Introduction to Spatial Optimization

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Content

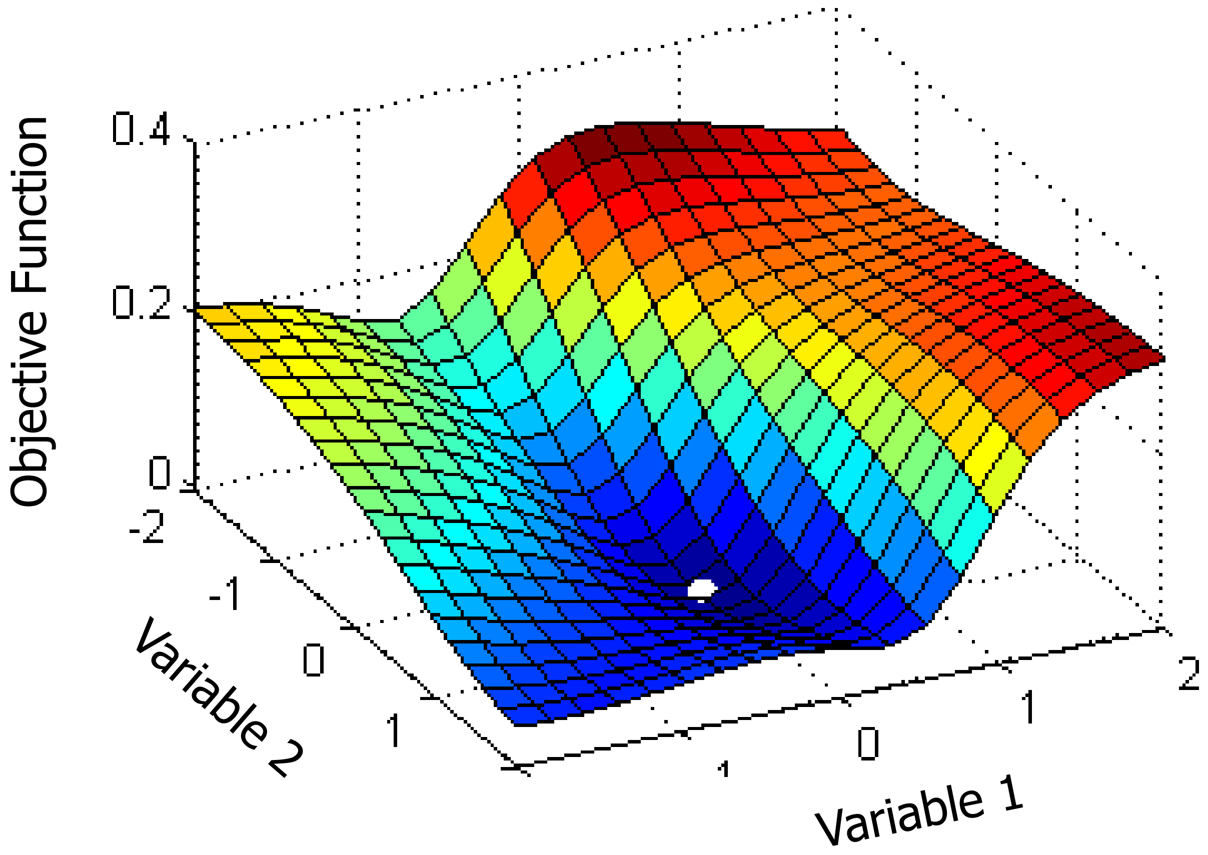
- Introduction to optimization concept and methods
- Linear Programming optimization method
- Introduction to spatial optimization
- Spatial Optimization in Practice

Optimization

- **Definition**: Optimization is the process of finding the best solution to a problem from a set of possible solutions.

- **Key Concepts:**
  - **Objective Function**: The function we want to maximize or minimize.
  - **Variables**: The parameters we can adjust to optimize the objective.
  - **Constraints**: The conditions that must be satisfied by the solution.

Optimization



Source: https://medium.com/@hakobavjyan/stochastic-gradient-descent-sgd-10ce70fea389

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Types of Optimization Problems

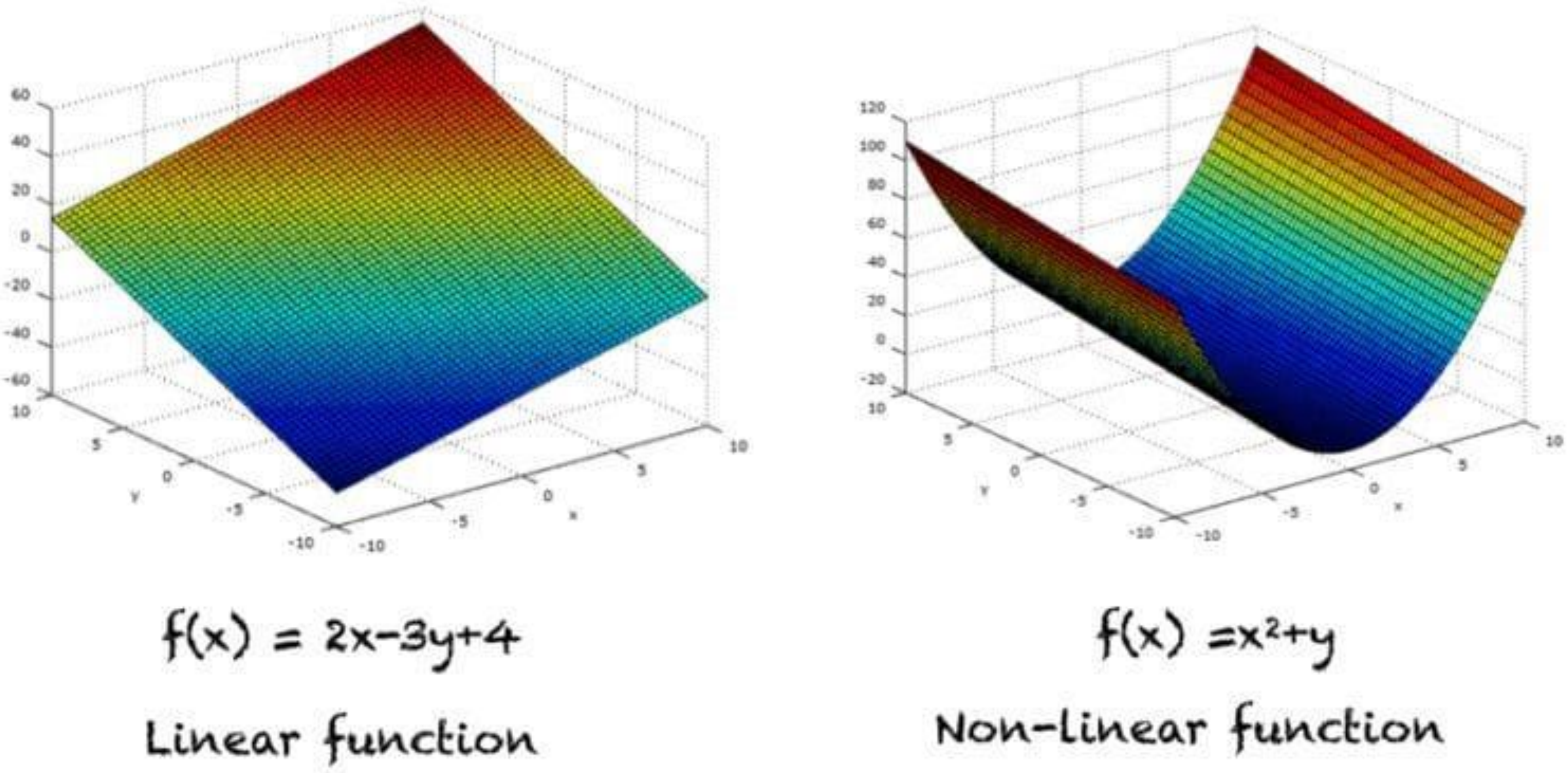
Based on Objective Function:

- Linear Optimization: Linear objective function and constraints.
- Non-linear Optimization: Non-linear objective function and/or constraints.

Based on Constraints:

- Constrained Optimization: Involves constraints on the variables.
- Unconstrained Optimization: No constraints on the variables.

Linear vs. Non-Linear Objective Function



Source: https://machinelearningmastery.com/a-gentle-introduction-to-optimization-mathematical-programming/

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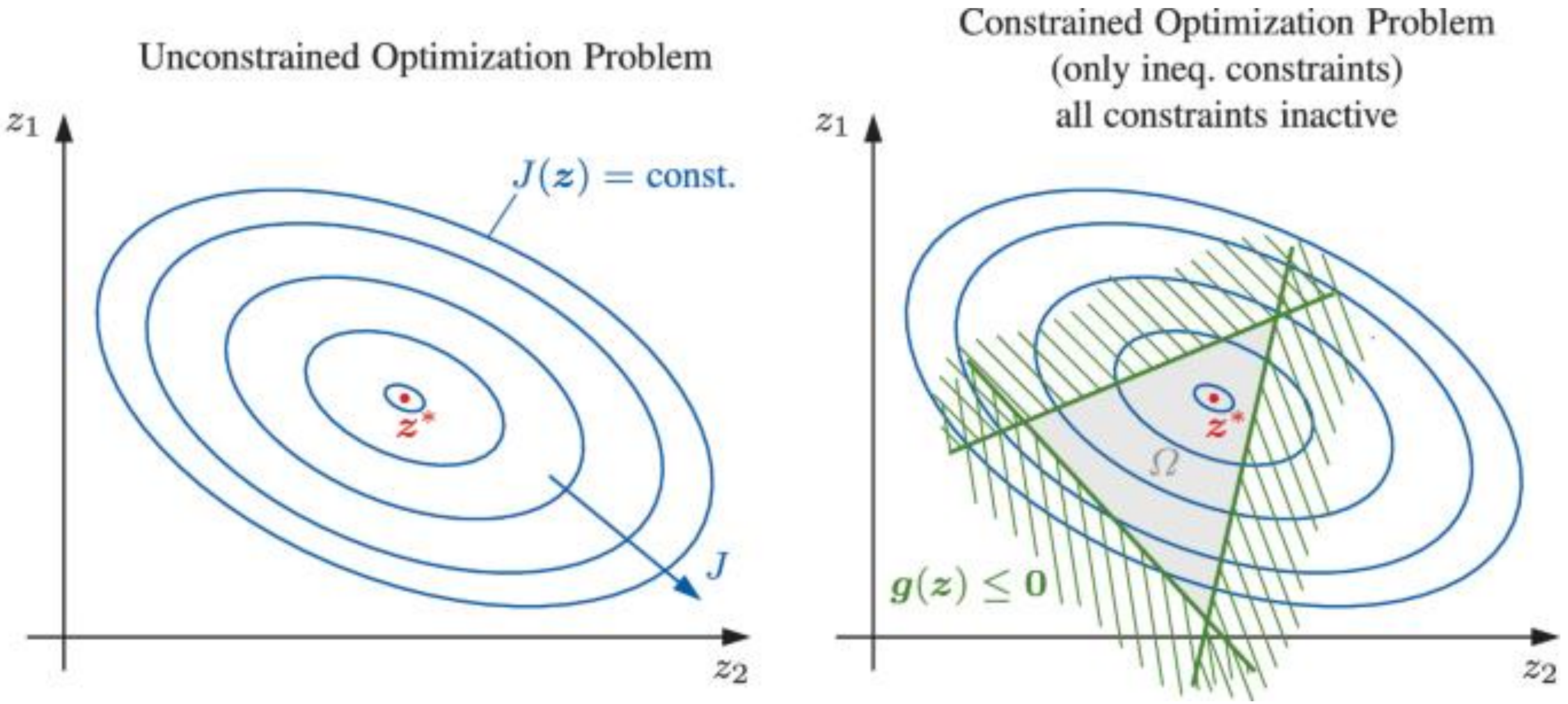
Constrained vs. Unconstrained Optimization



Source: Albin Rajasingham, T. (2021). Mathematical Fundamentals of Optimization. In: Nonlinear Model Predictive Control of Combustion Engines. Advances in Industrial Control. Springer, Cham. https://doi.org/10.1007/978-3-030-68010-7_3

Constrained Optimization

- Optimizing (maximizing or minimizing) an objective function **subject to** certain constraints. These constraints can take the form of equalities, inequalities, or bounds that limit the possible values the decision variables can take.

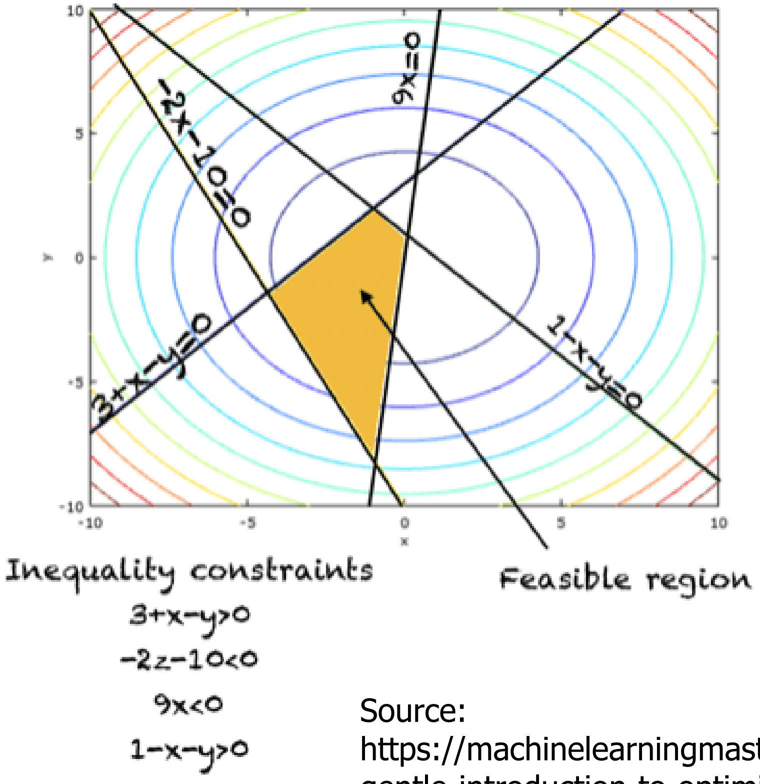
- **Example:** Find minimum of a function such that certain domain variables lie in a certain range.

- **Example:** $minimize\ x^2 + y^2$ $\boxed{\text{subject to: } x + y \leq 1}$

Constrained Optimization: Feasible Region

- The feasible region is the set of all points in space where the problem's constraints are satisfied. An optimization algorithm explores this feasible region to find the optimal points.

- For an unconstrained optimization problem, the entire domain of the function is a feasible region.



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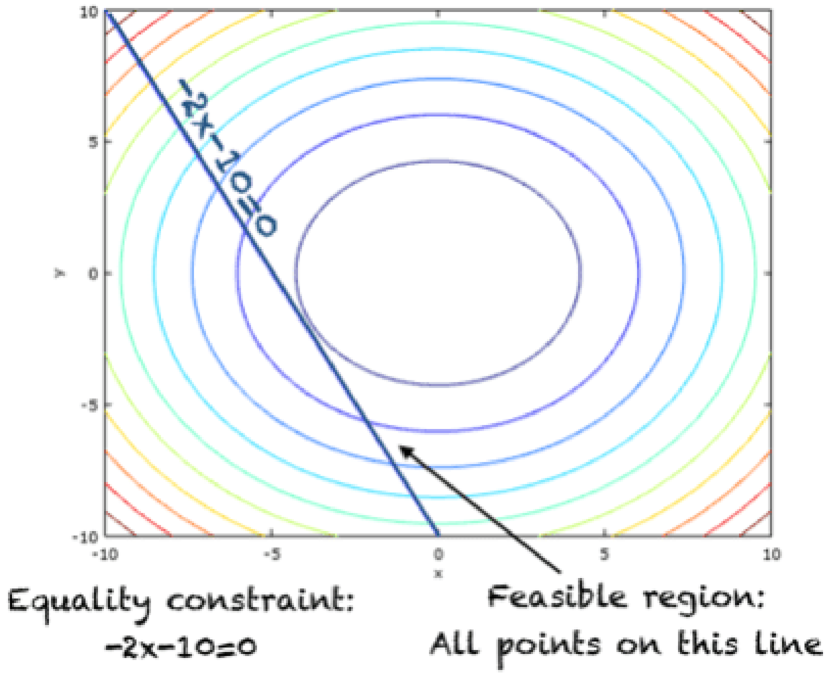
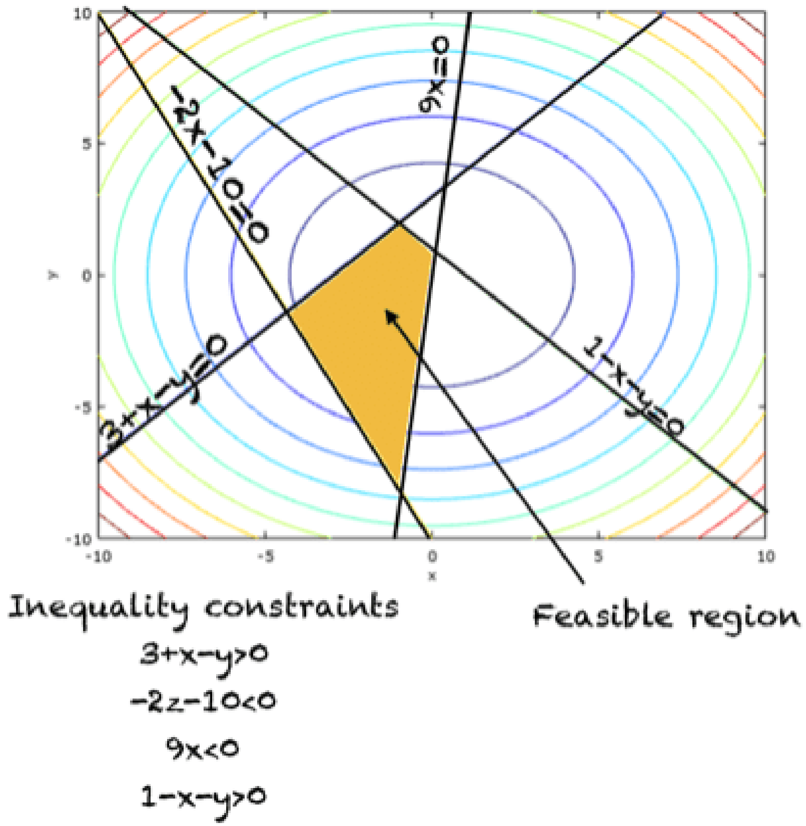
Equality Vs. Inequality Constraints





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Categories of Optimization Methods

- **Deterministic Methods:**
  Provide consistent results for the same input.

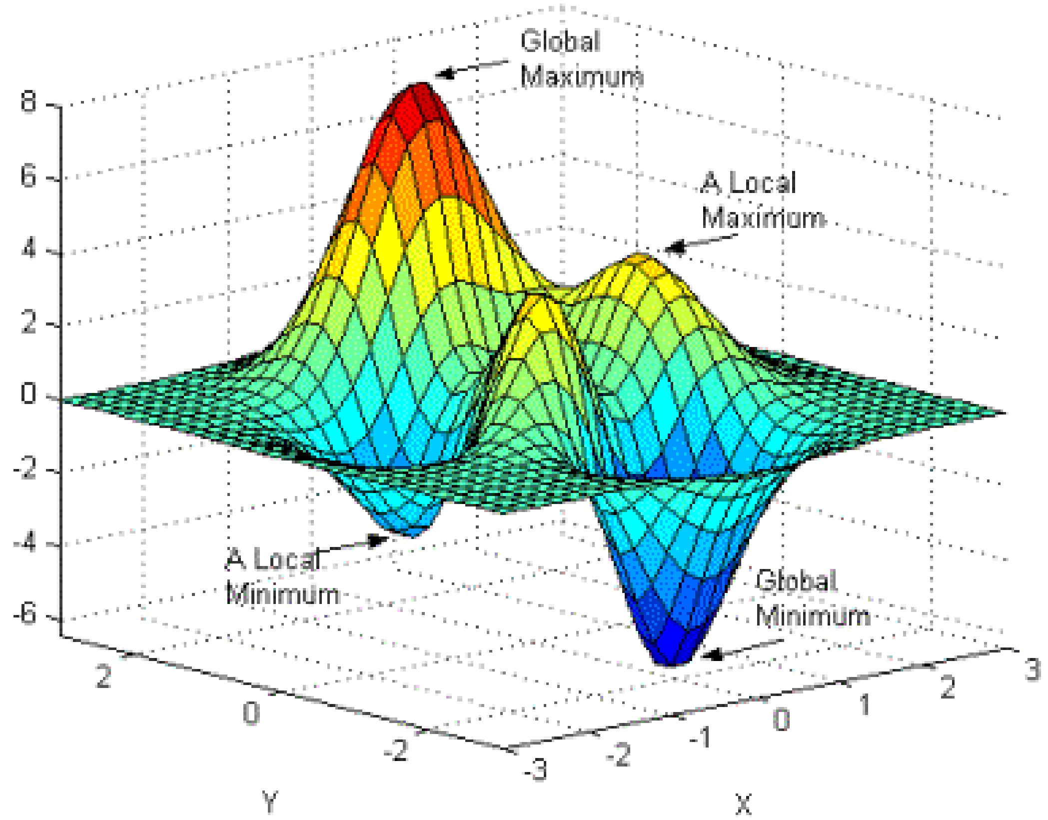
- **Stochastic Methods:**
  Incorporate randomness, can lead to different results on each run.

Optimization

- **Local vs. Global Optimum:**
  - **Local Optimum:** Best solution within a neighboring set of solutions.
  - **Global Optimum:** Best solution over the entire set of possible solutions.

- **Convex vs. Non-convex Problems:**
  - **Convex:** Any local optimum is a global optimum.
  - **Non-convex:** Multiple local optima exist.

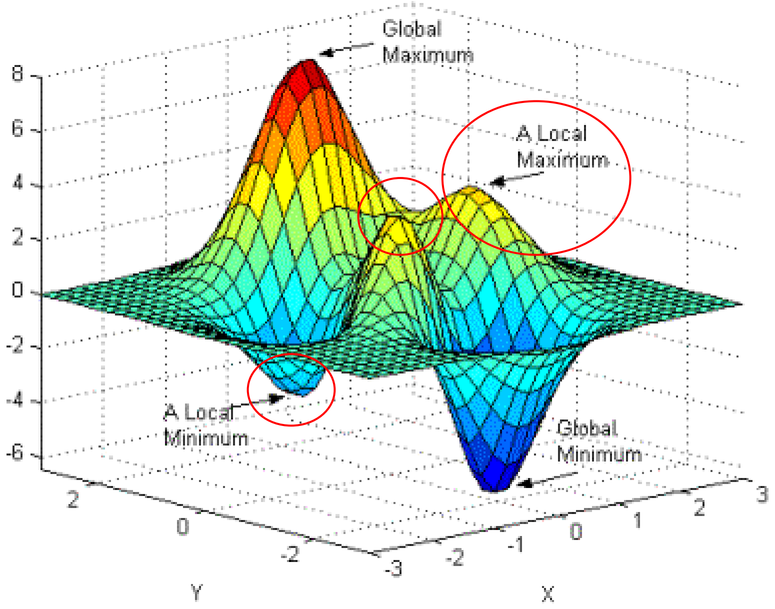
Optimization: Local vs. Global Optimum



Source: https://kharepratyush.medium.com/optimization-in-machine-learning-a-beginners-guide-f624d6f0764d

Local Optimum

- A local optimum (either a local minimum or a local maximum) is a point within a certain neighborhood of the feasible region where the objective function achieves its best value compared to other nearby points. However, it may not be the best value overall in the entire feasible region.



- **Local Minimum**: A point x^* is a local minimum if there exists some small region around x^* such that $f(x^*) \leq f(x)$ for all x **in that region**.

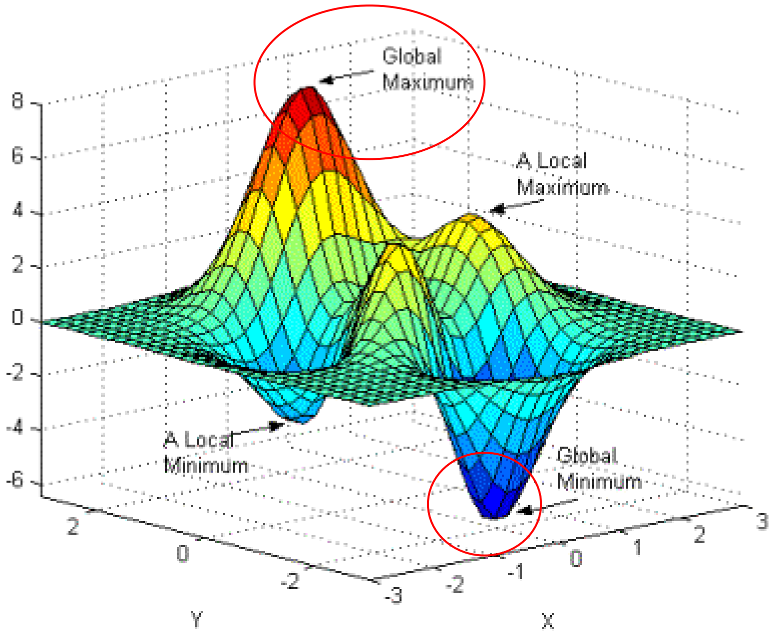
- **Local Maximum**: A point x^* is a local maximum if there exists some small region around x^* such that $f(x^*) \geq f(x)$ for all x **in that region**.

Global Optimum

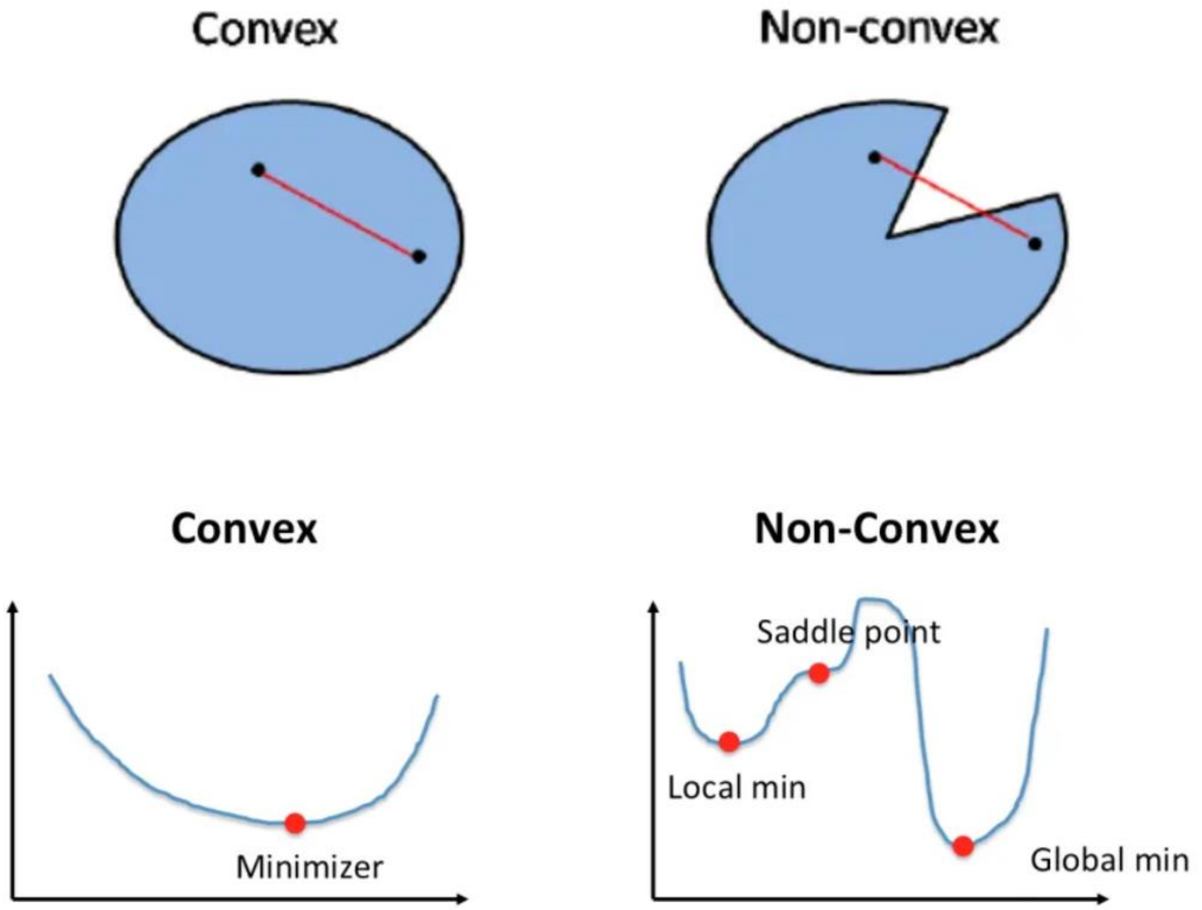
- A global optimum (either a global minimum or a local maximum) is a point where the objective function achieves the best possible value across the entire feasible region.

- **Global Minimum**: A point x^* is a global minimum if $f(x^*) \leq f(x)$ for all x **in the feasible region**.

- **Gobal Maximum**: A point x^* is a global maximum if $f(x^*) \geq f(x)$ for all x **in the feasible region**.



Optimization: Convex vs. Non-convex Problems



Source: https://ai.plainenglish.io/navigating-the-terrain-convex-vs-non-convex-functions-in-optimization-86812e9a1989

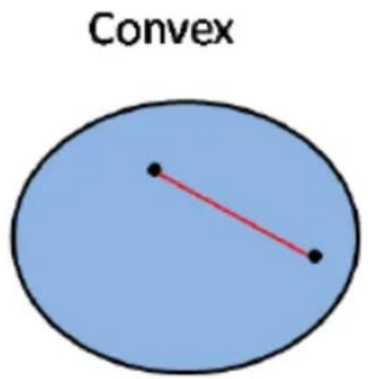
Optimization: Convex Problems

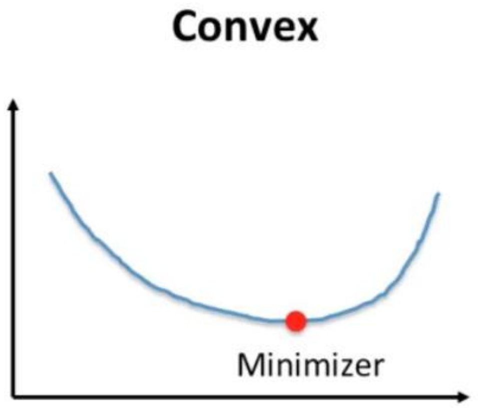
Definition:
A function is convex if, for any two points in its domain, the line segment connecting them lies above the graph of the function.

Characteristics:
- Single global minimum.
- No local minima.
- All saddle points are global minima.

Advantages:
- Simplicity in optimization.
- Guaranteed convergence to global minimum.

Challenges:
Limited representation power for complex problems.





Source: https://ai.plainenglish.io/navigating-the-terrain-convex-vs-non-convex-functions-in-optimization-86812e9a1989

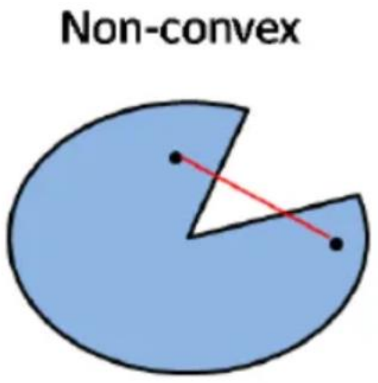
Optimization: Non-convex Problems

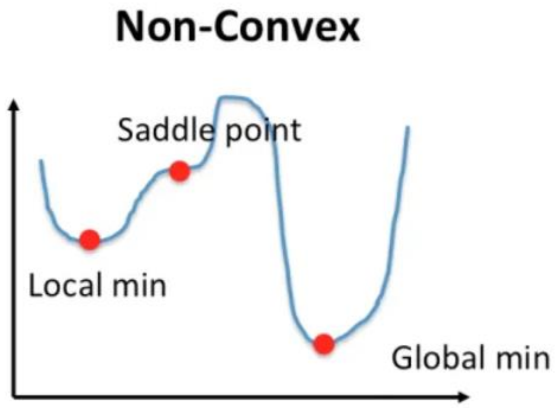
Definition:
A function is non-convex if it is not convex, meaning there exist points where the line segment connecting them can dip below the function's graph.

Characteristics:
- Multiple local minima.
- Presence of saddle points.
- Complexity varies widely.

Advantages:
- Ability to represent complex relationships.

Challenges:
- Convergence to global minimum not guaranteed.
- Vulnerable to getting stuck in local minima.





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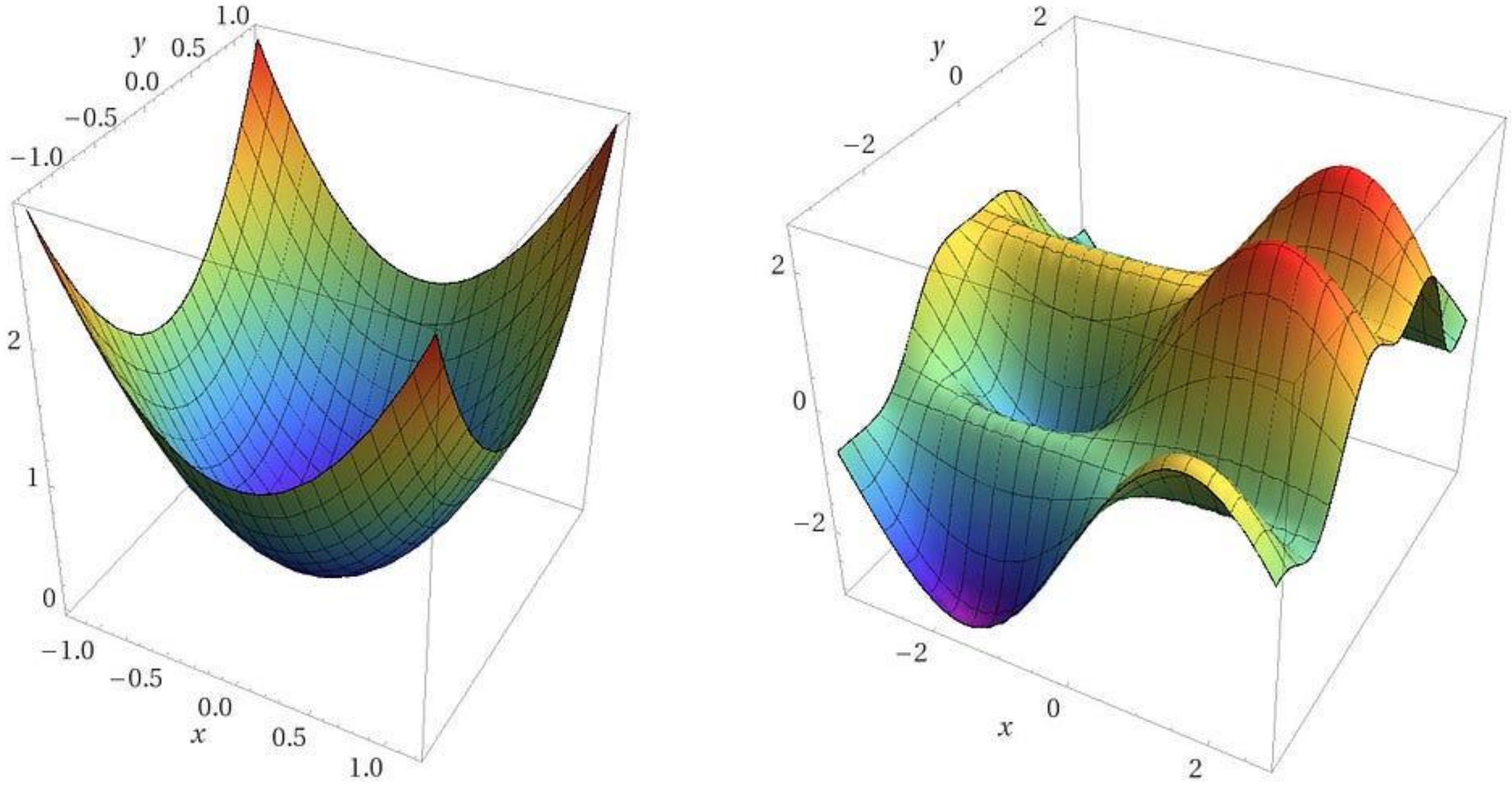
Optimization: Convex vs. Non-convex Problems



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Optimization methods

- Numerical Optimization
- Heuristic Methods
- Meta-Heuristic Methods

Optimization methods

- **Numerical Optimization**
- Heuristic Methods
- Meta-Heuristic Methods

Numerical Optimization

- Rely on mathematical formulas and deterministic procedures to find optimal solutions.
- They are generally used when the problem is well-defined with an objective function that is continuous and differentiable.
- These methods aim to provide precise solutions and often require good mathematical properties (e.g., convexity) of the objective function.

Numerical Optimization Examples

- **Gradient-Based Methods:**
  - Gradient Descent, Newton's Method, Conjugate Gradient Method.
- **Linear Programming:**
  - Simplex Method, Interior-Point Methods.
- **Quadratic Programming:**
  - Active Set Method.
- **Dynamic Programming:**
  - Bellman’s Principle of Optimality.

Optimization methods

- Numerical Optimization
- **Heuristic Methods**
- Meta-Heuristic Methods

Heuristic Methods

- Heuristics are rule-of-thumb strategies designed to find good enough solutions quickly, often for problems that are too complex or time-consuming for exact methods.

- They do not guarantee an optimal solution but can often provide satisfactory solutions in a reasonable amount of time.

- Heuristics are often problem-specific and are designed to exploit the structure of the problem to find good solutions efficiently.

Heuristic Methods
Examples

- **Greedy Algorithms**:
  - Huffman Coding, Kruskal's Algorithm for Minimum Spanning Tree.

- **Local Search Methods**:
  - Hill Climbing, Simulated Annealing (when not considered a meta-heuristic).

Meta-Heuristic Methods

- Meta-heuristics are higher-level strategies that guide underlying heuristics to explore the search space more effectively.
- They are often used for complex, non-linear, and combinatorial problems where traditional methods may struggle.
- Meta-heuristics are often problem-agnostic and can be applied to a wide range of optimization problems.
- They are designed to avoid getting trapped in local optima and explore the search space more globally.

Meta-Heuristic Methods Examples

- **Genetic Algorithms**: Evolutionary processes inspired by natural selection.
- **Particle Swarm Optimization:** Simulates social behavior of birds or fish.
- **Ant Colony Optimization:** Mimics the foraging behavior of ants.
- **Simulated Annealing:** Combines probabilistic moves with gradual cooling of the system.
- **Tabu Search:** Uses memory structures to avoid cycles and escape local optima.

Numerical Optimization Examples

- **Gradient-Based Methods:**
  - Gradient Descent, Newton's Method, Conjugate Gradient Method.
- **Linear Programming:**
  - Simplex Method, Interior-Point Methods.
- **Quadratic Programming:**
  - Active Set Method.
- **Dynamic Programming:**
  - Bellman’s Principle of Optimality.

Decision variables

$$\begin{matrix}\textbf{Min}\\\textbf{Max}\end{matrix}\quad Z = c_1x_1 + c_2x_2 + c_3x_3 + \ldots + c_nx_n = \sum_{i=1}^{n} c_ix_i$$

Subject to:

Constraints

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n \leq b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n \leq b_2 \\ \ldots \\ a_{m1}x_1 + a_{m2}x_2 + a_{m3}x_3 + \ldots + a_{mn}x_n \leq b_m \\ x_1 \geq 0, x_2 \geq 0, x_3 \geq 0, \ldots, x_n \geq 0 \end{cases}$$

Example

$$\boldsymbol{Max}\, Z = f(x, y) = 3x + 2y$$

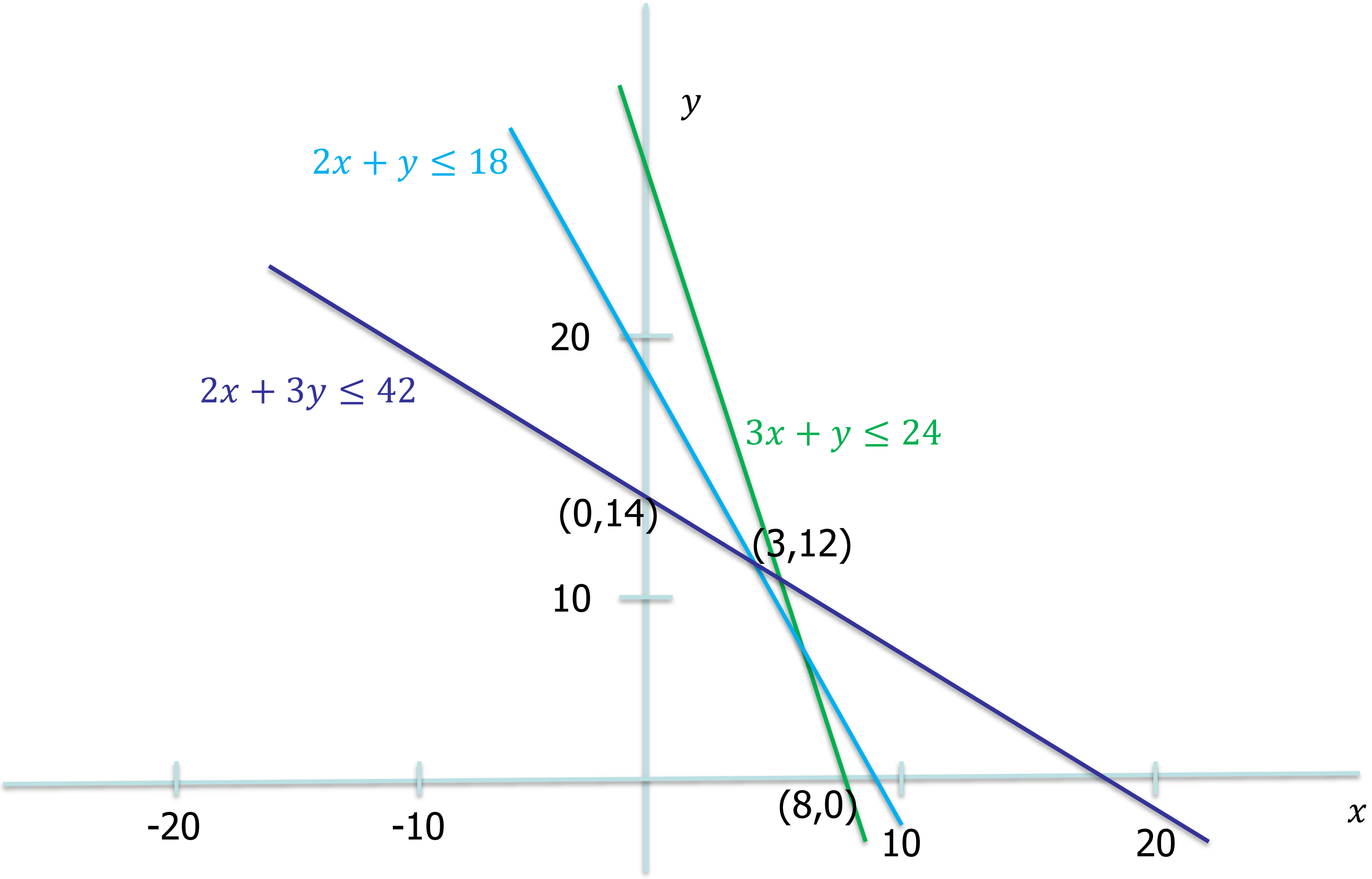
Constraints:

$$2x + 3y \leq 42$$

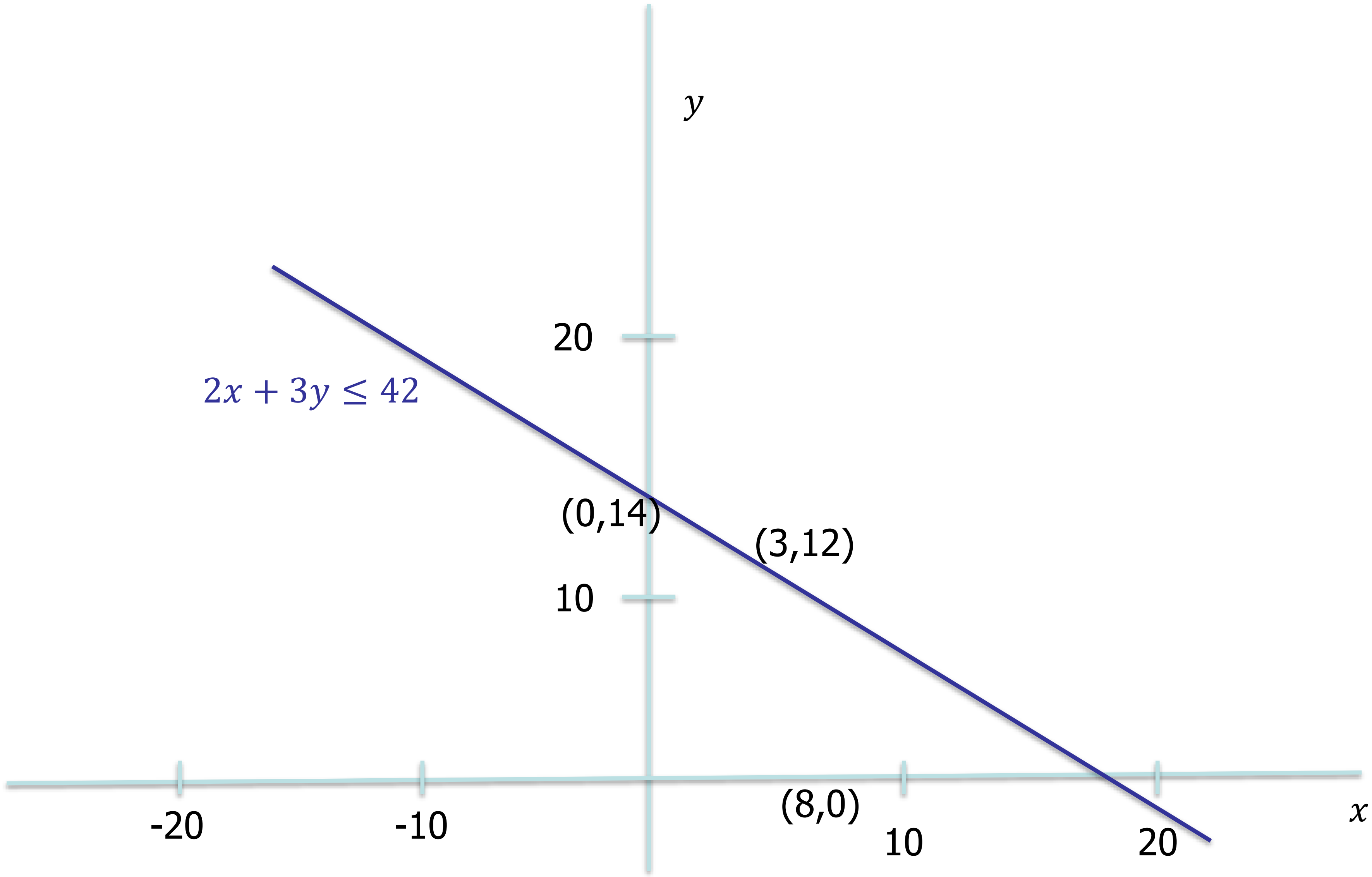
$$2x + y \leq 18$$

$$3x + y \leq 24$$

$$x > 0, y > 0$$

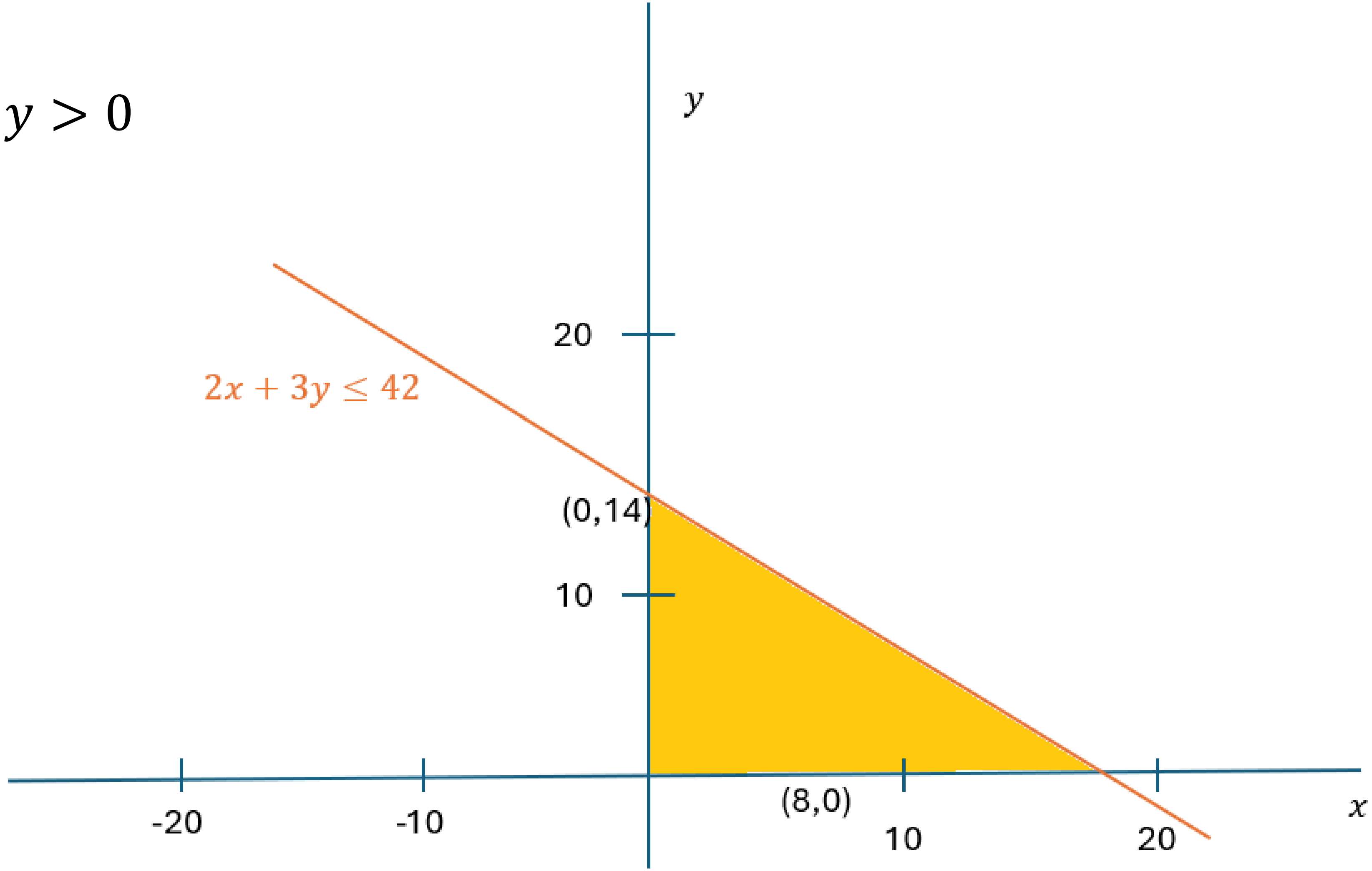


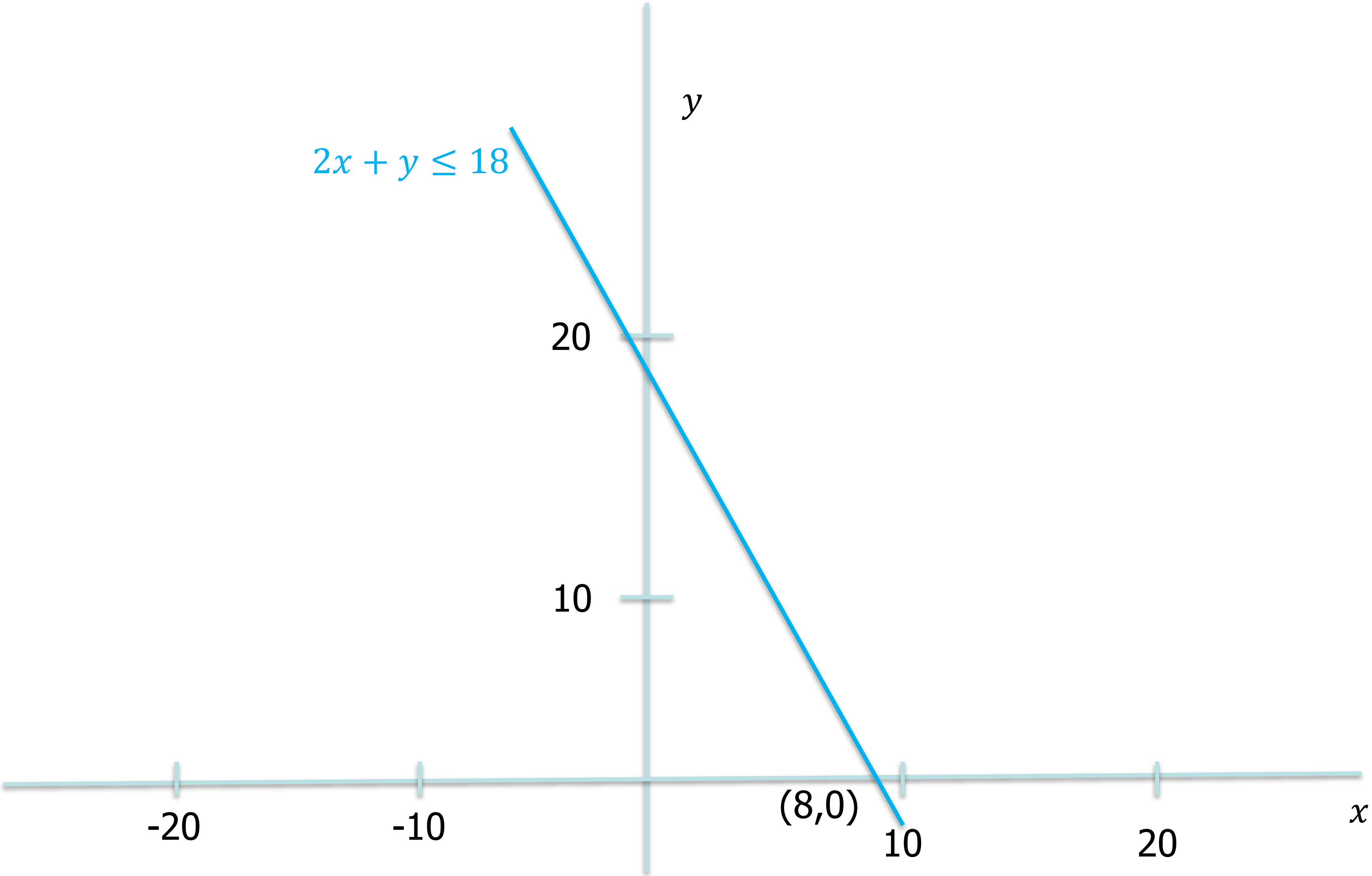
Source: https://www.shiksha.com/online-courses/articles/linear-programming-problem/



y
20
$2x + 3y \leq 42$
(0,14)
(3,12)
10
-20
-10
(8,0)
10
20
x

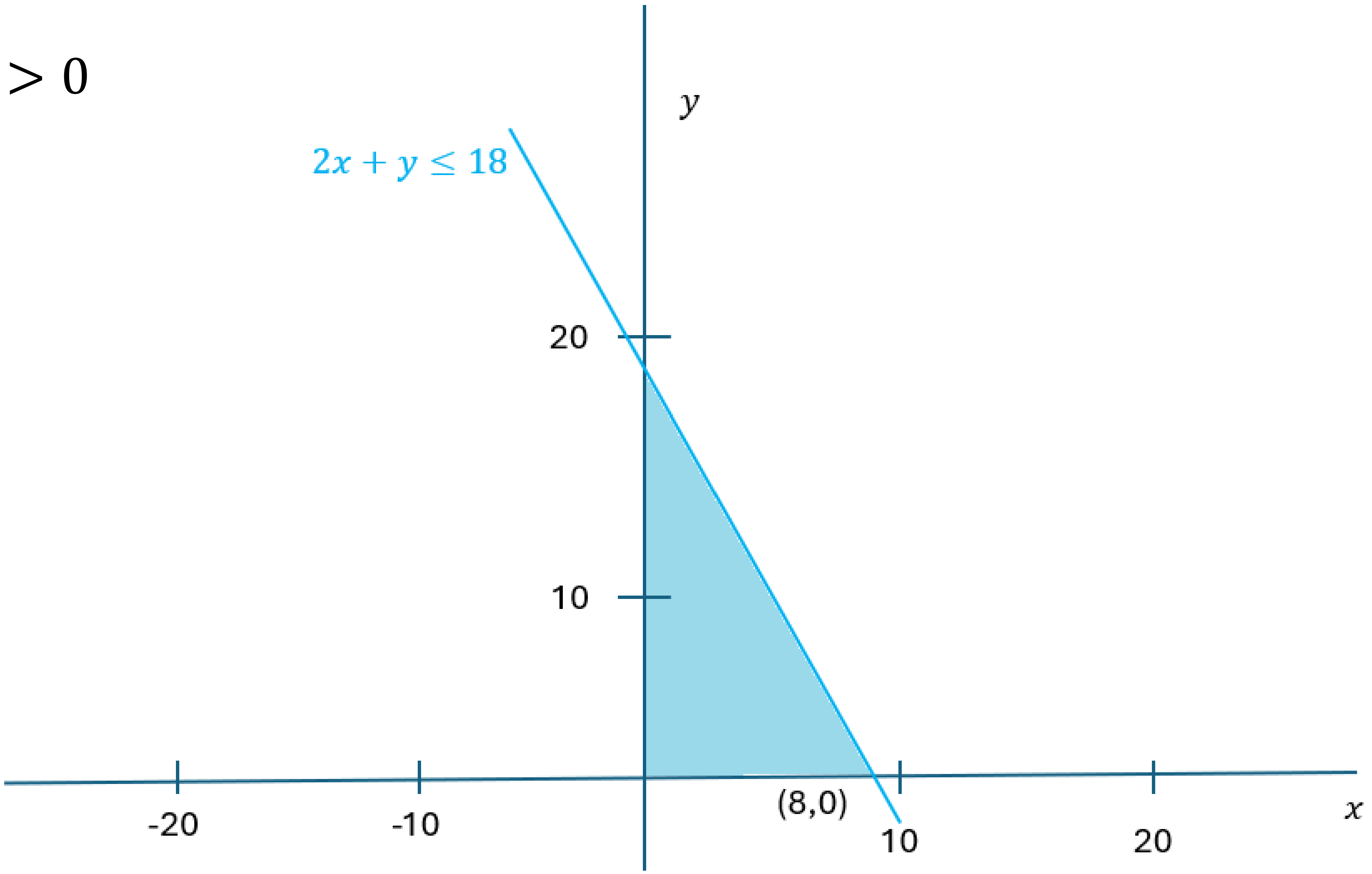
$x > 0, y > 0$

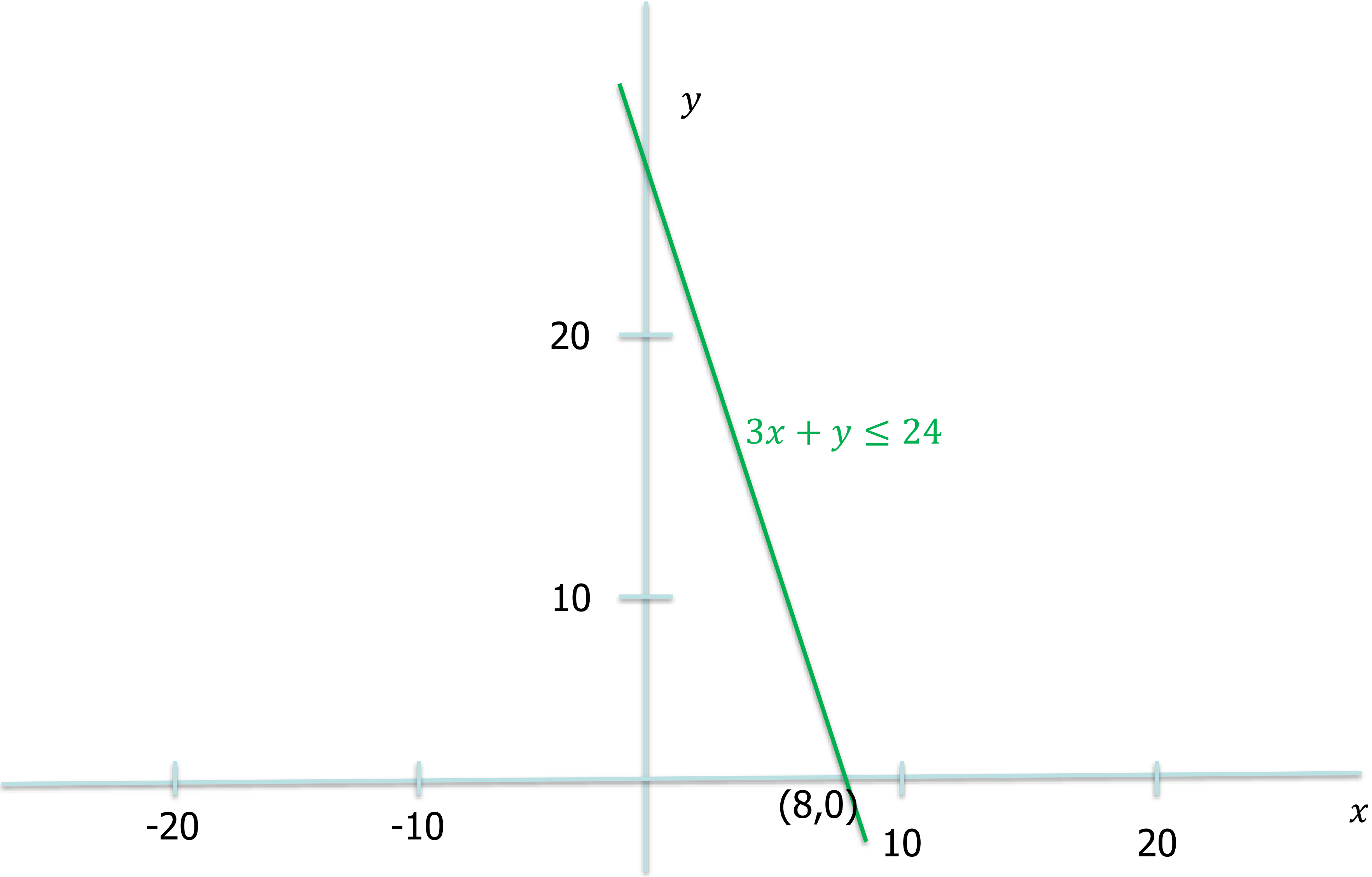




y
$2x + y \leq 18$
20
10
-20
-10
(8,0)
10
20
x

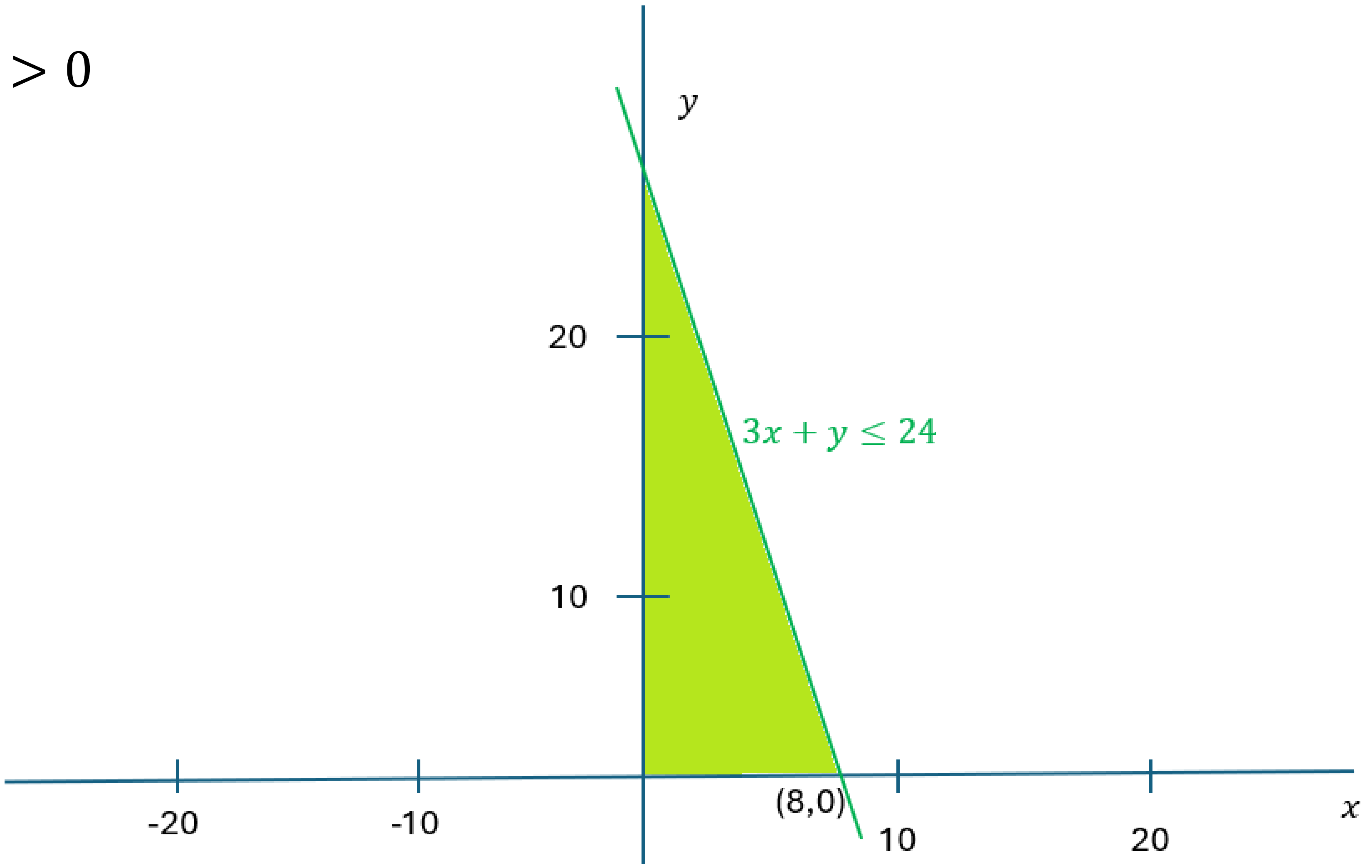
$x > 0, y > 0$

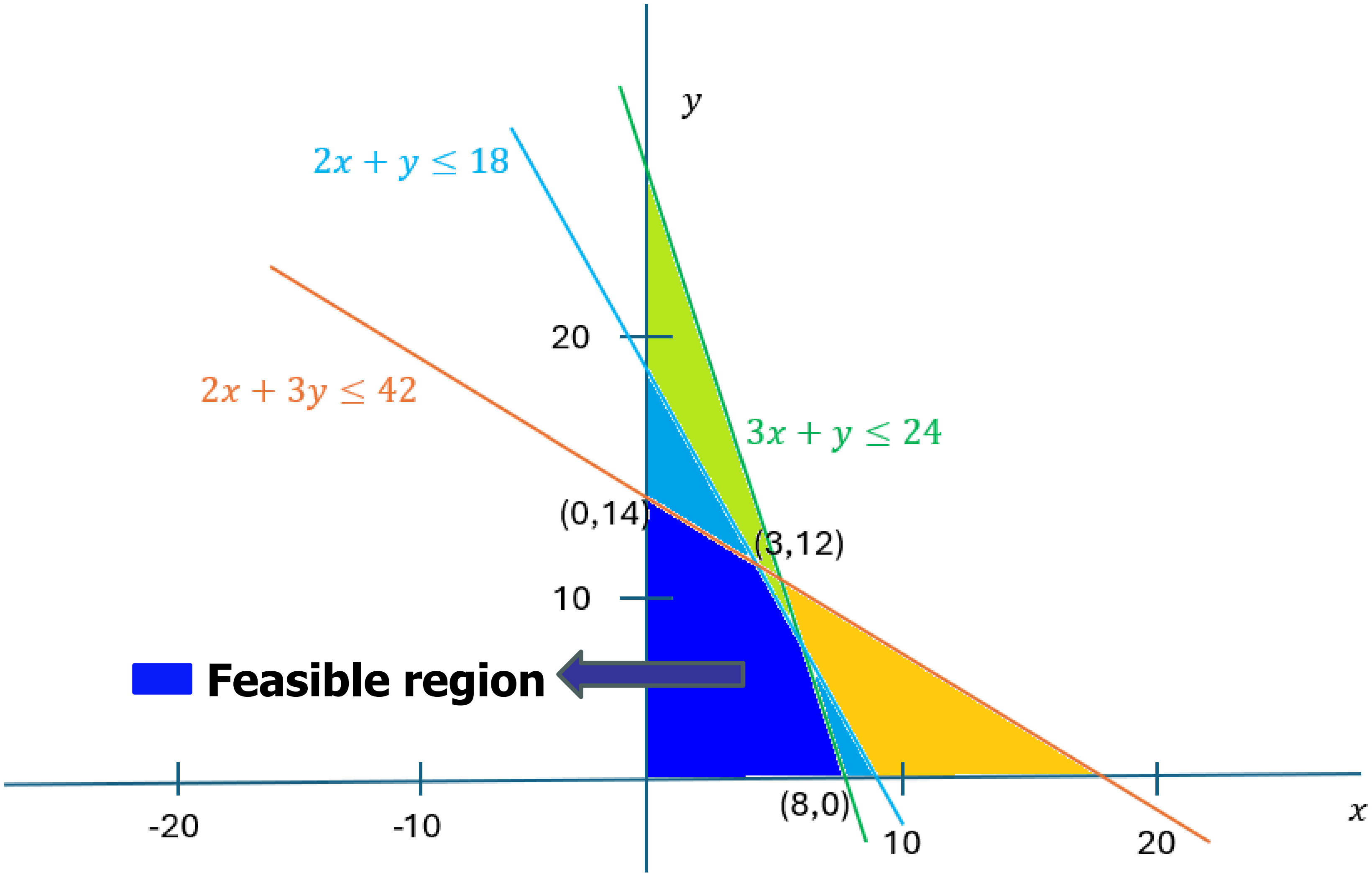




y
20
$3x + y \leq 24$
10
(8,0)
-20
-10
10
20
x

$x > 0, y > 0$





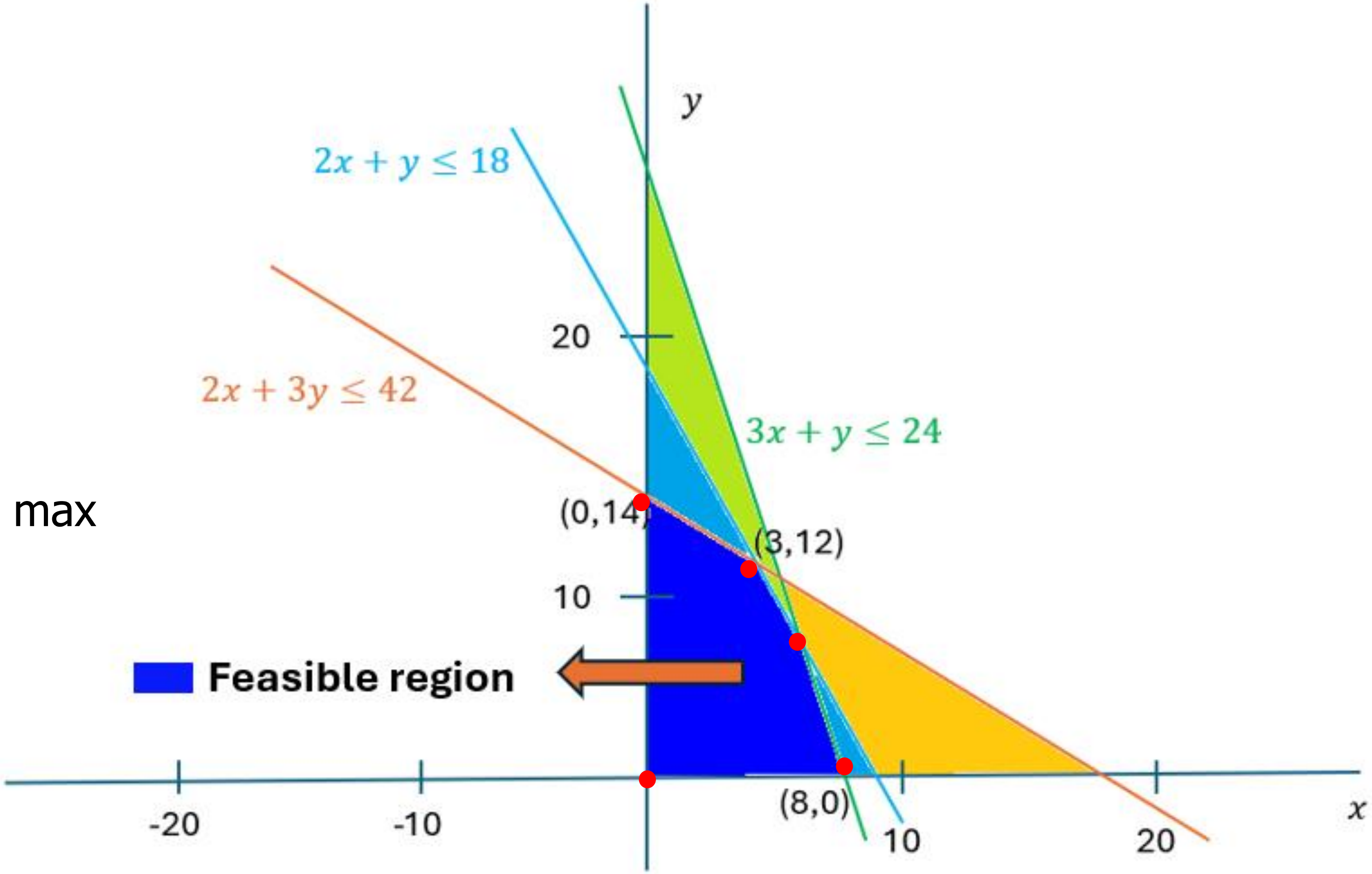
y
$2x + y \leq 18$
$2x + 3y \leq 42$
$3x + y \leq 24$
20
10
(0,14)
(3,12)
(8,0)
Feasible region
-20
-10
10
20
x

finding the value of the objective function at the corner points of the feasible region:

Corner Point	*f(x,y) = 3x+2y*
(0, 0)	0
(8, 0)	24
(6, 6)	30
(3, 12)	33
(0, 14)	28

max

$$\boldsymbol{Max}\, Z = f(x,y) = 3x + 2y$$



Spatial Optimization
Introduction

Source: Tong, D., & Murray, A. T. (2012). Spatial optimization in geography. Annals of the Association of American Geographers, 102(6), 1290-1309.

- Spatial Optimization: process of finding the most efficient arrangement or allocation of spatial elements within a given area to achieve specific objectives, considering constraints and utilizing spatial data.

- Various applications, for instance in:
  - Transportation
  - Retail geography
  - Urban planning
  - Landuse modelling

Characterizing a spatial optimization problem

Consist of three components:

- Objective, decisions variables, and constraining conditions.

- The problem objective is often structured using one or multiple **objective functions**

- objectives, decision variables and constraints are combined in some way to reflect the spatial problems of interest in either implicit or explicit terms, solved by exact or approximate techniques.

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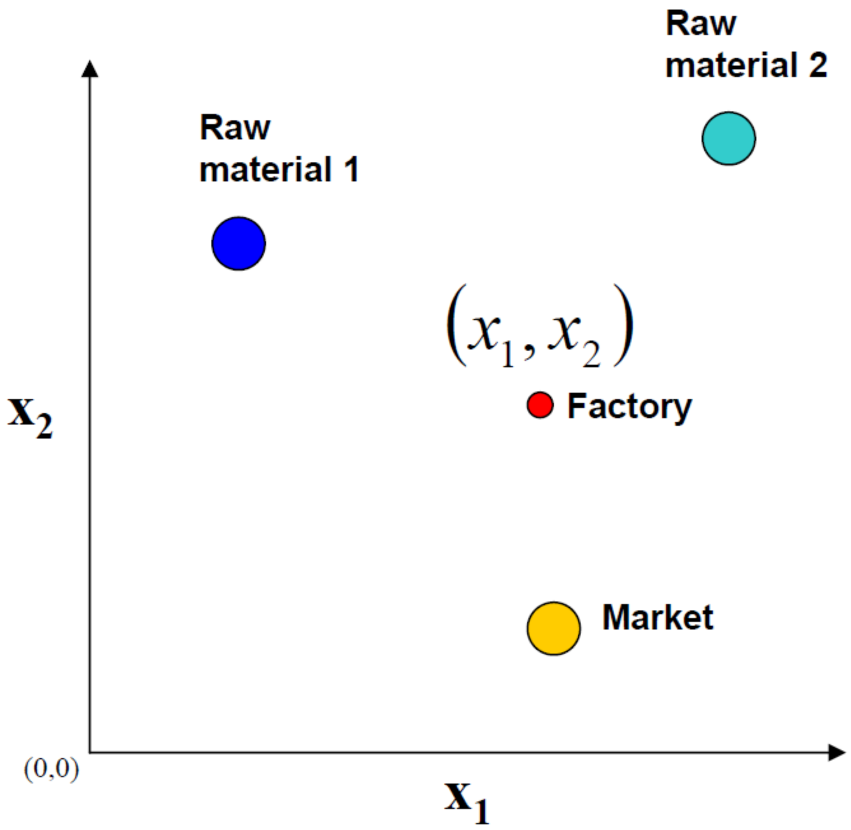
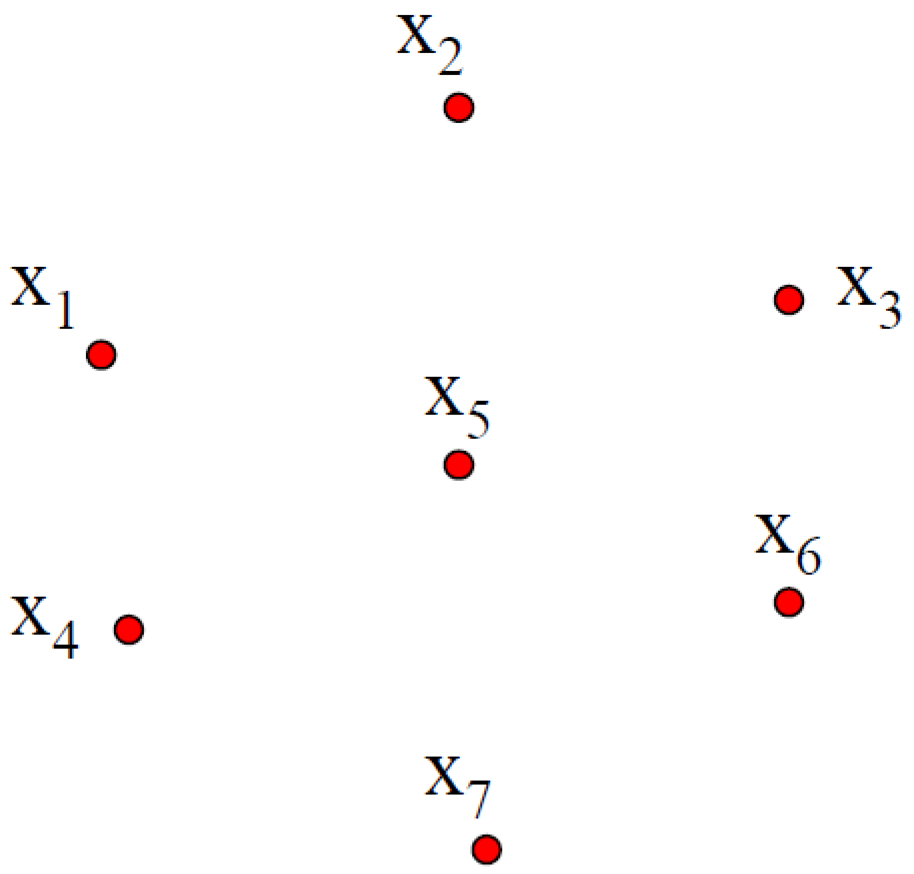
Spatial decision variables (continuous)

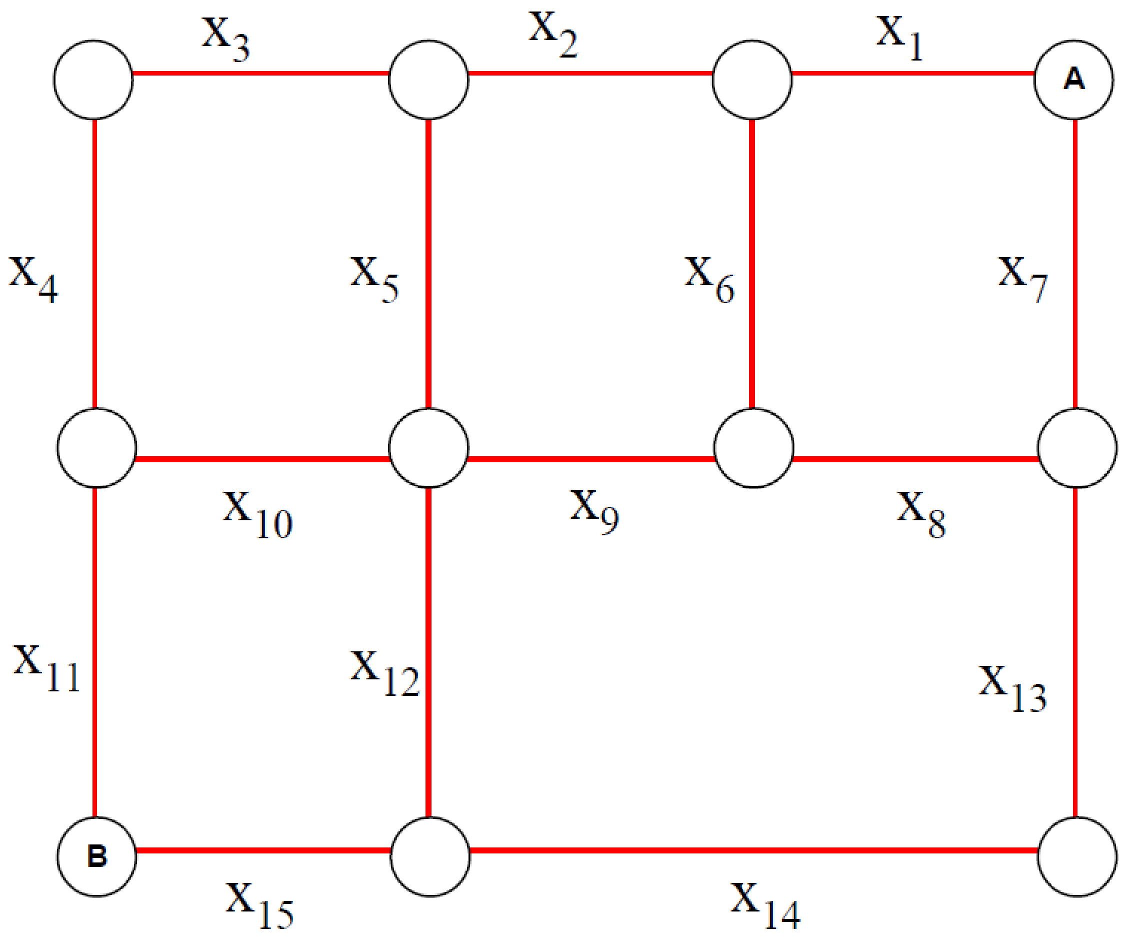


infinite number of potential locations

Spatial decision variables (discrete)



Spatial decision variables (discrete)



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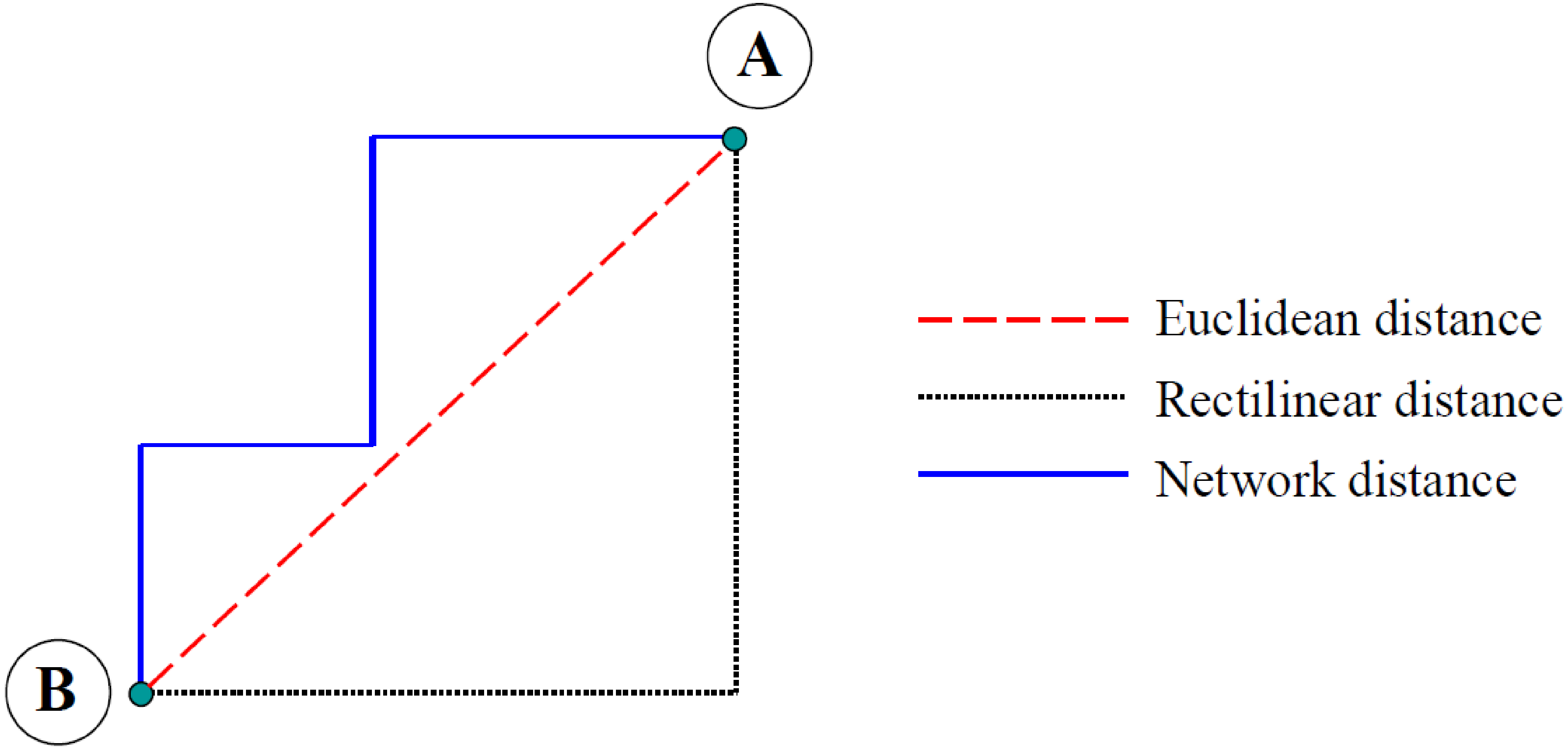
Characterizing a spatial optimization problem
Spatial relationships in functions/constraints

- Distance
- Adjacency
- Connectivity
- Containment
- Intersection
- Shape
- Districts
- Pattern

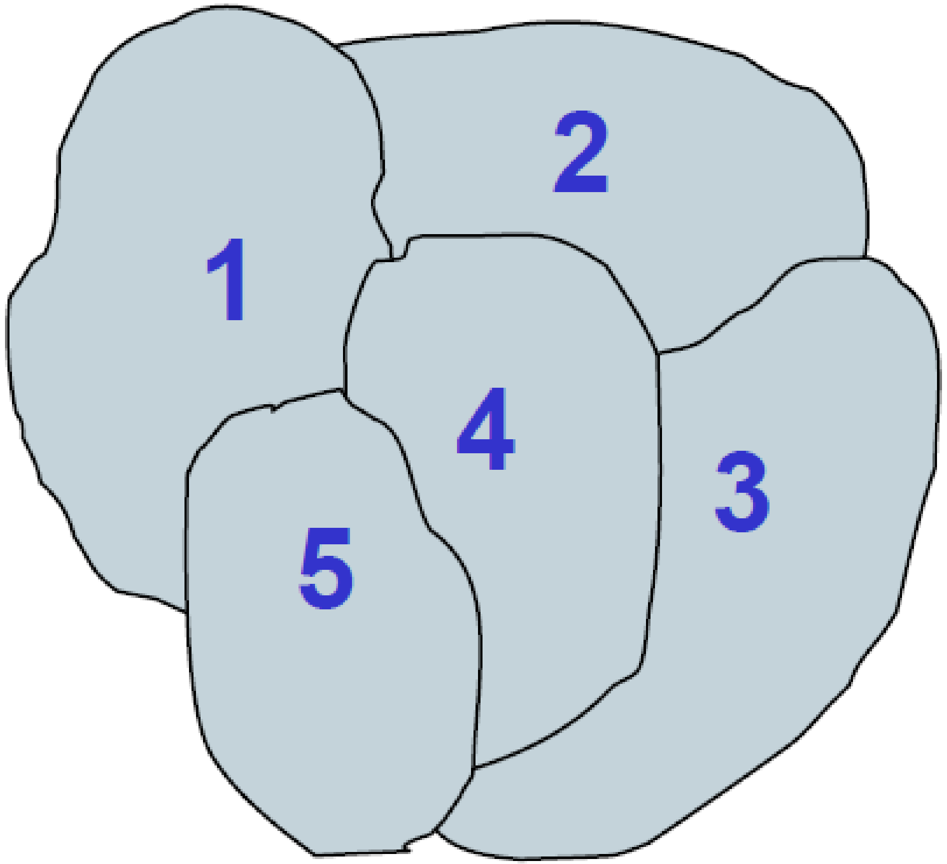
Distance

- Proximity between places, either in terms of physical distance or travel time



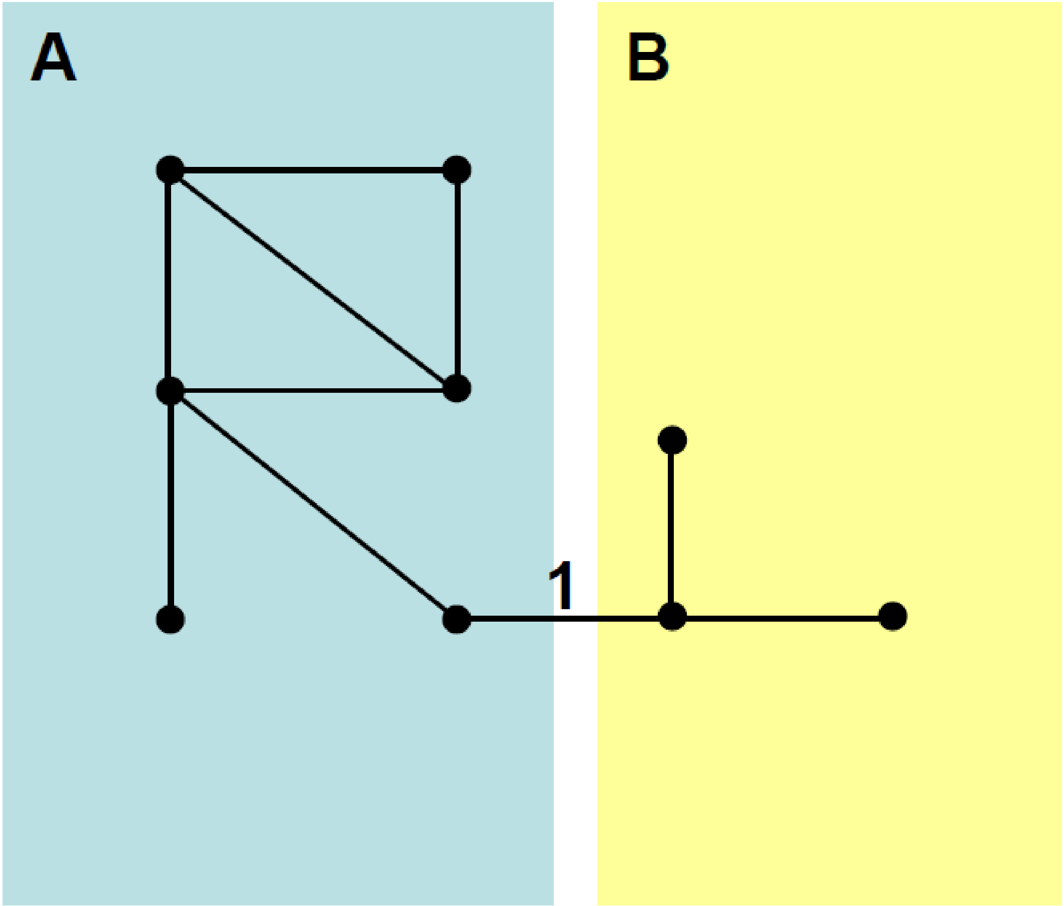
Adjacency of spatial units

when two polygons share a common edge or boundary



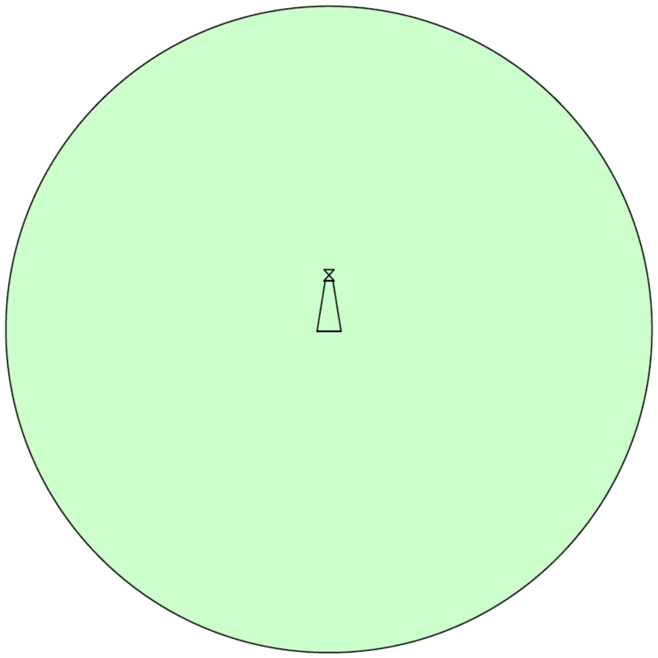
Connectivity

- The ability to get from one location to another or moving unimpeded from one location to Another
- Connectivity typically arises in a network, comprised of nodes and incident arcs, where one is interested in whether a path exists along arcs in the network between a given set of nodes (or locations)



Spatial containment

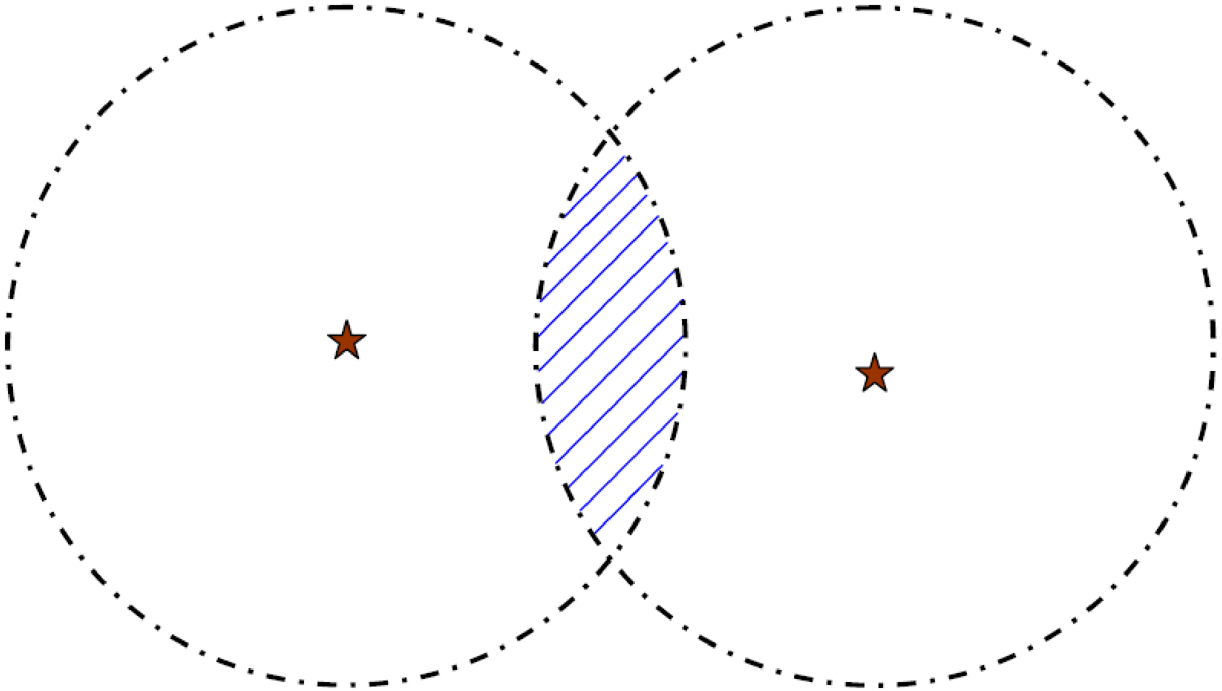
the condition where one object is completely within the other object is the containment relationship



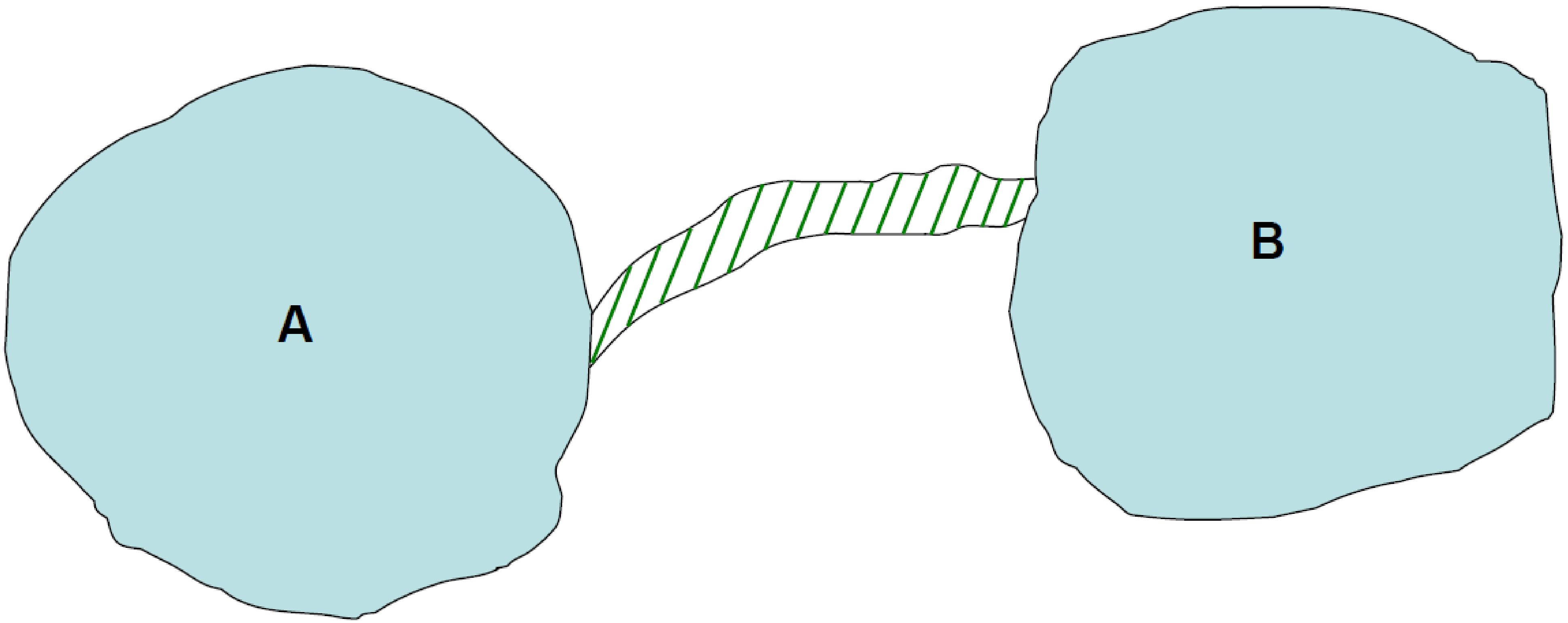
coverage of a warning siren

Intersection of spatial objects

a spatial location(s) where two objects simultaneously exist.



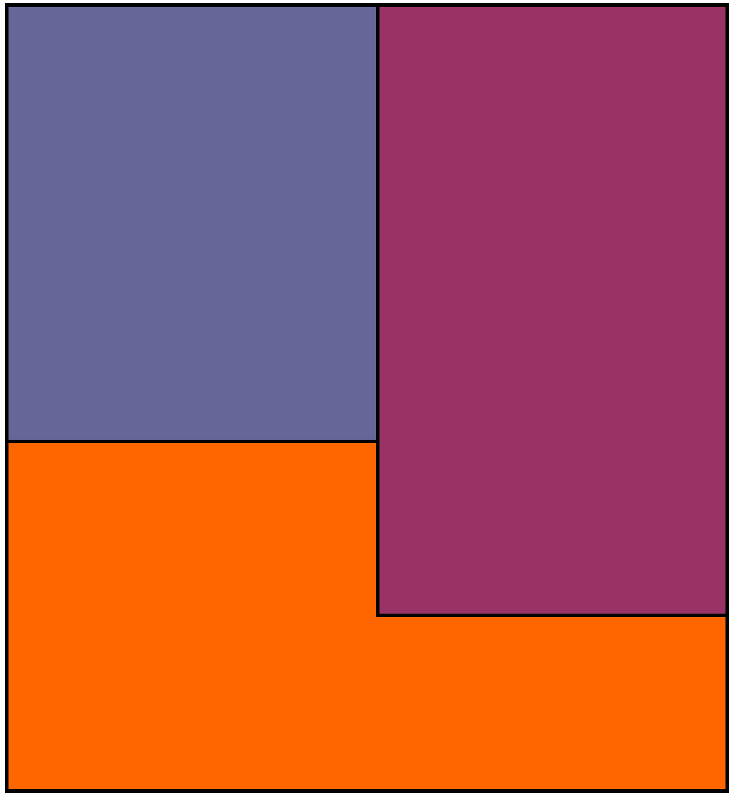
Shape



Elongated corridor

Districting

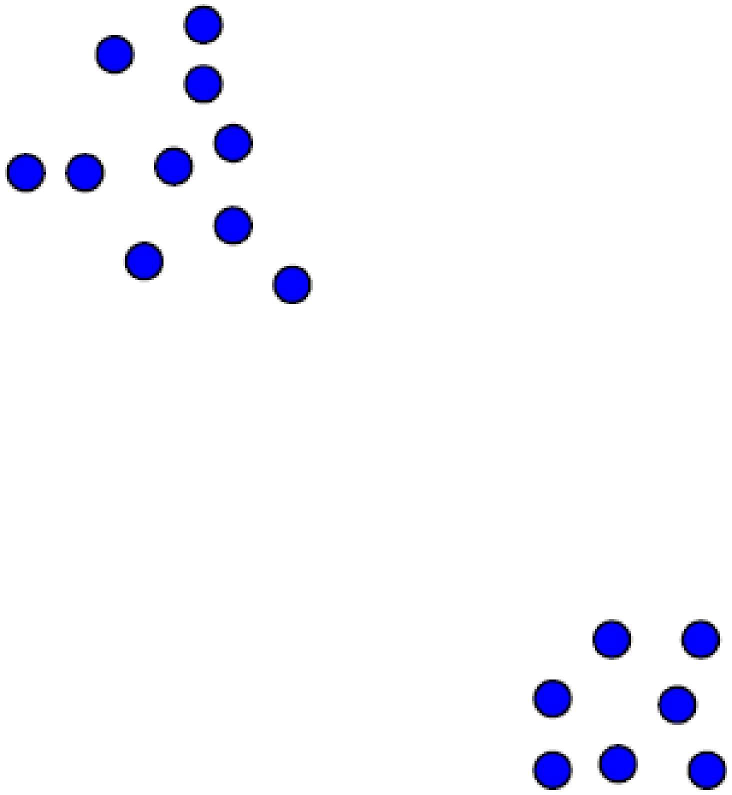
partitioning of space into a finite number of sub-regions



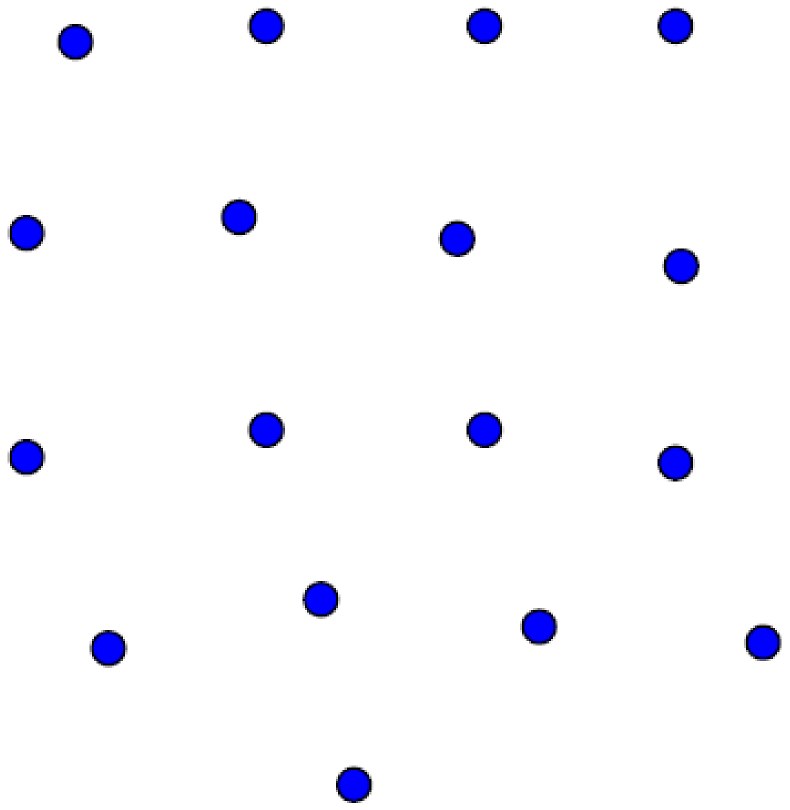
Pattern
Clustered

Pattern: A description of a distribution of spatial objects

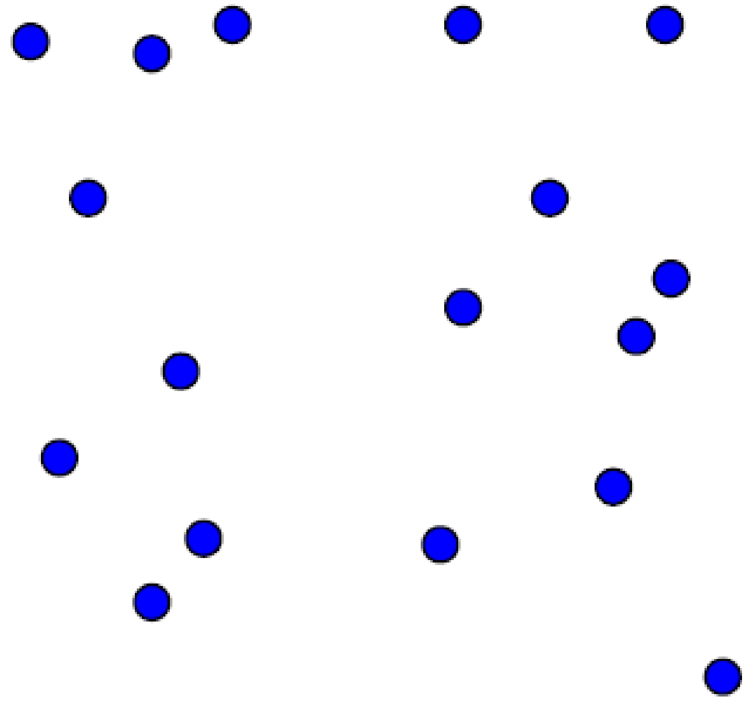
pattern reflects a property of how objects are organized across space, and in many cases is conceived of in terms of being **random**, **clustered** or **dispersed**.



Pattern
Dispersed



Pattern
Random



Solving spatial optimization problems

- **Exact methods**
- **(meta)Heuristics**

Exact methods

- The best possible, or optimal, solution is guaranteed to be identified
- Approaches: derivative based techniques, enumeration, linear programming, integer programming
- problem specific methods: the Hungarian algorithm, transportation simplex, out-of-kilter algorithm, Dijkstra's algorithm

(meta)Heuristics

- based on rules-of-thumb, strategies or ad hoc procedures to solve an optimization problem
- to explore the solution space in some way, identifying feasible solutions from which a best can be found.
- According to the specific search rule of the heuristic, a new solution(s) is identified and the current solution(s) is updated
- Many heuristics have been used for solving spatial optimization problems, including interchange, greedy, simulated annealing, tabu search, and population-based heuristics, such as genetic algorithms and ant colony heuristics.

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Multiple objectives and tradeoffs

- Spatial problems are complex, as they reflect real world issues to be addressed
- different aspects should be considered for most problems of interest, including social, environmental, economical, political, legal, etc.
- Given this, there is increasing recognition of multiple objectives that should be addressed
- For example, in land use planning, criteria for land acquisition can include proximity to transportation facilities, costs, environment impact, etc.
- As a result, problem solutions often reflect the tradeoffs between different objectives

Multiple objectives and tradeoffs

- Different objectives often conflict with each other and there rarely exists a solution that optimizes all the objectives simultaneously.
- Hence, a multi-objective optimization problem often has a set of optimal solutions, with each representing some tradeoff or compromise between objectives

Spatial Optimization in practice

Multiobjective linear programming method

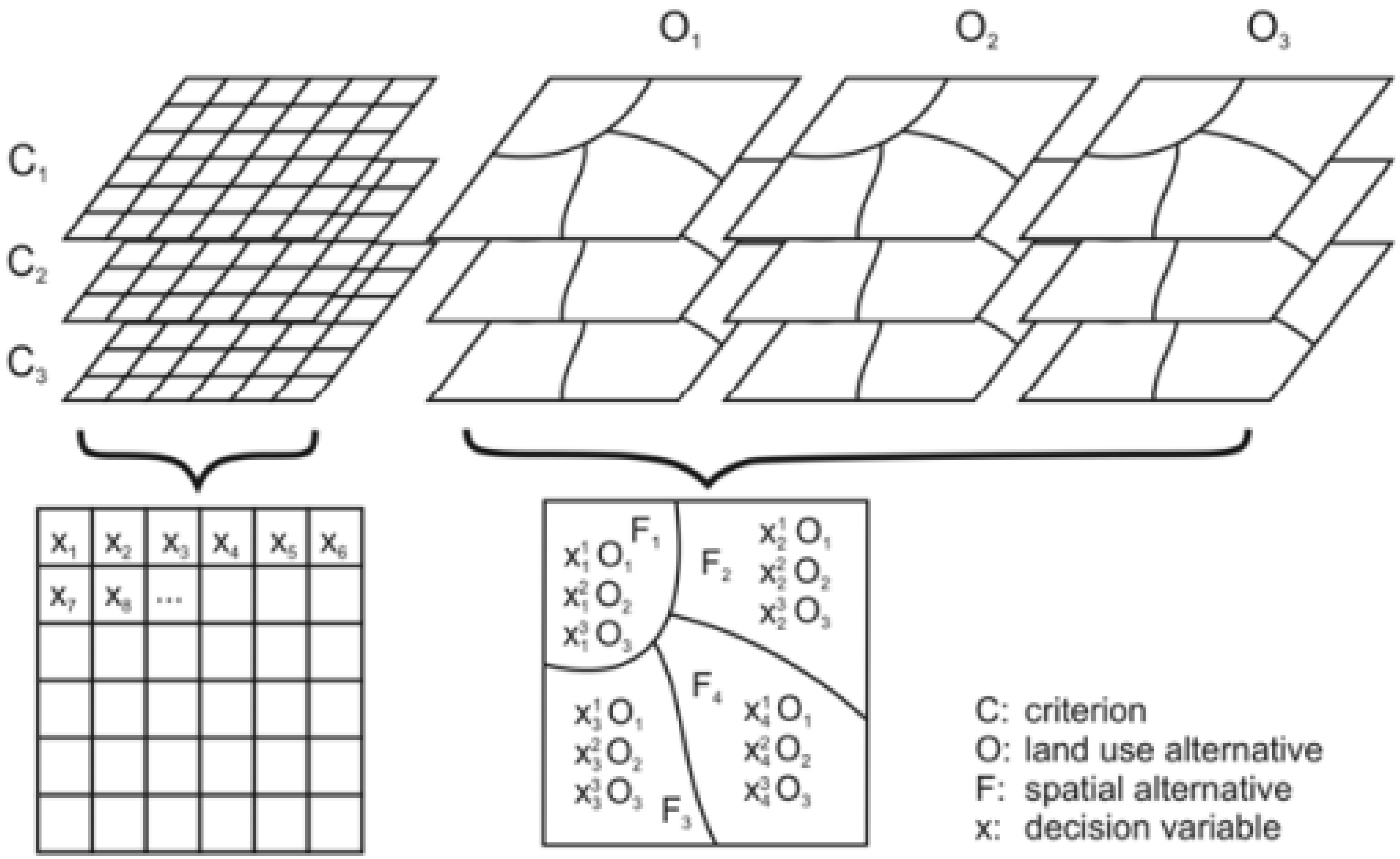
A GIS-based Module for the Multiobjective Optimization of Areal Resource Allocation

Alexander Herzig

Department of Geography, Division of Landscape Ecology and Geoinformation Sciences Christian-Albrechts-Universität zu Kiel

A GIS-based Module for the Multiobjective Optimization of Areal Resource Allocation

- Spatial decision support system LUMASS (Land Use Management Support System)
- Optimization of land use pattern with respect to ecological criteria and subject to given area shares of the individual land use alternatives



O1
O2
O3
C1
C2
C3
x1 x2 x3 x4 x5 x6
x7 x8 ...
F1
F2
F3
F4
C: criterion
O: land use alternative
F: spatial alternative
x: decision variable

Decision Problem

- How to allocate different land use alternatives O_r (e.g. arable land, pasture, wood, etc.) among the spatial alternatives F_i (i.e. polygons) with respect to the given criteria C_j and subject to given area shares of each land use O_r ?

- for example, criteria may be soil erosion and groundwater recharge. The overall objectives, in relation to the given criteria, may then be minimizing soil erosion and maximizing groundwater recharge.

Linear Programming

Criterion scores vector

Decision variables: The vector $\boldsymbol{x}$ holds the quantities of the given land use alternatives O_r in terms of the spatial alternatives F_i

Linear objective functions

$$max\ f_j(x) = z_j$$

$$
\left\{
\begin{array}{l}
max\ \boldsymbol{c}^1\boldsymbol{x} = z_1 \\
max\ \boldsymbol{c}^2\boldsymbol{x} = z_2 \\
\quad \dots \\
max\ \boldsymbol{c}^n\boldsymbol{x} = z_n
\end{array}
\right.
$$

As result of the decision problem, a point $x \in B$ is in demand, so that $z_j \in R$ is maximal for all j

matrix of coefficients

$$x \in B = \{x \in R^u \,|\, \boxed{\boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{b}}, \boxed{\boldsymbol{x} \geq 0}, \boldsymbol{b} \in R^q\}$$

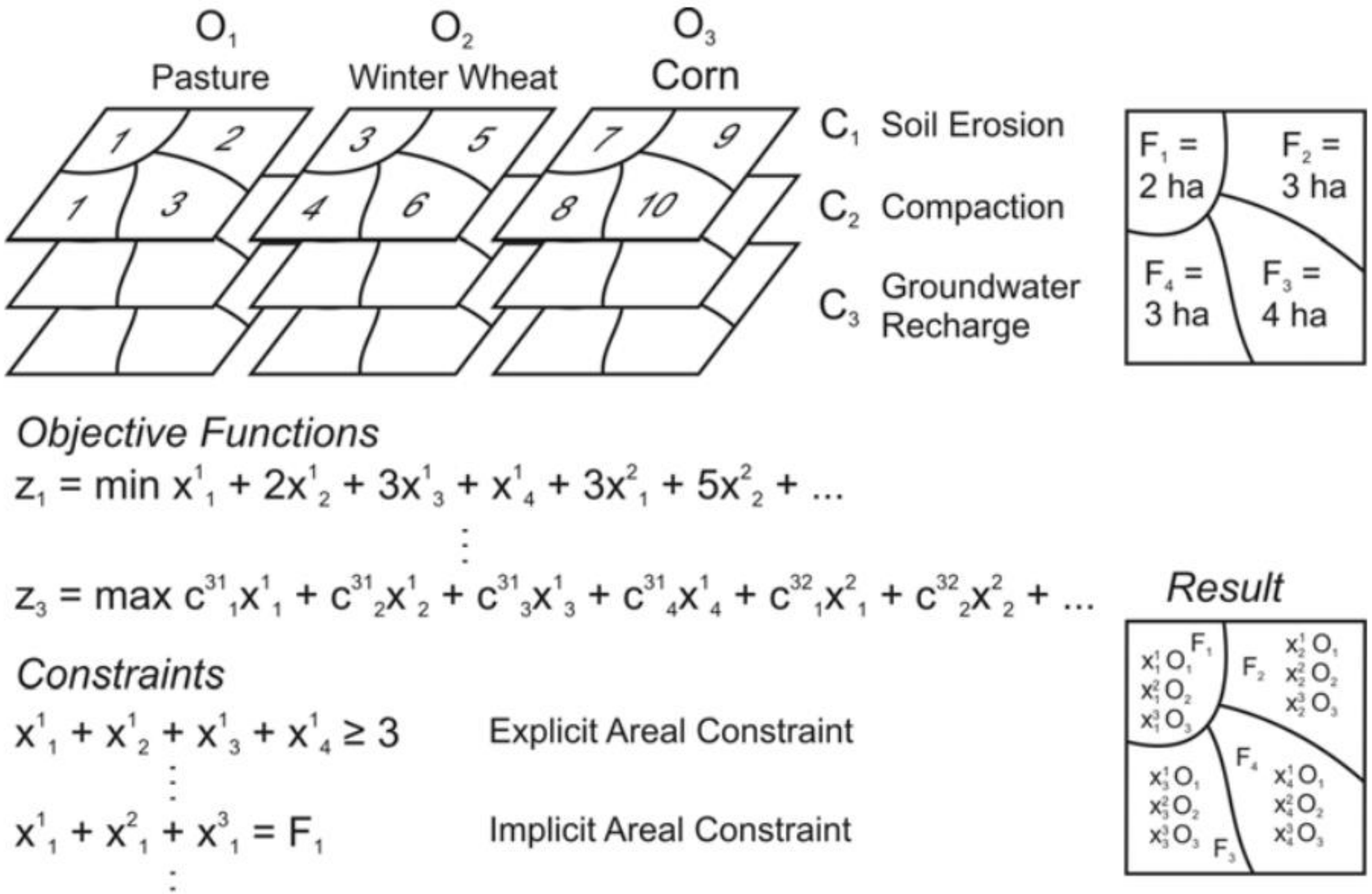
restricts the set of feasible solutions B

non-negative constraint

Here: ensures that no negative quantity of a land use alternative is allocated to a parcel

Problem

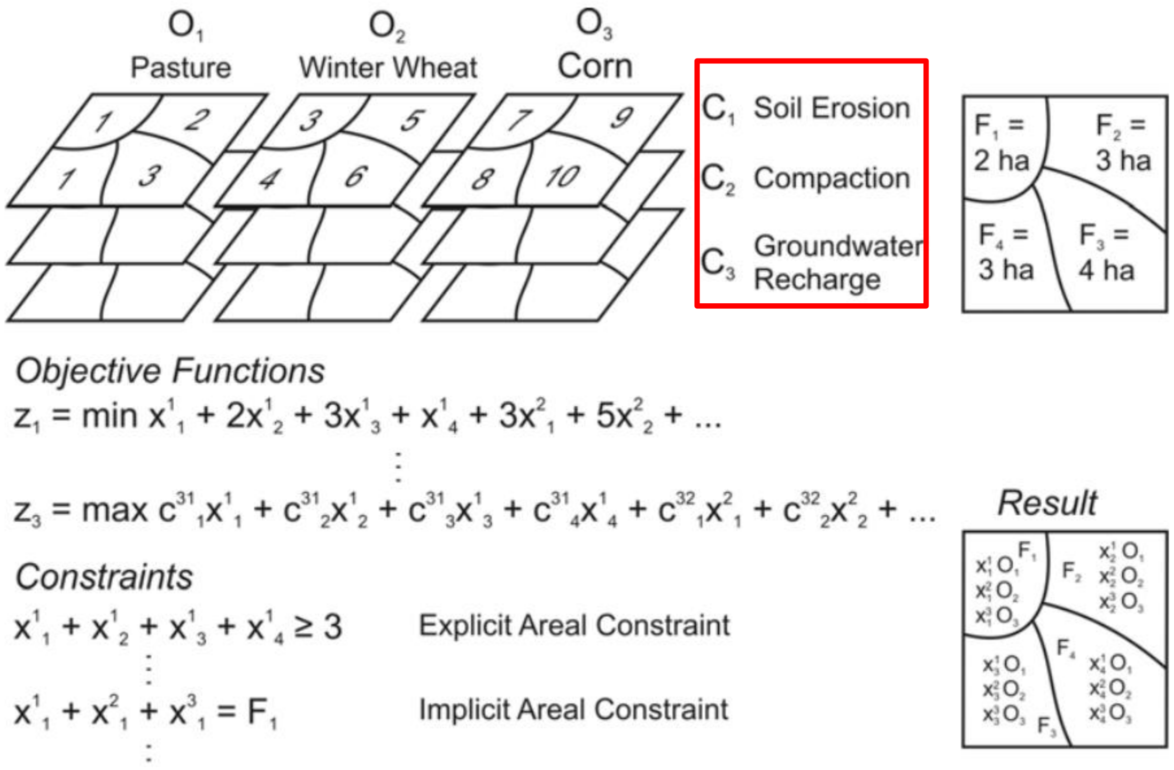
- Specifying the general frame of the allocation problem



Example of a typical optimization problem

Criteria

- Assignment of the modelled criterion scores to the land use alternatives



$$
\begin{array}{cccc}
 & \text{Pasture} & \text{Winter Wheat} & \text{Corn} \\
\text{Soil Erosion} & & & \\
\text{Compaction} & & \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} & \\
\text{Groundwater recharge} & & &
\end{array}
$$

Objectives

- Specification of the objective function; selection of the decision rule
- Solving multiobjective linear optimization problems is often done by transferring the multiobjective optimization problem into a single objective optimization problem.
- Well-known and efficient algorithms (e.g. simplex) may then be used to solve the problem

Objectives

- A simple method to scalarize the multiobjective linear problem is "Weighted Sum":

the given n objective functions are weighted by *j* and finally added to a single objective function :

$$\max \sum_{j=1}^{n} \lambda_j f_j(\mathbf{x})$$

with:

$$x \in B, \lambda \in R^n, \lambda_j > 0, \sum_{j=1}^{n} \lambda_j = 1$$

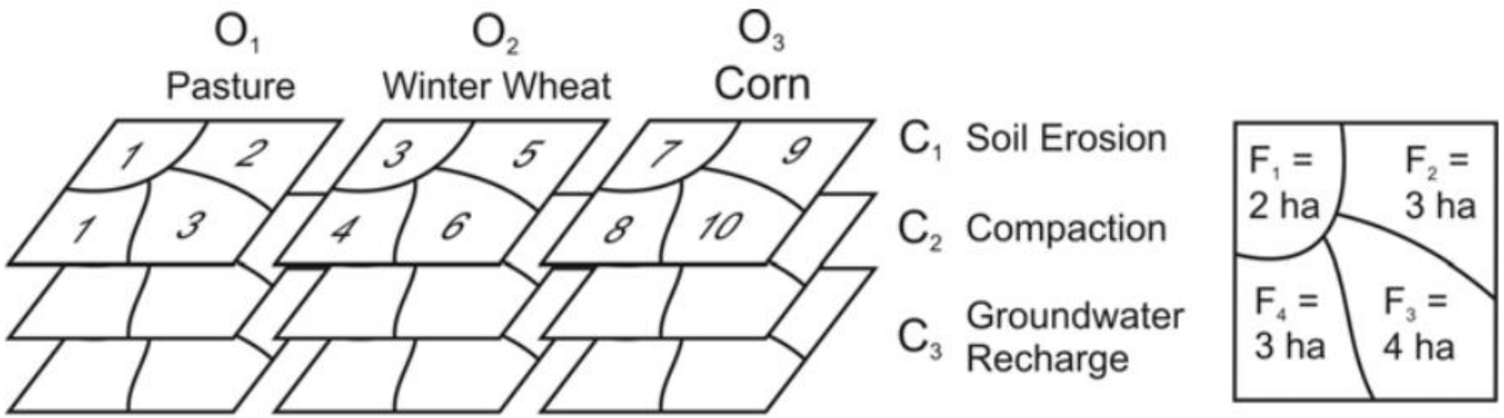
weights *j* are used to model the stakeholder's preferences in terms of the objective functions.

Constraints

- Specification of area shares in terms of the land use alternatives;
- specification of the objective constraints

- Mathematically “Constraints” serve to define the matrix **A** and the vector **b** of coefficients given by the inequality $\mathbf{Ax} \leq \mathbf{b}$, restricting the set of feasible solutions.

Constraints



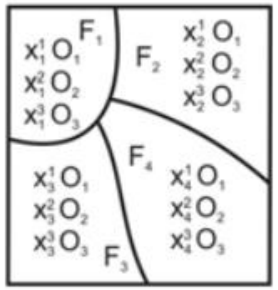
Objective Functions

$$z_1 = \min x^1_1 + 2x^1_2 + 3x^1_3 + x^1_4 + 3x^2_1 + 5x^2_2 + \ldots$$

$$\vdots$$

$$z_3 = \max c^{31}_1 x^1_1 + c^{31}_2 x^1_2 + c^{31}_3 x^1_3 + c^{31}_4 x^1_4 + c^{32}_1 x^2_1 + c^{32}_2 x^2_2 + \ldots$$

Result



Constraints

$x^1_1 + x^1_2 + x^1_3 + x^1_4 \geq 3$ Explicit Areal Constraint

$\vdots$

$x^1_1 + x^2_1 + x^3_1 = F_1$ Implicit Areal Constraint

$\vdots$

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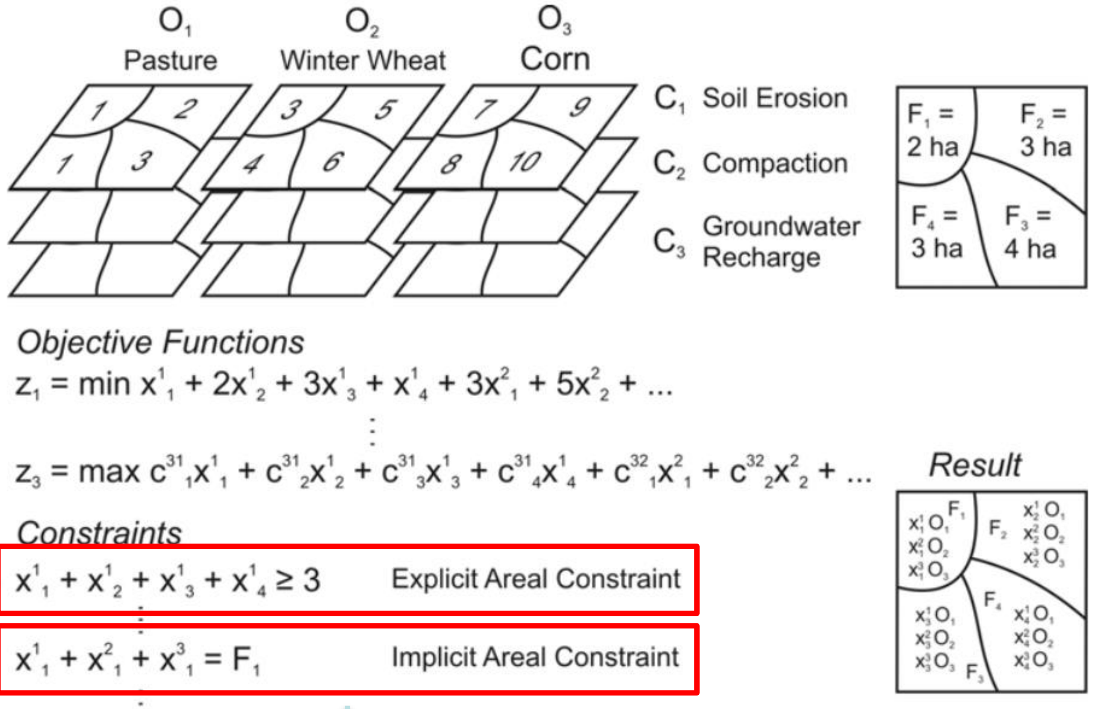
Constraints



user specified area shares expressed in map units

$$\sum_{i=1}^{m} x_i^r \leq b_w$$

continuous / integer

$$\sum_{i=1}^{m} G_i x_i^r \leq b_w$$

binary

the area of the spatial alternative (polygon) Fi

to ensure that the total quantity of land use alternatives Or allocated to a spatial alternative Fi does not exceed its area, these constraints (“Implicit Areal Constraint”) are additionally managed:

$$\sum_{r=1}^{p} x_i^r = G_i = b_w$$

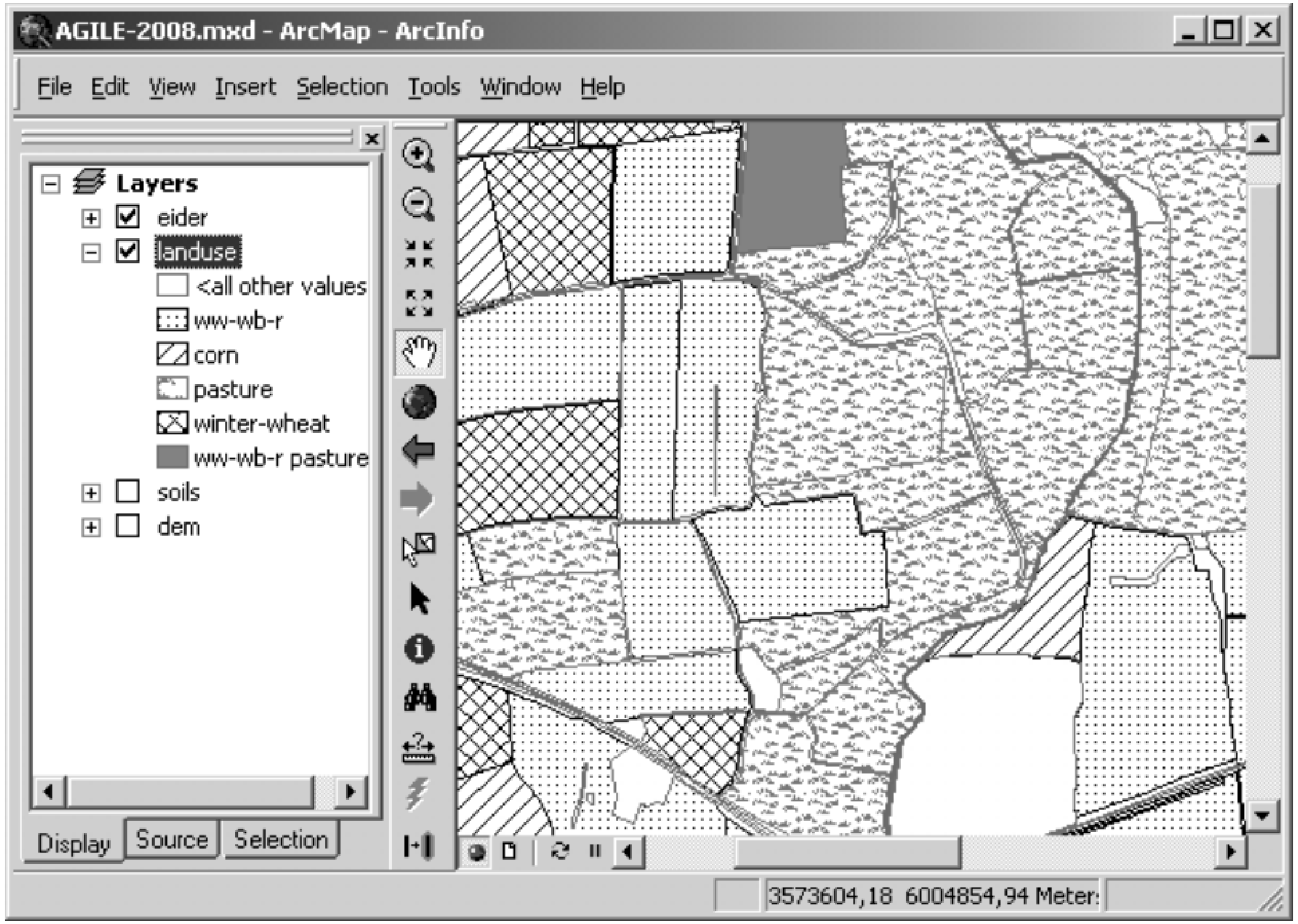
continuous / integer

$$\sum_{r=1}^{p} G_i x_i^r = G_i = b_w$$

binary

Solution

- Solve, evaluate and map the decision problem at hand



The automatically generated map as final result of a land use optimization problem