ITCS 6156/8156 Fall 2023
Machine Learning

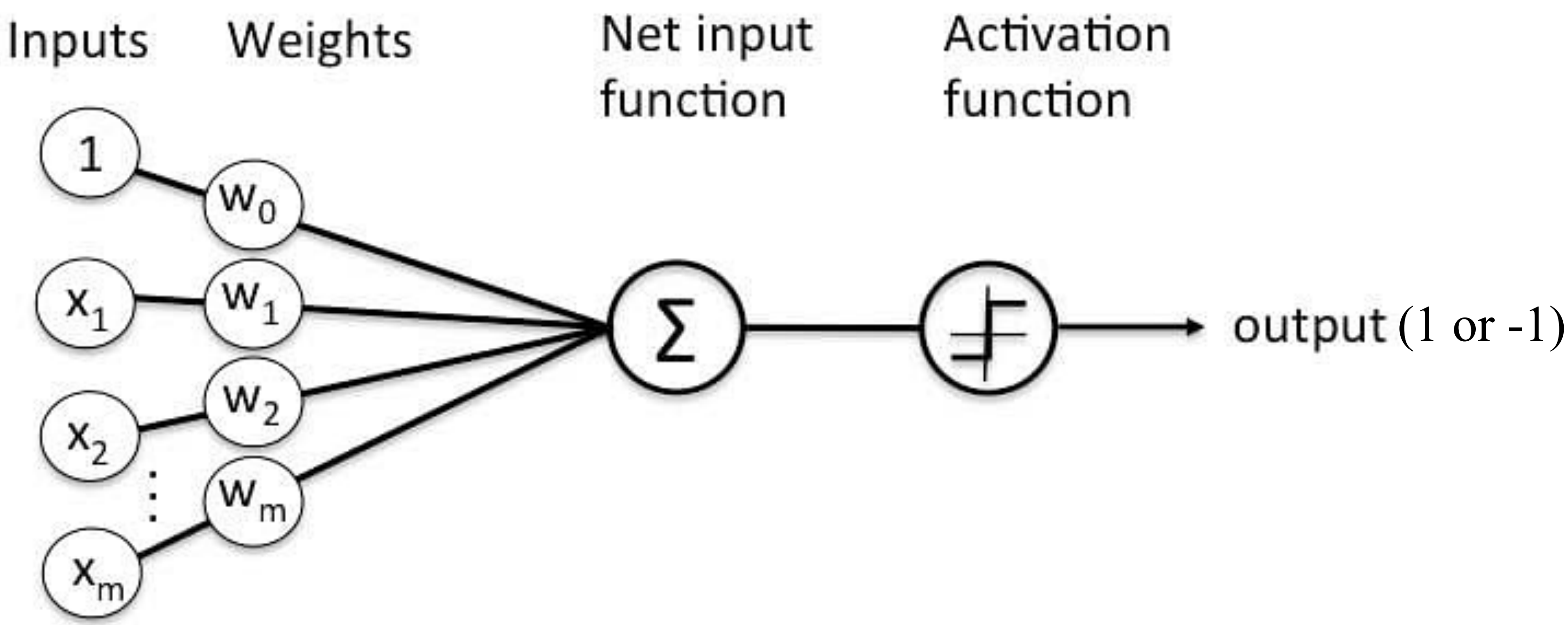
Support Vector Machine

Instructor: Hongfei Xue
Email: hongfei.xue@charlotte.edu
Class Meeting: Mon & Wed, 4:00 PM – 5:15 PM, CHHS 376

UNIVERSITY OF NORTH CAROLINA CHARLOTTE

Some content in the slides is based on Dr. Varun's lecture

Perceptron



- $h_{\mathbf{w}}(X) = \mathbf{w}^T X = [w_0, w_1, \ldots, w_d]^T [1, x, \ldots, x_d]$
  $= w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_d x_d$
- If $h_{\mathbf{w}}(X) > 0$, output will be 1; otherwise, output will be -1
- Activation function is $sign(z)$:

$$sign(z) = \begin{cases} 1, & if\ z > 0 \\ -1, & otherwise \end{cases}$$

Training

- Training algorithm:

initialize parameters $\mathbf{w} = 0$

for $n = 1 \ldots N$

$\quad h_n = \mathbf{w}^T \mathbf{x}_n$

$\quad$ **if** $h_n \geq 0$ and $t_n = -1$

$\quad\quad \mathbf{w} = \mathbf{w} - \mathbf{x}_n$

$\quad$ **if** $h_n \leq 0$ and $t_n = +1$

$\quad\quad \mathbf{w} = \mathbf{w} + \mathbf{x}_n$

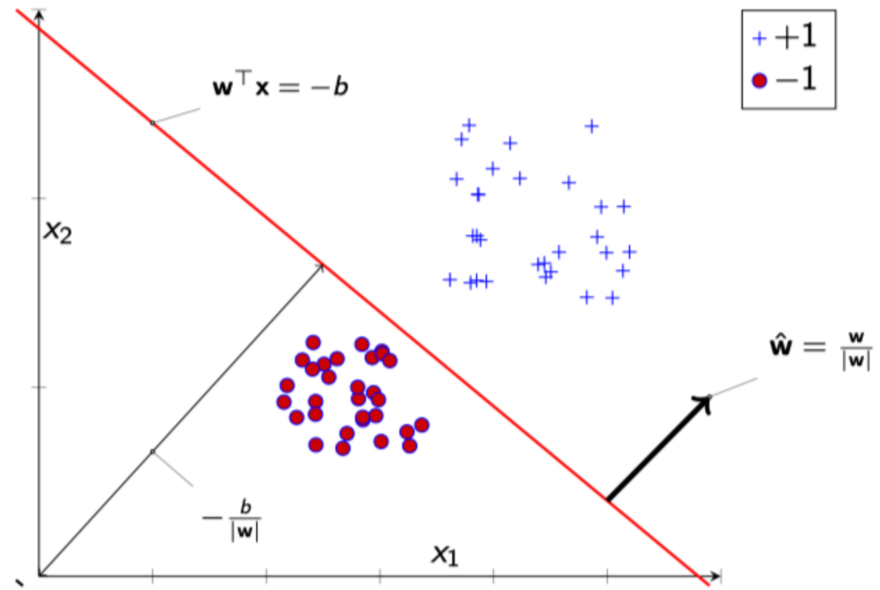
Repeat:
- until converge
- for a number of epochs

- Theorem:
  - If the training dataset is linearly separable, the perceptron learning algorithm is **guaranteed** to find a solution in a finite number of steps.

Maximum Margin Classifiers

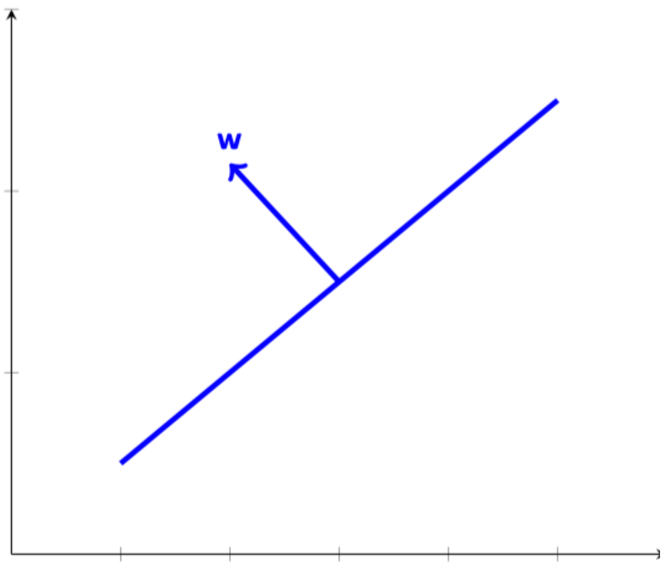
$$y = \mathbf{w}^\top \mathbf{x} + b$$

- Remember the Perceptron!
- If data is linearly separable
  - Perceptron training guarantees learning the decision boundary
- There can be other boundaries
  - Depends on initial value for $\mathbf{w}$
- **But what is the best boundary?**



Linear Hyperplane

- Separates a D-dimensional space into two half-spaces
- Defined by $\mathbf{w} \in \Re^D$
  - *Orthogonal* to the hyperplane
  - This $\mathbf{w}$ goes through the origin
  - How do you check if a point lies "above" or "below" $\mathbf{w}$?
  - What happens for points **on** $\mathbf{w}$?
- Add a bias b
- How to check if point lies above or below $\mathbf{w}$?
  - If $\mathbf{w}^\top \mathbf{x} + b > 0$ then $\mathbf{x}$ is *above*
  - Else, *below*



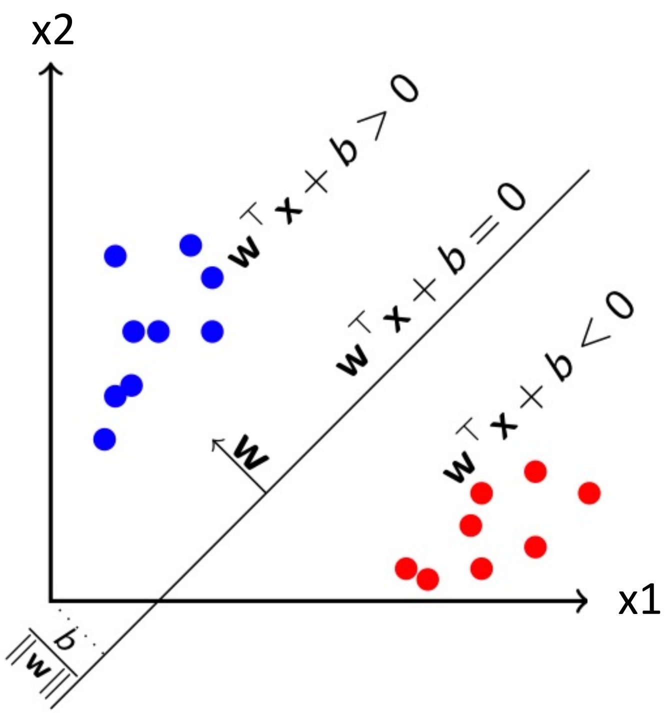
Line as a Decision Surface

- Decision boundary represented by the hyperplane $\mathbf{w}$
- For binary classification, $\mathbf{w}$ points **towards** the positive class

Decision Rule

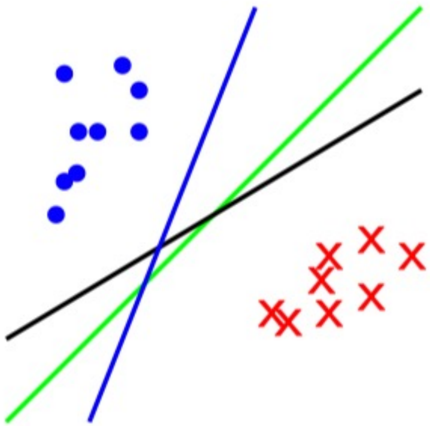
$$y = sign(\mathbf{w}^\top \mathbf{x} + b)$$

- $\mathbf{w}^\top \mathbf{x} + b > 0 \Rightarrow y = +1$
- $\mathbf{w}^\top \mathbf{x} + b < 0 \Rightarrow y = -1$



Best Hyperplane Separator

- **Perceptron** can find a hyperplane that separates the data
  - ... if the data is linearly separable
- But there can be many choices!
- Find the one with best separability (largest margin)
- Gives better generalization performance



Concept of Margin

- **Margin** is the distance between an example and the decision line
- Denoted by γ
- For a positive point:

$$\gamma = \frac{\mathbf{w}^\top \mathbf{x} + b}{||\mathbf{w}||}$$

- For a negative point:

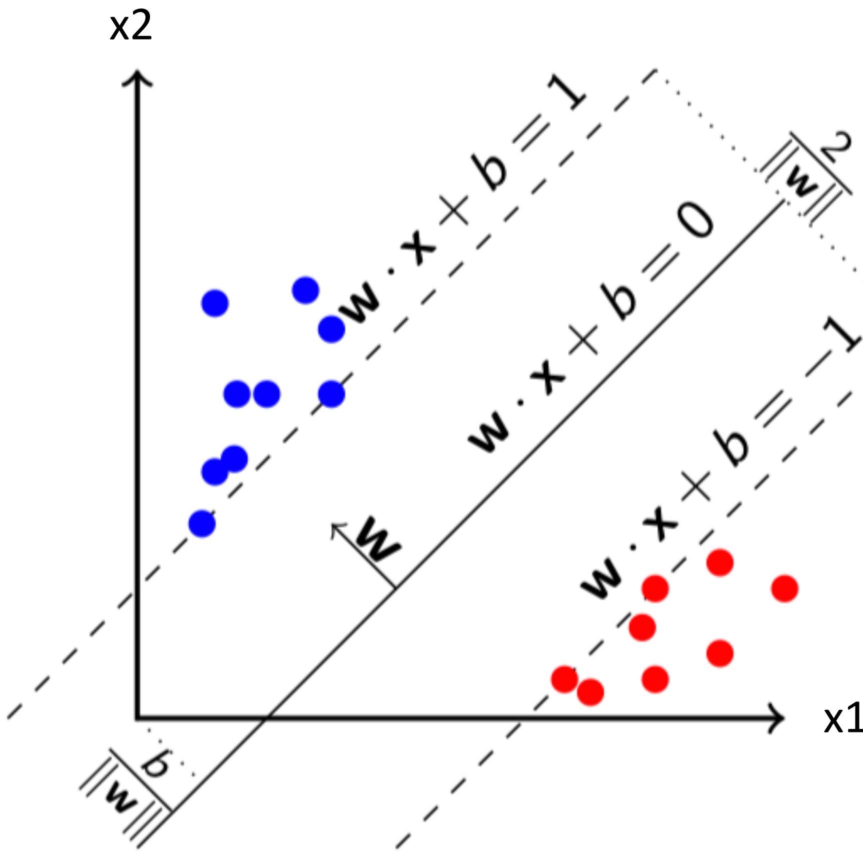
$$\gamma = -\frac{\mathbf{w}^\top \mathbf{x} + b}{||\mathbf{w}||}$$

Functional Interpretation

- Margin **positive** if prediction is **correct**; **negative** if prediction is **incorrect**

Maximum Margin Principle

- Figure after normalization:



From the figure one can note that the size of the margin is $\frac{2}{\|\mathbf{w}\|}$. We can show this as follows. Since the data is separable, we can get two parallel lines represented by $\mathbf{w}^\top \mathbf{x} + b = +1$ and $\mathbf{w}^\top \mathbf{x} + b = -1$. Using result from (1) and (2), the distance between the two lines is given by $2\gamma = \frac{2}{\|\mathbf{w}\|}$.

Support Vector Machines

- A hyperplane based classifier defined by **w** and b
- Like perceptron
- Find hyperplane with *maximum separation margin* on the training data
- Assume that data is linearly separable (will relax this later)
  - Zero training error (loss)

SVM Prediction Rule

$$y = sign(\mathbf{w}^\top \mathbf{x} + b)$$

SVM Learning

- **Input**: Training data $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}$
- **Objective**: Learn **w** and b that maximizes the margin

SVM Learning

- SVM learning task as an optimization problem
- Find $\mathbf{w}$ and b that gives zero training error
- Maximizes the margin ($= \frac{2}{\|w\|}$)
- Same as minimizing $\|\mathbf{w}\|$

Optimization Formulation

$$\underset{\mathbf{w},b}{\text{minimize}} \quad \frac{\|\mathbf{w}\|^2}{2}$$
$$\text{subject to} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, \; i = 1, \ldots, n.$$

- **Optimization** with N linear inequality constraint

A Different Interpretation of Margin

- What impact does the margin have on $\mathbf{w}$?
- Large margin $\Rightarrow$ Small $\|\mathbf{w}\|$
- Small $\|\mathbf{w}\| \Rightarrow$ regularized/simple solutions
- Simple solutions $\Rightarrow$ Better generalizability (*Occam's Razor*)

Optimization Problem

Optimization Formulation

$$\underset{\mathbf{w},b}{\text{minimize}} \quad \frac{\|\mathbf{w}\|^2}{2}$$

$$\text{subject to} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, \; i = 1, \ldots, n.$$

- There is an quadratic objective function to minimize with N inequality constraints
- "Off-the-shelf" packages - quadprog (MATLAB), CVXOPT
- Is that the best way?

An Optimization Problem

- An optimization problem without constraint:

$$\boxed{\underset{x,y}{\text{minimize}} \quad f(x,y) = \quad x^2 + 2y^2 - 2}$$

- An optimization problem with constraint:

$$\boxed{\begin{aligned} \underset{x,y}{\text{minimize}} \quad & f(x,y) = \quad x^2 + 2y^2 - 2 \\ \text{subject to} \quad & h(x,y) = \quad x + y - 1 = 0. \end{aligned}}$$

An Optimization Problem

- Tool for solving constrained optimization problems of differentiable functions

$$\boxed{\begin{array}{lll} \underset{x,y}{\text{minimize}} & f(x,y) = & x^2 + 2y^2 - 2 \\ \text{subject to} & h(x,y): & x + y - 1 = 0. \end{array}}$$

- A Lagrangian multiplier (β) lets you combine the two equations into one

$$\boxed{\underset{x,y,\beta}{\text{minimize}} \quad L(x,y,\beta) = \quad f(x,y) + \beta h(x,y)}$$

An Optimization Problem

Solution 1. *Writing the objective as Lagrangian.*

$$L(x, y, \beta) = x^2 + 2y^2 - 2 + \beta(x + y - 1)$$

Setting the gradient to 0 with respect to x, y *and* β *will give us the optimal values.*

$$\frac{\partial L}{\partial x} = 2x + \beta = 0$$

$$\frac{\partial L}{\partial y} = 4y + \beta = 0$$

$$\frac{\partial L}{\partial \beta} = x + y - 1 = 0$$

Multiple Constraints

$$
\begin{aligned}
\underset{x,y,z}{\text{minimize}} \quad & f(x,y,z) = & x^2 + 4y^2 + 2z^2 + 6y + z \\
\text{subject to} \quad & h_1(x,y,z): & x + z^2 - 1 = 0 \\
& h_2(x,y,z): & x^2 + y^2 - 1 = 0.
\end{aligned}
$$

$$
L(x,y,z,\boldsymbol{\beta}) = f(x,y,z) + \sum_i \beta_i h_i(x,y,z)
$$

Handling Inequality Constraints

$$\boxed{\begin{array}{lcc} \underset{x,y}{\text{minimize}} & f(x,y) = & x^3 + y^2 \\ \text{subject to} & g(x): & x^2 - 1 \leq 0. \end{array}}$$

- Inequality constraints are **transferred** as constraints on the Lagrangian, α

The Lagrangian in the above example becomes:

$$\begin{aligned} L(x,y,\alpha) &= f(x,y) + \alpha g(x,y) \\ &= x^3 + y^2 + \alpha(x^2 - 1) \end{aligned}$$

Handling Inequality Constraints

Solving for the gradient of the Lagrangian gives us:

$$\begin{aligned}\frac{\partial}{\partial x} L(x, y, \alpha) &= 3x^2 + 2\alpha x = 0 \\ \frac{\partial}{\partial y} L(x, y, \alpha) &= 2y = 0 \\ \frac{\partial}{\partial \alpha_1} L(x, y, \alpha) &= x^2 - 1 = 0\end{aligned}$$

Furthermore we require that:

$$\alpha \geq 0$$

From above equations we get $y = 0$, $x = \pm 1$ and $\alpha = \pm\frac{3}{2}$. But since $\alpha \geq 0$, hence $\alpha = \frac{3}{2}$. This gives $x = 1$, $y = 0$, and $f = 1$.

Generalized Lagrangian

Handling Both Types of Constraints

$$\begin{array}{lll} \underset{\mathbf{w}}{\text{minimize}} & f(\mathbf{w}) & \\ \text{subject to} & g_i(\mathbf{w}) \leq 0 & i = 1, \ldots, k \\ \text{and} & h_i(\mathbf{w}) = 0 & i = 1, \ldots, l. \end{array}$$

Generalized Lagrangian

$$L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\boldsymbol{w}) + \sum_{i=1}^{k} \alpha_i g_i(\mathbf{w}) + \sum_{i=1}^{l} \beta_i h_i(\mathbf{w})$$

subject to, $\alpha_i \geq 0, \forall i$

Primal and Dual Formulations

Primal Optimization

- Let θ_P be defined as:

$$\theta_P(\mathbf{w}) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

- One can prove that the optimal value for the original constrained problem is same as:

$$p^* = \min_{\mathbf{w}} \theta_P(\mathbf{w}) = \min_{\mathbf{w}} \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

Consider

$$\begin{aligned} \theta_P(\mathbf{w}) &= \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) \\ &= \max_{\boldsymbol{\alpha},\boldsymbol{\beta}:\alpha_i \geq 0} f(\mathbf{w}) + \sum_{i=1}^{k} \alpha_i g_i(\mathbf{w}) + \sum_{i-1}^{l} \beta_i h_i(\mathbf{w}) \end{aligned}$$

It is easy to show that if any constraints are not satisfied, i.e., if either $g_i(\mathbf{w}) > 0$ or $h_i(\mathbf{w}) \neq 0$, then $\theta_P(\mathbf{w}) = \infty$. Which means that:

$$\theta_P(\mathbf{w}) = \begin{cases} f(\mathbf{w}) & \text{if primal constraints are satisfied} \\ \infty & \text{otherwise,} \end{cases}$$

A Toy Example

Optimization Formulation

$$\underset{\mathbf{w},b}{\text{minimize}} \quad \frac{\|\mathbf{w}\|^2}{2}$$

$$\text{subject to} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, \; i = 1, \ldots, n.$$

A Toy Example

- $\mathbf{x} \in \Re^2$
- Two training points:

$$\mathbf{x}_1, y_1 = (1, 1), -1$$

$$\mathbf{x}_2, y_2 = (2, 2), +1$$

- Find the best hyperplane $\mathbf{w} = (w_1, w_2)$

A Toy Example

Optimization problem for the toy example

$$\begin{aligned} \underset{\mathbf{w}}{\text{minimize}} \quad & f(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{subject to} \quad & g_1(\mathbf{w}, b) = y_1(\mathbf{w}^\top \mathbf{x}_1 + b) - 1 \geq 0 \\ & g_2(\mathbf{w}, b) = y_2(\mathbf{w}^\top \mathbf{x}_2 + b) - 1 \geq 0. \end{aligned}$$

- Substituting actual values for $\mathbf{x}_1, y_1$ and $\mathbf{x}_2, y_2$.

$$\begin{aligned} \underset{\mathbf{w}}{\text{minimize}} \quad & f(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{subject to} \quad & g_1(\mathbf{w}, b) = -(\mathbf{w}^\top \mathbf{x}_1 + b) - 1 \geq 0 \\ & g_2(\mathbf{w}, b) = (\mathbf{w}^\top \mathbf{x}_2 + b) - 1 \geq 0. \end{aligned}$$

The above problem can be also written as:

$$\begin{aligned} \underset{w_1, w_2, b}{\text{minimize}} \quad & f(w_1, w_2) = \frac{1}{2}(w_1^2 + w_2^2) \\ \text{subject to} \quad & g_1(w_1, w_2, b) = -(w_1 + w_2 + b) - 1 \geq 0 \\ & g_2(w_1, w_2, b) = (2w_1 + 2w_2 + b) - 1 \geq 0. \end{aligned}$$

A Toy Example

To solve the toy optimization problem, we rewrite it in the Lagrangian form:

$$L(w_1, w_2, b, \alpha) \quad = \quad \frac{1}{2}(w_1^2 + w_2^2) + \alpha_1(w_1 + w_2 + b + 1) - \alpha_2(2w_1 + 2w_2 + b - 1)$$

Setting $\nabla L = 0$, we get:

$$\begin{aligned}
\frac{\partial}{\partial w_1} L(w_1, w_2, b, \alpha) &= w_1 + \alpha_1 - 2\alpha_2 = 0 \\
\frac{\partial}{\partial w_2} L(w_1, w_2, b, \alpha) &= w_2 + \alpha_1 - 2\alpha_2 = 0 \\
\frac{\partial}{\partial b} L(w_1, w_2, b, \alpha) &= \alpha_1 - \alpha_2 = 0 \\
\frac{\partial}{\partial \alpha_1} L(w_1, w_2, b, \alpha) &= w_1 + w_2 + b + 1 = 0 \\
\frac{\partial}{\partial \alpha_2} L(w_1, w_2, b, \alpha) &= 2w_1 + 2w_2 + b - 1 = 0
\end{aligned}$$

Solving the above equations, we get, $w_1 = w_2 = 1$ and $b = -3$.

Questions?

UNIVERSITY OF NORTH CAROLINA
CHARLOTTE