# Support Vector Machines

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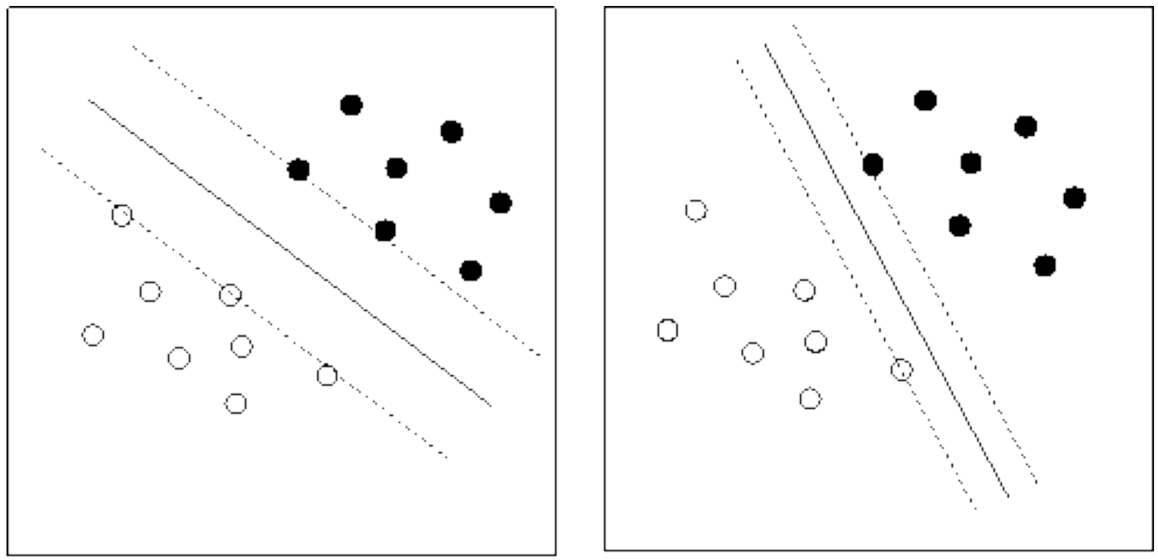
# Philosophy

- First formulate a classification problem as finding a separating hyper-plane that maximizes "the margin".
- Allow for errors in classification using "slack-variables".
- Convert problem to the "dual problem".
- This problem only depends on inner products between feature vectors which can be replaced with kernels.
- A kernel is like using an *infinite* number of features.

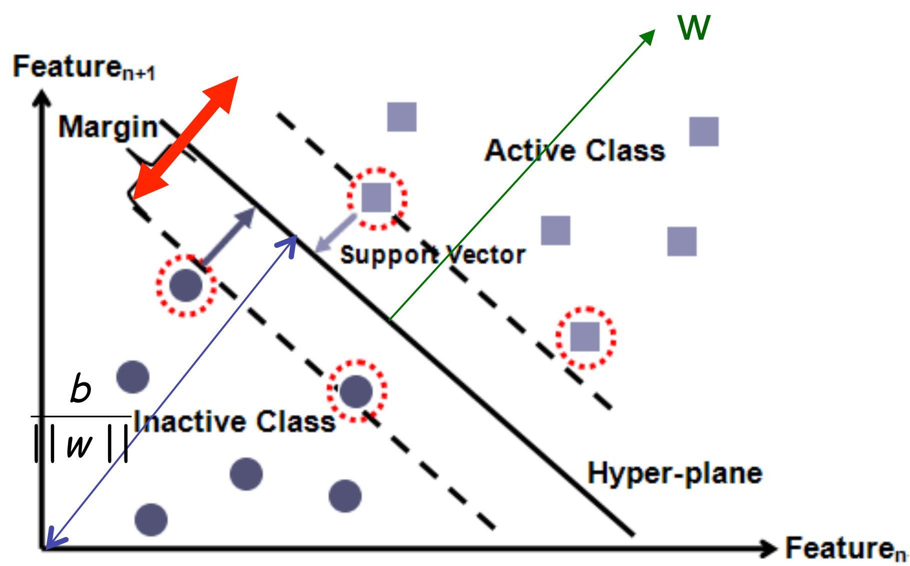
# The Margin



(a) Larger margin (b) Smaller margin

- Large margins are good for generalization performance (on future data).
- Note: this is very similar to logistic regression (but not identical).

# Primal Problem

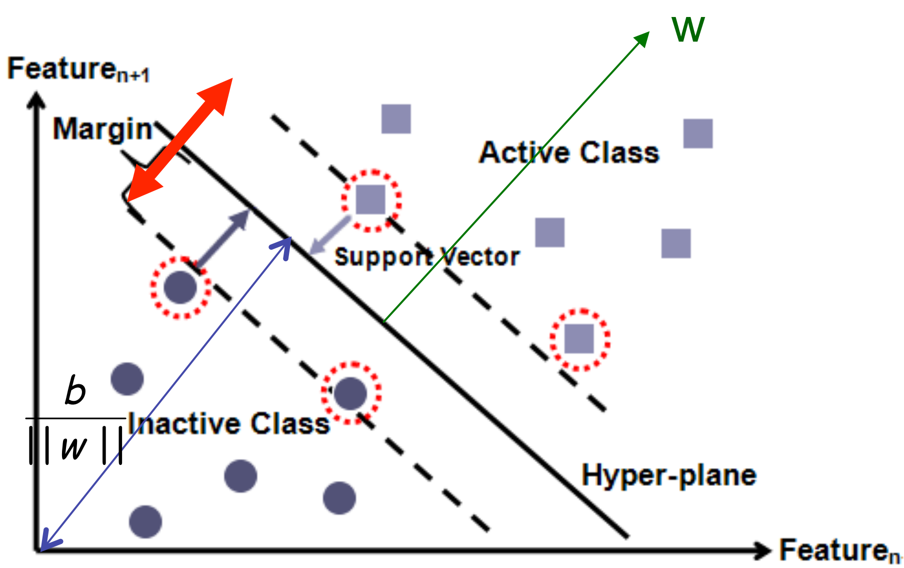



- We would like to find an expression for the margin (a distance).
- Points on the decision line satisfy: $w^T x - b = 0$
- First imagine the line goes through the origin: $w^T x = 0$

  Then shift origin: $w^T (x - a) = 0$

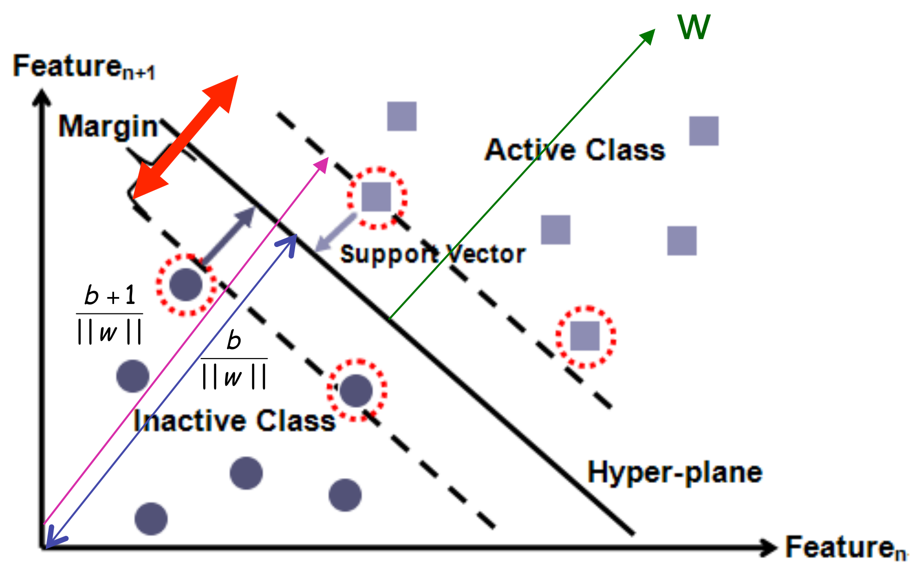
  Choose $a // w \Rightarrow b = w^T a = ||a|| \times ||w|| \Rightarrow ||a|| = \frac{b}{||w||}$

# Primal Problem




- Points on support vector lines (dashed) are given by: $$w^T x = b + \delta$$ $$w^T x = b - \delta$$
- If I change: $w \to \lambda w,\ b \to \lambda b,\ \delta \to \lambda\delta$ the equations are still valid. Thus we can choose $\delta = 1$ without loss of generality.

# Primal Problem



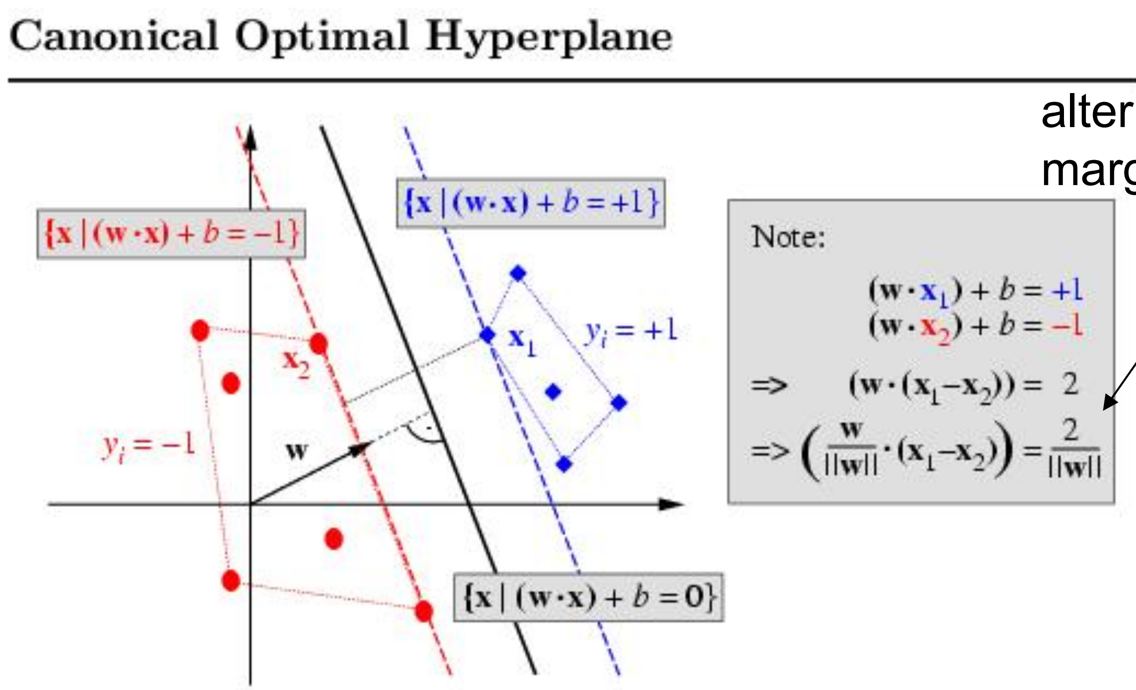

- We can express the margin as: $2\left(\frac{b+1}{||w||} - \frac{b}{||w||}\right) = \frac{2}{||w||}$

2/||w|| is always true. Check this also for b in (-1,0).

- Recall: we want to maximize the margin, such that all data-cases end up on the correct side of the support vector lines.

$$\min_{w,b} ||w||^2 \text{ subject to } \begin{cases} w^T x_n \geq b+1 \text{ if } y_n = +1 \\ w^T x_n \leq b-1 \text{ if } y_n = -1 \end{cases} \quad \forall n$$

# Primal problem (QP)




alternative derivation
margin

$$\min_{w,b} \ \frac{1}{2} || w ||^2$$

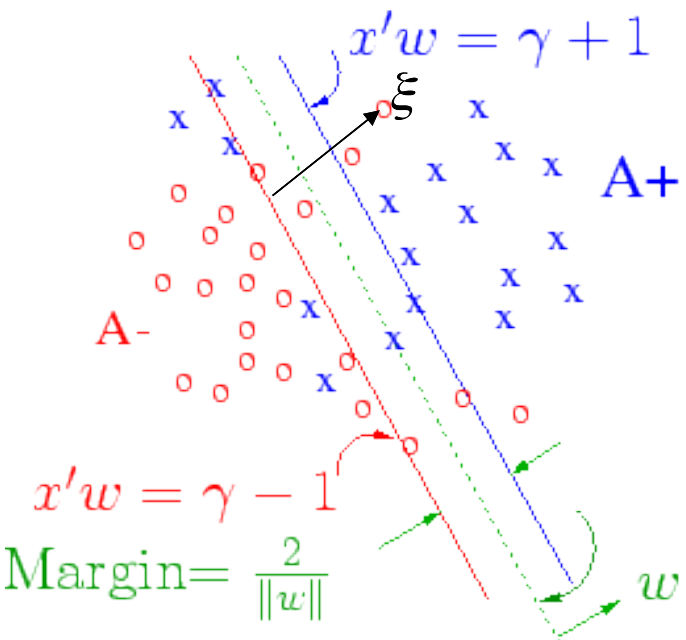
$$s.t. \ \ y_n(w^T x_n - b) - 1 \geq 0 \ \ \forall n$$

alternative primal
problem formulation

# Slack Variables

- It is not very realistic to assume that the data are perfectly separable.

- Solution: add slack variables to allow violations of constraints:




$$\begin{cases} w^T x_n \geq b + 1 - \xi_n & if \;\; y_n = +1 \\ w^T x_n \leq b - 1 + \xi_n & if \;\; y_n = -1 \end{cases} \quad \forall n$$

- However, we should try to minimize the number of violations. We do this by adding a term to the objective:

$$\min_{w,b,\xi} \; \frac{1}{2} || w ||^2 + C \sum_{n=1}^{N} \xi_n$$

$$s.t. \;\; y_n (w^T x_n - b) - 1 + \xi_n \geq 0 \quad \forall n$$

$$s.t. \;\; \xi_n \geq 0 \;\; \forall n$$

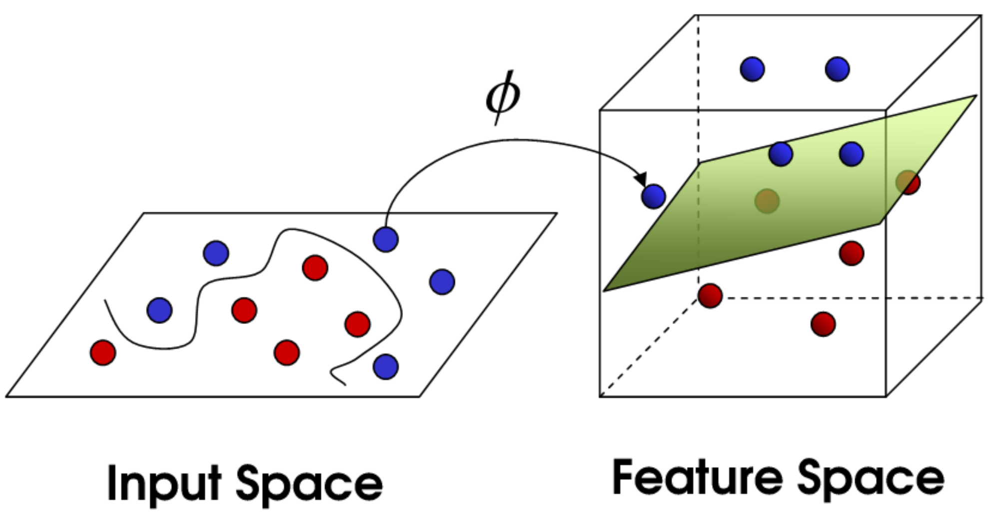
# Features

- Let's say we wanted to define new features: $\phi(x) = [x, y, x^2, y^2, xy, ....]$
  The problem would then transform to:

$$\min_{w,b,\xi} \frac{1}{2} || w ||^2 + C \sum_{n=1}^{N} \xi_n$$

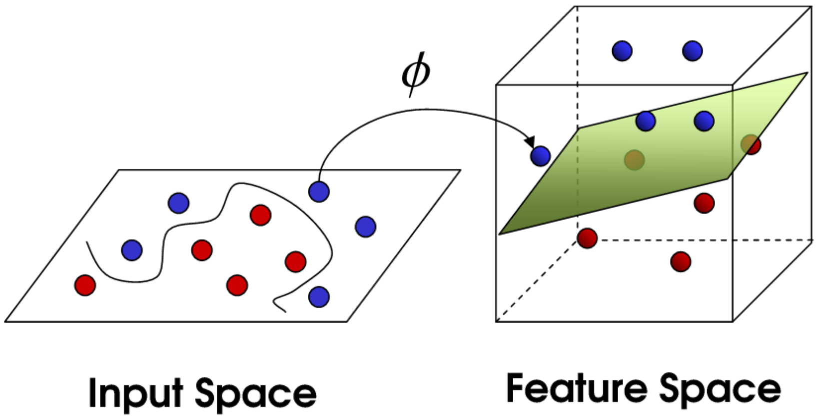
$$s.t.\ \ y_n(w^T \phi(x_n) - b) - 1 + \xi_n \geq 0 \quad \forall n$$

$$s.t.\ \ \xi_n \geq 0 \ \ \forall n$$




- Rationale: data that is linearly non-separable in low dimensions may become linearly separable in high dimensions (provided sensible features are chosen).

# Dual Problem




• Let's say we wanted very many features (F>>N), or perhaps *infinitely many features.*

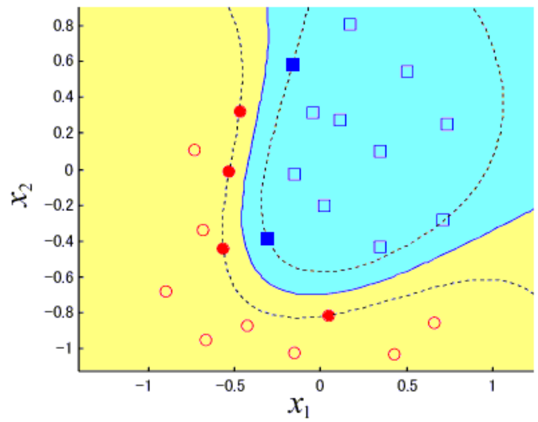
• In this case we have very many parameters w to fit.

• By converting to the *dual problem,* we have to deal with exactly N parameters.

• This is a change of basis, where we recognize that we only need dimensions inside the space spanned by the data-cases.

• The transformation to the dual is rooted in the theory of *constrained convex optimization*.
For a convex problem (no local minima) the dual problem is equivalent to the primal problem (i.e. we can switch between them).

# Dual Problem (QP)




$$\max_{\alpha} \sum_n \alpha_n - \frac{1}{2}\sum_{n,m} \alpha_n \alpha_m y_n y_m \phi_n^T \phi_m$$

$$s.t. \sum_n \alpha_n y_n = 0, \quad \alpha_n \in [0,C] \; \forall n$$

$\alpha_n \geq 0$
if no slack
variables

- The $\alpha_n$ should be interpreted as forces acting on the data-items.
  Think of a ball running down a hill (optimizing w over ||w||^2).
  When it hits a wall, the wall start pushing back, i.e. the force is active.

If data-item is on the correct side of the margin: no force active: $\alpha_n = 0$

If data-item is on the support-vector line (i.e. it is a support vector!)
The force becomes active: $\alpha_n \in [0,C]$

If data-item is on the wrong side of the support vector line, the force is fully engaged: $\alpha_n = C$

# Complementary Slackness

- The complementary slackness conditions come from the KKT conditions in convex optimization theory.

$$\alpha_n(y_n(w^T\phi_n - b) - 1 + \xi_n) = 0$$

- From these conditions you can derive the conditions on alpha (previous slide)

- The fact that many alpha's are 0 is important for reasons of efficiency.

# Kernel Trick

- Note that the dual problem only depends on $\phi_n^T \phi_m$

- We can now move to infinite number of features by replacing:

$$\phi(x_n)^T \phi(x_m) \rightarrow K(x_n, x_m)$$

- As long as the kernel satisfies 2 important conditions you can forget about the features

$$v^T K v \geq 0 \quad \forall v \quad (\textit{positive semi definite, positive eigenvalues})$$
$$K = K^T \qquad (\textit{symmetric})$$

- Examples: $K_{pol}(x, y) = (r + x^T y)^d$

$$K_{rbf}(x, y) = c \exp(-\beta \, || x - y ||^2)$$

# Prediction

- If we work in high dimensional feature spaces or with kernels, b has almost no impact on the final solution. In the following we set b=0 for convenience.

- One can derive a relation between the primal and dual variables (like the primal dual transformation, it requires Lagrange multipliers which we will avoid here. But see notes for background reading).

- Using this we can derive the prediction equation:

$$y_{test} = sign\left[w^T x_{test}\right] = sign\left[\sum_{n \in SV} \alpha_n y_n K(x_{test}, x_n)\right]$$

- Note that it depends on the features only through their inner product (or kernel).

- Note: prediction only involves support vectors (i.e. those vectors close to or on wrong side of the boundary). This is also efficient.

# Conclusions

- kernel-SVMs are non-parametric classifiers:
  It keeps all the data around in the kernel-matrix.

- Still we often have parameters to tune (C, kernel parameters).
  This is done using X-validation or by minimizing a bound on the generalization error.

- SVMs are state-of-the-art (given a good kernel).

- SVMs are also slow (at least O(N^2)). However approximations are available to elevate that problem (i.e. O(N)).