Lecture 7: Support Vector Machines (SVM), scikit-learn

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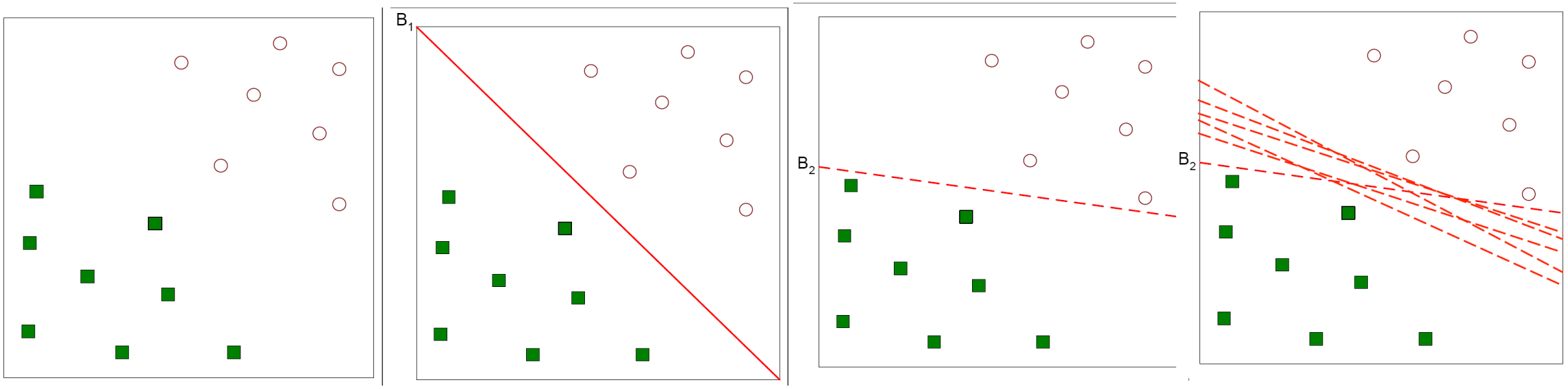
Support Vector Machines - introduction

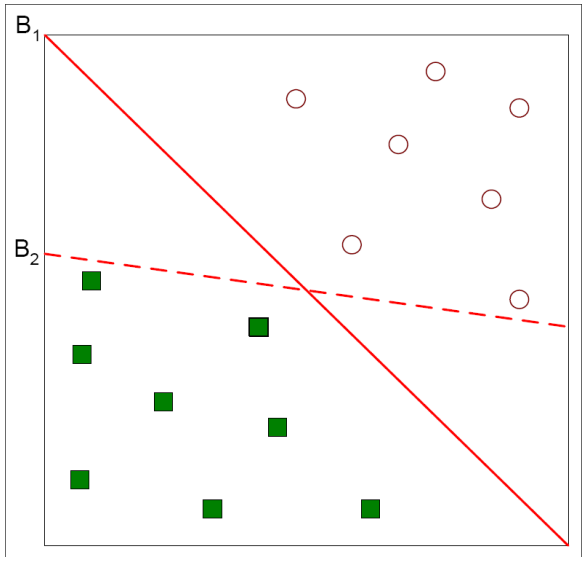
- SVM is an extension of perceptron. The perceptron model minimizes the misclassification error. SVM **maximizes the margin.**
- Find a linear hyperplane (decision boundary) that will separate the data.

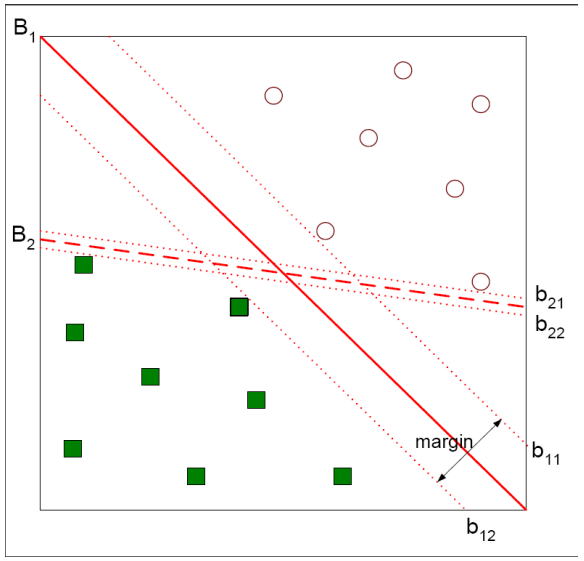


(a) dataset (b) Solution B1 (c) Solution B2 (d) Solution B3

Support Vector Machines - idea

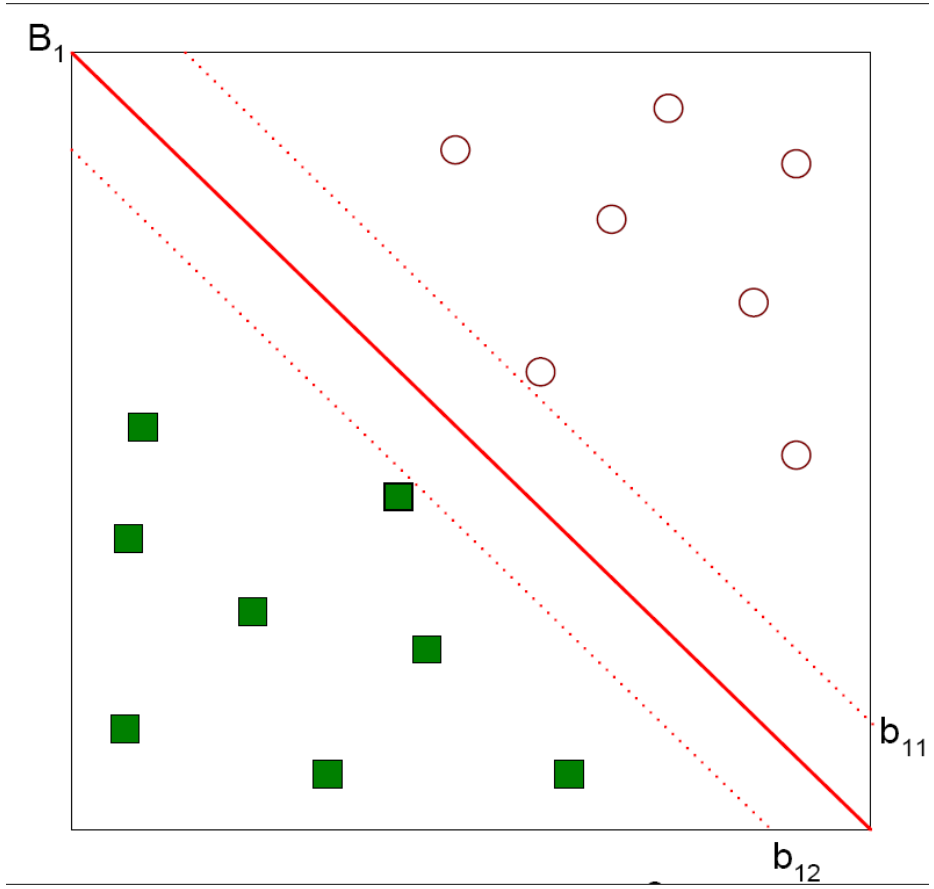
- Which one is better? B1 or B2?
- The bigger the margin, the better.
- Find hyperplane that maximizes the margin; so B1 is better than B2





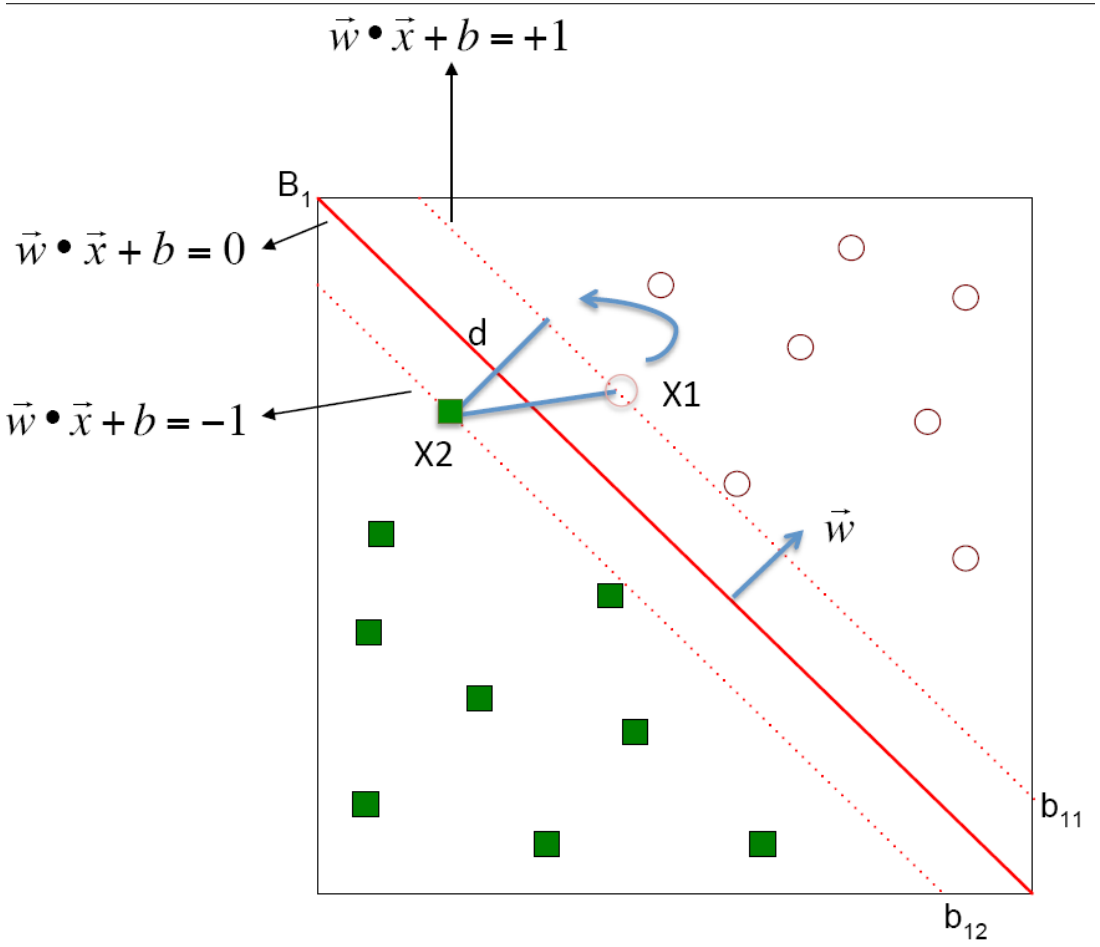
Support Vector Machines - formulation

- How do we formulate B1 and its margin, *b*11, and *b*12?



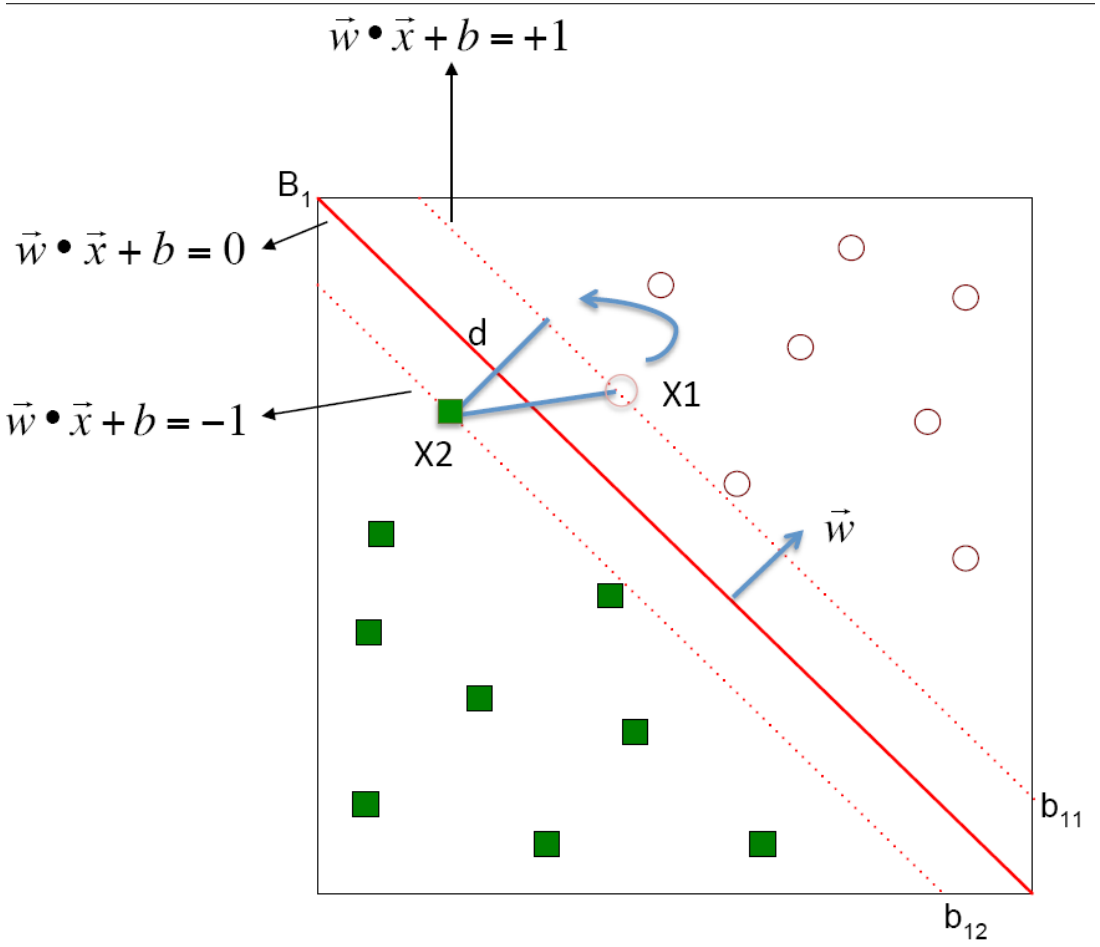
Support Vector Machines - Concepts

- **Decision boundary:** the separating hyperplane
- **Margin**: the distance between the decision boundary and the training samples that are closest to the decision boundaries
- **Support vectors**: the samples that are closest to the decision boundaries.



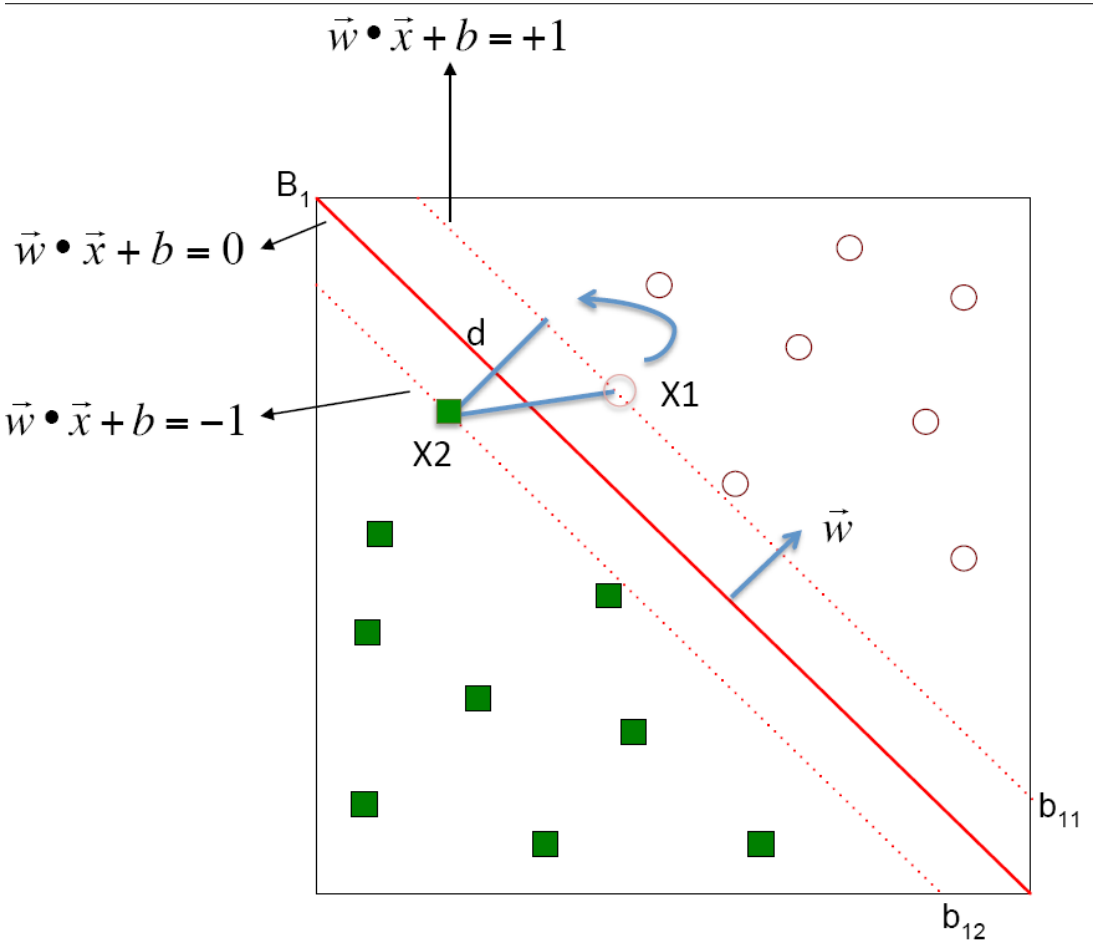
Support Vector Machines - formulation

- **Decision boundary**
  - B_1: $\mathbf{w}^\intercal \mathbf{x} + b = 0$
- Hyperplanes defining margins
  - b_{11} $(positive\ hyperplane)$
  - $\mathbf{w}^\intercal \mathbf{x} + b = 1$
  - b_{12} $(negative\ hyperplane)$
  - $\mathbf{w}^\intercal \mathbf{x} + b = -1$



Margin of the decision boundaries

- Let d be the distance between the two hyperplanes b11 and b12
- The margin of the decision boundaries
- b_{11}: $\mathbf{w}^T\mathbf{x} + b = 1$
- b_{12}: $\mathbf{w}^T\mathbf{x} + b = -1$
- Let x_1 be on b_{11} and x_2 be on b_{12}. Then, we have $\mathbf{w}^T x_1 + b = 1$ and $\mathbf{w}^T x_2 + b = -1$. Thus, $\mathbf{w}^T(x_1 - x_2) = 2$
- $\mathbf{w}^T(x_1 - x_2) = \| \mathbf{w} \| \times \| (\mathbf{x}_1 - \mathbf{x}_2) \| \times \cos(\theta)$ where $\|\cdot\|$ is the norm of a vector
- $\| \mathbf{w} \| \times \| (\mathbf{x}_1 - \mathbf{x}_2) \| \times \cos(\theta) = \| \mathbf{w} \| \times d$, where d is the length of vector $\mathbf{x}_1 - \mathbf{x}_2$ in the direction of vector $\mathbf{w}$.
- $\| \mathbf{w} \| \times d = 2$
- $d = \frac{2}{\|\mathbf{w}\|}$



Learn a linear SVM Model

- The training phase of SVM is to estimate the parameters **w** and b.
- The parameters must follow two conditions

$$y^{(i)} = \begin{cases} 1, & if\ \mathbf{w}^\intercal \mathbf{x}^{(i)} + b \geq 1 \\ -1, & if\ \mathbf{w}^\intercal \mathbf{x}^{(i)} + b \leq -1 \end{cases}$$

- These two conditions mean: all negative samples should fall on one side of the negative hyperplane, whereas all the positive samples should fall behind the positive hyperplane.

Formulate the problem

- We want to maximize the margin $d = \frac{2}{\|\mathbf{w}\|}$
  - This is equivalent to minimize $L(\mathbf{w}) = \frac{\|\mathbf{w}\|^2}{2}$
- Subjected to the following constraints:

$$y^{(i)} = \begin{cases} 1, & if\ \mathbf{w}^\intercal \mathbf{x}^{(i)} + b \geq 1 \\ -1, & if\ \mathbf{w}^\intercal \mathbf{x}^{(i)} + b \leq -1 \end{cases}$$

  - which is equivalent to $y^{(i)}\left(\mathbf{w}^\intercal \mathbf{x}^{(i)} + b\right) \geq 1, i \ldots, n$

Formulate the problem

- Constrained optimization problem.
  - Objective function: $Minimize\ \frac{\|\mathbf{w}\|^2}{2}$
  - subject to $y^{(i)}\left(\mathbf{w}^\intercal \mathbf{x}^{(i)} + b\right) \geq 1, i \ldots, n$
- **Convex** optimization problem
  - Objective function is quadratic
  - Constraints are linear
  - Can be solved using the standard **Lagrange multiplier** method, which is skipped.

Get **w** and b

- Solving the optimization problem
- We can get **w** and b

Prediction

- Given a test data point **z**, we can calculate
  - $y_z = sign(\mathbf{w}^\intercal \mathbf{z} + b)$
- If $y_z = 1$, the test instance is classified as positive class
- If $y_z = -1$, the test instance is classified as negative class

Different implementations in scikit-learn

- **SVC** class uses the LIBSVM library (which is an equivalent C/C++ library)

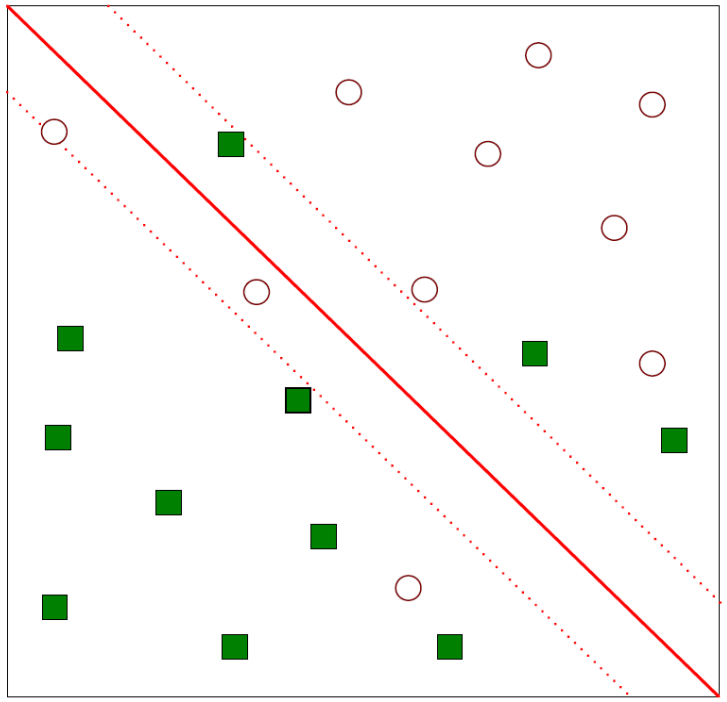
```
from sklearn.svm import SVC

svm = SVC(kernel='linear', C=1.0, random_state=1)
svm.fit(X_train_std, y_train)
```

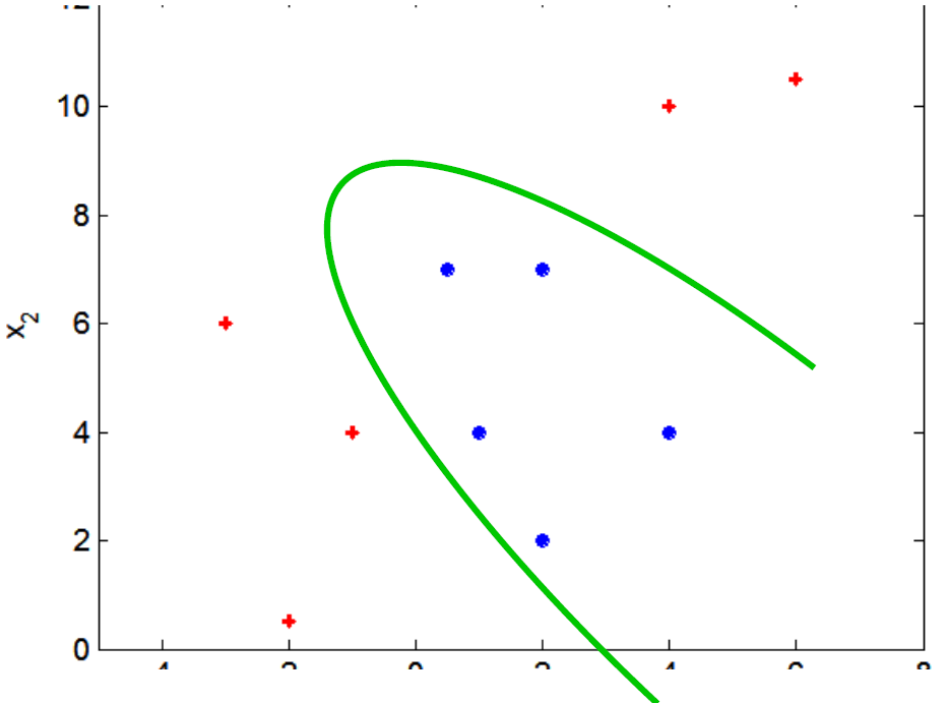
Different implementations in scikit-learn

- **SGDClassifier** class
  - It is a linear classifier (SVM, logistic regression) with SGD training.
  - Datasets are too large to fit into computer memory
  - Online learning via partial_fit method

```
from sklearn.linear_model import SGDClassifier

ppn = SGDClassifier(loss='perceptron')
svm = SGDClassifier(loss='hinge')
```

What is the problem if not linearly separable?





Dealing with a nonlinearly separable case using slack variables

- Introduce a slack variable ξ, to generate the so-called **soft-margin classification**.
- Subjected to the following constraints:

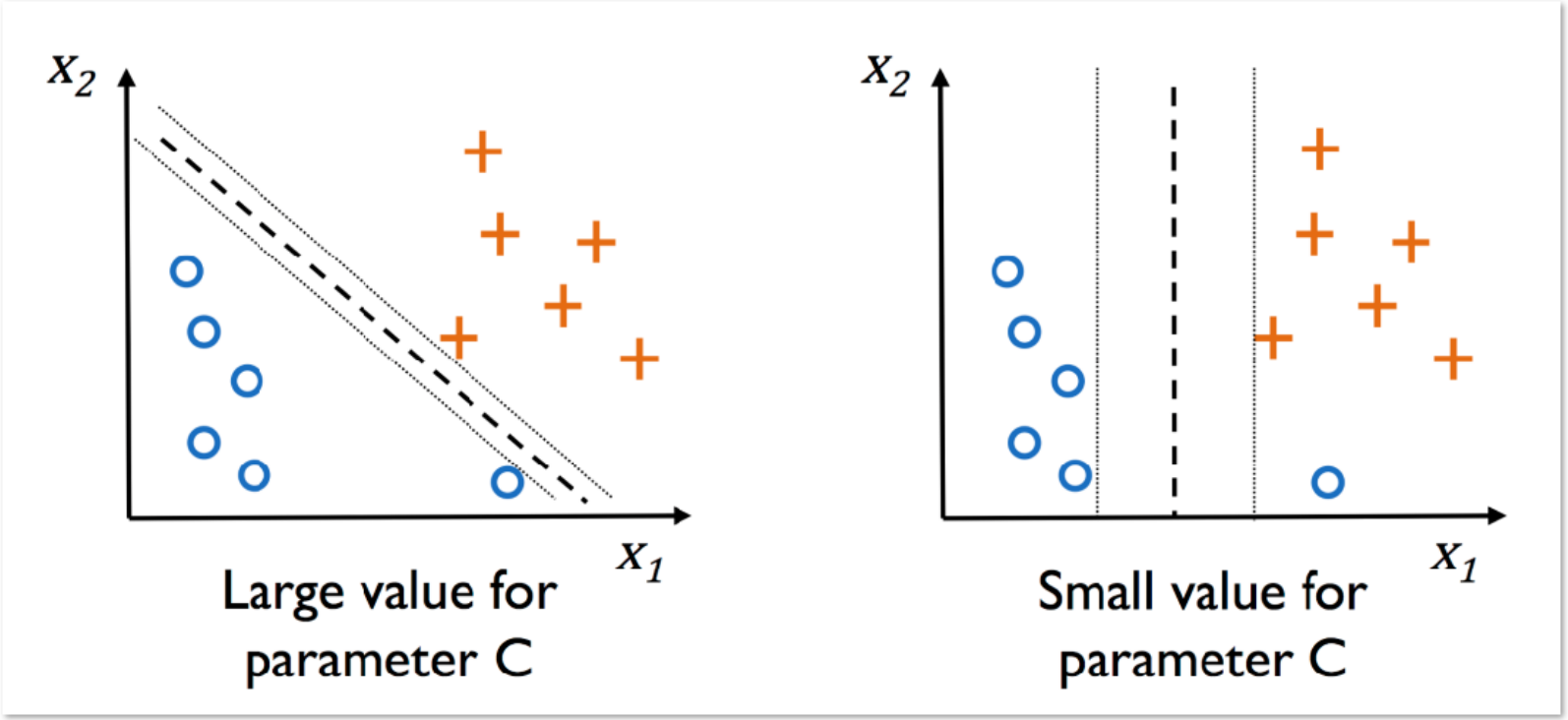
$$y^{(i)} = \begin{cases} 1, & if\ \mathbf{w}^\intercal \mathbf{x}^{(i)} + b \geq 1 - \xi^{(i)} \\ -1, & if\ \mathbf{w}^\intercal \mathbf{x}^{(i)} + b \leq -1 + \xi^{(i)} \end{cases}$$

- Objective function:

$$Minimize\ \frac{\| \mathbf{w} \|^2}{2} + C\left(\sum_{i=1}^{N} \xi^{(i)}\right)$$

Effect of C

- Control the penalty for misclassification
  - Larger value of C: for large error penalty
  - Smaller value of *C*: less strict about misclassification errors.



Kernel SVM: Use SVM to solve nonlinear problems

- SVM can be **kernelized** to solve nonlinear classification problem.
- **Kernel SVM**. The basic idea behind kernel methods is to create nonlinear combinations of the original features ($\boldsymbol{X}$ space) to project data points onto a higher-dimensional space (**Z** space) via a mapping function φ. In the higher-dimensional space, the data becomes linearly separable. We can train a linear SVM model to classify the data in the new space.
  - In particular, in the quadratic programming (QP) task, the SVM model replaces the dot product $\left(\mathbf{x}^{(i)}\right)^{\mathsf{T}}\mathbf{x}^{(j)}$ with $\phi\left(\mathbf{x}^{(i)}\right)^{\mathsf{T}}\phi(\mathbf{x}^{(j)})$.
- Support vectors live in **Z** space.

Kernel SVM

- During prediction, we use the same mapping function to transform the new data point to the new space and classify it using the linear SVM model.
  - E.g., $\phi(x_1, x_2) = (z_1, z_2, z_3) = (x_1, x_2, {x_1}^2 + {x_2}^2)$
- **Issue with the mapping approach**: It is relatively expensive to calculate the new features, especially for high-dimensional data.

Kernel trick

- **Kernel trick** is to address this issue.
- Define a kernel function $\mathcal{K}\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \phi(\mathbf{x}^{(i)})^{\mathsf{T}}\, \phi(\mathbf{x}^{(j)})$
- **Radial Basis Function (RBF) kernel** (also called Gaussian kernel)
  - $\mathcal{K}\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = \exp\left(-\frac{|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}|^2}{2\sigma^2}\right)$
  - Let $\gamma = \frac{1}{2\sigma^2}$, this kernel function is represented as
  - $\mathcal{K}\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = exp(-\gamma|x^{(i)} - x^{(j)}|^2)$
- RBF kernel is formed by taking an infinite sum over polynomial kernels (proof)

Explanation $\mathcal{K}\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = exp(-\gamma|x^{(i)} - x^{(j)}|^2)$

- $|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}|^2$ measures distance, then $-|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}|^2$ measures similarity
- Due to the exponential term, the similarity score is in the range of 0 (dissimilar) to 1 (similar).
- The extreme case is $\mathbf{x}^{(i)} = \mathbf{x}^{(j)}$, where $\mathcal{K}\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) = exp(0) = 1$
- When the distance is bigger, $\mathcal{K}\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)$ is smaller

Prediction

- In kernel SVM, we map the data points into a possibly infinite dimension Hilbert space *Z*. It turns out that w has the form

$$w = \sum_{i=1}^{n} \lambda_i y_i \varphi(x^{(i)})$$

  - where $\varphi(x^{(i)})$ is the mapped data point in the feature space
  - the $\lambda_i s$ are from the optimization solver (and if $x^{(i)}$ is not a support vector then λ_i=0).
- One of the things that makes SVM practical is that w is a finite linear combination of $\varphi\left(x^{(i)}\right)$.

Prediction

- We classify a new data point **x** by determining which side of the hyperplane x is on.
- Given the kernel function K, the calculation:

$$sign(\mathrm{b} + \boldsymbol{w}^T \mathbf{x}) = sign\left(b + \left(\sum_{i=1}^{n} \lambda_i y_i \varphi\left(x^{(i)}\right) \right)^T \varphi(x) \right)$$

$$= sign\left(b + \left(\sum_{i=1}^{n} \lambda_i y_i \varphi\left(x^{(i)}\right)^T \right) \varphi(x) \right)$$

$$= sign\left(b + \sum_{i=1}^{n} \lambda_i y_i K(x^{(i)}, x) \right)$$

Discussions

- Note that we never actually need to calculate any $\phi(x)$. We instead only need inner products which are provided by K. There is no way around computing this, but for certain kernels there may be tricks to compute it faster.
- Time calculation: the prediction of one data point needs to use all consuming the training instances.

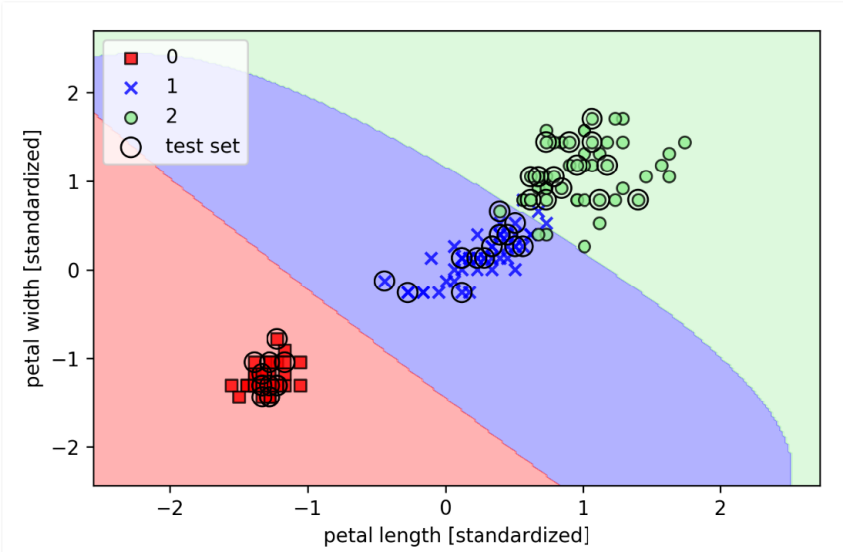
Scikit-learn implementation

- Parameter **kernel**='rbf' to represent the radial basis function 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. If a callable is given it is used to pre-compute the kernel matrix from data matrices; that matrix should be an array of shape (n_samples, n_samples).
- Parameter **gamma**: kernel coefficient for 'rbf', 'poly', and 'sigmoid'.

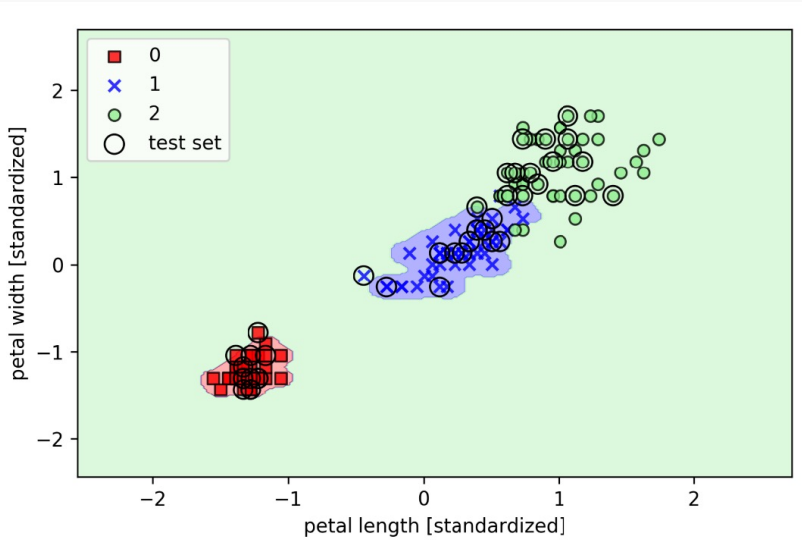
```
from sklearn.svm import SVC

svm = SVC(kernel='rbf', random_state=1, gamma=0.10, C=10.0)
svm.fit(X, y)
```

γ parameter

- γ parameter is treated as a cut-off parameter. The higher value leads to a tighter and bumpier decision boundary. A smaller value leads to a relatively soft boundary.



$\gamma = 0.2$



$\gamma = 100.0$

References

- Sebastian Raschka, Yuxi Liu, Vahid Mirjalili: Machine Learning with PyTorch and scikit-learn. 3rd Edition. ISBN 978-1-80181-931-2. Publisher: Packt Publishing Ltd. **Chapter 3**