Optimization and Complexity

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Aim

- Give you an intuition of what is meant by
  - Optimization
  - P and NP problems
  - NP-completeness
  - NP-hardness
- Enable you to recognize formals of complexity theory, and its usefulness

Overview

- Motivating example
- Formal definition of a problem
- Algorithm and problem complexity
- Problem reductions
  - NP-completeness
  - NP-hardness
- Glimpse of approximation algorithms and their design

What is optimization?

- Requires a *measure* of optimality
  - Usually modeled using a mathematical function
- Finding the solution that yields the globally best value of our measure

What is the problem?

- Nike: Just do it
- Not so simple:
  - Even problems that are simple to formally describe can be intractable
  - Approximation is necessary
  - Complexity theory is a tool we use to describe and recognize (intractable) problems

Example: Variable Selection

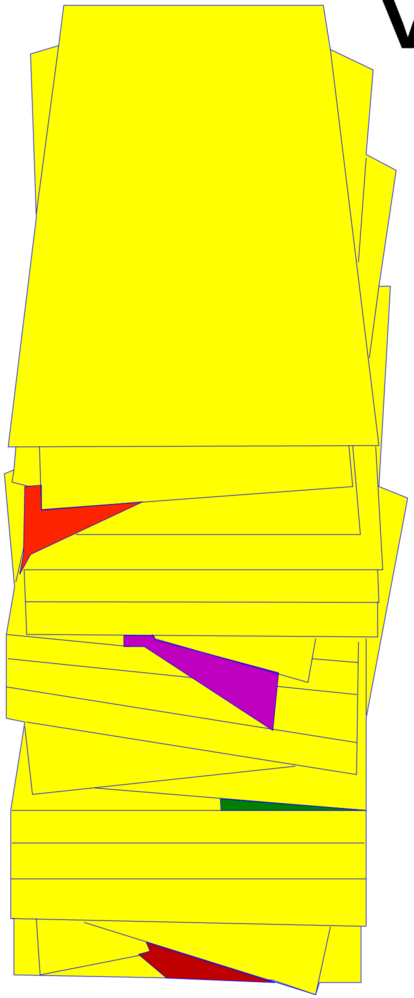
- Data tables T and V have n predictor columns and one outcome column. We use machine learning method L to produce predictive model L(T) from data table T. We can evaluate L(T) on V, producing a measure E(L(T),V).

- We want to find a maximal number of predictor columns in T to delete, producing T', such that

$$E(L(T'),V) = E(L(T), V)$$

- There is no known method of solving this problem optimally (e.g, NP-hardness of determining a minimal set of variables that maintains discernibility in training data, aka the rough set reduct finding problem).

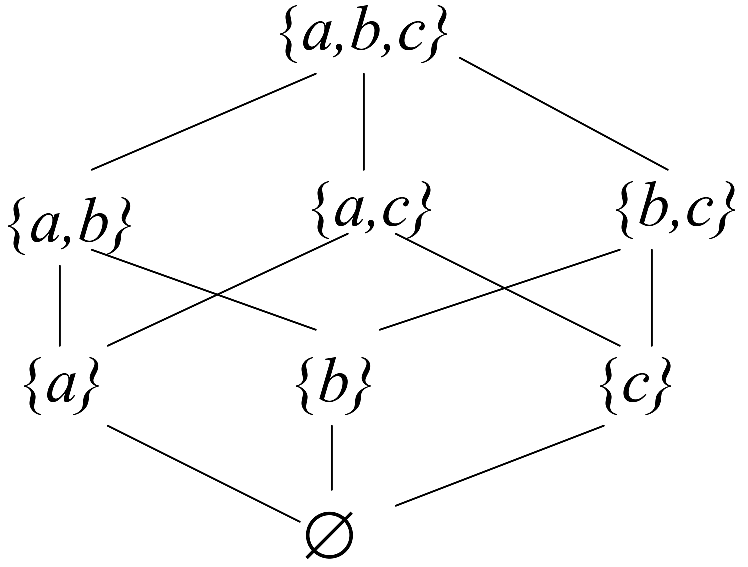
Search for Optimal Variable Selection



- The space of all possible selections is huge
- 43 variables, 2^{43} -1 possibilities of selecting a non-empty subset, each being a potential solution
- one potential solution pr. post-it gives a stack of post-its reaching more than half way to the moon

Search for Optimal Variable Selection

- Search space
  - discrete
  - structure that lends itself to *stepwise search* (add a new or take away one old)
  - optimal point is not known, nor is optimal evaluation value



Popular Stepwise Search Strategies

- Hill climbing:
  - select starting point and always step in the direction of most positive change in value

Popular Stepwise Search Strategies

- Simulated annealing:
  - select starting point and select next stepping direction stochastically with increasing bias towards more positive change

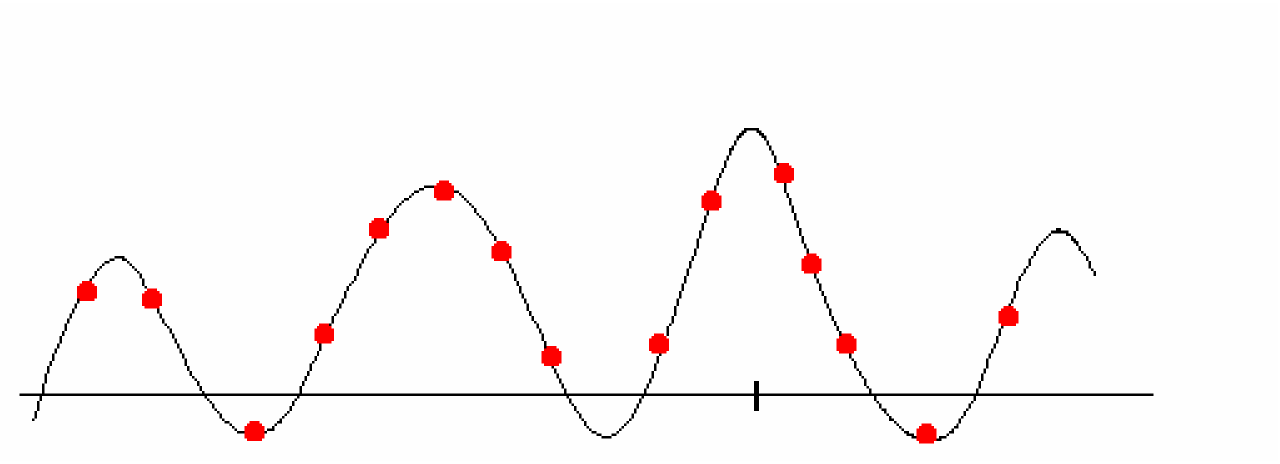
Problems

- Exhaustive search: generally intractable because of the size of the search space (exponential in the size of variables)
- Stepwise: no consideration of synergy effects
  – Variables *a* and *b* considered in isolation from each other are excluded, but their combination would not be

Genetic Algorithm Search

- population of solutions
- Stochastic selection of parents with bias towards “fitter” individuals
- “mating” and “mutation” operations on parents
- Merging of old population with offspring
- Repeat above until no improvement in population

GA Optimization Animation



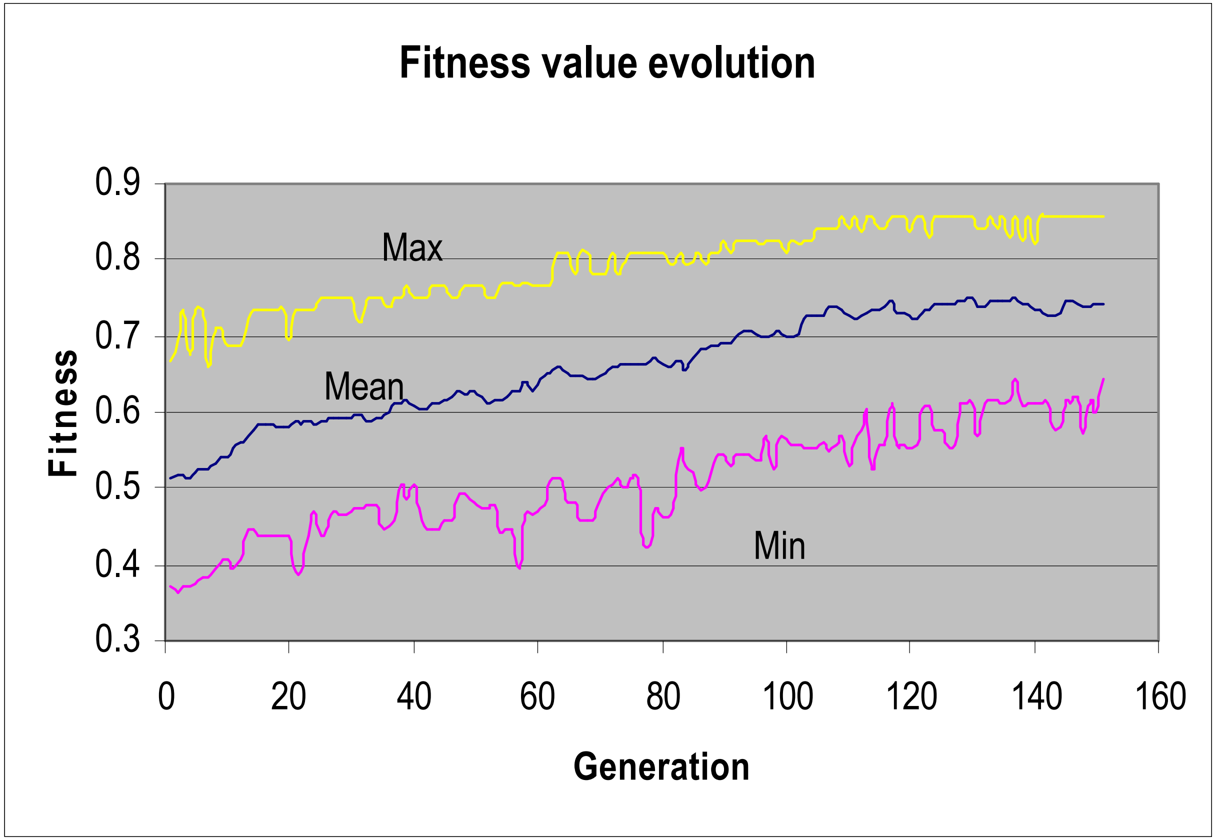
Addressing the Synergy Problem of Stepwise Search

- Genetic algorithm search
  - Non-stepwise, non-exhaustive
  - Pros:
    - Potentially finds synergy effects
    - Does not a priori exclude any parts of the search space
  - Cons:
    - Computationally expensive
    - Difficult to analyze, no comprehensive theory for parameter specification

Variable Selection for Logistic Regression using GA

- Data:
  - 43 predictor variables
  - Outcome: MI or not MI (1 or 0)
  - Training (*T*, 335 cases) and Holdout (*H*, 165 cases) from Sheffield, England
  - External validation (*V*, 1253 cases) from Edinburgh, Scotland

GA Variable Selection for LR: Generational Progress



GA Variable Selection for LR: Results

- Table presenting results on validation set E, including SAS built-in variable selection methods (removal/entry level 0.05)

Selection	Size	ROC AUC
Genetic	6	0.95
none	43	0.92
Backward	11	0.92
Forward	13	0.91
Stepwise	12	0.91

$P < 0.05$

Problem Example

- Boolean formula f (with variables)
  - Is there a truth assignment such that f is true?
  - Does this given truth assignment make f true?
  - Find a satisfying truth assignment for f
  - Find a satisfying truth assignment for f with the minimum number of variables set to true

Problem Formally Defined

- A problem P is a relation from a set I of instances to a set S of solutions: $P \subseteq I \times S$
  - Recognition: is $(x,y) \in P$?
  - Construction: for x find y such that $(x,y) \in P$
  - Optimization: for x find the *best* y such that $(x,y) \in P$

Solving Problems

- Problems are solved by an algorithm, a finite description of steps, that compute a result given an instance of the problem.

Algorithm Cost

- Algorithm cost is measured by
  - How many operations (steps) it takes to solve the problem (time complexity)
  - How much storage space the algorithm requires (space complexity)

  on a particular machine type as a function of input length (e.g., the number of bits needed to store the problem instance).

O-Notation

- O-notation describes an upper bound on a function
- let g,f: $N \rightarrow N$

$$f(n) \text{ is } O(g(n))$$

if there exists constants a,b,m such that for all n=m

$$f(n) = a * g(n) + b$$

O-Notation Examples

$f(n) = 9999999999999999$
is $O(1)$

$f(n) = 1000000n + 100000000$
is $O(n)$

$f(n) = 3n^2 + 2n - 3$
is $O(n^2)$

(Exercise: convince yourselves of this please)

Worst Case Analysis

- Let $t(x)$ be the running time of algorithm A on input x
- Let $T(n) = \max\{t(x) \mid |x| = n\}$
  - I.e., T(n) is the worst running time on inputs not longer than n.
- A is of time complexity O(g(n)) if

$$T(n) \text{ is } O(g(n))$$

Problem Complexity

- A problem P has a time complexity O(g(n)) if there exists an algorithm that has time complexity O(g(n))
- Space complexity is defined analogously

Decision Problems

- A *decision problem* is a problem P where the set of Instances can be partitioned into Y_P of positive instances and N_P of non-positive instances, and the problem is to determine whether a particular instance is a positive instance
- Example: satisifiability of Boolean CNF formulae, does a satisfying truth assignment exist for a given instance?

Two Complexity Classes for Decision Problems

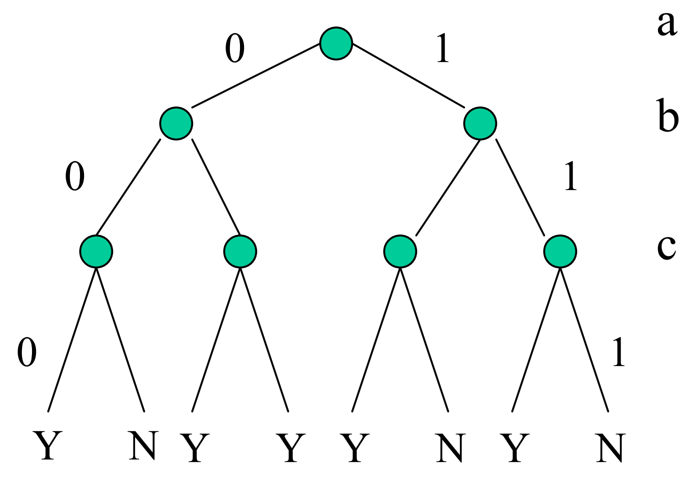
- P – all decision problems of time complexity $O(n^k)$, $0 = k = \infty$
- NP – all decision problems for which there exists a non-deterministic algorithm with time complexity $O(n^k)$, $0 = k = \infty$

What is a non-deterministic algorithm?

- Algorithm: finite description (program) of steps.
- Non-deterministic algorithm: an algorithm with “guess” steps allowed.

Computation Tree

- Each guess step results in a “branching point” in a computation tree
- Example: satisfying a Boolean formula with 3 variables



$$((\sim a \wedge b) \vee \sim c)$$

Non-deterministic algorithm time complexity

- A ND algorithm A solves the decision problem P in time complexity t(n) if, for any instance x with |x| = n, A halts for any possible guess sequence and $x \in Y_P$ if and only if there exists at least one sequence which results in YES in time at most t(n)

P and NP

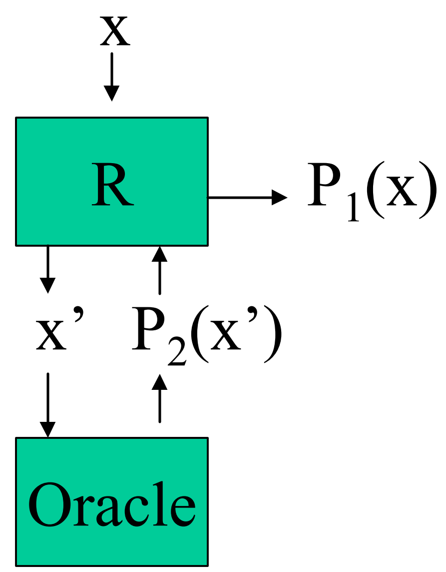
- We have that
  - $P \subseteq NP$
- If there are problems in NP that are not in P is still an open problem, but it is strongly believed that this is the case.

Problem Reduction

- A reduction from problem P_1 to problem P_2 presents a method for solving P_1 using an algorithm for P_2.
  - P_2 is then intuitively at least as difficult as P_1

Problem Reduction

- Problem P_1 is *reducible* to P_2 if there exists an algorithm R which solves P_1 by querying an *oracle* for $P_{2.}$ In this case, R is said to be a *reduction* from P_1 to P_2, and we write $P_1 = P_2$
- If R is of polynomial time complexity we write $P_1 =^p P_2$



NP-completeness

- A decision problem P is NP-complete if
  - It is in NP, and
  - For any other problem P' in NP we have that $P' =^p P$,
- This means that any NP problem can be solved in polynomial time if one finds a polynomial time algorithm for NP-complete P
- There are problems in NP for which the best known algorithms are exponential in time usage, meaning that NP-completeness is a sign of problem intractability

Optimization Problems

- Problem P is a quadruple (I_P, S_P, m_P, g_P)
  - I_P is the set of instances
  - S_P is a function that for an instance x returns the set of feasible solutions $S_P(x)$
  - $m_P(x,y)$ is the positive integer measure of solution quality of a feasible solution y of a given instance x
  - g_P is either min or max, specifying whether P is a maximization or minimization problem
- The optimal value for m_P for x over all solutions is denoted $m_P(x)$. A solution y for which $m_P(x,y) = m_P(x)$ is called optimal and is denoted $y^*(x)$.

Optimization Problem Example

- Minimum hitting set problem
  - $I = \{ C \mid C \subseteq 2^U \}$
  - $S = \{ H \mid H \cap c \neq \emptyset, c \in C \}$
  - $m(C,H) = |H|$
  - $g = \min$

Complexity Class NPO

An optimization problem (I, S, m, g) is in NPO if

1. An element of I is recognizable as such in polynomial time
2. Solutions of x are bounded in size by a polynomial q(|x|), and are recognizable as such in q(|x|) time
3. m is computable in polynomial time

Theorem: For an NPO problem, the decision problem whether m(x) = K (g=min) or m(x) = K (g=max) is in NP

Complexity Class PO

- An optimization problem P is said to be in PO if it is in NPO and there exists an algorithm that for each x in I computes an element y*(x) and its value m(x) in polynomial time

NP-hardness

- NP-completeness is defined for decision problems
- An optimization problem P is NP-hard if we for every NP decision problem P’ we have that $P' =^{p} P$
- Again, NP-hardness is a sign of intractability

Approximation Algorithms

- An algorithm that for an NPO problem P always returns a feasible solution is called an *approximation algorithm* for P
- Even if an NPO problem is intractable it might not be difficult to design a polynomial time approximation algorithm

Approximate Solution Quality

- Any feasible solution is an approximate solution, and is characterized by the distance from its value to the optimal one.
- An approximation algorithm is characterized by its complexity, and by the ratio of the distance above to the optimum, and the growth of this performance ratio with input size
- An algorithm is a p-approximate algorithm if the performance ratio is bounded by the function p in input size

Some Design Techniques for Approximation Algorithms

- Local search
  - Given solution, search for better “neighbor” solution
- Linear programming
  - Formulate problem as a linear program
- Dynamic Programming
  - Construct solution from optimal solutions to sub-problems
- Randomized algorithms
  - Algorithms that include random choices
- Heuristics
  - Exploratory, possibly learning strategies that offer no guarantees

Thank you

That’s all folks