# CS540 Introduction to Artificial Intelligence
# Lecture 5

Young Wu
Based on lecture slides by Jerry Zhu and Yingyu Liang

June 3, 2019

# Correction for Lecture 3 Slides

## Review

- The gradient descent step formula in Lecture 3 Slides should have $a_i - y_i$ instead of $y_i - a_i$.

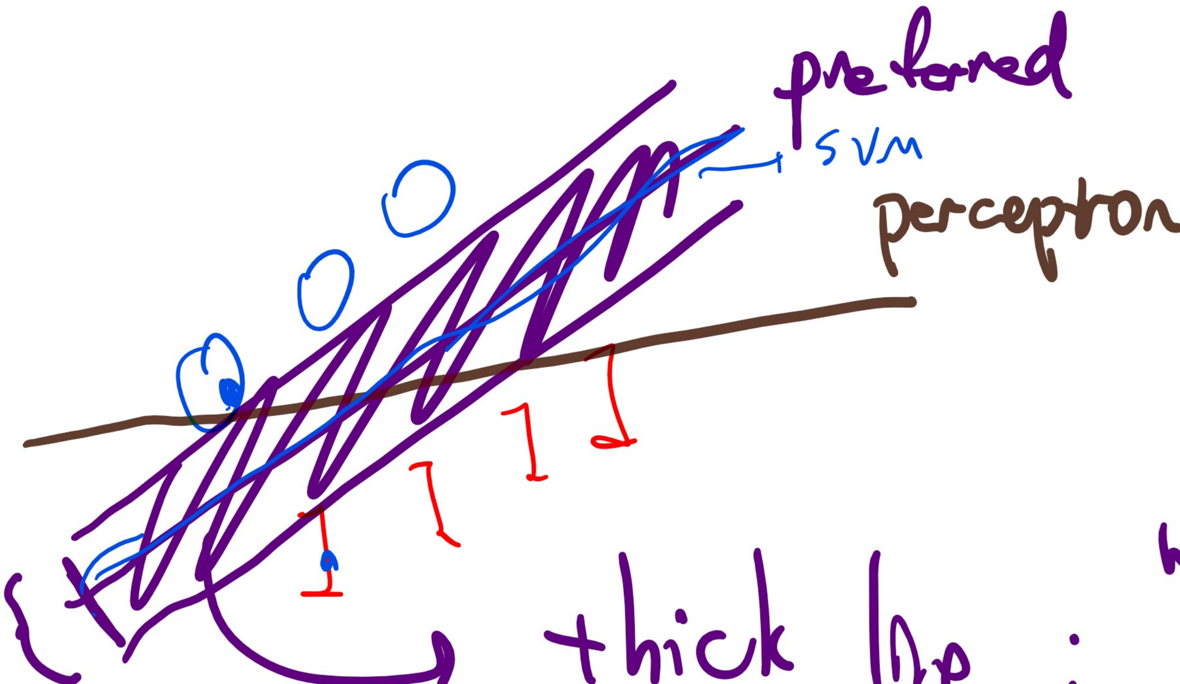
$$C = \frac{1}{2}\sum_{i=1}^{n}(a_i - y_i)^2 = \frac{1}{2}\sum_{i=1}^{n}(y_i - a_i)^2$$

$$\frac{\partial C}{\partial a_i} = (y_i - a_i) \cdot (-1) = a_i - y_i$$

- The slides are updated.

# Maximum Margin Diagram

## Motivation




widest
thick line : want thickest

line not touch data point

margin

goal : max margin s.t. all pts classified correctly.

SVM

# Margin and Support Vectors

## Motivation

- The perceptron algorithm finds any line $(w, b)$ that separates the two classes.

$$\hat{y}_i = \mathbb{1}_{\{w^T x_i + b \geqslant 0\}}$$

- The margin is the maximum width (thickness) of the line before hitting any data point.
- The instances that the thick line hits are called support vectors.
- The model that finds the line that separates the two classes with the widest margin is call support vector machine (SVM).

# Support Vector Machine

## Description

- The problem is equivalent to minimizing the norm of the weights subject to the constraint that every instance is classified correctly (with the margin).
- Use subgradient descent to find the weights and the bias.

# Finding the Margin

## Definition

- Define two planes: plus plane $w^T x + b = 1$ and minus plane $w^T x + b = -1$.
- The distance between the two planes is $\frac{2}{\sqrt{w^T w}}$.
- If all of the instances with $y_i = 1$ are above the plus plane and all of the instances with $y_i = 0$ are below the minus plane, then the margin is $\frac{2}{\sqrt{w^T w}}$.

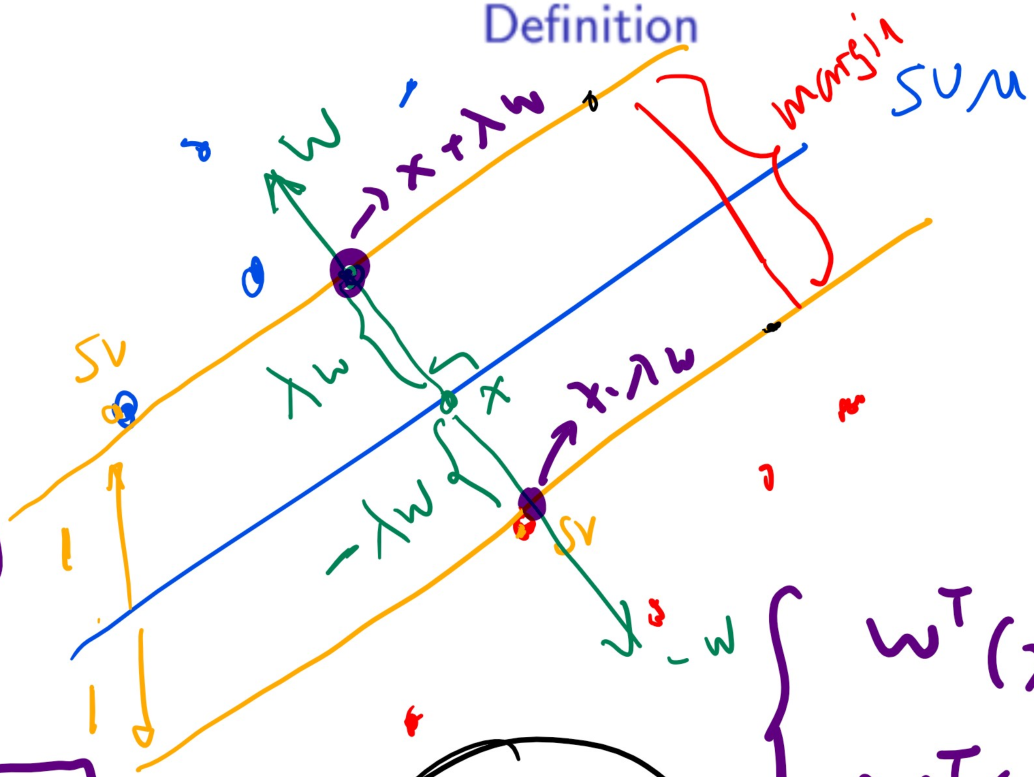
# Constrained Optimization Derivation

## Definition

$\boxed{w^Tx+b=1}$

$w^Tx+b=0$

$\boxed{w^Tx+b=-1}$




eg

$w=\binom{1}{1}$

$b=0$

$\oplus$ $x_1+x_2=1$

$\ominus$ $x_1+x_2=-1$

$x_2=1-x_1$

$x_2=-1-x_1$

$$\begin{cases} w^T(x+\lambda w)+b=1 \\ w^T(x-\lambda w)+b=-1 \end{cases}$$

$$w^Tx = 1-b-\lambda w^Tw$$

$$w^Tx = -1-b+\lambda w^Tw$$

diff

$$0 = 2-2\lambda w^Tw$$

margin $\frac{2}{\sqrt{w^Tw}}$

//

$$\lambda = \frac{1}{w^Tw}$$

length of $w$

$$\text{margin} = 2\lambda\|w\| = \frac{2}{w^Tw}\cdot\sqrt{w^Tw}$$

# Constrained Optimization

## Definition

- The goal is to maximize the margin subject to the constraint that the plus plane and the minus plane separates the instances with $y_i = 0$ and $y_i = 1$.

$$\underbrace{\max_w \frac{2}{\sqrt{w^T w}}}_{\text{margin}} \text{ such that } \underbrace{\begin{cases} (w^T x_i + b) \leqslant -1 & \text{if } y_i = 0 \\ (w^T x_i + b) \geqslant 1 & \text{if } y_i = 1 \end{cases}}_{\text{classified correctly by + plane, − plane}}, i = 1, 2, \ldots, n$$

- The two constrains can be combined.

$$\max_w \frac{2}{\sqrt{w^T w}} \text{ such that } (2y_i - 1)\left(w^T x_i + b\right) \geqslant 1, i = 1, 2, \ldots, n$$

label classes ; 0, 1

in textbook −1, 1

$y_i = 0 \quad = -1$

$y_i = 1 \quad = 1$

# Hard Margin SVM

## Definition

$$\max_{w} \frac{2}{\sqrt{w^T w}} \text{ such that } (2y_i - 1)\left(w^T x_i + b\right) \geqslant 1, i = 1, 2, \dots, n$$

- This is equivalent to the following minimization problem, called hard margin SVM.

data must be linearly separable.

$$\min_{w} \frac{1}{2} w^T w \text{ such that } (2y_i - 1)\left(w^T x_i + b\right) \geqslant 1, i = 1, 2, \dots, n$$

$$\max f(w) \Rightarrow \min \frac{1}{f(w)} \geqslant 0 \Rightarrow \min \left(\frac{1}{f(w)}\right)^2 \rightarrow \min 2\left(\frac{1}{f(w)}\right)^2$$

# Hard Margin SVM

## Quiz (Participation)

- Fall 2014 Final Q17
- Which of the following transformations can make a hard margin SVM that is working no longer work?
- A: $x_i = x_i + c, c \in \mathbb{R}^m$ for all $i = 1, 2, ..., n$
- B: $x_i = x_i \cdot c, c \in \mathbb{R}$ for all $i = 1, 2, ..., n$
- C: Rotated the instances in $\mathbb{R}^m$ around the origin.
- D: Swap 1st and 2nd coordinates, $x_{i1} \Leftrightarrow x_{i2}$ for all $i = 1, 2, ..., n$
- E: Do not choose this.

# SVM Weights

## Quiz (Graded)

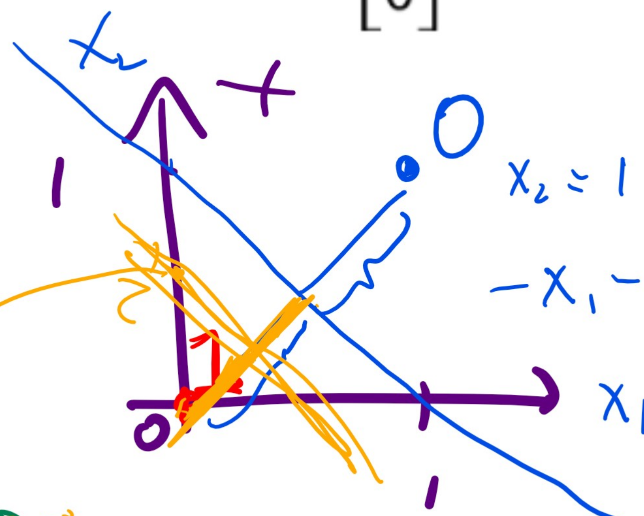
Q3

- Fall 2005 Final Q15 and Fall 2006 Final Q15
- Find the weights $w_1, w_2$ for the SVM classifier $\mathbb{1}_{\{w_1 x_{i1} + w_2 x_{i2} + 1 \geq 0\}}$ given the training data $x_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ and $x_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ with $y_1 = 1, y_2 = 0$.

put on midterm

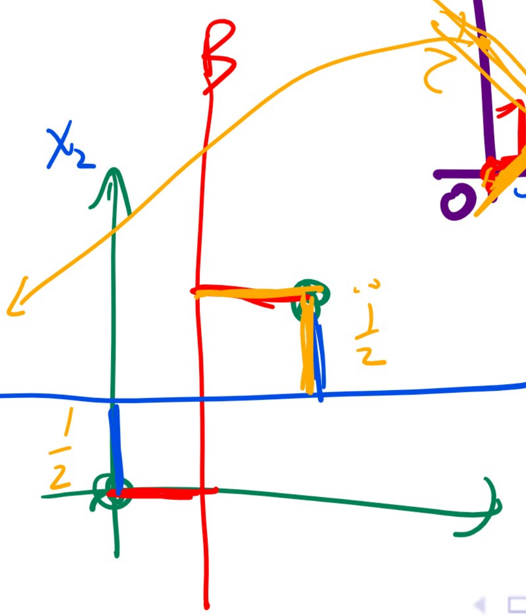
$0 \quad -2$

- A: $w_1 = 0, w_2 = -2$
- B: $w_1 = -2, w_2 = 0$
- C: $w_1 = -1, w_2 = -1$
- D: $w_1 = -2, w_2 = -2$
- E: none of the above




$x_2 = 1 - x_1$

$-x_1 - x_2 + 1 = 0$




A

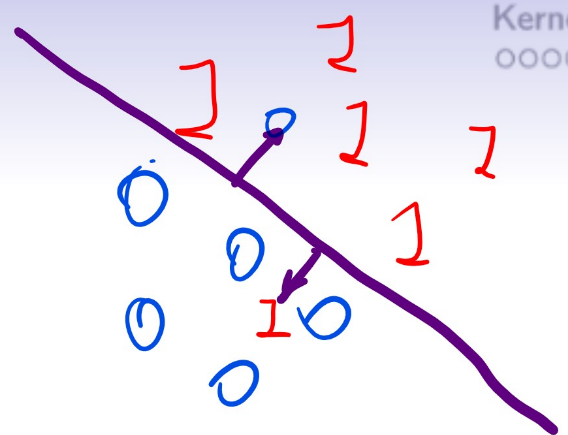
$-2x_{i2} + 1 = 0$

$x_{i2} = \frac{1}{2}$

allow misclassification → add cost,

# Soft Margin

## Definition



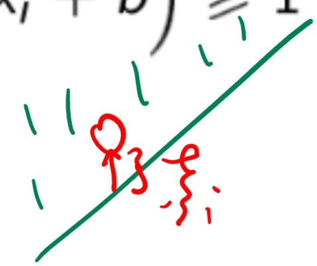
- To allow for mistakes classifying a few instances, slack variables are introduced.
- The cost of violating the margin is given by some constant $\frac{1}{\lambda}$.
- Using slack variables $\xi_i$, the problem can be written as the following.

cost for average mistake

mistake = how far to the margin in wrong direction

$$\min_w \frac{1}{2} w^T w + \frac{1}{\lambda}\frac{1}{n}\sum_{i=1}^{n} \xi_i$$

such that $(2y_i - 1)\left(w^T x_i + b\right) \geqslant 1 - \xi_i, \xi_i \geqslant 0, i = 1, 2, ..., n$



# Soft Margin SVM

## Definition

$$\min_{w} \frac{1}{2} w^T w + \frac{1}{\lambda}\frac{1}{n}\sum_{i=1}^{n} \xi_i$$

such that $(2y_i - 1)\left(w^T x_i + b\right) \geqslant 1 - \xi_i, \xi_i \geqslant 0, i = 1, 2, ..., n$

$\lambda$

- This is equivalent to the following minimization problem, called soft margin SVM.

L2 regularization

hinge loss.

$$\min_{w} \frac{\lambda}{2} w^T w + \frac{1}{n}\sum_{i=1}^{n} \max\left\{0, 1 - (2y_i - 1)\left(w^T x_i + b\right)\right\}$$

?

# Subgradient Descent

## Definition

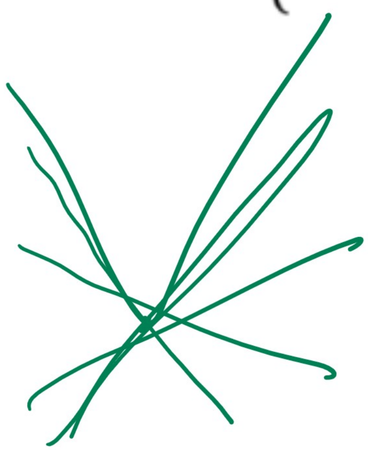
$$\min_{w} \frac{\lambda}{2} w^T w + \frac{1}{n} \sum_{i=1}^{n} \max \left\{0, 1 - (2y_i - 1)\left(w^T x_i + b\right)\right\}$$

- The gradient for the above expression is not defined at points with $1 - (2y_i - 1)\left(w^T x_i + b\right) = 0$.
- Subgradient can be used instead of gradient.

# Subgradient

- The subderivative at a point of a convex function in one dimension is the set of slopes of the lines that are tangent to the function at that point.
- The subgradient is the version for higher dimensions.
- The subgradient $\partial f(x)$ is formally defined as the following set.

$$\partial f(x) = \left\{ v : f(x') \geqslant f(x) + v^T (x' - x) \ \forall\, x' \right\}$$

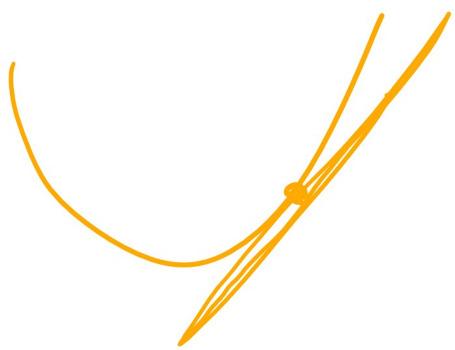


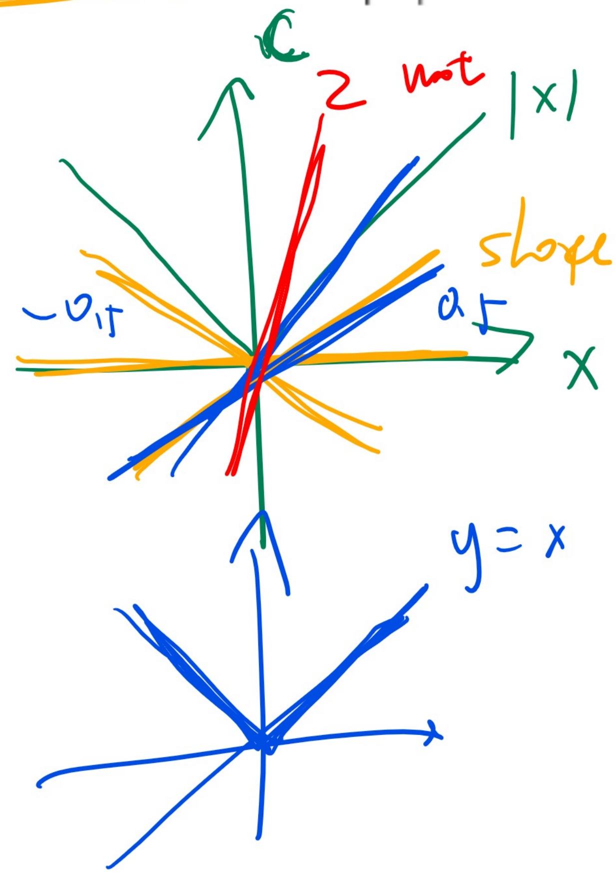
# Subgradient, Part I

## Quiz (Participation)

$\partial |x| = [-1, 1]$

- Which ones (multiple) are subderivatives of $|x|$ at $x = 0$?
- A: -1
- B: -0.5
- C: 0
- D: 0.5
- E: 1





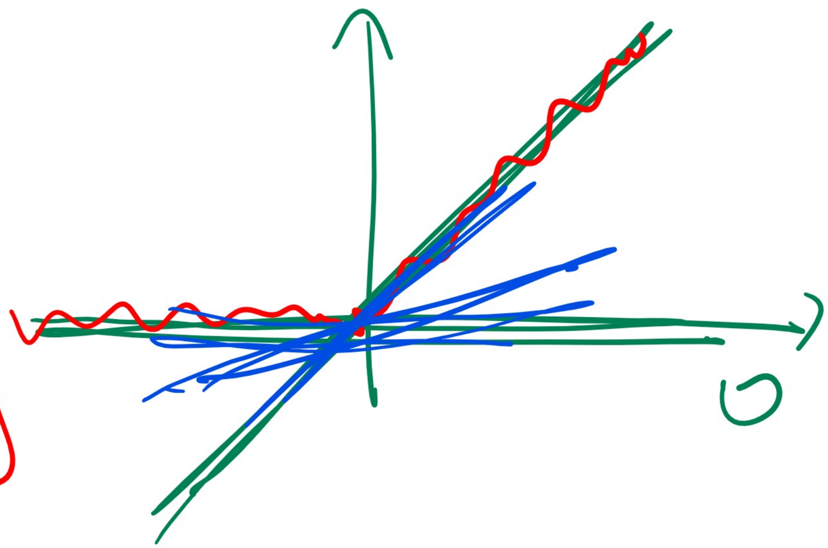
# Subgradient, Part II

## Quiz (Graded)

5

$\partial \max\{x, 0\} = [0, 1]$

- Which ones (multiple) are subderivatives of $\max\{x, 0\}$ at $x = 0$?
- A: -1
- B: -0.5
- C: 0
- D: 0.5
- E: 1

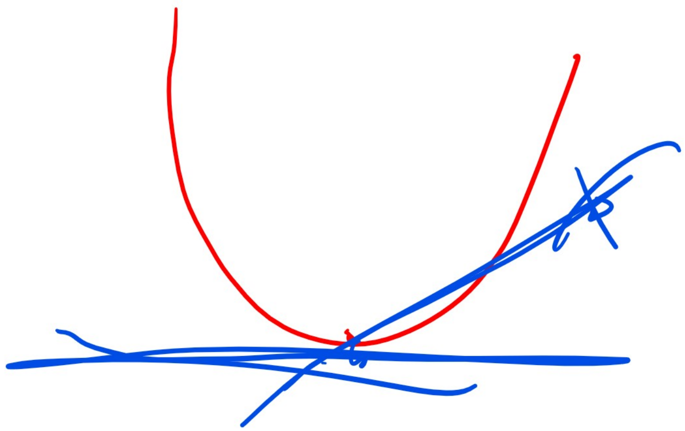


# Subgradient, Part II

## Quiz (Graded)

Q6

- Which ones (multiple) are subderivatives of $\max\{x^2, 0\}$ at $x = 0$?
- A: -1
- B: -0.5
- C: 0
- D: 0.5
- E: 1



$x^2$

# Subgradient Descent Step

## Definition

- One possible set of subgradients with respect to $w$ and $b$ are the following.

$x \in S$

$$\partial_w C \ni \lambda w - \sum_{i=1}^{n} (2y_i - 1)\, x_i \mathbb{1}_{\{(2y_i-1)(w^T x_i+b) \geqslant 1\}}$$

set

$$\partial_b C \ni - \sum_{i=1}^{n} (2y_i - 1)) \mathbb{1}_{\{(2y_i-1)(w^T x_i+b) \geqslant 1\}}$$

- The gradient descent step is the same as usual, using one of the subgradients in place of the gradient.

# Class Notation and Bias Term

## Definition

- Usually, for SVM, the bias term is not included and updated. Also, the classes are -1 and +1 instead of 0 and 1. Let the labels be $z_i \in \{-1, +1\}$ instead of $y_i \in \{0, 1\}$. The gradient steps are usually written the following way.

want $b$

$$w = (1 - \lambda)\, w - \alpha \sum_{i=1}^{n} z_i x_i \mathbb{1}_{\{z_i w^T x_i \geqslant 1\}}$$

add $x_j = 1$

constant feature

$$z_i = 2y_i - 1, i = 1, 2, ..., n$$

# Regularization Parameter

## Definition

$$w = (1 - \lambda)\, w - \alpha \sum_{i=1}^{n} z_i x_i \mathbb{1}_{\{z_i w^T x_i \geqslant 1\}}$$

$$z_i = 2y_i - 1, i = 1, 2, ..., n$$

- The parameter $\lambda$ is slightly different from the one from the previous slides. $\lambda$ is usually called the regularization parameter because it reduces the magnitude of $w$ the same way as the parameter $\lambda$ in L2 regularization.

NOT Name

# Pegasos Algorithm

Primal
Estimated
subGrAdient
SOlver
for
Svm

## Algorithm

- Inputs: instances: $\{x_i\}_{i=1}^{n}$ and $\{z_i = 2y_i - 1\}_{i=1}^{n}$
- Outputs: weights: $\{w_j\}_{j=1}^{m}$
- Initialize the weights.

$$w_j \sim \text{ Unif } [0, 1]$$

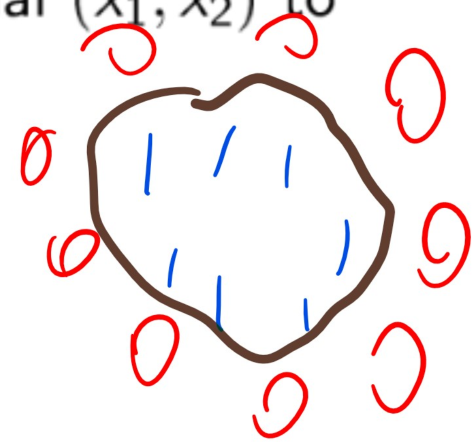
- Update the weights using subgradient descent for a fixed number of iterations.

$$w = (1 - \lambda)\, w - \alpha \sum_{i=1}^{n} z_i x_i \mathbb{1}_{\{z_i w^T x_i \geqslant 1\}}$$

# Kernel Trick

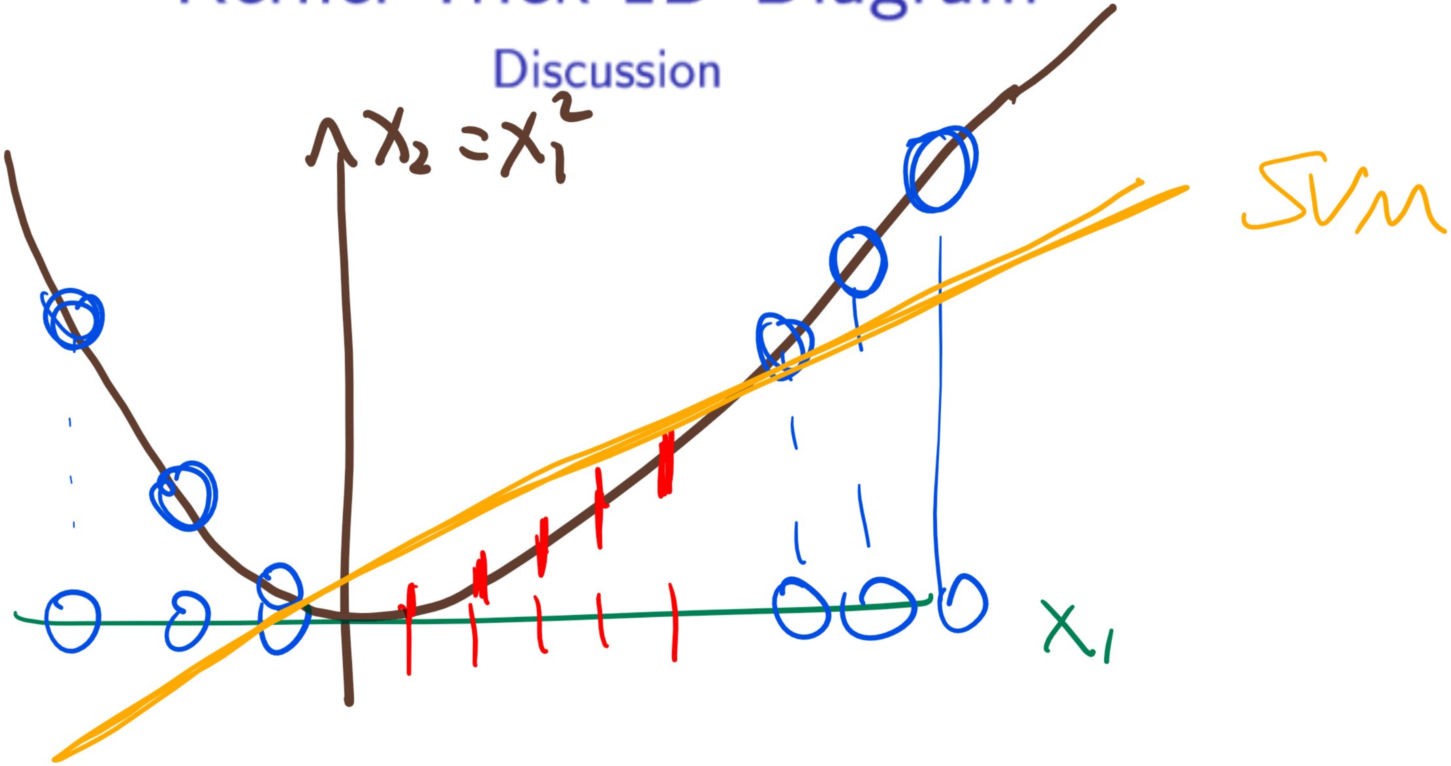
## Discussion

- If the classes are not linearly separable, more features can be created.
- For example, a 1 dimensional $x$ can be mapped to $\phi(x) = (x, x^2)$.
- Another example is to map a 2 dimensional $(x_1, x_2)$ to $\phi(x = (x_1, x_2)) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$.



# Kernel Trick 1$D$ Diagram

## Discussion



# Kernelized SVM

## Discussion

- With a kernel $\phi$, the SVM can be trained on new data points $\left\{\left(\phi\left(x_1\right), y_1\right), \left(\phi\left(x_2\right), y_2\right), ..., \left(\phi\left(x_n\right), y_n\right)\right\}$.
- The weights $w$ correspond to the new features $\phi\left(x_i\right)$.
- Therefore, test instances are transformed to have the same new features.

$$\hat{y}_i = \mathbb{1}_{\{w^T \phi(x_i) \geqslant 0\}}$$

# Kernel Matrix

## Discussion

- The kernel is usually represented by a $n \times n$ matrix $K$ called the Gram matrix.

100 instances

$\phi(x_1)^T \phi(x_1)$

$\phi(x_1)^T \phi(x_2)$

$$K_{ij} = \phi(x_i)^T \phi(x_j)$$

instance i

instance j

# Examples of Kernel Matrix

## Discussion

- For example, if $\phi(x) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$, then the kernel matrix can be simplified.

$$K_{ij} = \left(x_i^T x_j\right)^2$$

- Another example is the quadratic kernel $K_{ij} = \left(x_i^T x_j + 1\right)^2$. It can be factored to have the following feature representations.

$$\phi(x) = \left(x_1^2, x_2^2, \sqrt{2}x_1x_2, x_1, x_2, 1\right)$$

# Kernel Matrix Characterization

## Discussion

- A matrix $K$ is kernel (Gram) matrix if and only if it is symmetric positive semidefinite.

# Popular Kernels

## Discussion

- Other popular kernels include the following.

1. Linear kernel: $K_{ij} = x_i^T x_j$ linear SVM
2. Polynomial kernel: $K_{ij} = (x_i^T x_j + 1)^d$
3. Radial Basis Function (Gaussian) kernel:

$$K_{ij} = \exp\left(-\frac{1}{\sigma^2}(x_i - x_j)^T (x_i - x_j)\right)$$

- Gaussian kernel has infinite dimensional feature representations. There are dual optimization techniques to find $w$ and $b$ for these kernels.

# Kernel Trick for XOR

## Quiz (Graded)

- March 2018 Final Q17
- SVM with quadratic kernel $\phi\left(x\right) = \left(x_1^2, \sqrt{2}x_1 x_2, x_2^2\right)$ can correctly classify the training set for XOR.
- A: True.
- B: False.
- C: Do not choose this.
- D: Do not choose this.
- E: Do not choose this.

# Kernel Matrix

## Quiz (Graded)

- Fall 2009 Final Q2
- What is the feature vector $\phi(x)$ induced by the kernel $K_{ij} = \exp(x_i + x_j) + \sqrt{x_i x_j} + 3$?
- A: $(\exp(x), \sqrt{x}, 3)$
- B: $(\exp(x), \sqrt{x}, \sqrt{3})$
- C: $\left(\sqrt{\exp(x)}, \sqrt{x}, 3\right)$
- D: $\left(\sqrt{\exp(x)}, \sqrt{x}, \sqrt{3}\right)$
- E: None of the above