CSE 417T
Introduction to Machine Learning

Lecture 17
Instructor: Chien-Ju (CJ) Ho

Logistics

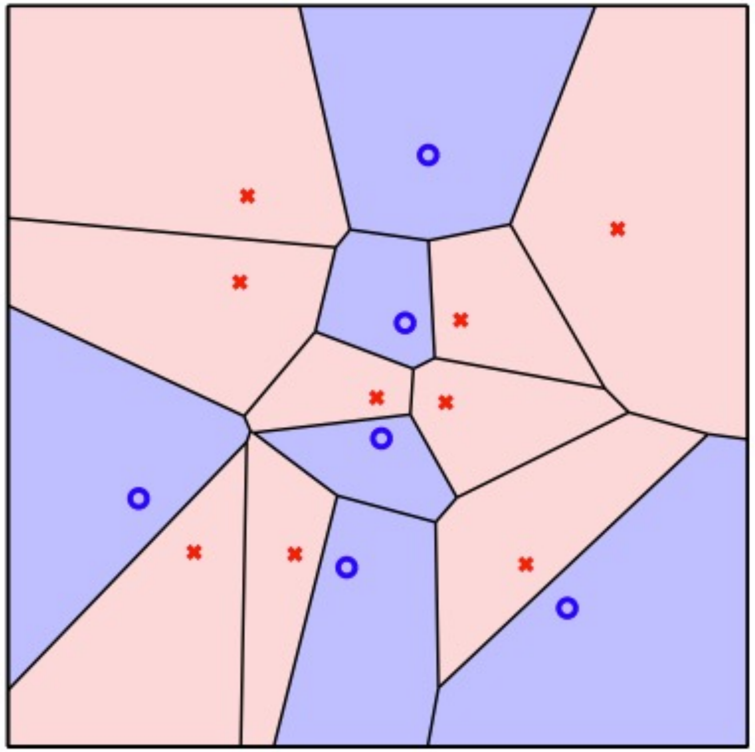
- Homework 4 is due April 1 (Friday)

- 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

$g(\vec{x})$ 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?
- Nearest Neighbor is 2-Optimal
  - When $N \to \infty$, with high probability, $E_{out} \leq 2E_{out}^*$

k-Nearest Neighbor (K-NN)

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

- 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 $E_{out}(g) \to E_{out}(g^*)$
    - E.g., $k(N) = \sqrt{N}$
  - Other practical rules of thumb:
    - $k = 3$ is often a good enough choice
    - Using validation to choose k

With suitable choice of k, when $N \to \infty$, we can recover the optimal hypothesis.

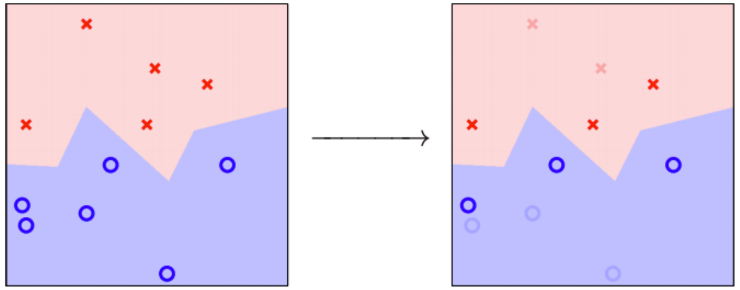
Summary of k-NN Properties

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

- Cons
  - Curse of dimensionality
    - When dimensionality is high, most points won’t be close to each other
    - For points to be close, they need to be close in every dimension
  - Computational issue
    - Each prediction requires heavy computation

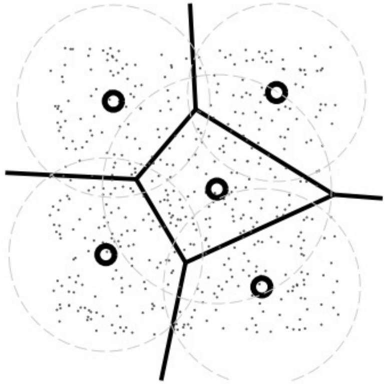
Dealing with Computational Issues

- Reduce the number of data points



  - Intuition: remove points that will not impact the decision boundary.
  - Generally a hard problem. But there are heuristic approaches (e.g., Condensed Nearest Neighbor).

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



  - Intuition: Clustering data points
  - For a new data point, we might be able to "ignore" some clusters when searching for nearest neighbor.

Radial Basis Function (RBF)

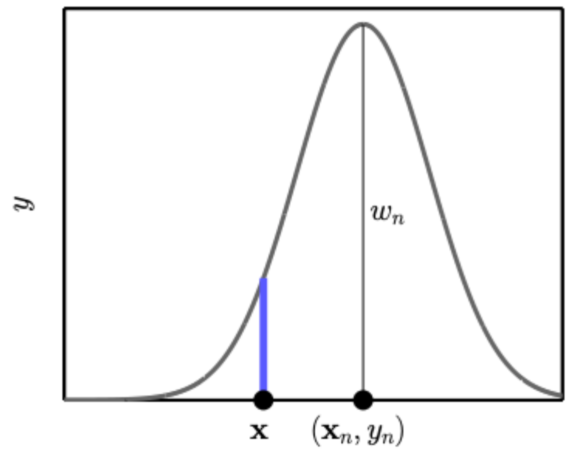
- Using distance to the points as the basis function to form hypothesis

- 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
    - Gaussian RBF (we have seen this in SVM): $\phi(s) = e^{-s}$

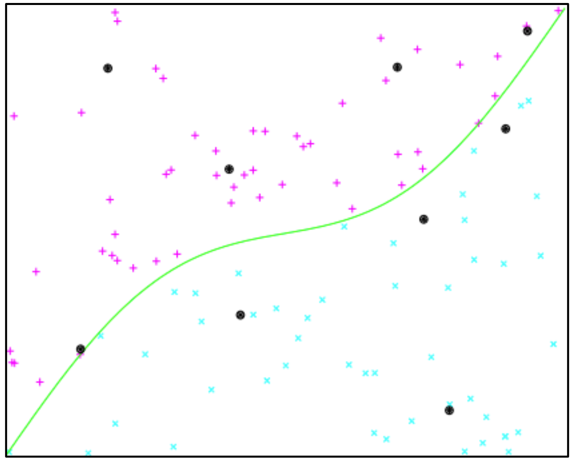
- This is for regression. We can take a sign and make it a classification.
- $Z(\vec{x}) = \sum_{m=1}^{N} \phi\left(\frac{\|\vec{x}-\vec{x}_m\|}{r}\right)$ is for normalization

Nonparametric and 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
  - $h(\vec{x}) = \sum_{k=1}^{K} w_k\, \phi\left(\frac{\|\vec{x}-\vec{\mu}_k\|}{r}\right)$
  - Find K reprensented points (e.g., clustering) $\vec{\mu}_1, \ldots, \vec{\mu}_K$
  - Learn w_k from data



Connection to Other Hypothesis Sets

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

- Connection to linear models
  - Parametric RBF is essentially linear models with nonlinear transformation
- Connection to nearest neighbor
  - RBF is based on the similarity to a set of points
- Connection to SVM with RBF Kernel
  - Using K representative points vs. using support vectors
- Connection to Neural Networks
  - RBF can be graphically represented as a one-hidden layer network

Today’s Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.

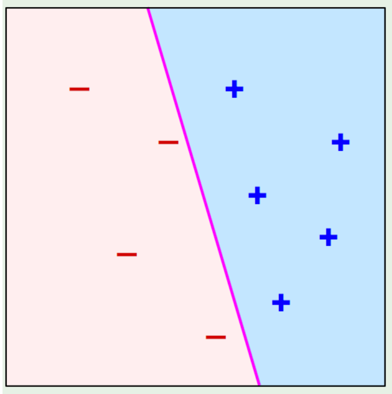
Let me know if you spot errors.

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.

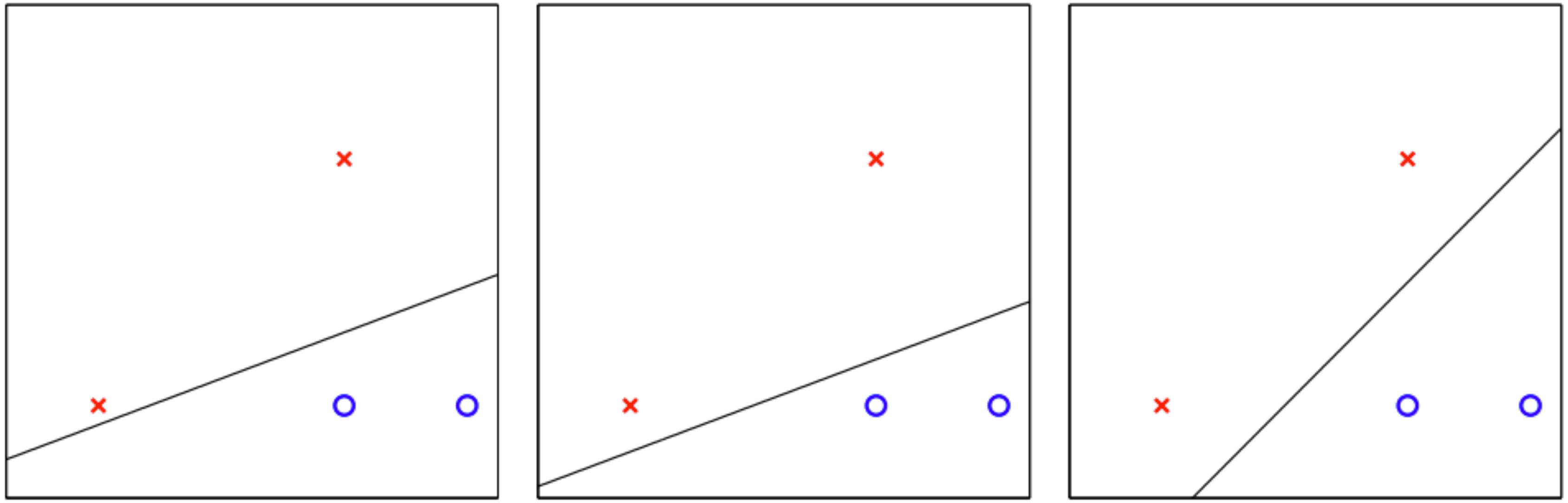
- Challenges
  - Binary classification error is hard to optimize
  - We cannot use “gradient descent” type of algorithm minimize E_{in}.



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

Linear Classification

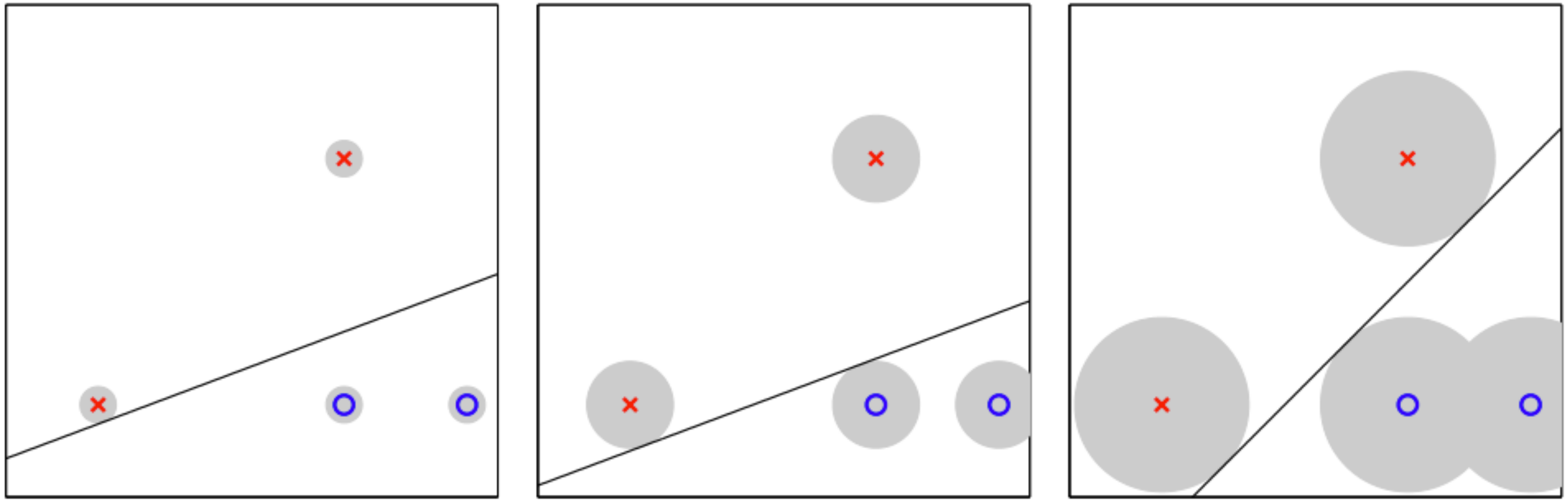
- Which separator would you choose?



Probably the right one.
Why?

Linear Classification

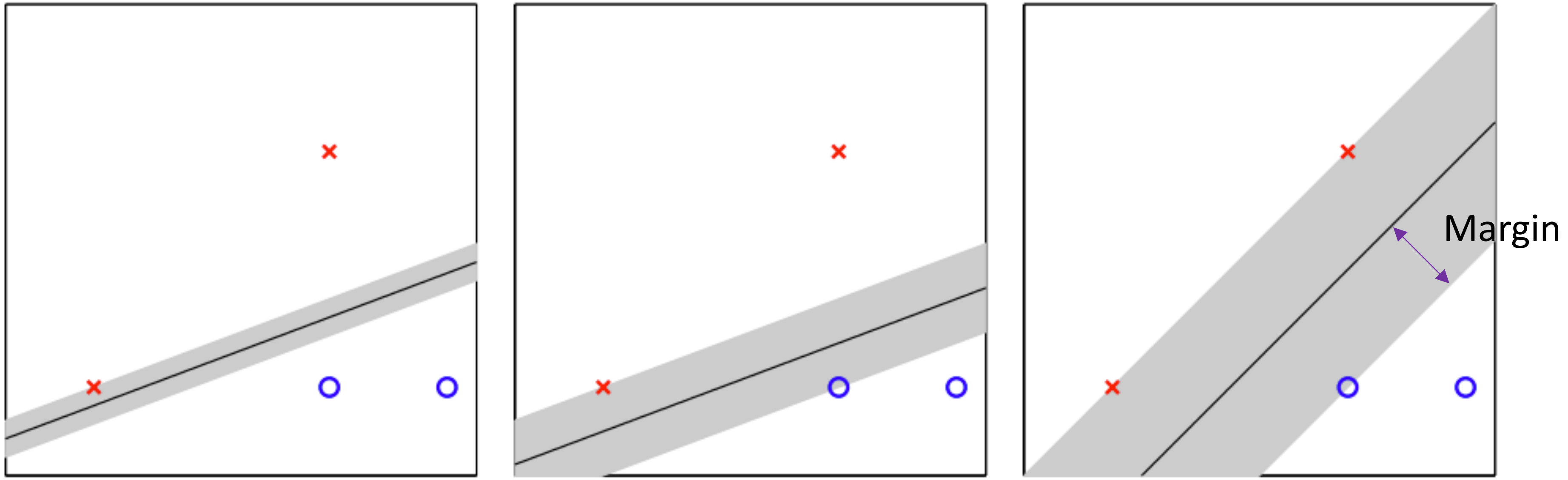
- Which separator would you choose?



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

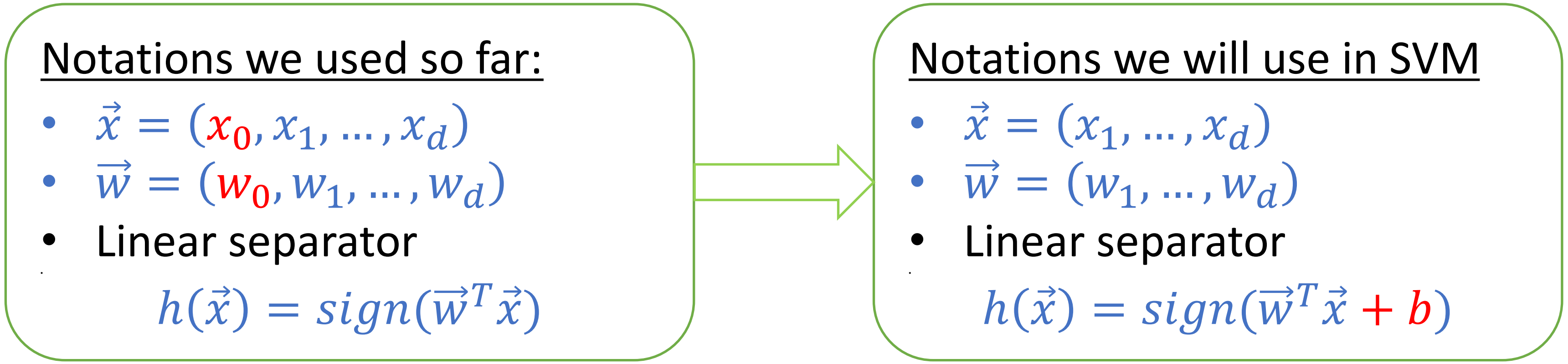
(Informal argument)

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

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

Notations we will use in SVM

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

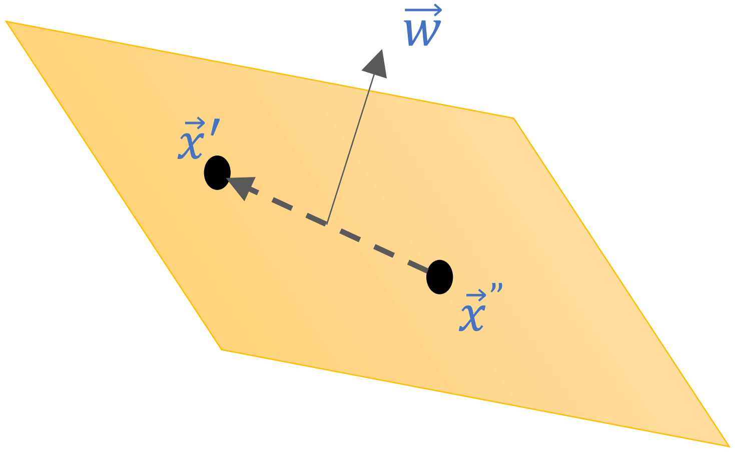
$$h(\vec{x}) = sign(\vec{w}^T\vec{x} + b)$$

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

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

Relevant Review of Linear Algebra

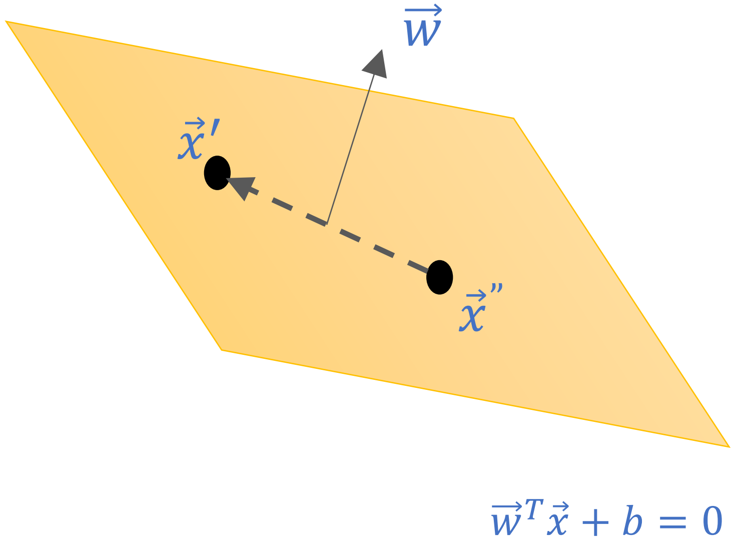
- Claim: $\vec{w}$ is the norm vector of the hyperplane $\vec{w}^T\vec{x} + b = 0$



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

Relevant Review of Linear Algebra

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



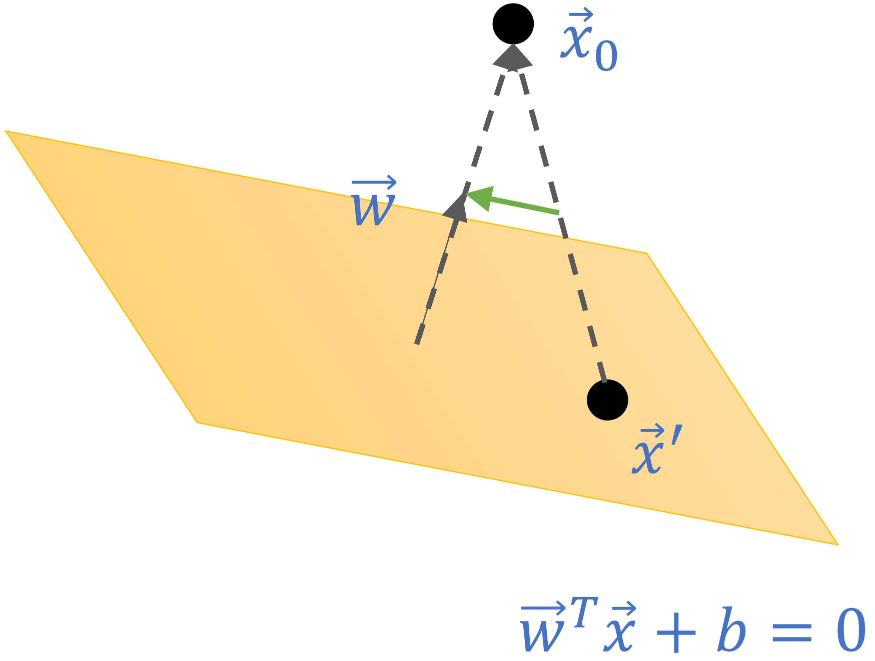
- Consider any two points $\vec{x}'$ and $\vec{x}''$ on the hyperplane
  - $\vec{w}^T\vec{x}' + b = 0$
  - $\vec{w}^T\vec{x}'' + b = 0$

- 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

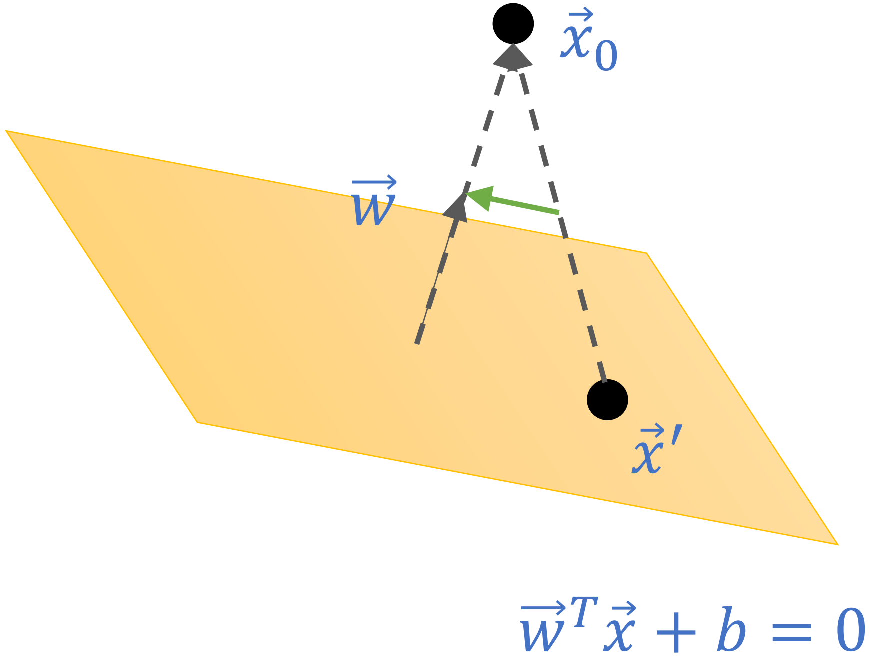
Relevant Review of Linear Algebra

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



Relevant Review of Linear Algebra

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



- 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 for SVM

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

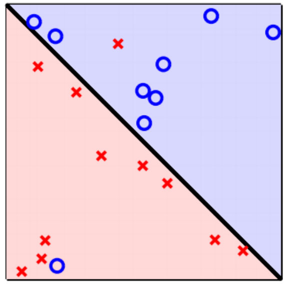
Given D, find separator $(\vec{w}, b)$ that

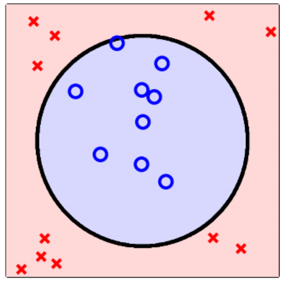
maximize margin$(\vec{w}, b)$

s.t. all points in D is correctly classified

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

- 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)

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

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

$y_n \in \{-1, +1\}$ 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

- $(\vec{w}, b)$ 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

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

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

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

Hard-Margin SVM

- Goal
  - Given $D = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_N, y_N)\}$ 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

$$\begin{array}{ll} \text{maximize}_{\vec{w},b} & \text{margin}(\vec{w}, b) \\ \text{subject to} & y_n(\vec{w}^T \vec{x}_n + b) \geq 0, \forall n \\ & \text{margin}(\vec{w}, b) = min_n \dfrac{1}{||\vec{w}||} y_n(\vec{w}^T \vec{x}_n + b) \end{array}$$

Hard-Margin SVM

- The constrained optimization problem

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

- 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 $min_n\, y_n(\vec{w}^T\vec{x}_n+b)=1$
    - $\text{margin}(\vec{w},b)=\frac{1}{\|\vec{w}\|}$
    - $y_n(\vec{w}^T\vec{x}_n+b) \geq 1, \forall n$

Hard-Margin SVM

- The constrained optimization problem

$$\begin{aligned}&\text{maximize}_{\vec{w},b} && \frac{1}{||\vec{w}||}\\ &\text{subject to} && y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n\end{aligned}$$

- Some final adjustments

$$\begin{aligned}&\text{minimize}_{\vec{w},b} && \frac{1}{2}\vec{w}^T\vec{w}\\ &\text{subject to} && y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n\end{aligned}$$

Final Form of Hard-Margin SVM

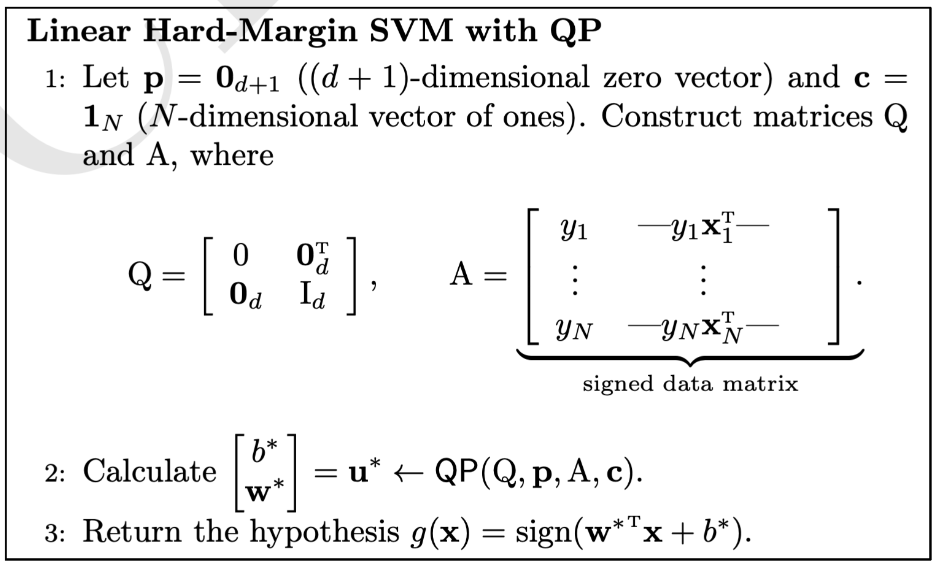
$$\begin{aligned} &\text{minimize}_{\vec{w},b} && \frac{1}{2}\vec{w}^T\vec{w} \\ &\text{subject to} && y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n \end{aligned}$$

Short Break and Questions:
How to construct QP for hard-margin SVM

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

$$\begin{aligned} &\text{minimize}_{\vec{u}} && \frac{1}{2}\vec{u}^T Q\vec{u} + \vec{p}^T\vec{u} \\ &\text{subject to} && A\vec{u} \geq \vec{c} \end{aligned}$$

  - There exist efficient QP solvers we can utilize



Linear Hard-Margin SVM with QP

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1: Let $\mathbf{p} = \mathbf{0}_{d+1}$ (($d+1$)-dimensional zero vector) and $\mathbf{c} = \mathbf{1}_N$ ($N$-dimensional vector of ones). Construct matrices Q and A, where
   $\mathrm{Q} = \begin{bmatrix} 0 & \mathbf{0}_d^{\mathrm{T}} \\ \mathbf{0}_d & \mathrm{I}_d \end{bmatrix}, \quad \mathrm{A} = \underbrace{\begin{bmatrix} y_1 & \text{—}y_1\mathbf{x}_1^{\mathrm{T}}\text{—} \\ \vdots & \vdots \\ y_N & \text{—}y_N\mathbf{x}_N^{\mathrm{T}}\text{—} \end{bmatrix}}_{\text{signed data matrix}}.$
2: Calculate $\begin{bmatrix} b^* \\ \mathbf{w}^* \end{bmatrix} = \mathbf{u}^* \leftarrow \mathrm{QP}(\mathrm{Q}, \mathbf{p}, \mathrm{A}, \mathbf{c})$.
3: Return the hypothesis $g(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^{*\mathrm{T}}\mathbf{x} + b^*)$.
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Connection to Regularization

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

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

- Another way to look at SVM

minimize $\vec{w}^T\vec{w}$

subject to $E_{in}(\vec{w}) = 0$

- Weight decay regularization

minimize $E_{in}(\vec{w})$

subject to $\vec{w}^T\vec{w} \leq C$

- Maximizing margin is similar to applying regularization!

- You'll see that these two interpretations are somewhat "equivalent" when we introduce Lagragian next lecture.

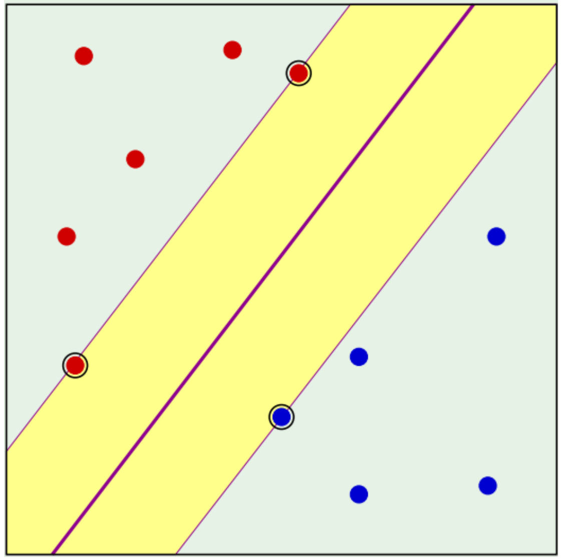
Support Vectors

We'll more formally define support vectors next lecture.

- We call the points closest to the separator (candidate) support vectors
  - Since they support the separator

- What are the math properties of support vectors?
  - They are the points that the equality holds in the constraints
    - If $\vec{x}_n$ is a support vector, $y_n(\vec{w}^T\vec{x}_n + b) = 1$ (the reverse might not be true)

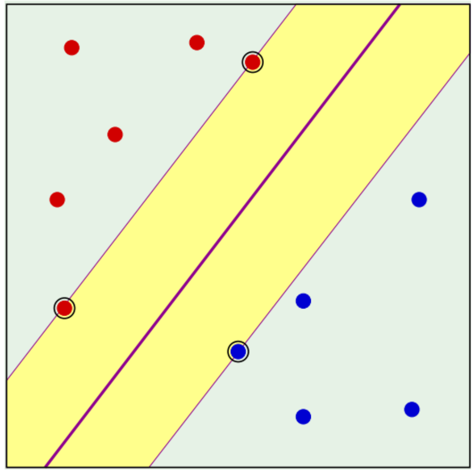
$$\begin{aligned} &\text{minimize}_{\vec{w},b} && \frac{1}{2}\vec{w}^T\vec{w} \\ &\text{subject to} && y_n(\vec{w}^T\vec{x}_n + b) \geq 1, \forall n \end{aligned}$$



  - Removing the non-support vectors will not impact the linear separator

Leave-One-Out Cross Validation (LOOCV)

- Two things we know so far
  - Removing non-support vectors will not impact the separator
  - LOOCV error (when not used for model selection) is an unbiased estimate of $E_{out}(N-1)$ (E_{out} when trained on $N-1$ points)

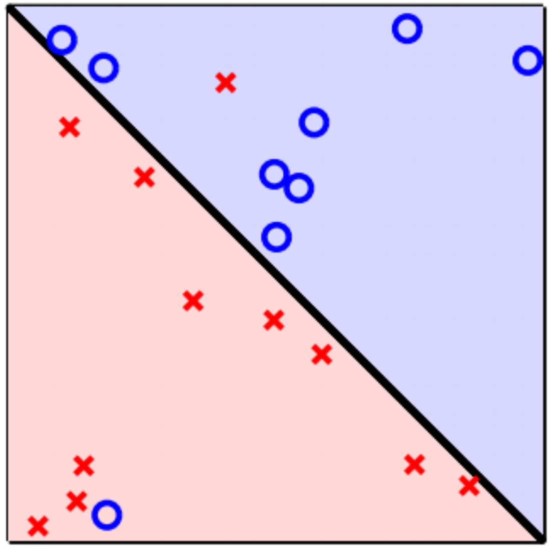


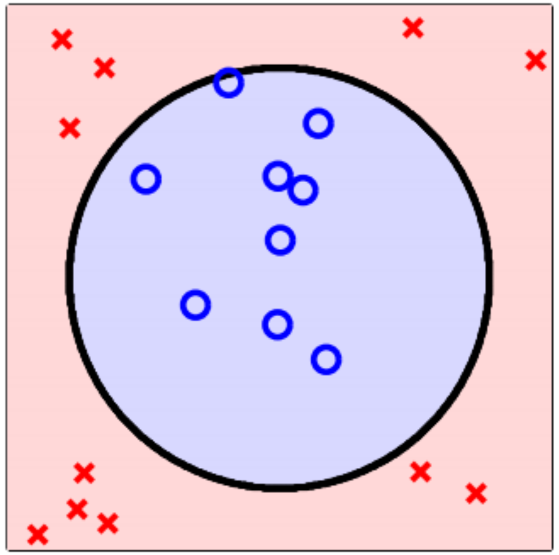
- What's the upper bound of LOOCV error for SVM?
  - $E_{LOOCV} \leq \frac{\#\,\text{support vectors}}{N}$
- Note that we know # support vectors after training
  - Count # points that satisfy $y_n(\vec{w}^T\vec{x}_n + b) = 1$
- Another method to estimate/bound E_{out} (counting # support vectors)

What if Data is Not Linearly Separable

Non-Separable Data

- Two scenarios





- Tolerate some noise
  - Soft-Margin SVM

- Nonlinear transform
  - Dual formulation and kernel tricks

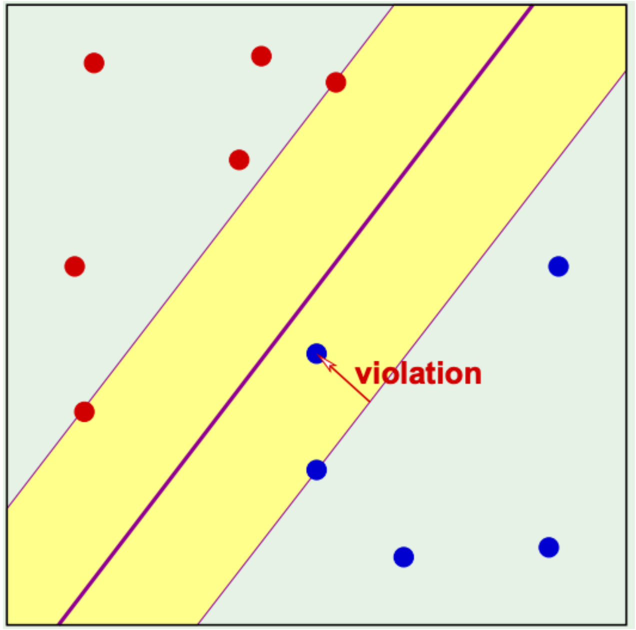
Soft-Margin SVM

- Intuition: We want to tolerate small noises when maintaining large margin

- For each point $(\vec{x}_n, y_n)$, we allow a deviation $\xi_n \geq 0$
  - Instead of requiring $y_n(\vec{w}^T \vec{x}_n + b) \geq 1$
  - The constraint becomes

$$y_n(\vec{w}^T \vec{x}_n + b) \geq 1 - \xi_n$$

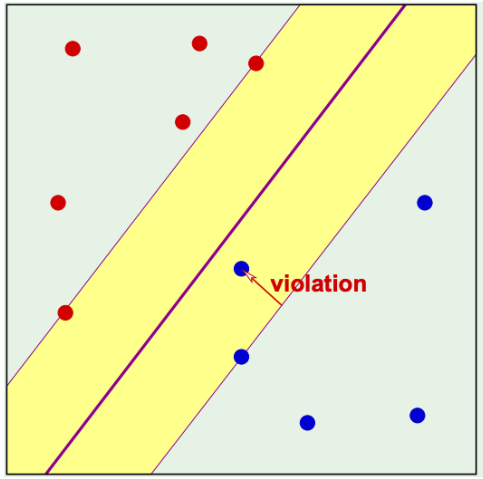
- We add a penalty for each deviation
  - Total penalty $C \sum_{n=1}^{N} \xi_n$



Soft-Margin SVM

- The constraint becomes: $y_n(\vec{w}^T\vec{x}_n + b) \geq 1 - \xi_n$
- We add a penalty for each deviation: Total penalty $C\sum_{n=1}^{N}\xi_n$

$$\begin{aligned} &\text{minimize}_{\vec{w},b,\vec{\xi}} && \frac{1}{2}\vec{w}^T\vec{w} + C\sum_{n=1}^{N}\xi_n \\ &\text{subject to} && y_n(\vec{w}^T\vec{x}_n + b) \geq 1 - \xi_n, \forall n \\ & && \xi_n \geq 0, \forall n \end{aligned}$$

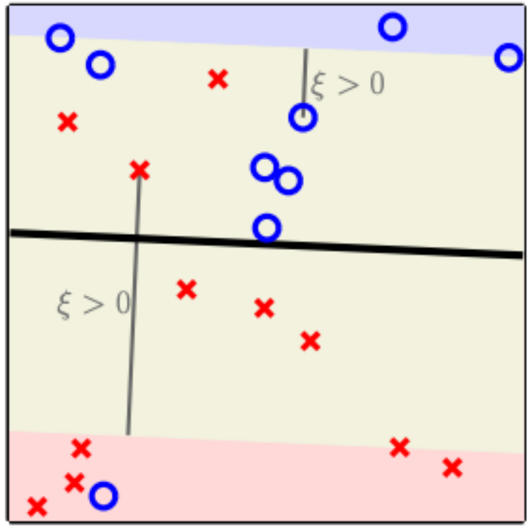


Remarks:

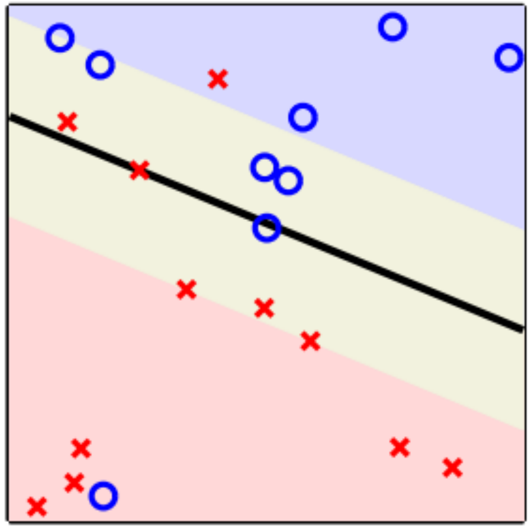
- C is a hyper-parameter we can choose, e.g., using validation
- Soft-margin SVM is still a Quadratic Program, with efficient solvers

Impacts of C in Soft-Margin SVM

- What happens when C is larger
  - less tolerate to noise, having smaller margin



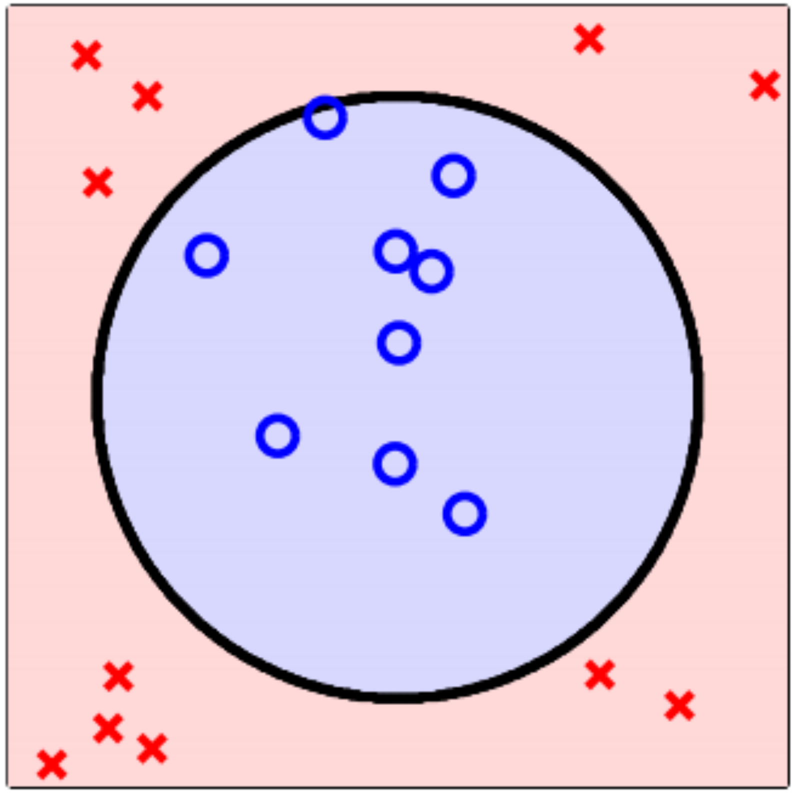
$C = 1$



$C = 500$

$$\begin{aligned}
&\text{minimize}_{\vec{w},b,\vec{\xi}} && \frac{1}{2}\vec{w}^T\vec{w} + C\sum_{n=1}^{N}\xi_n \\
&\text{subject to} && y_n(\vec{w}^T\vec{x}_n + b) \geq 1 - \xi_n, \forall n \\
& && \xi_n \geq 0, \forall n
\end{aligned}$$

What if Tolerating Small Noises Is Not Enough



Nonlinear transform

We can apply standard nonlinear transformation procedure we talked about before

In SVM, we can combine the ideas of dual formulation and kernel tricks for the transformation

This is one of the key ingredients that makes SVM powerful

Nonlinear Transform: $\vec{z} = \Phi(\vec{x})$

- Consider hard-margin SVM in the $\vec{z}$ space

$$\begin{aligned} &\text{minimize}_{\vec{w},b} && \frac{1}{2}\vec{w}^T\vec{w} \\ &\text{subject to} && y_n(\vec{w}^T\vec{z}_n + b) \geq 1, \forall n \end{aligned}$$

Involves changing $\vec{w}$ and $\vec{z}$.
The computation grows as the dimension of the $\vec{z}$ space grows

- There exists a corresponding dual formulation (more next lecture)

$$\begin{aligned} &\text{maximize}_{\vec{\alpha}} && \textstyle\sum_{n=1}^{N} \alpha_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n\alpha_m y_n y_m \vec{z}_n^T\vec{z}_m \\ &\text{subject to} && \textstyle\sum_{n=1}^{N} \alpha_n y_n = 0 \\ & && \alpha_n \geq 0, \forall n \end{aligned}$$

The only difference for the nonlinear transformation is from calculating $\vec{x}_n^T\vec{x}_m$ to $\vec{z}_n^T\vec{z}_m$

- Why dual
  - The optimal primal is the same as the optimal dual
  - We can infer the optimal primal solutions from the optimal dual solutions

Next Lecture

- Primal-dual formulations using Lagrangian

$$\begin{aligned} &\text{minimize}_{\vec{w},b} && \frac{1}{2}\vec{w}^T\vec{w} \\ &\text{subject to} && y_n(\vec{w}^T\vec{z}_n + b) \geq 1, \forall n \end{aligned}$$

$$\begin{aligned} &\text{maximize}_{\vec{\alpha}} && \textstyle\sum_{n=1}^{N} \alpha_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \vec{z}_n^T \vec{z}_m \\ &\text{subject to} && \textstyle\sum_{n=1}^{N} \alpha_n y_n = 0 \\ & && \alpha_n \geq 0, \forall n \end{aligned}$$

- Kernel tricks
  - Intuition: If we can find an efficient way to calculate $\vec{z}_n^T\vec{z}_m$, we can efficiently derive the optimal dual to infer the optimal primal.
  - Doing nonlinear transform without sacrificing much about computation.