

SVC and SVR

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In Previous Lectures

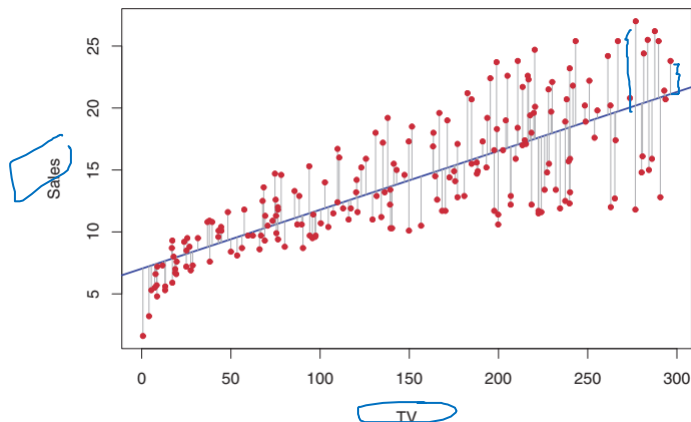
- Linear Regression
- Polynomial Regression
- Training and test error
- Bias and Variance Tradeoff
- Classification
- KNN
- Logistic Regression



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Review- Regression

- A simple, useful and widely used tool for predicting a quantitative response.
- It serves as a starting point for more complex approaches



An Introduction to Statistical Learning. James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani, 2013, ISBN: 978-1-461-47137-0



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SVR - Key Idea

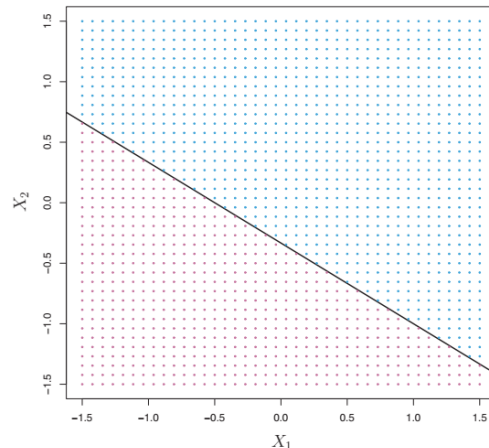
- Instead of minimizing the observed training error, Support Vector Regression (SVR) attempts to minimize the generalization error bound so as to achieve generalized performance. How?



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Basic Notions - Hyperplane

- In a p -dimensional space, a hyperplane is a flat affine subspace of dimension $p-1$.
- In two dimensions, a hyperplane is a flat one-dimensional subspace (a line).
- In figure, the separating hyperplane is $1 + 2x_1 + 3x_2 = 0$



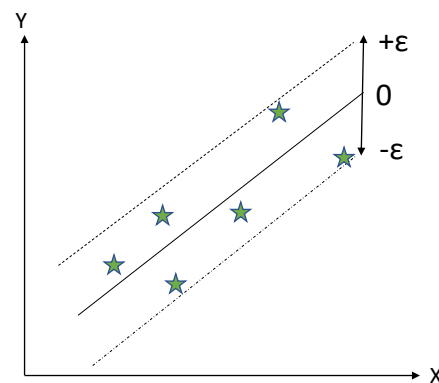
An Introduction to Statistical Learning. James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani, 2013, ISBN: 978-1-461-47137-0



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Support Vector Regression (Epsilon-Support Vector Regression)

- Using a margin of tolerance.
- Our goal is to find a function $f(x)$ that has at most ϵ deviation from the targets y_i for all the training data, and at the same time is as flat as possible.
- In other words, we do not care about errors as long as they are less than ϵ but will not accept any deviation larger than this.
- $f(x)$ is the **maximal margin hyperplane**

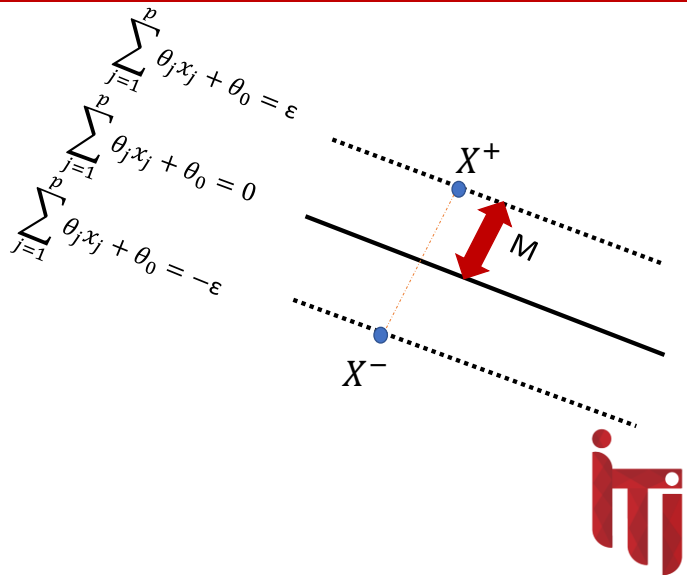


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Construction of the Maximal Margin Hyperplane

- Choose the values of the model parameters θ that maximize the margin M : $\max_{\theta_0, \theta_1, \dots, \theta_p} M$
- The vector θ is orthogonal to the maximal margin hyperplane (**why?**)
- We can say

$$X^+ = \lambda \theta + X^-$$
- (i.e. we can get from X^- to X^+ by moving in the direction of θ for an unknown distance determined by λ)



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- $A=(-3,10)$, $B = (b_1, b_2)$
- $-3b_1+10b_2=0$
- $b_2=0.3 b_1$



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Construction of the Maximal Margin Hyperplane (Cont.)

- We know that at X^+

$$\sum_{j=1}^p \theta_j x_j + \theta_0 = \varepsilon$$

- Using the augmented form $\theta^T X^+ = \varepsilon$

- But, $X^+ = \lambda \theta + X^-$

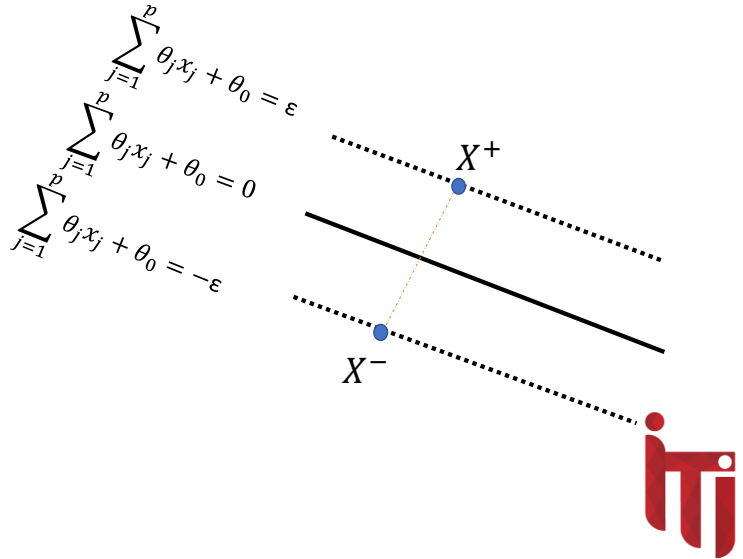
- $\theta^T (\lambda \theta + X^-) = \varepsilon$

- $\lambda \theta^T \theta + \theta^T X^- = \varepsilon$

- But we know $\theta^T X^- = -\varepsilon$

- $\lambda \theta^T \theta - \varepsilon = \varepsilon$

$$\lambda = \frac{2\varepsilon}{\theta^T \theta} = \frac{2\varepsilon}{\|\theta\|^2}$$



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Construction of the Maximal Margin Hyperplane (Cont.)

- $M = \frac{1}{2} (X^+ - X^-) = \frac{1}{2} \|\lambda \theta\| = \frac{1}{2} \frac{2\varepsilon \|\theta\|}{\|\theta\|^2} = \frac{\varepsilon}{\|\theta\|}$

- To maximize M, To maximize, we can maximize λ

- That is minimize $\frac{1}{2} \|\theta\|^2$, subject to constraints

$$\sum_{j=1}^p \theta_j x_j + \theta_0 \leq \varepsilon$$

$$\sum_{j=1}^p \theta_j x_j + \theta_0 \geq -\varepsilon$$

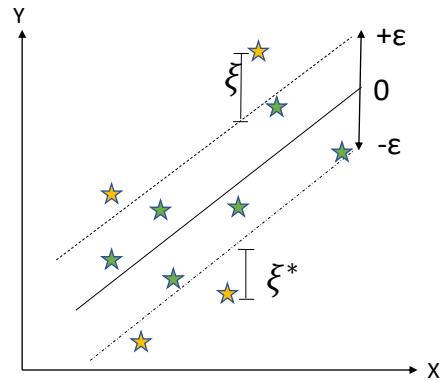
- Constrained Optimization Problem (solved using Lagrange multipliers)
- Solution of this optimization equation is out of the scope of this course



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Support Vector Regression – Using Soft Margin

- The assumption we had before it that there is a function that approximates all pairs (x_i, y_i) with ε precision.
- Sometimes, this is not the case.
- We may want to allow for some errors (How?).
- One can introduce slack variables ξ_i , ξ_i^* to cope with otherwise infeasible constraints of the optimization problem.



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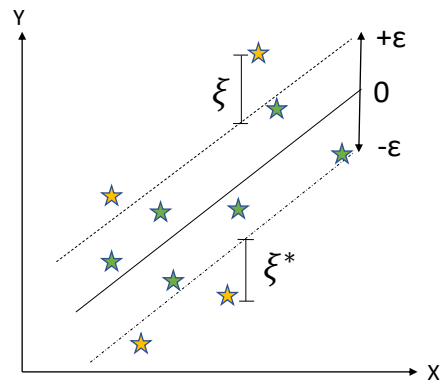
Support Vector Regression – Using Soft Margin (Cont.)

- minimize $\frac{1}{2} \|\theta\|^2 + \underline{C} \sum_{i=1}^N (\xi_i + \xi_i^*)$
- N: number of examples in the dataset
- Subject to

$$\sum_{j=1}^p \theta_j x_j + \theta_0 \leq \varepsilon + \xi_i$$

$$\sum_{j=1}^p \theta_j x_j + \theta_0 \geq -(\varepsilon + \xi_i^*)$$

$$\xi_i, \xi_i^* \geq 0$$
- Again, a constrained optimization problem



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Tuning the Hyperparameter C

- The constant $C > 0$ determines the trade-off between the flatness of f and the amount up to which deviations larger than ε are tolerated.
- Decreasing C , increases bias, reduces the variance (we become more tolerant of violations to the margin, margin will widen)
- Increasing C , reduces bias, increases variance (we become less tolerant of violations to the margin, margin narrows)
- C is generally chosen via [cross-validation](#).



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Solution of the constrained optimization problem

$$\max_{\alpha_i, \alpha_i^*} \left\{ \frac{1}{2} \sum_{i,j=0}^N (\alpha_i - \alpha_i^*)(\alpha_i - \alpha_j^*) \langle X^{(i)}, X^{(j)} \rangle - \varepsilon \sum_{i=1}^N (\alpha_i + \alpha_i^*) + \sum_{i=1}^N y_i (\alpha_i - \alpha_i^*) \right\}$$

Subject to $\sum_{i=1}^N (\alpha_i - \alpha_i^*) = 0$ and $\alpha_i, \alpha_i^* \in [0, C]$



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Solution of the constrained optimization problem

$$\theta = \sum_{i=1}^N (\alpha_i - \alpha_i^*) X^{(i)}$$

Linear SVR

$$f(X) = \sum_{i=1}^N (\alpha_i - \alpha_i^*) \cdot \langle X^{(i)}, X \rangle + b$$

$\langle X^{(i)}, X^{(j)} \rangle$ is the dot product between the two observations $X^{(i)}, X^{(j)}$

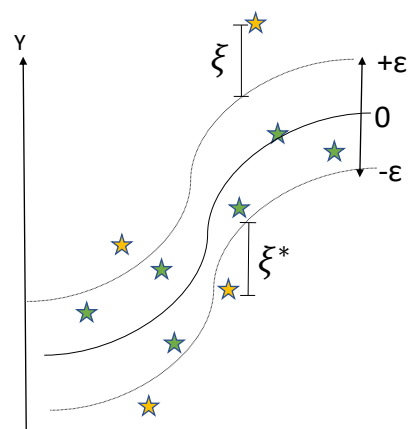
- The solution has $2N$ parameters $\alpha_1, \alpha_1^*, \alpha_2, \alpha_2^* \dots \alpha_n, \alpha_n^*$
- The majority of these parameters will equal zero. Few (at support vectors) will have a value greater than 0
- The complexity of a function's representation by SVs is independent of the dimensionality of the input space X , and depends only on the number of SVs.



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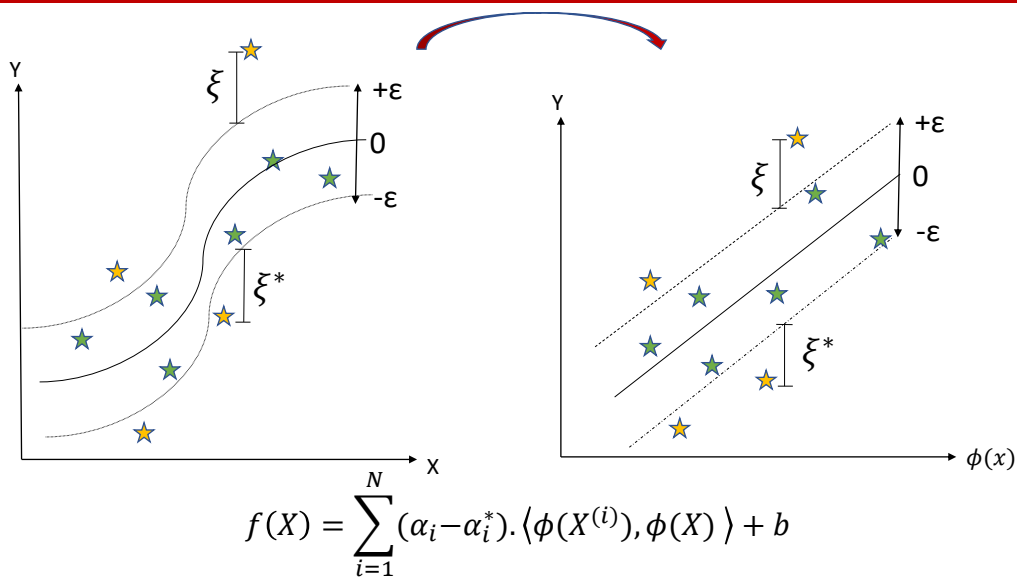
How about non-linear relationships

- Idea: we can transform the training data x_i by a map $\phi : \mathcal{X} \rightarrow \mathcal{F}$ into some feature space \mathcal{F} in which we can do the linear separation.



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Transformation



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Transformation - Implicit mapping via kernels

$$f(X) = \sum_{i=1}^N (\alpha_i - \alpha_i^*) \cdot \langle \phi(X^{(i)}), \phi(X) \rangle + b$$

- Knowing $\phi(X)$ is not easy.
- Do we need to know $\phi(X)$ explicitly?
- the SV algorithm only depends on dot products between patterns x_i . Hence it suffices to know the **kernel function** $k(x, x') := \langle \phi(x), \phi(x') \rangle$ rather than $\phi(X)$ explicitly
- **Kernel:** function that quantifies the similarity of two observations.
- There are conditions for kernel functions. The discussion of which is out of the scope of this course

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Common Kernel

- Polynomial kernel of degree d ($d > 1$)

$$K(X^{(i)}, X^{(j)}) = \left(1 + \sum_{l=1}^p x_{il} x_{jl} \right)^d$$

- Gaussian Radial Basis Function

$$K(X^{(i)}, X^{(j)}) = \exp \left(-\gamma \sum_{l=1}^p (x_{il} - x_{jl})^2 \right)$$



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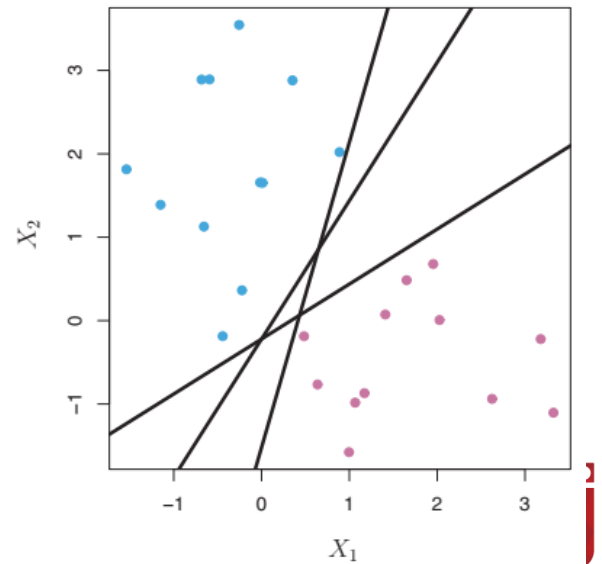
DEMO



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Classification

- Same dataset can be separated with many hyperplanes. Which one shall we choose?

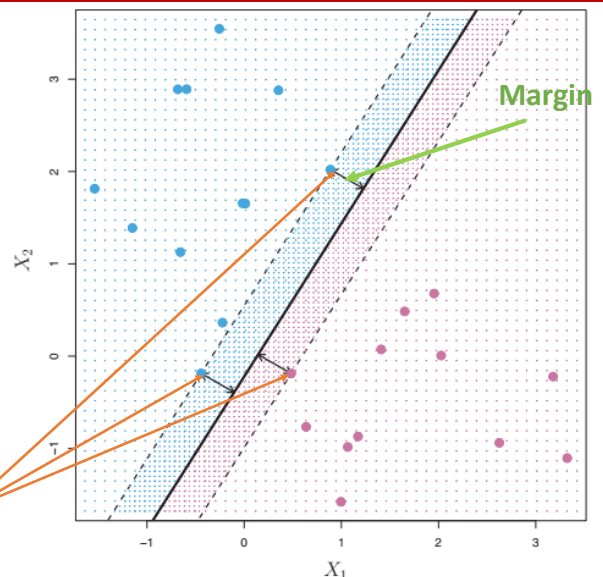


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The Maximal Margin Classifier

- **Margin**: the minimal distance from the observations to the hyperplane (the distance from the solid line (separating hyperplane) to either of the dashed lines (defined by the support vectors)).
- A natural choice is the **maximal margin hyperplane** (also known as the *optimal separating hyperplane*), which is the separating hyperplane that is farthest from the training observations.
- This is known as the **maximal margin classifier**.

Support Vectors



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Review –Linear Algebra

- If you have a line $-3b_1 + 10b_2 = 0$ then you can say that vector $[-3, 10]$ is orthogonal to this line



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Construction of the Maximal Margin Classifier (Cont.)

- The vector θ is orthogonal to the separating hyperplane

- We can say

$$X^+ = \lambda \theta + X^-$$

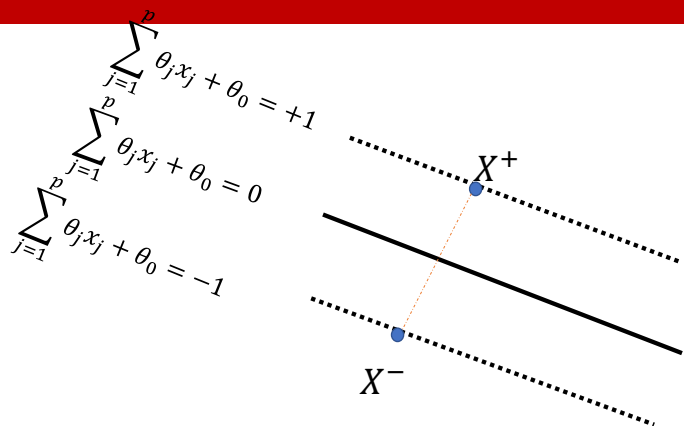
(i.e. we can get from X^- to X^+ by moving in the direction of θ for an unknown distance determined by λ)

Using the augmented form

$$\begin{aligned}\theta^T X^+ &= 1 \\ \theta^T (\lambda \theta + X^-) &= 1 \\ \lambda \theta^T \theta + \theta^T X^- &= 1\end{aligned}$$

But we know $\theta^T X^- = -1$

$$\begin{aligned}\lambda \theta^T \theta - 1 &= 1 \\ \lambda &= \frac{2}{\theta^T \theta} = \frac{2}{\|\theta\|^2}\end{aligned}$$



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Construction of the Maximal Margin Classifier (Cont.)

However

$$M = \frac{1}{2}(X^+ - X^-) = \frac{1}{2} \|\lambda \theta\| = \frac{1}{2} \frac{2\|\theta\|}{\|\theta\|^2} = \frac{1}{\|\theta\|}$$

- To maximize M

$$\max_{\theta_0, \theta_1, \dots, \theta_p} M$$

- We can minimize $\|\theta\|$ subject to constraint $t_i \left(\sum_{j=1}^p \theta_j x_j + \theta_0 \right) \geq 1$

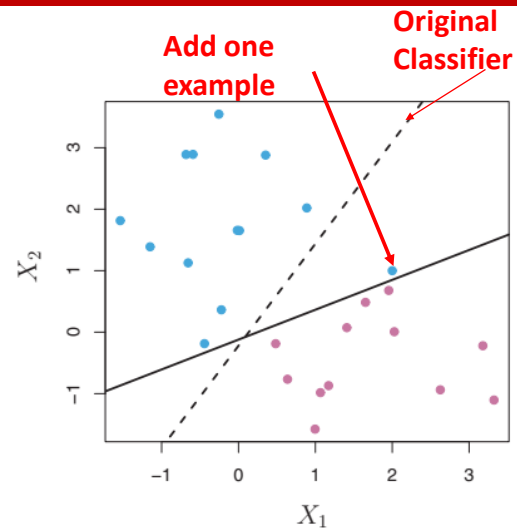
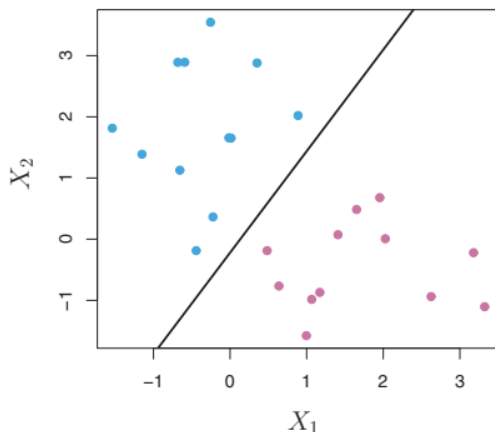
- That is minimize $\|\theta\|^2$ such that $t_i \left(\sum_{j=1}^p \theta_j x_j + \theta_0 \right) \geq 1$ for each observation (training example) i.

- The solution of this optimization problem is not in the scope of this course



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The Need for Support Vector Classifiers- reduce sensitivity to individual observations



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Support Vector Classifier

- Use a soft margin constraint
- Instead of

$$t_i \left(\sum_{j=1}^p \theta_j x_j + \theta_0 \right) \geq 1$$

- Let's use

$$t_i \left(\sum_{j=1}^p \theta_j x_j + \theta_0 \right) \geq (1 - \epsilon_i)$$

- $\epsilon_1, \epsilon_2, \dots, \epsilon_n$: Slack variables
- Where

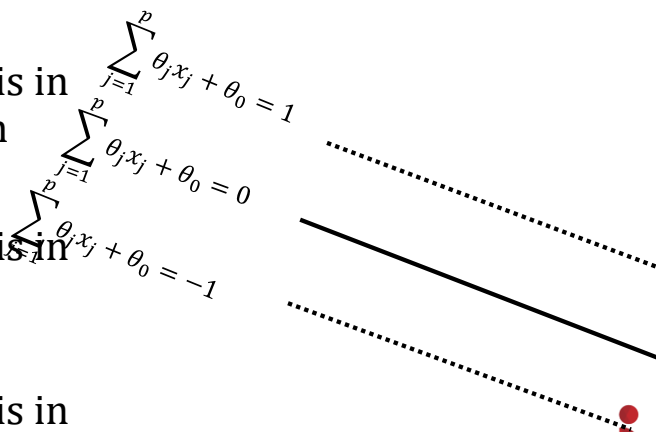
$$\epsilon_i \geq 0, \sum_{i=1}^n \epsilon_i \leq C$$



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Support Vector Classifier

- ϵ_i is a learnable parameter
- If $\epsilon_i = 0$, the i th observation is in the correct side of the margin
- If $\epsilon_i > 0$, the i th observation is in the wrong side of the margin
- If $\epsilon_i > 1$, the i th observation is in the wrong side of the hyperplane



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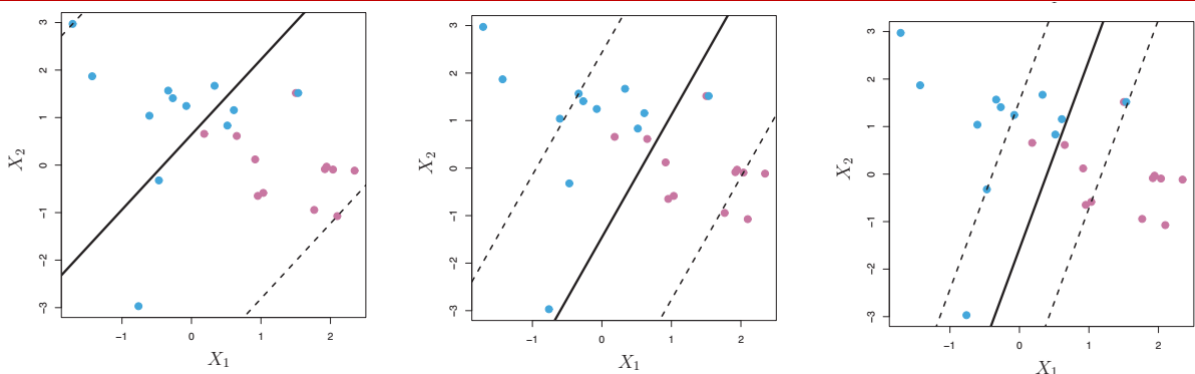
Tuning C hyperparameter

- C is a nonnegative tuning parameter.
- C bounds the sum of the ϵ_i 's, and so it determines the number and severity of the violations to the margin (and to the hyperplane) that we will tolerate.
- Increasing C, increases bias, reduces the variance (we become more tolerant of violations to the margin, margin will widen)
- Decreasing C, reduces bias, increases variance (we become less tolerant of violations to the margin, margin narrows)
- C is generally chosen via [cross-validation](#).



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Using different values of the tuning parameter C



Decreasing C



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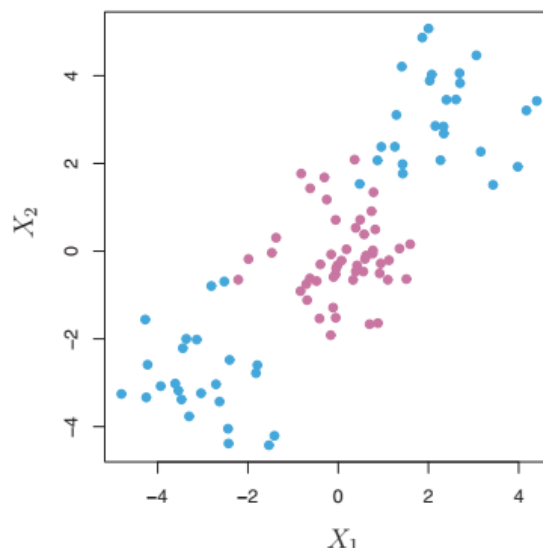
Using different values of the tuning parameter C

- For Unbalanced datasets, you may use a different C for each class.
- Assign a smaller C value for classes that have smaller number of examples (the model gives more importance to these classes)



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Non-linear Decision Boundaries



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Support Vector Machines (SVM)

- The support vector machine (SVM) is an extension of the support vector classifier that results from enlarging the feature space in a specific way, using kernels.
- The kernel approach allows us to accommodate a non-linear boundary between the classes
- Before discussing kernels, let's discuss the solution in case of the Maximal Margin Classifier



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Solution to the optimization problem introduced earlier

- Using Lagrange multipliers, you get that

$$\theta = \sum_{i=1}^n \alpha_i t^{(i)} X^{(i)}$$

To calculate $\alpha_1, \alpha_2, \dots, \alpha_n$, n : number of training examples

$$\max_{\alpha_i} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=0}^n t^{(i)} t^{(j)} \alpha_i \alpha_j \langle X^{(i)}, X^{(j)} \rangle$$

$\langle X^{(i)}, X^{(j)} \rangle$ is the dot product between the two observations $X^{(i)}, X^{(j)}$

Subject to

$$\alpha_i \geq 0, \sum_{i=0}^n \alpha_i t^{(i)} = 0$$



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Solution to the optimization problem introduced earlier

- The solution has n parameters $\alpha_1, \alpha_2, \dots, \alpha_n$
- The majority of these parameters will equal zero. Few (at support vectors) will have a value greater than 0



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Using Kernels

- Instead of the dot product $\langle X^{(i)}, X^{(j)} \rangle$, we use $K(X^{(i)}, X^{(j)})$
- $K(X^{(i)}, X^{(j)})$, the kernel function: a function that quantifies the similarity of two observations.

- Take

$$K(X^{(i)}, X^{(j)}) = \sum_{l=1}^p x_{il}x_{jl}$$

- It gives us the support vector classifier (linear)



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Common Kernels

- Polynomial kernel of degree d ($d > 1$)

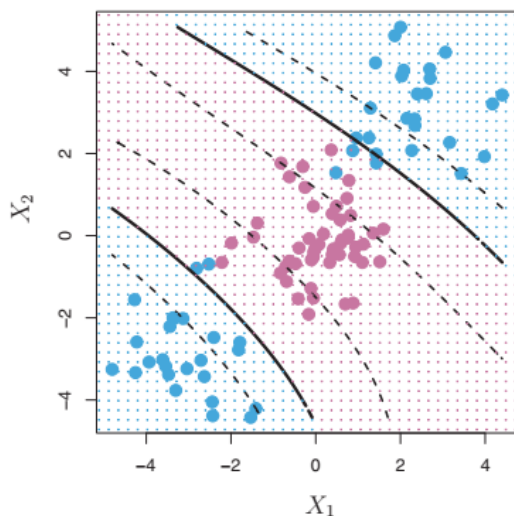
$$K(X^{(i)}, X^{(j)}) = \left(1 + \sum_{l=1}^p x_{il} x_{jl} \right)^d$$

- Radial Kernel

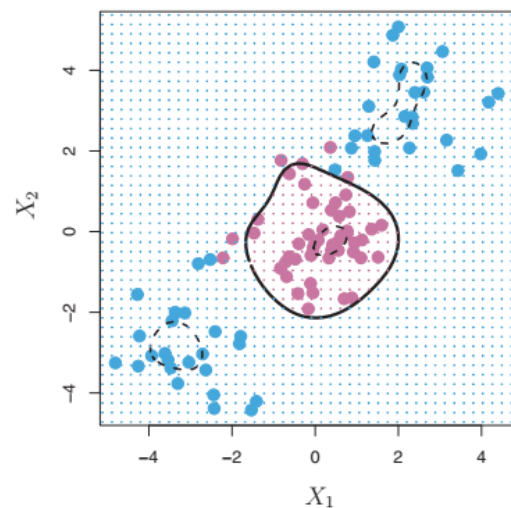
$$K(X^{(i)}, X^{(j)}) = \exp \left(-\gamma \sum_{l=1}^p (x_{il} - x_{jl})^2 \right)$$



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Polynomial kernel of degree 3



Radial Kernel



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