Machine Learning

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2. Supervised Learning
   - Linear Regression, Logistic Regression, Support Vector Machines, Trees, Random Forests, Boosting, Artificial Neural Networks
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Supervised Learning

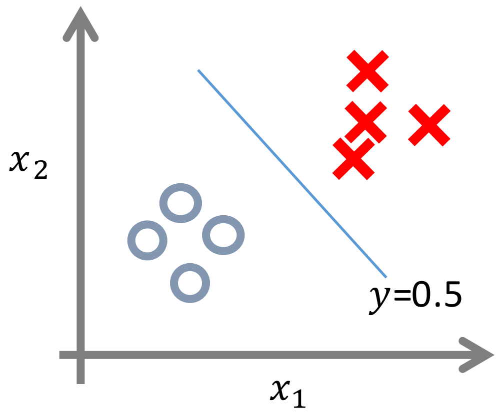
- Linear Regression
- **Logistic Regression**
- Support Vector Machines
- Trees (Decision and Regression)
- Random Forests
- Boosting
- Artificial Neural Networks

Logistic Regression

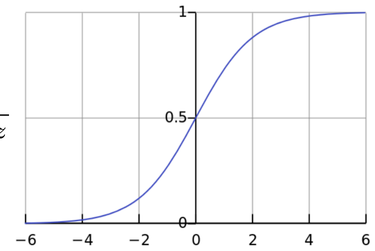
- The output y is discrete
- Classify X with a line $y = \boldsymbol{g}(w_0 + w_1 x_1 + w_2 x_2)$
- The best line is the one with minimum loss

$$\mathrm{L}(w) = \frac{1}{m}\sum_{i=1}^{m}[\hat{y}^{(i)}\log(y^{(i)}) + (1-\hat{y}^{(i)})\log(1-y^{(i)})]$$

- Solved with gradient descent



$$g(z) = \frac{1}{1+e^{-z}}$$

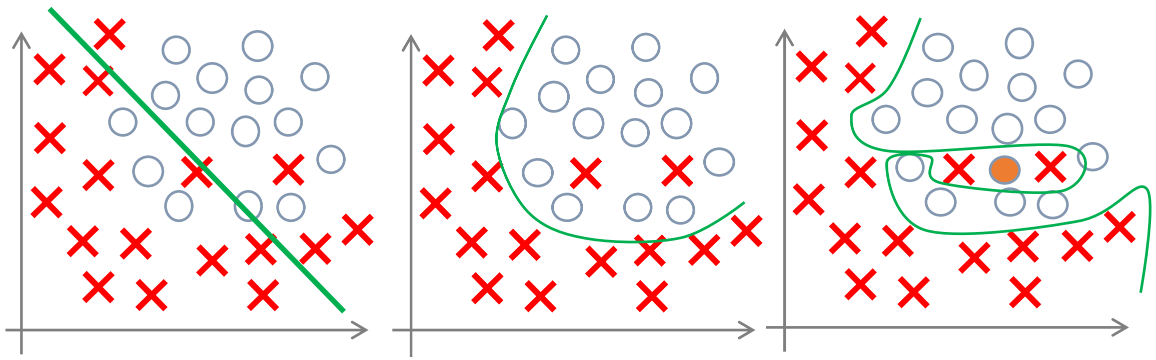


Overfitting vs. Underfitting

Underfitting
High Bias
Low variance

Trade-off

Overfitting
Low Bias
High Variance



Linear and Logistic Regression

- Hyper-Parameters Tuning
  - λ : regularization hyper-parameter
  - d: degree of polynomial

Supervised Learning

- Linear Regression
- Logistic Regression
- **Support Vector Machines**
- Trees (Decision and Regression)
- Random Forests
- Boosting
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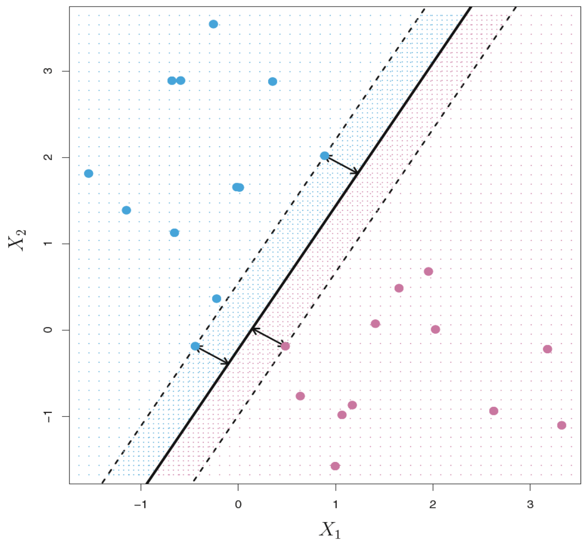
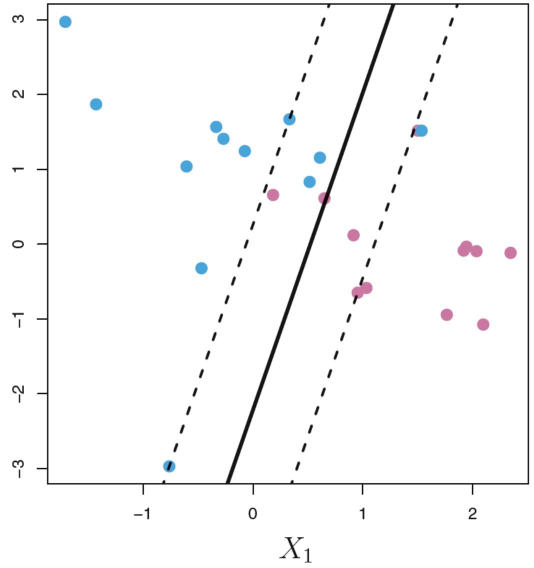
Support Vector Machines

Maximum Margin Classifier



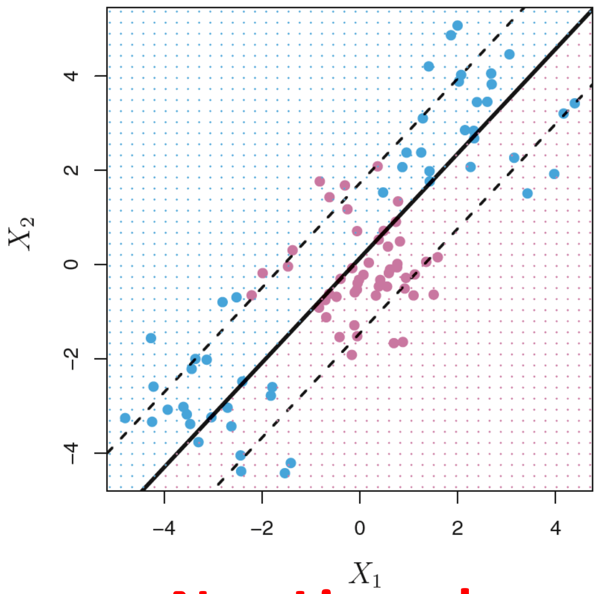
Linearly separable

Soft Margin Classifier



Slightly Linearly separable

Support Vector Machines



Non Linearly separable

Maximal Margin Classifier

- 2D: line

$$w_0 + w_1x_1 + w_2x_2 = 0$$

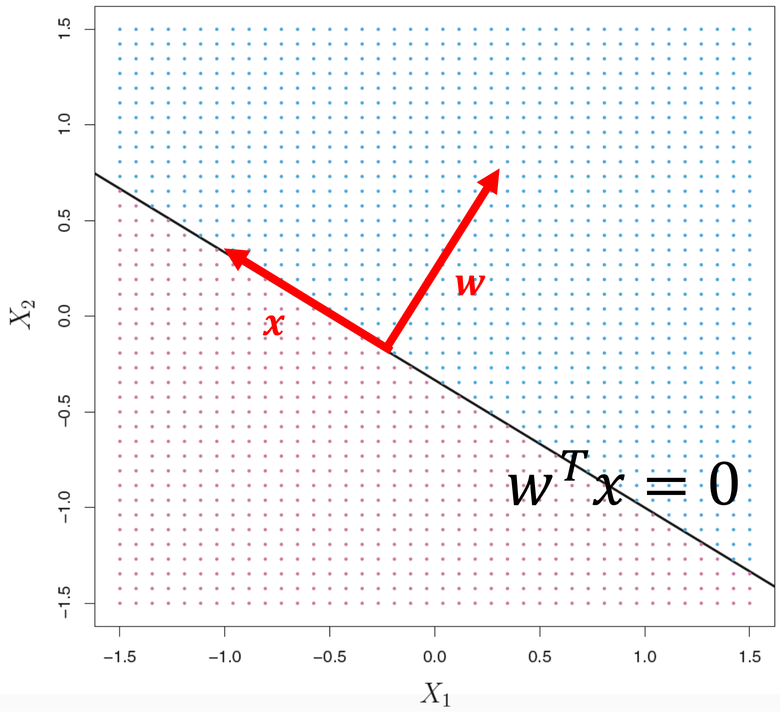
- 3D: plan

$$w_0 + w_1x_1 + w_2x_2 + w_3x_3 = 0$$

- nD: Hyperplane

$$w_0 + w_1x_1 + w_2x_2 + \cdots + w_nx_n = 0$$

$$w^Tx = 0$$



Maximal Margin Classifier

A separating hyperplane has the properties that:
for all i = 1, … m.

$$w^T x^{(i)} > 0 \;\; if \;\; y^{(i)} = +1$$

$$w^T x^{(i)} < 0 \;\; if \;\; y^{(i)} = -1$$

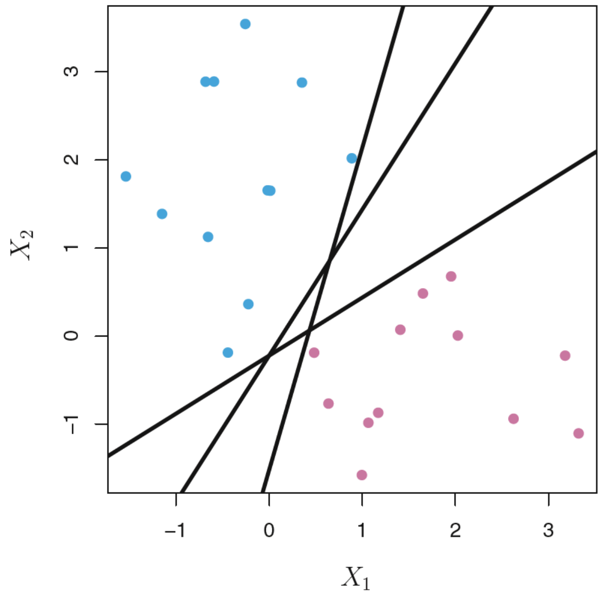
Equivalently

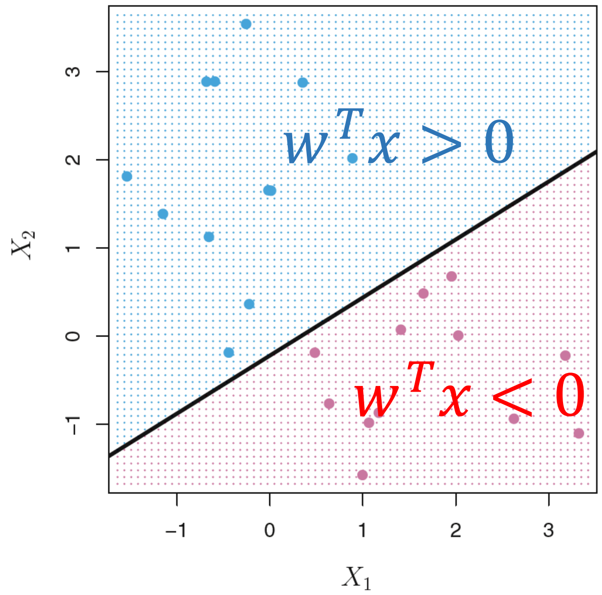
$$y^{(i)}(w^T x^{(i)}) > 0$$

$y^{(i)}$={1,-1}

2 classes

$$w \begin{bmatrix} w_0 \\ w_1 \\ \dots \\ w_n \end{bmatrix} \qquad x^{(i)} \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \dots \\ x_n^{(i)} \end{bmatrix}$$





Many hyperplanes
Which is the best?

Maximal Margin Classifier

The optimization problem

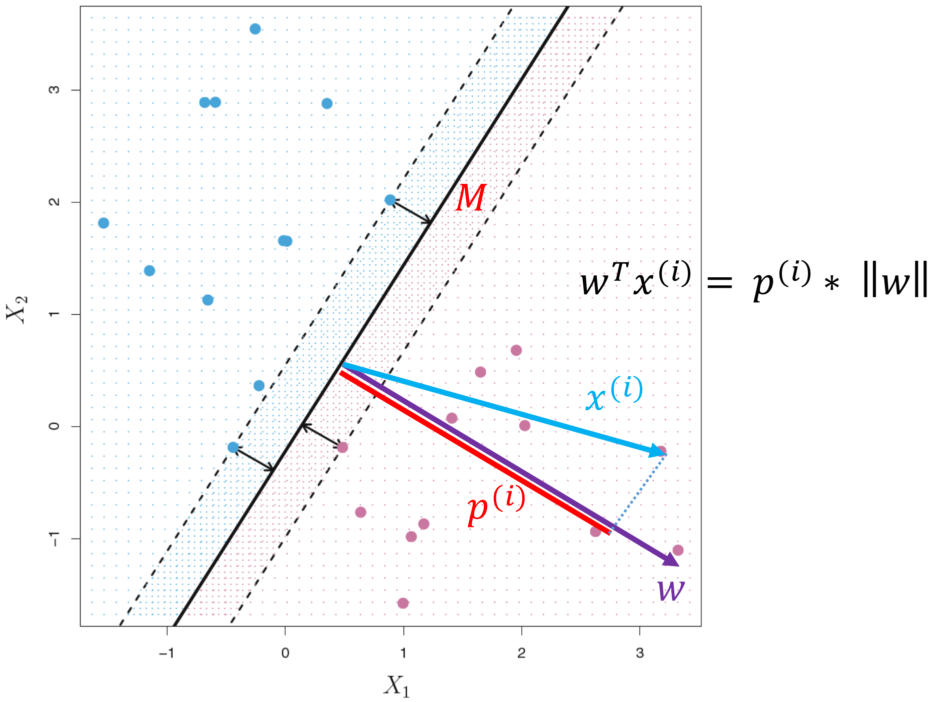
$$\underset{w}{\text{maximize}}\, M$$

Subject to: $\|w\| = \sum_{j=1}^{n} w_j^2 = 1,$

$$y^{(i)}(w^T x^{(i)}) \geq M, \forall\, i = 1 \ldots m$$

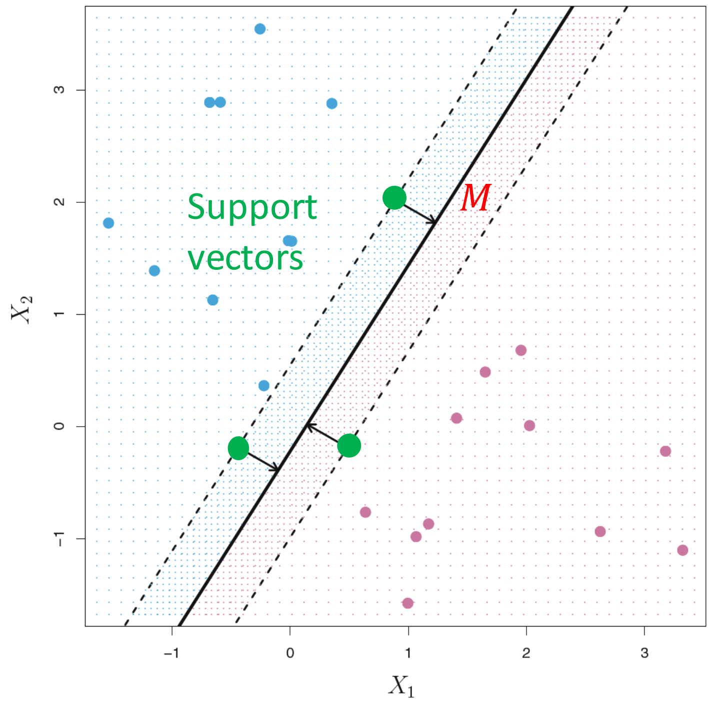
These equations ensure that each example is on the correct side of the hyperplane and at least a distance M from it.

Intuitively, pick the hyperplane with Maximum margin



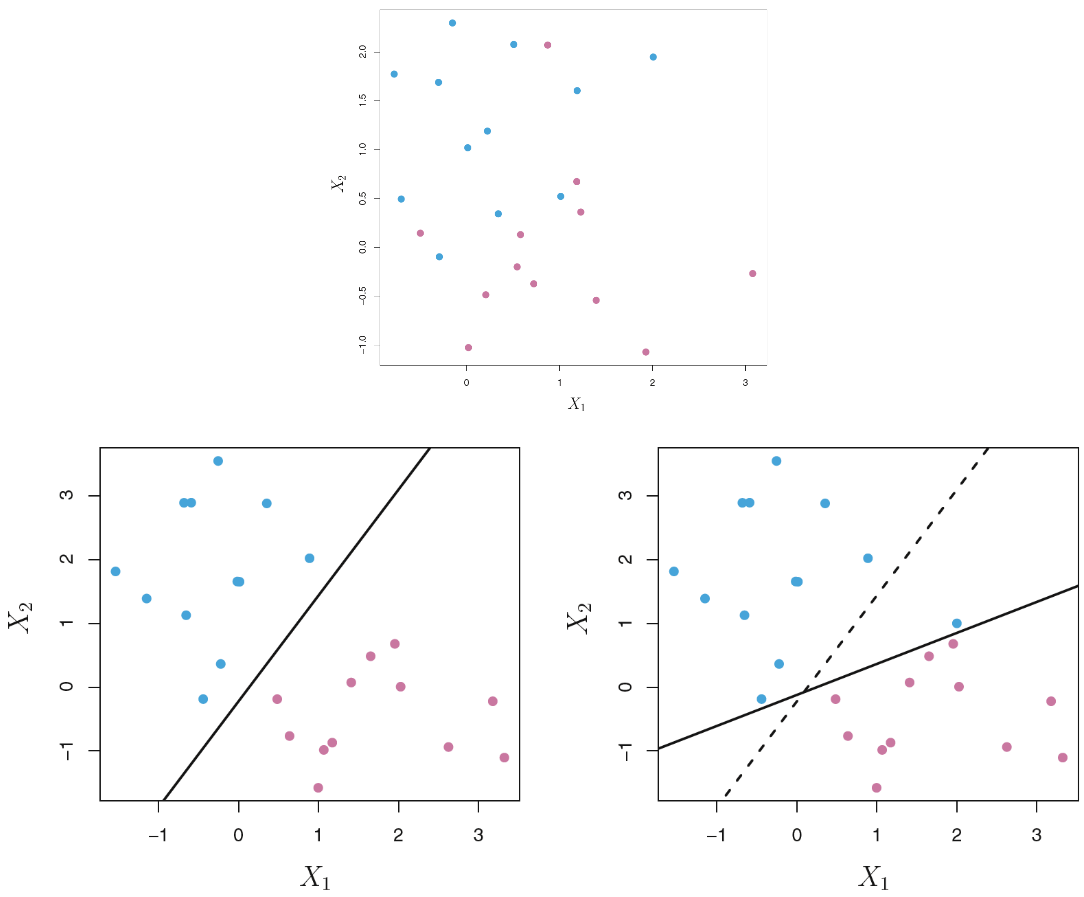
Maximal Margin Classifier

- Support vectors: examples supporting the margin (equidistant from the maximal margin hyperplane)
- If Support vectors were moved slightly, then the maximal margin hyperplane would move as well.
- The non-support vectors have no impact on the hyperplane !



Soft Margin Classifier

- The Non-linearly separable case
- Soft margin: can be violated by some of the training examples.
- It could be better to misclassify a few training examples in order to do a better job in classifying the remaining ones.



Soft Margin Classifier

The optimization problem

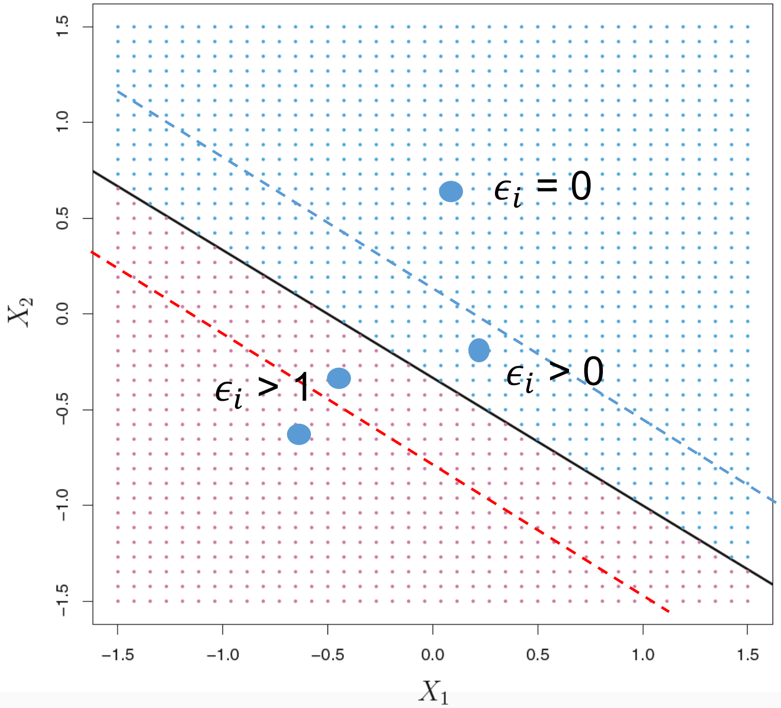
$$\underset{w,\epsilon}{\text{maximize}}\, M$$

Subject to: $\|w\| = \sum_{j=1}^{n} w_j^2 = 1,$

$$y^{(i)}(w^T x^{(i)}) \geq M(1 - \epsilon_i), \forall\, i = 1 \ldots m$$

$$\epsilon_i \geq 0, \quad \|\epsilon\| = \sum_{i=1}^{m} \epsilon_i^2 \leq C,$$

slack variables



- If $\epsilon_i = 0$, then example i is on the correct side of the margin,
- If $\epsilon_i > 0$, then example i is on the wrong side of the margin.
- If $\epsilon_i > 1$, then it is on the wrong side of the hyperplane.

Soft Margin Classifier

The optimization problem

$$\underset{w,\epsilon}{\text{maximize}}\, M$$

Subject to: $\|w\| = \sum_{j=1}^{n} w_j^2 = 1,$

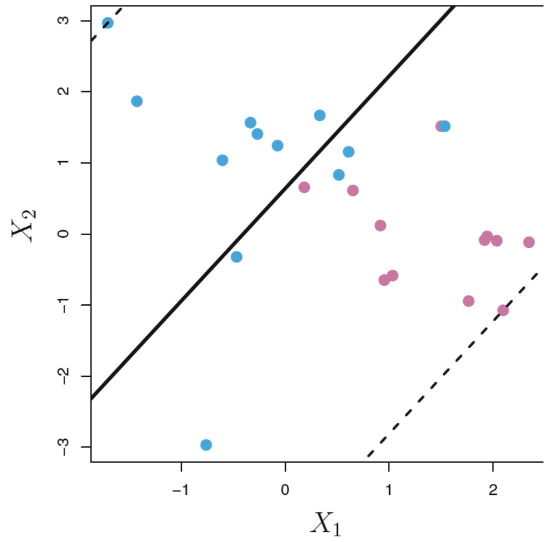
$$y^{(i)}(w^T x^{(i)}) \geq M(1-\epsilon_i), \forall\, i = 1 \ldots m$$

$$\epsilon_i \geq 0, \quad \|\epsilon\| = \sum_{i=1}^{m} \epsilon_i^2 \leq C,$$

slack variables

Hyper parameter ≥ 0

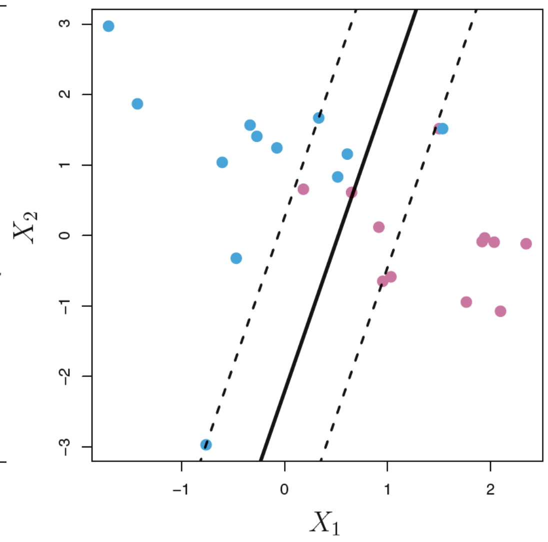
C is large



High tolerance for examples being on the wrong side of the margin ($\epsilon_i > 0$)

Underfitting:
(high bias, low variance)

C is small



Low tolerance for examples being on the wrong side of the margin ($\epsilon_i > 0$)

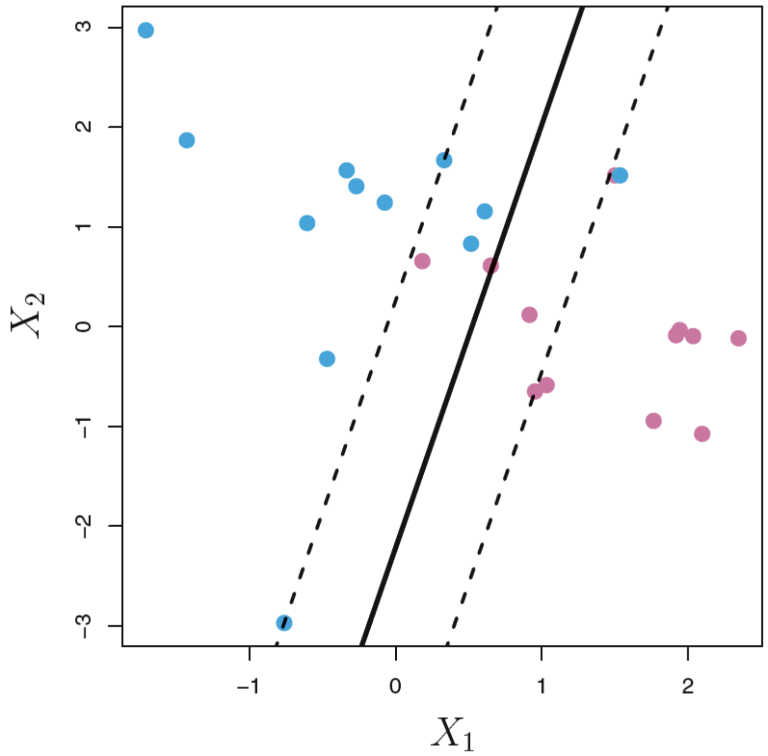
Overfitting:
(low bias, high variance)

Soft Margin Classifier

- It turns out that, the solution is :

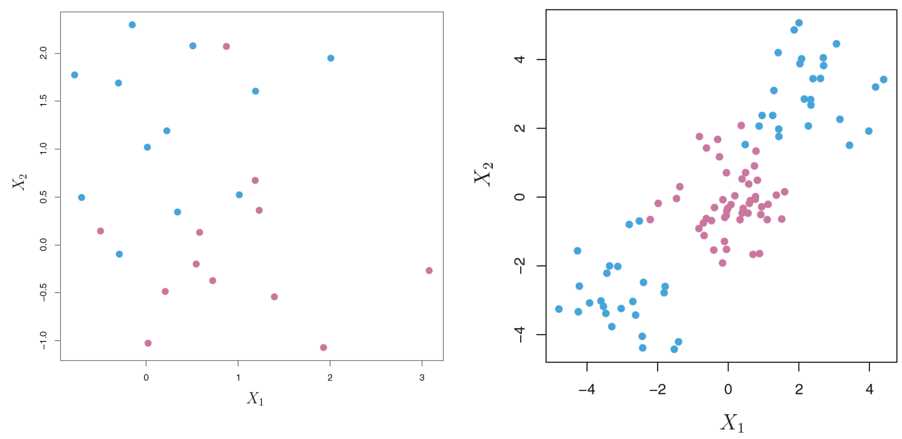
$$f(x) = w_0 + \alpha_i \sum_{i=1}^{m} x^T x^{(i)}$$

- Where α_i are Lagrange multipliers
- $x^{(i)}$ where $\alpha_i > 0$ are called Support Vectors
- They are examples that lie directly on the margin, or on the wrong side of the margin for their class.
- Only those examples can affect the hyperplane, and hence the support vector classifier f.



Support Vector Machines

- Highly non-linearly separable case
- Use feature mapping $\varphi(x)$ to address this non-linearity.
- Example: high order polynomials



$$x = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix} -> \varphi(x) = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_N \end{bmatrix}$$

N is the number of
features in the new space

Support Vector Machines

The optimization problem

$$\underset{w,\epsilon}{\text{maximize}}\, M$$

Subject to: $\|w\| = \sum_{j=1}^{N} w_j^2 = 1,$

$y^{(i)}(w^T \varphi(x^{(i)})) \geq M(1-\epsilon_i),$
$\forall\ i = 1 \ldots m$

$\epsilon_i \geq 0,$ $\quad \|\epsilon\| = \sum_{i=1}^{m} \epsilon_i^2 \leq C,$

If S is the set of support vectors, then:

$$f(x) = w_0 + \alpha_i \sum_{i \epsilon S} \varphi(x)^T \varphi(x^{(i)})$$

N could be very large → the computations would become unmanageable!

→ Use Kernel Trick

Support Vector Machines

- Non linearly separable data become separable in higher space!
- So, first go to higher feature space $x -> \varphi(x)$
- To solve SVM, you have to compute the Kernel $K(u, v) = \varphi(u)^T \varphi(v)$
  - But: very costly !!!
- Kernel Trick: If you chose φ carefully, you end up getting K, without calculating the very costly dot product $\varphi(u)^T \varphi(v)$

Support Vector Machines

- Exemple
  - Assume each example $x = [x_1, x_2]^T$ is mapped to the quadratic feature space $\varphi(x) = \left[x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1\right]^T$
  - We can then show that $K(x, x')$ = $\varphi(x)^T\varphi(x')$ = $(1 + x^Tx')^2$
  - In this way, the computation in the higher dimensional space is performed implicitly in the original input space !

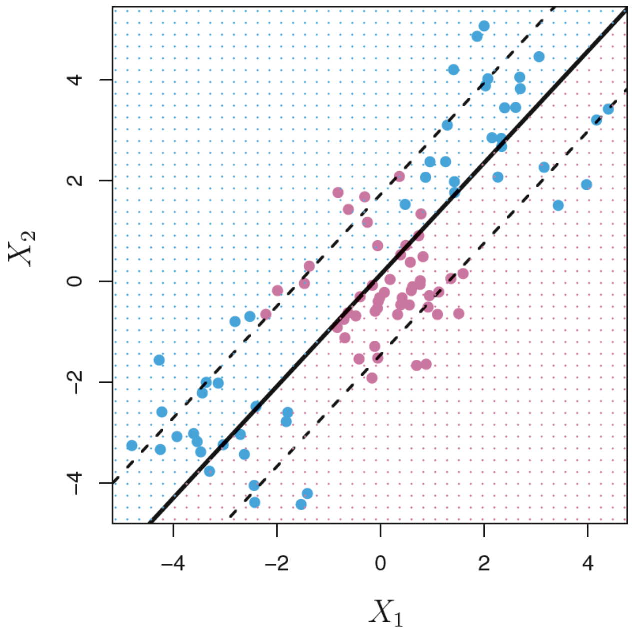
Support Vector Machines

- Kernel Examples
  - Linear Kernel $K(u, v) = u^T v$,
  - Polynomial Kernel: $K(u, v) = (c + u^T v)^d$,
  - Radial Basis Function (RBF) Kernel (Gaussian Kernel) :

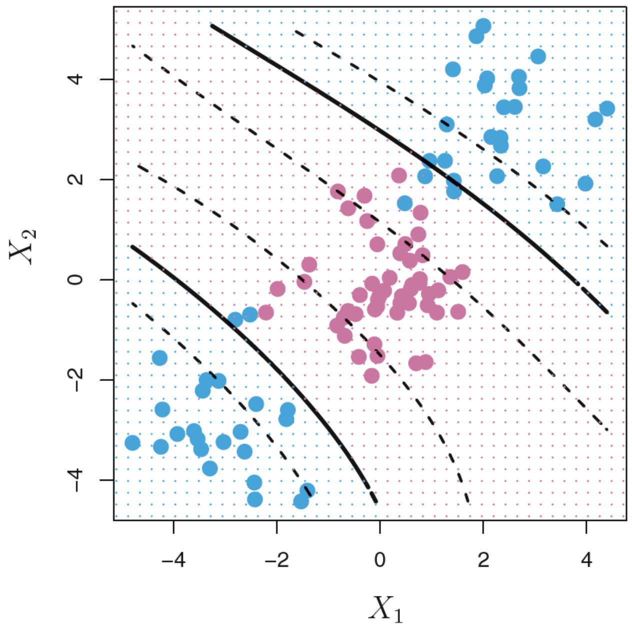
    $$K(u, v) = \exp(-\gamma \|u - v\|^2),$$ (infinite feature space!)
  - And many others: Sigmoid Kernel, String kernel, chi-square kernel, histogram intersection kernel, etc.

    (d, c and γ are hyper-parameters)
- Kernels need to satisfy technical conditions called "Mercer's conditions"

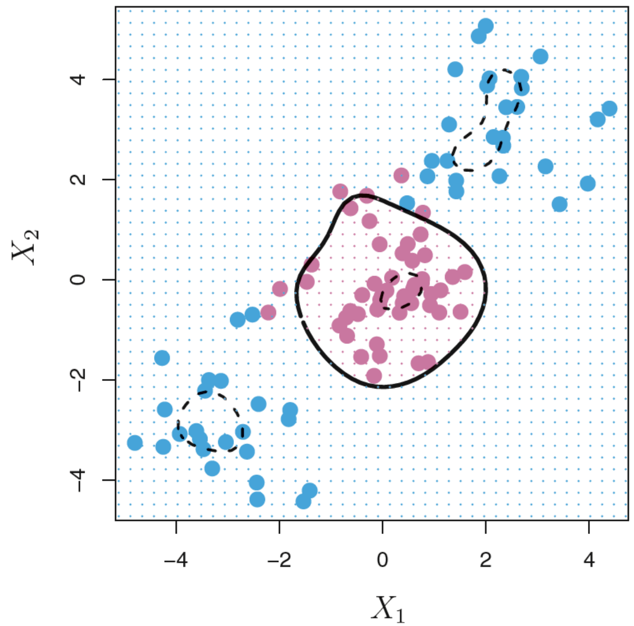
Support Vector Machines



Linear Kernel



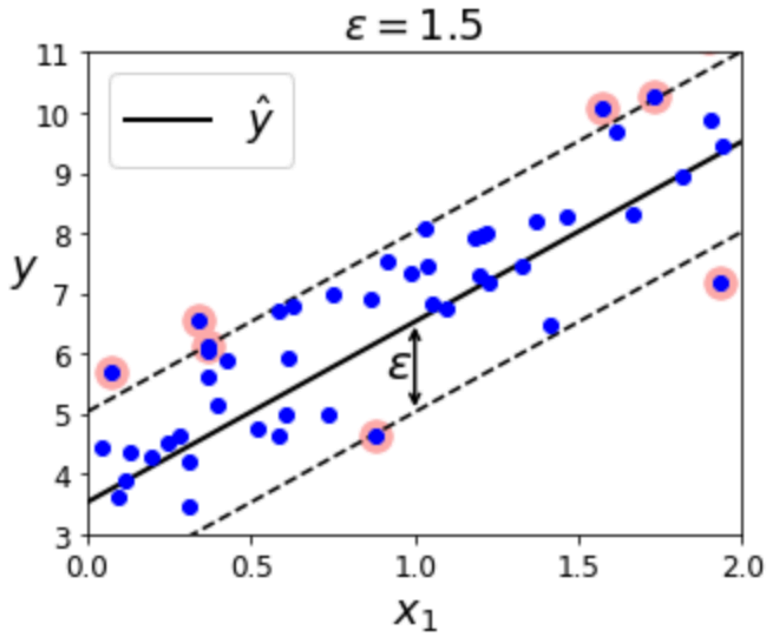
Polynomial Kernel
d=3



Radial Kernel
γ =0.1

Support Vector Machines

- Regression
  - Fit as many points as possible on the street while limiting margin violations.
  - The width of the street is controlled by a hyper-parameter ϵ



Support Vector Machines

- Hyper-Parameters Tuning
  - C, d: polynomial Kernel
  - γ: RBF kernel
  - ϵ: for regression
  - Etc.