DM811 – Autumn 2013 Heuristics for Combinatorial Optimization

### Lecture 1 Course Introduction Combinatorial Optimization and Modeling

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# Outline

- 1. Course Introduction
- 2. Combinatorial Optimization Combinatorial Problems Solution Methods
- 3. Exercise
- 4. Problem Solving

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### 1. Course Introduction

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# Schedule and Material

- Class schedule:
  - Monday 08:15-10:00
  - Tuesday 14:15-18:00
  - Last class: Tuesday, October 11, 2012

Intro phase (Introfase) 12 classes Skills training phase (Træningsfase) 10 timer Study phase: (Studiefase)

- Communication tools
  - Course Public Webpage (WWW) ⇔ BlackBoard (BB) (link from http://www.imada.sdu.dk/~marco/DM811/)
  - Announcements in BlackBoard
  - Course Documents (for photocopies) in (BB)
  - Discussion Board (anonymous) in (BB)
  - Personal email

### Contents

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



### Evaluation

- Obligatory Assignments, pass/fail, evaluation by teacher (1+3 handins) Work in pairs, submit individually
   → Feedback
- Evaluation: final individual project, 7-grade scale, external examiner) ~ NEW: Based on the obligatory assignments
  - 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, chp. 3,4,6). Third Edition. Prentice Hall, 2010.
  - B4 P.V. Hentenryck and L. Michel. Constraint-Based Local Search. The MIT Press, Cambridge, USA, 2005. (In BlackBoard)
  - B5 H. Hoos and T. Stuetzle, Stochastic Local Search: Foundations and Applications, 2005, Morgan Kaufmann
    - https://class.coursera.org/optimization-001
- Literature Collection (from Course Documents left menu of BlackBoard)
- R notes from the Webpage
- Lecture slides
- Assignments
- Examples and Exercises (take notes in class)

# Active participation

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

- Be prepared for:
  - Problem solving in class
  - Assignments for hands on experience ~>> programming
  - Experimental analysis of performance
  - Group discussions
  - Exercise Sheets

Required study phase (= work outside the classes)

# Former students' feedback (1/2)

On the course:

- the course bulids on 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
- unexpected heavy workload
- the assignments are really an important preparation to the final projects

### Word cloud



# Former students' feedback (2/2)

On the exam:

 hardest part is the design of the heuristics the content of the course is vast → many possibilities without clue on what will work best.

In general:

• Examples are relevant, would be nice closer look at source code.

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

- non competitive local search procedures
- bad descriptions
- mistaken data aggregation in instance set analysis.

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# Combinatorial Problems (1/6)

### 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
- auction winner determination
- portfolio selection

• ...

# Combinatorial Problems (2/6)

Simplified models are often used to formalize real life problems

- coloring graphs (GCP)
- finding models of propositional formulae (SAT)
- finding variable assignment that satisfy constraints (CSP)
- finding shortest/cheapest round trips (TSP)
- 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 (3/6)

Combinatorial problems are characterized by an input, *i.e.*, a general description of conditions (or constraints) 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.

Note:

in this course, (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 (4/6) Examples

Grouping:

Given a finite set  $N = \{1, ..., n\}$ , weights  $c_j$  for each  $j \in N$ , and a set  $\mathcal{F}$  of feasible subsets of N, find a minimum weight feasible subset of N, ie,

 $\min_{S \subseteq N} \{ \sum_{j \in S} c_j \mid S \in \mathcal{F} \}$ 

- candidate solution: one of the  $2^{|N|}$  possible subsets of N.
- solution: the feasible subset of minimal cost

# Combinatorial Problems (5/6)

Ordering:

### Traveling Salesman Problem

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

- 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 exist
- Search variant: Find a solution for given problem instance (or determine that no solution exists)

# **Optimization problems**

### Traveling Salesman Problem

- $\bullet$  Given: edge-weighted, undirected complete graph G
- Task: find a minimum-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 (6/6)

General problem vs problem instance:

General problem  $\Pi$ :

- $\bullet\,$  Given any set of points X in a square, find a shortest Hamiltonian cycle
- Solution: Algorithm that finds shortest Hamiltonian cycle for any X

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

- $\bullet\,$  Given a specific set of points I in the square, find a shortest Hamiltonian cycle
- Solution: Shortest Hamiltonian cycle for I

Problems can be formalized on sets of problem instances  $\mathcal{I}$  (instance classes)

# **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 only 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 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 (eg, branch and bound)

### 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
- $\mathbb{R}$  Do not achieve same performance as specific algorithms

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# The Vertex Coloring Problem

**Given:** A graph G and a set of colors  $\Gamma$ .

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



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

### Exercise

Map coloring:



# Timetabling as a graph coloring problem

#### Definition

Find an assignment of lectures to time slots and rooms which is

#### Feasible

rooms are only used by one lecture at a time, each lecture is assigned to a suitable room, no student has to attend more than one lecture at once, lectures are assigned only time slots where they are available;

#### and Good

no more than two lectures in a row for a student, unpopular time slots avoided (last in a day), students do not have one single lecture in a day. Hard Constraints

Soft Constraints

ID	year	lecs	studs	rooms	ecs/stud	studs/lec	rooms/le	degree	slots/lec	slots/lec	slots/lec	Prec.	Rel. Prec.
1	2007	400	500	10	21.02	26.27	4.08	0.34	16	25.34	34	40	14
2	2007	400	500	10	21.03	26.29	3.95	0.37	17	25.69	33	36	14
3	2007	200	1000	20	13.38	66.92	5.04	0.47	19	25.54	33	20	11
4	2007	200	1000	20	13.40	66.98	6.40	0.52	15	25.66	33	20	9
5	2007	400	300	20	20.92	15.69	6.80	0.31	16	25.43	34	120	43
6	2007	400	300	20	20.73	15.54	5.07	0.30	13	25.39	36	119	32
7	2007	200	500	20	13.47	33.66	1.57	0.53	9	17.86	26	20	10
8	2007	200	500	20	13.83	34.58	1.92	0.52	11	17.17	26	21	13
9	2007	400	500	10	21.43	26.79	2.91	0.34	17	25.42	34	41	18
10	2007	400	500	10	20.98	26.23	3.20	0.38	14	25.47	34	40	13
11	2007	200	1000	10	13.61	68.04	3.38	0.50	17	25.32	35	21	17
12	2007	200	1000	10	13.61	68.03	3.35	0.58	15	25.67	35	20	13
13	2007	400	300	20	21.19	15.89	8.68	0.32	17	25.75	34	116	34
14	2007	400	300	20	20.86	15.64	7.56	0.32	17	25.44	36	118	46
15	2007	200	500	10	13.05	32.63	2.23	0.54	11	17.38	24	21	13
16	2007	200	500	10	13.64	34.09	1.74	0.46	10	17.57	25	19	10

### A look at the instances

These are large scale instances.

### A look at the basic Graph Model (vertices correspond to lectures)



### Exercise

### N-Queens problem

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

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



### Exercise

### $N^2$ 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  $\iff$  a corresponding conflict graph admits a coloring with N colors

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# Heuristics

### Get inspired by approach to problem solving in human mind

[A. Newell and H.A. Simon. "Computer science as empirical inquiry: symbols and search." Communications of the ACM, ACM, 1976, 19(3)]

- effective rules
- trial and error



Applications:

- Optimization, Timetabling, Routing, Scheduling
- But also in Psychology, Economics, Management [Tversky, A.; Kahneman, D. (1974). "Judgment under uncertainty: Heuristics and biases". Science 185]

Basis on empirical evidence rather than mathematical logic. Getting things done in the given time.

### 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?	Мар	
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 <sup>[3]</sup>	
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

# Summary

- 1. Course Introduction
- 2. Combinatorial Optimization
  - Combinatorial Problems, Terminology
  - Solution Methods, Overview
  - Travelling Salesman Problem
- 3. Problem Solving
  - Example: Graph Coloring Problem
  - Polya's view about Problem Solving
- 4. Basic Concepts from Algorithmics (Review slides and Cormen, Leiserson, Rivest and Stein. *Introduction to algorithms*. 2001)