Introduction to Optimization

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Outline of Presentation

- What is optimization and what are its main elements?
- What are some of the main types optimization problems?
- What are the main approaches for solving optimization problems?
- What types of modeling software are available for optimization?

What is Optimization?

- An **optimization problem** involves finding the "best" solution from the set of all feasible solutions.
  - Criteria for "best" depend on the decision context
- Optimization is a mathematical approach for analyzing and solving this type of decision problem
- Optimization should be thought of as support tool for decision making rather than as a substitute for professional judgment

Example of a Bay TMDL optimization problem:

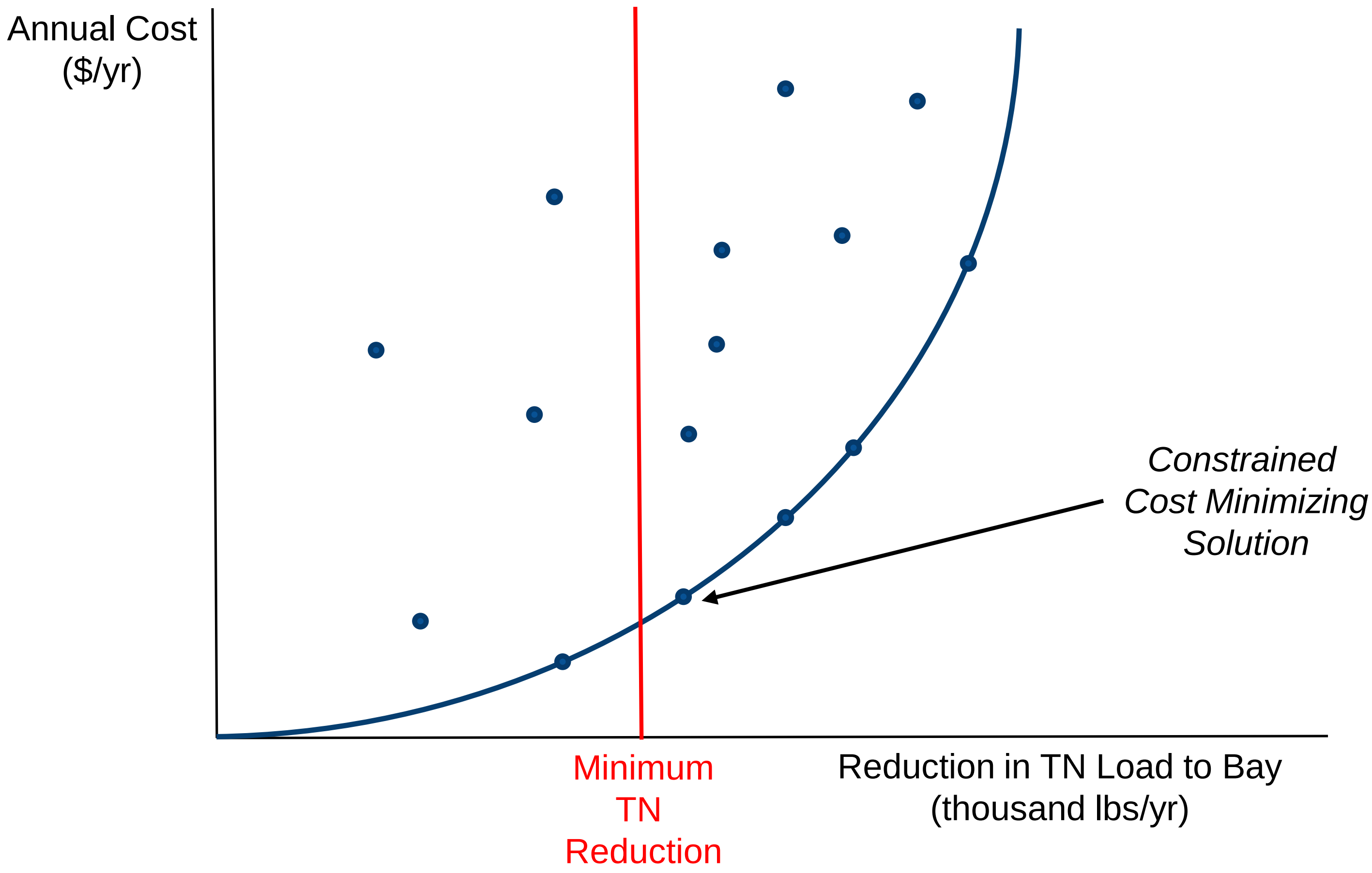
- Of all the possible types and combinations of feasible BMPs, which mix of BMPs will allow us to meet the TMDL load allocations at the lowest total cost?

Key Elements of an Optimization Model

Solving an optimization problem requires a model that expresses the following elements in mathematical terms

- An ***objective*** is a quantitative measure of the outcome we want to minimize or maximize.
  - Total annual cost of implementing and maintaining new BMPs in the county
- The ***variables*** are the components of the system for which we want to find values
  - Number or percent of acres in a county that are treated with each BMP (by land-use type)
- The ***constraints*** are functions that define the allowable values for the variables.
  - Allowable annual TN, TP, and sediment loads from the county to the Bay (TMDL constraint)

Constrained Cost Minimization Example



Optimization Methods

- Scoring Methods
  - This simple approach is feasible when there is a relatively small number of discrete alternatives
    1. Develop method for scoring each possible alternative
    2. Rank all alternatives based on their score
    3. Select alternative with highest score

- Mathematical Optimization Methods
  - When the set of feasible alternatives and/or constraints is very large (or infinite), more advanced modeling and computational methods are needed

Alternative Types of Optimization Problems

- Equality vs. Inequality constrained optimization
- Linear vs. Non-linear optimization
- Continuous vs. Discrete optimization
- Single- vs. Multi-Objective optimization
- Stochastic vs. Deterministic optimization
- Static vs. Dynamic optimization

Types of Constraints

- **"Inequality" constraints** set upper (≤) or lower (≥) limits
  - on the variables themselves
    - The number of acres of early drilled rye cover crop cannot exceed total acres of cropland in the county

  OR

  - on functions of the variables
    - Total loads of TN cannot exceed the TMDL limit
    - No more than 300 acres of active cropland can be converted to forest or wetlands (i.e., <u>sum</u> of converted acres ≤ 300 acres)

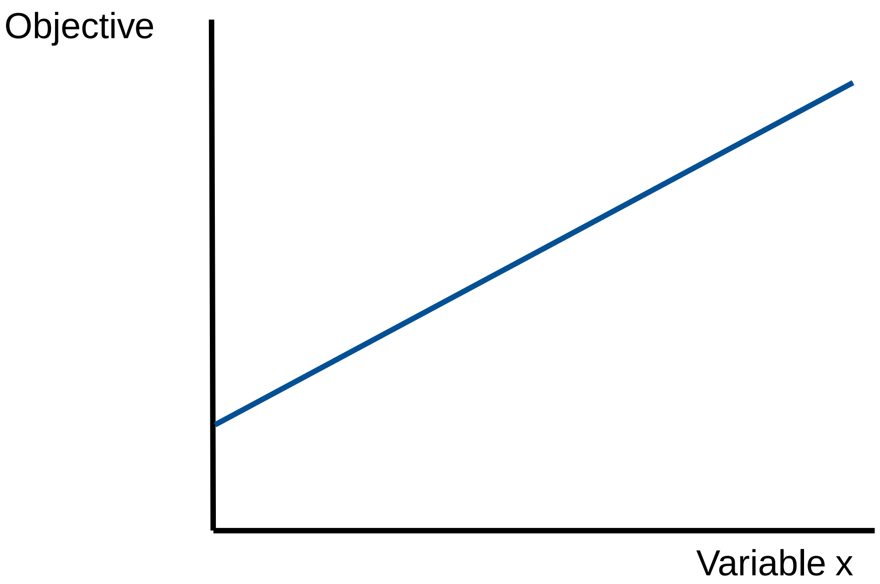
- **"Equality" constraints** set exact values on functions of the variables

Linear vs. Non-linear Optimization

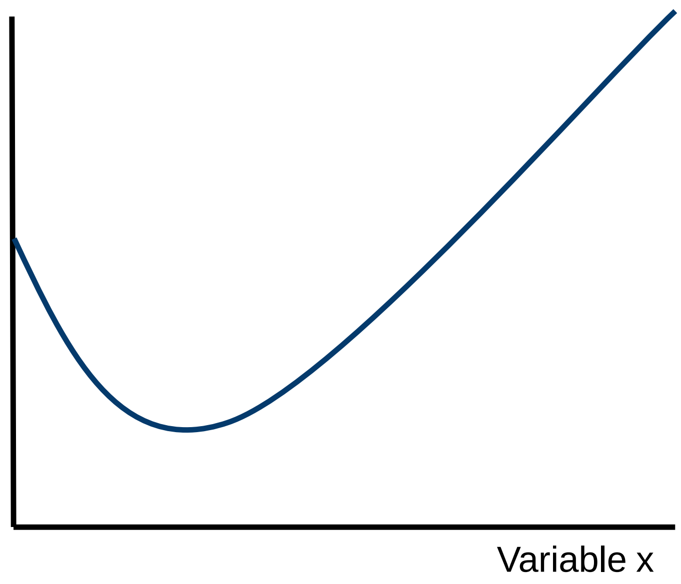
- Linear model: A one unit change in a variable will always have the same effect on the objective (or constraints) regardless of
  - (1) the starting point for the variable and
  - (2) the level of all other variables
- Well established and robust methods exist for solving large "linear programming" problems
- Non-linear models are more complex and require specialized approaches, depending on the shape and smoothness of the response surface

Linear vs. Non-linear Optimization

LINEAR

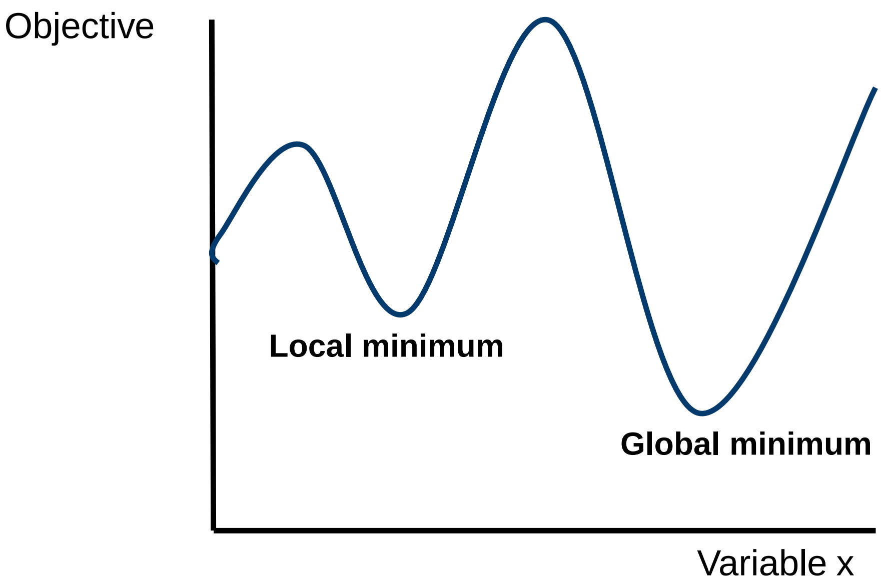


NON-LINEAR, CONVEX
- single (global) minimum

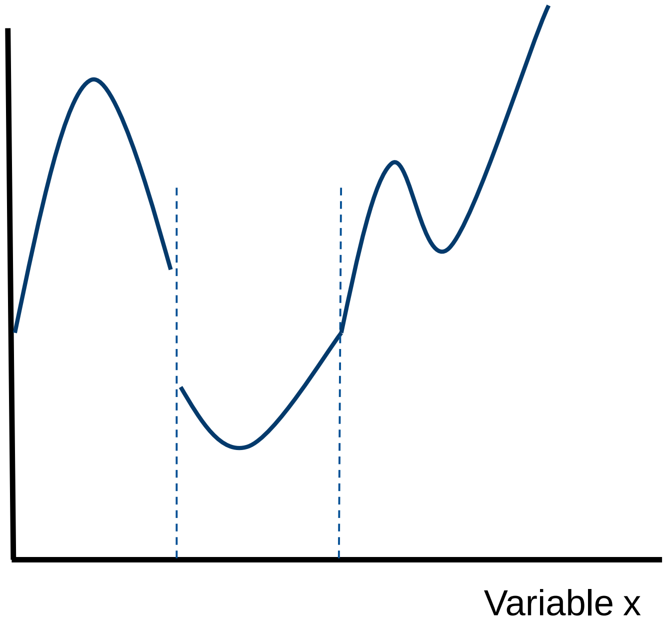


Linear vs. Non-linear Optimization

NON-LINEAR, NON-CONVEX, SMOOTH
- local and global minima



NON-LINEAR, NON-CONVEX, NON-SMOOTH, DISCONTINUOUS
- local and global minima
- breaking points



Examples of Non-Linearities

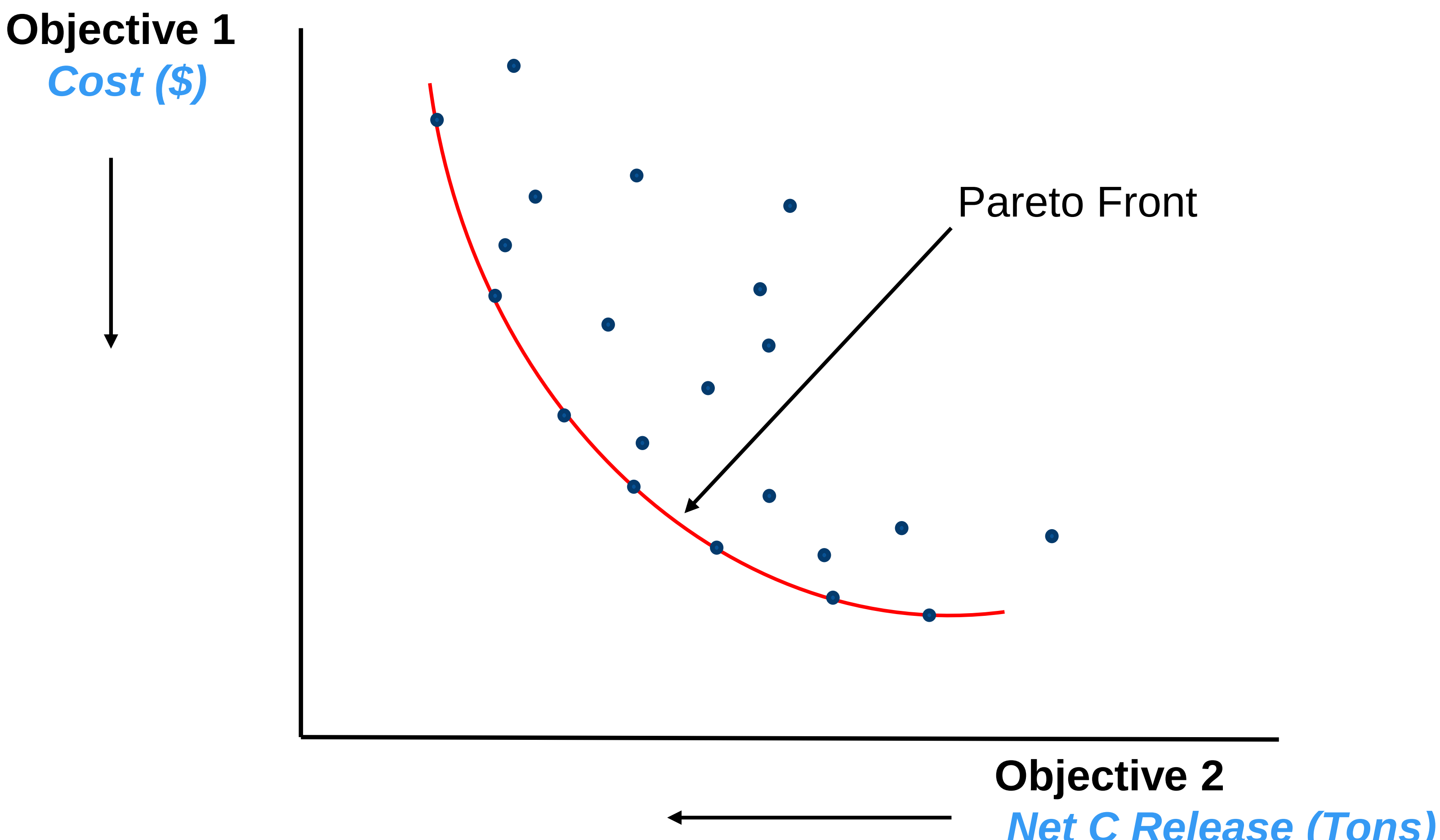
- Economies of scale: the average cost per acre for a BMP declines with the number of acres
- Load reductions achieved by one BMP depend on presence of other BMPs
  - Example 1: The application of animal BMPs at AFOs not only reduces loads from these sources but can also increase nutrient loads on manure-receiving land uses
  - Example 2: The load reduction achieved by installing a grass buffer on cropland is lower if cover crops are applied on the land

Continuous vs. Discrete Optimization

- Example
  - Continuous problem: on how many acres should cover crops be applied?
  - Discrete problem: which (if any) new wastewater treatment technology should be installed at each municipal facility?

- Continuous problems are often easier to solve because knowing the objective and constraint value at a point ***x*** can be used to deduce what they are in the neighborhood of ***x***

Multi-Objective Optimization



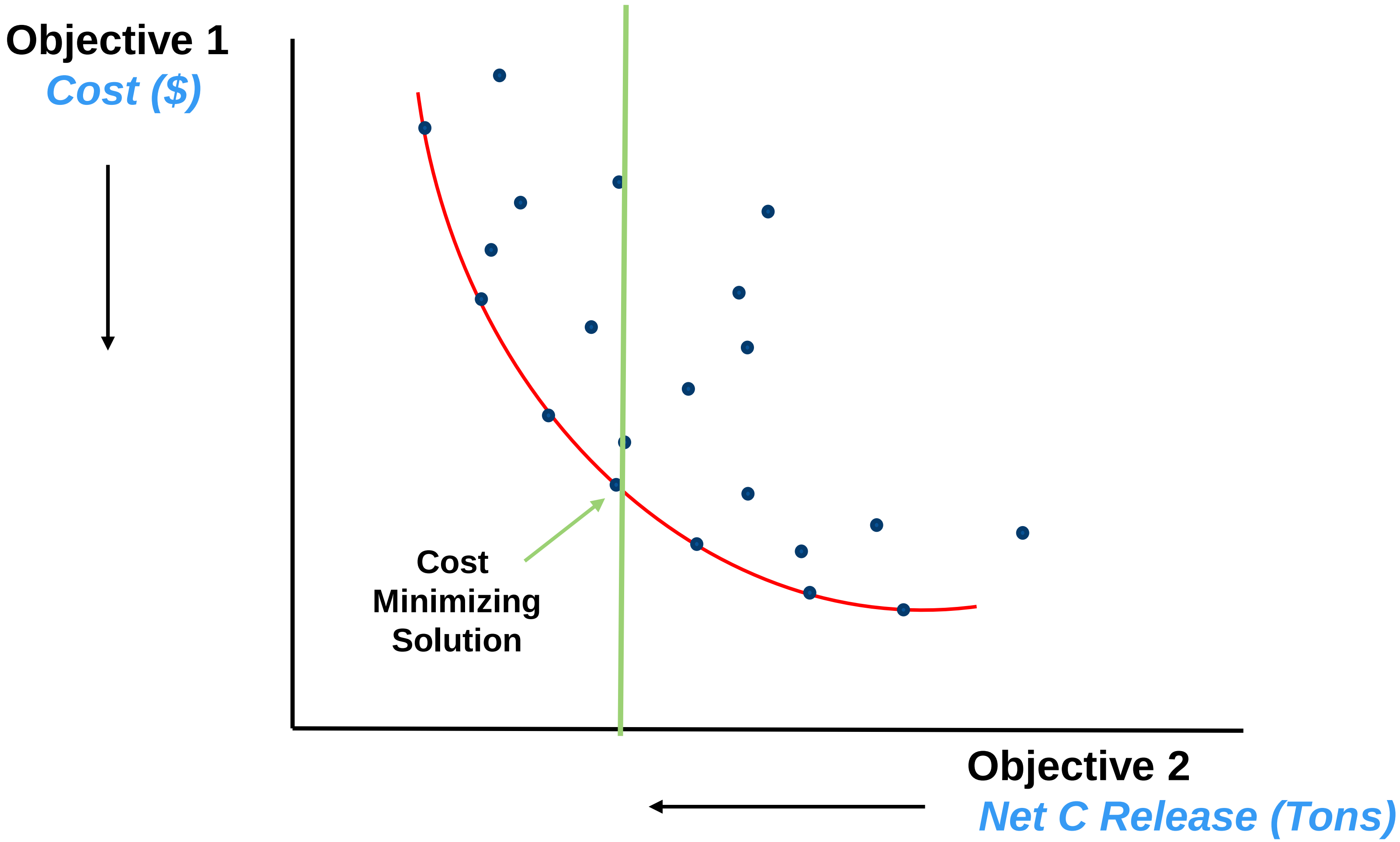
Approaches for Multi-Objective Optimization

- Combine objectives into a single objective
  - Define a weighted combination of the individual objectives
  - Example 1: Weighted sum of costs and C releases
  - Example 2: Convert C releases into $ terms and add $s together

- Treat some objectives as constraints and solve for remaining objective
  - Example: Minimize cost of achieving C and nutrient reduction targets
  - Pareto front can be found by repeating this process for different constraint levels

- Directly solve for the multiple Pareto front solutions
  - Representing these solutions is particularly challenging with more than 3 objectives

Multi-Objective Optimization



Other Types of Optimization Problems

- Stochastic Optimization is optimization under uncertainty
  - Only know the probability of achieving certain objectives and/or constraints
  - Example: Minimize costs such that there is only a 5% probability that the nutrient load limits will be exceeded in a given year.
- Dynamic Optimization (optimal control) is optimization over time rather than at a point in time (static)
  - Need to define an optimal "time path" for the variables of interest
  - Example: At what rate should new BMPs and technologies be installed each year?

Types of Optimization Programs

- Optimization Solvers/Algorithms
  - Solvers are computerized routines for solving specific types of optimization problems
  - They use systematic search methods to find the minimum or maximum point
  - Examples include:
    - Simplex Methods for linear programming problems
    - Newton Methods for smooth continuous non-linear optimization
    - Genetic Algorithms for more complex non-linear non-smooth optimization
- Optimization Modeling Software Programs
  - Software packages that allow users formulate the optimization problem in mathematical terms and to draw from a menu of solvers depending on the type of problem
    - Examples: GAMS, MATLAB, Dakota, Excel

Types of Solver Search Methods

- Gradient-Based Methods
  - More traditional class of search methods.
  - Various approaches that approximate the slope of the response surface to find the quickest way to the peak/trough
  - Most efficient when problem is “well-behaved” (i.e., smooth, continuous and with no or few local minima/maxima)

- Non-Gradient-Based Methods
  - Include pattern search methods and genetic algorithms (GA)
  - More computationally demanding and slower convergence rates but can be more robust for problems that are not “well-behaved”

Genetic Algorithms

- Most common alternative to traditional gradient-based methods
- Relatively well suited for finding global minima/maxima in problems that are highly non-linear or non-smooth, but can be very computationally intensive
- Modeled on natural selections processes in biological evolution
  - Generates a population of potential solutions at each iteration (rather than a single point).
  - Selects best points from these populations, which they use as “parents” for defining next iteration

Optimization Modeling Software

- Commercial/proprietary software is usually more reliable and robust but also more expensive.

Examples include:

  - General Algebraic Modeling System (GAMS)
  - MATLAB
  - Mathematica

- Open Source Resources
  - Computational Infrastructure for Operations Research (COIN-OR) (http://www.coin-or.org/)
  - Dakota toolkit (https://dakota.sandia.gov/)
  - NEOS Server (http://www.neos-server.org/neos/)

Thank you

- Questions?