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3253 - Analytic Techniques and Machine Learning

Module 6: Support Vector Machines

Course Plan

Module Titles
Module 1 – Introduction to Machine Learning
Module 2 – End to End Machine Learning Project
Module 3 – Classification
Module 4 – Clustering and Unsupervised Learning
Module 5 – Training Models and Feature Selection
Module 6 – Current Focus: Support Vector Machines
Module 7 – Decision Trees and Ensemble Learning
Module 8 – Dimensionality Reduction
Module 9 – Introduction to TensorFlow
Module 10 – Introduction to Deep Learning and Deep Neural Networks
Module 11 – Distributing TensorFlow, CNNs and RNNs
Module 12 – Final Assignment and Presentations (no content)

Learning Outcomes for this Module

- Apply linear and non-linear Support Vector Machine (SVM) to classification problems
- Use SVM for regression problems
- Explore how SVM works

Topics for this Module

- **6.1** Introduction to Support Vector Machines (SVM)
- **6.2** Linear classification with SVM
- **6.3** Non-linear classification
- **6.4** SVM regression
- **6.5** How SVM works
- **6.6** Resources and Wrap-up

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Module 6 – Section 1

Introduction to Support Vector Machines (SVM)

SVM

- An ML algorithm for either classification or regression
- It can model both linear and non-linear patterns
- Most appropriate for small or mid-size data sets
- Training points (x, y) have labels +1 or -1

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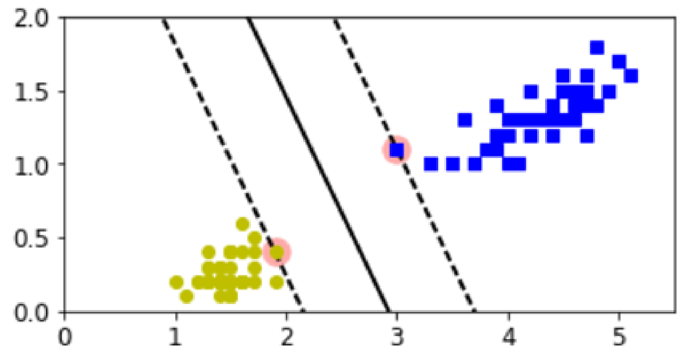
Module 6 – Section 2

Linear Classification with SVM

Linear Classification

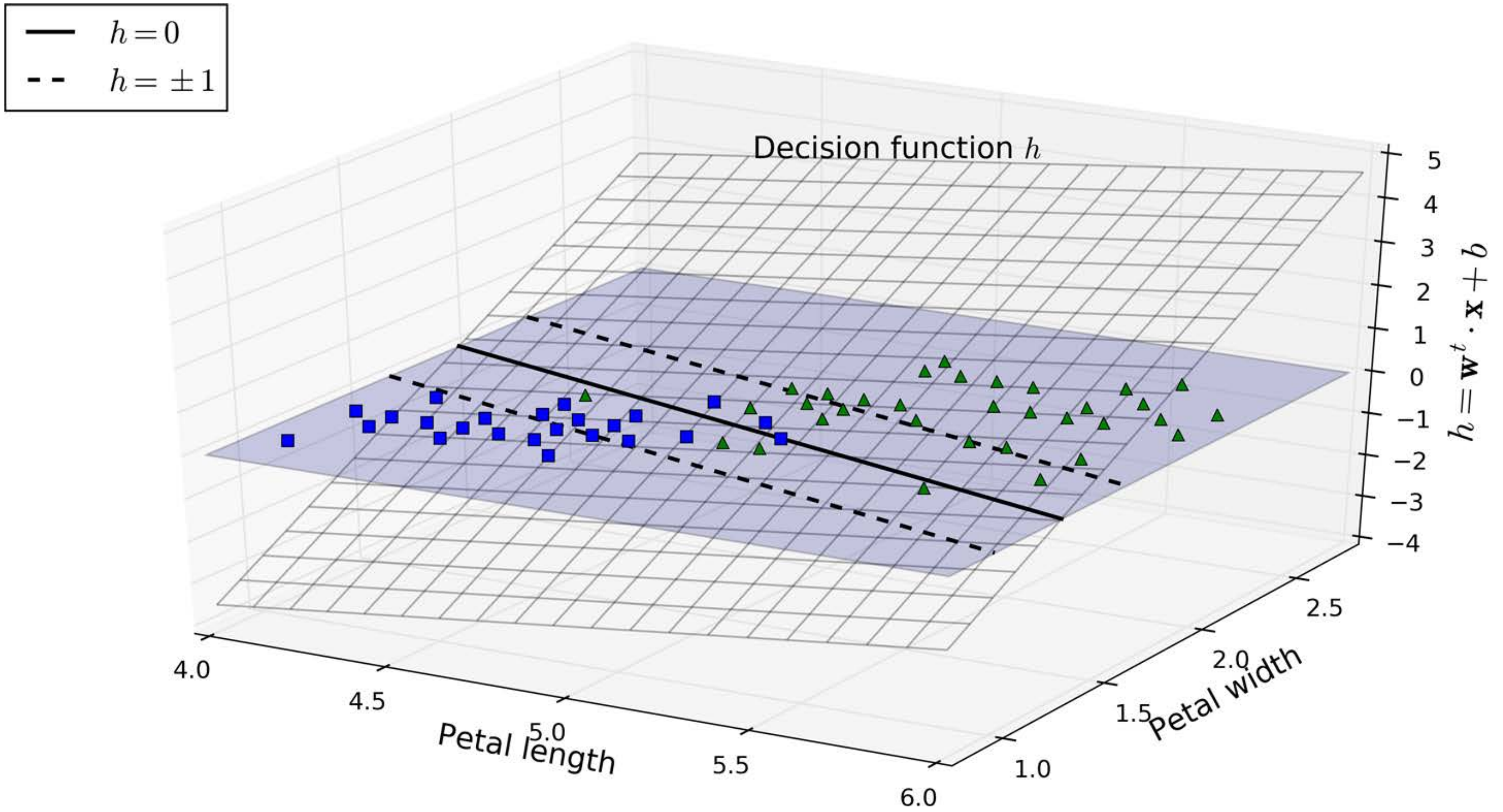
- A training set is linearly separable if a hyperplane leaves class +1 on one side and class -1 on the other side
- SVM finds the hyperplane that leaves the largest possible margin on both sides, until the first examples are found



Linear Classification (cont'd)

- A hyperplane in the plane is a line
- The points (x_1, x_2) in the line satisfy the equation $w_1 x_1 + w_2 x_2 + b = 0$ with w_1, w_2, b constants
- (w_1, w_2) is $\perp$ to the line
- A hyperplane in 3D space is a plane described as $w_1 x_1 + w_2 x_2 + w_3 x_3 + b = 0$
- In n-dimensions (features), a hyperplane is $w_1 x_1 + \ldots + w_n x_n + b = w^T \cdot x + b = 0$

Linear Classification (cont'd)



Linear Classification (cont'd)

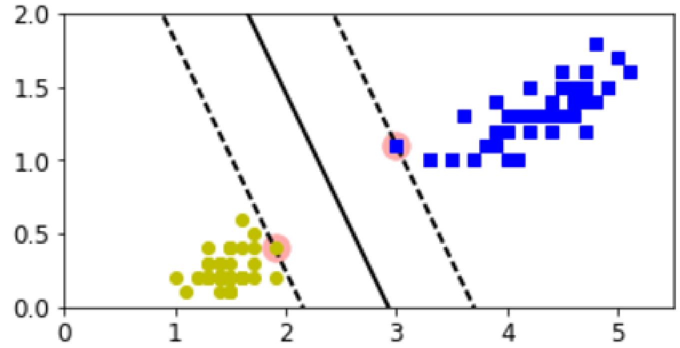
- If the data is linearly separable, the SVM algorithm finds w and b, so that class +1 satisfies $w^T \cdot x + b \geq 1$ and class -1 satisfies $w^T \cdot x + b \leq -1$

- Once w, b are known, new points x are classified by:

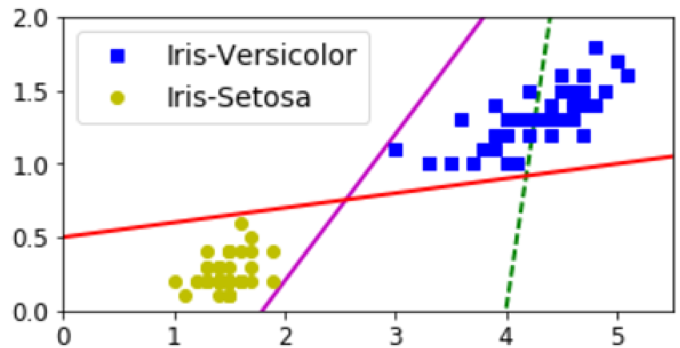
$$y = \begin{cases} +1, & if\ w^T \cdot x + b > 0 \\ -1, & if\ w^T \cdot x + b < 0 \end{cases}$$

Linear Classification (cont'd)

- What does an SVM solution look like?

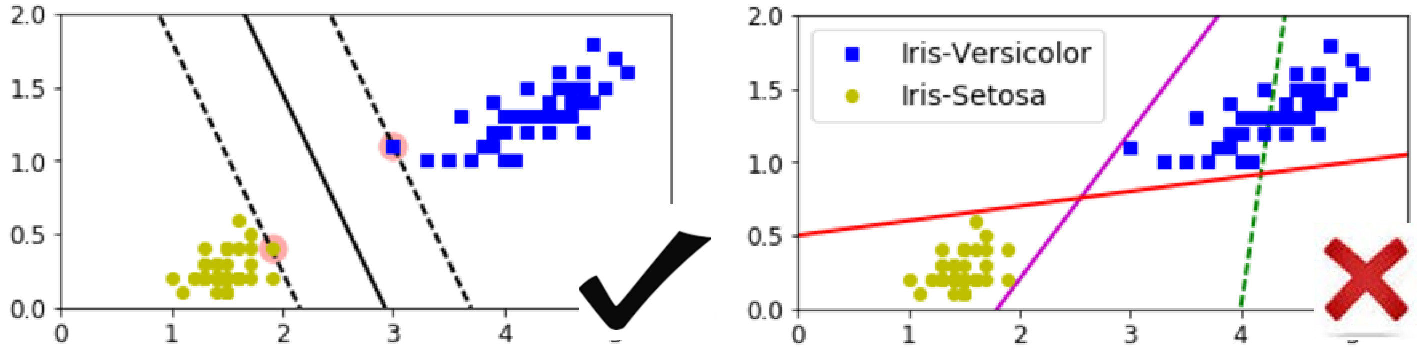


- What does it *not* look like?



Linear Classification (cont'd)

- What does an SVM solution look like?



- The vectors on the dashed lines are the *support vectors,* and determine the solution
- Neither Setosa examples to the far left, or Versicolor examples to the far right, determine the solution

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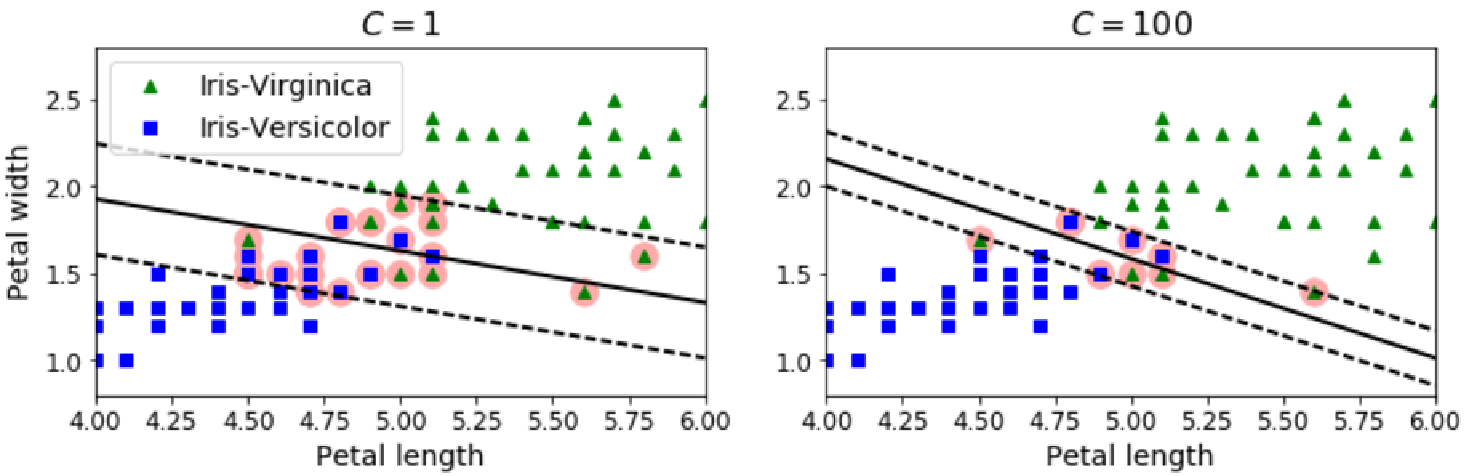
Linear Classification (cont'd)

- SVM described above is *hard margin*, no examples between dashed lines
- *Soft margin* SVM allows violations of this: examples within the dashed lines
- The solution finds a balance between wide margin and number of violations
- This is managed by a hyperparameter C
- Low C ⇔ big margin & more violations

Linear Classification (cont'd)

- C can be used for regularization
- If SVM overfits, decrease C. It allows violations, less aggressively fitting the data



- Violations may not be misclassifications

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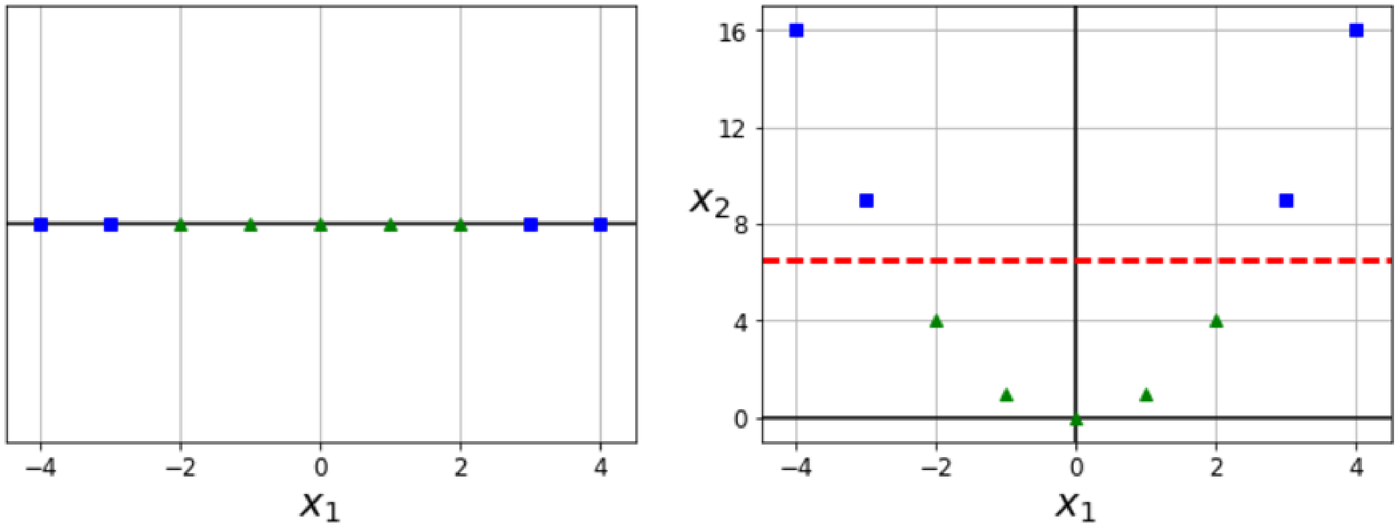
Module 6 – Section 3

Non-Linear Classification

Non-Linear Classification

- Non linearly-separable datasets can become so by adding new features
- A non linearly separable 1-feature set can become separable by transforming the feature (in this example, by squaring it)



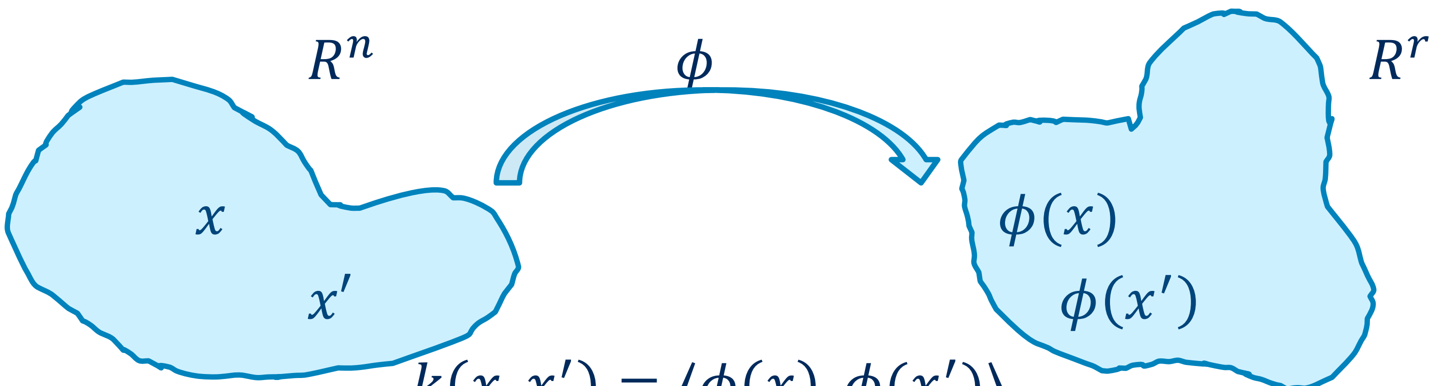
Non-Linear Classification (cont'd)

- Adding non-linear features manually is not the best approach. There's a better way!
- The algorithm works as if the original features are transformed non-linearly into a high dimensional space $\phi: R^n \rightarrow R^r, r \gg n$
- In R^r the dataset (hopefully) becomes separable, and linear SVM is applied
- The transformation ϕ is unknown. The algorithm does not actually use it

Non-Linear Classification (cont'd)

- All that is needed to do linear SVM is to apply inner product, with which geometry can be done, and w, b be found
- To do linear SVM is the transformed space we only need inner product $\langle \phi(x), \phi(x') \rangle$
- Kernel trick: only need a kernel in the original space $k: R^n \times R^n \rightarrow R$. Mercer's Thm. assures there exists $\phi: R^n \rightarrow R^r$ (for some r) such that $k(x, x') = \langle \phi(x), \phi(x') \rangle$

Non-Linear Classification (cont'd)



$$\underbrace{k(x, x')}_{\text{Doable}} = \underbrace{\langle \phi(x), \phi(x') \rangle}_{\text{Wanted}}$$

Non-linear SVM requires specifying the kernel

There are many possible kernels (hyperparameter)

Popular kernels: polynomial, gaussian, linear

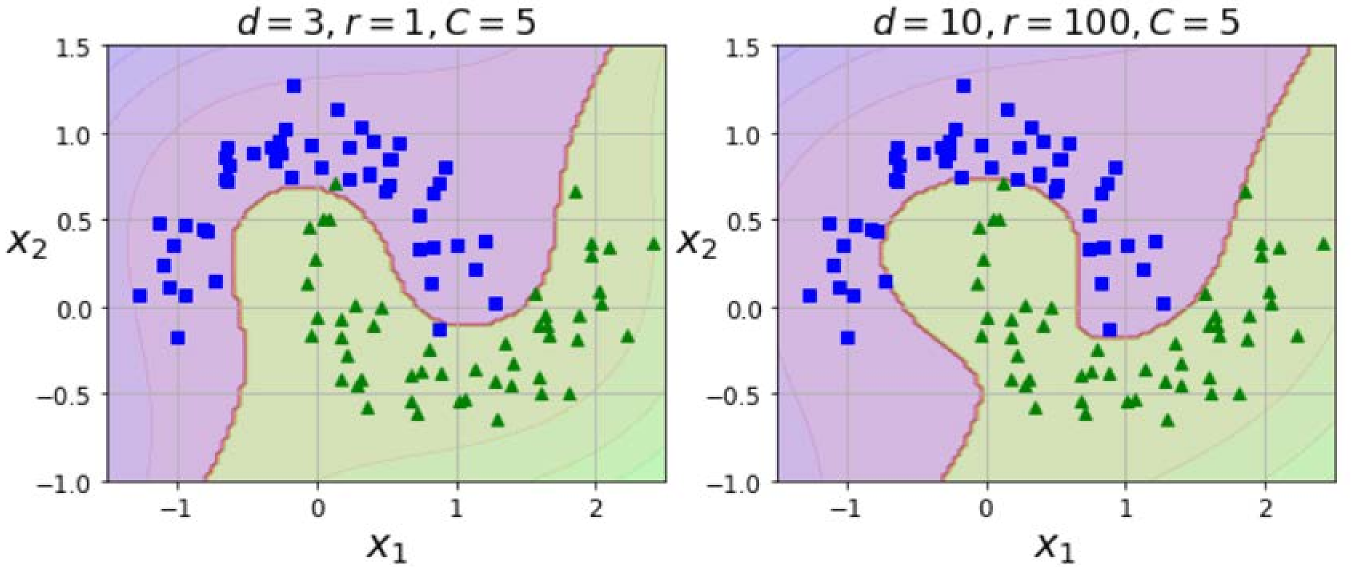
Non-Linear Classification (cont'd)

- Linear: $k(x, x') = \langle x, x' \rangle$
- Polynomial: $k(x, x') = (\langle x, x' \rangle + r)^d$
- Gaussian: $k(x, x') = \exp\left(-\gamma \left|\left|x - x'\right|\right|^2\right) = \exp(-\gamma\langle x -$

Non-Linear Classification (cont'd)

- Polynomial kernel is analogous to replacing the original features by many polynomial transformations of them

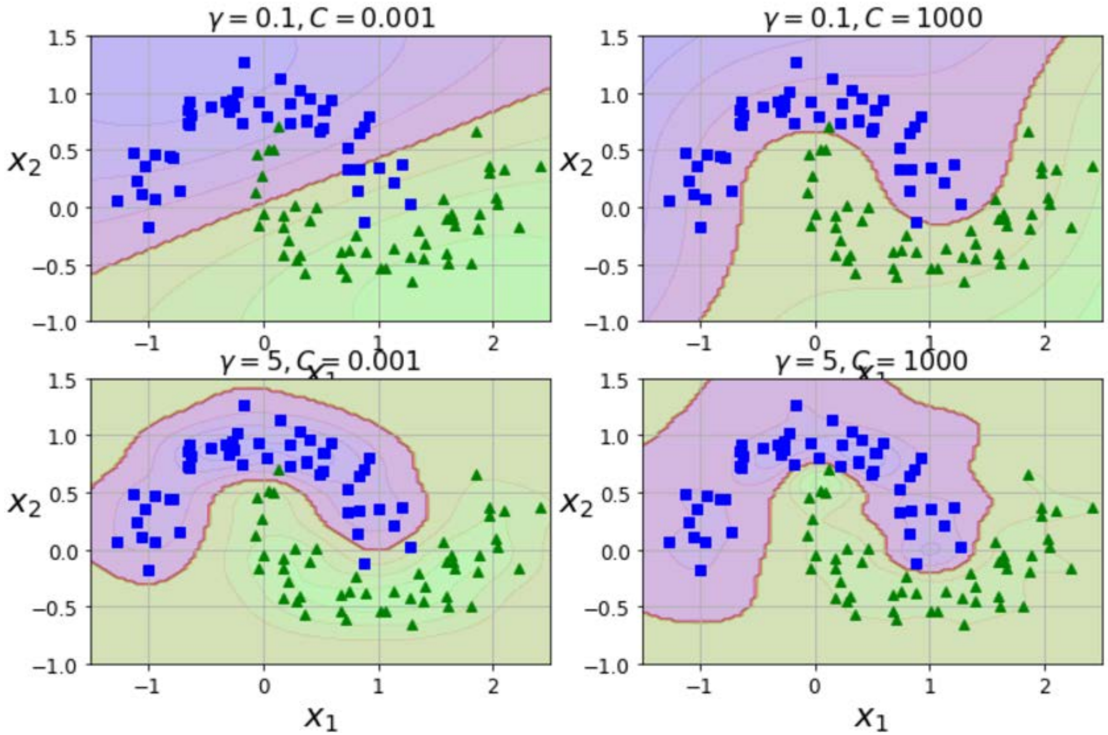
$$k(x, x') = (\langle x, x' \rangle + r)^d$$



Non-Linear Classification (cont'd)

- Gaussian Kernel

$$k(x, x') = \exp(-\gamma \left|\left| x - x' \right|\right|^2)$$



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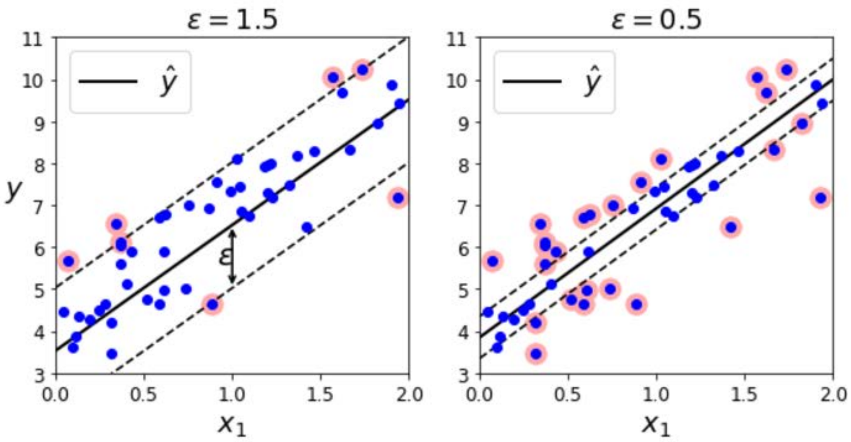
Module 6 – Section 4

SVM Regression

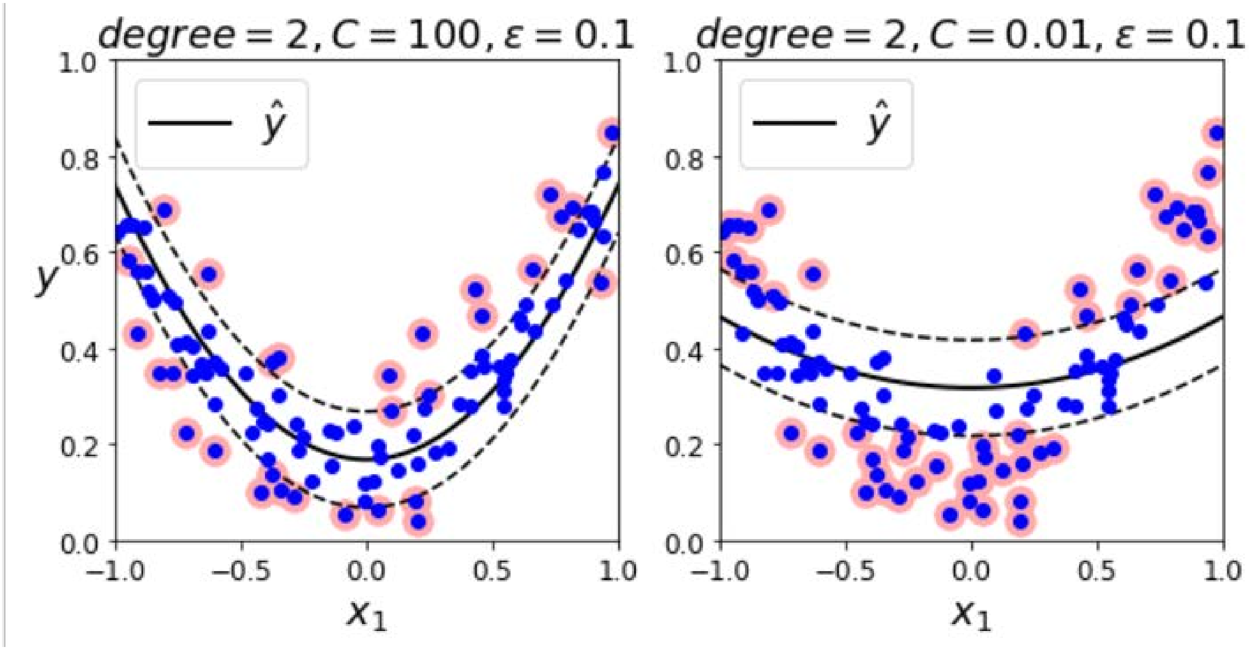
SVM Regression

- Classification goal: find parallel dashed lines as far as possible and containing few points between them
- Regression goal: find parallel dashed lines that are close to each other and contain as many points as possible
- Instead of C the regularization hyperparameter is ϵ



SVM Regression (cont'd)

- Non linear SVM Regression, same kernels
- E.g., polynomial kernels:



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Module 6 – Section 5

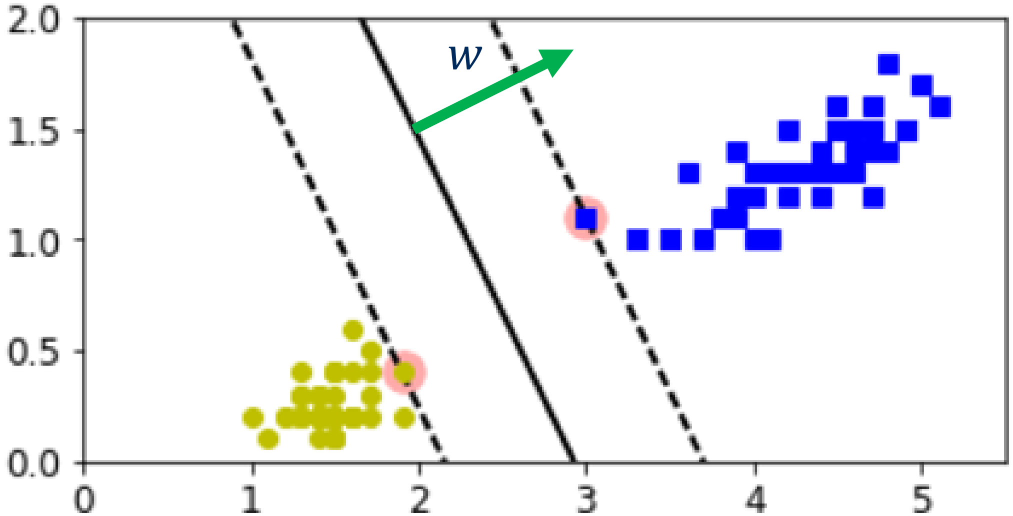
How SVM Works

How SVM works

- Linear SVM classifies points by:

$$y = \begin{cases} +1, & if\ w^T \cdot x + b > 0 \\ -1, & if\ w^T \cdot x + b < 0 \end{cases}$$

- The algorithm finds w $(\perp\ to\ line)$ and b



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How SVM works (cont'd)

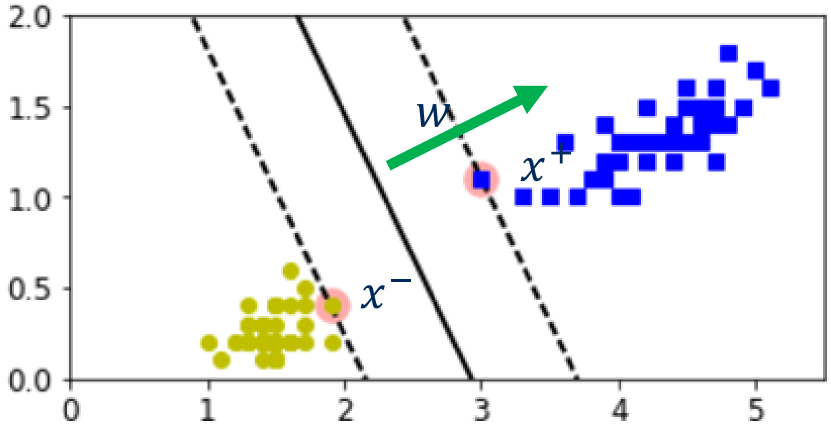
- Linear SVM classifies points by:

$$y = \begin{cases} +1, & if\ w^T \cdot x + b > 0 \\ -1, & if\ w^T \cdot x + b < 0 \end{cases}$$

- The algorithm finds w ($\perp\ to\ line$) and b

- Distance between margins: $\frac{w}{||w||}(x^+ - x^-) = \frac{2}{||w||}$

x^+, x^- are supports



How SVM works (cont'd)

- Optimization problem that yields w, b

$$\begin{cases} minimize: \dfrac{1}{2} w^T \cdot w \\ subject\ to: \ y^{(i)}\left(w^T \cdot x^{(i)} + b\right) \geq 1, for\ all\ i \end{cases}$$

- For soft margin: add slack variables

$$\begin{cases} minimize: \dfrac{1}{2} w^T \cdot w + C \displaystyle\sum_i \xi^{(i)} \\ subject\ to: y^{(i)}\left(w^T \cdot x^{(i)} + b\right) \geq 1 - \xi^{(i)} \end{cases}$$

How SVM works (cont'd)

- These formulations (*Primal*) are cases of Quadratic Programming

$$\begin{cases} minimize\ (variable\ u)\text{: } \dfrac{1}{2}u^T \cdot H \cdot u + f^T \cdot u \\ subject\ to\text{: } A \cdot u \leq d \end{cases}$$

where: $u, f \in R^{q\times 1}, H\ symmetrix\ q \times q, d \in R^{m\times 1}, A \in R^{m\times q}$

- With appropriate values for H, f, A, d, the primal formulation can be solved as QP problems (well studies)

How SVM works (cont'd)

- There is an equivalent formulation (same solution) to the Primal, called *Dual*

$$\begin{cases} minimize\ (variable\ \alpha): \sum_{i=1}^{m} \alpha_i y^{(i)} - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y^{(i)} y^{(j)} \langle x^{(i)}, x^{(j)} \rangle \\ subject\ to: \alpha_i \geq 0, \sum_{i=1}^{m} \alpha_i y^{(i)} = 0 \end{cases}$$

- Once α is found, it can be used to obtain w and b from the Primal formulation, and build the classifier

$$b = \frac{1}{n_s} \sum\nolimits_{i:\alpha_i > 0} (1 - y^{(i)} \langle w, x^{(i)} \rangle)$$

$$w = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}$$

How SVM works (cont'd)

- The Dual formulation is also applicable for the non linear case, using any kernel: replace $\langle _, _ \rangle$by k

$$\begin{cases} minimize\ (variable\ \alpha)\text{:} \sum_{i=1}^{m} \alpha_i y^{(i)} - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y^{(i)} y^{(j)} (k(x^{(i)}, x^{(j)})) \\ subject\ to\text{:} \alpha_i \geq 0, \sum_{i=1}^{m} \alpha_i y^{(i)} = 0 \end{cases}$$

- Once α is found, b can be found, and the classifier can be computed $y = w^T \cdot \phi(x) + b$:

$$b = \frac{1}{n_s} \sum_{i:\alpha_i > 0} \left(1 - y^{(i)} \sum_{j=1}^{m} \alpha_j y^{(j)} k(x^{(j)}, x^{(i)}) \right)$$

$$y = w^T x + b = \sum_{i=1}^{m} \alpha_i y^{(i)} k(x^{(i)}, x) + b$$

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Module 6 – Section 6

Resources and Wrap-up

Resources

- Hands-On Machine Learning with Scikit-Learn and Tensorflow

Assessment

- See Jupyter Notebook

Next Class

- Decision Trees

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Any questions?

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