CSE 417T
Introduction to Machine Learning

Lecture 16

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Logistics

- Homework 4 is due November 14 (Monday)
- Keep track of your own late days
  - Gradescope doesn’t allow separate deadlines
  - Your submissions won’t be graded if you exceed the late-day limit

Recap

Nearest Neighbor

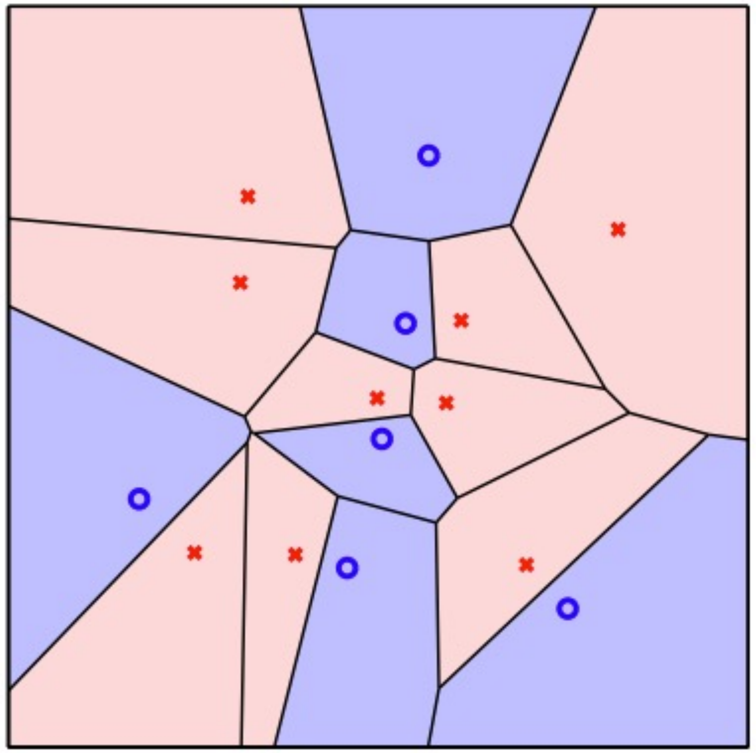
- Predict $\vec{x}$ according to its nearest neighbor
  - Given $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \dots, (\vec{x}_N, y_N)\}$; $y_n \in \{+1, -1\}$
  - Let $\vec{x}_{[1]}$ be $\vec{x}$'s nearest neighbor, i.e., the closest point to $\vec{x}$ in D
  - Let $y_{[i]}(\vec{x})$ or $y_{[i]}$ be the label of $\vec{x}_{[i]}$

- Nearest neighbor hypothesis

$$g(\vec{x}) = y_{[1]}(\vec{x})$$

Nearest Neighbor

$g(\vec{x})$ looks like a Voronoi diagram



- Properties of Nearest Neighbor (NN)
  - No training is needed
  - Good interpretability
  - In-sample error $E_{in} = 0$
  - VC dimension is ∞
- This seems to imply bad learning models from what we talk about so far? Why we care?
- What we really care about is E_{out}
  - VC analysis: $E_{out} \leq E_{in} +$ Generalization error
    - We can infer E_{out} through E_{in} and model complexity
  - NN has nice guarantees outside of VC analysis

Nearest Neighbor is 2-Optimal

- Given mild conditions, for nearest neighbor, when $N \to \infty$, with high probability,

$$E_{out} \leq 2E_{out}^{*}$$

- That is, we can not infer E_{out} from E_{in}, but we know it cannot be much worse than the best anyone can do.

<u>Informal intuitions:</u>

Assumption for nearest neighbor:
- Target function is continuous
- That is, nearby points have similar label distributions

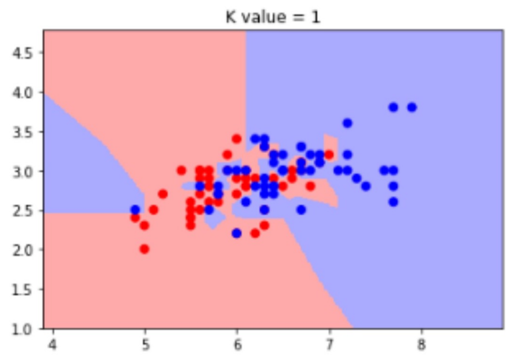
As N goes large, there are “close enough” points for prediction

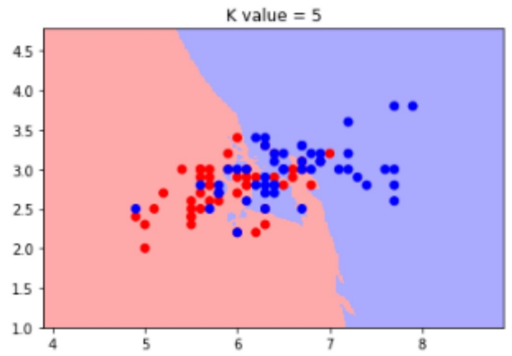
Today’s Lecture

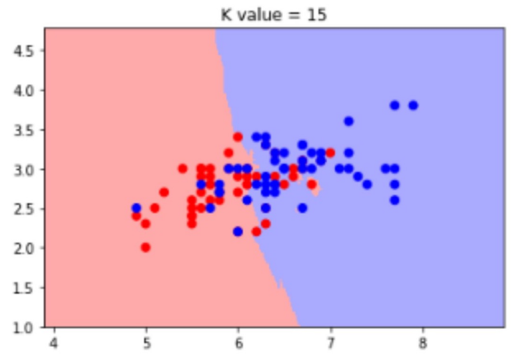
k-Nearest Neighbor (K-NN)

- Nearest neighbor
  - Influenced heavily by noisy data

- k-nearest neighbor (K-NN)
  - $g(\vec{x}) = sign\left(\sum_{i=1}^{k} y_{[i]}(\vec{x})\right)$
  - (k is often odd for binary classification)

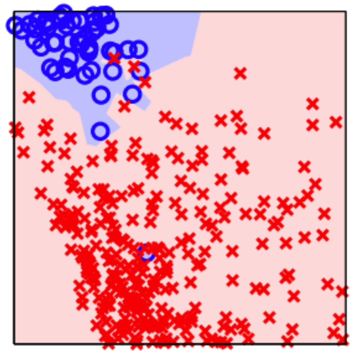


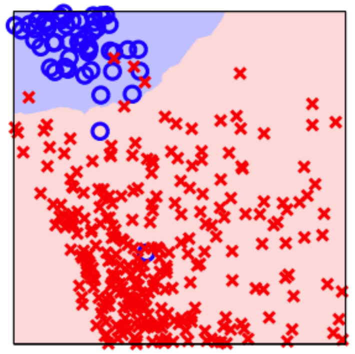


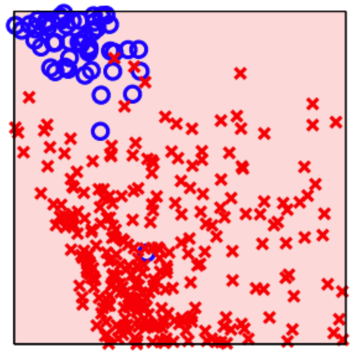


Impacts of k in k-Nearest Neighbor

- $k = 1$: the nearest neighbor hypothesis
  - many, complicated decision boundaries; may overfit
- $k = N$, g predicts the most common label in the training dataset
  - no decision boundaries; may underfit
- k controls the complexity of the hypothesis set
  - k affects how well the learned hypothesis will generalize


1-NN rule


21-NN rule


127-NN rule

How to Choose k

- Making the choice of k a function of N, denoted by $k(N)$
- Theorem:
  - For $N \to \infty$, if $k(N) \to \infty$ and $\frac{k(N)}{N} \to 0$
  - Then $E_{in}(g) \to E_{out}(g)$ and $E_{out}(g) \to E_{out}(g^*)$

- Example: $k(N) = \sqrt{N}$ satisfies the condition

<u>Informal intuitions:</u>

$\frac{k(N)}{N} \to 0$: all the nearest neighbors are next to $\vec{x}$

$k(N) \to \infty$: select infinitely many neighbors

=> We can almost reconstruct the target function

How to Choose k

- Making the choice of k a function of N, denoted by $k(N)$
- Theorem:
  - For $N \to \infty$, if $k(N) \to \infty$ and $\frac{k(N)}{N} \to 0$
  - Then $E_{in}(g) \to E_{out}(g)$ and $E_{out}(g) \to E_{out}(g^*)$
- Example: $k(N) = \sqrt{N}$ satisfies the condition
- Practical rules of thumb:
  - Small k $(\mathrm{e.g.}, \mathrm{k} = 3)$ is often a good enough choice
  - Using validation to choose k

Summary of k-NN So Far

- Pros
  - Simple algorithm
  - Good interpretations
  - Nice theoretical guarantee
  - Easy to adapt to regression (average of nearest neighbors) and multi-class classification (majority voting)

- Cons
  - Curse of dimensionality
  - Computational issue
    - each prediction requires $O(N)$ computation

Curse of Dimensionality

- Generally, higher dimensionality implies harder learning (think VC)
- Things are worse with similarity-based methods
  - Rely on assumptions that nearby points have similar labels
  - As the dimension grows, most of the points will not be nearby to each other…

Illustration of Curse of Dimensionality

- Think about Euclidean distance: $d(\vec{x}, \vec{x}') = \|\vec{x} - \vec{x}'\|$

- Illustration
  - Consider the space $[0,1]^d$ (a hypercube with length of each side = 1)
  - What's the side length ℓ of a hypercube that takes up 1% of the space?
    - $d = 1$: $\ell = 0.01$
    - $d = 2$: $\ell = 0.1$
    - …
    - $d = 100$: $\ell^d = 0.01 \Rightarrow \ell \approx 0.95$
    - $d = 1000$: $\ell^d = 0.01 \Rightarrow \ell \approx 0.9954$

Illustration of Curse of Dimensionality

- Consider the distance to the origin when $d = 100$
  - Consider the case that the value of each dimension is uniformly drawn
  - Only 1% of the points will be in the hypercube $[0,0.95]^{100}$
  - Most of the points will be far away from the origin
  - Most of the points will be far away from each other

- No simple solutions….
  - Getting more data
  - Reduce dimensions (see LFD 9.2)

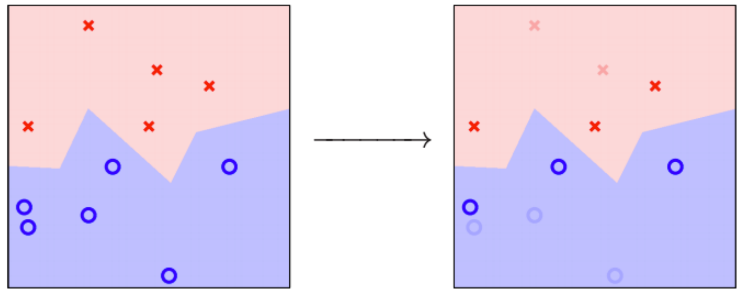
Computational Issues for k-NN

Computational Issues

- k-Nearest Neighbor is computationally demanding
  - Need to store all data points: space complexity $O(Nd)$
  - For each prediction for $\vec{x}$
    - Calculate the distance to every point in D
    - Find the k closest points
    - Time complexity $O(Nd + Nlogk)$
- Two general approaches:
  - Reduce the number of data points
  - Store the data in some data structure to speed up searching
  - See LFD 6.2.3 for more discussion

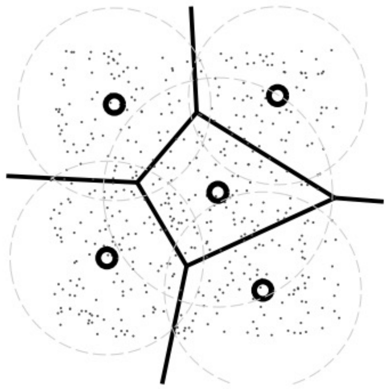
Computational Issues: Potential Solutions

- Reduce the number of data points



- Intuition: remove points that will not impact the decision boundary.
- Generally a hard problem. But there are some heuristic approaches.

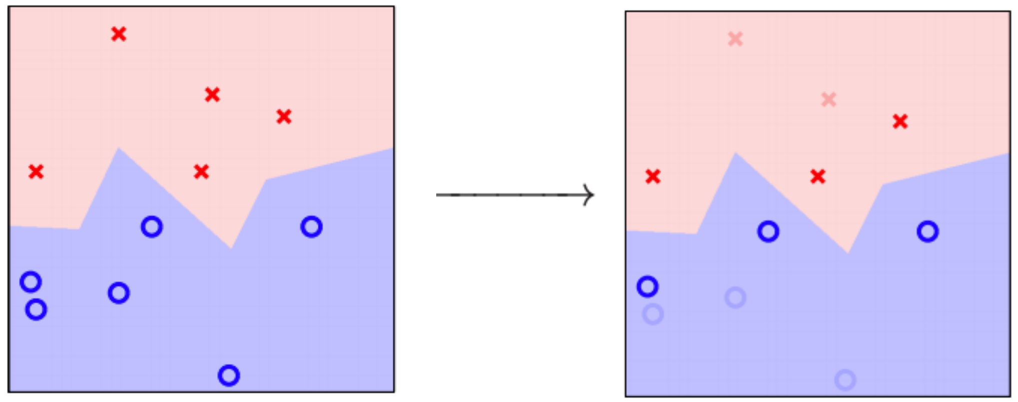
- Store the data in some data structure to speed up searching



- Intuition: Cluster data points
- For a new data point, first find a nearest cluster. Then find the nearest points within that cluster

Reduce the Amount of Data

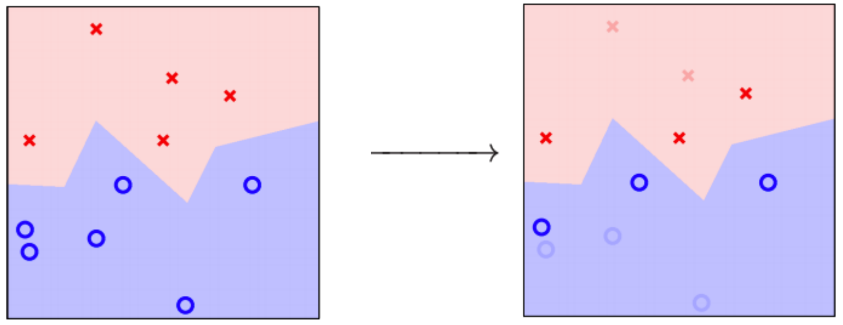
- Consider the following example



- Goal: Drop data that doesn't impact the decision boundary
  - Find $S \subseteq D$, such that $g_S(\vec{x}) = g_D(\vec{x})\ \forall \vec{x}$
  - Generally a hard goal to achieve

A Probably Easier Goal

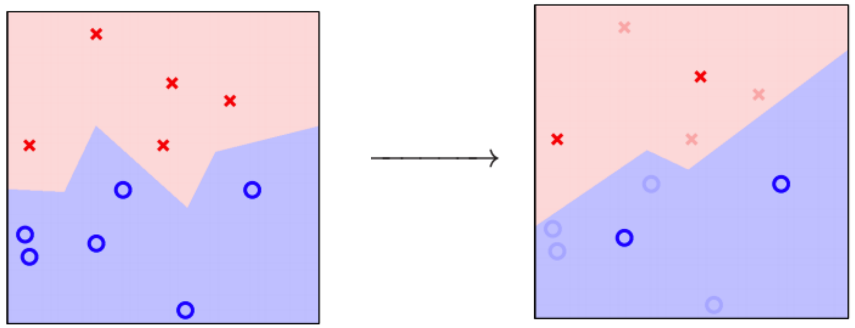
- Instead of making the decision boundary consistent



$g_D(\vec{x})$ $g_S(\vec{x})$

Find $S \in D$, such that $g_S(\vec{x}) = g_D(\vec{x})\ \forall \vec{x}$

- Aim for making the prediction on the training data consistent

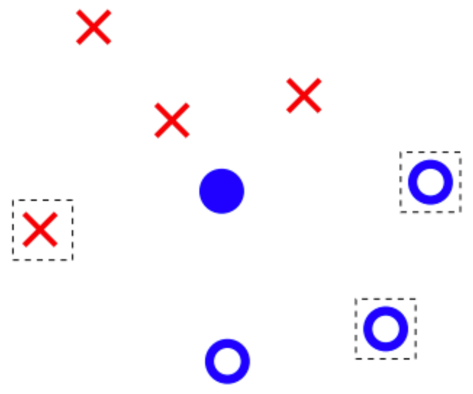


$g_D(\vec{x})$ $g_S(\vec{x})$

Find $S \in D$, such that $g_S(\vec{x}) = g_D(\vec{x})\ \forall \vec{x} \in D$

Condensed Nearest Neighbor (CNN)

- Goal: Find $S \in D$, such that $g_S(\vec{x}) = g_D(\vec{x}) \; \forall \vec{x} \in D$

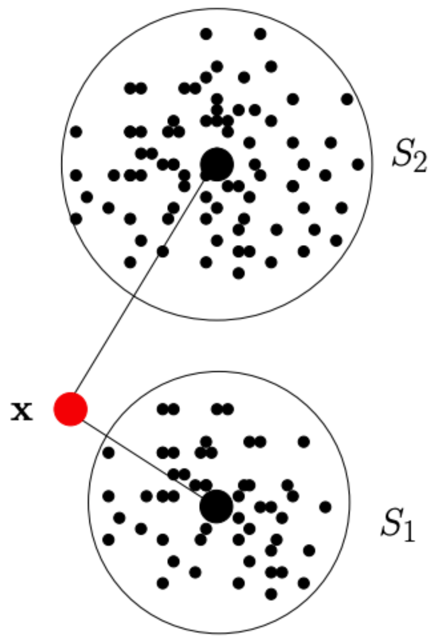


- CNN: An iterative algorithm
  - Random initialize a subset of data points S
  - While (there exists point $\vec{x}_* \in D$ such that $g_S(\vec{x}_*) \neq g_D(\vec{x}_*)$)
    - Let y_* be $g_D(\vec{x}_*)$
    - Find the nearest point $\vec{x}' \in D \backslash S$ with the label y_*
    - Insert $\vec{x}'$ to S

- No theoretical guarantees
- Reasonable empirical performance

Speed Up the Search for Nearest Neighbor

- For each prediction for $\vec{x}$, we need to find the nearest point in D
- Can we speed up this process?



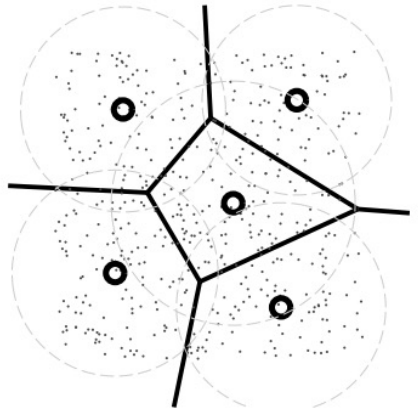
- S_1 and S_2 are two clusters
  - Centers $\vec{\mu}_1, \vec{\mu}_2$ and radii r_1, r_2

- Let S_1 be the nearest cluster for $\vec{x}$
- Let $\vec{x}'_{[1]}$ be the nearest point in S_1

- Distance from $\vec{x}$ to any point in S_2 is at least $\|\vec{x} - \vec{\mu}_2\| - r_2$
- If $\left\|\vec{x} - \vec{x}'_{[1]}\right\| \leq \|\vec{x} - \vec{\mu}_2\| - r_2$
  - we don't need to search points in S_2

Lloyd’s Algorithm: Construct Clusters

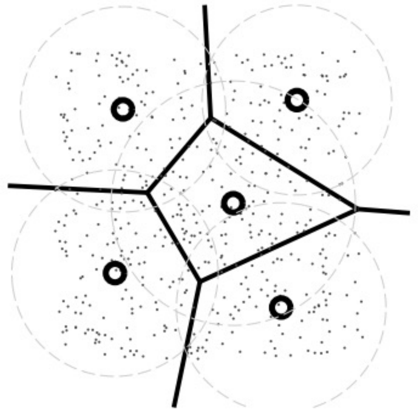
- Goal: Cluster data into K clusters
  - Again, hard in general, but we can use greedy-based approaches



Lloyd’s Algorithm: Construct Clusters

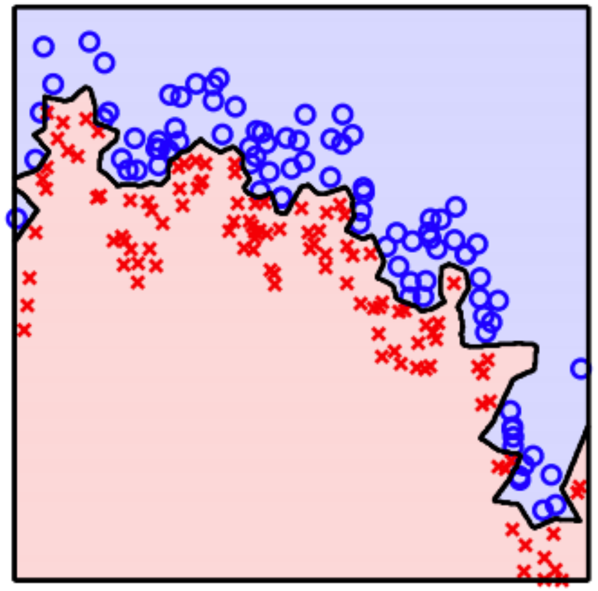
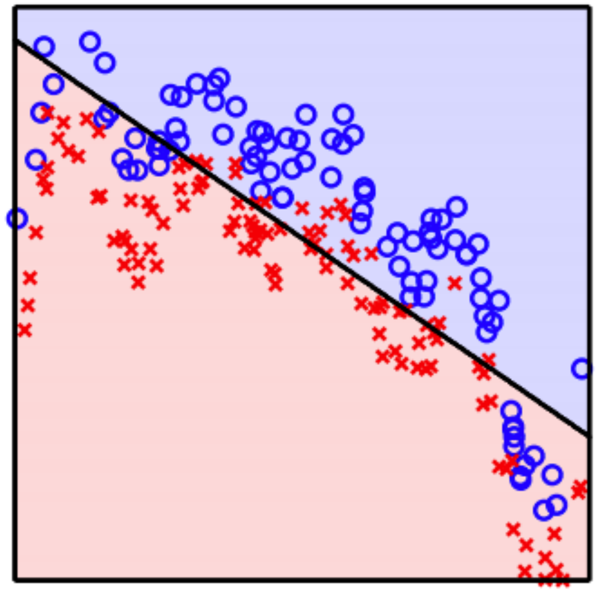
- Goal: Cluster data into K clusters
  - Again, hard in general, but we can use greedy-based approaches

- Lloyd’s Algorithm
  1. Randomly pick K points as centers
  2. Create the Voronoi regions as clusters
  3. Update the centers (calculating the mean)
  4. Update the region
  5. Repeat 3 and 4



- This is the first (and probably the only) unsupervised learning algorithm we talk about in this course.

Final Remark:
Nearest Neighbor is Nonparametric

Nearest Neighbor	Linear models
	
no parameters	$(d+1)$ parameters
expressive/flexible	rigid, always linear
$g(\mathbf{x})$ needs data	$g(\mathbf{x})$ needs only weights
generic, can model anything	specialized

Radial Basis Functions (RBF)

Instance-Based Learning

- Make predictions based on data instances

- k-nearest neighbor (K-NN)
  - $g(\vec{x}) = sign\left(\sum_{i=1}^{k} y_{[i]}(\vec{x})\right)$
  - Predict according to the nearest neighbors

- Radial Basis Functions (RBF)
  - Focus of today

- Kernel SVM (Topic of Next Week)
  - $g(\vec{x}) = sign\left(\sum_{\alpha_n^*>0} \alpha_n^* y_n K(\vec{x}_n, \vec{x}) + b^*)\right)$
  - Predict according to support vectors

Radial Basis Functions

- Think about k-nearest neighbor (K-NN) again
  - $g(\vec{x}) = sign\left(\sum_{i=1}^{k} y_{[i]}(\vec{x})\right)$

  - Make predictions based on k nearest data points
  - Each of the k data points has the same weight

- Natural questions:
  - Can we use more (or even all) data?
  - Weight them based on how close data points are to $\vec{x}$

Radial Basis Functions

- Given dataset $D = \{\vec{x}_1, \dots, \vec{x}_N\}$
- Task: Make a prediction on $\vec{x}$

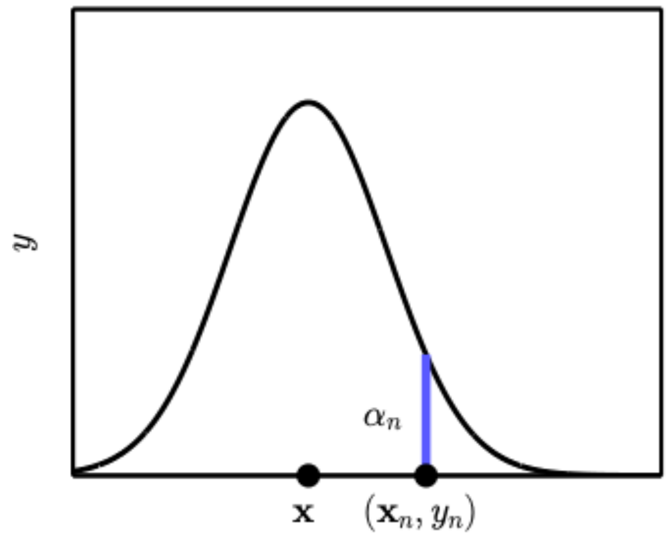
- Radial Basis Function:
  - $g(\vec{x}) = \frac{1}{Z(\vec{x})} \sum_{n=1}^{N} \phi\left(\frac{\|\vec{x}-\vec{x}_n\|}{r}\right) y_n$
  - $\phi(s)$: a monotonically decreasing function

- This is for regression. We can take a sign and make it a binary classification.
- $Z(\vec{x}) = \sum_{m=1}^{N} \phi\left(\frac{\|\vec{x}-\vec{x}_m\|}{r}\right)$ is for normalization

- It's called radial basis function since it takes the distance to the points as the basis function

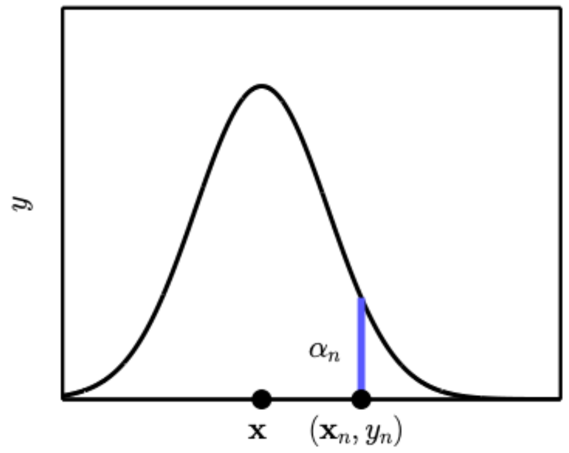
Radial Basis Functions

- Radial Basis Function:
  - $g(\vec{x}) = \sum_{n=1}^{N} \frac{1}{Z(\vec{x})} \phi\left(\frac{\|\vec{x}-\vec{x}_n\|}{r}\right) y_n$
  - Example of ϕ
    - Gaussian RBF: $\phi(s) = e^{-s}$
- Intuitions
  - The impact of $\vec{x}_n$ to $\vec{x}$ is higher if it's closer to $\vec{x}$
  - The role of r is similar to k in k-NN
    - $r \to 0$: 1-NN
    - $r \to \infty$: N-NN (i.e., $k = N$)



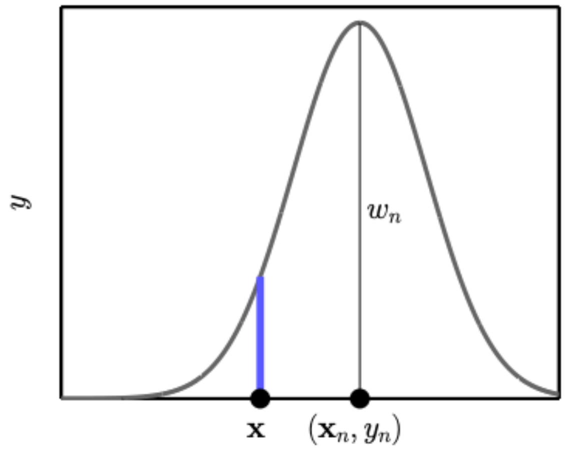
Changing the Viewpoints

- ϕ centered around $\vec{x}$



$$g(\vec{x}) = \sum_{n=1}^{N} \frac{y_n}{Z(\vec{x})} \phi\left(\frac{\|\vec{x} - \vec{x}_n\|}{r}\right)$$

- ϕ centered around $\vec{x}_n$



$$g(\vec{x}) = \sum_{n=1}^{N} w_n(\vec{x})\, \phi\left(\frac{\|\vec{x} - \vec{x}_n\|}{r}\right)$$

From Nonparametric to Parametric RBF

- Nonparametric RBF
  - $g(\vec{x}) = \sum_{n=1}^{N} \frac{y_n}{Z(\vec{x})} \phi\left(\frac{\|\vec{x}-\vec{x}_n\|}{r}\right)$
  - $g(\vec{x}) = \sum_{n=1}^{N} w_n(\vec{x})\, \phi\left(\frac{\|\vec{x}-\vec{x}_n\|}{r}\right)$
  - The hypothesis is defined by dataset

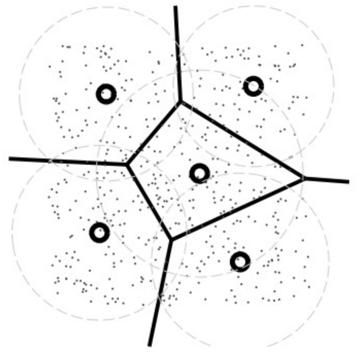
- Parametric RBF hypothesis set
  - $h(\vec{x}) = \sum_{n=1}^{N} w_n\, \phi\left(\frac{\|\vec{x}-\vec{x}_n\|}{r}\right)$
  - Learn w_n from data

Parametric RBF => Linear Models

- Parametric RBF is linear model with nonlinear transformation
  - $h(\vec{x}) = \sum_{n=1}^{N} w_n \, \phi\left(\frac{\|\vec{x}-\vec{x}_n\|}{r}\right)$
  - The projection $\Phi(\vec{x}) = \begin{bmatrix} \phi\left(\frac{\|\vec{x}-\vec{x}_1\|}{r}\right) \\ \phi\left(\frac{\|\vec{x}-\vec{x}_2\|}{r}\right) \\ \vdots \\ \phi\left(\frac{\|\vec{x}-\vec{x}_N\|}{r}\right) \end{bmatrix}$
- We can apply what we learned in linear models to learn w_n
- However, this seems to be overfitting (N parameters for N points)

From N points to K points

- Use only K points $(\vec{\mu}_1, \dots, \vec{\mu}_K)$
  - $h(\vec{x}) = \sum_{k=1}^{K} w_k \, \phi\left(\frac{\|\vec{x}-\vec{\mu}_k\|}{r}\right)$
- Which K points?
  - We can find K representative points
  - Use clustering algorithms, e.g., Lloyd algorithm as introduced earlier
    1. Randomly pick K points as centers
    2. Create the Voronoi regions as clusters
    3. Update the centers (calculating the mean)
    4. Update the region
    5. Repeat 3 and 4



More Discussion on RBF

- $h(\vec{x}) = \sum_{k=1}^{K} w_k \, \phi\left(\frac{\|\vec{x} - \vec{\mu}_k\|}{r}\right)$

- Connection to linear models
  - Parametric RBF is essentially linear model with nonlinear transformation

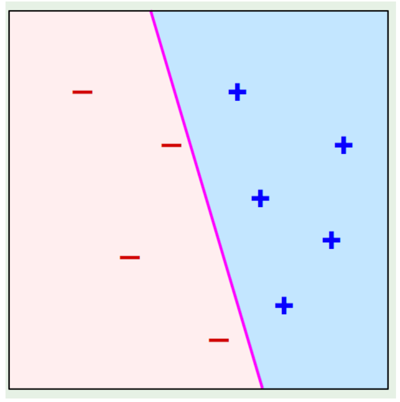
- Connection to nearest neighbor
  - Radial Basis Function is defined by “similarity
  - A prediction for a point is based on the “similarity” of the points to be predicted and other points

Support Vector Machines (SVM)

What Do We Know about Linear Classification?

- What we discussed so far:
  - PLA: Find a linear separator that separates the data within finite steps, if data is linear separable.
  - Pocket algorithm: empirically keep the best separator during PLA.
  - Surrogate loss: Using logistic regression for linear classification.

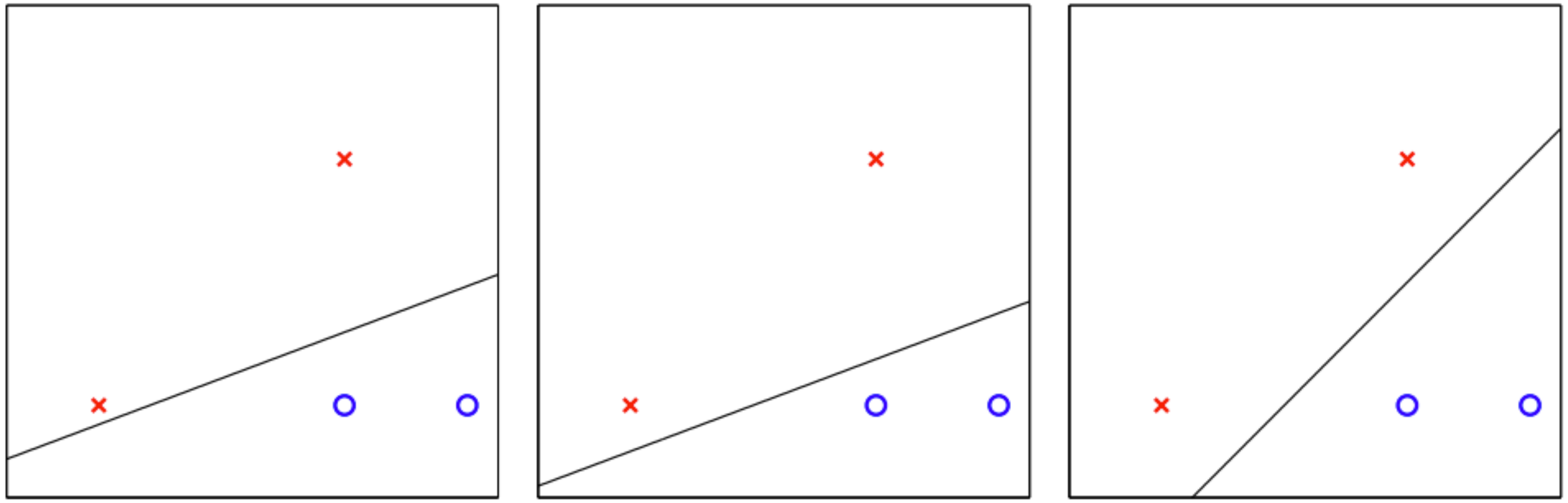
- Challenges
  - Binary classification error is hard to optimize
  - We cannot use "gradient descent" type of algorithm minimize E_{in}.



- Support vector machines (SVM) tries to look at things a bit differently.

Linear Classification

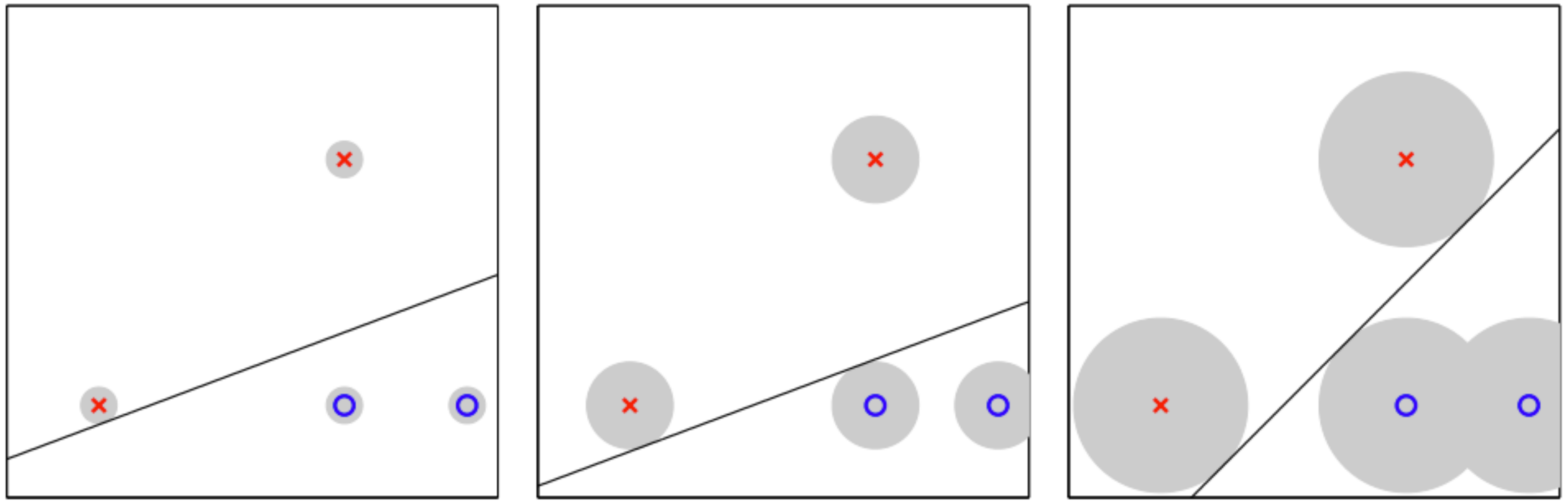
- Which separator would you choose?



Probably the right one.
Why?

Linear Classification

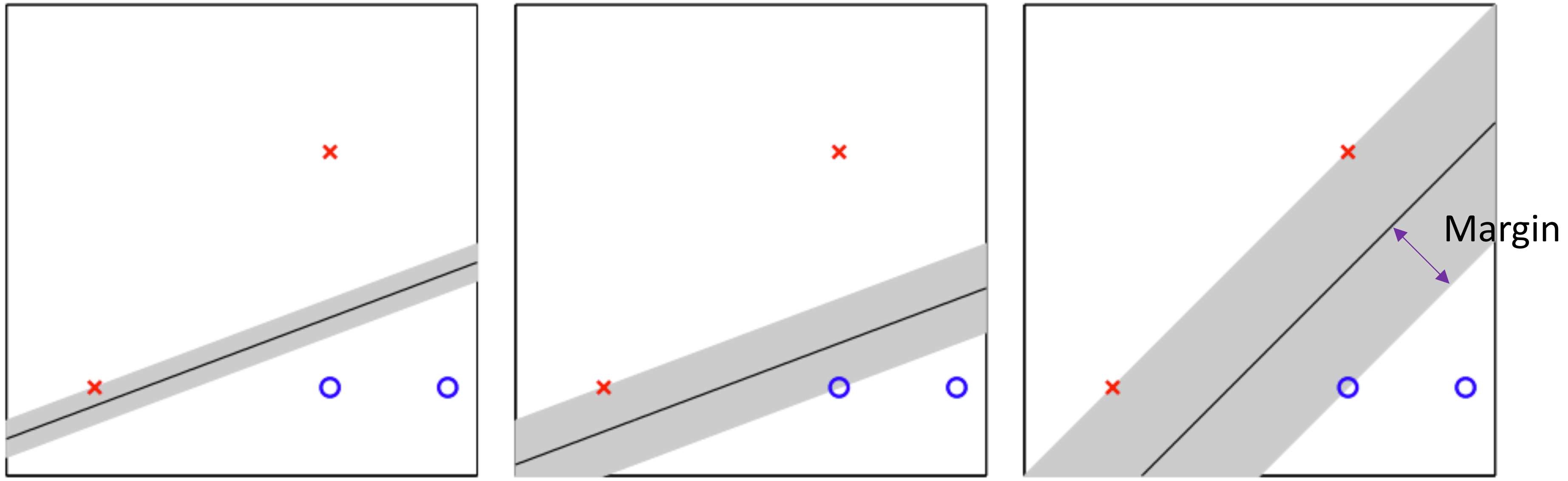
- Which separator would you choose?



More robust to noise (e.g., measurement error of $\vec{x}$)

Linear Classification

- Which separator would you choose?



Margin: shortest distance from the separator to the points in D

(Informal argument)

Higher margin => more “constrained” hypothesis => lower VC dimension

Support Vector Machine

- Goal:
  - Find the max-margin linear separator that separates the data
  - Recall the goal of PLA: Find the linear separator that separates the data

- Notations:

Notations we used so far:

- $\vec{x} = (x_0, x_1, \dots, x_d)$
- $\vec{w} = (w_0, w_1, \dots, w_d)$
- Linear separator

$$h(\vec{x}) = sign(\vec{w}^T \vec{x})$$

$\Rightarrow$

Notations we will use in SVM

- $\vec{x} = (x_1, \dots, x_d)$
- $\vec{w} = (w_1, \dots, w_d)$
- Linear separator

$$h(\vec{x}) = sign(\vec{w}^T \vec{x} + b)$$

Separating the bias/intercept b is important for us to characterize the margin.

We will use $(\vec{w}, b)$ to characterize the hypothesis