DM811 – Fall 2010

Heuristics for Combinatorial Optimization

Lecture 1

Course Introduction
Combinatorial Optimization and Problem Solving

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Outline

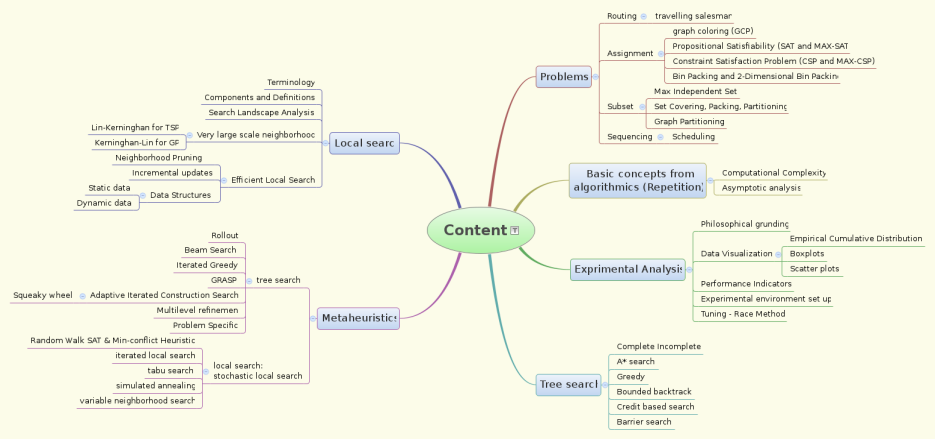
Outline

Schedule and Material

- Schedule (28 lecture hours):
  - Monday 12.15-14
  - Wednesday 12.15-14
  - Friday 12.15-14 (exercises ➨ you work)
  - Last lecture: Wednesday, 22th December, 2010
- Communication tools
  - Course Public Webpage (Wp) ⇔ Blackboard (Bb)
  - Announcements (Bb)
    (link from `http://www.imada.sdu.dk/~marco/DM811/`)
  - Documents (Photocopies) in Bb
  - Discussion board in Bb
  - Personal email in Bb
  - You are welcome to visit me in my office in working hours (8-16).

Contents

Heuristic algorithms: compute, efficiently, good solutions to a problem with no guarantee of optimality.



Evaluation

- Evaluation: final individual project (internal examiner)
  - Algorithm design
  - Implementation (deliverable and checkable source code)
  - (Analytical) and experimental analysis
  - Written description
  - Performance counts

References

- Main References:

  B1 W. Michiels, E. Aarts and J. Korst. Theoretical Aspects of Local Search. Springer Berlin Heidelberg, 2007

  B2 S. Russell and P. Norvig. Artificial Intelligence: A Modern Approach. (Part II) Prentice Hall, 2003.

  B3 Comet Tutorial (see doc in Comet Application)

  B4 P.V. Hentenryck and L. Michel. Constraint-Based Local Search. The MIT Press, Cambridge, USA, 2005.

  B5 H. Hoos and T. Stuetzle, Stochastic Local Search: Foundations and Applications, 2005, Morgan Kaufmann

- Photocopies (from Course Documents left menu of Blackboard)
- Articles from the Webpage
- R notes from the Webpage
- Lecture slides
- Assignments
- Lecture notes collaborative project

- ...but take notes in class!

Active participation

Practical experience is important to learn to use heuristics
Implementation details play an important role.

- Friday exercise sessions
  - Problem solving in class
  - Hands on with Comet
  - Implementation of heuristics for a certain problem
  - Experimental analysis of performance
  - Groups in competition
  - Require home preparation!
  - (worthwhile in preparation of the project!)
- Theme posted in assignment sheets linked from the webpage

Collaborative project

Lecture Notes:

- Write lecture notes for future students in an appropriate language
- Wiki page in Bb (but use LaTex style)
- In turn each one will be in charge of editing the past lecture
- Comments open to everybody

Functions:

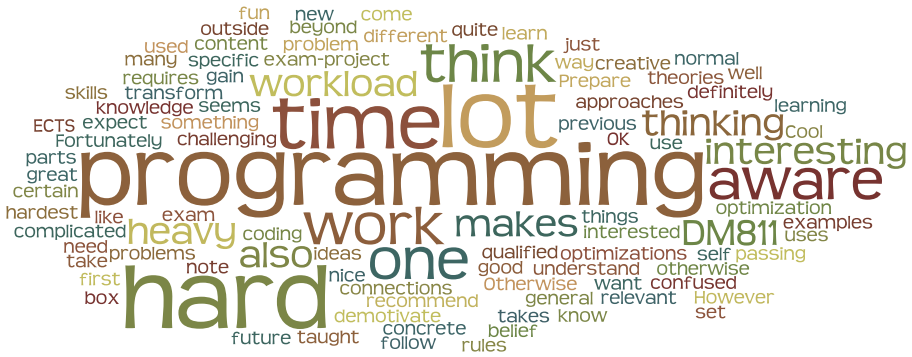
- Revise the lecture
- Providing me with feedback on whether the goals of the lecture have been achieved
- Getting yourself feedback
- Practicing scientific writing
- Contribute to make next editions of the course better

Former students' feedback (1/2)

On the course:

- a lot of knowledge from previous courses
- programming
- practical drive
- taught on examples
- no sharp rules are given and hence more space left to creativity
- heavy workload

Word cloud



Former students' feedback (2/2)

On the exam:

- the hardest part is the design of the heuristics because the content of the course is wide and there are many possibilities without clue on what will work best.

In general:

- They all felt the relevance of hands-on examples possibly with explanation of every algorithmic iteration.

From my side, mistakes I would like to see avoided:

- Among them: non competitive local search procedures and mistaken data aggregation in instance set analysis.

Outline

Combinatorial Problems (1/5)

Combinatorial problems

They arise in many areas
of Computer Science, Artificial Intelligence and Operations Research:

- allocating register memory
- planning, scheduling, timetabling
- Internet data packet routing
- protein structure prediction
- combinatorial auctions winner determination
- portfolio selection
- ...

Combinatorial Problems (2/5)

Simplified models are often used to formalize real life problems

- finding shortest/cheapest round trips (TSP)
- finding models of propositional formulae (SAT)
- coloring graphs (GCP)
- finding variable assignment which satisfy constraints (CSP)
- partitioning graphs or digraphs
- partitioning, packing, covering sets
- finding the order of arcs with minimal backward cost
- ...

Example Problems

- They are chosen because conceptually concise, intended to illustrate the development, analysis and presentation of algorithms
- Although real-world problems tend to have much more complex formulations, these problems capture their essence

Combinatorial Problems (3/5)

Combinatorial problems are characterized by an input,
i.e., a general description of conditions and parameters and
a question (or task, or objective) defining
the properties of a solution.

They involve finding a grouping, ordering, or assignment
of a discrete, finite set of objects that satisfies given conditions.

(Candidate) solutions are combinations of objects or solution components
that need not satisfy all given conditions.

Solutions are candidate solutions that satisfy all given conditions.

Combinatorial Problems (4/5)

Classical Example

Traveling Salesman Problem

- **Given:** edge-weighted, undirected graph G
- **Task:** find a minimal-weight Hamiltonian cycle in G.

Note:

- **solution component:** segment consisting of two points that are visited one directly after the other
- **candidate solution:** one of the $(n-1)!$ possible sequences of points to visit one directly after the other.
- **solution:** Hamiltonian cycle of minimal length

Decision problems

Hamiltonian cycle problem

- **Given:** undirected graph G
- **Question:** does G contain a Hamiltonian cycle?

solutions = candidate solutions that satisfy given *logical conditions*

Two variants:

- Existence variant: Determine whether solutions
  for given problem instance exists
- Search variant: Find a solution for given problem instance
  (or determine that no solution exists)

Optimization problems

Traveling Salesman Problem

- **Given:** edge-weighted, undirected graph G
- **Task:** find a minimal-weight Hamiltonian cycle in G.

- objective function measures solution quality
  (often defined on all candidate solutions)
- find solution with optimal quality, *i.e.*, minimize/maximize obj. func.

Variants of optimization problems:

- Evaluation variant: Determine optimal objective function
  value for given problem instance
- Search variant: Find a solution with optimal
  objective function value for given problem instance

Remarks

- Every optimization problem has an associated decision problem:
  Given a problem instance and a fixed solution quality bound b,
  find a solution with objective function value $\leq b$ (for minimization problems) or determine that no such solution exists.
- Many optimization problems have an objective function as well as constraints (= logical conditions) that solutions must satisfy.
- A candidate solution is called feasible (or valid) iff it satisfies the given constraints.
- Approximate solutions are feasible candidate solutions that are not optimal.
- **Note:** Logical conditions can always be captured by an objective function such that feasible candidate solutions correspond to solutions of an associated decision problem with a specific bound.

Combinatorial Problems (5/5)

General problem *vs* problem instance:

General problem Π:

- Given *any* set of points X, find a Hamiltonian cycle
- *Solution:* Algorithm that finds shortest Hamiltonian cycle for any X

Problem instantiation $\pi = \Pi(I)$:

- Given a specific set of points I, find a shortest Hamiltonian cycle
- *Solution:* Shortest Hamiltonian cycle for I

Problems can be formalized on sets of problem instances $\mathcal{I}$

Traveling Salesman Problem

Types of TSP instances:

- Symmetric: For all edges uv of the given graph G, vu is also in G, and $w(uv) = w(vu)$.
  Otherwise: asymmetric.
- Euclidean: Vertices = points in an Euclidean space,
  weight function = Euclidean distance metric.
- Geographic: Vertices = points on a sphere,
  weight function = geographic (great circle) distance.

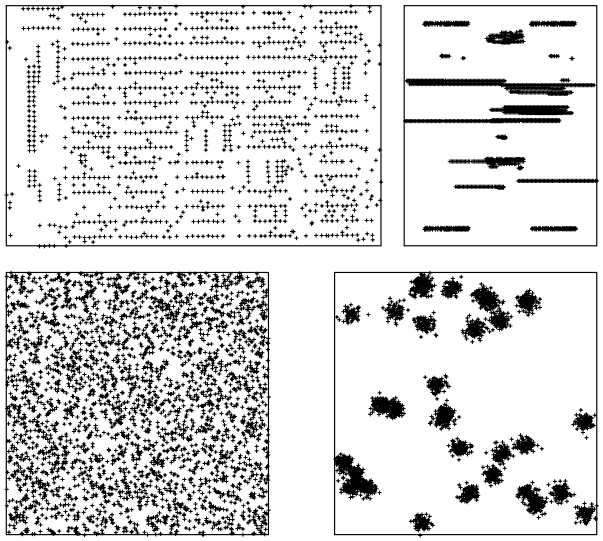
TSP: Benchmark Instances

Instance classes

- Real-life applications (geographic, VLSI)
- Random Euclidean
- Random Clustered Euclidean
- Random Distance

Available at the TSPLIB (more than 100 instances upto 85.900 cities)
and at the 8th DIMACS challenge

TSP: Instance Examples



Methods and Algorithms

A Method is a general framework for the development of a solution algorithm. It is not problem-specific.

An Algorithm (or algorithmic model) is a problem-specific template that leaves some practical details unspecified.
The level of detail may vary:

- minimally instantiated (few details, algorithm template)
- lowly instantiated (which data structure to use)
- highly instantiated (programming tricks that give speedups)
- maximally instantiated (details specific of a programming language and computer architecture)

A Program is the formulation of an algorithm in a programming language.

An algorithm can thus be regarded as a class of computer programs (its implementations)

Solution Methods

- **Exact methods** (complete)
  guaranteed to eventually find (optimal) solution,
  or to determine that no solution exists (eg, systematic enumeration)
  - Search algorithms (backtracking, branch and bound)
  - Dynamic programming
  - Constraint programming
  - Integer programming
  - Dedicated Algorithms
- **Approximation methods**
  worst-case solution guarantee
  `http://www.nada.kth.se/~viggo/problemlist/compendium.html`
- **Heuristic (Approximate) methods** (incomplete)
  not guaranteed to find (optimal) solution,
  and unable to prove that no solution exists

Problem specific methods:

- Dynamic programming (knapsack)
- Dedicated algorithms (shortest path)

General methods:

- Integer Programming
- Constraint Programming

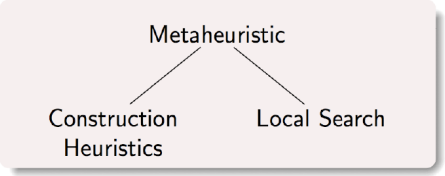
Generic methods:

- 👍 Allow to save development time
- 👎 Do not achieve same performance as specific algorithms

Heuristics

Get inspired by approach to problem solving in human mind (more on this later) [Newell and Simon, 1976]

- effective rules
- trial and error



Applications:

- Optimization, Timetabling, Routing, Scheduling
- But also in Psychology, Economics, Management

Side aspects: basis on empirical evidence rather than mathematical logic. Getting things done in the given time. Good having creativity in problem solving and criticism.

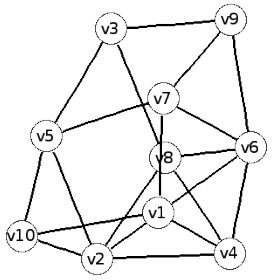
Outline

The Vertex Coloring Problem

Given: A graph G and a set of colors Γ.

A proper coloring is an assignment of one color to each vertex of the graph such that adjacent vertices receive different colors.

Decision version (k-coloring)
Task: Find a proper coloring of G that uses at most k colors.
Optimization version (chromatic number)
Task: Find a proper coloring of G that uses the minimal number of colors.



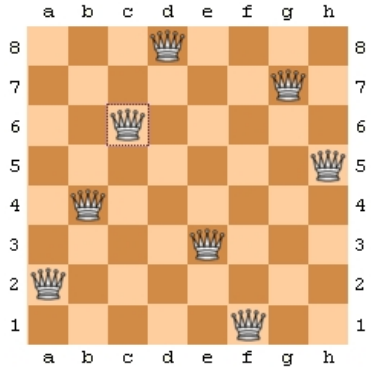
Design an algorithm for solving general instances of the graph coloring problem.

Home Assignment

N-Queens problem

Input: A chessboard of size N × N

Task: Find a placement of n queens on the board such that no two queens are on the same row, column, or diagonal.



Home Assignment

N^2 Queens

Input: A chessboard of size $N \times N$

Question: Given such a chessboard, is it possible to place N sets of N queens on the board so that no two queens of the same set are in the same row, column, or diagonal?

0	5	9	6	3	8	4	1	10	11	7	2
7	11	4	2	1	6	10	3	0	8	9	5
8	1	10	9	5	2	0	7	11	6	3	4
10	0	3	8	7	11	9	5	4	1	2	6
5	6	11	4	2	1	3	0	8	9	10	7
11	7	0	1	10	4	8	6	3	2	5	9
2	8	6	3	9	5	7	11	1	10	4	0
3	4	5	0	11	10	6	9	2	7	8	1
9	2	1	10	4	7	5	8	6	3	0	11
4	10	7	11	0	3	1	2	9	5	6	8
6	3	2	5	8	9	11	4	7	0	1	10
1	9	8	7	6	0	2	10	5	4	11	3

The answer is yes $\iff$ an opportune conflict graph admits a coloring with N colors

The Mathematical Perspective

Beside psychologists, also mathematicians reflected upon problem solving processes:

- George Pólya, *How to Solve it*, 1945
- J. Hadamard, *The Mathematician's Mind - The Psychology of Invention in the Mathematical Field*, 1945

Mathematical Problem Solving

George Pólya

George Pólya's 1945 book *How to Solve It*:

1. Understand the problem.
2. Make a plan.
3. Carry out the plan.
4. Look back on your work. How could it be better?

`http://en.wikipedia.org/wiki/How_to_Solve_It`

Pólya's First Principle: Understand the Problem

- Do you understand all the words used in stating the problem?
- What are you asked to find or show?
- Is there enough information to enable you to find a solution?
- Can you restate the problem in your own words?
- Can you think of a picture or a diagram that might help you to understand the problem?

Pólya's Second Principle: Devise a plan

There are many reasonable ways to solve problems.

- Guess and check
- Make an orderly list
- Eliminate possibilities
- Use symmetry
- Consider special cases
- Use direct reasoning

Also suggested:

- Look for a pattern
- Draw a picture
- Solve a simpler problem
- Use a model
- Work backward

Choosing an appropriate strategy is best learned by solving many problems.

Pólya's Third Principle: Carry out the plan

"Needed is care and patience, given that you have the necessary skills. Persist with the plan that you have chosen. If it continues not to work discard it and choose another. Don't be misled, this is how mathematics is done, even by professionals."

Pólya's Fourth Principle: Review/Extend

"Much can be gained by taking the time to reflect and look back at what you have done, what worked and what didn't. Doing this will enable you to predict what strategy to use to solve future problems."

Heuristic	Informal Description	Formal analogue
Analogy	Can you find a problem analogous to your problem and solve that?	Map
Generalization	Can you find a problem more general than your problem?	Generalization
Induction	Can you solve your problem by deriving a generalization from some examples?	Induction
Variation of the Problem	Can you vary or change your problem to create a new problem (or set of problems) whose solution(s) will help you solve your original problem?	Search
Auxiliary Problem	Can you find a subproblem or side problem whose solution will help you solve your problem?	Subgoal
Here is a problem related to yours and solved before	Can you find a problem related to yours that has already been solved and use that to solve your problem?	Pattern recognition Pattern matching Reduction
Specialization	Can you find a problem more specialized?	Specialization
Decomposing and Recombining	Can you decompose the problem and "recombine its elements in some new manner"?	Divide and conquer
Working backward	Can you start with the goal and work backwards to something you already know?	Backward chaining
Draw a Figure	Can you draw a picture of the problem?	Diagrammatic Reasoning [3]
Auxiliary Elements	Can you add some new element to your problem to get closer to a solution?	Extension

Inspiration can strike anytime, particularly after an individual had worked hard on a problem for days and then turned the attention to another activity.

The Mathematician's Mind - The Psychology of Invention in the Mathematical Field, J. Hadamard, 1945

Outline

Summary

1. Course Introduction

2. Combinatorial Optimization
   - Combinatorial Problems, Terminology
   - Solution Methods, Overview
   - Travelling Salesman Problem

3. Problem Solving
   - Example: Graph Coloring Problem
   - Mathematical Perspective, Polya's view
   - Psychological Perspective

4. Basic Concepts from Algorithmics

Outlook

Next Time:

- Constraint Satisfaction Problem
- Generalitis on Heuristics
- Setting up the Working Environment

In preparation:

- Lecture notes
- Revise basic concepts in algorithmics (see slides available in Wp and deepening in [B8])
- Reading material
- Download assignment