Support Vector Machines(SVMs)

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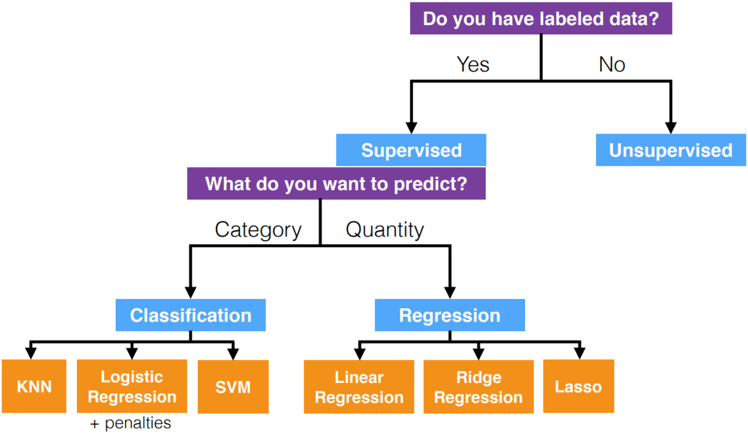
Agenda

- Hyperplanes
- Maximal margin classifier
- Support vector classifier
- Support vector machine

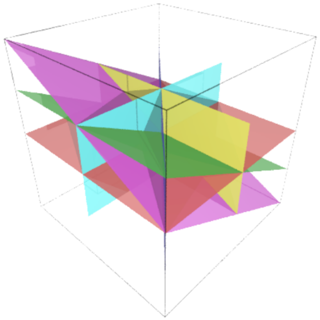

Do you have labeled data?
Yes
No
Supervised
Unsupervised
What do you want to predict?
Category
Quantity
Classification
Regression
KNN
Logistic Regression
SVM
Linear Regression
Ridge Regression
Lasso
+ penalties

Support vector machine (SVM) is a supervised method for binary classification (two class). It is a generalization of 1 and 2 below.

1. **Maximal margin classifier:** only applicable to linearly separable data.
2. **Support vector classifier:** can be applied to data that is not linearly separable. Decision boundary still linear.
3. **Support vector machine:** non-linear decision boundary.

What is a hyperplane?

- In p-dimensional space, a hyperplane is a $(p-1)$-dimensional affine subspace.
- In 2D, a hyperplane is a flat 1D subspace, aka a line.
- In 3D, a hyperplane is a flat 2D subspace, aka a plane.



Mathematical Definition

- A 2D hyperplane is defined by the equation:

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 = 0$$

- "Define" means any $\mathbf{X} = (X_1, X_2)$ for which the above equation holds is a point on the hyperplane.
- The above equation describes a line, which is a hyperplane in 2D.

Mathematical Definition

- In p dimensions, a hyperplane is defined by the equation:

$$\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p = 0$$

- Similarly, any $\mathbf{X} = (X_1, X_2, \ldots, X_p)$ for which the above equation holds is a point on the hyperplane.

Separating Hyperplane

- Instead of a point on the hyperplane, consider $\mathbf{X}$ for which

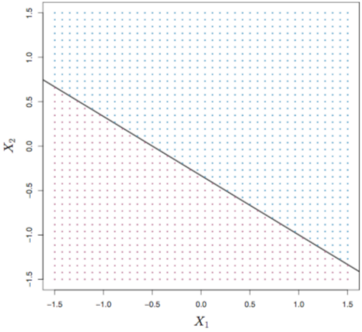
$$\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p > 0$$

- This point lies on one side of the hyperplane. An $\mathbf{X}$ for which

$$\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p < 0$$

  lies on the other side of the hyperplane.
- We can think of the hyperplane as dividing the p-dimensional space into two halves.

Separating Hyperplane



ISL (8th printing, 2017)

- This hyperplane in 2 dimensions is the line

$$1 + 2X_1 + 3X_2 = 0$$

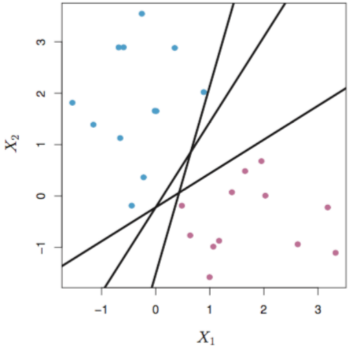
- The blue region is the set of points for which

$$1 + 2X_1 + 3X_2 > 0$$

- The purple region is the set of points for which

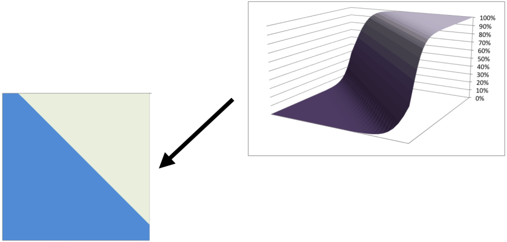
$$1 + 2X_1 + 3X_2 < 0$$

- **Idea:** Use a separating hyperplane for binary classification.
- **Key assumption:** Classes can be separated by a linear decision boundary.



ISL (8th printing, 2017)

- **Aside:** Logistic regression effectively finds a separating hyperplane.



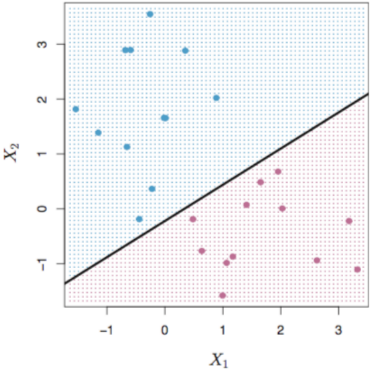
- Maximal margin classifiers and SVMs do this differently.

Separating Hyperplane Classifier

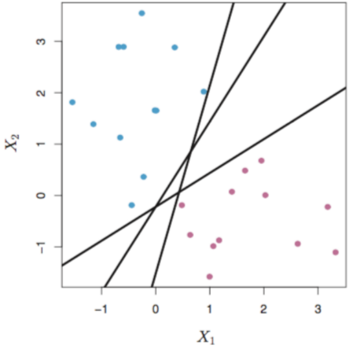
- **To classify new data points:**
- Assign class by location of new data point with respect to the hyperplane.

$$\hat{y} = \text{sign}(\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p)$$

- The farther away a point is from the separating hyperplane, the more confident we are about its class assignment.



- Notice that for a linearly separable dataset, there are many possible separating hyperplanes that divide the dataset into two classes (in fact, an infinite number).



Which decision boundary?

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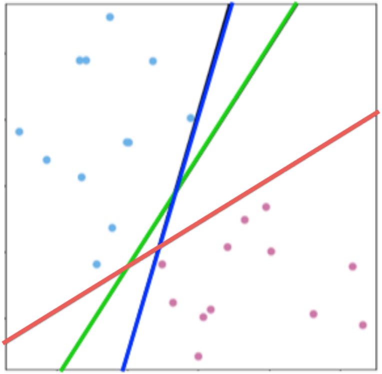
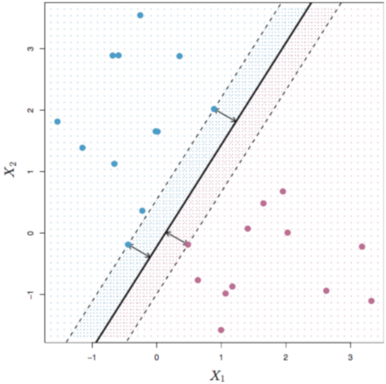
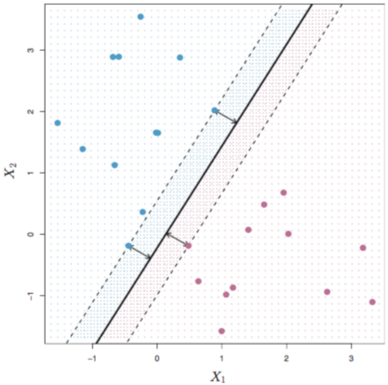
- Multiple decision boundaries can perfectly separate the data.
- Which one should we choose?
- Some boundaries may generalize better than others.



- Which of the infinite separating hyperplanes should we choose?
- A natural choice is the **maximal margin hyperplane**.
- It is the separating hyperplane that is farthest from the training samples.



- Margin: smallest distance between any training observation and the hyperplane.
- Support vectors: training observations whose distance to the hyperplane is equal to the margin



Why is it called a support vector?

- "Support": maximal margin hyperplane only depends on these observations.
- "Vector": points are vectors in p-dimensional space.
- If support vectors are perturbed, then MM hyperplane will change.
- If other training observations perturbed (provided not perturbed within margin distance of hyperplane), then MM hyperplane not affected.

Finding Maximal Margin Classifier

- To find the maximal margin hyperplane on data $(\vec{x}^{(i)}, y^{(i)})$, where $y^{(i)} \in \{-1, 1\}$, solve:

$$\max_{\beta_0,\ldots,\beta_p} M$$

- maximize the margin, M

$$\text{subject to} \quad \sum_{j=0}^{p} \beta_j^2 = 1$$

- constraint necessary for well-defined optimization problem

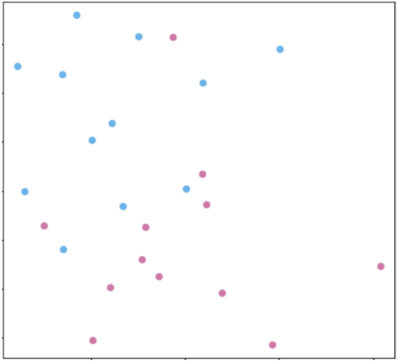
$$y^{(i)} \left(\beta_0 + \beta_1 x_1^{(i)} + \ldots + \beta_p x_p^{(i)} \right) \geq M, \quad \forall i$$

- all training points must be at least distance M from hyperplane

Finding Maximal Margin Classifier

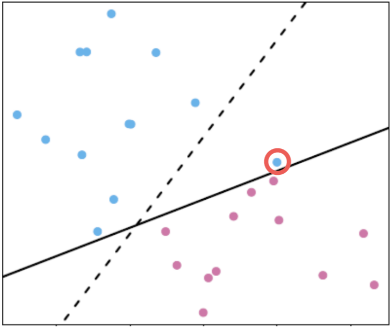
- To find the maximal margin hyperplane on data $(\vec{x}^{(i)}, y^{(i)})$, where $y^{(i)} \in \{-1, 1\}$, solve:
- $$\max_{\beta_0,\ldots,\beta_p} M$$
- subject to $\sum_{j=0}^{p} \beta_j^2 = 1$
- $y^{(i)} \left(\beta_0 + \beta_1 x_1^{(i)} + \ldots + \beta_p x_p^{(i)}\right) \geq M, \quad \forall i$
- Can be written as a convex optimization problem.
- We know how to solve convex optimization problems efficiently to find M and β.

- Recall the assumption: Classes can be separated by a linear decision boundary.
- What if there is no separating hyperplane?



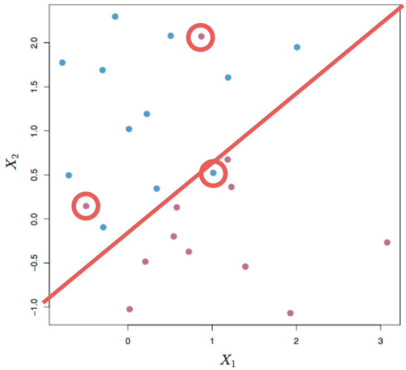
Maximal Margin Classifier

- Furthermore, notice a disadvantage of the maximal margin classifier:
  - Can be sensitive to individual observations
  - May overfit training data

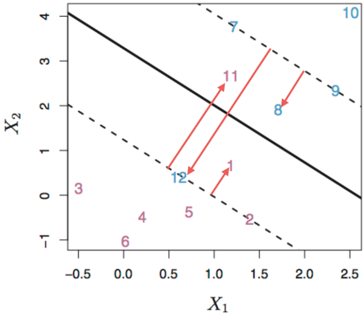


Support Vector Classifier

- Like the maximal margin classifier, it looks for a hyperplane to perform classification.
- However, training samples are allowed to be on the “wrong side” of the margin or hyperplane.
- This hyperplane *almost* separates the classes using a “soft margin”.

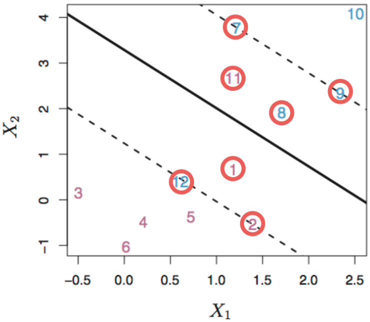


Support Vector Classifier



- Some points are allowed to violate the margin.

Support Vector Classifier



- Support vector classifiers also have support vectors.
- They are points lying directly on the margin, or on the wrong side of the margin for their class.
- These observations affect the hyperplane.

To find the support vector classifier hyperplane, solve:

$$\max_{\beta_0,\ldots,\beta_p,\epsilon_1,\ldots,\epsilon_n} M$$

$$\text{subject to } \sum_{j=0}^{p} \beta_j^2 = 1$$

$$y^{(i)}\left(\beta_0 + \beta_1 x_1^{(i)} + \ldots + \beta_p x_p^{(i)}\right) \geq M(1-\epsilon_i), \quad \forall i$$

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

Support Vector Classifier

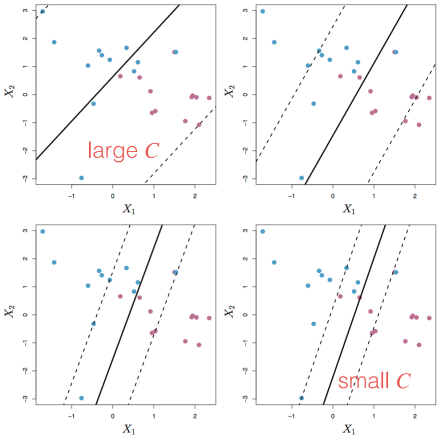
- Slack variables ϵ_i allow for violations of the margin.
  - $\epsilon_i = 0$: training point is on correct side of margin
  - $\epsilon_i > 0$: training point violates the margin
  - $\epsilon_i > 1$: training point is misclassified (wrong side of hyperplane)
- Penalty parameter C is the total "budget" for violations.
  - Allows at most C misclassifications on training set.

How do we choose C?

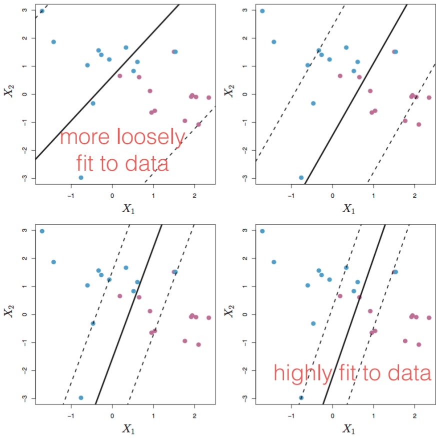
- As with many things we don't know *a priori* in machine learning, C is a hyperparameter that we tune using cross-validation.
- Note that it must be non-negative.
- If $C = 0$, we recover the maximal margin classifier (if one exists).
- As C goes from small to large, there is a bias-variance tradeoff.

Bias, Variance and C

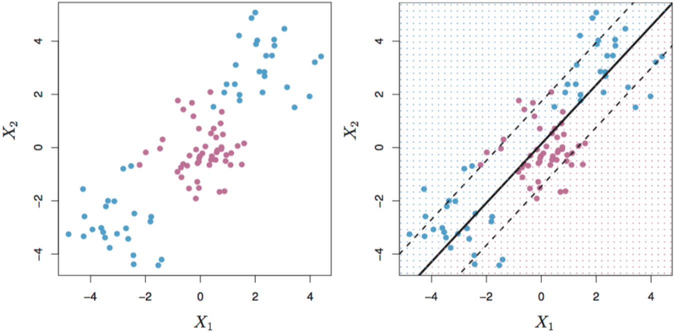
- **Large** C
  - Large violation budget
  - Large margin
  - Many support vectors
- **Small** C
  - Small violation budget
  - Small margin
  - Few support vectors



- **Large** C
  - High bias
  - Low variance
- **Small** C
  - Low bias
  - High variance



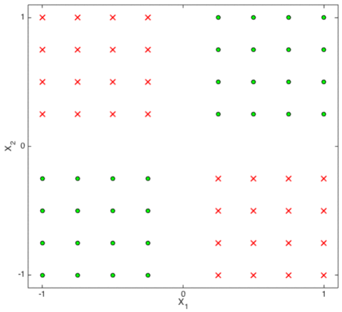
We are still using a **linear** *decision boundary.*



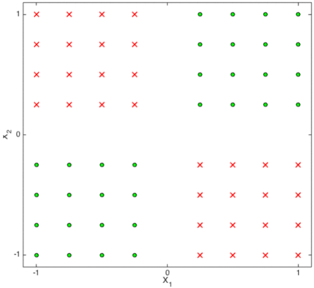
Expanding Feature Space

Some datasets are not linearly separable, but they *become* linearly separable when transformed into a *higher* dimensional space.

(Note: Yes, higher dimension also increases chance of overfitting. But in some cases the tradeoff is worthwhile.)

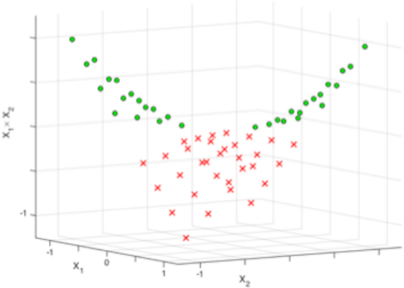


Original feature space



variables x_1, x_2

New feature space



variables x_1, x_2, $x_1 x_2$

Expanding Feature Space

- In linear regression, we created new features to capture non-linearity of data.
- For example:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \epsilon$$

- We can apply the same technique to support vector classifiers.

- Suppose our original data has p features.

$$\vec{X} = (X_1, X_2, \ldots, X_p)$$

- We can expand the feature space to include e.g. $2p$ features.

$$\vec{X} = (X_1, X_1^2, X_2, X_2^2, \ldots, X_p, X_p^2)$$

$$= (\tilde{X}_1, \tilde{X}_2, \tilde{X}_3, \tilde{X}_4, \ldots, \tilde{X}_{2p-1}, \tilde{X}_{2p})$$

Expanding Feature Space

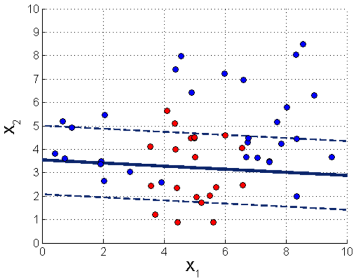
- Support vector classifier will find a hyperplane in $2p$ dimensions:

$$\beta_0 + \beta_1 \tilde{X}_1 + \beta_2 \tilde{X}_2 + \cdots + \beta_{2p-1} \tilde{X}_{2p-1} + \beta_{2p} \tilde{X}_{2p} = 0$$

- Hyperplane will be non-linear in *original* feature space. In this case, it is an ellipse:

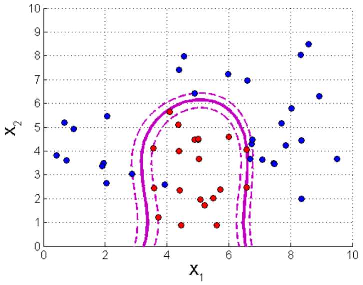
$$\beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \cdots + \beta_{2p-1} X_p + \beta_{2p} X_p^2 = 0$$

Non-linear Decision Boundary

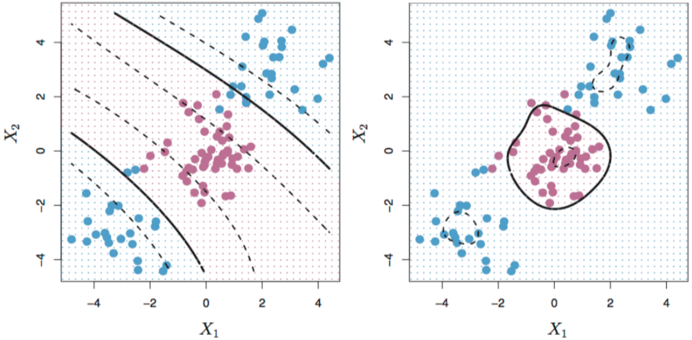


Expanding Feature Space

- Can imagine adding higher-order polynomial terms, quotients, and more to expand feature set.
- Large number of features becomes computationally challenging.
- We need an efficient way to work with large number of features.



- Extends the support vector classifier by using **kernel functions** to achieve non-linear decision boundaries.



- **Kernel function:** generalization of inner product. It takes in two arguments and *implicitly* computes their inner product in some feature space.
- Kernels are an efficient computational approach to create non-linear decision boundaries.
- They (implicitly) map data into a higher-dimensional space.
- We then apply a support vector classifier in this high-dimensional space with a linear decision boundary (hyperplane).

It can be shown that a support vector classifier can be represented as:

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i \langle x, x_i \rangle$$

- $f(x) > 0$ is one class, $f(x) < 0$ is another
- S is the set of support vectors
- $\langle x, x_i \rangle$ is the **inner product**

Where:

$$\langle \vec{u}, \vec{v} \rangle = \sum_{j=1}^{p} u_j v_j$$

General SVM

It can be shown that a support vector classifier can be represented as:

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i \langle x, x_i \rangle$$

In SVM, we replace the inner product with a kernel function:

$$f(x) = \beta_0 + \sum_{i \in S} \alpha_i K\left(x^{(i)}, x\right)$$

Properties of Kernels

- **Generalization of inner product:**

  for an explicit feature map $\phi : \mathcal{X} \to \mathcal{X}^{\phi}, \quad x \mapsto \phi(x)$

  $$K(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{X}^{\phi}}$$

- **Symmetric:** $K(x, x') = K(x', x)$
- **Gives a measure of similarity** between X and X'
  - If X and X' are close together, then $K(X, X')$ is large
  - If X and X' are far apart, then $K(X, X')$ is small

For a more formal definition: http://mlweb.loria.fr/book/en/constructingkernels.html

Common SVM Kernels

- **Linear kernel**

$$K(x, x') = \langle x, x' \rangle$$

- **Polynomial kernel** (degree p)

$$K(x, x') = (1 + \langle x, x' \rangle)^p$$

- **Radial basis kernel**

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

(an infinite-dimensional feature map!)

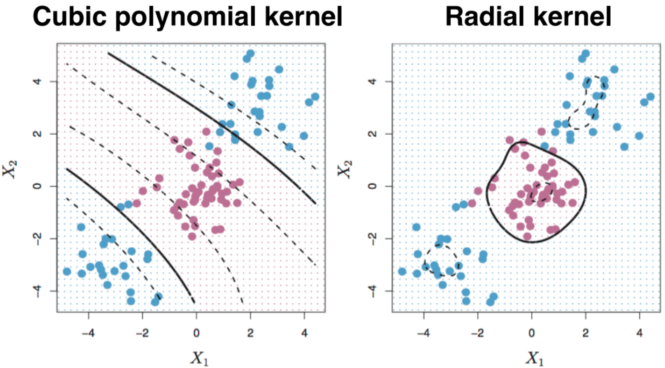
Why use kernels?

- Why use kernels instead of explicitly constructing a larger feature space?
- Computational advantage:

$$\phi : \mathbb{R}^p \rightarrow \mathbb{R}^P, \quad p \ll P$$

$$K(x, x') = \langle \phi(x), \phi(x') \rangle \quad \text{in } \mathcal{O}(p)$$

SVM with Non-Linear Kernels



SVM Summary

Pros:

- Regularization parameter C helps avoid overfitting
- Use of kernel gives flexibility in shape of decision boundary
- Optimization problem is convex — unique solution

Cons:

- Must tune hyperparameters (e.g. C, kernel function)
- Must formulate as binary classification
- Difficult to interpret

SVM with 3+ Classes

- SVMs are designed for binary classification, given the nature of a separating hyperplane.
- We can adapt SVMs to perform classification when we have more than 2 classes.
- Popular approaches:
  - One-versus-one
  - One-versus-all

- Construct an SVM for each pair of classes.
- For k classes, this requires training $k(k-1)/2$ SVMs.
- To classify a new observation:
  - Apply all $k(k-1)/2$ SVMs to the observation.
  - Take the most frequent class among the pairwise results as the predicted class.
- **Con:** computationally expensive for large k.

One-versus-all Classification

- Construct an SVM for each class against the $k - 1$ other classes pooled together.
- For k classes, this requires training k SVMs.
- Distance to separating hyperplane is a proxy for classification confidence.
- To classify a new observation:
  - Choose the class with the highest confidence (i.e., farthest from the hyperplane).
- **Con:** may exacerbate class imbalances; distance to hyperplane may not correspond well to confidence.

[1] Sherrie Wang et al. *CME250: Introduction to Machine Learning*. Stanford University, Winter 2019. https://web.stanford.edu/class/cme250/.