CSE 417T
Introduction to Machine Learning

Lecture 16
Instructor: Chien-Ju (CJ) Ho

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
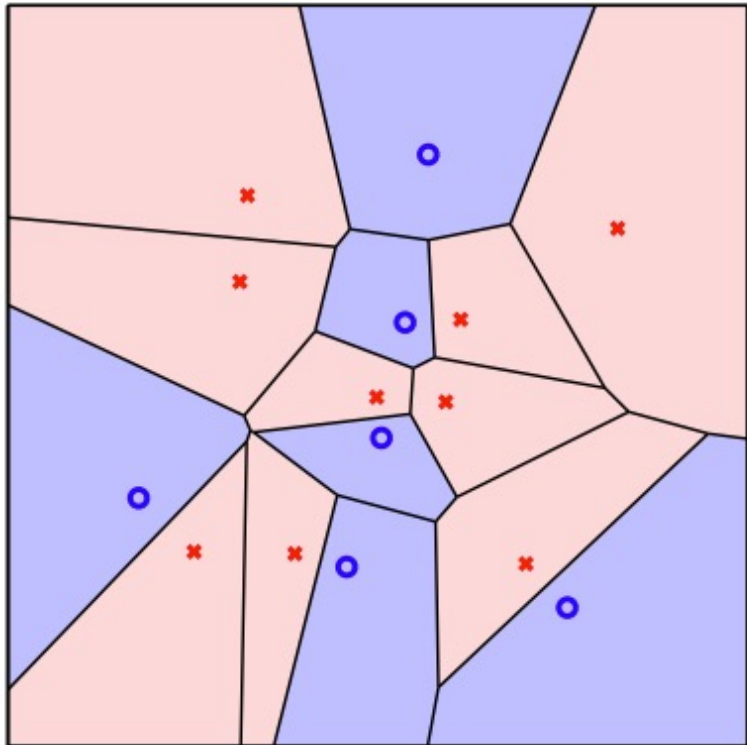
Nearest Neighbor

- Predict $\vec{x}$ according to its nearest neighbor

  - Given $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_N, y_N)\}$; $y_n \in \{+1, -1\}$

  - 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 (similar $\vec{x}$ have similar label distribution, input distribution has non-zero support in all space), 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.

Informal intuitions:

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

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook. Let me know if you spot errors.
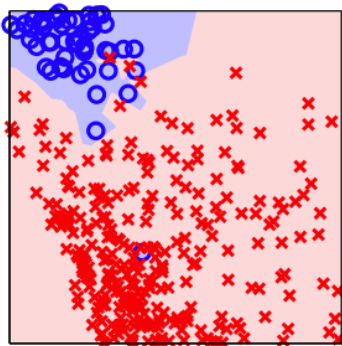
k-Nearest Neighbor

"Stabilize" the Hypothesis

- Making predictions according to k nearest neighbors
  - Instead of using a "single" nearest neighbor

- k-nearest neighbor (K-NN)
  - $g(\vec{x}) = sign\left(\sum_{i=1}^{k} y_{[i]}(\vec{x})\right)$
 - (k is often chosen to be an odd number for binary classification)
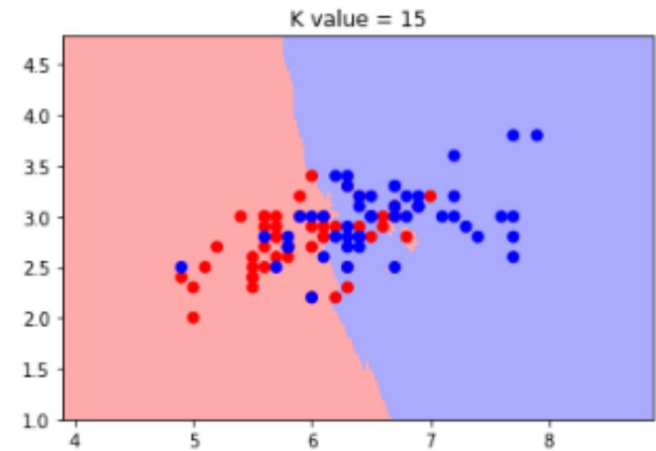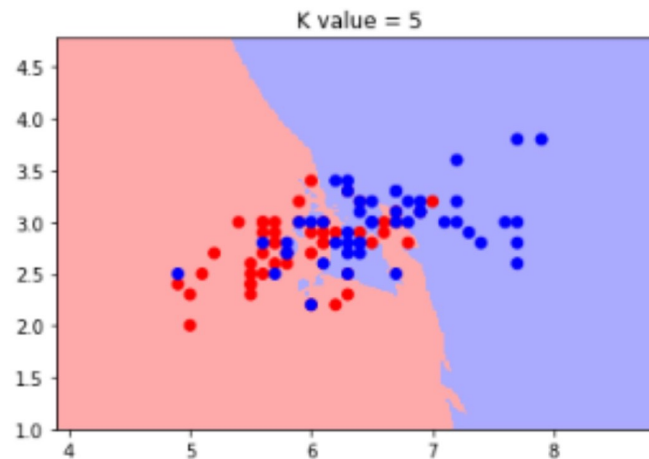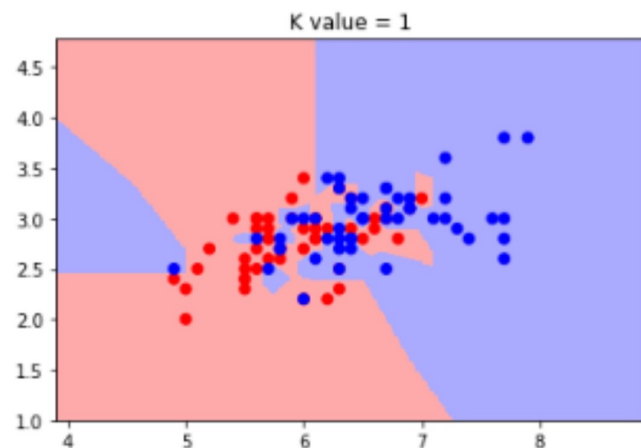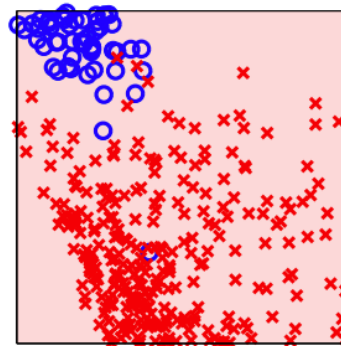
Impacts of k in k-Nearest Neighbor

- $k = 1$: 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
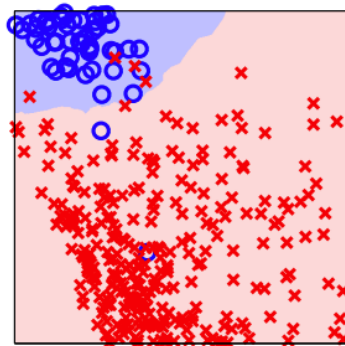
1-NN rule   21-NN rule   127-NN rule

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 $\dfrac{k(N)}{N} \to 0$

  - Then $E_{in}(g) \to E_{out}(g)$ and $E_{out}(g) \to E_{out}(g^*)$

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

Informal intuitions:

$\dfrac{k(N)}{N} \to 0$: 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 $\dfrac{k(N)}{N} \to 0$
  - 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 $(e.\,g.\,, k = 3)$ 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 label distributions
    - 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
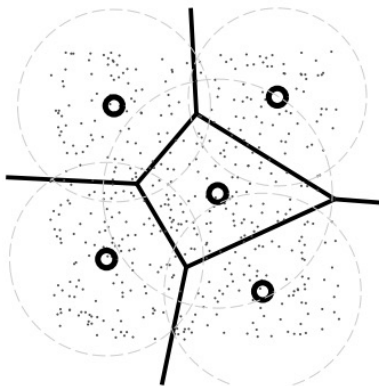 - See LFD 6.2.3 for more discussion

Computational Issues: Potential Solutions

- Reduce the number of data points
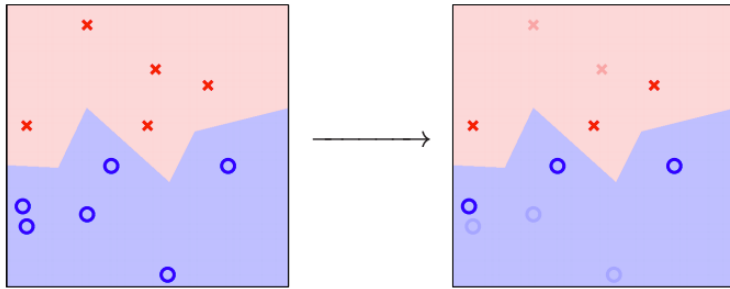
  - Intuition: remove points that will not impact the decision boundary.

  - Generally a hard problem. But there are some heuristic approaches.
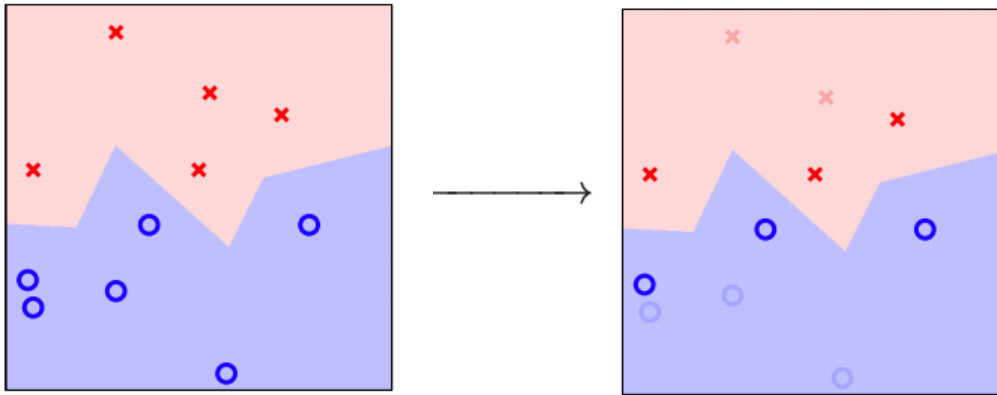
- Store the data in some data structure to speed up searching

  - Intuition: Cluster data points

  - For a new data point, first find a nearest cluster. Then find the nearest points within that cluster
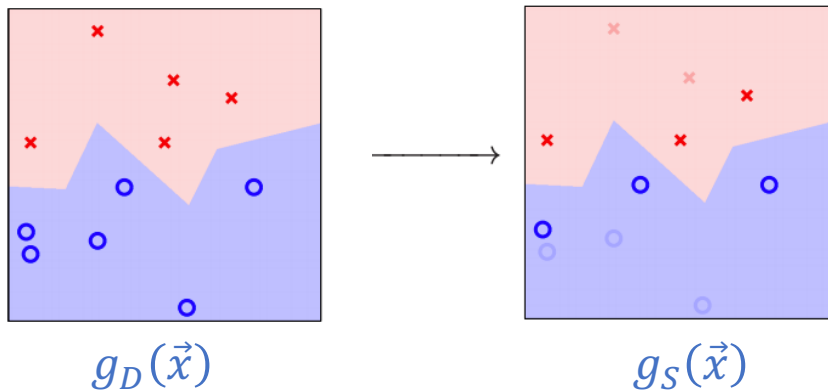
Reduce the Amount of Data

- Consider the following example

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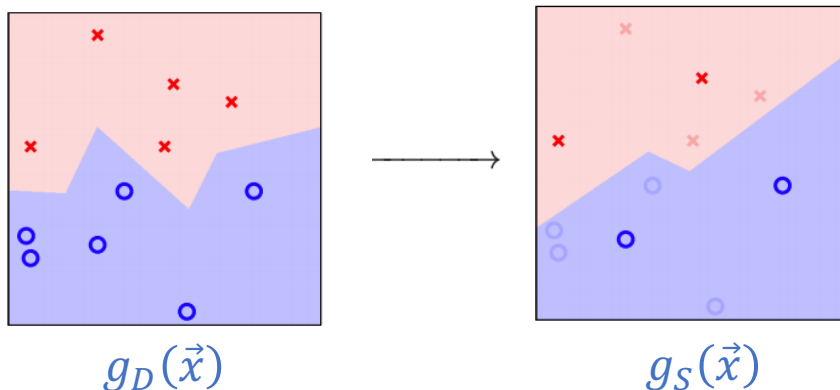 - Generally a hard goal to achieve

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

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

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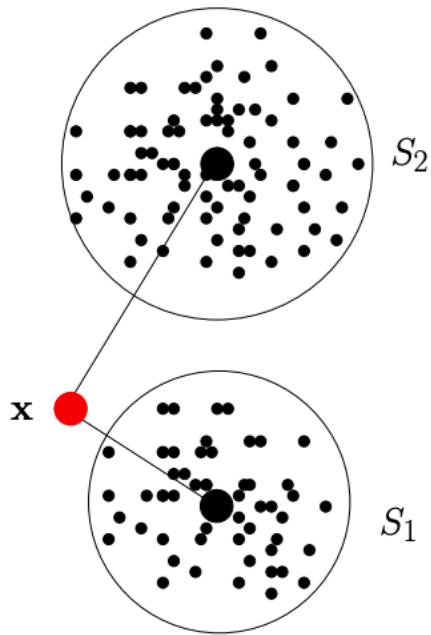
- S_1 and S_2 are two clusters
  - Centers $\vec{\mu}_1, \vec{\mu}_2$ and radii r_1, r_2

- 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 $\left\|\vec{x} - \vec{x}'_{[1]}\right\| \le \|\vec{x} - \vec{\mu}_2\| - r_2$
  - we don't need to search points in S_2

Lloyd's Algorithm: Construct Clusters

- Goal: Cluster data into K clusters
  - Split points into K sets $S_1, \dots, S_N$
  - Such that the sum of distance from each point to its center is the smallest

  - 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 unsupervised learning algorithm we talk about in this course
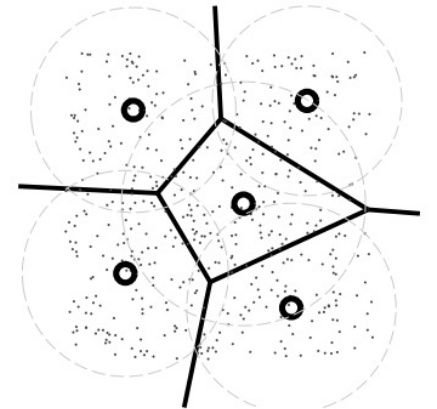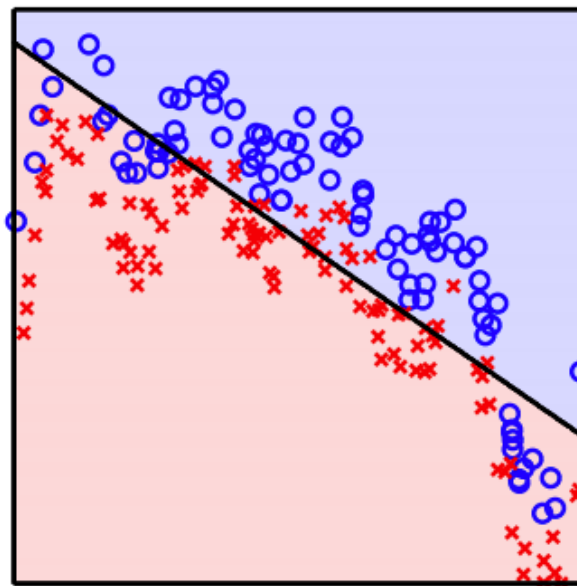
Final Remark:
Nearest Neighbor is Nonparametric

Nearest Neighbor
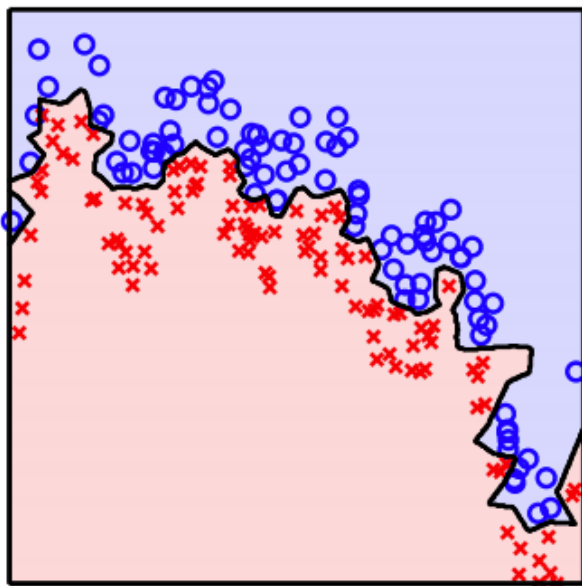
Linear models

no parameters

expressive/flexible

$g(\mathbf{x})$ needs data

generic, can model anything

$(d+1)$ parameters

rigid, always linear

$g(\mathbf{x})$ needs only weights

specialized

Radial Basis Functions (RBF)

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

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
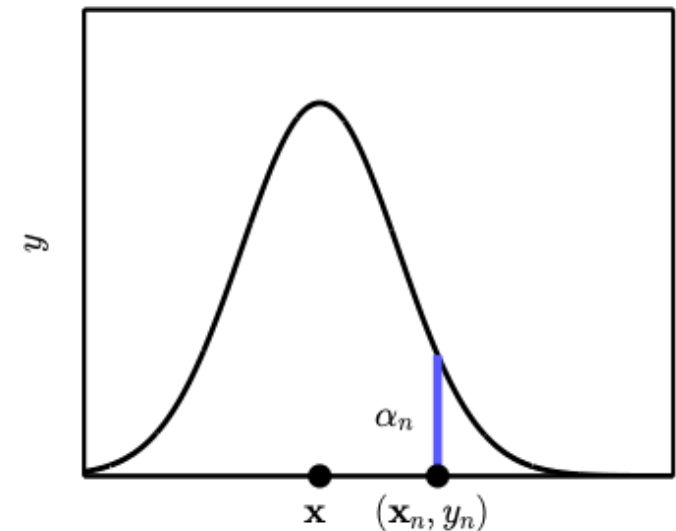
Radial Basis Functions

- 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., $k = N$)

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 $(\vec{\mu}_1, \ldots, \vec{\mu}_K)$

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

- 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
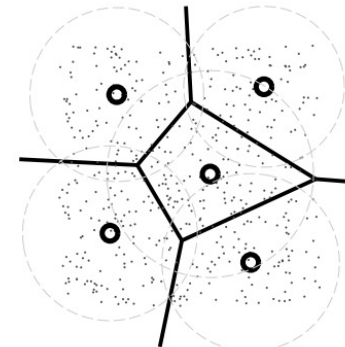
Dual Views of RBF

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

- 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

- Also have some connection to SVM and neural network that we'll discuss

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 to minimize E_{in}.

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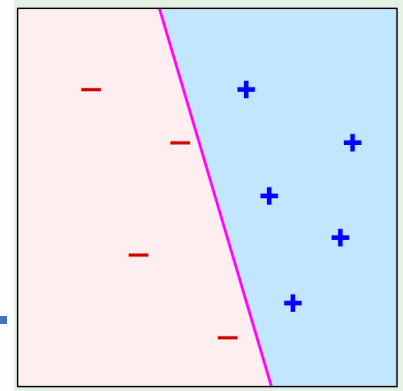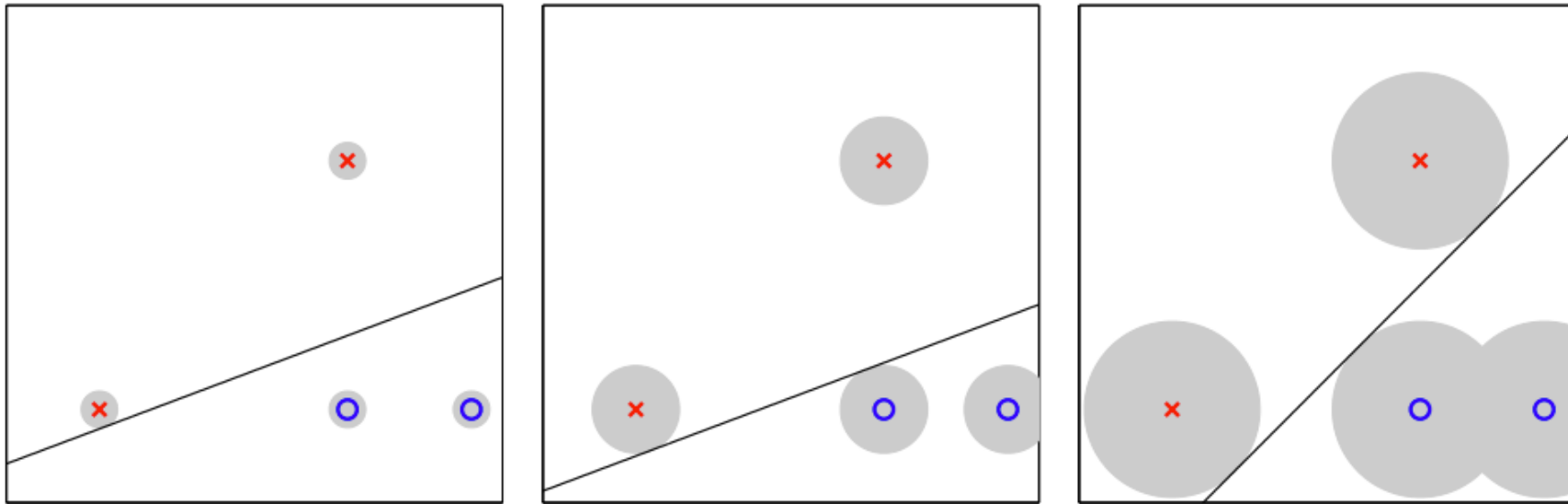
Linear Classification

- Which separator would you choose?
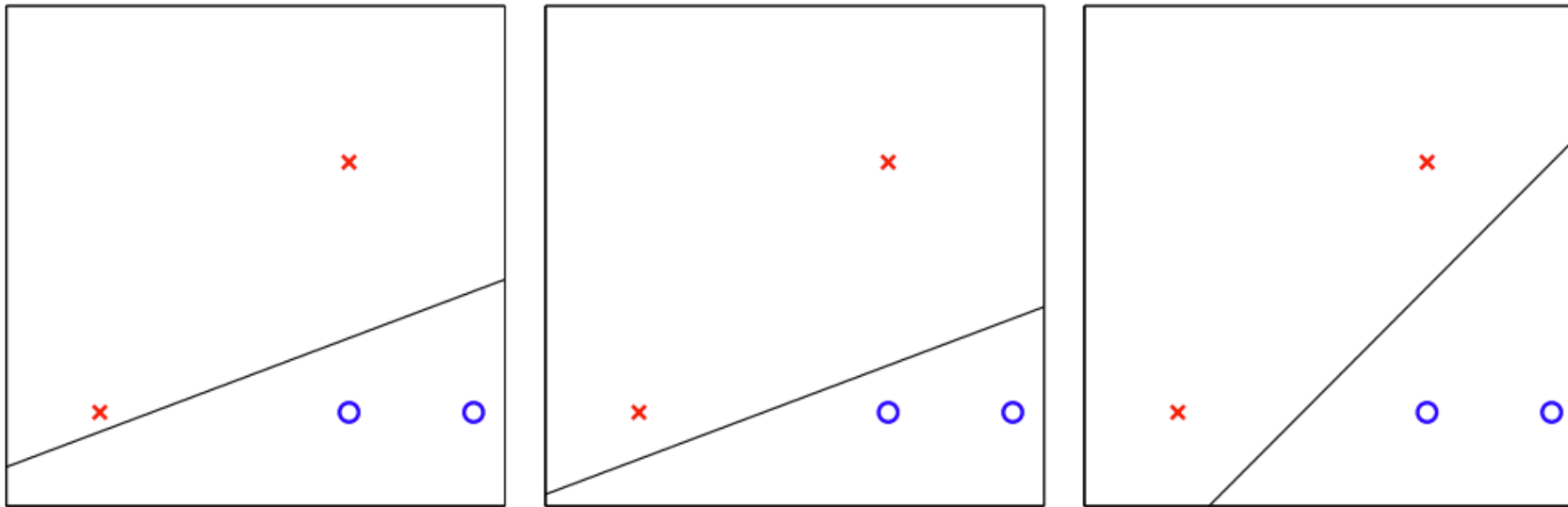
Probably the right one.
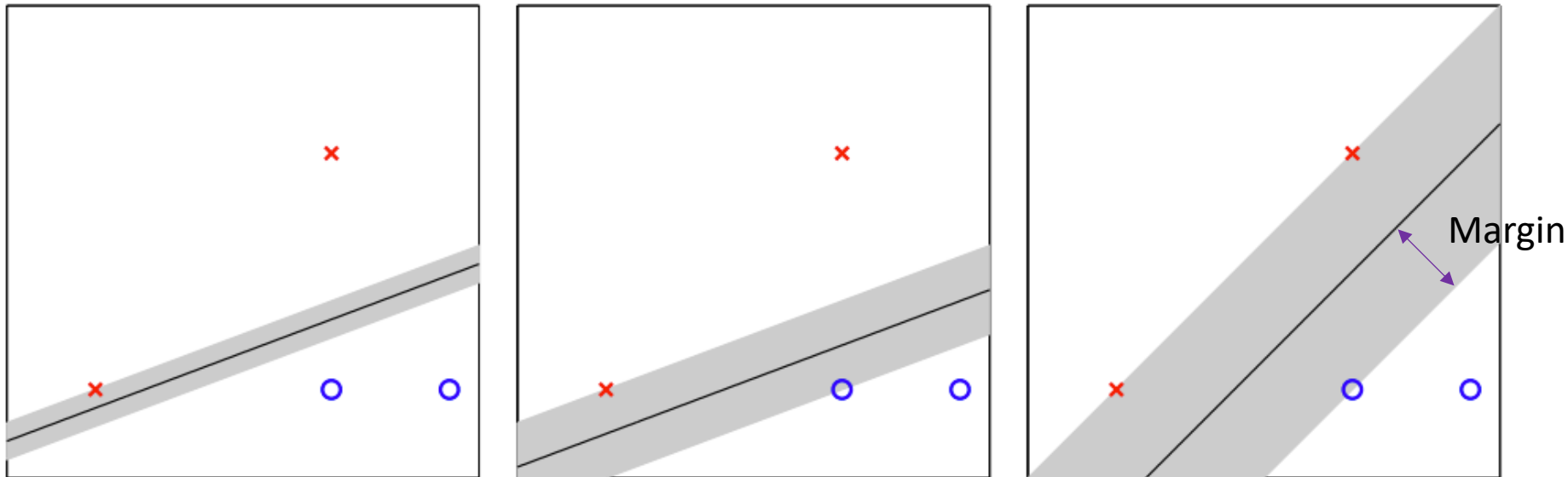Why?

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:
- $\vec{x} = (x_0, x_1, \ldots, x_d)$
- $\vec{w} = (w_0, w_1, \ldots, w_d)$
- Linear separator
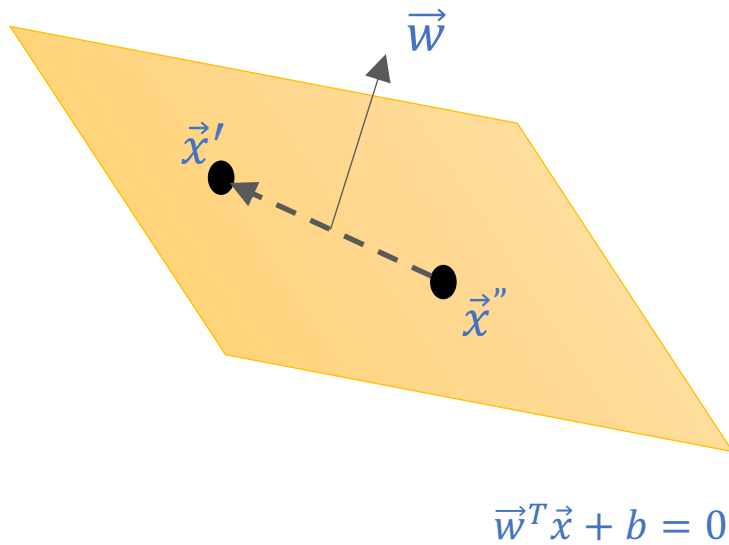 $$h(\vec{x}) = sign(\vec{w}^T \vec{x})$$

Notations we will use in SVM
- $\vec{x} = (x_1, \ldots, x_d)$
- $\vec{w} = (w_1, \ldots, w_d)$
- 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.

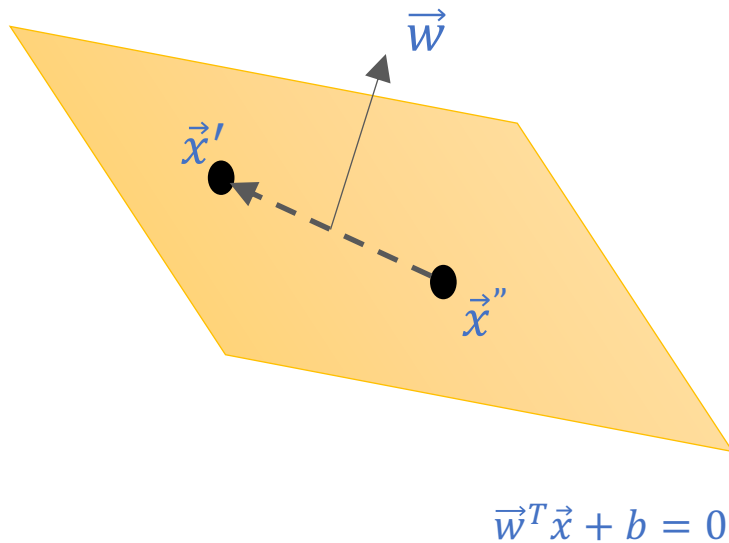We will use $(\vec{w}, b)$ to characterize the hypothesis

Relevant Review of Linear Algebra

- Claim: $\vec{w}$ is the norm vector of the hyperplane $\vec{w}^T\vec{x} + b = 0$

$$\vec{w}$$

$$\vec{x}'$$

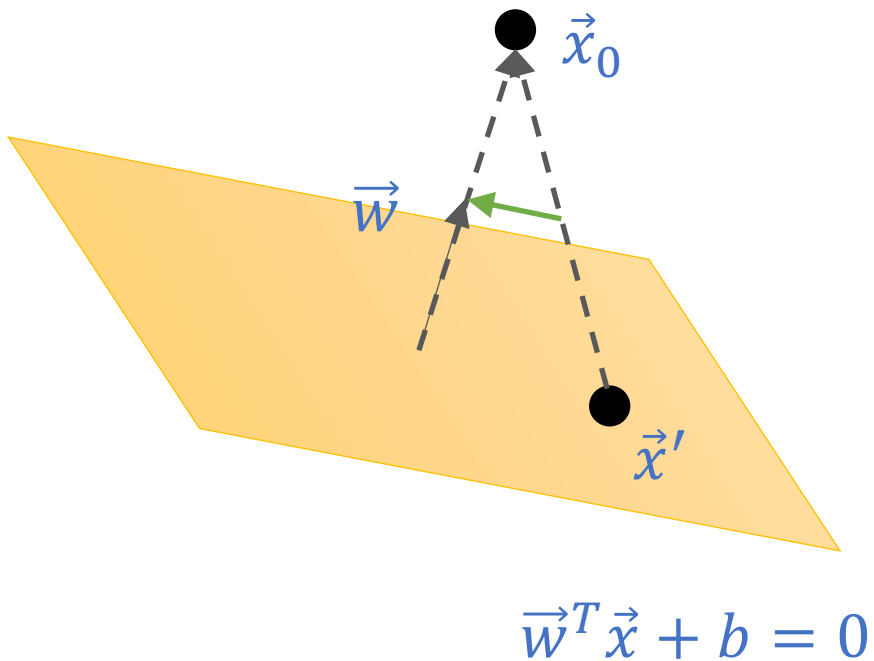$$\vec{x}''$$

$$\vec{w}^T\vec{x} + b = 0$$

Relevant Review of Linear Algebra

- Claim: $\vec{w}$ is the norm vector of the hyperplane $\vec{w}^T \vec{x} + b = 0$

$\vec{w}^T \vec{x} + b = 0$

- Consider any two points $\vec{x}'$ and $\vec{x}''$ on the hyperplane
  - $\vec{w}^T \vec{x}' + b = 0$
  - $\vec{w}^T \vec{x}'' + b = 0$

- Combining the above
  - $\vec{w}^T (\vec{x}' - \vec{x}'') = 0$

- $\vec{w}$ is orthogonal to the hyperplane
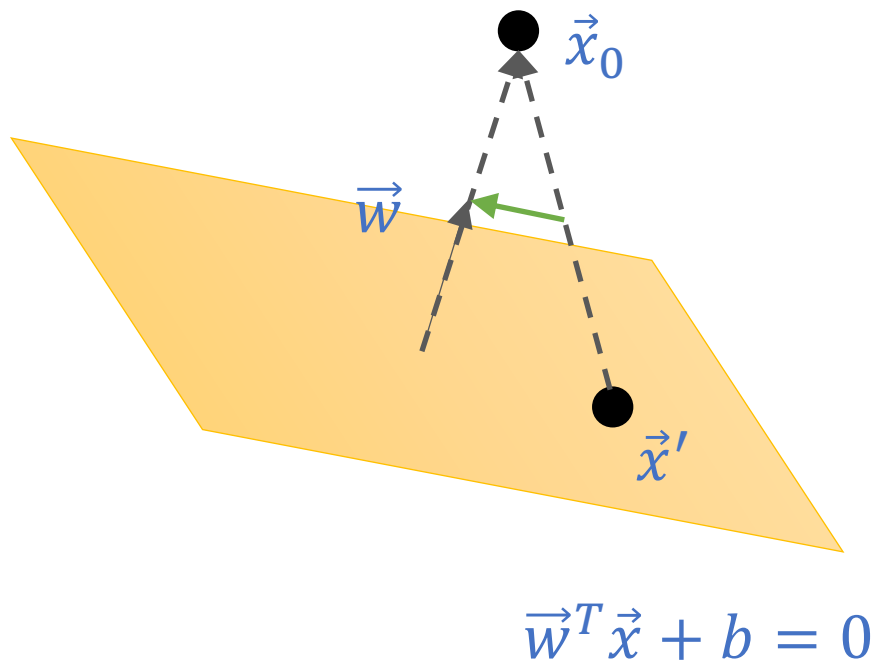- $\vec{w}$ is the norm vector of the hyperplane

Relevant Review of Linear Algebra

- What is the distance between a point $\vec{x}_0$ and a hyperplane $\vec{w}^T\vec{x} + b = 0$

$$\vec{x}_0$$

$$\vec{w}$$

$$\vec{x}'$$

$$\vec{w}^T\vec{x} + b = 0$$

Relevant Review of Linear Algebra

- What is the distance between a point $\vec{x}_0$ and a hyperplane $\vec{w}^T\vec{x} + b = 0$

$$\vec{w}^T\vec{x} + b = 0$$

- Consider an arbitrary point $\vec{x}'$ on the hyperplane

- Distance between the point $\vec{x}_0$ and the hyperplane

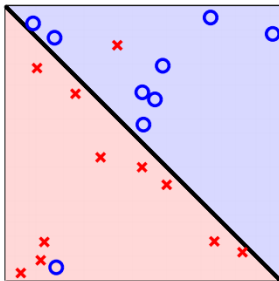$$dist(\vec{x}_0, \vec{w}, b) = \left| \frac{\vec{w}^T}{\|\vec{w}\|}(\vec{x}_0 - \vec{x}') \right|$$

$$\left| \frac{1}{\|\vec{w}\|}(\vec{w}^T\vec{x}_0 - \vec{w}^T\vec{x}') \right|$$

$$\left| \frac{1}{\|\vec{w}\|}(\vec{w}^T\vec{x}_0 + b) \right|$$

Outline of Our Discussion

- Assume data is linearly separable
  - Formulate the hard-margin SVM

  > Given D, find separator $(\vec{w}, b)$ that
  >
  > maximize   margin$(\vec{w}, b)$
  >   s.t.   all points in D is correctly classified

- When data is not linearly separable
  - Tolerate some noise
    - Soft-margin SVM

  - Nonlinear transform
    - Dual formulation and kernel tricks
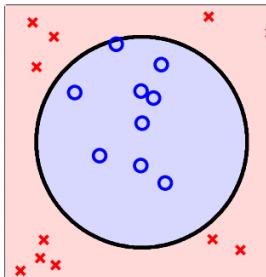
Hard-Margin SVM

Hard-Margin SVM

- Goal
  - Given $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$ that is linearly separable
  - Find separator $(\vec{w}, b)$ that (1) maximizes the margin and (2) separates D

- $(\vec{w}, b)$ separates D (making correct predictions for all points in D)
  - $y_n = sign(\vec{w}^T \vec{x}_n + b)$ for all n
  - $y_n(\vec{w}^T \vec{x}_n + b) \geq 0$ for all n

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

$$\text{margin}(\vec{w}, b) = min_n \, dist(\vec{x}_n, \vec{w}, b)$$
$$= min_n \left| \frac{1}{\|\vec{w}\|} (\vec{w}^T \vec{x}_n + b) \right|$$
$$= min_n \frac{1}{\|\vec{w}\|} y_n(\vec{w}^T \vec{x}_n + b)$$

$$dist(\vec{x}_0, \vec{w}, b) = \left| \frac{1}{\|\vec{w}\|} (\vec{w}^T \vec{x}_0 - b) \right|$$

$y_n \in \{-1, +1\}$ and
$y_n(\vec{w}^T \vec{x}_n + b) \geq 0$

Hard-Margin SVM

- Goal
  - Given $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$ that is linearly separable
  - Find separator $(\vec{w}, b)$ that (1) maximizes the margin and (2) separates D

- Formulate it as a constrained optimization problem

$$\text{maximize}_{\vec{w}, b} \quad \text{margin}(\vec{w}, b)$$
$$\text{subject to} \quad y_n(\vec{w}^T \vec{x}_n + b) \geq 0, \forall n$$
$$\text{margin}(\vec{w}, b) = min_n \frac{1}{\|\vec{w}\|} y_n(\vec{w}^T \vec{x}_n + b)$$

Hard-Margin SVM

- The constrained optimization problem

$$\text{maximize}_{\vec{w},b} \quad \text{margin}(\vec{w}, b)$$
$$\text{subject to} \quad y_n(\vec{w}^T \vec{x}_n + b) \geq 0, \forall n$$
$$\text{margin}(\vec{w}, b) = min_n \frac{1}{\|\vec{w}\|} y_n(\vec{w}^T \vec{x}_n + b)$$

- normalizing $(\vec{w}, b)$
  - Note that $\vec{w}^T \vec{x} + b = 0$ is equivalent to $c\vec{w}^T \vec{x} + cb = 0$ for any c
  - We will normalize $(\vec{w}, b)$ such that $min_n \ y_n(\vec{w}^T \vec{x}_n + b) = 1$
    - margin$(\vec{w}, b) = \frac{1}{\|\vec{w}\|}$
    - $y_n(\vec{w}^T \vec{x}_n + b) \geq 1, \forall n$

Hard-Margin SVM

- The constrained optimization problem

$$\text{maximize}_{\vec{w},b} \quad \frac{1}{\|\vec{w}\|}$$

$$\text{subject to} \quad y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n$$

- Some final adjustments

$$\text{minimize}_{\vec{w},b} \quad \frac{1}{2}\vec{w}^T\vec{w}$$

$$\text{subject to} \quad y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n$$

Final Form of Hard-Margin SVM

$$\text{minimize}_{\vec{w},b} \quad \frac{1}{2}\vec{w}^T\vec{w}$$

$$\text{subject to} \quad y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n$$

- How to solve it?
  - Hard-margin SVM is a Quadratic Program
  - Standard form of Quadratic Program (QP)

$$\text{minimize}_{\vec{u}} \quad \frac{1}{2}\vec{u}^T Q\vec{u} + \vec{p}^T\vec{u}$$

$$\text{subject to} \quad A\vec{u} \geq \vec{c}$$

  - There exist efficient QP solvers we can utilize