Numerical Optimization
Mathematical Formulation

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Mathematical Formulation

Definition

Optimisation is the minimisation or maximisation of a function subject to constraints on its variables.

The Mathematical Framework (Components of an Optimisation Problem)

- X is a vector of variables, also called unknowns or parameters;
- f is the objective function; a function of X that we want to optimise (maximise or minimise).
- C is the vector function of constraints that must be satisfied by the unknowns X.

Formal Definition

The optimisation problem can be stated as:

$$\min_{x \in \mathbb{R}^n} f(x) \qquad \text{subject to} \qquad \begin{cases} c_i(x) & = 0, \quad i \in \mathscr{E} \\ c_j(x) & \geq 0, \quad j \in \mathscr{I} \end{cases} \tag{1}$$

- $f : \mathbb{R}^n \to \mathbb{R}$, (a scalar valued function)
- $c_i : \mathbb{R}^n \to \mathbb{R}$
- $\mathscr{E}$: set of indices for equality constraints
- $\mathscr{I}$: set of indices for inequality constraints

Optimisation Problem

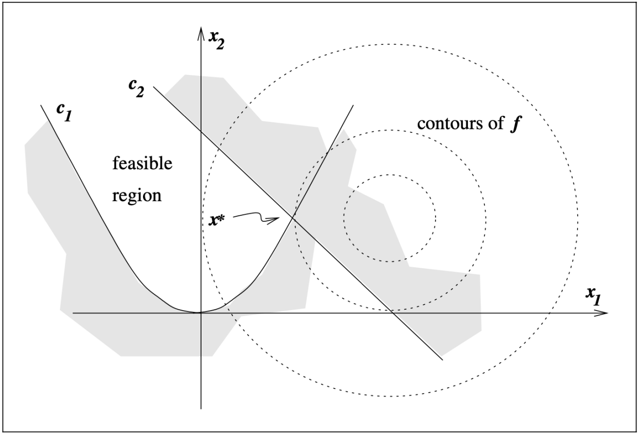


Figure: (a) Shows the contours of objective function f and (b) feasible region i.e the region satisfying all the constraints.

A Simple Example

$$\min_{x\in\mathbb{R}^2} (x_1-2)^2 + (x_2-1)^2 \quad \text{subject to} \quad \begin{cases} x_1^2 - x_2 & \leq 0, \\ x_1 + x_2 & \leq 2. \end{cases} \tag{2}$$

The above problem can be morphed into the following:

$$\begin{aligned} f(x) &= (x_1-2)^2 + (x_2-1)^2, && \textit{the objective function} \\ x &= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} && \textit{unknowns or variables} \\ c(x) &= \begin{bmatrix} c_1(x) \\ c_2(x) \end{bmatrix} = \begin{bmatrix} -x_1^2 + x_2 \\ -x_1 - x_2 + 2 \end{bmatrix}, && \textit{inequality constraints} \\ \mathscr{I} &= \{1,2\}, \quad \mathscr{E} = \phi \end{aligned}$$

Modelling an Optimisation Problem

A transport problem:

A chemical company has two factories F_1 and F_2 and a dozen of retail outlets $R_1, \ldots, R_{12}$.

- F_i produces a_i tons of chemicals per week i.e. a_i is the capacity of the plant.
- Each outlet R_j has a weekly demand of b_j tons of chemicals.
- cost of shipping one ton from F_i to R_j is c_{ij}.

Challenge:

Figure out how much product to ship from each factory to each outlet while satisfying all requirements but still minimising the costs.

TRANSPORTATION PROBLEM

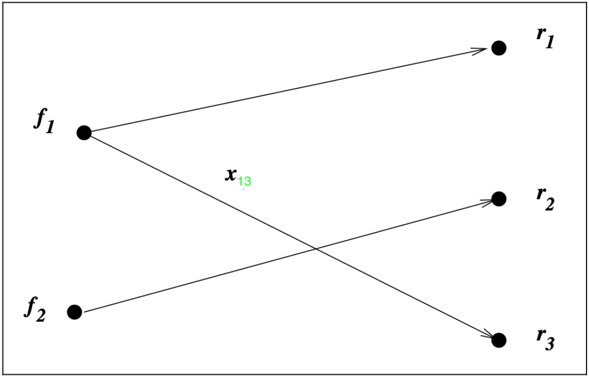


Figure: A transportation problem: Showing the no. of tons shipped from factory F_i to outlet R_j

Modelling the Transport Problem

Objective:

- Let x_{ij} be variables: no. of tons of chemicals shipped from F_i to outlet R_j ($i = 1, 2$ and $j = 1, 2, \ldots, 12$).
- The objective function to be minimised can now be written as

$$f(x) = \sum c_{ij} x_{ij}$$

- **Constraints**:

$$\begin{aligned}
\sum_{j=1}^{12} x_{ij} &\leq a_i \quad \text{for} i = 1, 2. \\
\sum_{i=1}^{2} x_{ij} &\geq b_j \quad \text{for} j = 1, \ldots, 12 \\
x_{ij} &\geq 0, \text{for} i = 1, 2 \quad j = 1, \ldots, 12.
\end{aligned} \tag{3}$$

Modelling the transport problem

- A more applicable model factors cost of manufacturing, profit from different stores, etc.
- Linear programming problems (LPP) (Objective and constraints linear)
- The variables in this case to be optimised were volumes to chemicals, which can take continuously positive values.
- If for example one has to figure out the manufacturing and transport of tractors from a factory to outlet, the answer 5.6 tractors to be sent to some outlet looks absurd.
- One could naively suggest to round up to the nearest integer value.
- Now, there is no guaranty that the modified solution is optimal in any sense.
- Problems of the first type are called continuous optimisation problems where as the second one falls in the category of discrete optimisation problems.

Discrete Vs Continuous Optimisation Problems

Continuous

$x_{ij} \in D$, $D \subset \mathbb{R}$ union of connected sets.

Discrete

$x_{ij} \in Z$, for all i, j (integer programming problem).
or

- The restriction of the domain (atleast for the discrete case) can be added into the constraints.
- The generic term discrete optimisation stands for problems where the solution is seeked within a finite set (possibly too large though).
- Continuous problems are easier solver (owing to smoothness of function).
- one may get the idea to explore through all the values to find the optimal solution for a discrete problem, but this might not be feasible owing to the size of the domain.

Some models may contain variables that are allowed to vary continuously and other that can only attain integer values;

these are referred to as mixed integer programming problems

Other Criterias to Group Optimisation Problems

There are many other categories into which optimisation problems can be put into, some of them are:

1. based on the nature of the objective function and constraints
   (*linear, non-linear, convex*)
2. based on number of variables (*large or small*).
3. the smoothness of the function (*differentiable or non-differentiable*) and so on.

Categories are formed as well, based on (types of) algorithms that can be employed some method may be very well suited for large scale problems but not for small.
Some algorithm may need to use certain order derivative of the objective function (smoothness)

Global Vs Local Optimisation

Local Optimisation problem: a maximum or minimum is seeked in a vicinity of a particular point of interest.

Advantage:

Can be solved very fast, owing to its local nature.

Disadvantage:

Suffers miserably to give any kind of indication about the global solution.

- For some application problems global solutions are highly desirable or necessary, but they are extermely difficult to identify.
- Convex programming (is a special case), where all local solutions are also global solutions.
- We focus on local optimisation and will just see through some global algorithms as well.

Stochastic Vs Deterministic Optimisation

- For some optimisation problems the model could not be specified completely at the time of formulation owing to the unavailability of full picture about a few of the variables in time.
- For example in the transportation problem, let the customer deman b_j at the retail outlets cannot be specified precisely in advance.
- In proctice, problems arising from financial and economic models, which depend on future interest rates and behaviour of the economy cannot be modelled simply.
- Modelers try to predict these unknown parameters with some degree of confidence by assigning some probability, based on previous experience.
- Stochastic Optimisation algorithms use these quantifications of the uncertainity to produce solutions that optimise the expected performance of the model.
- Deterministic Optimisation problems are thise in which the model is fully specified.

Convexity

- The concept of convexity is quite fundamental in optimisation.
- Many practical problems posses it, making them theoretically and in practice to be solved conveniently.
- The term "*Convexity*" can be realised for both sets(domains) and functions (Objective, Constraints).

Definition (Convex Set)

A set $\mathbb{S} \in \mathbb{R}^n$ is said to be convex, if the line segment joining any two points in $\mathbb{S}$ lie entirely inside $\mathbb{S}$ i.e.

$$x,\; y \in \mathbb{S} \implies \alpha y + (1-\alpha)x \in \mathbb{S} \quad \text{for all} \quad \alpha \in [0,1] \tag{4}$$

Example:

1. unit ball
2. Any polyhedron, which is a set defined by linear equalities and inequalities

Convexity

Definition (Convex function)

A function $f : \mathbb{S} \to \mathbb{R}^n$, $\mathbb{S} \subset \mathbb{R}^n$ is said to be convex, if $\mathbb{S}$ is convex and for any two points x and y in $\mathbb{S}$ the graph of f lies below the straight line connecting $(x, f(x))$ and $(y, f(y))$ in the space $\mathbb{R}^{n+1}$. That is we have the following:

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y), \text{ for all } \alpha \in [0,1]$$

- When f is smooth as well as convex and the dimension n is 1 or 2, the graph of f is bowl-shaped and its contours define convex sets.
- A function f is said to be concave if $-f$ is convex.

A Convex Function

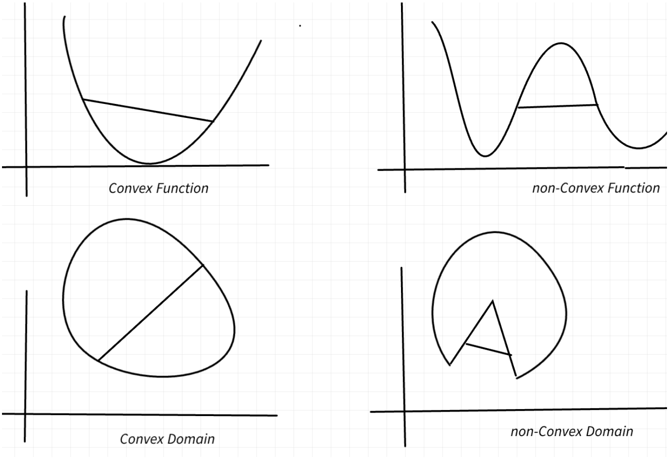
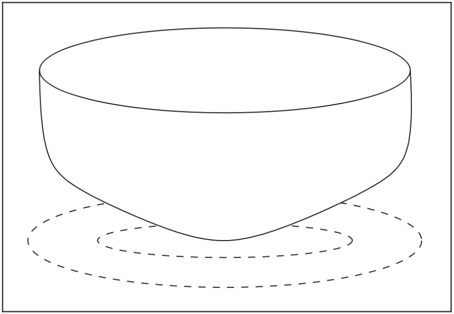


Figure: A Convex Function.

Convex Optimisation



The convex function $f(x) = (x_1 - 6)^2 + \frac{1}{25}(x_2 - 4.5)^4$.

Figure: A Convex Function.

- *Convex optimisation problem:* the objective function and the feasible set are both convex.
- Ex.: linear programming (LP).
- Easier to solve because every local min is a global min.