

Deep Learning

Vijaya Saradhi

IIT Guwahati

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Knowledge Representation

Definition

Stored information or models used by a person or a machine to interpret, predict and appropriately respond to the outside world.

Knowledge Representation

Discussion

Knowledge of the world consists of two kinds of information:

- **Prior Information** the known facts.
- Class related prior information example: 20% of emails belong to spam;
- Feature related prior information example 2: 90% of spam emails contain the word "Free Free Free"

Knowledge Representation

Four main points

- Rule 1 Similar inputs from similar classes should produce similar representations inside the network
- Rule 2 Inputs to be categorized as separate classes should be given widely different representation in the network
- Rule 3 Importance to specific features is given through involving large number of neurons
- Rule 4 Prior information is achieved through design of neural network.

Introduction

- Obtain **best result** under given circumstance
- In engineering discipline the goal is to **minimize** the effort required or **maximize** the desired benefit
- These are expressed as **function** of certain **decision variables**
- Optimization can be defined as the process of finding conditions that gives maximum or minimum value of a function

Introduction

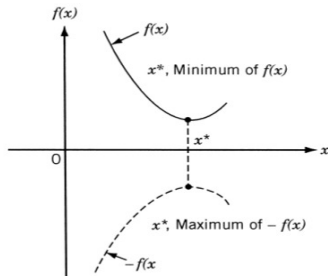
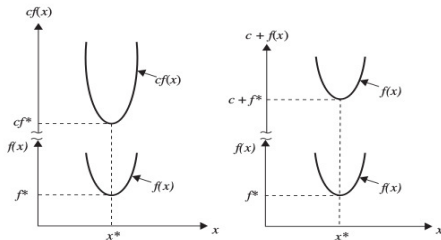


Figure 1.1 Minimum of $f(x)$ is same as maximum of $-f(x)$.



Statement Of Optimization Problem

- Optimization problem

$$\begin{array}{ll} \underset{\mathbf{x}}{\text{minimize}} & f(\mathbf{x}) \\ \text{subject to} & g_j(\mathbf{x}) \leq 0 \quad \forall j = 1, 2, \dots, m \\ & l_j(\mathbf{x}) = 0 \quad \forall j = 1, 2, \dots, p \end{array}$$

- \mathbf{x} : Design variables/ design vector
- $f(\mathbf{x})$: objective function
- $g_j(\mathbf{x})$ inequality constraints
- $l_j(\mathbf{x})$ equality constraints
- Constrained optimization problem

Variations

- Design variables:
 - Single variable/Multi-variable
 - Continuous values/integer values
- objective function
 - Linear
 - Non-linear
 - Convex
 - Single objective/multi objective
 - Unimodal/multimodal
- Constraints
 - No constraints
 - only $l_j(\cdot)$ which are linear
 - both $g_j(\cdot)$ and $l_j(\cdot)$
 - Convex

Variables

Single Variable

$$f(x) = (x^2 - 2x + 7)$$

$$f(x) = x^2 + \frac{54}{x}$$

Multi Variable

$$f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2$$

$$f(x_1, x_2) = x_1 - x_2 + 2 \times x_1^2 + 2 \times x_1 \times x_2 + x_2^2$$

Continuous vs Integer

Continuous

$$\begin{aligned} f(x) &= x^2 + \frac{54}{x} \\ \text{s.t. } x &\in \mathbb{R} \end{aligned}$$

Continuous

Integer

$$\begin{aligned} f(x) &= (x^2 - 2x + 7) \\ \text{s.t. } x &\in \mathbb{N} \end{aligned}$$

Objective function

Linear

$$\text{Minimize } f(x_1, x_2) = c_1x_1 + c_2x_2 + \cdots + c_nx_n$$

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$

$$\vdots$$

$$a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n = b_m$$

Objective function

Matrix Form

Let

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

let

$$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}$$

Objective function

Objective function matrix Form

$$\text{Minimize } f(\mathbf{x}) = \mathbf{c}^T \mathbf{x}$$

Objective function

Constraints in matrix form

Let $\mathbf{A} =$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}$$

Let $\mathbf{b} =$

$$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Objective function

Constraints in matrix form

$$\mathbf{Ax} = \mathbf{b}$$

Objective function

Linear objective

$$\begin{aligned} & \text{Minimize } f(\mathbf{x}) = \mathbf{c}^T \mathbf{x} \\ & \text{subject to } \mathbf{Ax} = \mathbf{b} \\ & \mathbf{x} \geq 0 \end{aligned}$$

Inequality Constraints

Example

$$\begin{aligned} &\text{Minimize } f(x_1, x_2) = x_1^2 + x_2^2 \\ &\text{subject to } x_1 + 2x_2 \leq 15 \\ &1 \leq x_1 \leq 10 \\ &1 \leq x_2 \leq 10 \end{aligned}$$

Nature of objective functions

- When there are no constraints present the problem is an **unconstrained** optimization
- When there are constraints present the problem is known as **constrained** optimization
- **Linear Optimization** When $f(\mathbf{x})$ is linear and only **linear** constraints are present
- **Non Linear Optimization** when $f(\mathbf{x})$ is nonlinear
- **Convex Optimization** When $f(\mathbf{x})$ is convex and constraints are linear

Optimization Definition

Local optimal

$f(x)$ has a **minimum** at $x = x^*$ if $f(x^*) \leq f(x^* + h)$ for all sufficiently small positive and negative values of h .

$f(x)$ has a **maximum** at $x = x^*$ if $f(x^*) \geq f(x^* + h)$ for all sufficiently small positive and negative values of h .

Global optimal

$x = x^*$ found in the **interval** $[a, b]$ such that x^* minimizes $f(x)$

Introduction

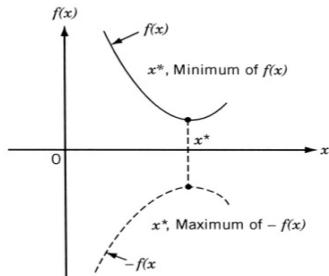
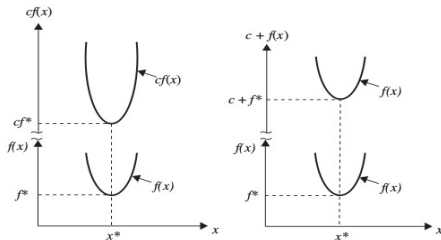


Figure 1.1 Minimum of $f(x)$ is same as maximum of $-f(x)$.



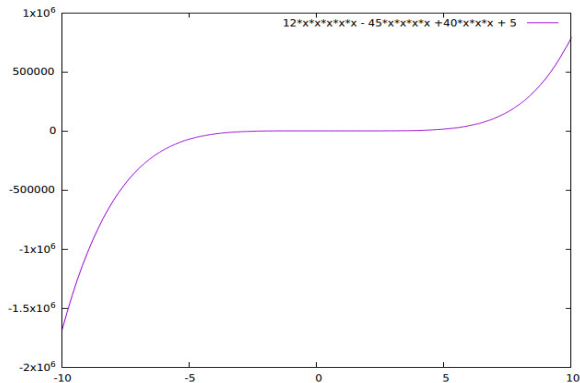
Single Variable

Necessary Condition

if $f(x)$ is defined in the interval $[a, b]$ and has a local minimum at $x = x^*$; let the first order derivative of $f(x)$ exists at $x = x^*$ then

$$\frac{df(x)}{dx} = 0$$

Example



Example

$$f'(x) = 60(x^4 - 3x^3 + 2x^2) = 60x^2(x - 1)(x - 2)$$

$f'(x) = 0$ at $x = 0, 1$ and 2 .

Multi Variable

Necessary Condition

Let $\mathbf{x} = (x_1, x_2, \dots, x_n)$

If $f(\mathbf{x})$ has a maximum or minimum point at $\mathbf{x} = \mathbf{x}^*$. Assume **partial derivatives** of $f(\mathbf{x})$ exists at \mathbf{x}^* then

$$\left. \frac{\partial f(\mathbf{x})}{\partial x_1} \right|_{x_1=x_1^*} = \left. \frac{\partial f(\mathbf{x})}{\partial x_2} \right|_{x_2=x_2^*} = \dots = \left. \frac{\partial f(\mathbf{x})}{\partial x_n} \right|_{x_n=x_n^*} = 0$$

$$\left. \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}^*} = \left[\begin{array}{c} \left. \frac{\partial f(\mathbf{x})}{\partial x_1} \right|_{\mathbf{x}=\mathbf{x}^*} \\ \left. \frac{\partial f(\mathbf{x})}{\partial x_2} \right|_{\mathbf{x}=\mathbf{x}^*} \\ \vdots \\ \left. \frac{\partial f(\mathbf{x})}{\partial x_n} \right|_{\mathbf{x}=\mathbf{x}^*} \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \\ \vdots \\ 0 \end{array} \right] = \mathbf{0}$$

Example

$$f(x_1, x_2) = x_1^3 + x_2^3 + 2x_1^2 + 4x_2^2 + 6$$

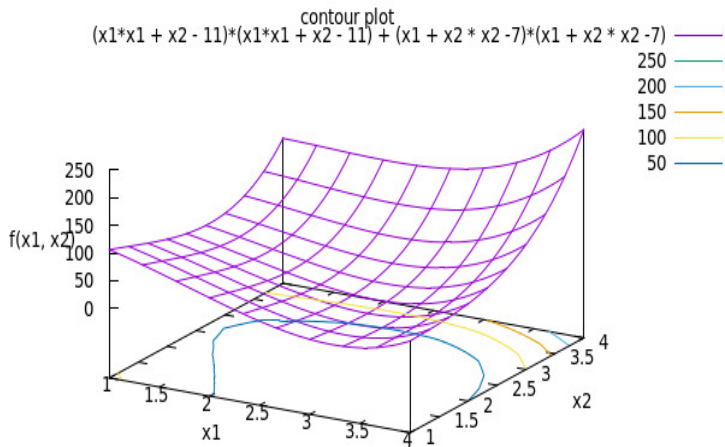
Necessary Condition

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 3x_1^2 + 4x_1 = x_1(3x_1 + 4) = 0$$

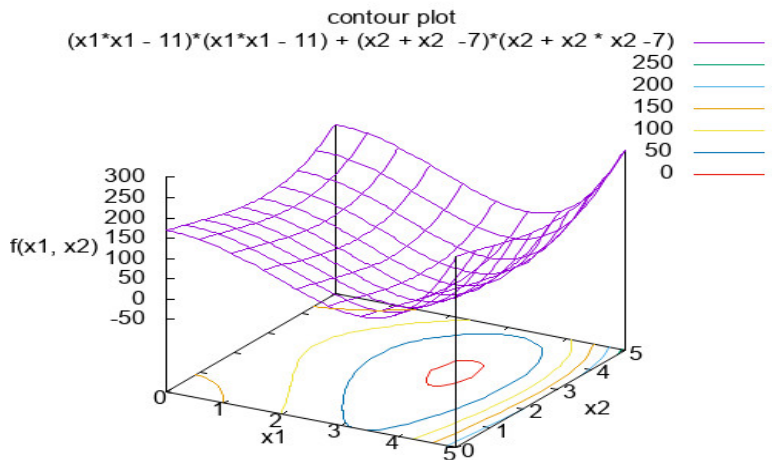
$$\frac{\partial f(x_1, x_2)}{\partial x_2} = 3x_2^2 + 8x_2 = x_2(3x_2 + 8) = 0$$

These equations satisfy at $(0, 0)$, $(0, -\frac{8}{3})$, $(-\frac{4}{3}, 0)$ and $(-\frac{4}{3}, -\frac{8}{3})$

Contours



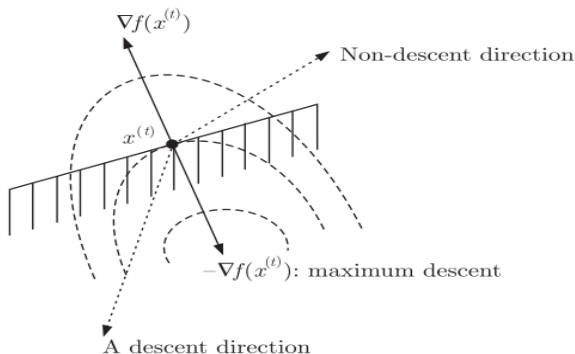
Contours



Descent Direction

Definition

A search direction \mathbf{d}^t is a descent direction at point \mathbf{x}^t if the condition $\nabla f(\mathbf{x}^t) \cdot \mathbf{d}^t \leq 0$ is satisfied



Descent Direction

Condition

$$\begin{aligned} f(\mathbf{x}^{(t+1)}) &< f(\mathbf{x}^t) \\ &< f(\mathbf{x}^t + \alpha \nabla f(\mathbf{x}^t) \cdot \mathbf{d}^t) \end{aligned} \quad (1)$$

That is function value at new point $\mathbf{x}^{(t+1)}$ is less than function value at the current point $\mathbf{x}^{(t)}$

Maximum Descent Direction

Condition

When $\mathbf{d}^t = -\nabla f(\mathbf{x}^t)$ maximum decrease in function value is obtained

Let $\mathbf{d}^t = (1, 0)^T$ Example: $f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2$

Let $\mathbf{x}^t = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Let $\mathbf{d}^t = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\nabla f \left(\begin{pmatrix} 1 \\ 1 \end{pmatrix} \right) = \begin{pmatrix} -46 \\ -38 \end{pmatrix}$$

$$(-46 - 38) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -46$$

Maximum Descent Direction

Condition

When $\mathbf{d}^t = -\nabla f(\mathbf{x}^t)$ maximum decrease in function value is obtained

Example: $f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2$

Let $\mathbf{x}^t = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

When $\mathbf{d}^t = -\nabla f(\mathbf{x}^t) = \begin{pmatrix} 46 \\ 38 \end{pmatrix}$

$\nabla f \left(\begin{pmatrix} 1 \\ 1 \end{pmatrix} \right) = \begin{pmatrix} -46 \\ -38 \end{pmatrix}$

$(-46 - 38) \begin{pmatrix} 46 \\ 38 \end{pmatrix} = -3560$

Gradient Descent

Algorithm

- Step 1** Choose: No. of iterations, $\mathbf{x}^{(0)}$, ϵ_1, ϵ_2 ; set $k = 0$
- Step 2** Calculate $\nabla f(\mathbf{x}^{(k)})$
- Step 3** if $\|\nabla f(\mathbf{x}^{(k)})\| \leq \epsilon_1$ then *terminate*
- Step 4** Perform *uni-directional search* to find $\alpha^{(k)}$ using ϵ_2
- such that $f(\mathbf{x}^{(k+1)}) = f(\mathbf{x}^{(k)} - \alpha^{(k)} \nabla f(\mathbf{x}^{(k)}))$ is minimum
 - Terminate when $\nabla f(\mathbf{x}^{(k+1)}) \cdot \nabla f(\mathbf{x}^{(k)}) \leq \epsilon_2$
- Step 5** Increment $k = k + 1$; Repeat steps 2 to 5

Gradient Descent

Example

minimize. $f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 + 7)^2$

Example

Step 1 Let $k = 0$; $\mathbf{x}^0 = (0, 0)^T$; $\epsilon_1 = \epsilon_2 = 0.001$

Gradient Descent

Example

minimize. $f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 + 7)^2$

Example

Step 1 Let $k = 0$; $\mathbf{x}^0 = (0, 0)^T$; $\epsilon_1 = \epsilon_2 = 0.001$

Step 2 $\nabla f(\mathbf{x}^{(0)}) = (-14, -22)^T$;
 $\|\nabla f(\mathbf{x}^{(0)})\| = ((-14)^2 + (-22)^2) = 680 > \epsilon_1$

Gradient Descent

Example

minimize. $f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 + 7)^2$

Example

Step 1 Let $k = 0$; $\mathbf{x}^0 = (0, 0)^T$; $\epsilon_1 = \epsilon_2 = 0.001$

Step 2 $\nabla f(\mathbf{x}^{(0)}) = (-14, -22)^T$;
 $\|\nabla f(\mathbf{x}^{(0)})\| = ((-14)^2 + (-22)^2) = 680 > \epsilon_1$

Step 4 In the direction $-\nabla f(\mathbf{x}^{(0)})$ perform unidirection search

- Steepest descent direction vector is: $(14, 22)^T$
- Find α^0 such that $f(\mathbf{x}^1) = f(\mathbf{x}^0 - \alpha^0 \nabla f(\mathbf{x}^{(0)}))$ is minimum
- Let us compute: $\mathbf{x}^1 = \mathbf{x}^0 - \alpha^0 \nabla f(\mathbf{x}^{(0)})$

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} - \alpha^0 \times \begin{pmatrix} -14 \\ -22 \end{pmatrix} = \begin{pmatrix} 14\alpha^0 \\ 22\alpha^0 \end{pmatrix}$$

Gradient Descent

Example

Step 4 To find α^0 , minimize the function $f\mathbf{x}^1$

- We have computed

$$\mathbf{x}^1 = \begin{pmatrix} 14\alpha^0 \\ 22\alpha^0 \end{pmatrix}$$

- Therefore

$$f(\mathbf{x}^1) = f \begin{pmatrix} 14\alpha^0 \\ 22\alpha^0 \end{pmatrix}$$

- Substituting in objective function

$f(x_1, x_2) = (x_1^+ x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2$ we have:

- $f(\mathbf{x}^1) =$

$$((14\alpha^0)^2 + (22\alpha^0) - 11)^2 + ((14\alpha^0) + (22\alpha^0)^2 - 7)^2$$

- Minimize $f(\mathbf{x}^1)$ to find best α^0

Gradient Descent

Example

Step 4 Using Golden section search or any other single variable optimization procedure we obtain $\alpha^0 = 0.127$. Compute $\mathbf{x}^1 = (\mathbf{x}^0 - \alpha^0 \nabla f(\mathbf{x}^0)) = (14\alpha^0, 22\alpha^0) = (1.788, 2.810)^T$

Step 4 Since the termination condition does not satisfy

- Terminate when $\nabla f(\mathbf{x}^{(1)}) \cdot \nabla f(\mathbf{x}^{(0)}) \leq \epsilon_2$
- $\nabla f(\mathbf{x}^{(1)}) = (30.707, -18.803)^T$
- $\nabla f(\mathbf{x}^{(0)}) = (-14, -22)^T$
-

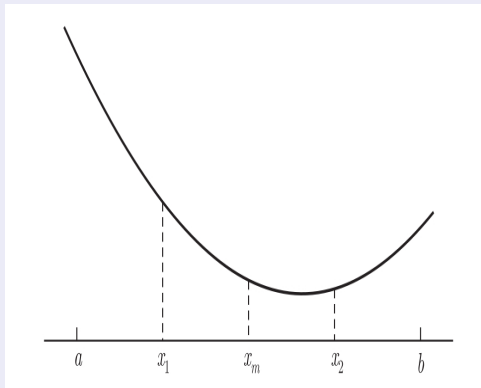
$$(30.707, -18.803) \begin{pmatrix} -14 \\ -22 \end{pmatrix} \leq \epsilon_2?$$

Step 5 increment $k = k + 1$; that is $k = 1$; Repeat the algorithm until termination criteria is met

The optimization obtains \mathbf{x}^* as $(3.008, 1.999)^T$

Single variable optimization

Interval halving method



Single variable optimization

Interval halving method

- Given interval (a, b)
- If $f(x_1) < f(x_m)$ then minimum cannot lie beyond x_m
That is $f(x_1) < f(x_{m+1}) < \dots < f(b)$
- The interval will reduce to (a, x_m)
- If $f(x_1) > f(x_m)$ then minimum cannot lie in (a, x_1)

Single variable optimization

Interval halving method - algorithm

- Step 1** Given interval (a, b) , choose ϵ . Let $x_m = \frac{(a+b)}{2}$; $L = (b - a)$
- Step 2** Initialize $x_1 = a + \frac{L}{4}$; $x_2 = b - \frac{L}{4}$; Compute $f(x_1), f(x_2)$
- Step 3** If $f(x_1) < f(x_m)$ then $b = x_m$; $x_m = x_1$; Go to step 5; else go to step 4
- Step 4** If $f(x_2) < f(x_m)$ then $a = x_m$; $x_m = x_2$; Go to step 5; else $a = x_1, b = x_2$; go to step 5;
- Step 5** Calculate $L = (b - a)$. If $(|L| < \epsilon)$ terminate else go to step 2

Text books to read

Optimization

- Engineering Optimization - Theory and Practice [Singiresu S Rao](#)
- Chapter 1 of the above book, sections 6.8 and 6.9
- mec.nit.ac.ir/file_part/master_doc/20149281833165301436305785.pdf
- Optimization for Engineering Design [Kalyanmoy Deb](#)
- Section 3.4 of the above book.