COMP 7990
Principles and Practices of Data Analytics

Lecture 3: Support Vector Machine and k Nearest Neighbors (k-NN) Algorithm

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Outline for Data Preprocessing and Data Mining

- **Data Preprocessing**
- **Supervised learning**

❖ Regression

1. Linear regression with one variable
2. Linear Regression with multiple variables

❖ Classification

1. Perceptron
2. Artificial Neural Network
3. Support Vector Machine
4. K Nearest Neighbor

- **Unsupervised learning**

1. K-means Clustering
2. Hierarchical Clustering

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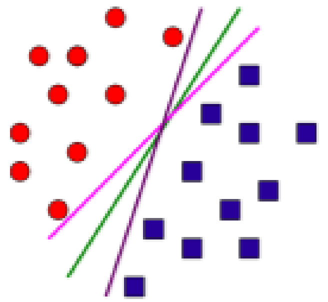
What Is the Best Hyperplane Separator?

- Perceptron finds one of many possible hyperplanes separating the data
  - If the hyperplane exist

- Among the many possible hyperplanes, which one is the best?

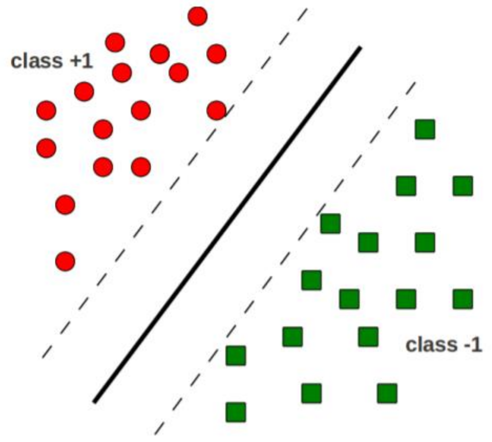


- Intuitively, we want the hyperplane not too close to each of the classes. In other words, the one with the maximum margin is preferred.

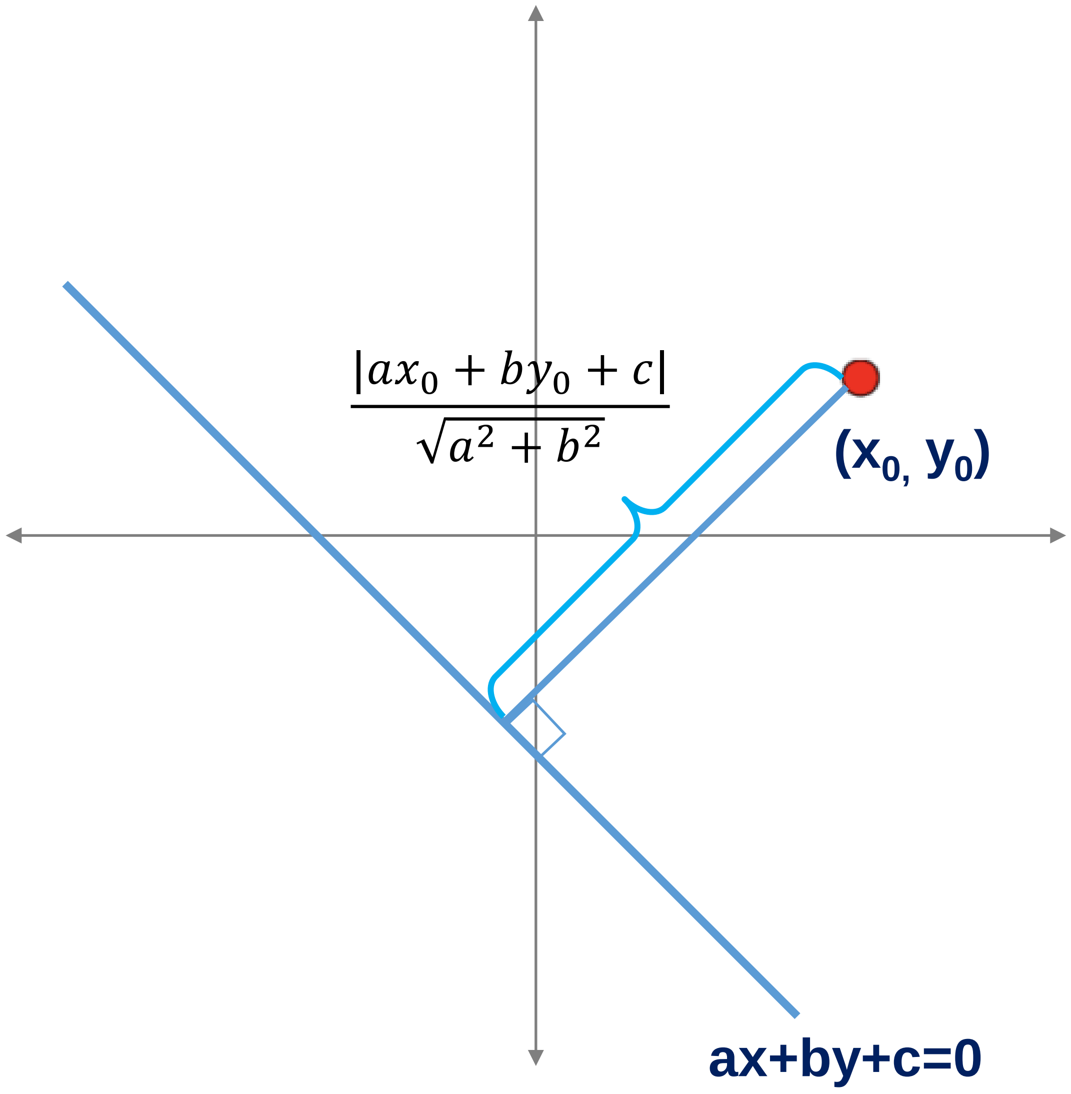
- A large margin can lead to good generalization on the test (unseen) data.

Support Vector Machine (SVM)

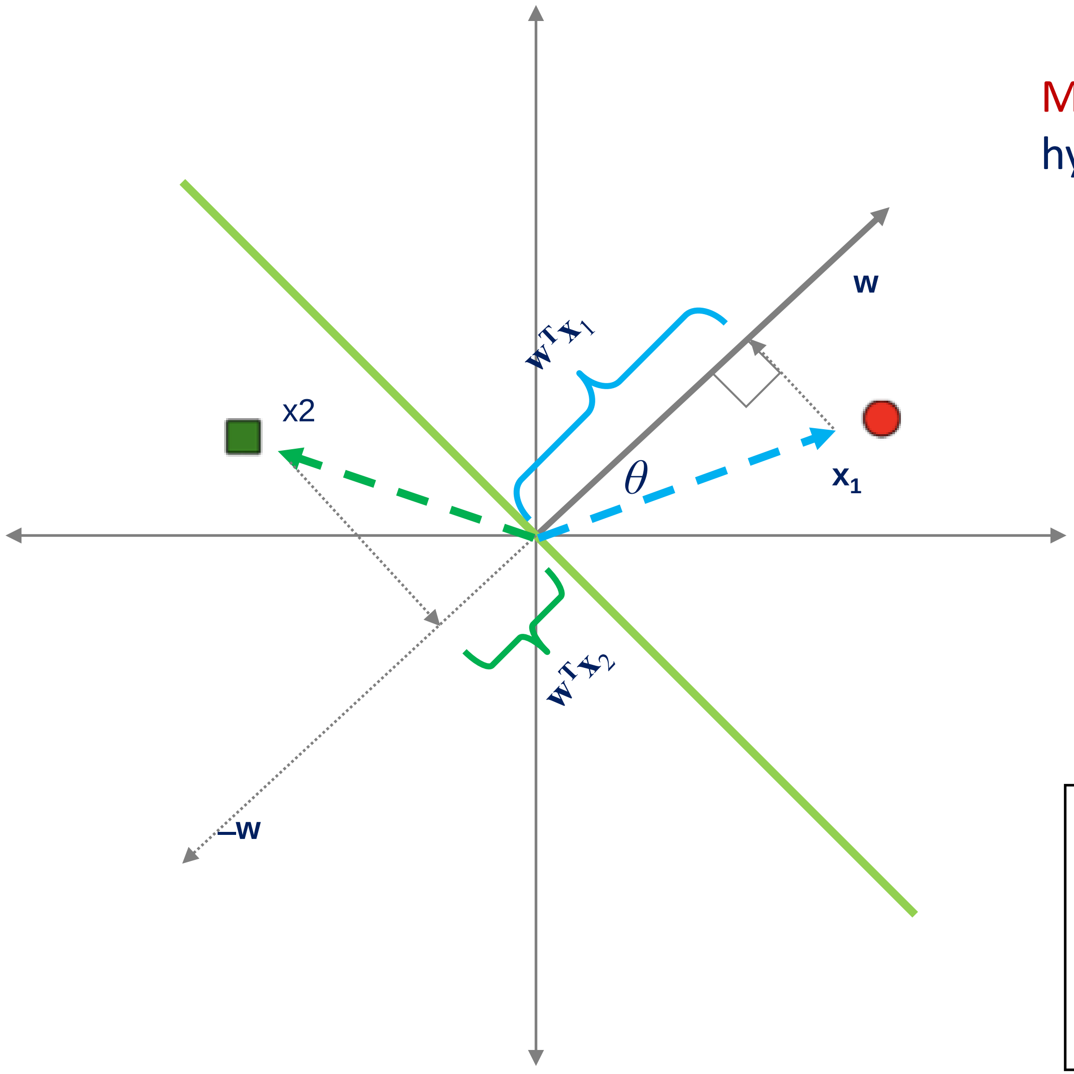
- Probably the most popular/influential classification algorithm
- Backed by solid theoretical groundings
- A hyperplane based classifier (like the Perceptron)
- Additionally uses the maximum margin Principle
  - Finds the hyperplane with maximum separation margin on the training data



Calculate distance from a point to a line



The Concept of Margins



Margin of a sample : γ_i of a sample $\mathbf{x}_i$ is its distance from the hyperplane

$$\|\boldsymbol{w}\| = \sqrt{\sum_{i=1}^{|\boldsymbol{w}|} {w_i}^2} \qquad \|\boldsymbol{w}\|^2 = \sum_{i=1}^{|\boldsymbol{w}|} {w_i}^2$$

$$\gamma_i = \frac{|\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b|}{\|\mathbf{w}\|}$$

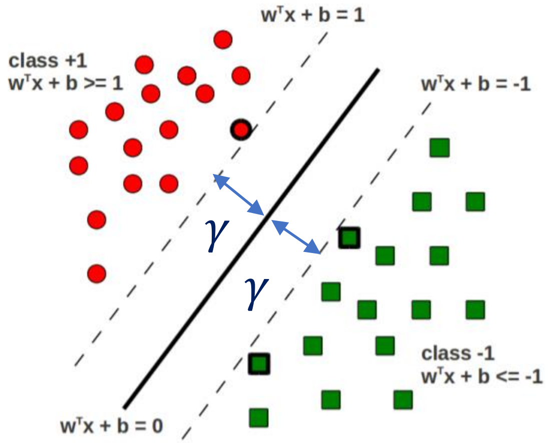
Margin of a set: is the minimum margin of all samples

$$\gamma = \min_{1\le i\le n} \gamma_i = \min_{1\le i\le n} \frac{|\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b|}{\|\mathbf{w}\|}$$

If we are asked to move the hyperplane to achieve better generalization, what should we do?

Support Vector Machine

- A hyperplane based linear classifier defined by **w** and *b*
- Prediction rule: $y = \text{sign}(\mathbf{w}^{\mathrm{T}}\mathbf{x} + b)$
- **Given:** Training data $\{\mathbf{x}_i, y_i\}_{i=1}^{m}$
- **Goal:** Learn **w** and *b* that achieve the maximum margin
- For now, assume the entire training data is linearly separable. We will handle linearly unseparable cases later



- Assume the hyperplane is such that
  - $\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b \geq 1$ for $y_i = +1$
  - $\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b \leq -1$ for $y_i = -1$
  - Equivalently, $y_i(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b) \geq 1$
  - The hyperplane's margin:

$$\min_{1 \leq i \leq m} |\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b| = 1$$

$$\gamma = \min_{1 \leq i \leq m} \gamma_i = \min_{1 \leq i \leq m} \frac{|\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}$$

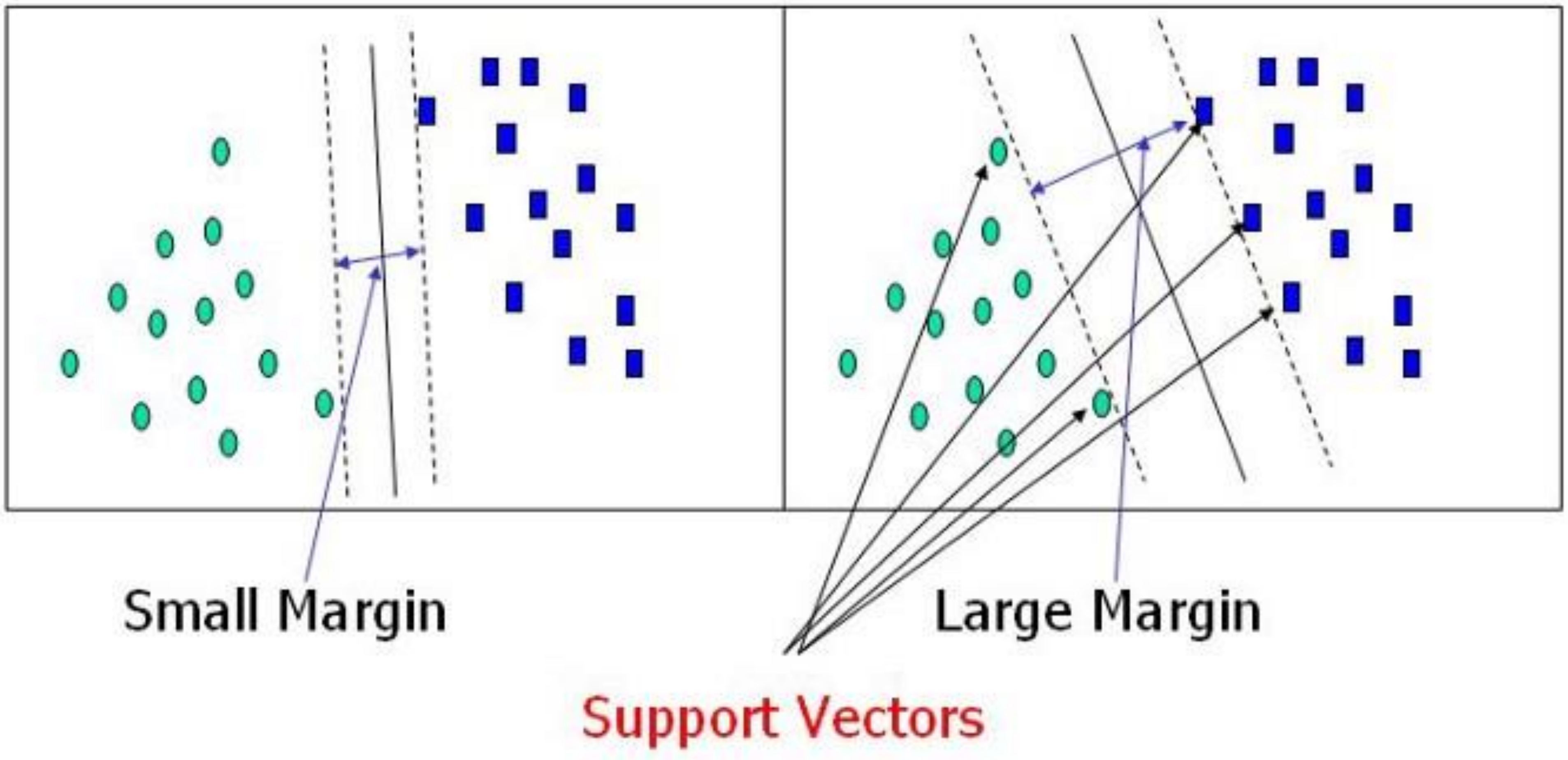
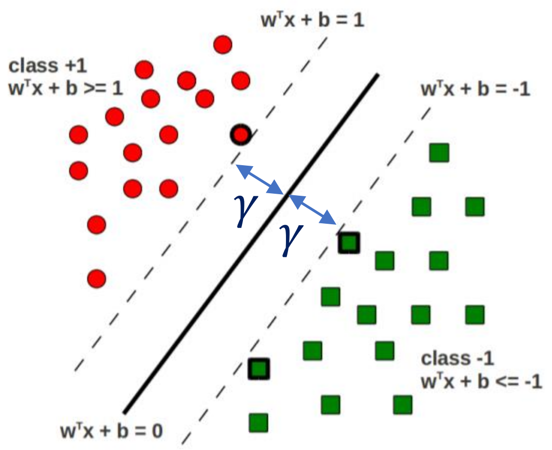


image credit: https://towardsdatascience.com/support-vector-machine-introduction-to-machine-learning-algorithms-934a444fca47

Support Vector Machine: the optimization problem

- We want to maximize the margin $\gamma = \frac{1}{\|\mathbf{w}\|}$, which is equivalent to minimize $\|\mathbf{w}\|$ or $\frac{\|\mathbf{w}\|^2}{2}$



- Therefore, the optimization problem of SVM for the *separable case* would be

$$\begin{aligned}&\min \frac{\|\mathbf{w}\|^2}{2}\\ &\text{subject to} \quad y_i(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b) \geq 1, i = 1, \ldots, m\end{aligned}$$

This is a Quadratic Program (QP) with *n* linear inequality constraints.

SVM: Solving the Optimization Problem (optional)

- The optimization problem is

$$\min \frac{\|\mathbf{w}\|^2}{2}$$
$$\text{subject to} \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1, i = 1, \dots, m$$

- Introducing Lagrange Multipliers α_i, one for each constraint, leads to the primal Lagrangian:

$$\min L_p = \frac{\|\mathbf{w}\|^2}{2} + \sum_{i=1}^{m} \alpha_i(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b))$$
$$\text{subject to} \quad \alpha_i \geq 0, i = 1, \dots, m$$

SVM: Solution! (optional)

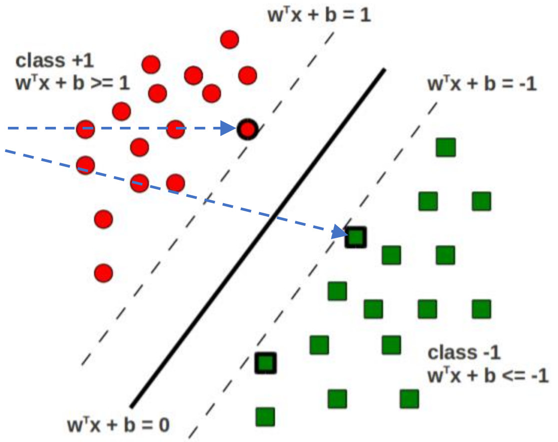
- Once we have the α_i, we can compute $\boldsymbol{w}$ and b as:

(duality optimization, KTT, Sequential Minimal Optimization)

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i \qquad b = y_i - \sum_{j=1}^{m} \alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i$$

$\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b = y_i$

any support vector will work



- An important consequence:
  - α_i is non-zero only if $\mathbf{x}_i$ lies on one of the two margin boundaries, i.e., for which

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) = 1$$

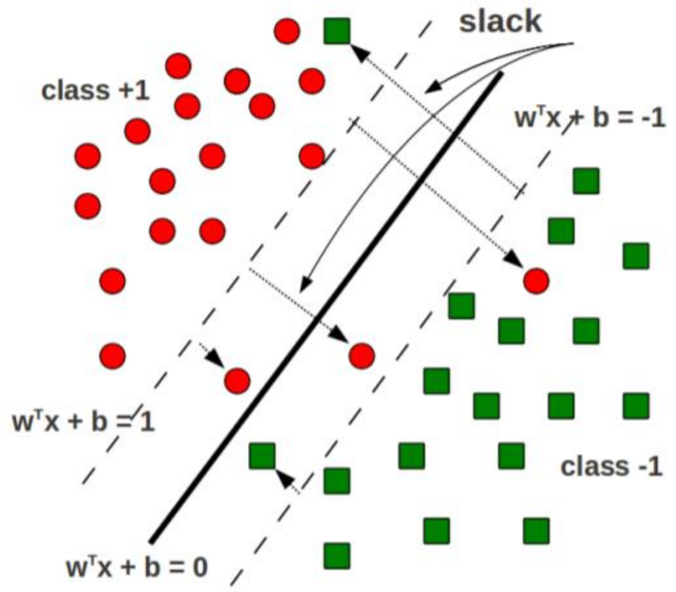
  - The samples are called **support vectors**.

SVM: Non-separable case

- Non-separable case: No hyperplane can separate the classes perfectly (common in practice).

- Still want to find the maximum margin hyperplane, but…
  - Allow some training samples to be misclassified (can you identify those points on the right?)

  - Allow some training samples to fall within the margin region (can you identify those points on the right?)



SVM: Use Slack Variables

- Solution: introduce slack variables

- Recall: for the separable case, the constraints are:

$$y_i(\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b) \geq 1, i = 1, \dots, m$$

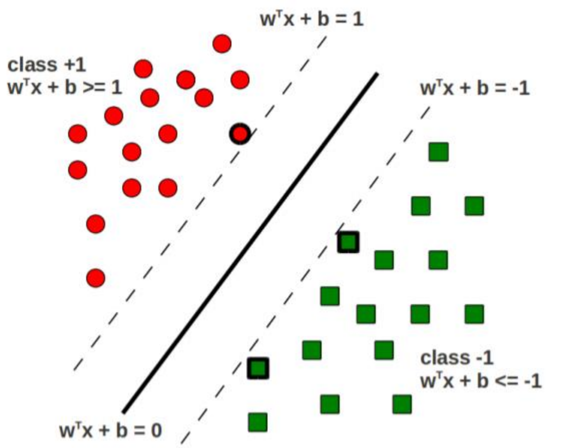
- For the non-separable case, we relax the constraints by adding slack variables

$$y_i(\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b) \geq 1 - \xi_i, i = 1, \dots, m$$

- $\xi_i \geq 0$ is required
- $\xi_i > 1$ for misclassified samples (for outside the margin)

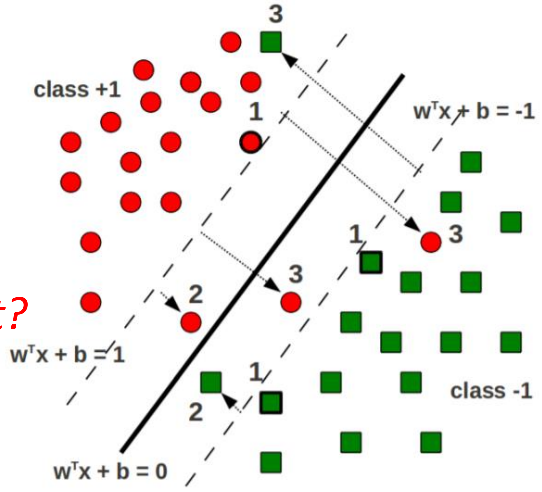
Support Vectors for non-separable cases

- Recall: the separable case has only one type of support vectors
  - Ones that lies on the margin boundaries $\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b = 1$ or $\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b = -1$



- The non-separable case has three types of support vectors
  1. Lying on the margin boundaries $\xi_i = 0$
  2. Lying with the margin region $0 < \xi_i < 1$ but still on the correct side
  3. Lying on the wrong side the hyperplane $\xi_i \geq 1$

Can you identify them on the right?



The Optimization Problem (optional)

- While we "allow" misclassified training samples
  - We want the number of misclassified training samples to be minimized
  - By minimizing the sum of slack variables $\sum_{i=1}^{m} \xi_i$

- Therefore, the new optimization problem for non-separable case will be

$$\min \frac{\|\mathbf{w}\|^2}{2} + \boldsymbol{C} \sum_{i=1}^{\mathrm{m}} \xi_i$$

$$\text{subject to} \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, i = 1, \dots, m$$
$$\xi_i \geq 0$$

$\boldsymbol{C}$ is a hyper-parameter to control the tradeoff between training errors and margins

- Large C, prefer low training errors
- Small C, prefer large margins

The Optimization Problem (optional)

- As in the linearly separable problem, by following the derivations, we will obtain the following dual problem

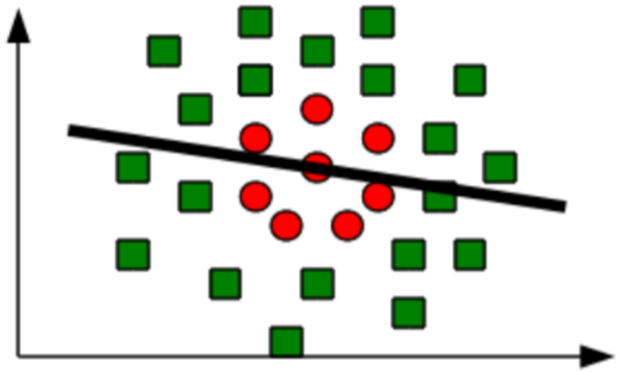
$$\max\ L_d = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{subject to} \quad \sum_{i=1}^{m} \alpha_i y_i = 0, 0 \le \alpha_i \le C, i = 1, \ldots, m$$

- Again a Quadratic Programming problem for α
- Given $\boldsymbol{\alpha}$, the solution $\mathbf{w}$, b has the same form as the separable case
- Note: $\boldsymbol{\alpha}$ is again sparse. Non-zero α_i corresponds to the **support vectors**

SVM for Nonlinear Classification

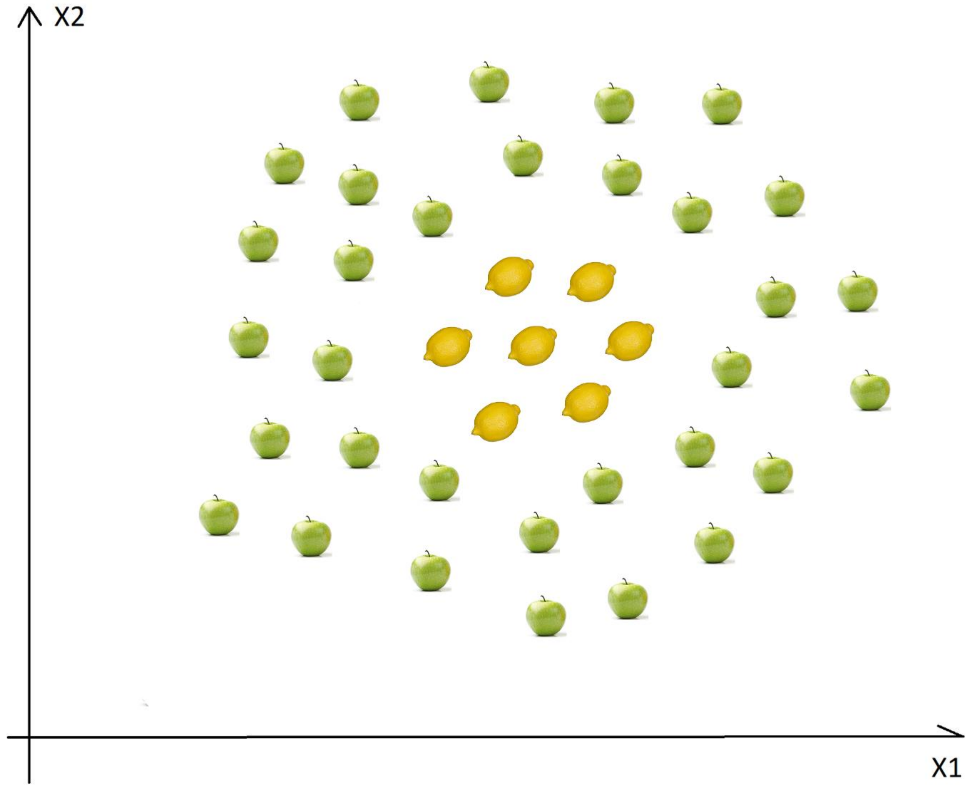
- Problem: SVM with linear function $\mathbf{w}^{\mathrm{T}}\mathbf{x} + b$ have very limited representation power. Therefore, it can not solve nonlinear classification problem.

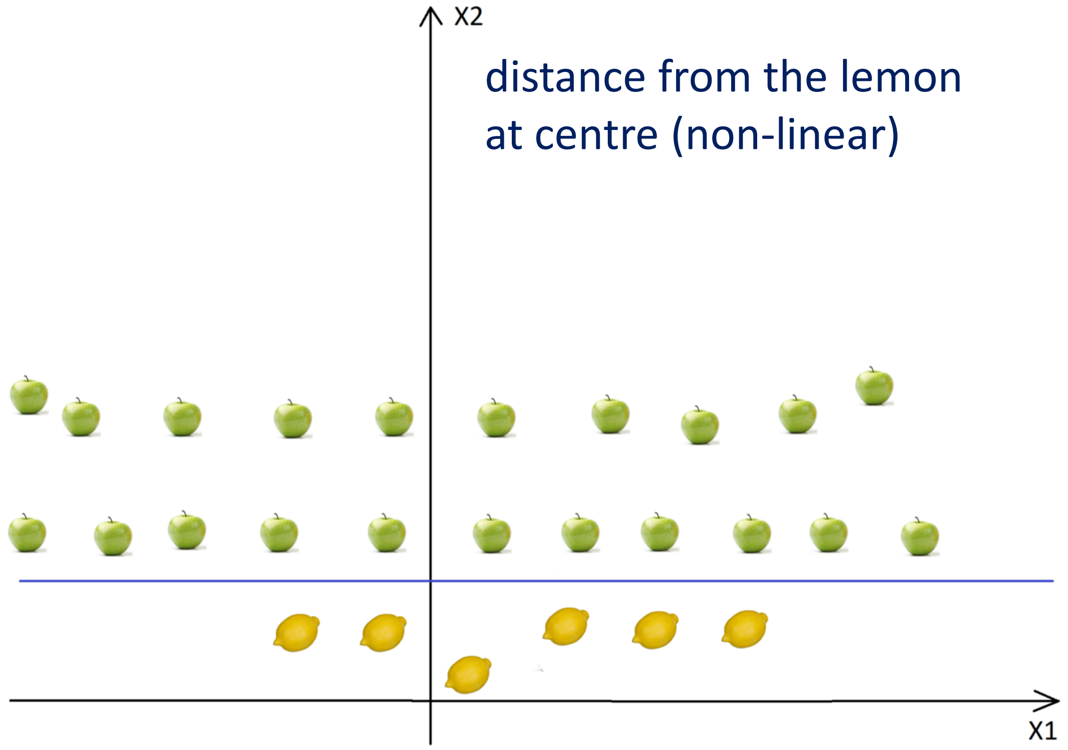


- Good news: With a slight modification using **kernel trick**, SVM can solve highly nonlinear classification problems.

Kernel SVM for Nonlinear Classification

- Key idea: Projecting the input to a high dimensional feature space so that non-linear classification problem becomes linearly separable again!

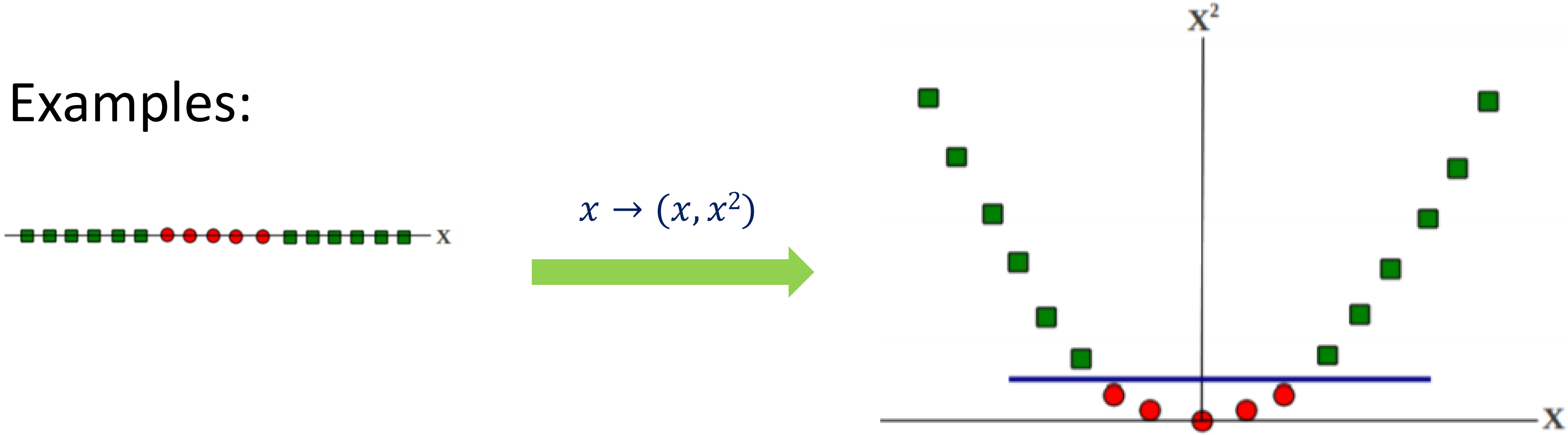




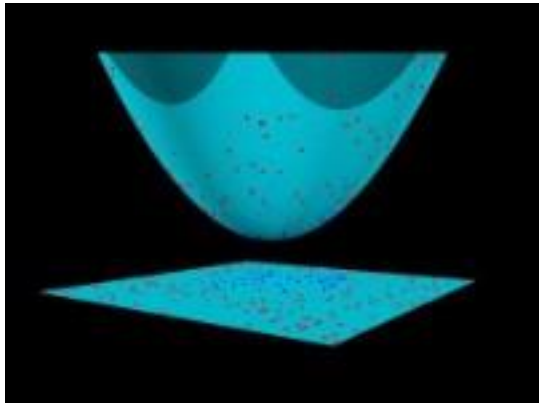
Kernels

- Kernels: Make linear models works in nonlinear settings
  - By mapping data to higher dimensions where it exhibits linear patterns.
  - Apply the linear model in the new input space
  - Mapping means changing the feature representation

- Examples:



Kernels



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  - By mapping data to higher dimensions where it exhibits linear patterns.
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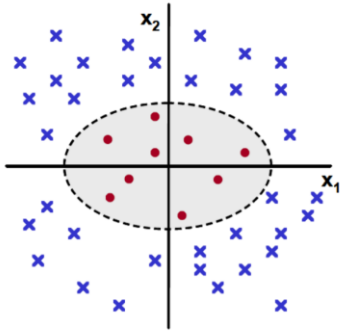
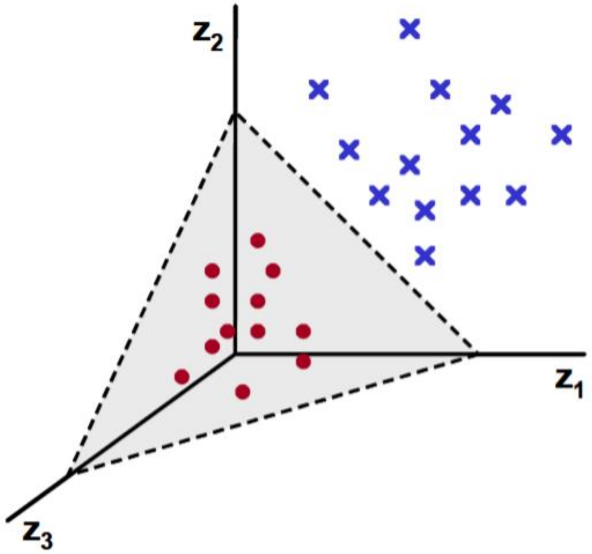
  - Mapping means changing the feature representation
  - https://www.youtube.com/watch?v=3liCbRZPrZA
- Examples:



$\mathbf{x}: [x_1, x_2] \rightarrow \mathbf{z}: [x_1^2, \sqrt{2}x_1x_2, x_2^2]$



Feature Mapping (optional)

- Consider the following mapping ϕ for a sample $\mathbf{x} = [x_1, x_2, \dots, x_n]$

$$\phi\colon \mathbf{x} \to [x_1^2, x_2^2, \dots, x_n^2, x_1x_2, x_1x_3 \dots, x_1x_n, \dots, x_{n-1}x_n]$$

- It is an example of quadratic mapping
  - Each new feature uses a pair of the original features

- Problem: Explicit mapping leads to the number of features blow up!

- Fortunately, kernel trick help us to avoid the problem.
  - The mapping does not have to be explicitly computed

Kernel as high dimensional feature mapping (optional)

- Consider two samples $\mathbf{x}$: $[x_1, x_2]$ and $\mathbf{z}$: $[z_1, z_2]$
- Let us assume there is a kernel function *k* that takes inputs **x** and **z**

$$\begin{aligned} k(\mathbf{x}, \mathbf{z}) &= (\mathbf{xz})^2 \\ &= (x_1 z_1 + x_2 z_2)^2 \\ &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 x_2 z_1 z_2 \\ &= \left(x_1^2, \sqrt{2}x_1 x_2, x_2^2\right)\left(z_1^2, \sqrt{2}z_1 z_2, z_2^2\right) \\ &= \phi(\mathbf{x})\phi(\mathbf{z}) \end{aligned}$$

$\phi(\mathbf{x})\phi(\mathbf{z})$ is computed efficiently in original input space.

- This kernel function k implicitly defines a mapping ϕ to a higher dimensional space

$$\phi(\mathbf{x}) = \left[x_1^2, \sqrt{2}x_1 x_2, x_2^2\right]$$

- Note that we do not have to define/compute this mapping. Simple defining the kernel is a certain way to give a higher dimensional mapping ϕ

Kernel: Formal definition (optional)

- ϕ takes input **x** in input space and maps to feature space

- Kernel k(**x**, **z**) takes two inputs and gives their similarity in feature space

$$k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})\phi(\mathbf{z})$$

- Some Examples of Kernels
  - Linear kernel $k(\mathbf{x}, \mathbf{z}) = \mathbf{xz}$
  - Quadratic Kernel $k(\mathbf{x}, \mathbf{z}) = (\mathbf{xz})^2$ or $k(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{xz})^2$
  - Polynomial Kernel $k(\mathbf{x}, \mathbf{z}) = (\mathbf{xz})^q$ or $k(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{xz})^q$
  - Radial Basis Function (RBF) kernel $k(\mathbf{x}, \mathbf{z}) = \exp(-\gamma||\mathbf{x} - \mathbf{z}||^2)$
    - The RBF kernel corresponds to an infinite dimensional feature space. We can not actually write down $\phi(\mathbf{x})$ for RBF kernel.

Using Kernel

- Kernel can turn a linear model into a nonlinear one
- Recall: Kernel $k(\mathbf{x}, \mathbf{z})$ represents a dot product in some high dimensional feature space.
- Any learning algorithm in which examples only appear as dot products $(\mathbf{x}_i \mathbf{x}_j)$ can be kernelized (i.e., non-linearized)
  - by replacing the $(\mathbf{x}_i \mathbf{x}_j)$ by $\phi(\mathbf{x}_i)\phi(\mathbf{x}_j) = k(\mathbf{x}_i, \mathbf{x}_j)$
- Most learning algorithms can be kernelized:
  - Perceptron, SVM, linear regression, logistic regression, etc

Kernelize SVM Training (optional)

- Recall the dual Lagrangian for linear SVM

$$\max L_d = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_\mathrm{i}\mathbf{x}_j)$$

$$\text{subject to} \quad \sum_{i=1}^{m} \alpha_i\, y_i = 0, 0 \le \alpha_i \le C, i = 1, \dots, m$$

- Replace $(\mathbf{x}_i\mathbf{x}_j)$ by $\phi(\mathbf{x}_i)\phi(\mathbf{x}_j) = k(\mathbf{x}_i, \mathbf{x}_j)$, where $k(,)$ is some kernel function

$$\max L_d = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j k(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{subject to} \quad \sum_{i=1}^{m} \alpha_i\, y_i = 0, 0 \le \alpha_i \le C, i = 1, \dots, m$$

- Now, SVM learns a linear separate in kernel defined feature space
    - This corresponds to non-linear separator in the original input space

Kernel SVM for Nonlinear Classification (optional)

- For a new input $\boldsymbol{x}$, the output will be:

$$y = \mathbf{w}^T\mathbf{x} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_{\boldsymbol{i}}^{\boldsymbol{T}} \mathbf{x}$$

Since $\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$

- For the non-linear classification, apply non-linear transformation $\Phi(\mathbf{x})$ to project $\mathbf{x}$ to a higher dimensional space and the inner product term becomes

$$y = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{\Phi}(\boldsymbol{xi})^{\boldsymbol{T}} \boldsymbol{\Phi}(\boldsymbol{x})$$

Kernel SVM for Nonlinear Classification (optional)

- As only the inner product is needed, we can apply the kernel trick. That is we care only the the way to measure distance between two points.

$$y = \sum_{i=1}^{m} \alpha_i y_i \boldsymbol{\Phi}(x_i)^T \boldsymbol{\Phi}(x)$$

$$y = \mathbf{w}^T\mathbf{x} = \sum_{i=1}^{m} \alpha_i y_i k(\mathbf{x_i}, \mathbf{x})$$

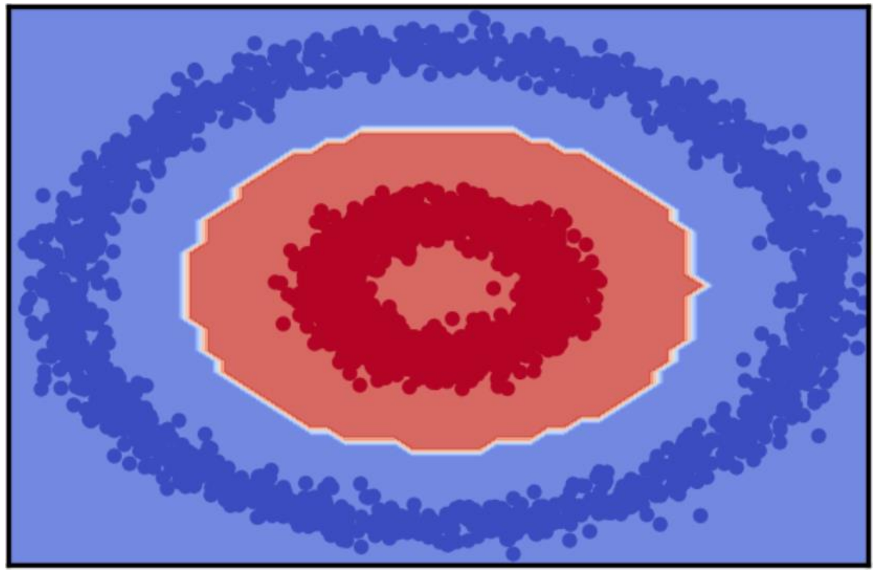
Note: We do not need to explicitly compute $\mathbf{w}$ and $\phi(\mathbf{x})$ for kernel SVM.

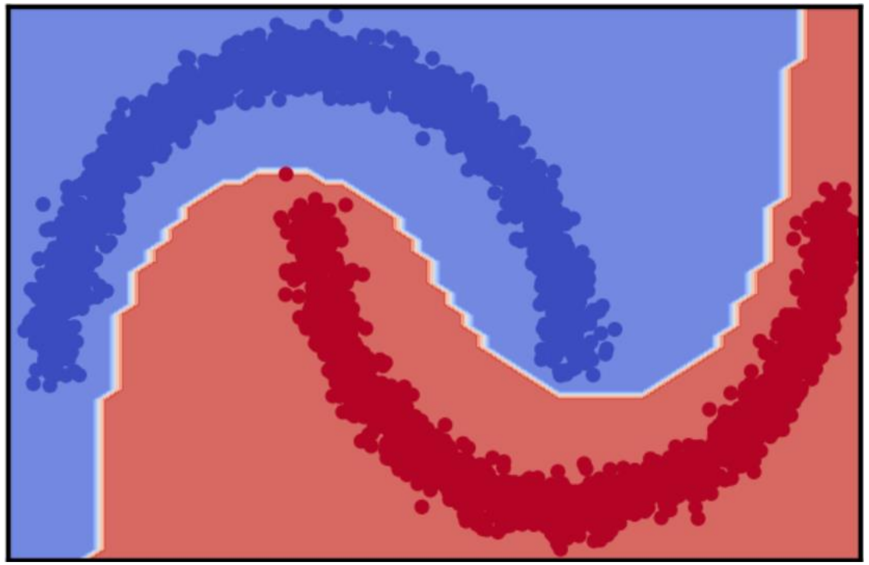
- One common kernel: Radial Basis Function (RBF)

$$k(\mathbf{x_i}, \mathbf{x}) = \exp(-\gamma\|\mathbf{x_i} - \mathbf{x}\|)$$

Gamma is for determining how the distance is considered influential.

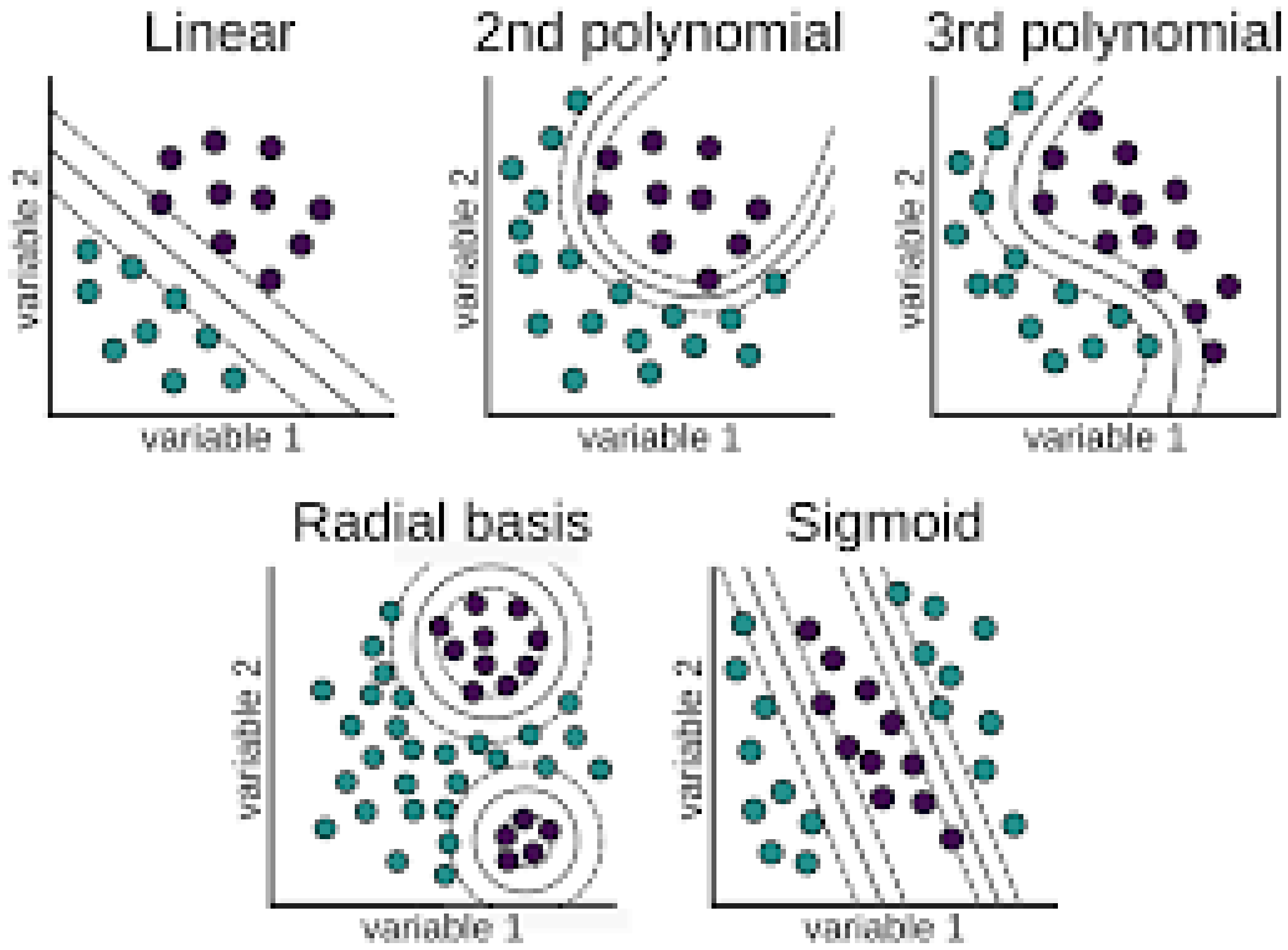
SVM with RBF kernel





The learned decision boundary by SVM with RBF kernel is nonlinear in the original space

SVM with Different Kernels and Decision Boundaries



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❖Regression

1. Linear regression with one variable
2. Linear Regression with multiple variables

❖Classification

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2. Artificial Neural Network
3. Support Vector Machine
4. K Nearest Neighbor

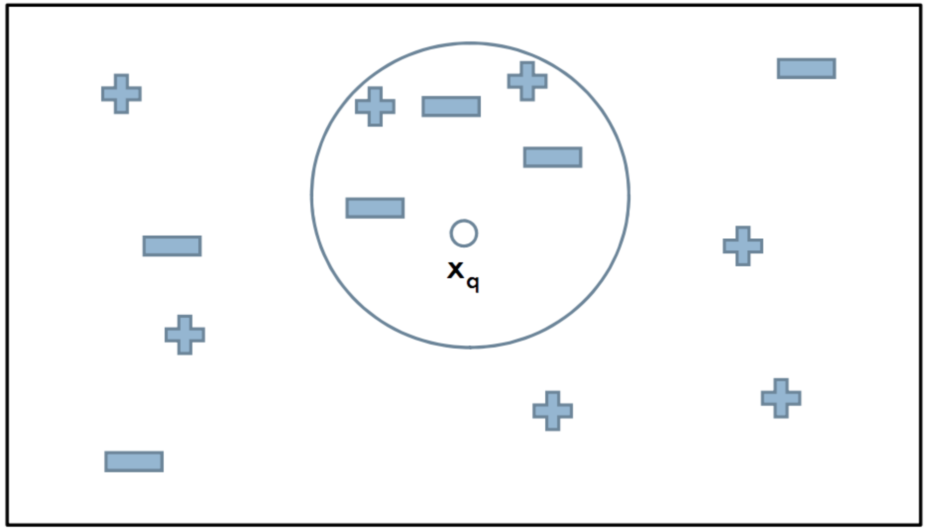
- **Unsupervised learning**

1. K-means Clustering
2. Hierarchical Clustering

k-NN Algorithm

- k Nearest Neighbor Algorithm
  - k is a user specified parameter, which means the number of nearest neighbors

- A Lazy Learning Algorithm
  - **Training:**
    - **No training process**, just store all training data in memory
  - **Prediction:**
    - Classify new samples based on most similar training samples via majority vote

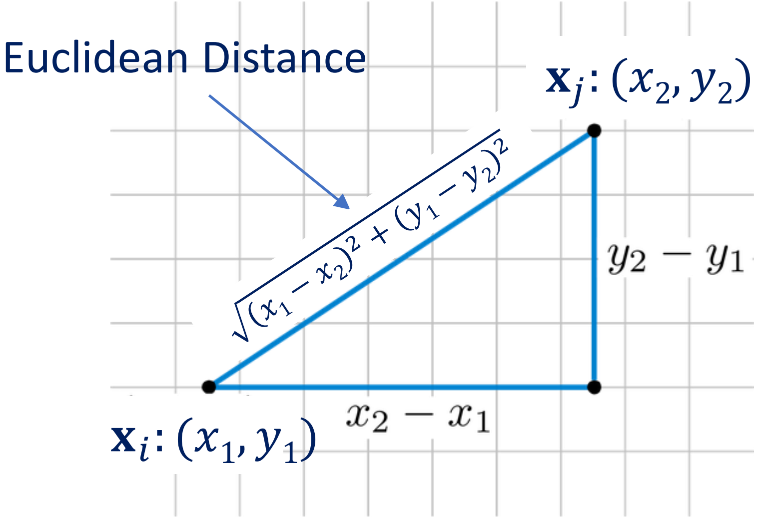


- $\mathbf{x}_q$ is the test sample.
- Assume k is equal to 5.
- Three out of its 5 nearest neighbors are from negative class.
- The predicted label for $\mathbf{x}_q$ is negative.

Nearest Neighbors

- Training Data {**X**, **y**}
- A test data point: $\mathbf{x}_{\text{test}}$
- Idea: the label of a test data point is estimated from the known label(s) of the nearest neighbors of $\mathbf{x}_{\text{test}}$ in the training data.
- Euclidean distance between feature vectors can be used to decide the nearest neighbors

$$\|\mathbf{x}_i - \mathbf{x}_j\|_2 = \sqrt{\sum_{k=1}^{n} (x_{ik} - x_{jk})^2}$$

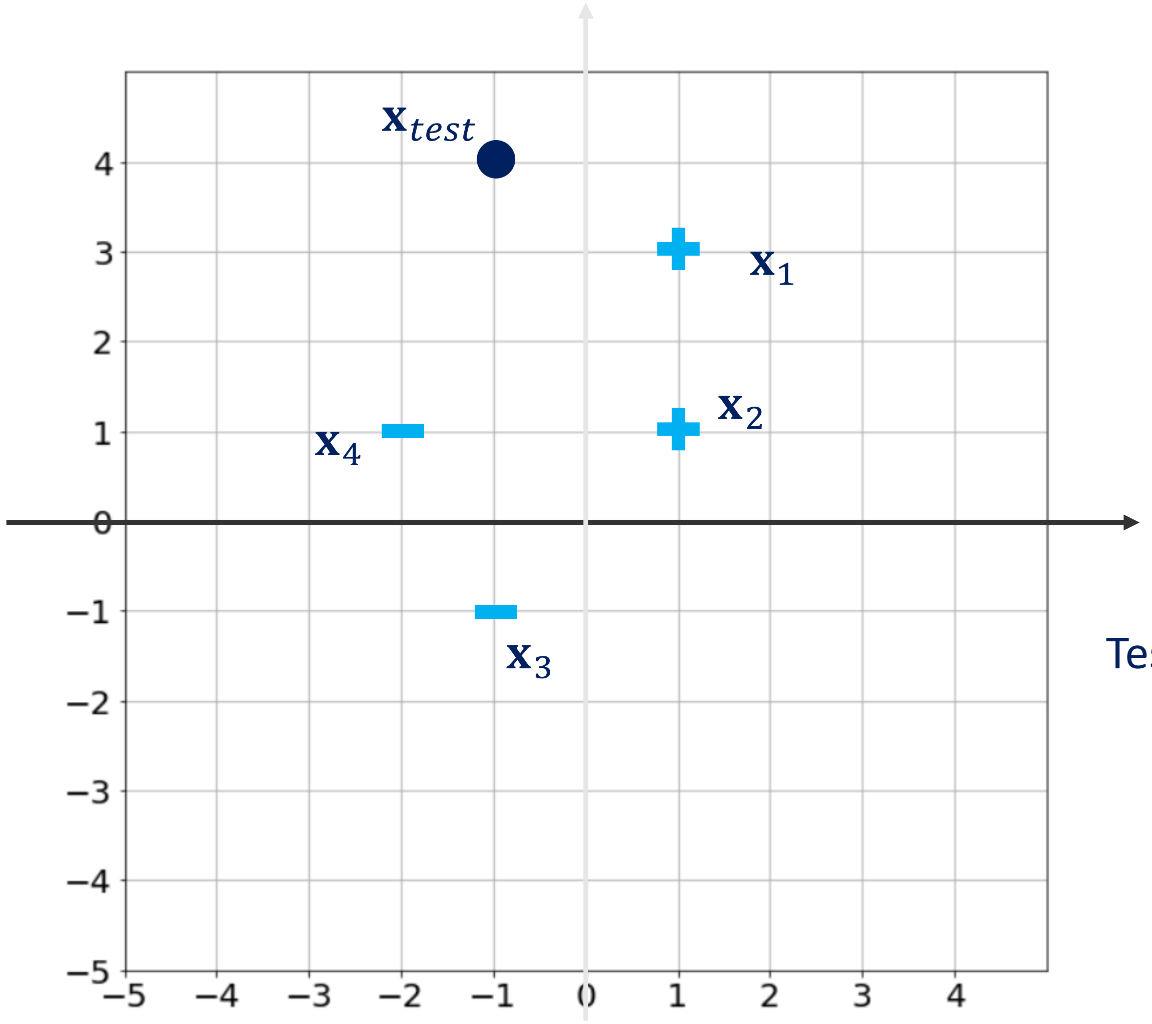


k -NN algorithm

- Input: training data {$\mathbf{X}$, y}, a test data sample $\mathbf{x}_{\text{test}}$, parameter k
  - Compute the distances between the test sample $\mathbf{x}_{\text{test}}$ and each training data sample
  - Sort by distances and get the k nearest neighbors of $\mathbf{x}_{\text{test}}$ (k is usually set to an odd number to prevent tie situations)
  - Use majority vote to predict the class label of $\mathbf{x}_{\text{test}}$

- Output: predicted class label of $\mathbf{x}_{\text{test}}$

k-Nearest Neighbors Example (k=3)



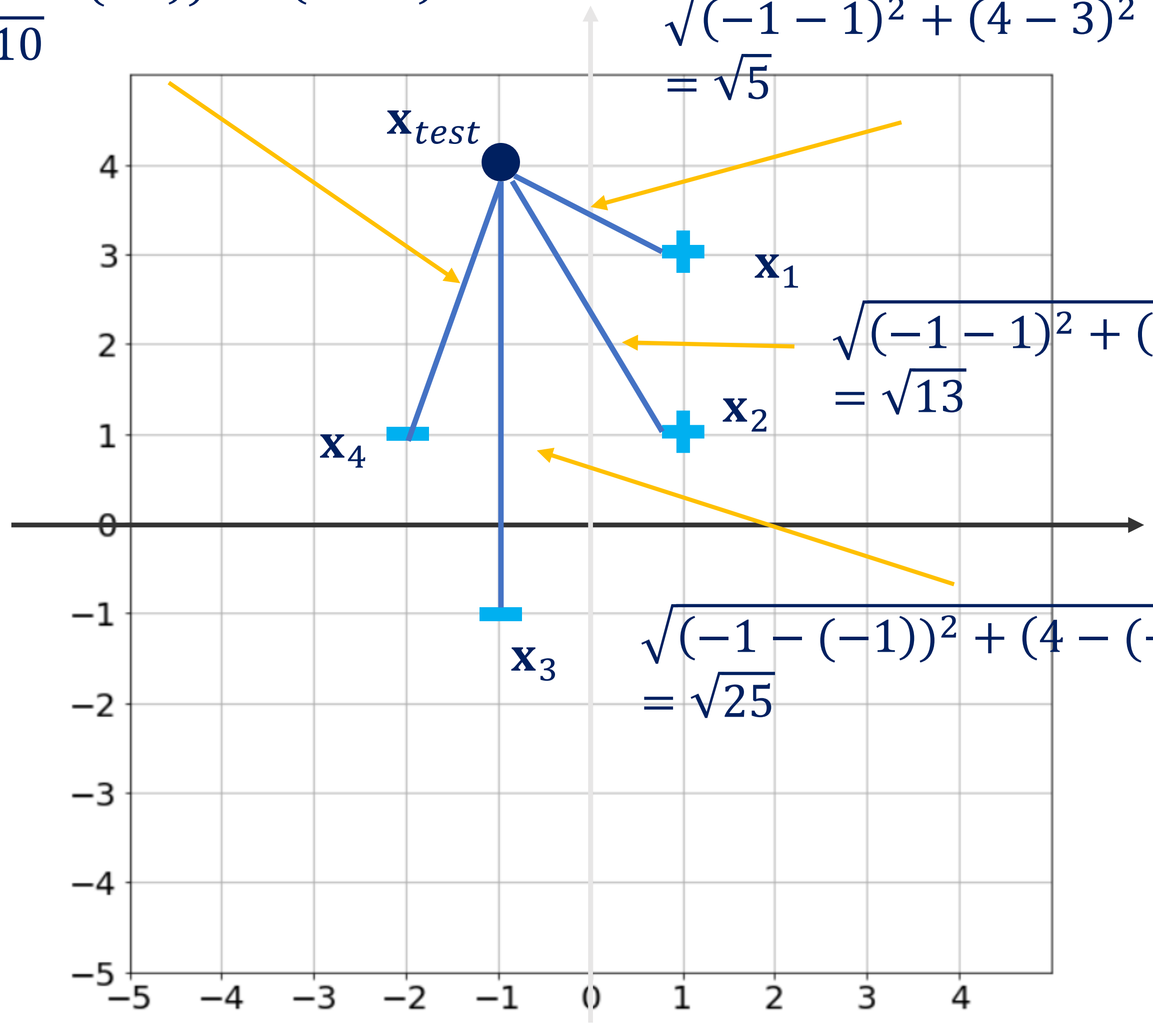
Training Data:

x_1	x_2	*label*
1	3	1
1	1	1
-1	-1	-1
-2	1	-1

Test Data:

x_1	x_2	*label*
-1	4	?

k-Nearest Neighbors Example (k=3)



Training Data:

x_1	x_2	*label*
1	3	1
1	1	1
-1	-1	-1
-2	1	-1

Test Data:

x_1	x_2	*label*
-1	4	1

	$\mathbf{x}_{test}$
$\mathbf{x}_1$	$\sqrt{5}$
$\mathbf{x}_2$	$\sqrt{13}$
$\mathbf{x}_3$	$\sqrt{25}$
$\mathbf{x}_4$	$\sqrt{10}$

Sort

	$\mathbf{x}_{test}$
$\mathbf{x}_1$	$\sqrt{5}$
$\mathbf{x}_4$	$\sqrt{10}$
$\mathbf{x}_2$	$\sqrt{13}$
$\mathbf{x}_3$	$\sqrt{25}$

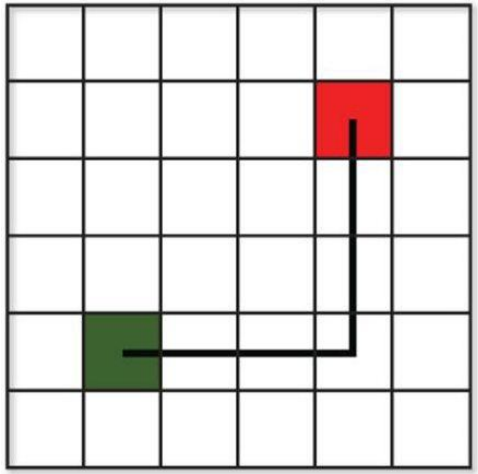
Other k-NN Distance metrics

Minkowski Distance

$$d = (\sum_{i=1}^{m} |x_i - y_i|^p)^{1/p}$$

Manhattan Distance

$$d = \sum_{i=1}^{m} |x_i - y_i|$$



Manhattan Distance

Other k-NN Distance metrics

Cosine Distance

$$\cos\theta = \frac{\vec{a}\cdot\vec{b}}{\|\vec{a}\|\cdot\|\vec{b}\|}$$

Jaccard Distance

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}$$

A = {X, Y, Z} , **B** = {W, X}, C = {X, Y}
J(A,B) = 1 / 4
J(A,C) = 2 / 3

k-NN - Generalize to multiple classes

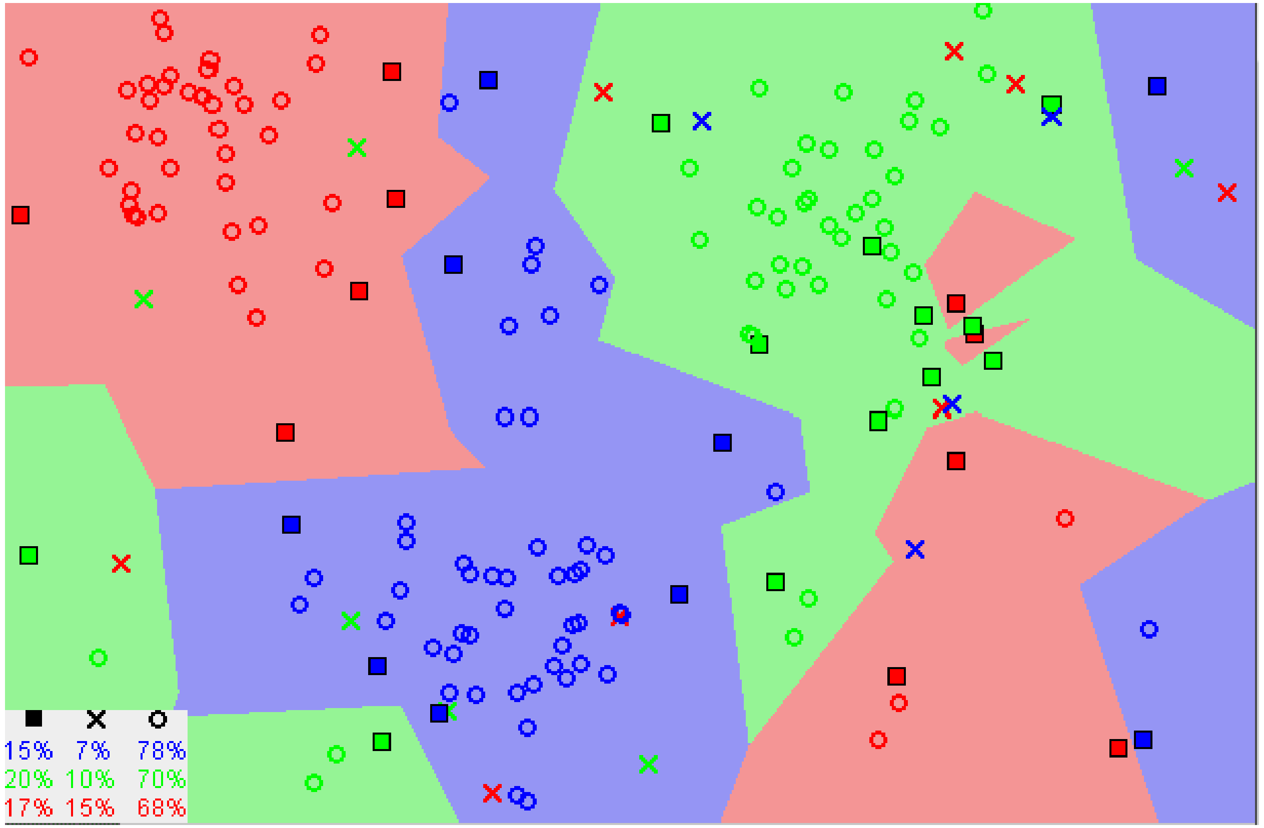


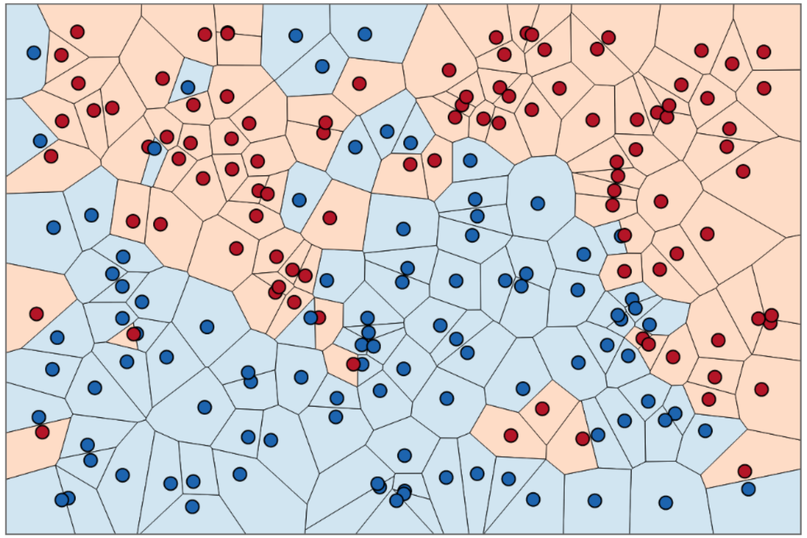
Image showing how similar data points typically exist close to each other

image credit: https://towardsdatascience.com/machine-learning-basics-with-the-k-nearest-neighbors-algorithm-6a6e71d01761

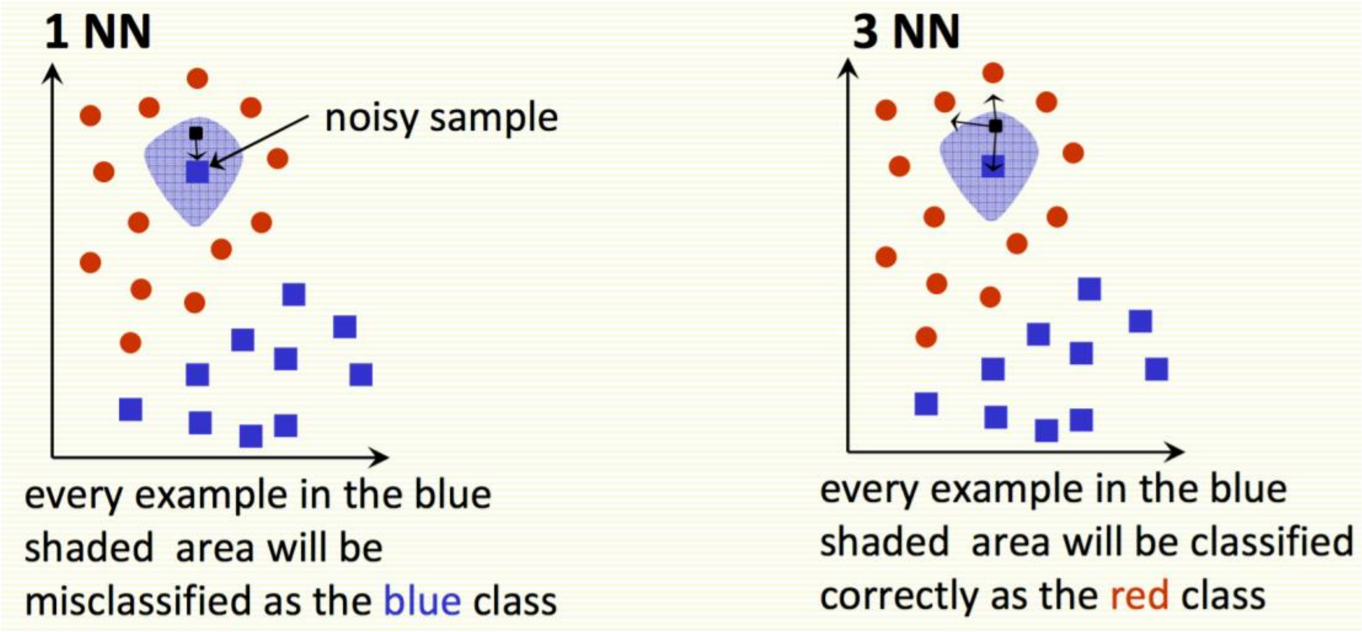
k-NN: Decision Boundaries

- k-NN algorithm does not explicitly compute decision boundaries, but the decision boundaries can be inferred.

- Decision boundaries of 1-NN: Voronoi diagram
  - Show how input space divided into classes
  - Each line segment is equidistant between two neighboring data points.

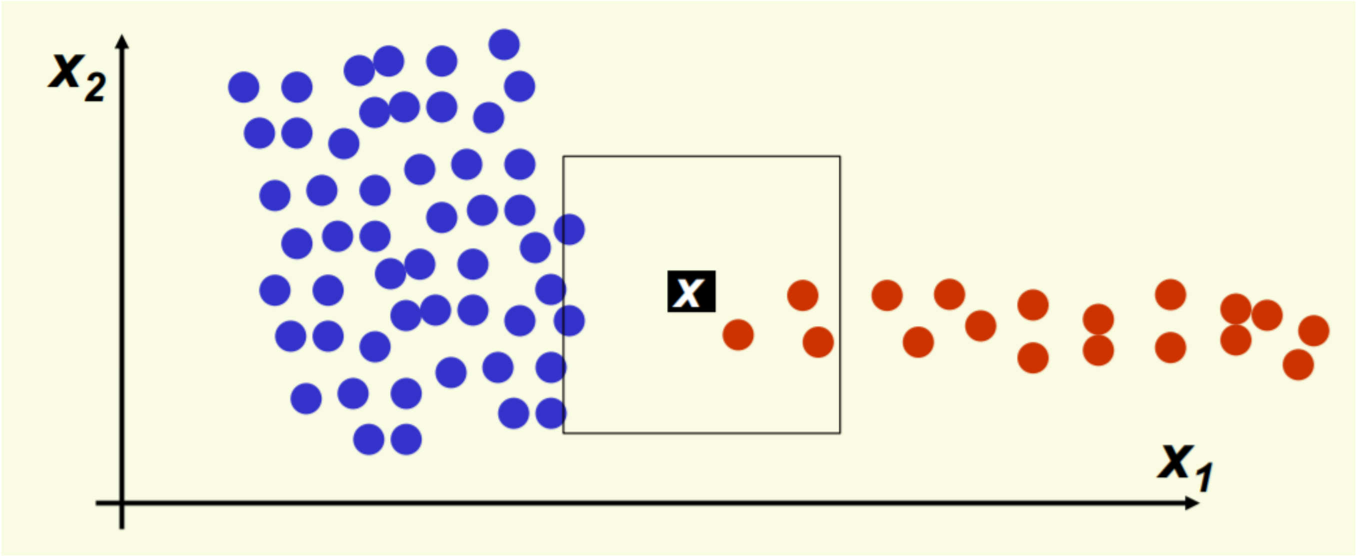


The Effect of k in k-NN



- If k is too small, k-NN will be very sensitive to “noisy samples” and lead to noisy decision boundaries.
- Large k will smooth the decision boundaries and may lead to better performance.

The Effect of k in k-NN



- If k is smaller than 5, data sample **x** is correctly predicted as red class.
- For larger k, data sample **x** is wrongly corrected as blue class.
- Therefore, if k is too large, we may end up with over-smoothed boundaries since it looks neighbors that are far away from the test data sample.

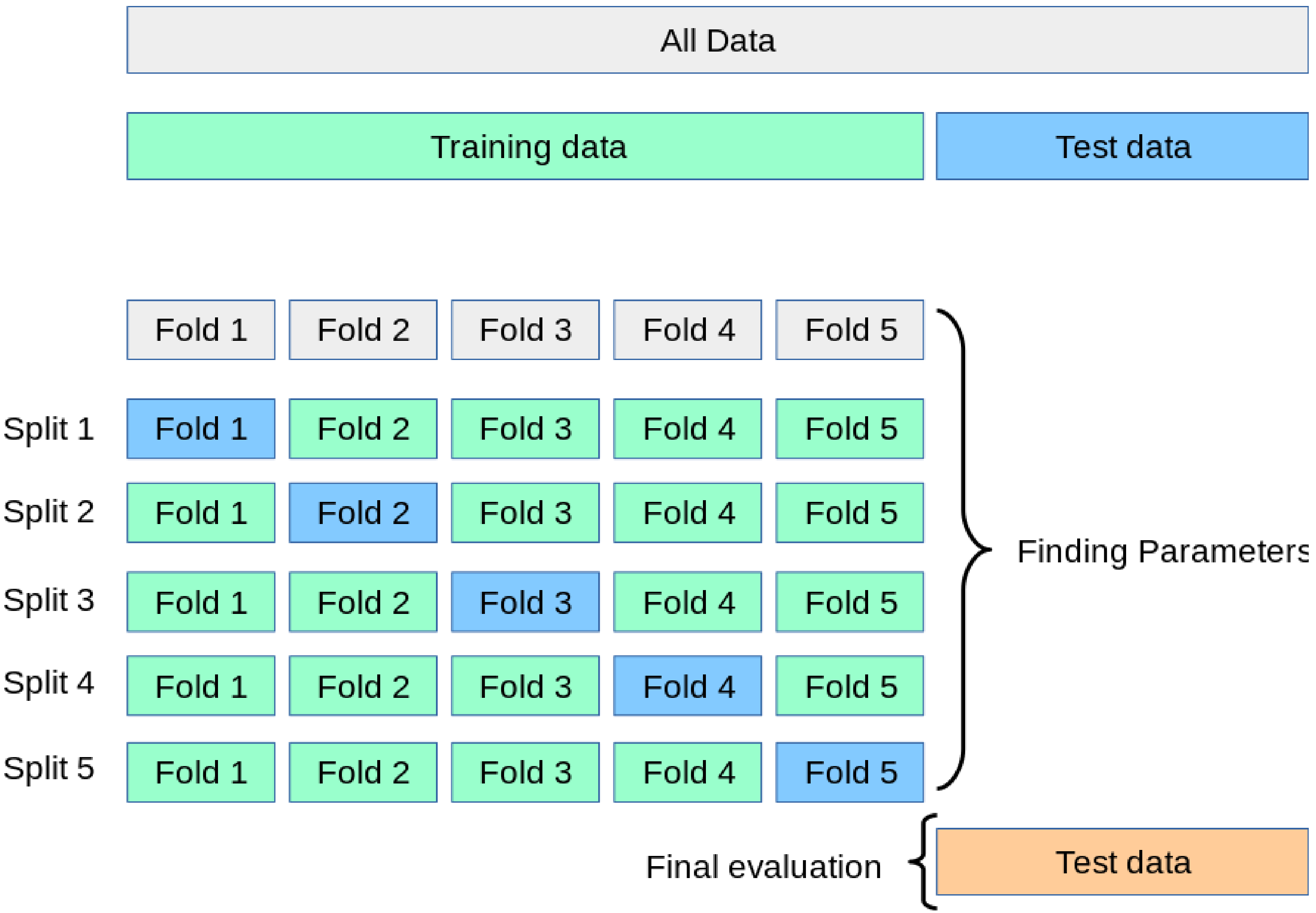
How to choose k?

- k being too small will be very sensitive to “noisy samples”, leading to noisy decision boundaries.

- k being too large will lead to over-smoothed boundaries since it looks neighbors that are far away from the test data sample.

- We can use cross validation to find k.
  - Try several values of k : {5, 10, 20, 30}
  - Select the best k based on cross validation.

Cross validation



k-NN: Some Issues and Remedies

- If some features (columns of data matrix) have large ranges, they will dominate the calculation of the distance.
  - Data Normalization
    - Min-max normalization: scale the range of each feature to be in range [0, 1]
    - Decimal normalization: scale each feature to be in range (-1, 1)
- Irrelevant, correlated features add noise to distance measures
  - Eliminate irrelevant features
  - Principal Component Analysis to reduce correlation among features
- Categorical Features, e.g., {‘red’, ’green’, ’blue’}
  - One-hot encoding