Numerical Optimization

Introduction

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NPTEL Course on Numerical Optimization

Introduction

Optimization : The procedure or procedures used to make a system or design as effective or functional as possible (adapted from `www.thefreedictionary.com`)

- Why Optimization?
  - Helps improve the quality of decision-making
  - Applications in Engineering, Business, Economics, Science, Military Planning etc.

Mathematical Program

- *Mathematical Program* : A mathematical formulation of an optimization problem:

$$\text{Minimize} \quad f(x) \quad \text{subject} \quad \text{to} \quad x \in S$$

- Essential Components of a Mathematical program:
  - x: *variables or parameters*
  - f: *objective function*
  - S: *feasible region*
- What is a solution of this Mathematical Program?

$$x^* \in S \text{ such that } f(x^*) \leq f(x) \; \forall \; x \in S$$

  - x^*: solution, $f(x^*)$: optimal objective function value
  - x^* may not be unique and may not even exist.
- Maximize $f(x) \equiv -$ Minimize $-f(x)$

Mathematical Optimization

The problem,

$$\text{Minimize} \;\; f(x) \;\; \text{subject to} \;\; x \in S$$

can be written as

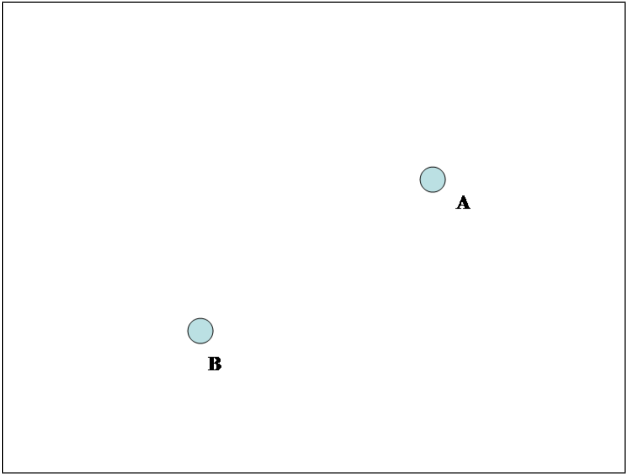
$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & x \in S \end{aligned} \tag{1}$$

Mathematical Optimization a.k.a. Mathematical programming

Study of problem formulations (1), existence of a solution, algorithms to seek a solution and analysis of solutions.

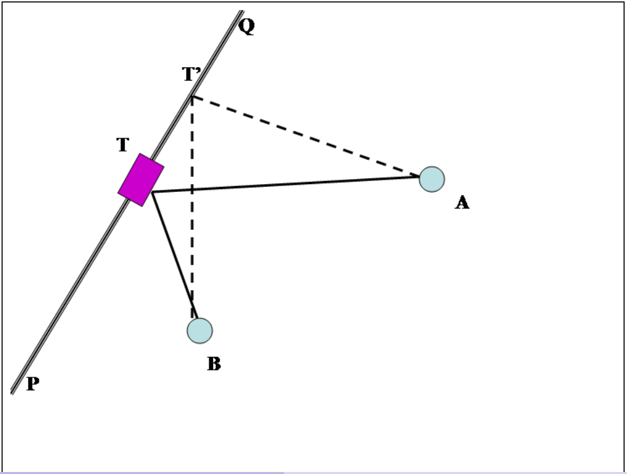
Some Optimization Problems

- Find the *shortest* path between the two points A and B in a horizontal plane

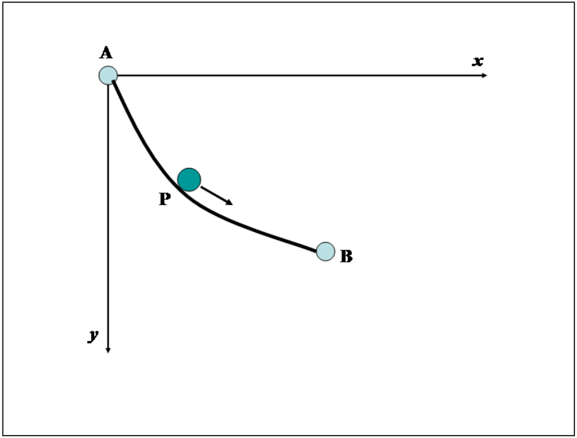


Some Optimization Problems

- Bus Terminus Location Problem: Find the location of the bus terminus T on the road segment PQ such that the lengths of the roads linking T with the two cities A and B is *minimum*.

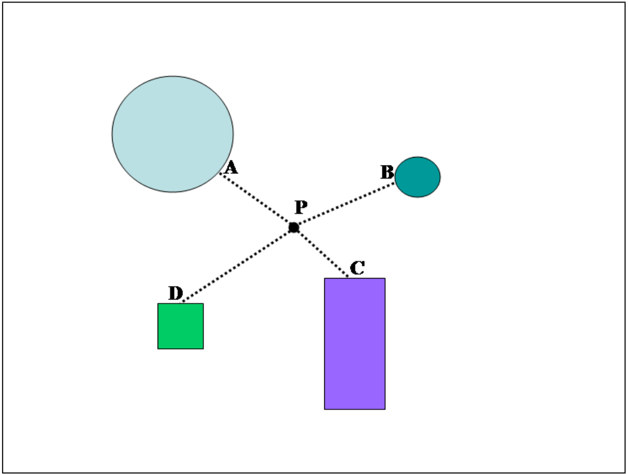


- Given two points A and B in a vertical plane, find a path APB which an object must follow, so that starting from A, it reaches B in the *shortest* time under its own gravity.



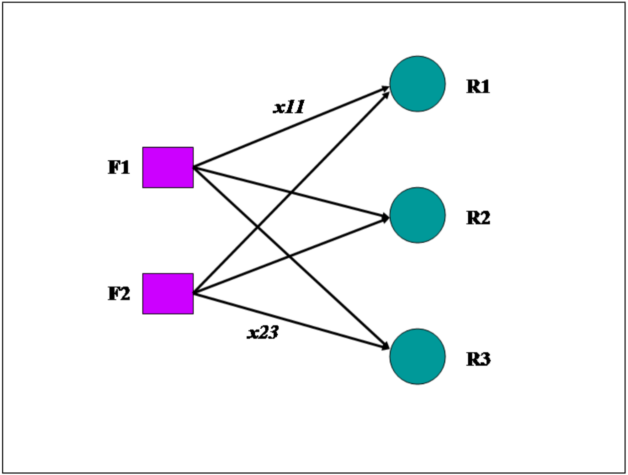
Some Optimization Problems

- Facility location problem: Find a location (within the boundary) that *minimizes* the sum of distances to each of the locations



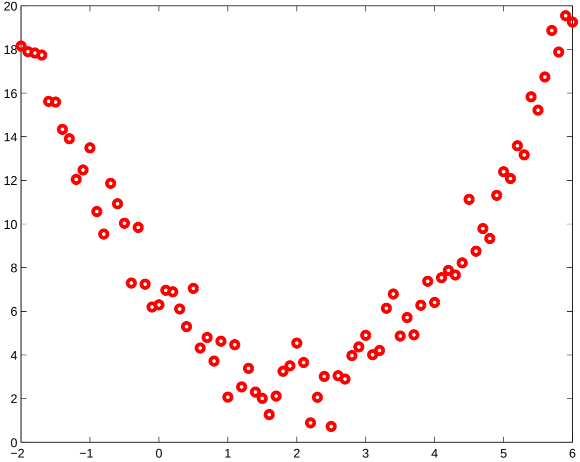
Some Optimization Problems

- Transportation Problem: Find the “best" way to satisfy the requirement of demand points using the capacities of supply points.



Some Optimization Problems

- Data Fitting Problem: From a family of potential models, find a model that “best" fits the observed data.



Some Optimization Problems

Application Domains

- Various disciplines in Engineering
- Science
- Economics and Statistics
- Business

Some Example Problems

- Scheduling problem
- Diet Problem
- Portfolio Allocation Problem
- Engineering Design
- Manufacturing
- Robot Path Planning
- ...

Some Optimization Problems

- Euclid's Problem (4th century B.C.): In a given triangle ABC, inscribe a parallelogram $ADEF$ such that $EF \| AB$ and $DE \| AC$ and the area of this parallelogram is *maximum*.
- AM (Arithmetic Mean)-GM (Geometric Mean) Inequality: For any two non-negative numbers a and b,

$$\sqrt{ab} \leq \frac{a+b}{2}$$

  Problem: Find the *maximum* of the product of two non-negative numbers whose sum is constant.
- Find the dimensions of the rectangular closed box of capacity V units which has the *least* surface area.

Mathematical Optimization Process

Typical steps for Solving Mathematical Optimization Problems

- Problem formulation
- Checking the existence of a solution
- Solving the optimization problem, if a solution exists
- Solution analysis
- Algorithm analysis

Mathematical Optimization Process

Typical steps for Solving Mathematical Optimization Problems

- Problem formulation

$$\min_x \quad f(x)$$
$$\text{s.t.} \quad x \in S$$

- Checking the existence of a solution
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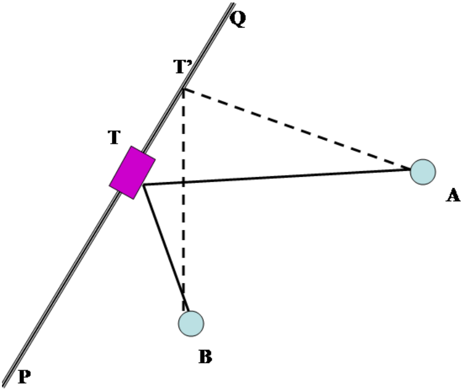
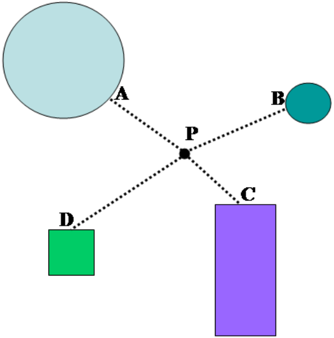
Formulation: Bus Terminus Location Problem



- Coordinates of A and B: $x_A = (x_{A1}, x_{A2})$ and $x_B = (x_{B1}, x_{B2})$
- Equation of line PQ: $ax_1 + bx_2 + c = 0$
- Use Euclidean distance
- $x_T = (x_{T1}, x_{T2})$ (variables)
- The objective is to *minimize* $d(x_A, x_T) + d(x_B, x_T)$
- T lies on PQ (constraint)

$$\begin{aligned} \min_{x_{T1}, x_{T2}} \quad & d(x_A, x_T) + d(x_B, x_T) \\ \text{s.t.} \quad & ax_{T1} + bx_{T2} + c = 0 \end{aligned}$$

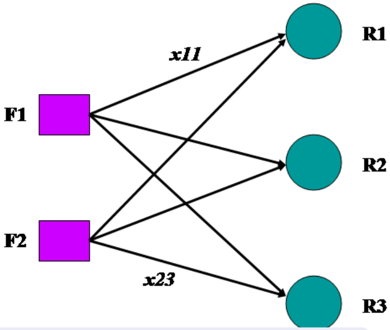
Formulation: Facility Location Problem



- x_A, x_B, x_C and x_D belong to the respective location boundaries
- Use Euclidean distance
- (x_{P1}, x_{P2}) (variables)
- The objective is to *minimize* $d(x_A, x_P) + d(x_B, x_P) + d(x_C, x_P) + d(x_D, x_P)$
- $x_A \in A, x_B \in B, x_C \in C$ and $x_D \in D$ (constraints)

$$\begin{array}{cc} \min\limits_{x_{P1}, x_{P2}} & d(x_A, x_P) + d(x_B, x_P) + d(x_C, x_P) + d(x_D, x_P) \\ \text{s.t.} & x_A \in A, x_B \in B, x_C \in C, x_D \in D \end{array}$$

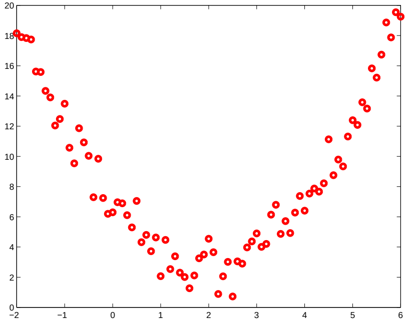
Formulation: Transportation Problem



- a_i : Capacity of the plant Fi
- b_j : Demand of the outlet Rj
- c_{ij} : Cost of shipping one unit of product from Fi to Rj
- x_{ij}: Number of units of the product shipped from Fi to Rj (variables)
- The objective is to *minimize* $\sum_{ij} c_{ij}x_{ij}$
- $\sum_{j=1}^{3} x_{ij} \leq a_i, \; i = 1,2$ (constraints)
- $\sum_{i=1}^{2} x_{ij} \geq b_j, \; j = 1,2,3$ (constraints)
- $x_{ij} \geq 0 \; \forall \; i,j$ (constraints)

$$
\begin{aligned}
\min_{\substack{x_{ij} \\ i=1,2;j=1,2,3}} \quad & \sum_{ij} c_{ij}x_{ij} \\
\text{s.t.} \quad & \sum_{j=1}^{3} x_{ij} \leq a_i, \; i = 1,2 \\
& \sum_{i=1}^{2} x_{ij} \geq b_j, \; j = 1,2,3 \\
& x_{ij} \geq 0 \; \forall \; i,j
\end{aligned}
$$

Formulation: Data Fitting Problem



- Given : $\{x_i, y_i\}_{i=1}^n$, n data points
- Given : Most probable model type, $f(x) = ax^2 + bx + c$
- a, b, c: variables
- Measure of misfit: $(y - f(x))^2$
- The objective is to *minimize* $\sum_i (y_i - (ax_i^2 + bx_i + c))^2$
- No constraints

$$\min_{a,b,c} \quad \sum_{i=1}^n (y_i - (ax_i^2 + bx_i + c))^2$$

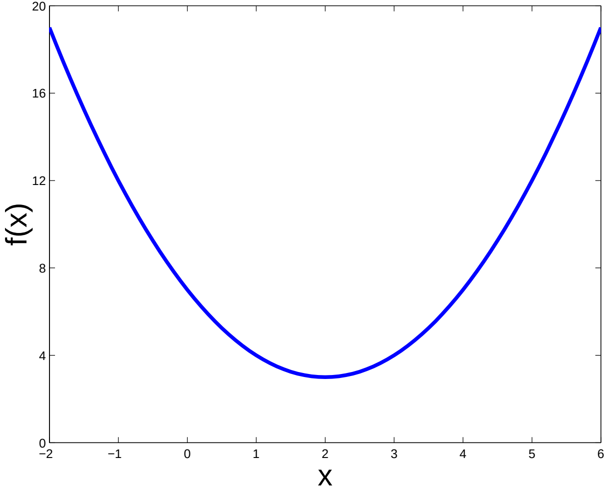
Mathematical Optimization Process

Typical steps for Solving Mathematical Optimization Problems

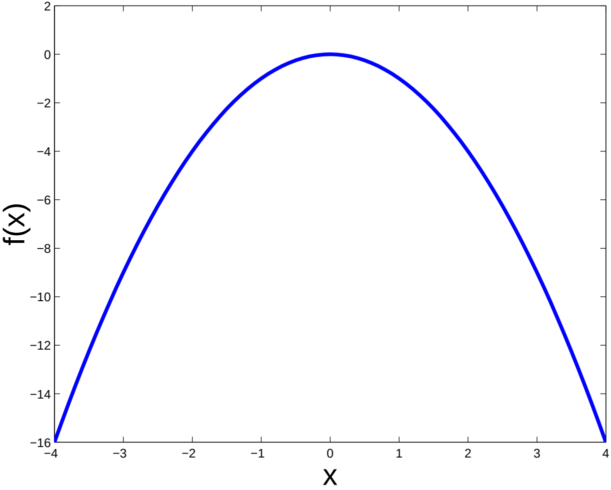
- Problem formulation
- Checking the existence of a solution
- Solving the optimization problem, if a solution exists
  - Graphical method
  - Analytical method
  - Numerical method
- Solution analysis
- Algorithm analysis

Functions of One Variable

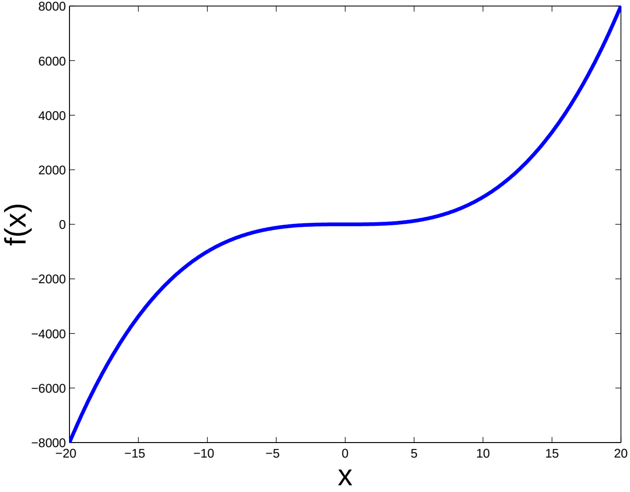
- $f(x) = (x-2)^2 + 3$
- Minimum at $x^* = 2$, minimum function value: $f(x^*) = 3$



- $f(x) = -x^2$
- Maximum at $x^* = 0$, maximum function value: $f(x^*) = 0$

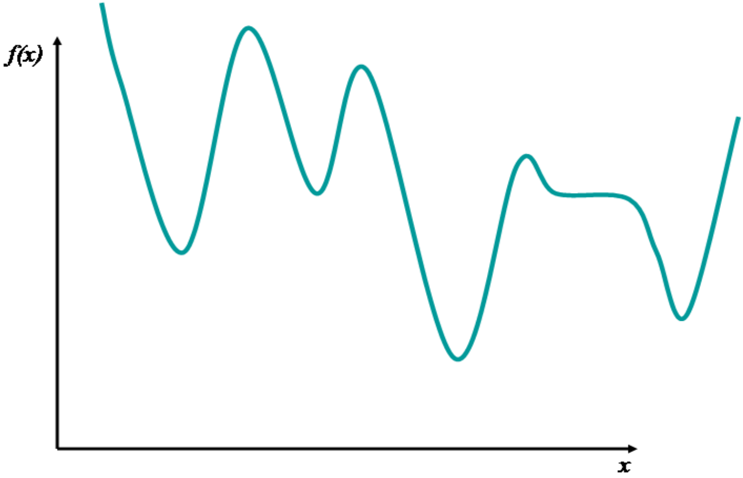


- $f(x) = x^3$
- Saddle Point at $x^* = 0$



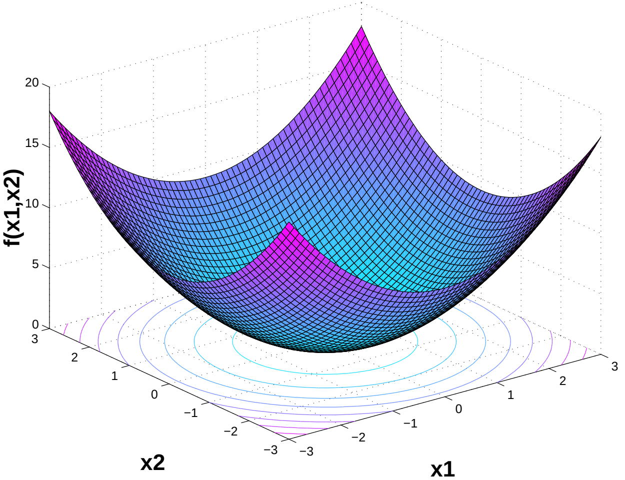
Functions of One Variable

- A typical nonlinear function



Functions of Two Variables: Surface Plots

- $f(x_1, x_2) = x_1^2 + x_2^2$
- Minimum at $x_1^* = 0$, $x_2^* = 0$; $f(x_1^*, x_2^*) = 0$



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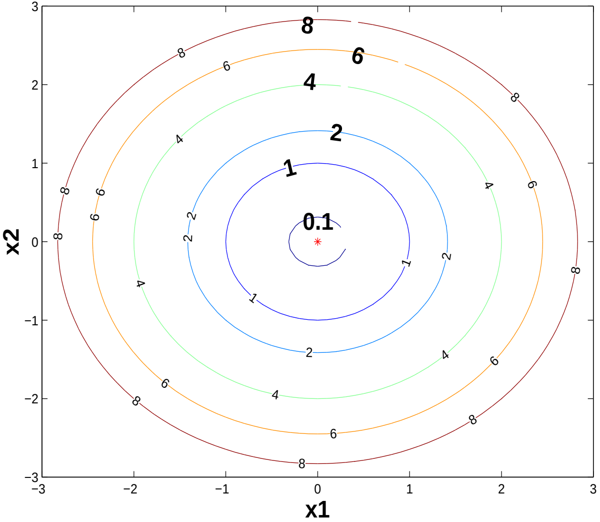
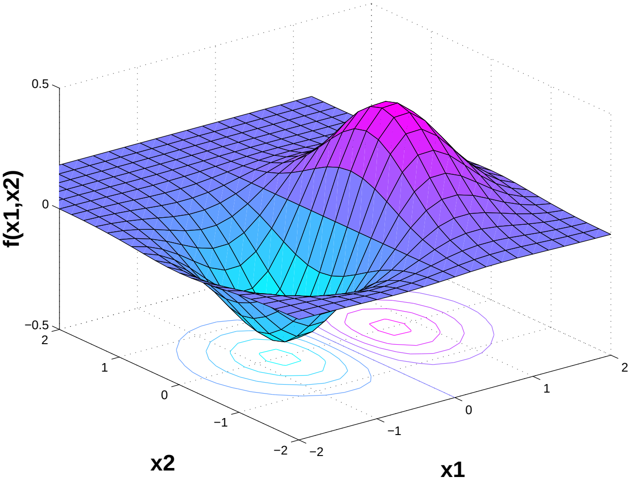
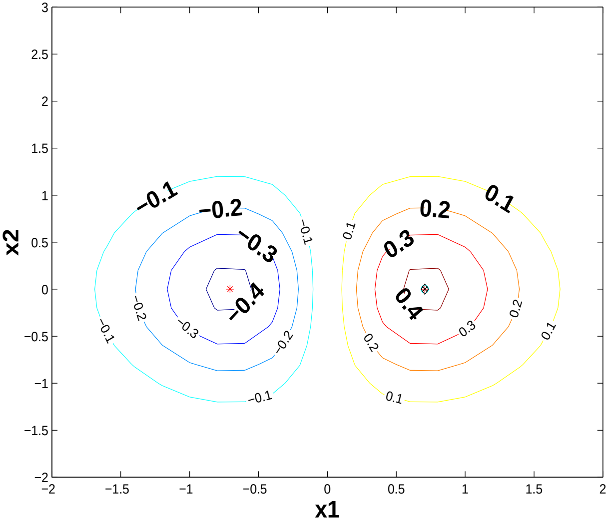


- $f(x_1, x_2) = x_1 \exp(-x_1^2 - x_2^2)$
- Minimum at $(-1/\sqrt{2}, 0)$, maximum at $(1/\sqrt{2}, 0)$



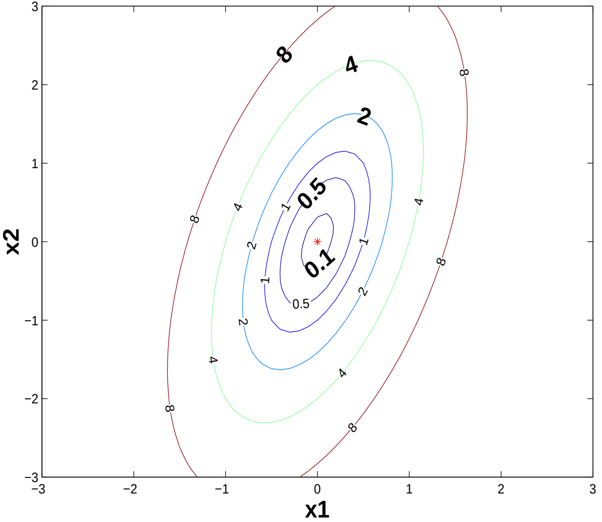
Functions of Two Variables: Contour Plots

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



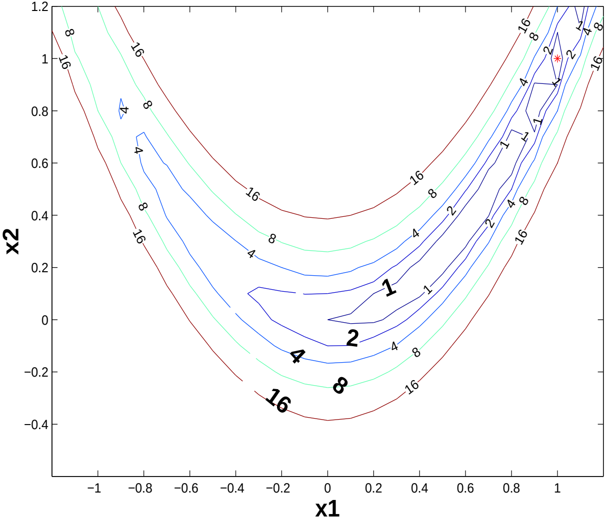
Functions of Two Variables: Contour Plots

- $f(x_1, x_2) = f(x_1, x_2) = 4x_1^2 + x_2^2 - 2x_1x_2$

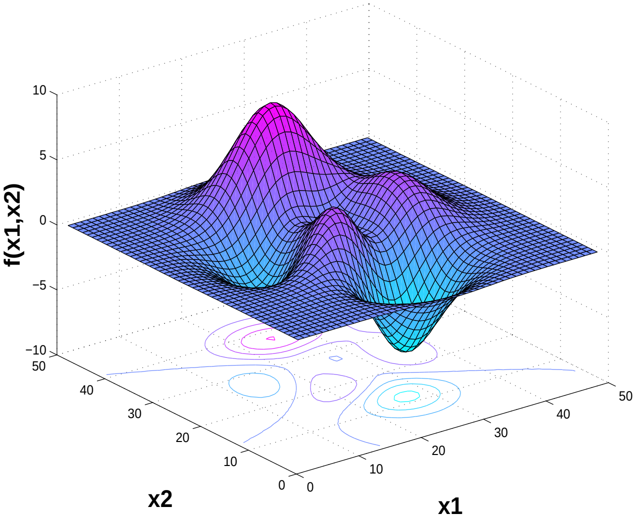


Functions of Two Variables: Contour Plots

- Rosenbrock function: $f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$
- Minimum at $(1, 1)$



Functions of Two Variables: Surface Plots



Mathematical Optimization Process

Typical steps for Solving Mathematical Optimization Problems

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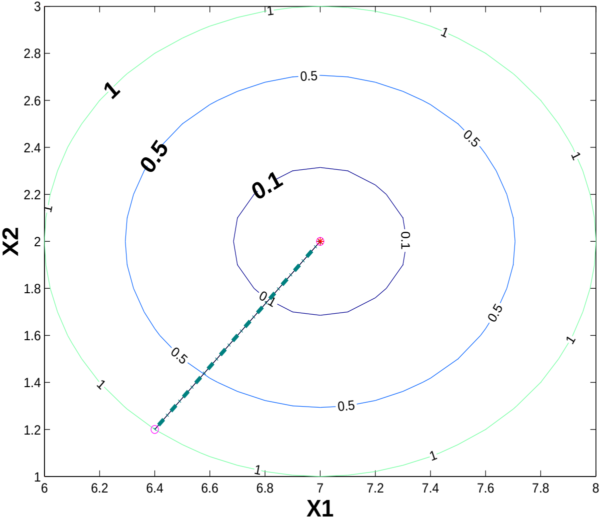
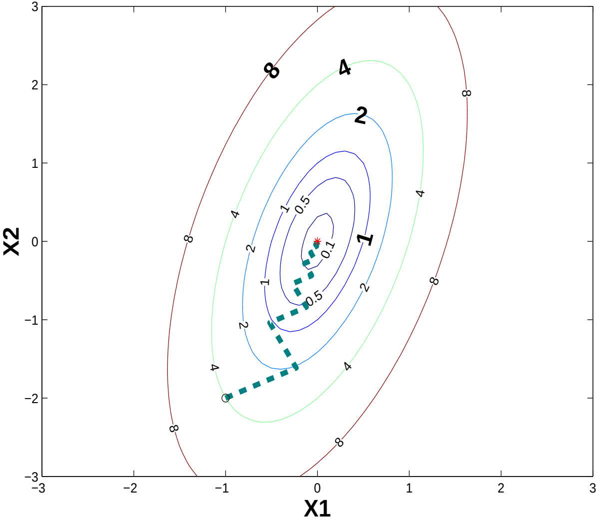
Iterates of an Optimization Algorithm

- $f(x_1, x_2) = (x_1 - 7)^2 + (x_2 - 2)^2$
- Initial Point: $(6.4, 1.2)$, Minimum at $(7, 2)$



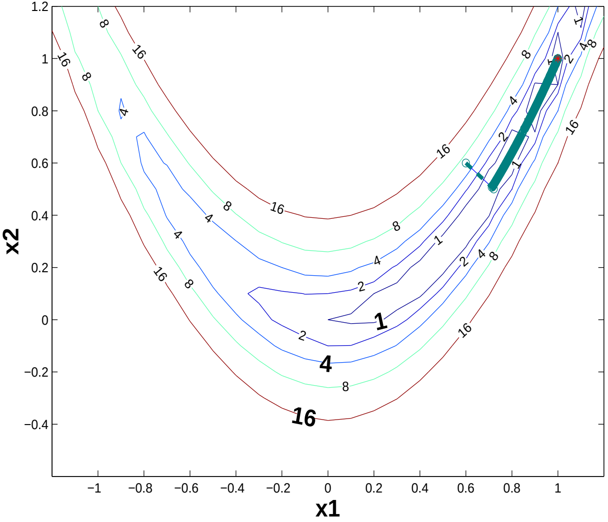
Iterates of an Optimization Algorithm

- $f(x_1, x_2) = 4x_1^2 + x_2^2 - 2x_1x_2$
- Initial Point: $(-1, -2)$, Minimum at $(0, 0)$



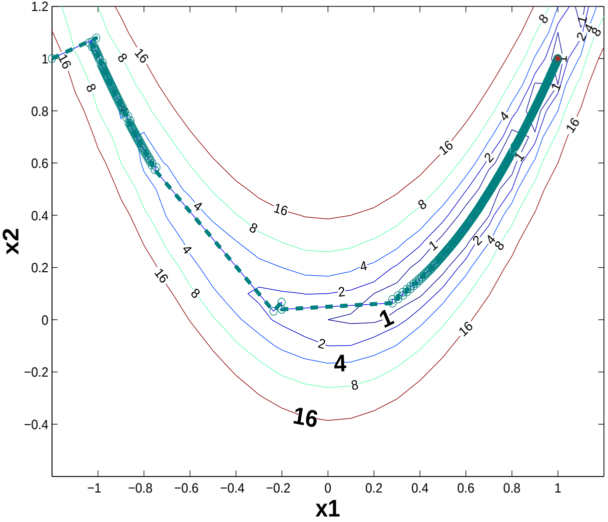
Iterates of an Optimization Algorithm

- $f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$
- Initial Point: $(0.6, 0.6)$, Minimum at $(1, 1)$

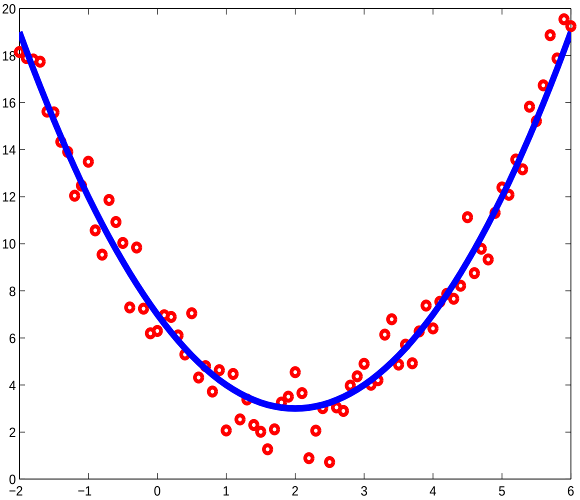


Iterates of an Optimization Algorithm

- $f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$
- Initial Point: $(-2, 1)$, Minimum at $(1, 1)$



A solution to Data Fitting Problem



Types of Optimization Problems

- Constrained and unconstrained optimization
- Continuous and discrete optimization
- Stochastic and deterministic optimization

Types of Optimization Problems

- Constrained optimization problem:

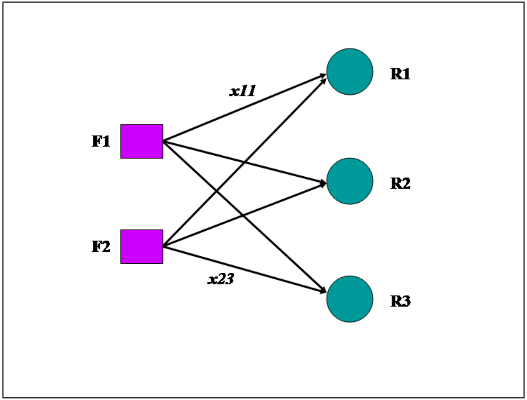
$$\begin{array}{ll} \min\limits_{x} & f(x) \\ \text{s.t.} & x \in S \end{array}$$

- Unconstrained optimization problem:

$$\min_{x} \quad f(x)$$

Types of Optimization Problems

- Continuous optimization
  - Variables are typically real-valued
- Discrete optimization
  - Variables are not real-valued: they take binary or integer values



Types of Optimization Problems

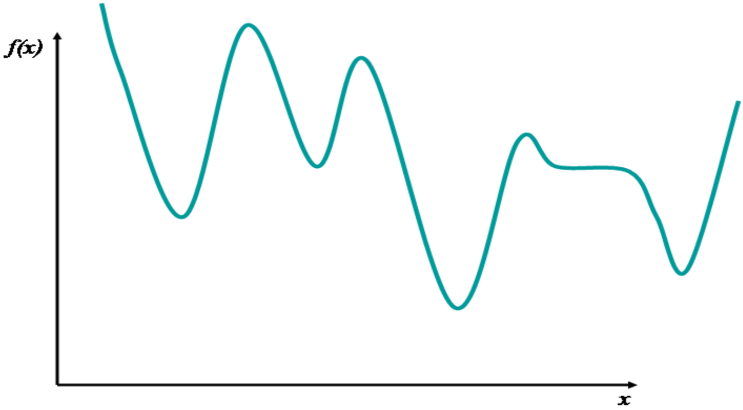
- Stochastic optimization
  - Some or all of the problem data are random
  - In some cases, the constraints hold with some probabilities
  - Need to define feasibility and optimality appropriately
- Deterministic optimization
  - No randomness in problem data and constraints

Types of Optimization Problems

- Constrained and unconstrained optimization
- Continuous and discrete optimization
- Stochastic and deterministic optimization

Types of Optimization Algorithms

- Local optimization algorithms
  - Find “locally" optimal solutions
- Global optimization algorithms
  - Find the “best" solution among all locally optimal solutions



Overview

- Mathematical Background
- One dimensional unconstrained optimization problems
- Algorithms for multi-dimensional unconstrained optimization problems
- Multi-dimensional Constrained optimization problems
- Active Set Methods
- Penalty and Barrier Function Methods

Some References

- Fletcher R., Practical Methods of Optimization, Wiley (2000)
- Kambo N. S., Mathematical Programming Techniques, Affiliated East-West Press (1984)
- Luenberger D., Linear and Nonlinear Programming, Addison-Wesley (1984)
- Nocedal J. and Wright M., Numerical Optimization, Springer (2000)
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Additional Reading List:

- Tikhomirov V. M., Stories About Maxima and Minima, The American Mathematical Society (1990), Universities Press (India) Limited (1998).