\langle \phi(x_i), \phi(x_j) \rangle$ looks impossible.

“The Kernel Trick”

- “Instead of defining $\phi(x)$, then computing $\phi(x_i)$ for each *i, and then* computing $\langle \phi(x_i), \phi(x_j) \rangle$ for each pair *(i,j),* simply define a kernel function

$$K(x,z) \overset{\text{def}}{=} \langle \phi(x), \phi(z) \rangle$$

  and work with it directly.”

- *K(x,z)* is called an inner product or dot-product kernel
- Since we only use the kernel, why bother to define $\phi(x)$?
- Just define the kernel *K(x,z)* directly!
- Then we never have to deal with the complexity of $\phi(x)$.
- This is usually called “the kernel trick”

Kernel Summary

1. *D* not easy to deal with in $\mathcal{X}$, apply feature transformation $\phi: \mathcal{X} \rightarrow \mathcal{Z}$, such that dim($\mathcal{Z}$) >> dim($\mathcal{X}$)

2. Constructing and computing ϕ(x) directly is too expensive:
   - Write your learning algorithm in inner product form
   - Then, instead of ϕ(x), we only need $\langle \phi(x_i), \phi(x_j) \rangle$ for all *i* and *j*, which we can compute by defining an "inner product kernel"

$$\boxed{K(x,z) = \langle \phi(x), \phi(z) \rangle}$$

   and computing $K(x_i,x_j)$ $\forall i,j$ directly

   - Note: the matrix

$$K = \begin{bmatrix} \vdots \\ \cdots K(x_i, z_j) \cdots \\ \vdots \end{bmatrix}$$

   is called the "Kernel matrix" or Gram matrix

3. Moral: Forget about ϕ(x) and instead use *K(x,z)* from the start!

Question?

- **What *is* a good inner product kernel?**
  - This is a difficult question (see Prof. Lenckriet's work)
- In practice, the usual recipe is:
  - Pick a kernel from a **library of known kernels**
  - some examples
    - the **linear kernel $K(x,z) = x^T z$**
    - the **Gaussian family**

$$K(x,z) = e^{-\frac{\|x-z\|^2}{\sigma}}$$

    - the **polynomial family**

$$K(x,z) = \left(1 + x^T z\right)^k, \quad k \in \{1, 2, \cdots\}$$

Kernelization of the SVM

- Note that all SVM equations depend only on $x_i^T x_j$
- The kernel trick is trivial: replace by $K(x_i, x_j)$
  - 1) Training:

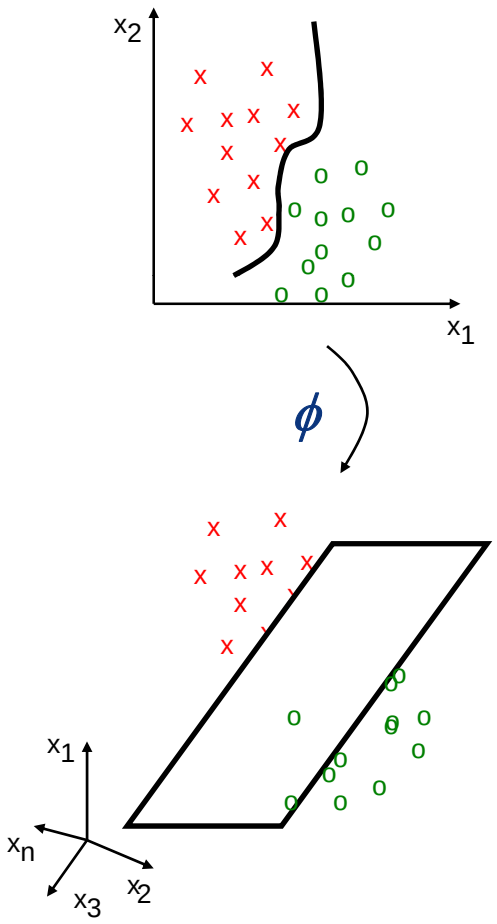
$$\max_{\alpha \geq 0} \left\{ -\frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j k\left(x_i, x_j\right) + \sum_{i} \alpha_i \right\}$$

$$\text{subject to} \quad \sum_{i} y_i \alpha_i = 0, \quad 0 \leq \alpha_i \leq C$$

$$b^* = -\frac{1}{2} \sum_{i \in \text{SV}} y_i \alpha_i^* \left(K\left(x_i, x^+\right) + K\left(x_i, x^-\right) \right)$$

  - 2) Decision function:

$$f(x) = \text{sgn}\left[\sum_{i \in \text{SV}} y_i \alpha_i^* K\left(x_i, x\right) + b^* \right]$$



Kernelization of the SVM

- **Notes:**
  - As usual, nothing we did really requires us to be in R^d.
    - We could have simply used $\langle x_i, x_j \rangle$ to denote for the inner product on a infinite dimensional space and all the equations would still hold
  - The only difference is that we can no longer recover w^* explicitly without determining the feature transformation ϕ, since

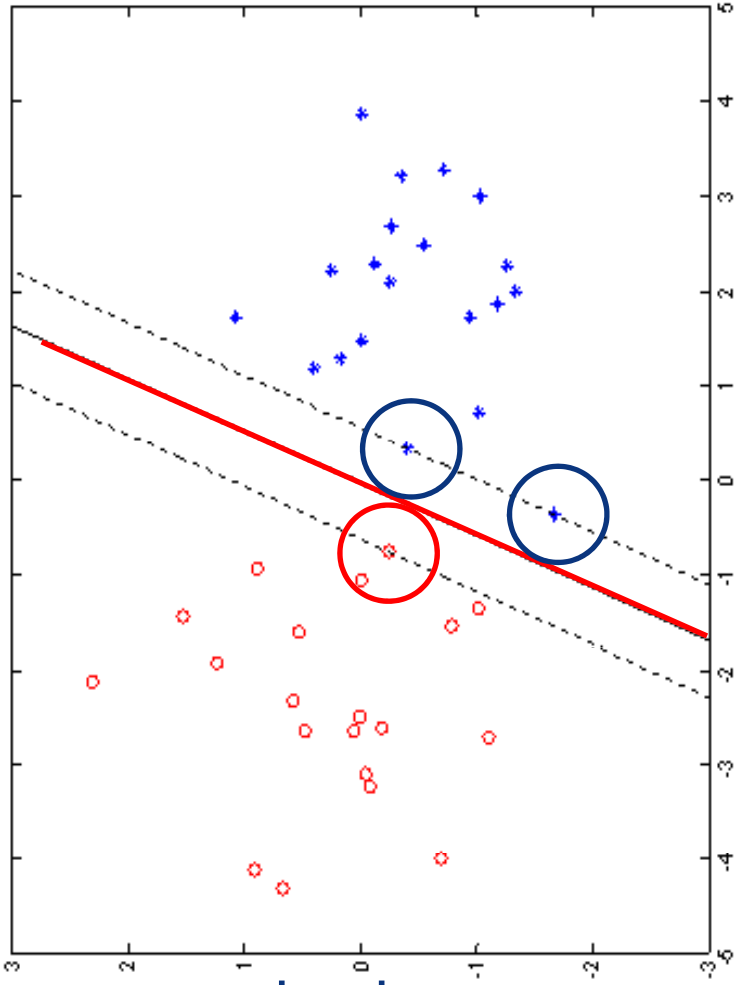
$$w^* = \sum_{i \in SV} \alpha_i^* y_i \phi(x_i)$$

  - This can be an infinite dimensional object. E.g., it is a sum of Gaussians ("lives" in an infinite dimensional function space) when we use the Gaussian kernel
  - Luckily, we don't need w^*, only the SVM decision function

$$f(x) = \text{sgn}\left[\sum_{i \in SV} y_i \alpha_i^* K(x_i, x) + b^* \right]$$

Limitations of the SVM

- The SVM is appealing, but there are some limitations:
  - A major problem is the selection of an appropriate kernel. There is no generic “optimal” procedure to find the kernel or its parameters
    - Usually we pick an arbitrary kernel, e.g. Gaussian
    - Then, determine kernel parameters, e.g. variance, by trial and error
  - *C* controls the importance of outliers (larger *C* = less influence)
    - Not really intuitive how to choose *C*



- SVM is usually tuned and performance-tested using cross-validation. There is a need to cross-validate with respect to both *C* and kernel parameters

Practical Implementation of the SVM

- In practice, we need an algorithm for solving the optimization problem of the training stage
  - This is a complex problem
  - There has been a large amount of research in this area
    - Therefore, writing “your own” algorithm is not going to be competitive
  - Luckily there are various packages available, e.g.:
    - libSVM: http://www.csie.ntu.edu.tw/~cjlin/libsvm/
    - SVM light: http://www.cs.cornell.edu/People/tj/svm_light/
    - SVM fu: http://five-percent-nation.mit.edu/SvmFu/
    - various others (see http://www.support-vector.net/software.html)
  - There are also many papers and books on algorithms (see e.g. B. Schölkopf and A. Smola. Learning with Kernels. MIT Press, 2002)

END