HPE DSI 311
Introduction to Machine Learning

Spring 2023

Instructor: Ioannis Konstantinidis

Overview

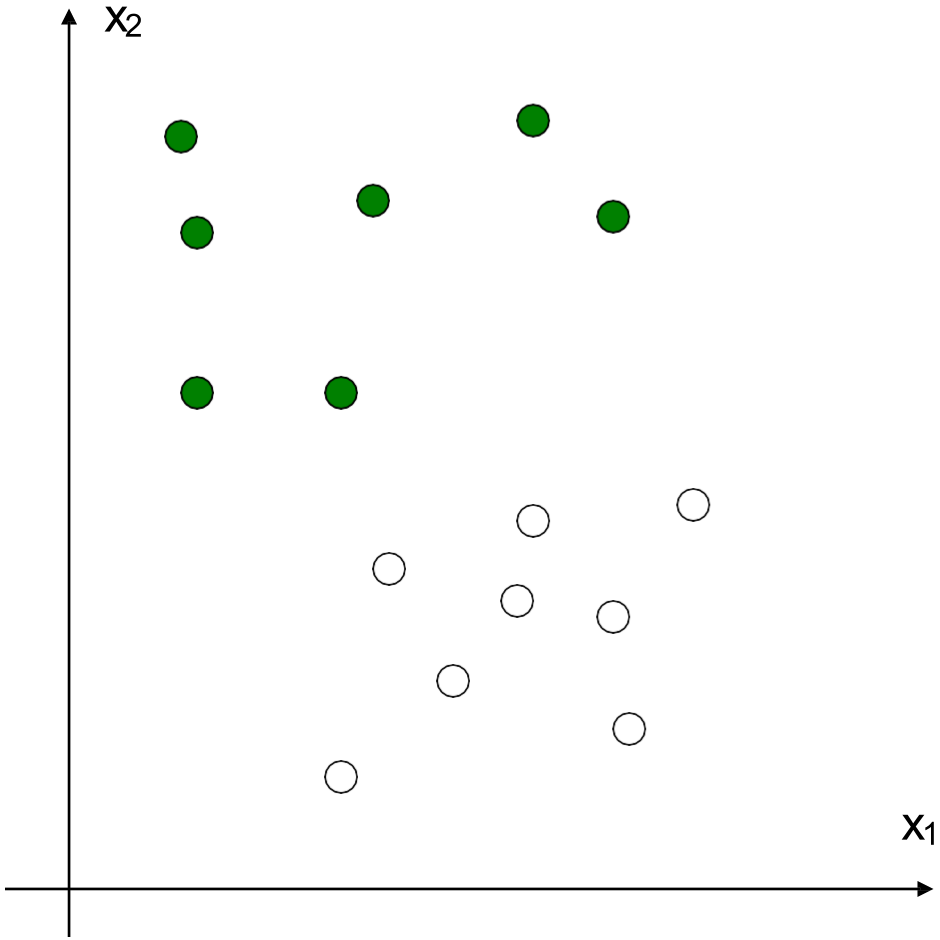
Support Vector Machines

Generalizations

- Kernels
- Regularization

New method: Support Vector Machines

- How would you classify these points to minimize error?



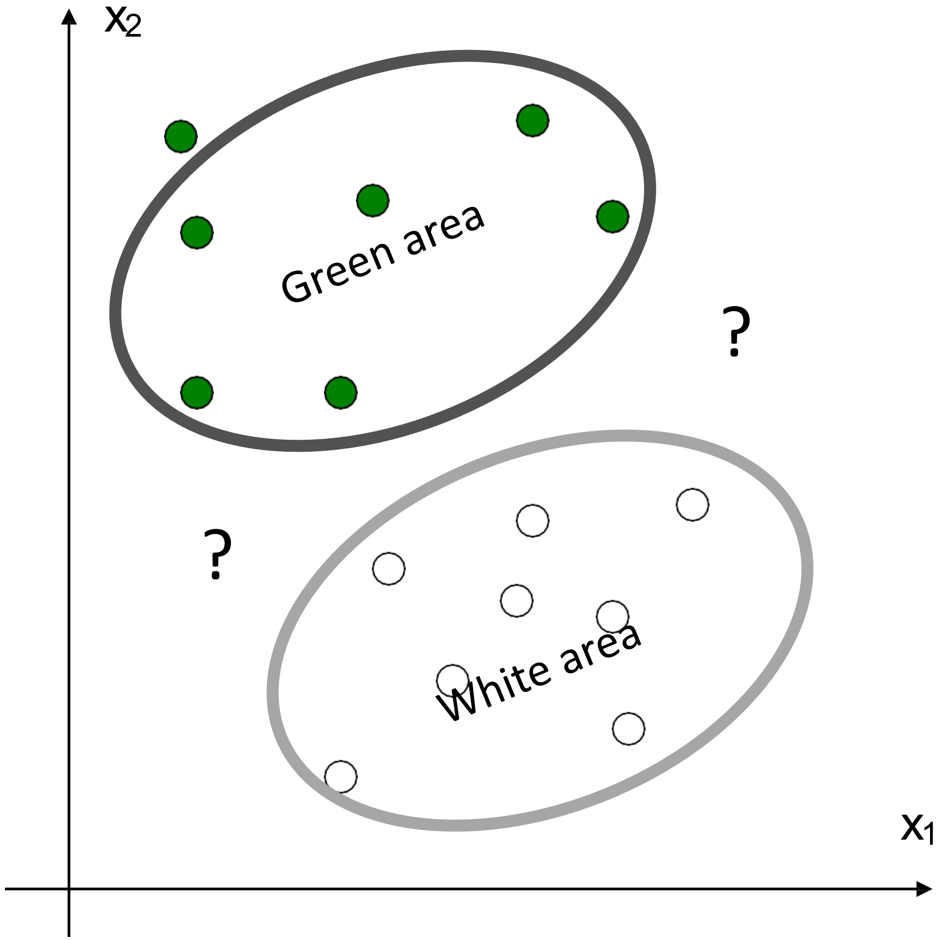
K-NN

- How would you classify these points to minimize error?

- Match to the color of the nearest neighbors

$$g(\mathbf{x}) = \sum_{i \in \mathrm{kNN}(\mathbf{x})} weight(\mathbf{x}_i, \mathbf{x})\, y_i$$

- Computation based on only k training points, but they differ based on where the test point is located
- Distant points (outliers?) don't affect decision



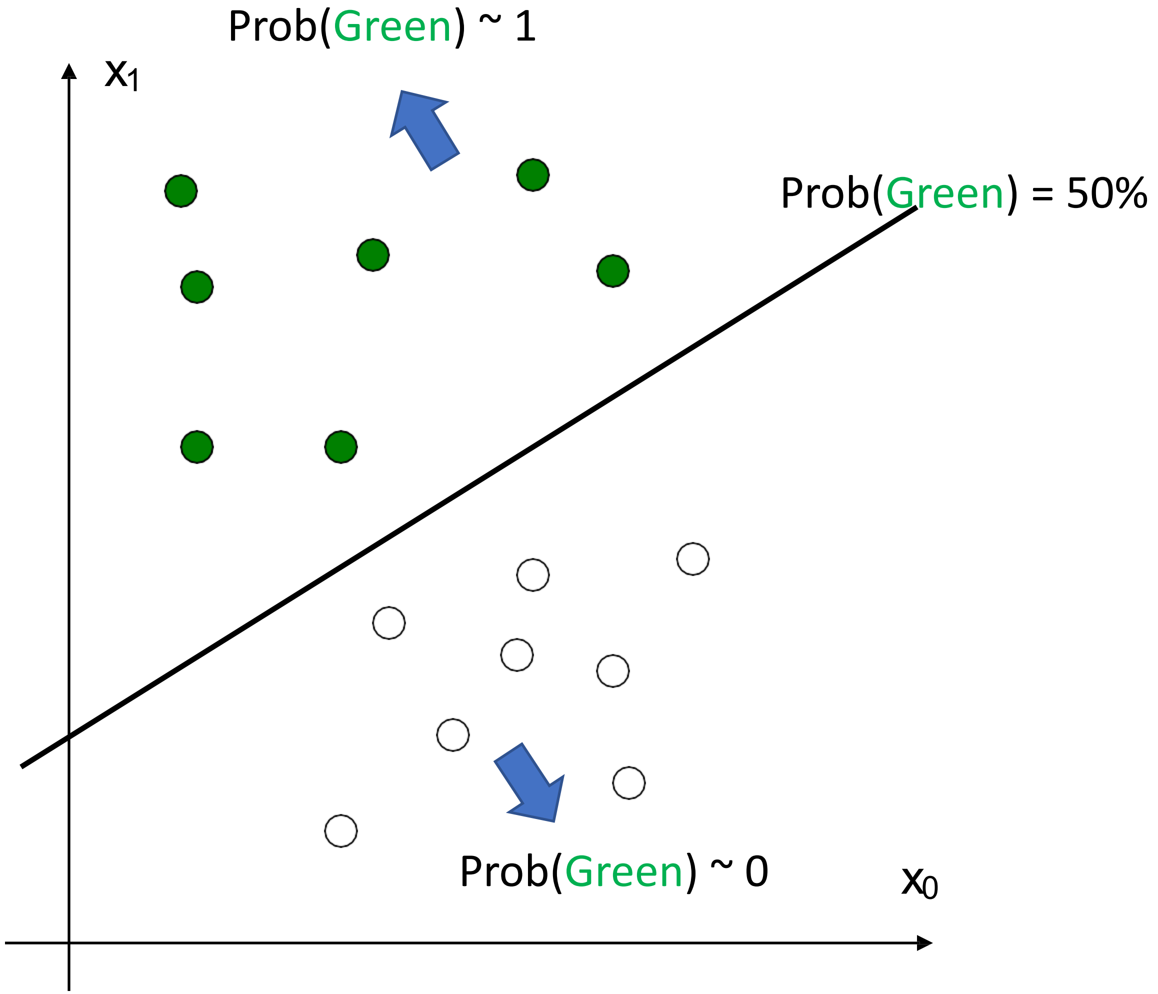
Logistic regression

- How would you classify these points to minimize error?

- Compute probability of match

- Computation based on ALL training points

$$Prob(Green) \sim w_0 x_0 + w_1 x_1 + b = \mathbf{w}^T \mathbf{x} + b$$



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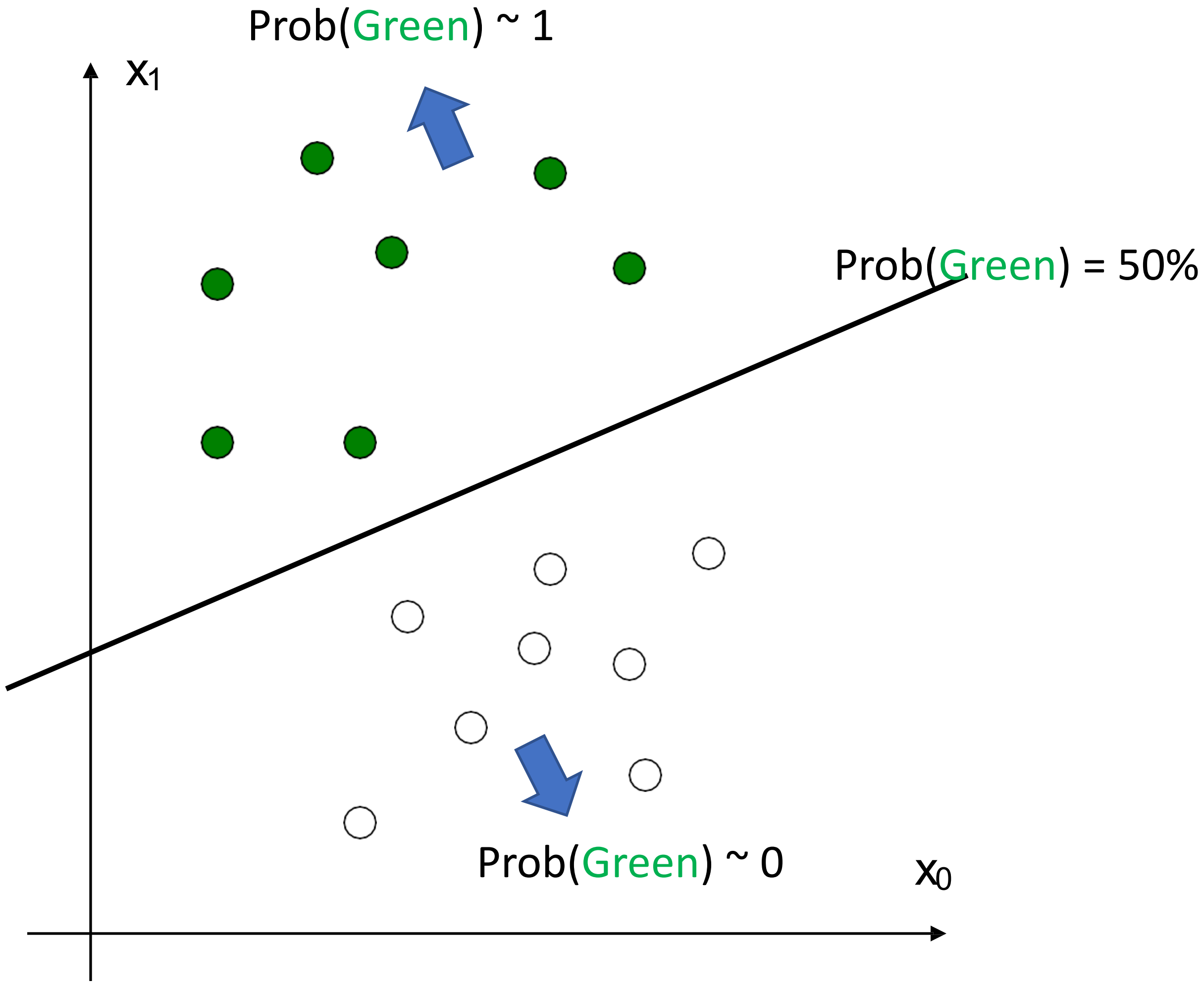
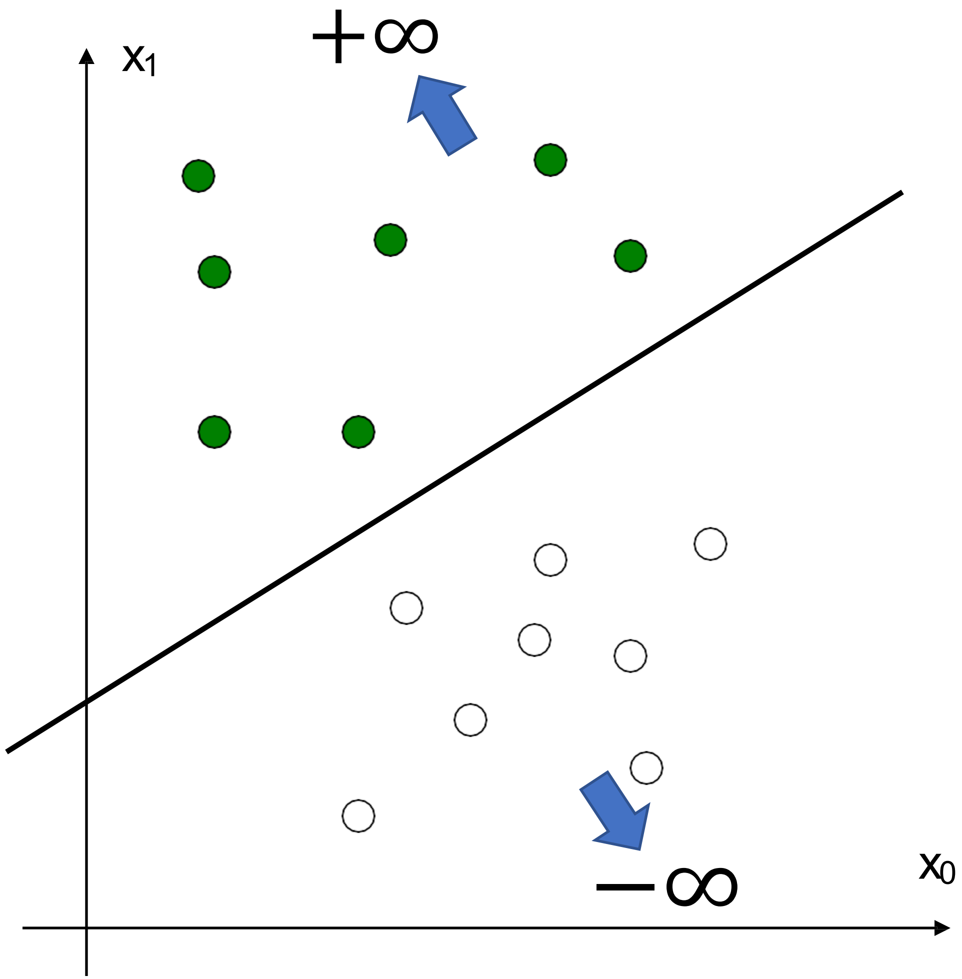


Linear Classifiers

- New method:



- Use a linear function as boundary (signed distance)
- Binary cut-off, not a probability

Linear Classifiers

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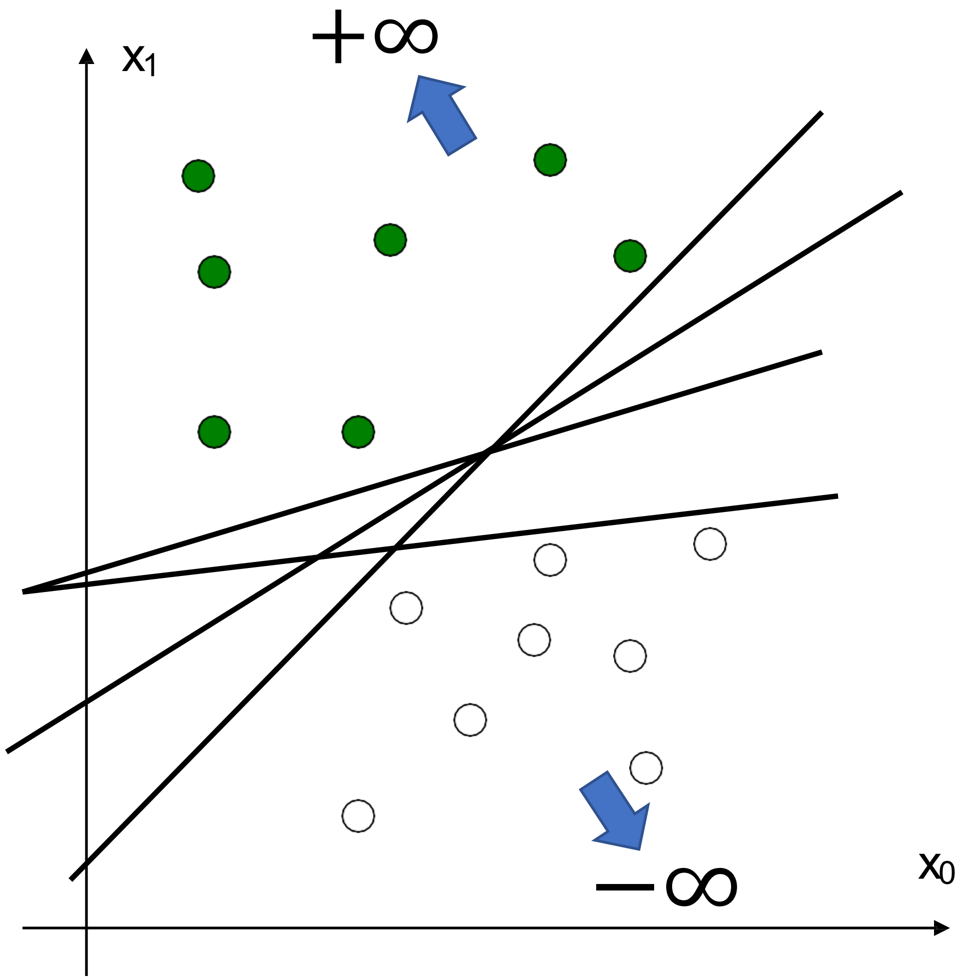
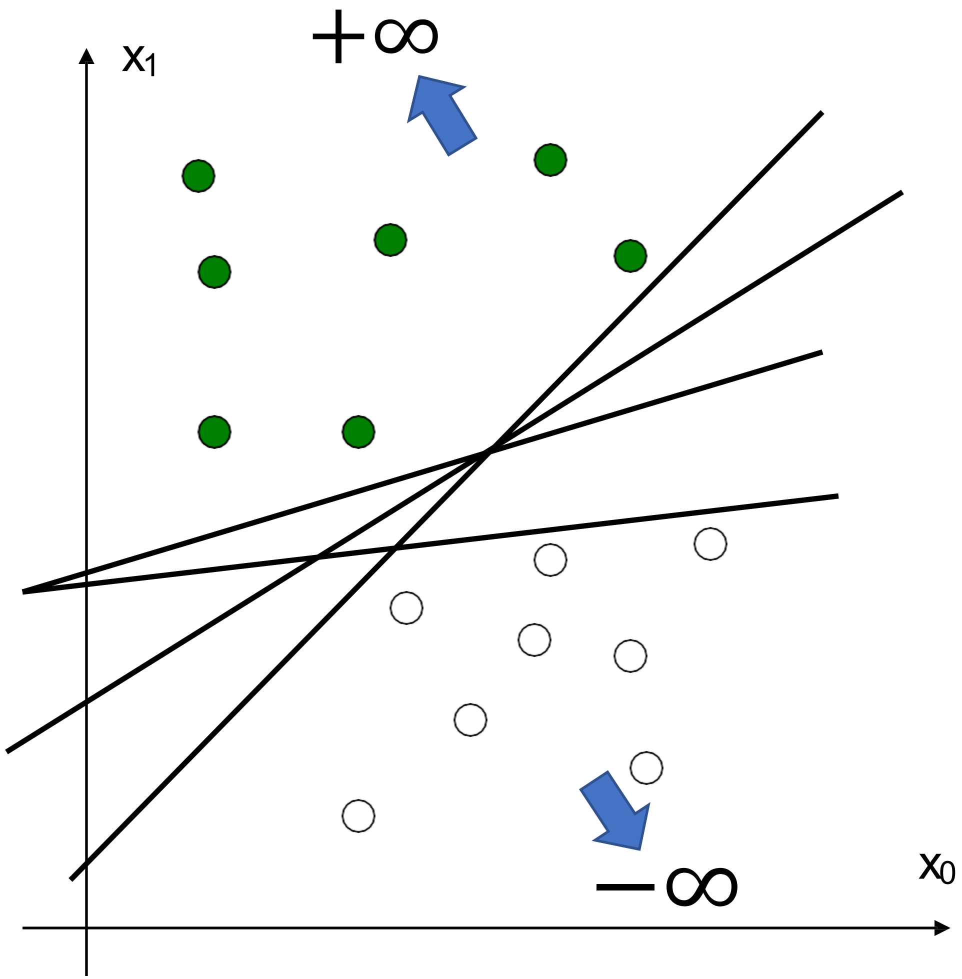


- Use a linear function as boundary (signed distance)
- MANY choices! (infinitely many)

Linear Classifiers

- New method:

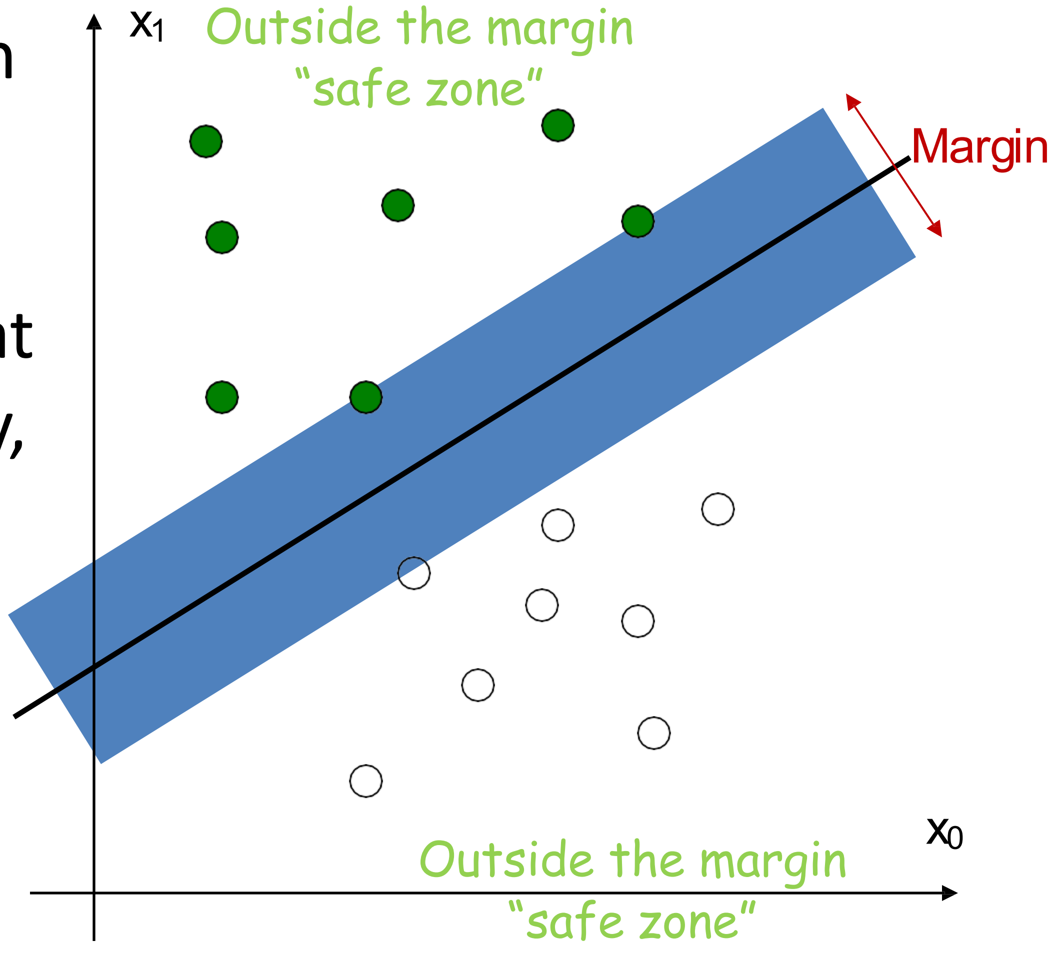


- Use a linear function as boundary (signed distance)
- MANY choices! (infinitely many)
- How to pick one?

The Largest Margin Linear Classifier

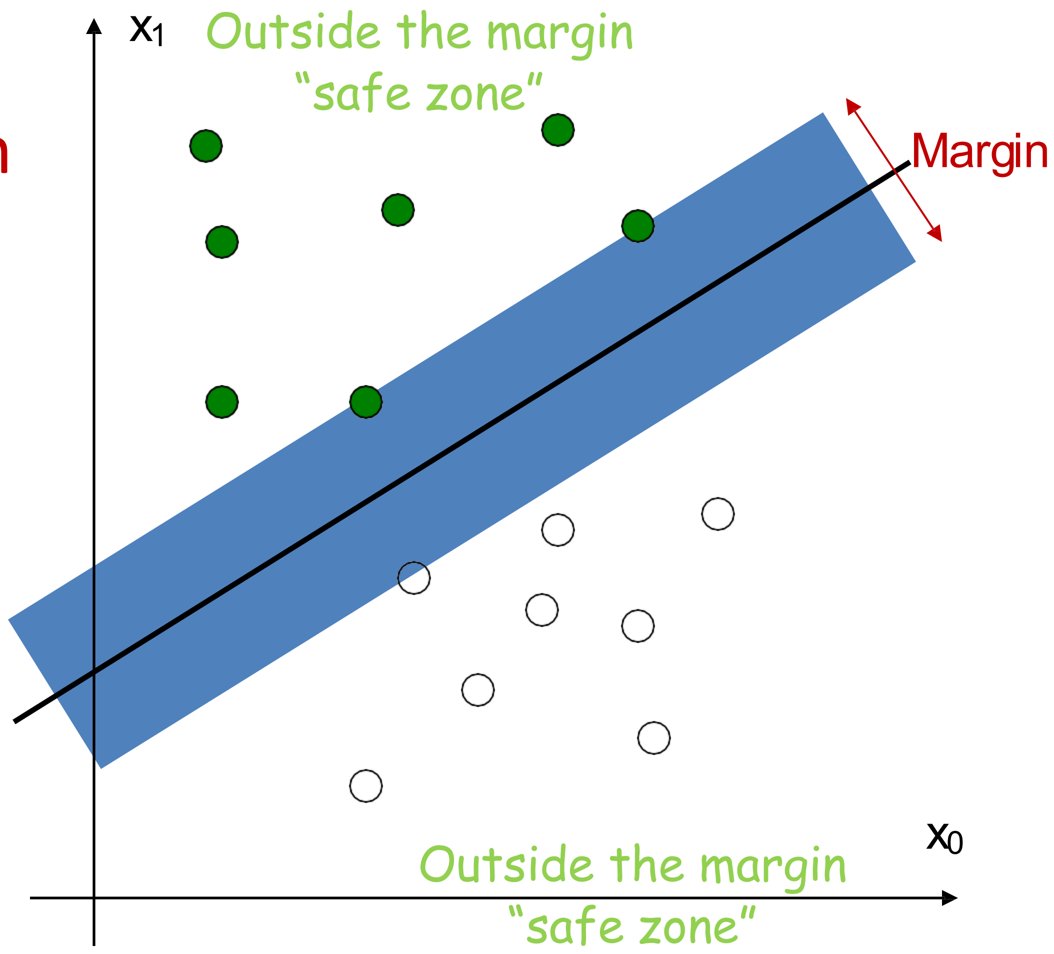
Pick the linear discriminant function with the maximum margin

- Margin is defined as the width that the boundary could be increased by, before hitting a data point



The Largest Margin Linear Classifier

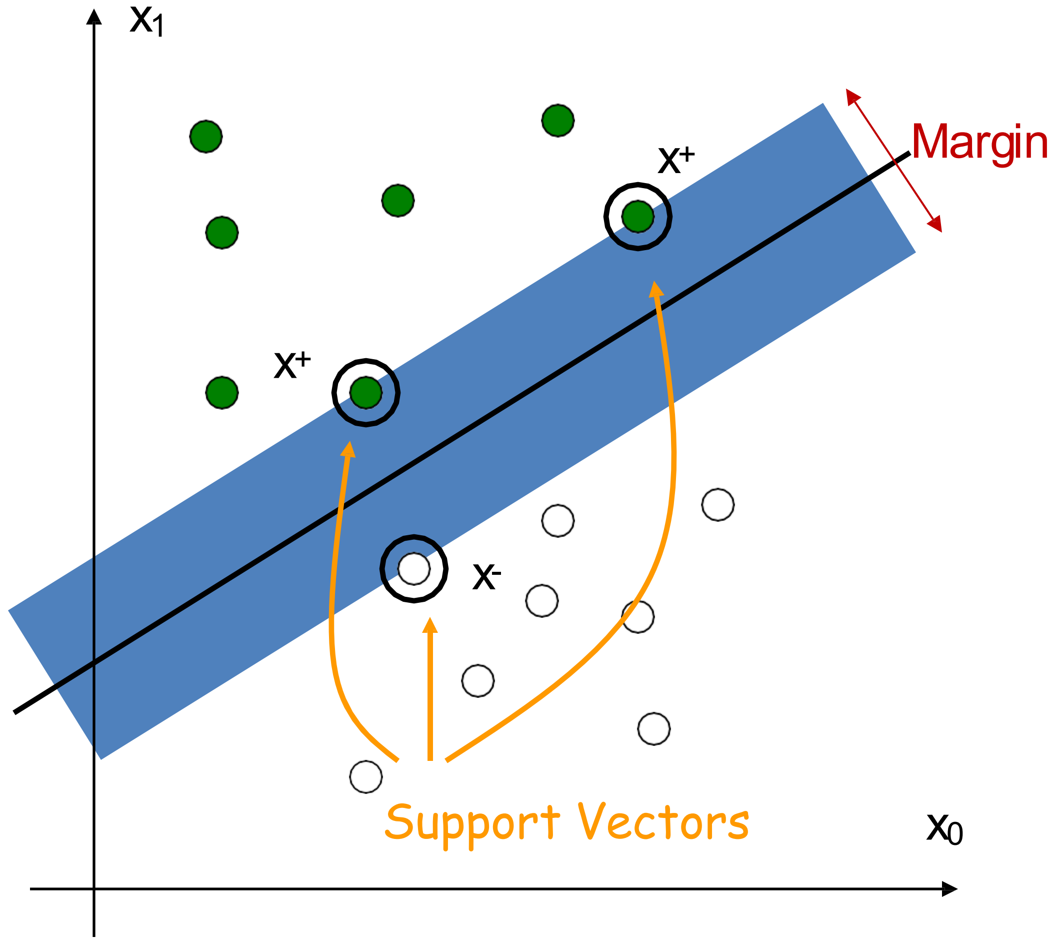
- Pick the linear discriminant function with the maximum margin



- Computation based only on a few "difficult" points that are near the boundary
- Robust to outliners (moving any other point does not change the separating line) and thus strong generalization ability

The Largest Margin Linear Classifier

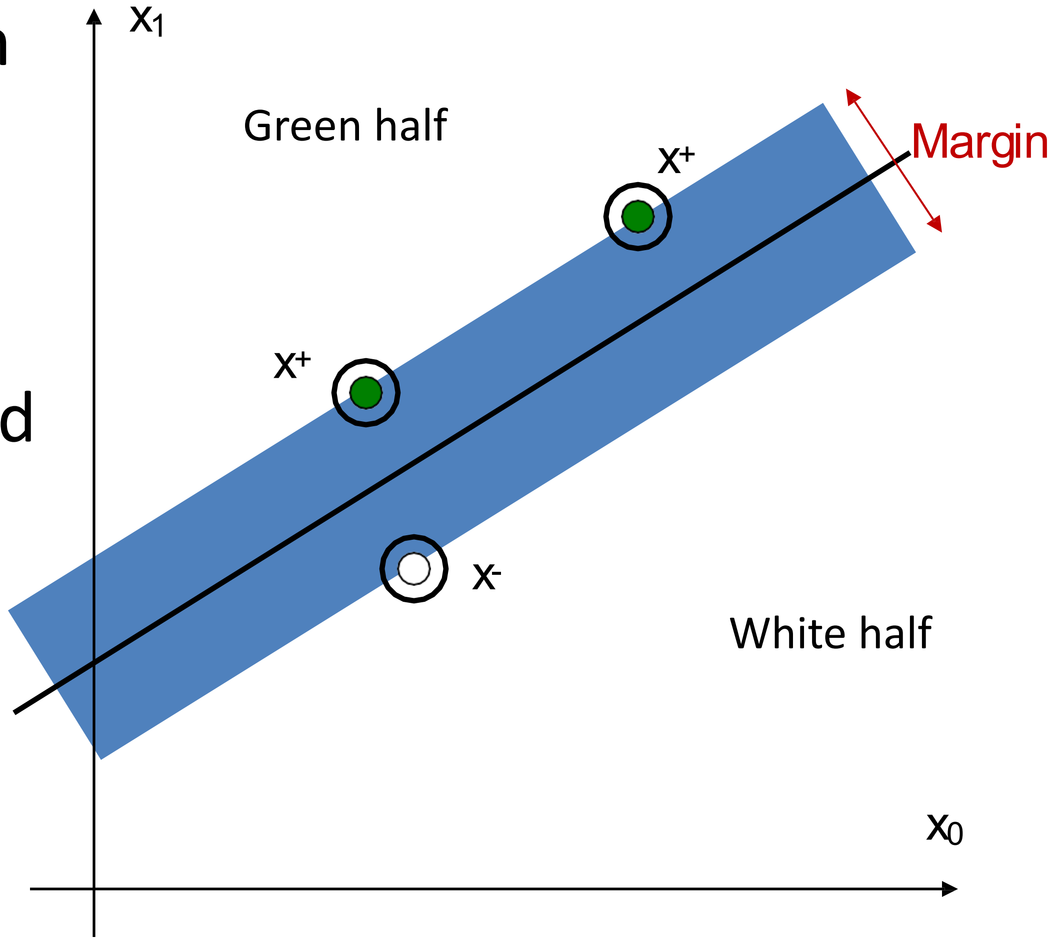
- These data points that define the margin are called support vectors



The Largest Margin Linear Classifier

- The data points further away from the margin do not count

- Fitting the model is about identifying the support vectors and throwing away the rest



The Largest Margin Linear Classifier

- Points on the decision boundary:

$$\mathbf{w}^T \mathbf{x}^+ + b = 0$$

Points on the edge of the margin (support vectors):

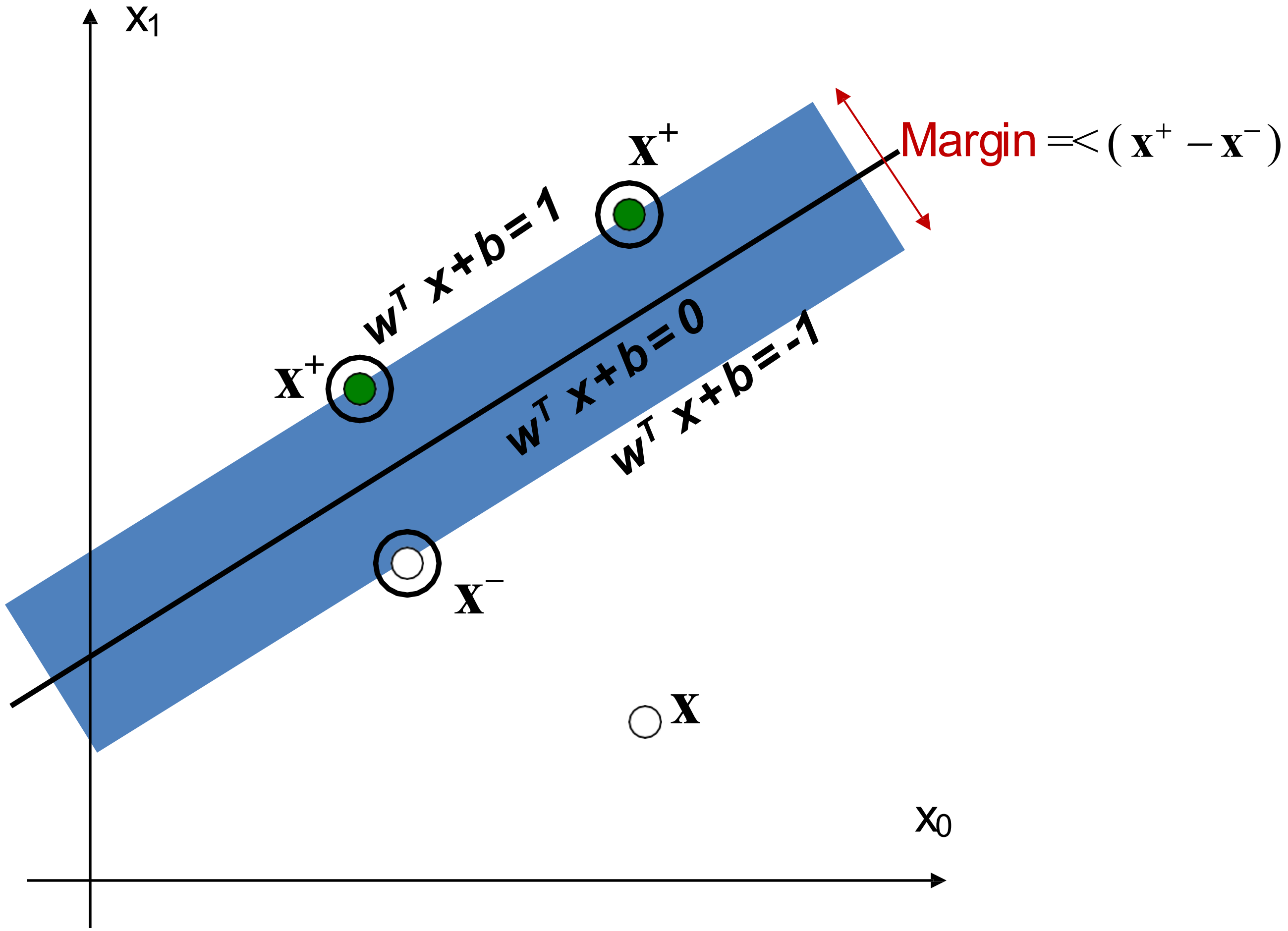
$$\mathbf{w}^T \mathbf{x}^+ + b = 1$$

$$\mathbf{w}^T \mathbf{x}^- + b = -1$$

Points elsewhere:

$\mathbf{w}^T \mathbf{x} + b > 0$ implies label=green

$\mathbf{w}^T \mathbf{x} + b < 0$ implies label=white



Optimization Problem: computing w

Quadratic programming with linear constraints

$$\text{minimize} \quad \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{s.t.} \quad y_i\,(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$$

Lagrangian Function

$$\text{minimize} \quad \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \lambda_i \left(y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1 \right)$$

$$\text{s.t.} \quad \lambda_i \geq 0$$

In the end:

$$\mathbf{w} = \sum_{i \in \mathrm{SV}} \lambda_i\, y_i\, \mathbf{x}_i$$

The Largest Margin Linear Classifier

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$$\mathbf{w} = \sum_{i \in \mathrm{SV}} \lambda_i \, \mathbf{x}_i y_i$$

$$\mathbf{w}^T \mathbf{x} + \mathrm{b} = \sum_{i \in \mathrm{SV}} \lambda_i \, \mathbf{x}_i^T \mathbf{x} \, y_i + \mathbf{b}$$

$\mathbf{w}^T \mathbf{x} + b > 0$ implies label=green

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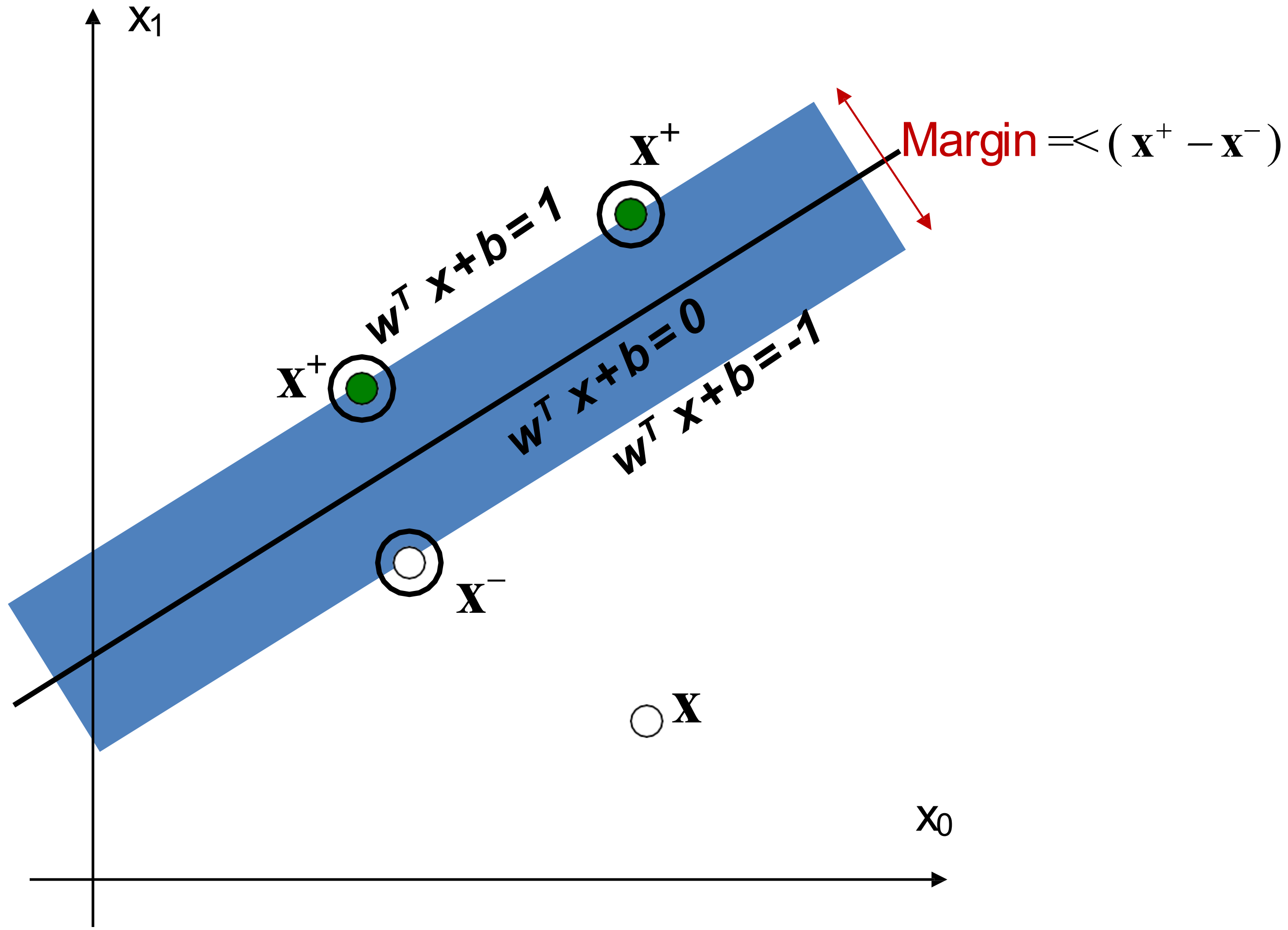


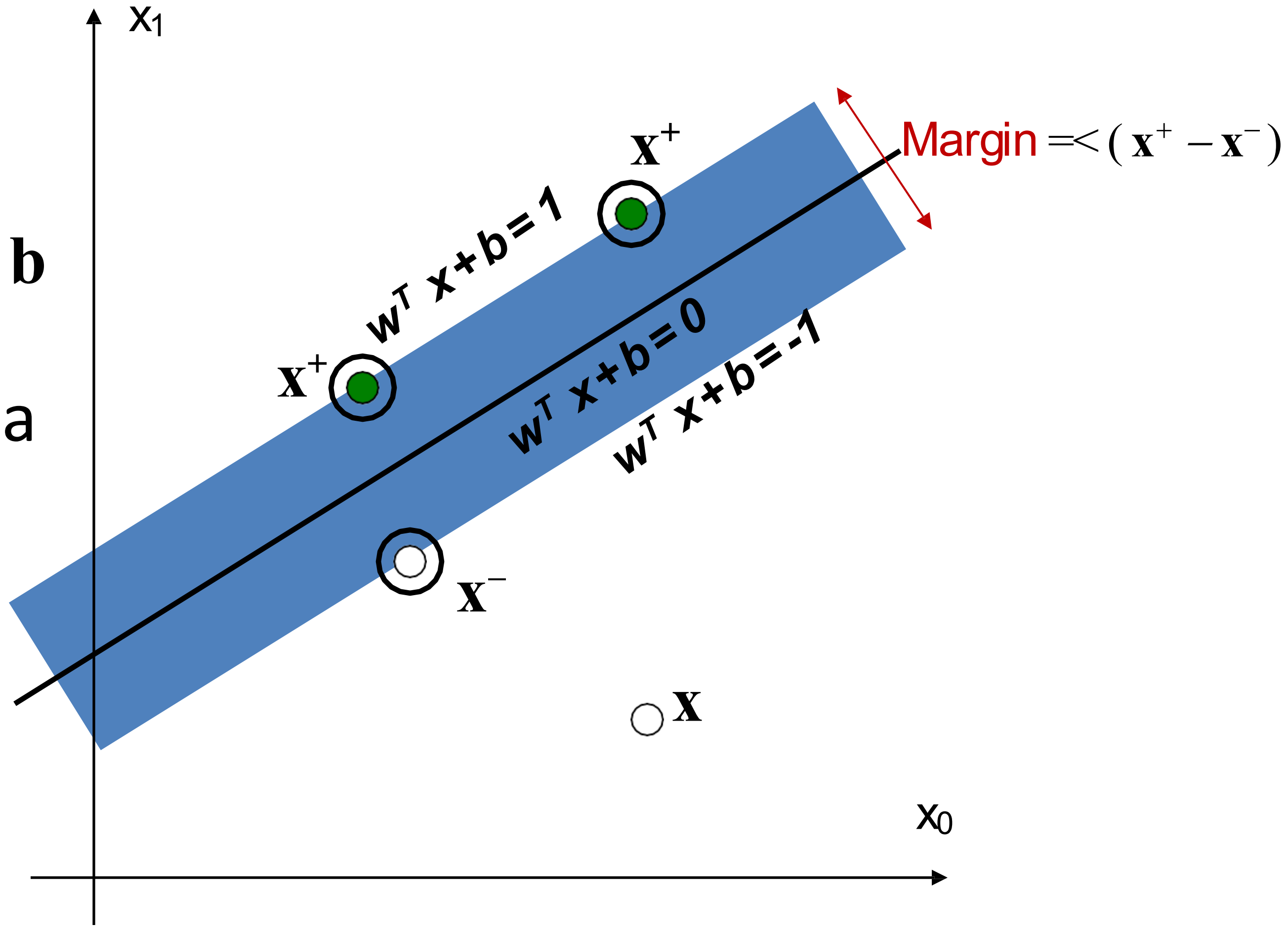
The Largest Margin Linear Classifier

- Similar to kNN, it is a weighted average of labels

$$\sum_{i \in \mathrm{SV}} \lambda_i \mathbf{x}_i^T \mathbf{x} \, y_i + \mathbf{b} = \sum_{i \in \mathrm{SV}} weight(\mathbf{x}_i, \mathbf{x}) \, y_i + \mathbf{b}$$

- Similar to Logistic Regression, it is a linear classifier $\mathbf{w}^T \mathbf{x} + b$

- but we only consider the training points that define the margin, not the training points close to the test point



SVM = Weighted Neighbors Nearest to Margin

For training

Data points outside the margin are redundant:

- all get a zero weight, and
- support vectors get to represent all of them in the voting process

Data points on the margin boundary are important:

- they become support vectors on either side of the boundary margin

For testing

Support vectors that are similar to the test point count more

- If $\mathbf{x}_i^T\mathbf{x}$ is small, it does not contribute much to the sum

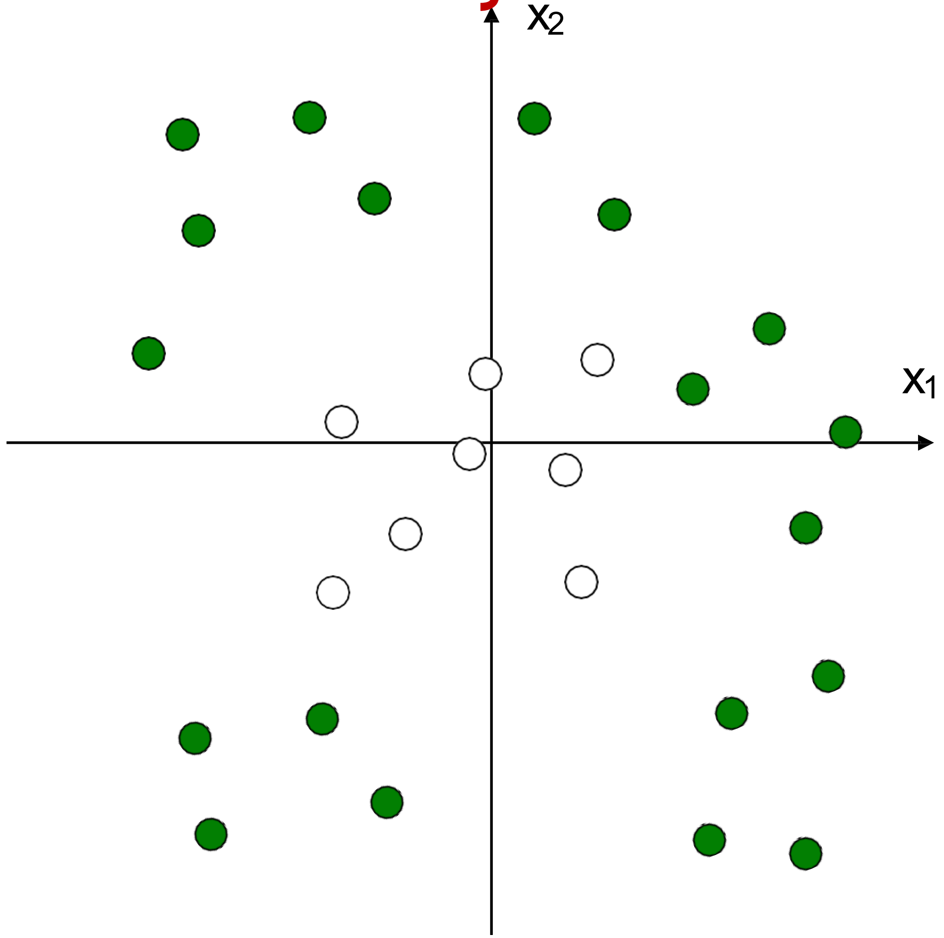
Hands-on Example:

SVC

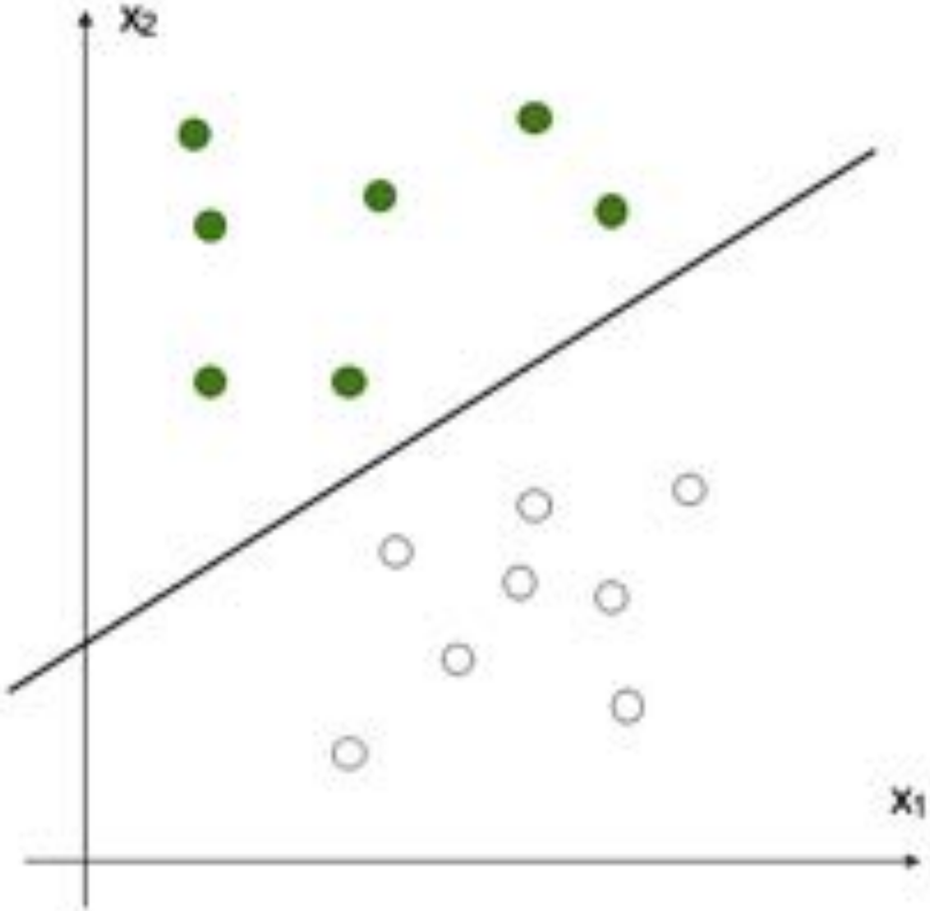
What if the points don’t line up exactly?

The kernel trick

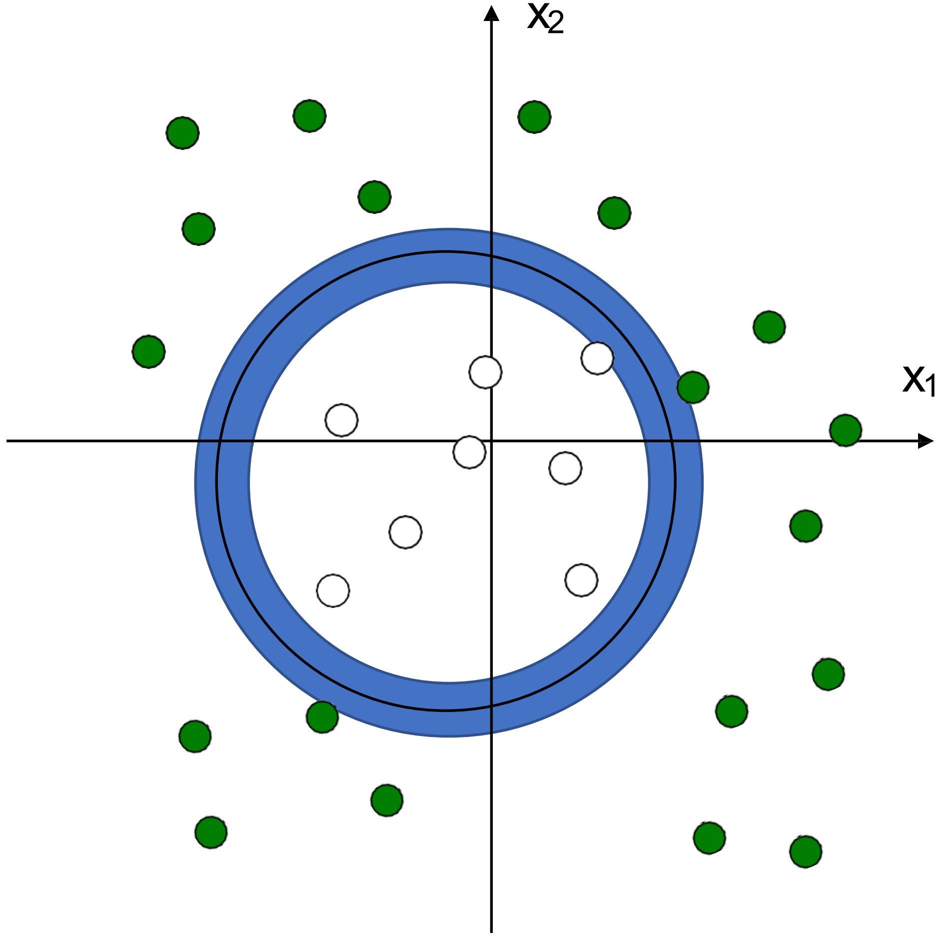
Non-linearity



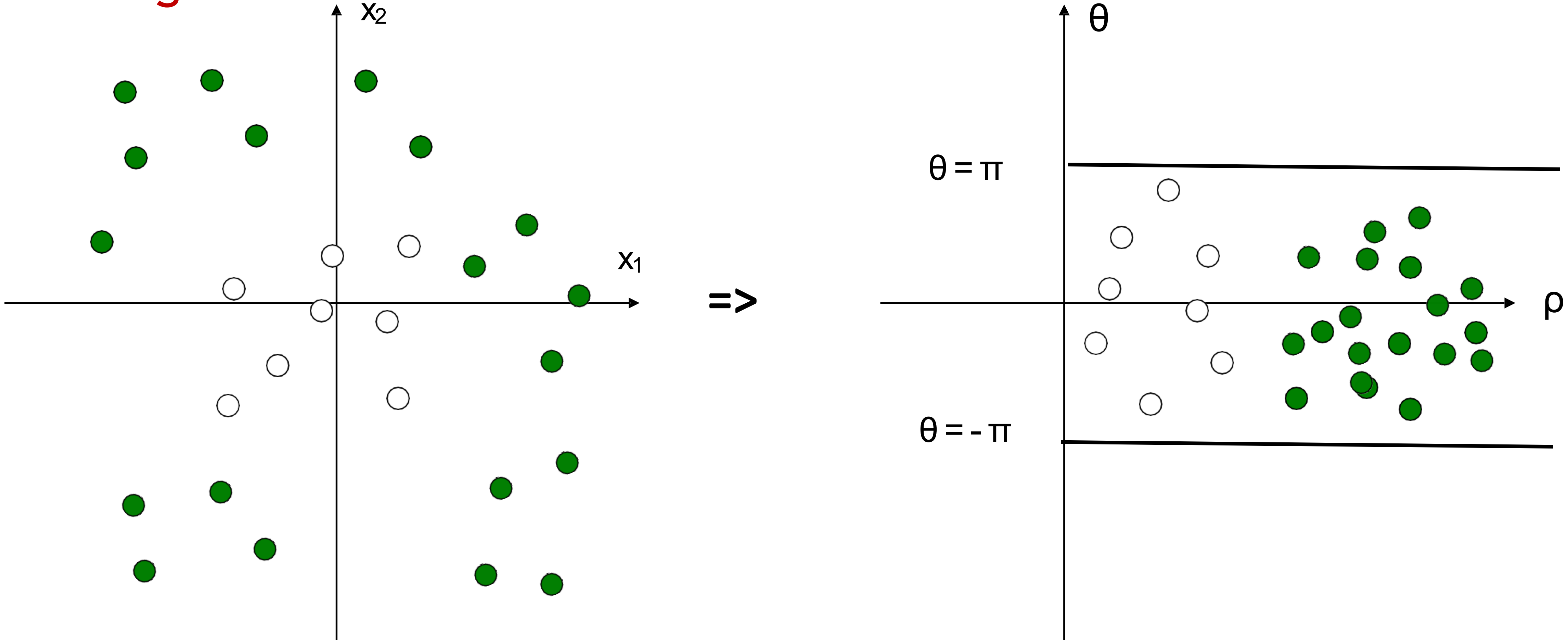
vs.



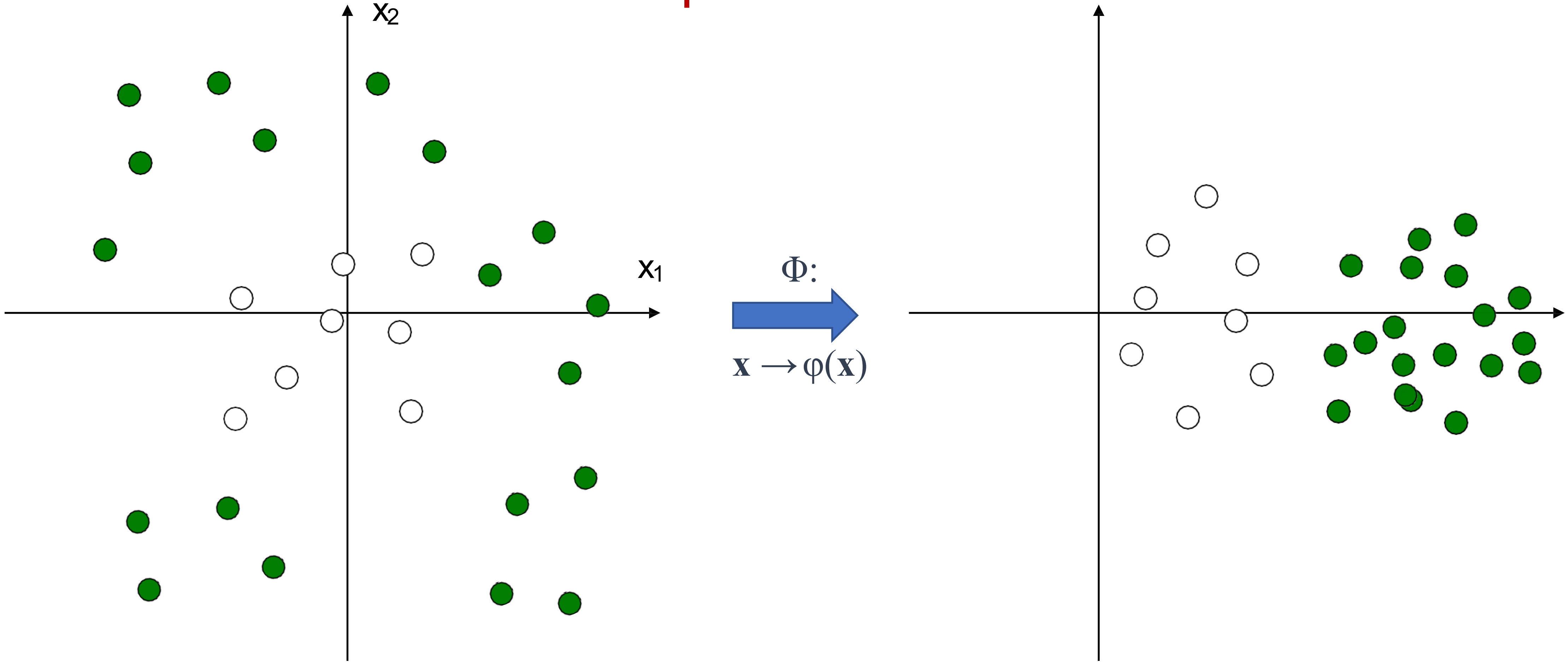
Circle Machines / Discriminant Analysis?



Change coordinates!



Non-linear SVMs: Feature Space



General idea: the original input space can be mapped to some transformed feature space where the training set is linearly separable

Solving the Optimization Problem

- The linear discriminant function is:

$$g(\mathbf{x}) = \sum \lambda_i \boxed{\varphi(\mathbf{x_i})^T \varphi(\mathbf{x})} y_i + b$$

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- No need to know this mapping $\boldsymbol{\varphi}$ explicitly, because we only use the new dot product of feature vectors in both the training and test.

- A *kernel function* is defined as a function that corresponds to a dot product of two feature vectors in some expanded feature space:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x_i})^T \varphi(\mathbf{x_j})$$

Nonlinear SVMs: similarity, not distance!

- Example of commonly used kernel functions:

- Linear $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$

- Polynomial $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$

- Gaussian (Radial Basis Function, or RBF) $K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\left\|\mathbf{x}_i - \mathbf{x}_j\right\|^2}{2s^2}\right)$

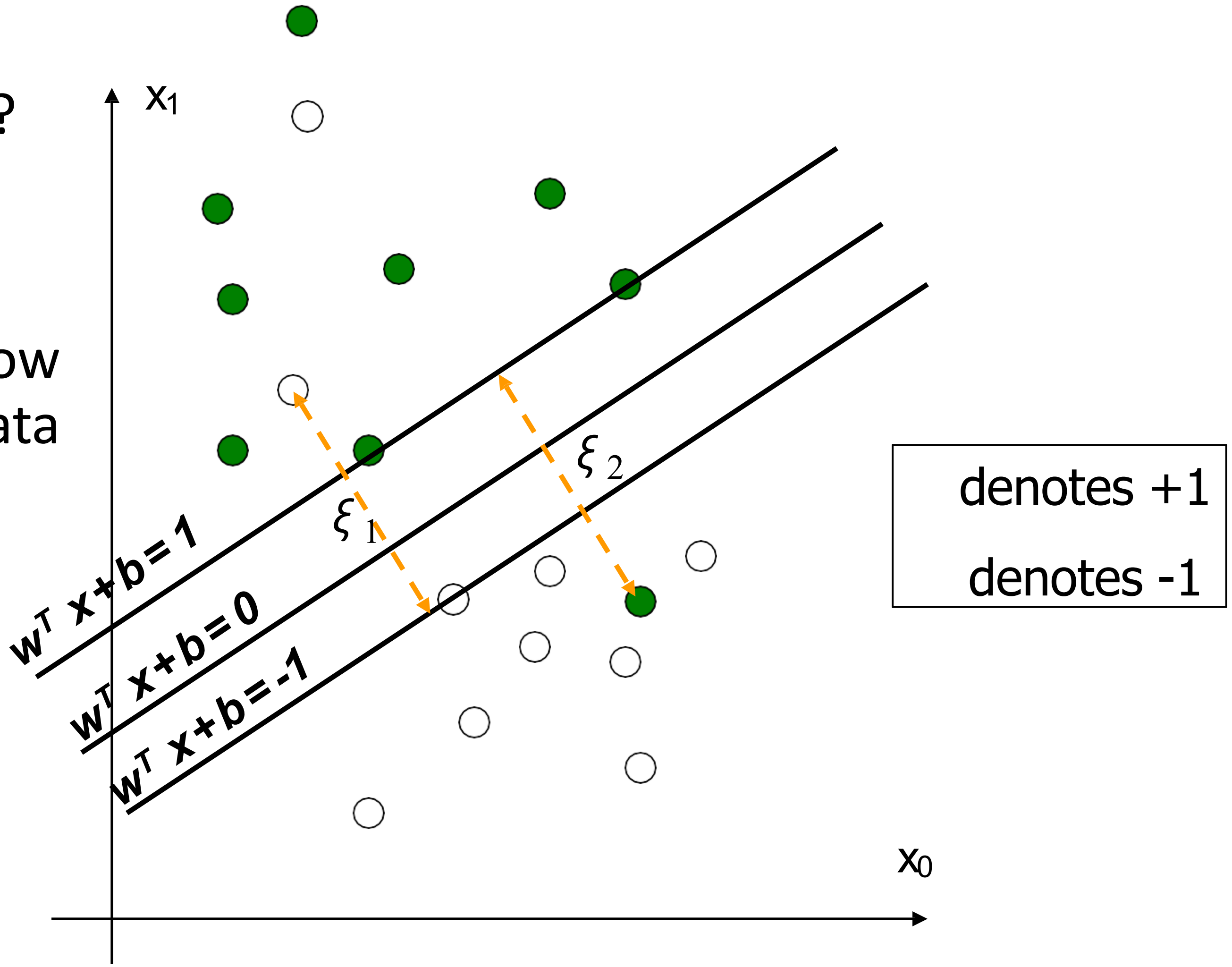
- Sigmoid $K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(b_0 \mathbf{x}_i^T \mathbf{x}_j + b_1)$

The regularization trick

The Largest Margin Linear Classifier

- What if data is not "cleanly" separable? (noisy data, outliers, etc.)

- Slack variables ξ_i can be added to allow misclassification of difficult or noisy data points



Optimization Problem: computing w

Quadratic programming with linear constraints

$$\text{minimize} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum \xi_i$$

$$\text{s.t.} \quad y_i\,(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i \qquad \xi_i \geq 0$$

Parameter C can be viewed as a way to control over-fitting

Hands-on Example:

SVC

SVC()

- ***C*** Regularization parameter. The strength of the regularization is inversely proportional to C. Must be strictly positive. The penalty is a squared l2 penalty.

- ***Kernel*** Specifies the kernel type to be used in the algorithm. It must be one of ‘linear’, ‘poly’, ‘rbf’, ‘sigmoid’, ‘precomputed’ or a callable. If none is given, ‘rbf’ will be used.
- ***Degree*** Degree of the polynomial kernel function (‘poly’). Ignored by all other kernels.
- ***Gamma*** Kernel coefficient for ‘rbf’, ‘poly’ and ‘sigmoid’.
  - if gamma='scale' (default) is passed then it uses 1 / (n_features * X.var()) as value of gamma,
  - if ‘auto’, uses 1 / n_features.
- ***Coef*** Independent term in kernel function. It is only significant in ‘poly’ and ‘sigmoid’.

SVC()

- ***Probability*** Whether to enable probability estimates. This must be enabled prior to calling fit, will slow down that method as it internally uses 5-fold cross-validation

- ***class_weight***
- ***max_iter***
- ***random_state***

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What if there are more than two classes?

The Problem with Multiple Classes

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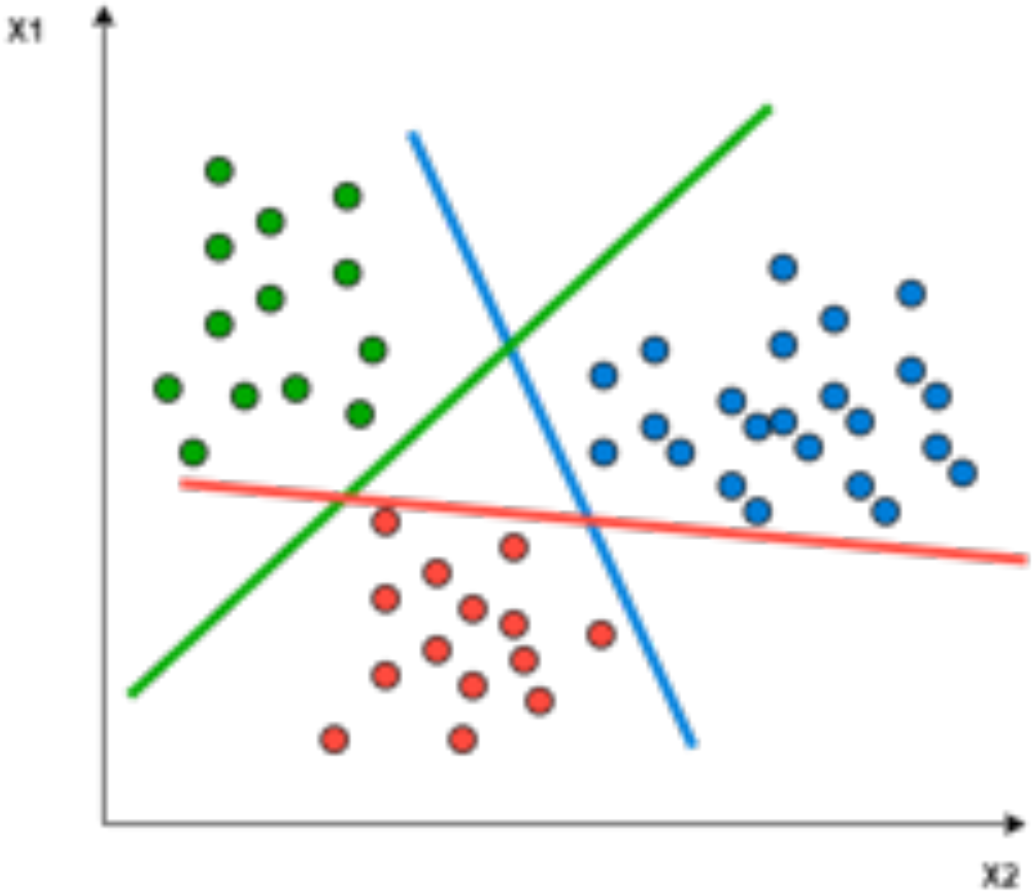
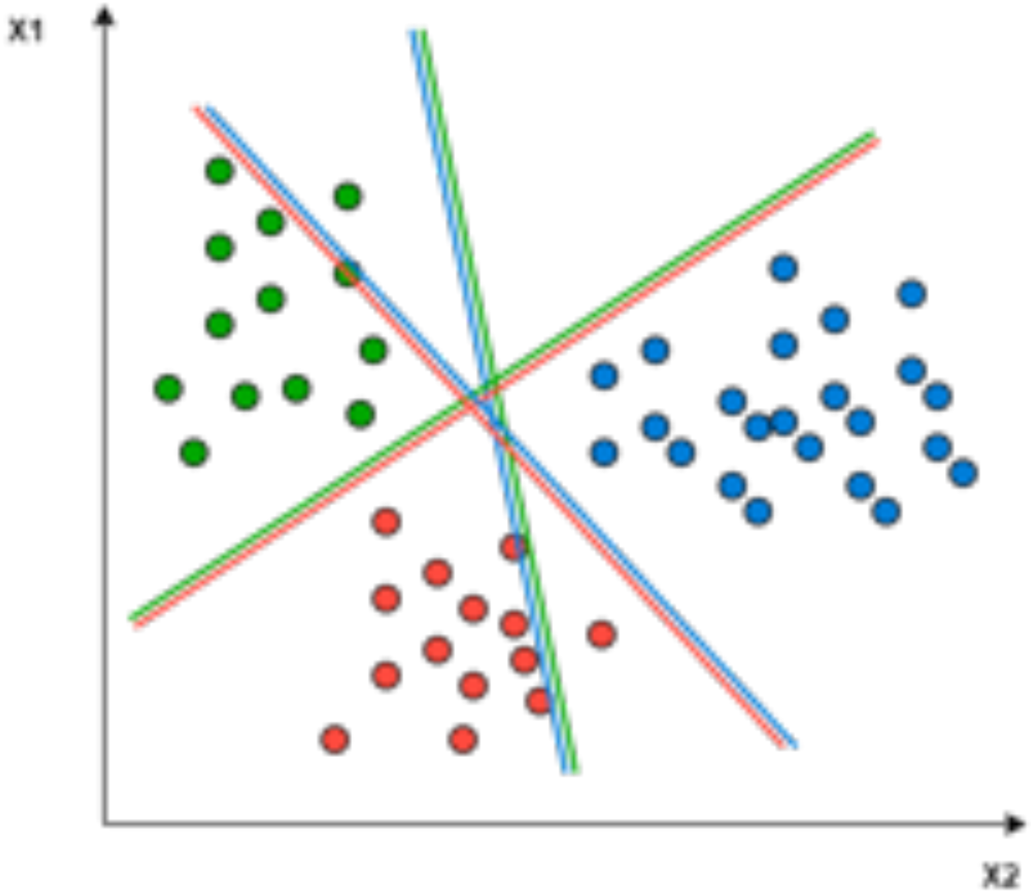
- Learn one discriminant function
  - for EVERY CLASS
- (one vs. rest/all, OvR/OvA)



Learn a discriminant function
for EVERY PAIR of classes
(one vs. one, or OvO)



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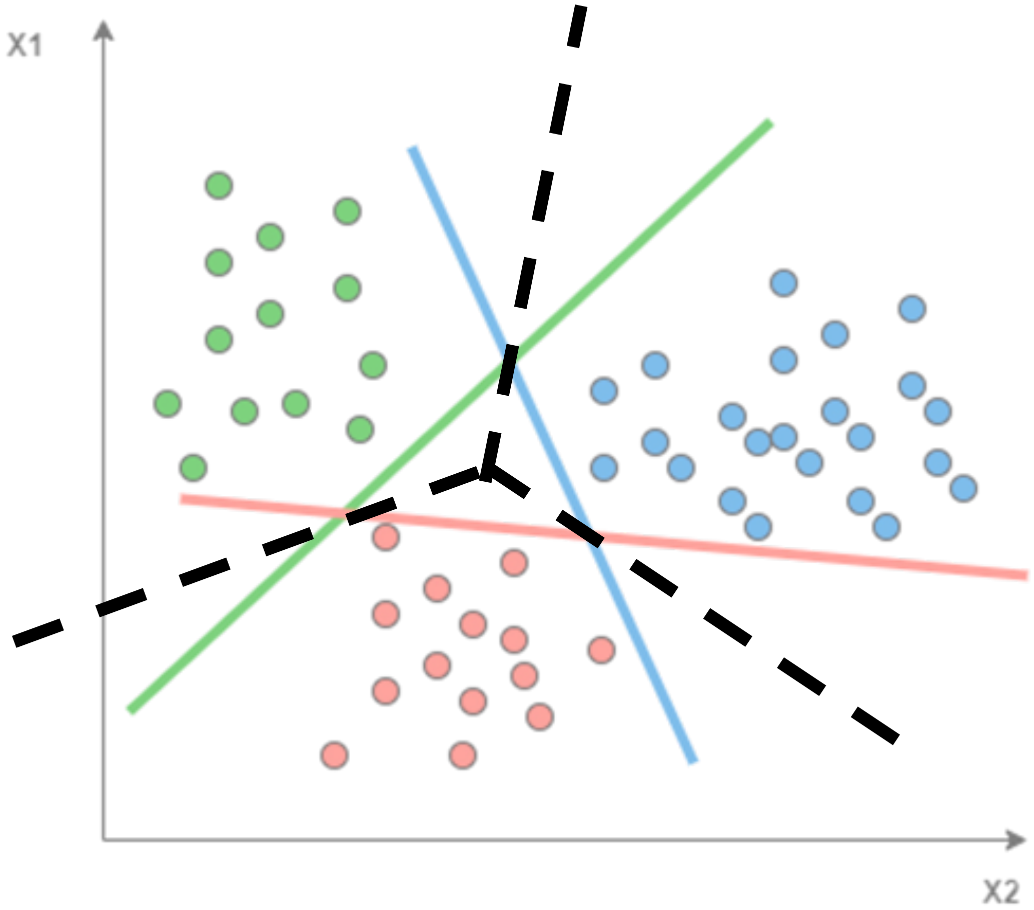

linear discriminant functions:

$g_k(x) = \mathbf{w}^T_k\, x + \mathbf{w}_0 \qquad k = 1, \ldots, c$

For each point x,

pick the largest value $g_k(x)$