CS 474/574 Machine Learning
4. Support Vector Machines (SVMs)

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Agenda

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- Soft-margin SVMs

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- Think about the error-based loss function for a classifier: $\sum_i (\hat{y} - y)^2$ where y is the ground truth label and $\hat{y}$ is the prediction.
- If $y = +1$ and $\hat{y} = +1.5$, should the error be 0.25 or 0 (because properly classified)?

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- Batch perceptron algorithm: In each batch, computer $\nabla J(\mathbf{w})$ for all samples misclassified using the same current $\mathbf{w}$ and then update.

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  1. Initially, $\mathbf{w}$ has arbitrary values. $k = 1$.
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- Note that $\mathbf{x}_k$ is not necessarily the k-th training sample due to the loop.

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   Need to update $\mathbf{W}$: $\mathbf{W}_2 = \mathbf{W}_1 + \rho \cdot \mathbf{x}_1 y_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

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2. $\mathbf{W}_2^T \cdot \mathbf{x}_2 y_2 = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = 1 > 0$. No updated need. But since $\mathbf{w}$ so far does not classify all samples correctly, we need to keep going. Just let $\mathbf{w}_3 = \mathbf{w}_2$.

An example of preceptron algorithm (cond.)

Continue in perceptron.ipynb

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- What is $\mathbf{w}$ exactly? A linear composition of all training samples!
- Do all samples contribute to $\mathbf{w}$? Not really!

Now let's begin the SVM journey.

Getting ready for SVMs

- Earlier our discussion used the augmented definition of linear binary classifier: the feature vector $\mathbf{x} = (x_1, \ldots, x_n, 1)^T$ and the weight vector $\mathbf{w} = (w_1, \ldots, w_n, w_b)^T$. The hyperplane is an equation $\mathbf{w}^T\mathbf{x} = 0$. If $\mathbf{w}^T\mathbf{x} > 0$, then the sample belongs to one class. If $\mathbf{w}^T\mathbf{x} < 0$, the other class.

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- Let's go back to the un-augmented version. Let $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$ and $\mathbf{w} = [w_1, w_2, \ldots, w_n]^T$. If $\mathbf{w}^T\mathbf{x} + w_b > 0$ then $\mathbf{x} \in C_1$. If $\mathbf{w}^T\mathbf{x} + w_b < 0$ then $\mathbf{x} \in C_2$. The equation $\mathbf{w}^T\mathbf{x} + w_b = 0$ is the hyperplane, where $\mathbf{w}$ only determines the direction of the hyperplane. To build a classifier is to search for the values for $w_1, \ldots, w_n$ and w_b, the bias/threshold.

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- For convenience, we denote $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$.
- We have proved that $\mathbf{w}$, augmented or not, is perpendicular to the hyperlane.

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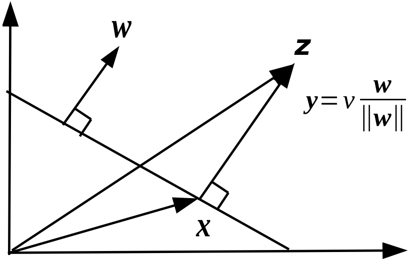

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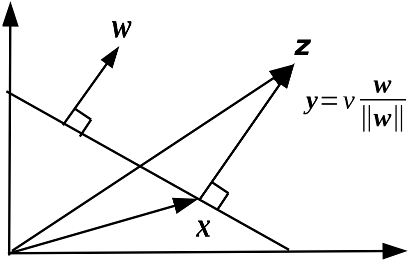

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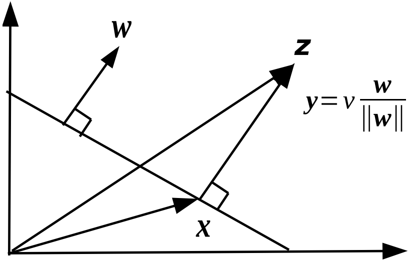

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3. Therefore, $\mathbf{z} = \mathbf{x} + v\frac{\mathbf{w}}{||\mathbf{w}||}$.

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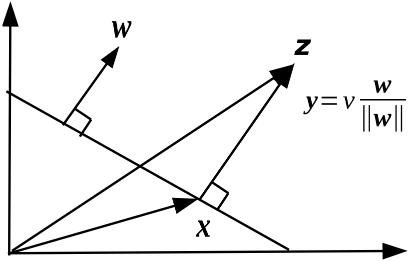

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3. Therefore, $\mathbf{z} = \mathbf{x} + v\frac{\mathbf{w}}{||\mathbf{w}||}$.
4. The prediction for $\mathbf{z}$ is then (subsituting into linear classifier equation):

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\begin{aligned}
& \mathbf{w}^T\mathbf{z} + w_b \\
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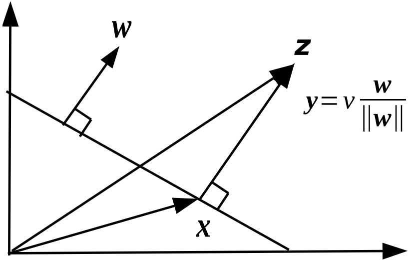
What is the distance from a sample $\mathbf{z}$ to the hyperplane?



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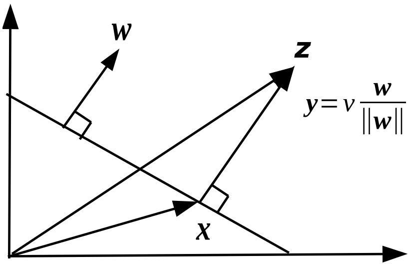

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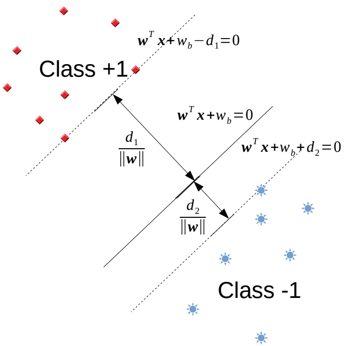
5. Finally, $v = \overbrace{\mathbf{w}^T\mathbf{z} + w_b}^{prediction}/||\mathbf{w}||$.
6. **Conclusion**: a sample $\mathbf{z}$'s distance to a hyperplane $\mathbf{w}^T\mathbf{x} + w_b = 0$ is $d/||\mathbf{w}||$ **if and only if** the prediction for it $\mathbf{w}^T\mathbf{z} + w_b$ is $\pm d$. (The sign ahead of d depends on which side the sample is on.)

Hard margin linear SVM (for two linearly separable classes)



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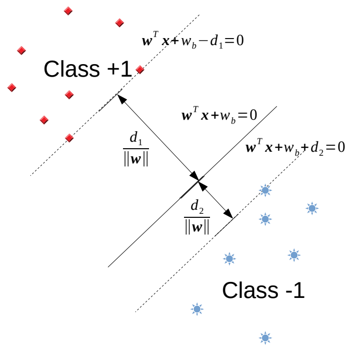

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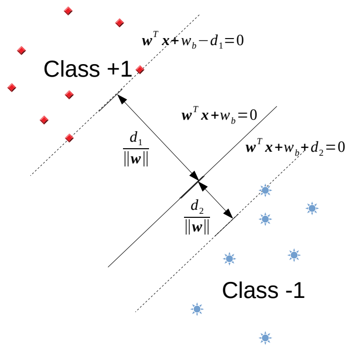

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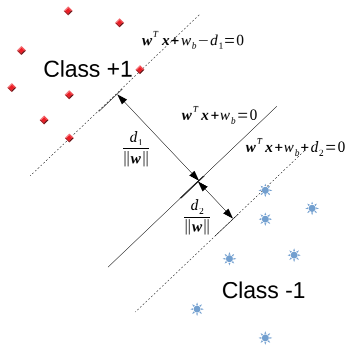

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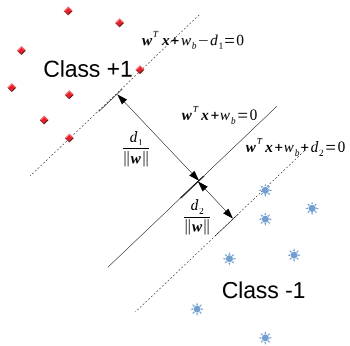

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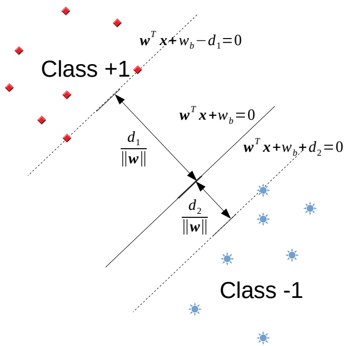

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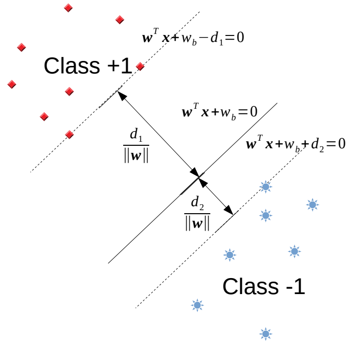

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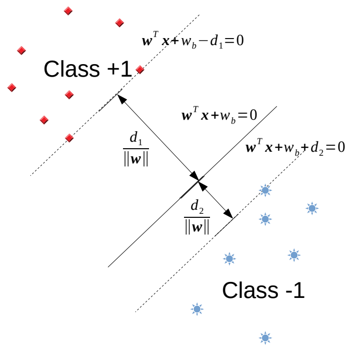

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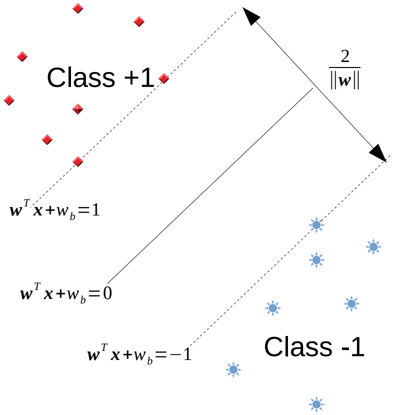
- We want to maximize margin width:

$$\begin{cases} \max & \frac{d_1}{||\mathbf{w}||} + \frac{d_2}{||\mathbf{w}||} \\ s.t. & \mathbf{w}^T\mathbf{x} + w_b - d_1 \geq 0, \forall \mathbf{x} \in C_{+1} \\ & \mathbf{w}^T\mathbf{x} + w_b + d_2 \leq 0, \forall \mathbf{x} \in C_{-1} \end{cases}$$

Hard margin linear SVM (cond.)



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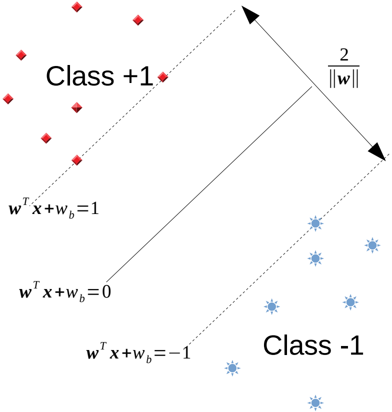

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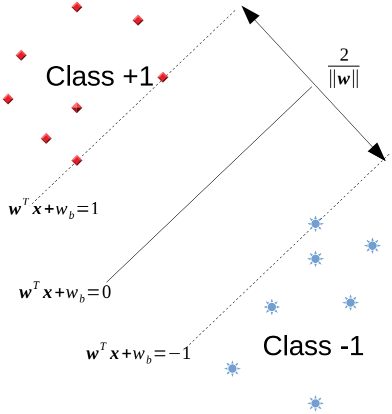

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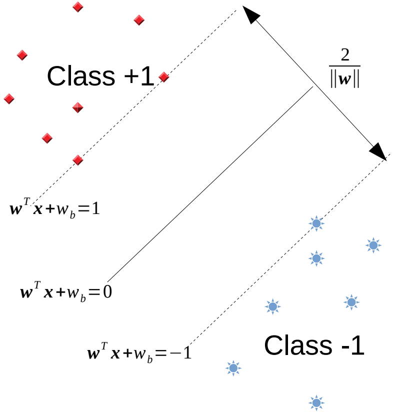

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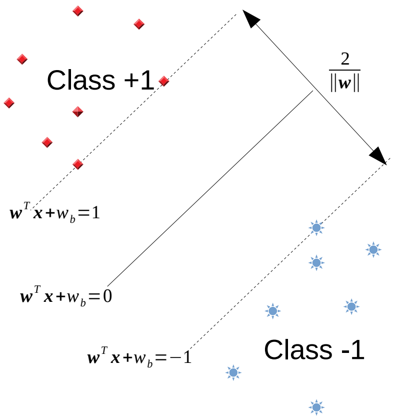

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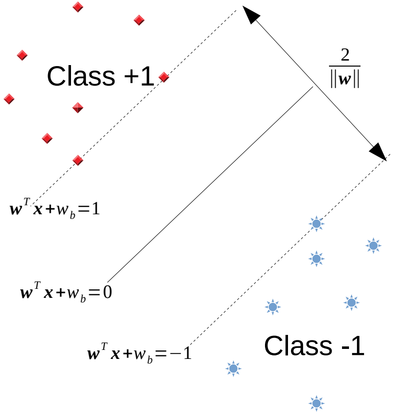

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- Why square $||\mathbf{w}||$?

Recap: the Karush-Kuhn-Tucker (KKT) conditions

- Given a nonlinear optimization problem

$$\begin{cases} \min & f(\mathbf{x}) \\ s.t. & h_k(\mathbf{x}) \geq 0, \forall k \in [1..K], \end{cases}$$

where $\mathbf{x}$ is a vector, and $h_k(\cdot)$ is linear, its Lagrangian function is:

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \sum_{k=1}^{K} \lambda_k h_k(\mathbf{x})$$

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- The necessary conditions that the problem above has a solution are KKT conditions:

$$\begin{cases} \frac{\partial L}{\partial \mathbf{x}} = \mathbf{0}, & \\ \lambda_k \geq 0, & \forall k \in [1..K] \\ \lambda_k h_k(\mathbf{x}) = 0, & \forall k \in [1..K] \end{cases}$$

The last condition is sometimes written in the equivalent form $\sum_k \lambda_k h_k(\mathbf{x}) = 0$.

The Lagrangian function of a hard-margin linear SVM

- Given a nonlinear optimization problem $\begin{cases} \min & f(\mathbf{x}) \\ s.t. & h_k(\mathbf{x}) \geq 0, \forall k \in [1..K], \end{cases}$ where $\mathbf{x}$ is a vector, and $h_k(\cdot)$ is linear, its Lagrangian function is:

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- Thus, given the primal form of SVMs: $\begin{cases} \min & \frac{1}{2}||\mathbf{w}||^2 = \frac{1}{2}\mathbf{w}^T\mathbf{w} \\ s.t. & y_k(\mathbf{w}^T\mathbf{x}_k + w_b) \geq 1, \forall \mathbf{x}_k. \end{cases}$ its Lagrangian function is:

$$L(\mathbf{w}, \lambda) = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{k=1}^{K} y_k(\mathbf{w}^T\mathbf{x}_k + w_b) - 1$$

where K is the total number of samples.

The KKT conditions and properties of hard margin linear SVM

For an SVM problem, the KKT conditions thus are:

$$\begin{cases} A : \frac{\partial L}{\partial w} = \mathbf{0}, & \\ B : \frac{\partial L}{\partial w_b} = 0, & \\ C : \lambda_k \geq 0, & \forall k \in [1..K] \\ D : \lambda_k [y_k(\mathbf{w}^T \mathbf{x_k} + w_b) - 1] = 0, & \forall k \in [1..K] \end{cases}$$

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From Eqs. A and B,

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{k=1}^{K} \lambda_k y_k \mathbf{x_k} \Rightarrow \mathbf{w} = \sum_{k=1}^{K} \lambda_k y_k \mathbf{x_k}$$

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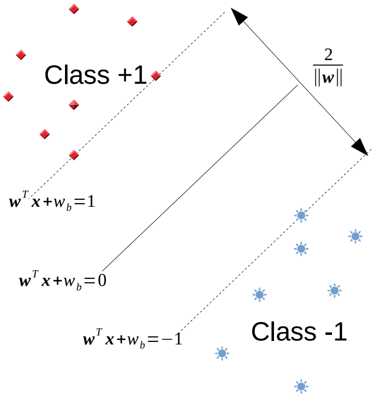
Because λ_k is either positive or 0, the solution of the SVM problem is only associated with samples whose $\lambda_k \neq 0$. Denote them as $N_s = \{\mathbf{x}_k | \lambda_k \neq 0, k \in [1..K]\}$.

Properties of hard margin linear SVM (cont.)

- Therefore, Eq. A can be rewritten into

$$\mathbf{w} = \sum_{\mathbf{x}_k \in N_s} \lambda_k y_k \mathbf{x_k}$$



Properties of hard margin linear SVM (cont.)

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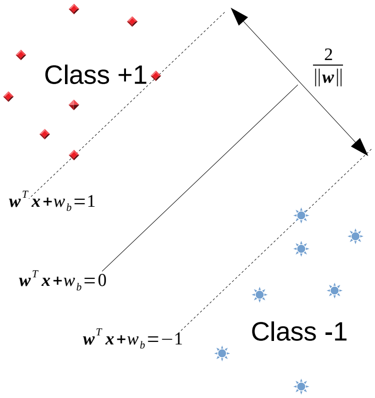
- The samples $\mathbf{x}_k \in N_s$ collectively determine the $\mathbf{w}$, and thus called **support vectors**, supporting the solution.



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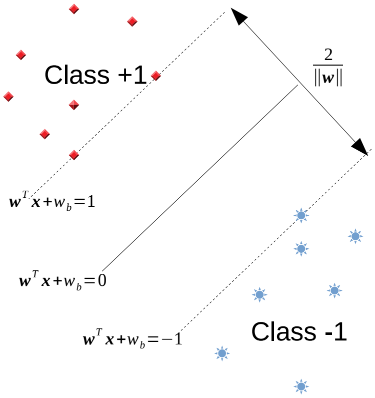

Properties of hard margin linear SVM (cont.)

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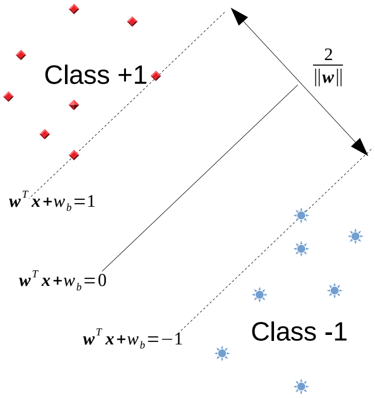

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Kernel tricks: achieving non-linearity on SVMs

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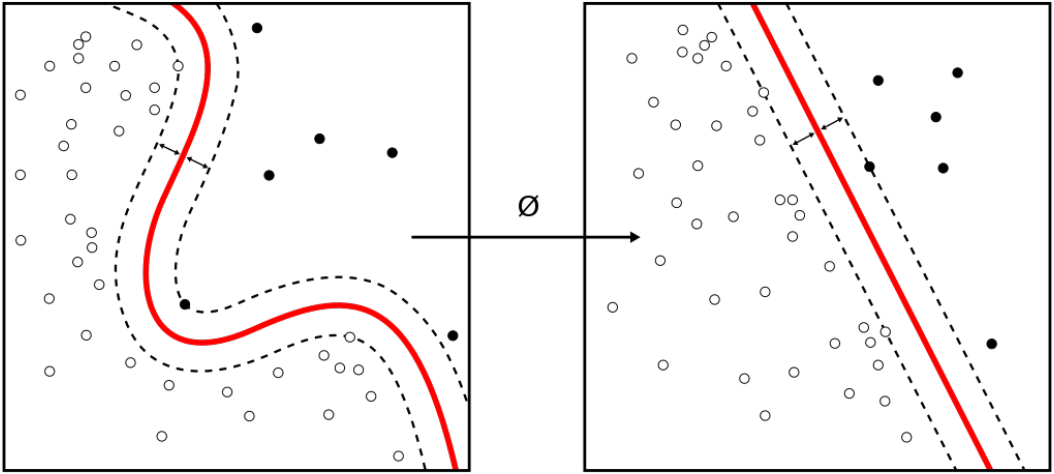
- Usually linear and Gaussian are good enough. A Gaussian kernel can be decomposed into many polynomial terms.

Transforming a nonlinearly separable problem to a linearly separable one



Source: Wikipedia/SVM.

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- Essentially, we are building a new hyperplane $g(\mathbf{x}) = 0$ such that $g(\mathbf{x}) = w_b + \sum_{p=1}^{P} w_p f_p(\mathbf{x})$. Instead of computing the weighted sum of elements of feature vector, we compute that of elements of the transformed vector.

Creating features from input features

- For example, $g(\mathbf{x}) = w_b + w_1 x_1 + w_2 x_2 + w_{12} x_1 x_2 + w_{11} x_1^2 + w_{22} x_2^2$

$$\Phi : R^2 \to R^3$$
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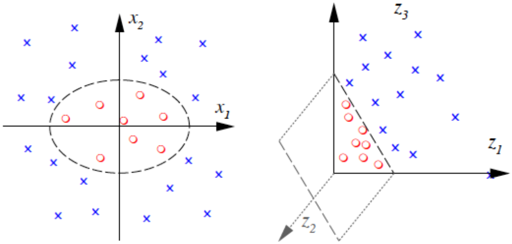

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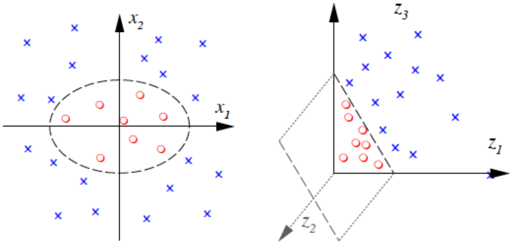

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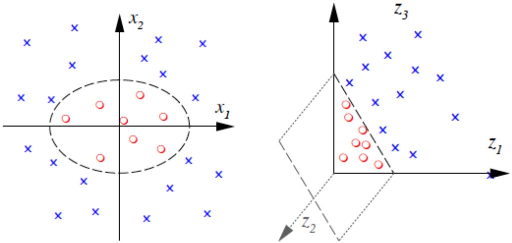
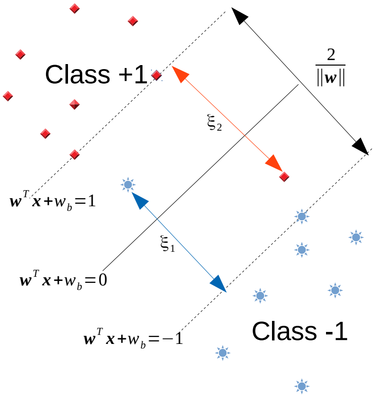


- A good explanation on StackOverflow: https://stats.stackexchange.com/questions/46425/what-is-feature-space

Soft margin linear SVM



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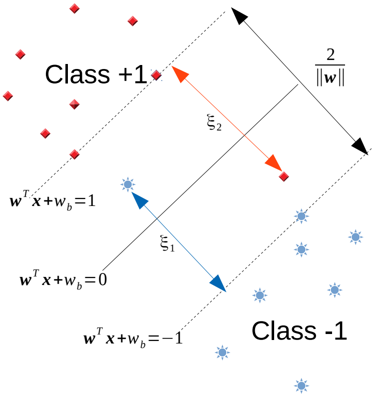

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- Therefore, we have a new optimization problem:

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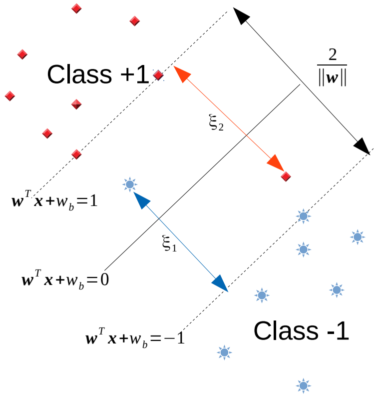

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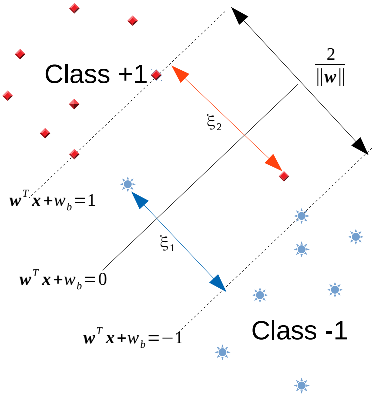

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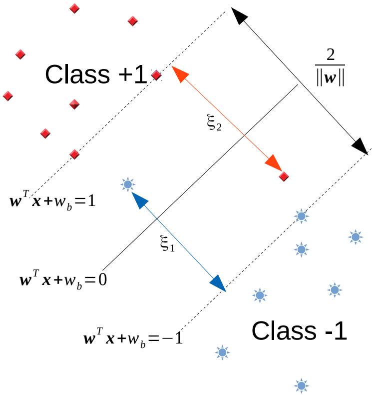

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- Such SVM is called *soft-margin*.
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- Next: How to find C and why is slack variable defined so.

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- But, is just one test set good?

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- leave-N-out CV (LNOCV): A special case of k-fold CV that only N samples are the test set. When $N = 1$, it becomes leave-one-out CV (LOOCV).

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- In that case, the constraint is the same as that for hard margin linear SVMs: $y_k(\mathbf{w}^T\mathbf{x} + w_b) \geq 0$.
- The expression $\max(0, 1 - y \cdot \hat{y})$ where $y \in \{+1, -1\}$ is the ground truth label and $\hat{y}$ is prediction for a classifier, is called a **hinge loss**. It's "hinge" because as long as the classification is correct, the loss/error is (capped at) 0.

Extended reading

- A Gentle Introduction to Support Vector Machines in Biomedicine, Statnikov et al., AIMA 2019