IE 607 Heuristic Optimization

Introduction to Optimization

- **Objective Function**

Max (Min) some function of *decision variables*

Subject to (s.t.)

equality (=) *constraints*

inequality ($<, >, \leq, \geq$) *constraints*

- **Search Space**

  Range or values of decisions variables that will be searched during optimization. Often a calculable size in combinatorial optimization

Types of Solutions

- A *solution* to an optimization problem specifies the values of the decision variables, and therefore also the value of the objective function.
- A *feasible solution* satisfies all constraints.
- An *optimal solution* is feasible and provides the best objective function value.
- A *near-optimal solution* is feasible and provides a superior objective function value, but not necessarily the best.

Continuous vs Combinatorial

- Optimization problems can be *continuous* (an infinite number of feasible solutions) or *combinatorial* (a finite number of feasible solutions).
- Continuous problem generally maximize or minimize a function of continuous variables such as min 4x + 5y where x and y are *real numbers*
- Combinatorial problems generally maximize or minimize a function of discrete variables such as min 4x + 5y where x and y are *countable items* (e.g. integer only).

Definition of Combinatorial Optimization

- Combinatorial optimization is the mathematical study of finding an optimal arrangement, grouping, ordering, or selection of discrete objects usually finite in numbers.

  - *Lawler*, 1976

- In practice, combinatorial problems are often more difficult because there is *no derivative information* and the *surfaces are not smooth*.

Constraints

- Constraints can be *hard* (must be satisfied) or *soft* (is desirable to satisfy).

  Example: In your course schedule a hard constraint is that no classes overlap. A soft constraint is that no class be before 10 AM.

- Constraints can be *explicit* (stated in the problem) or *implicit* (obvious to the problem).

- **TSP** (Traveling Salesman Problem)

  Given the coordinates of n cities, find the *shortest closed tour* which visits each *once and only once* (i.e. exactly once).

  Example: In the TSP, an implicit constraint is that all cities be visited once and only once.

Aspects of an Optimization Problem

- Continuous or Combinatorial
- **Size** – number of decision variables, range/count of possible values of decision variables, search space size
- **Degree of constraints** – number of constraints, difficulty of satisfying constraints, proportion of feasible solutions to search space
- *Single* or *Multiple* objectives

Aspects of an Optimization Problem

- *Deterministic* (all variables are deterministic) or *Stochastic* (the objective function and/or some decision variables and/or some constraints are random variables)
- **Decomposition** – decomposite a problem into series problems, and then solve them independently
- **Relaxation** – solve problem beyond relaxation, and then can solve it back easier

<u>Simple</u>	<u>Hard</u>
Few decision variables	Many decision variables
Differentiable	Discontinuous, combinatorial
Single modal	Multi modal
Objective easy to calculate	Objective difficult to calculate
No or light constraints	Severely constraints
Feasibility easy to determine	Feasibility difficult to determine
Single objective	Multiple objective
deterministic	Stochastic

- For Simple problems, enumeration or exact methods such as *differentiation* or *mathematical programming* or *branch and bound* will work best.

- For Hard problems, differentiation is not possible and enumeration and other exact methods such as math programming are not computationally practical. For these, *heuristics* are used.

Search Basics

- **Search** is the term used for constructing/improving solutions to obtain the optimum or near-optimum.

Solution Encoding (representing the solution)

Neighborhood Nearby solutions (in the encoding or solution space)

Move Transforming current solution to another (usually neighboring) solution

Evaluation The solutions' feasibility and objective function value

- **Constructive** search techniques work by constructing a solution step by step, evaluating that solution for (a) feasibility and (b) objective function.
- **Improvement** search techniques work by constructing a solution, moving to a neighboring solution, evaluating that solution for (a) feasibility and (b) objective function.

- Search techniques may be *deterministic* (always arrive at the same final solution through the same sequence of solutions, although they may depend on the initial solution). Examples are LP (simplex method), tabu search, simple heuristics like FIFO, LIFO, and greedy heuristics.

- Search techniques may be *stochastic* where the solutions considered and their order are different depending on random variables. Examples are simulated annealing, ant colony optimization and genetic algorithms.

- Search techniques may be *local*, that is, they find the nearest optimum which may not be the real optimum. Example: greedy heuristic (local optimizers).

- Search techniques may be *global*, that is, they find the true optimum even if it involves moving to worst solutions during search (non-greedy).

Heuristics

- Heuristics are rules to search to find optimal or near-optimal solutions. Examples are FIFO, LIFO, earliest due date first, largest processing time first, shortest distance first, etc.

- Heuristics can be *constructive* (build a solution piece by piece) or *improvement* (take a solution and alter it to find a better solution).

- Many constructive heuristics are *greedy* or *myopic*, that is, they take the best thing next without regard for the rest of the solution.

  Example: A constructive heuristic for TSP is to take the nearest city next. An improvement heuristic for TSP is to take a tour and swap the order of two cities.

Meta-Heuristics

An iterative generation process which guides a subordinate heuristic by combining intelligently different concepts derived from classical heuristics, artificial intelligence, biological evolution, natural and physical sciences for exploring and exploiting the search spaces using learning strategies to structure information in order to find efficiently near-optimal solutions.

- *Osman and Kelly*, 1996

- This course will focus on **meta-heuristics** inspired by *nature*.
- Meta-heuristics are not tied to any special problem type and are general methods that can be altered to fit the specific problem.
- The inspiration from nature is:

  Simulated Annealing (SA) – molecule/crystal arrangement during cool down

  Evolutionary Computation (EC) – biological evolution

  Tabu Search (TS) – long and short term memory

  Ant Colony and **Swarms** - individual and group behavior using communication between agents

Advantages of Meta-Heuristics

- Very flexible
- Often global optimizers
- Often robust to problem size, problem instance and random variables
- May be only practical alternative

Disadvantages of Meta-Heuristics

- Often need problem specific information / techniques
- Optimality (convergence) may not be guaranteed
- Lack of theoretic basis
- Different searches may yield different solutions to the same problem (stochastic)
- Stopping criteria
- Multiple search parameters

Algorithm Design & Analysis

Steps:

- Design the algorithm
- Encode the algorithm
    - Steps of algorithm
    - Data structures
- Apply the algorithm

Algorithm Efficiency

- Run-time
- Memory requirements
- Number of elementary computer operations to solve the problem in the worst case

Study increased in the 70's

Complexity Analysis

- Seeks to classify problems in terms of the mathematical order of the computational resources required to solve the problems via computer algorithms

- **Problem** is a collection of instances that share a mathematical form but differ in size and in the values of numerical constants in the problem form (i.e. *generic model*) Example: shortest path.
- **Instance** is a special case of problem with specified data and parameters.
- An algorithm *solves* a problem if the algorithm is guaranteed to find the optimal solution for any instance.

Complexity Measures

- **Empirical Analysis**
  - see how algorithms perform in practice
  - write program, test on classes of problem instances
- **Average Case Analysis**
  - determine expected number of steps
  - choose probability distribution for problem instances, use statistical analysis to derive asymptotic expected run times

Complexity Measures

- **Worst Case Analysis**

  - provides upper bound (UB) on the number of steps an algorithm can take on *any* instance

  - count largest possible number of steps

  - provides a "guarantee" on number of steps the algorithm will need

Complexity Measures

- **CONs of Empirical Analysis**
  - algorithm performance depends on computer language, compiler, hardware, programmer’s skills
  - costly and time consuming to do
  - algorithm comparison can be inconclusive

Complexity Measures

- **CONs of Average Case Analysis**
  - depends heavily on choice of probability distribution
  - hard to pick the probability distribution of realistic problems
  - analysis often very complex
  - assumes analyst solving multiple problem instances

Complexity Measures

- **Worst Case Analysis**

  PROs

  - independent of computing environment

  - relatively easy

  - guarantee on steps (time)

  - definitive

  CONs

  - simplex method exception

  - algorithm comparisons can be inconclusive

Big “O” Notation

- A theoretical measure of the execution of an algorithm given the problem size n.
- An algorithm is said to run in O(g(n)) time if f(n) = O(g(n)) (of order g(n)) and there are positive constants c and k, such that $0 \le f(n) \le cg(n)$ for all $n \ge k$ (i.e. the time taken by the algorithm is at most cg(n) for all $n \ge k$)

Big "O" Notation

- Usually interested in performance on large instances
- Only consider the dominant term

Example: $100n + 1000n^2 + 0.01n^3$

$\rightarrow$ $O(n^3)$

Polynomial vs Exponential-Time Algorithms

- What is a “good” algorithm?
- It is commonly accepted that worst case performance bounded by a polynomial function of the problem parameters is “good”. We call this a *Polynomial-Time Algorithm*

  Example: $O(n^3)$
- Strongly preferred because it can handle arbitrarily large data

Polynomial vs Exponential-Time Algorithms

- In Exponential-Time Algorithms, worst case run time grows as a function that cannot be polynomially bounded by the input parameters.

  Example: $O(2^n)$ $O(n!)$
- Why is a polynomial-time algorithm better than an exponential-time one?

  →Exponential time algorithms have an explosive growth rate

	n=5	n=10	n=100	n=1000
n	5	10	100	1000
n^2	25	100	10000	1000000
n^3	125	1000	1000000	10^9
2^n	32	1024	1.27×10^{30}	1.07×10^{301}
n!	120	3.6×10^6	9.33×10^{157}	4.02×10^{2567}

Optimization vs Decision Problems

- **Optimization Problem**

  A computational problem in which the object is to find the best of all possible solutions. (i.e. find a solution in the feasible region which has the minimum or maximum value of the objective function.)
- **Decision Problem**

  A problem with a “yes” or “no” answer.

- **Convert Optimization Problems into equivalent Decision Problems**

  What is the optimal value?

  →Is there a feasible solution to the problem with an objective function value equal to or superior to a specified threshold?

Class P

- The class of decision problems for which we can find a solution in *polynomial* time.

  i.e. **P** includes all decision problems for which there is an algorithm that halts with the correct yes/no answer in a number of steps bounded by a polynomial in the problem size n.
- The **Class P** in general is thought of as being composed of relatively "easy" problems for which efficient algorithms exist.

Examples of Class P Problems

- Shortest path
- Minimum spanning tree
- Network flow
- Transportation, assignment and transshipment
- Some single machine scheduling problems

Class NP

- **NP** = Nondeterministic Polynomial
- **NP** is the class of decision problems for which we can *check* solutions in polynomial time.

  i.e. *easy to verify but not necessarily easy to solve*

Class NP

- Formally, it is the set of decision problems such that if *x* is a "yes" instance then this could be *verified* in *polynomial* time if a **clue** or **certificate** whose size is polynomial in the size of *x* is appended to the problem input.
- **NP** includes all those decision problems that could be polynomial-time solved if the right (polynomial-length) clue is appended to the problem input.

Class P vs Class NP

- **Class P** contains all those that have been conquered with well-bounded, constructive algorithms.
- **Class NP** includes the decision problem versions of virtually all the widely studied combinatorial optimization problems.
- **P** is a subset of **NP**.

Polynomial Reduction

- Problem **P** reduces in polynomial-time to another problem **P´**, if and only if,

  - there is an algorithm for problem **P** which uses problem **P´** as a subroutine,

  - each call to the subroutine of problem **P´** counts as a single step,

  - this algorithm for problem **P´** runs in polynomial-time.

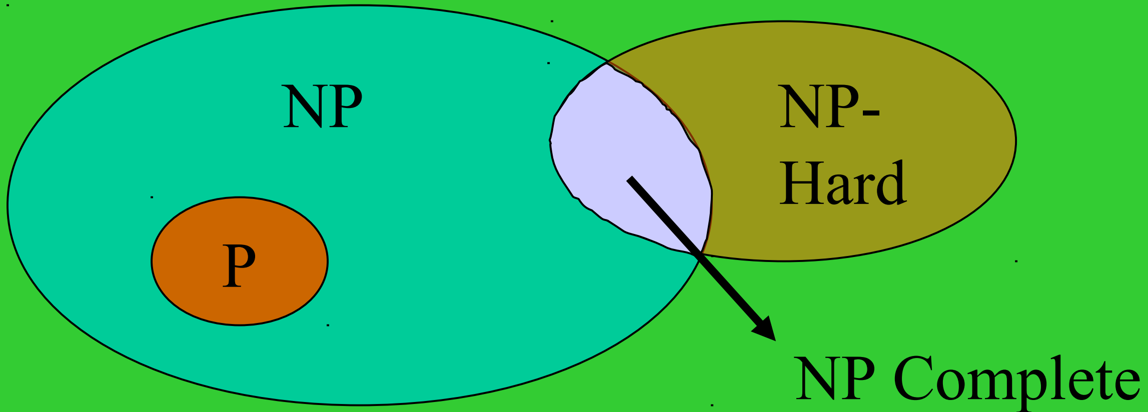
Polynomial Reduction

- If problem **P** *polynomially reduces* to problem **P´** and there is a polynomial-time algorithm for problem **P´**, then there is a polynomial-time algorithm for problem **P**.

  →Problem **P´** is at least as hard as problem **P**!

NP Hard vs NP Complete

- A problem **P** is said to be ***NP-Hard*** if all members of **NP** *polynomially reduce* to this problem.
- A problem **P** is said to be ***NP-Complete*** if (a) **P** ∈**NP**, and (b) **P** is ***NP-Hard.***



- If there is an efficient (i.e. polynomial) algorithm for some **NP-Complete** problem, then there is a polynomial algorithm existing for all problems in **NP**.→ **P = NP**

- Examples of NP-Hard problems:

  TSP, graph coloring, set covering and partitioning, knapsack, precedence-constrained scheduling, etc.