Heuristics an overview

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Deel heuristieken Patrick De Causmaecker

- Overzicht van metaheuristieken
 - Simulated annealing, Tabu Search, Variable
 Neighborhood Search, Hyperheuristieken,...
- Link met data
 - Parameter tuning, Algoritme configuratie,
 Stochastische kosten

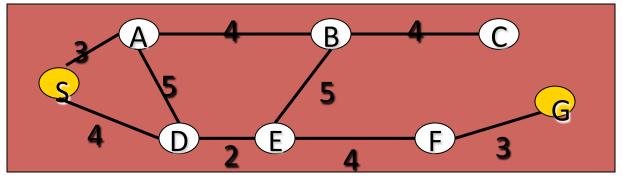
Content (lecture 1)

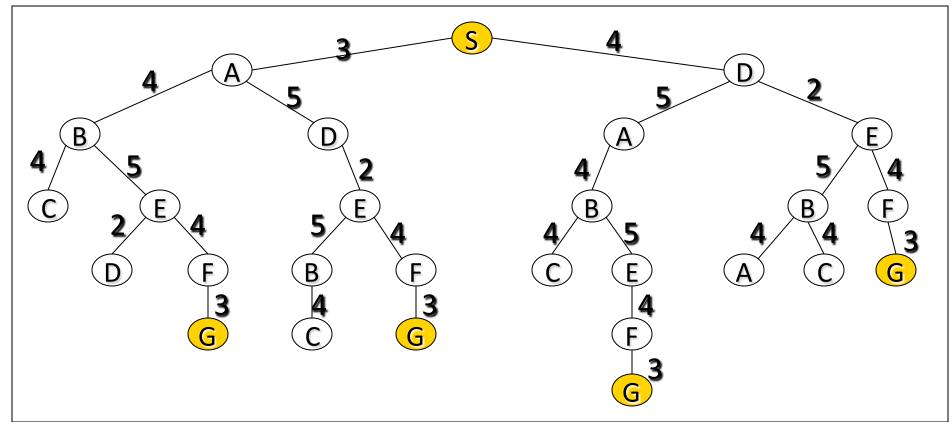
- An early example (what this talk is not about)
- What is may be about
- What it is about
- Genetic algorithms
- Tabu search
- Variable neighborhood search
- Hyper heuristics

Content (lecture 2)

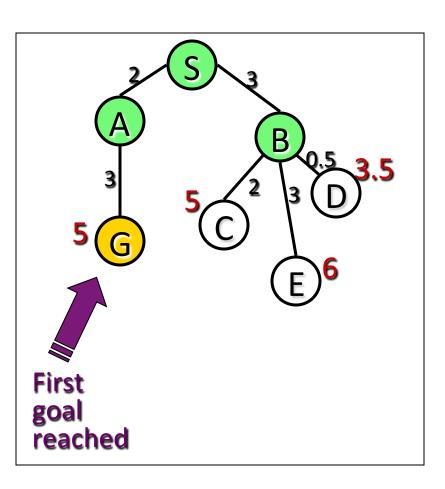
- Examples of real applications
- Detailed solution procedure

An early Example (what it is not about)



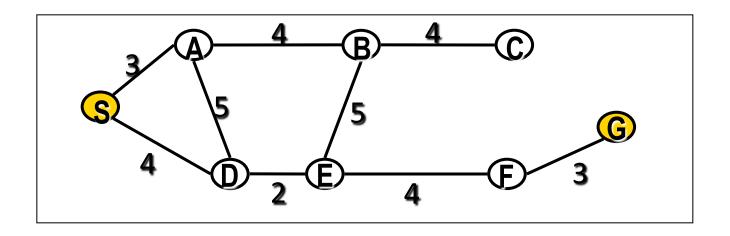


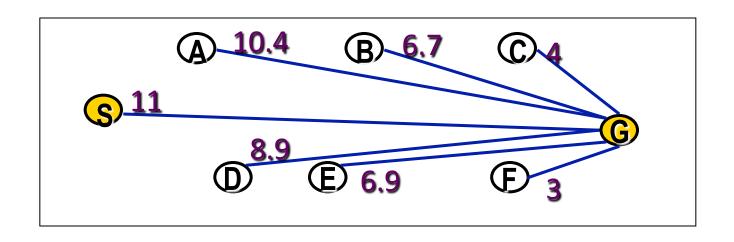
Branch and bound



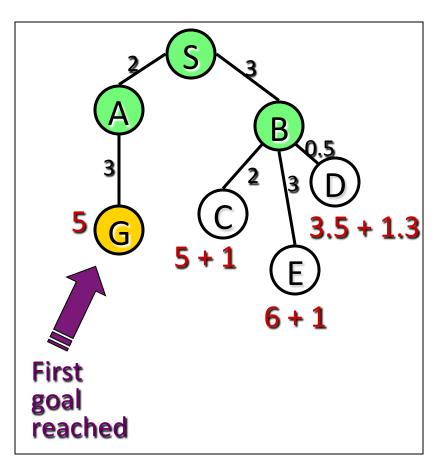
- Use any (complete) search method to find <u>a path</u>.
- Remove all partial paths that have an accumulated cost larger or equal than the found path.
- Continue search for the next path.
- Iterate.

Heuristic estimates





Search using heuristic estimates



- Use any (complete) search method to find a path.
- Remove all partial paths that have an *estimated* accumulated cost larger or equal than the found path.
- Continue search for the next path.
- Iterate.
- Finds the optimal path if the heuristic is an underestimate

Another example 8-puzzle

• f1(T) = the number correctly placed tiles on the

board:

- f2(T) = number of incorrectly placed tiles on board:
 - → gives (rough!) estimate of how far we are from goal

$$f2 \begin{bmatrix} 1 & 3 & 2 \\ 8 & 4 \\ 5 & 6 & 7 \end{bmatrix} = 4$$

Most often, 'distance to goal' heuristics are more useful!

Another example: 8 puzzle

- f3(T) = the sum of (the horizontal + vertical distance that each tile is away from its final destination):
 - gives a better estimate of distance from the goal node

Linear programming

maximize
$$3x_1 + 5x_2 + 4x_3$$

subject to

$$7.5x_1 + 8x_2 + 4x_3 \leq 10000$$

 $12x_1 + 9x_2 + 8x_3 \leq 18000$
 $3x_1 + 4x_2 + 2x_3 \leq 9000$
 $x_1 \geq 1000$

General (Canonical) form

$$max(min) \sum_{i=1}^{n} c_i x_i$$

subject to

$$\sum_{i=1}^{n} a_{1i} x_i \sim b_1$$

Ī

$$\sum_{i=1}^{n} a_{mi} x_i \sim b_m$$

$$x_i \geq 0$$

 $max \ CX$

subject to

$$AX = b$$

$$X \geq 0$$

Duality

 $max \ CX$

subject to

AX = b

 $X \geq 0$

 $min \ b^T Y$

subject to

$$A^TY \geq C^T$$

$$Y \geq 0$$

Facility location: mixed integer problem (MIP)

$$min$$
 $52.(25x_{11} + 20x_{12} + 15x_{13})$
 $+ 25x_{11} + 20x_{12} + 15x_{13}$
 $+ 15x_{21} + 25x_{22} + 20x_{23}$
 $+ 20x_{31} + 15x_{32} + 25x_{33})$
 $+ 500000.(y1 + y2 + y3)$

subject to $x_{11} + x_{21} + x_{31} \le 1500y_1$
 $x_{11} + x_{12} + x_{13} = 1000$
 $x_{21} + x_{22} + x_{23} = 1000$
 $x_{31} + x_{32} + x_{33} = 500$
 $x_{ij} \ge 0$
 $y_i \in \{0, 1\}$

Relaxation

Remove integer constraint from the MIP

$$y_j \in \{0,1\}$$

- The new problem (LR) is 'easier', a (linear) relaxation
 - Optimal value is 'better'
 - LR infeasible -> MIP is infeasible
 - Optimal solution of LR with integer values is optimal for MIP
 - Floor/ceiling property (min problem with integer c)

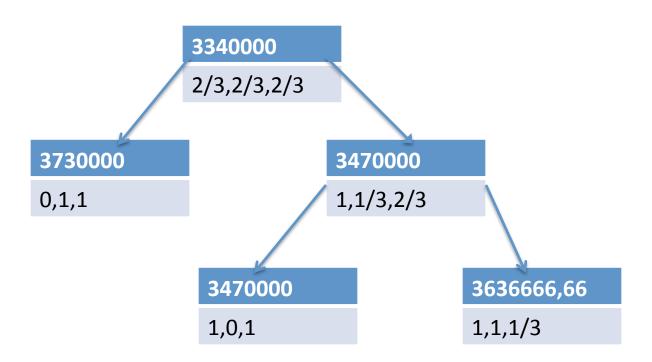
$$\lceil LR \rceil \leq MIP$$

Optimum of LR for the facility location

$$y_1 = \frac{2}{3} = y_2 = y_3$$
 $Optimum = 3340000$ $Round to y_1 = 1 = y_2 = y_3(feasible!) o 3840000$

- Rather good, but is it optimal?
- Hence: branching: $IP(y_1 = 1) \& IP(y_1 = 0)$
- This has lead to a rich research area with remarkable advances in both theory and practice.

Full tree



Heuristics in complete search

- Bring in domain/expert knowledge
- More accurate heuristics deliver better
- Reduce the search time/do not reduce worst case complexity

Combinatorial problems

- Hamilton cycle
- Set covering
- Knapsack
- Assignment
- Bin packing
- Scheduling

- Travelling salesperson
- Knapsack
- Assignment
- Max clique
- Shortest path
- Bin packing
- Vehicle routing
- Scheduling

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Heuristic search

- Nearest neighbor for TSP and Hamilton
- New-best-in heuristic for max clique
- Best fit for bin packing
- Worst fit for bin packing
- Earliest due date for scheduling
- Shortest job for scheduling

• ...

Complex? Complete/Optimal?

- Fast: typically O(n^2)
- Not exactly optimal, e.g. TSP with NN:
 - N cities randomly distributed on a plane:
 - average = 1.25 * exact_shortest_length
 - Special constructions
 - Worst route can be found
- If the triangle inequality is satisfied:
 - NN: O(log | V |) (Rozenkrantz, 1977)
 - Christofides algorithm guarantees
 1.5*exact_shortest_length

Are exact/complete solutions feasible? Take TSP

- Enumeration (O(n!))
- Dynamic programming (O(n^2*2^n)) (exponential space)
- Branch and bound (40-60 cities)
- Lagrangian relaxation (100)
- Linear/integer programming (200)
- Benchmarks: TSPLIB
 - 15112 German towns: 22.6 years, 100 processors, 2001
 - 24978 Swedish cities: 2004
 - Recent: 33810 (2005), 85900 (2006) cities...

Live with (incomplete/non exact) algorithms/heuristics But there are some problems

- Problem specific:
 - No generality
 - Application to real world problems?
- Improvement
 - Heuristics often run in a fixed time,
 - giving it more time does not result in better results
 - Stochastic behavior delivers better results faster.
 - Heuristics are often deterministic in nature. If there is a stochastic element, it is localized and it is hard to manipulate its impact

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Move from problem specific heuristics to general heuristic schemata

- 1986: 'metaheuristic' (Fred Glover)
- Recipe to build a heuristic
- developer can insert problem specific information at certain points
- Attempt to find a general approach that works for a large set of problems
- Bears on general principles and ideas
 - Sometimes with hard mathematical underpinning
- Can be considered designer guidelines

Some examples

- Genetic algorithms
- Evolutionary algorithms
- Tabu search
- Simulated annealing
- Great deluge
- Hyperheuristics

- Variable neighbourhood search
- Late acceptance
- Extreme optimisation
- Neural networks
- Electrostatic potential

METAPHORS

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Genetic algorithms

- Initialisation: Set up a population of individuals
 - Random across search space or guided by domain knowledge

Evaluation:

fitness values of the candidate solutions

Selection:

favour the better solutions

Recombination:

combine parts of solutions

Mutation:

random changes in each recombination

Replacement:

offspring replaces parental

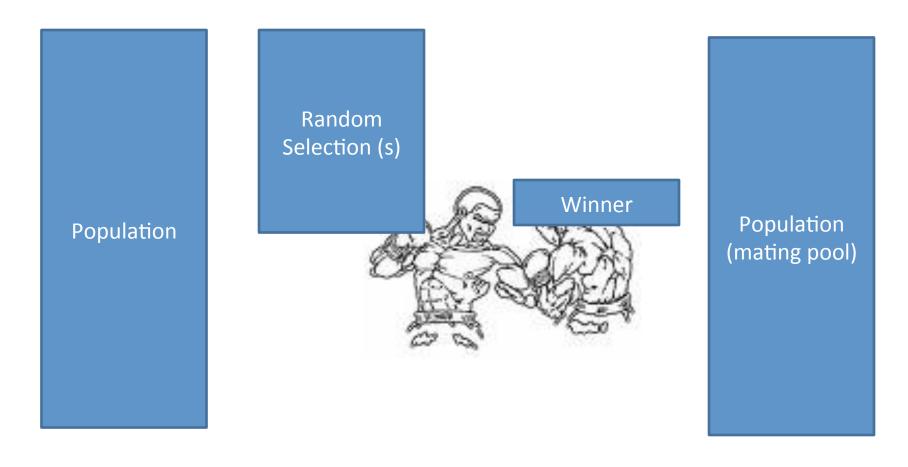
Genetic algorithms

- Selection
 - Fitness proportional, e.g. biased roulette wheel

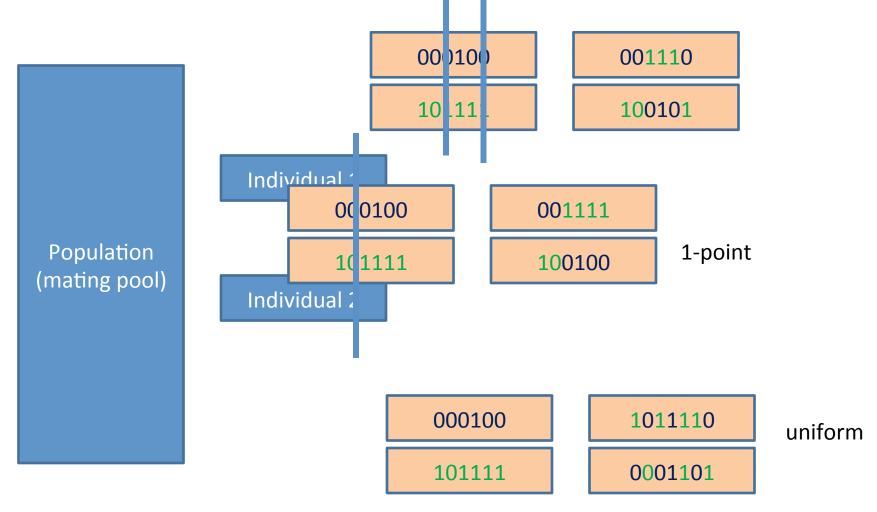


Genetic algorithms

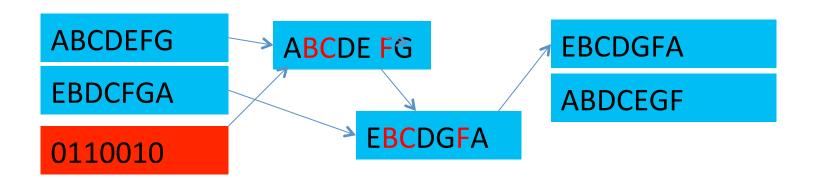
Tournament selection



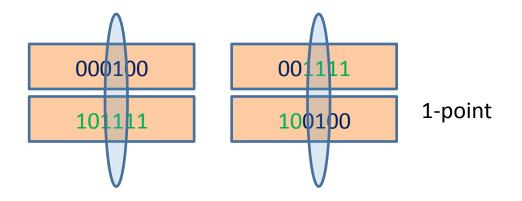
Genetic algorithms: Crossover (recombination): k-point



Genetic algorithms: crossover permutations: uniform order based



Genetic algorithms Mutation



Some genes never change Diversity

Mutation (at a low probability when compared to crossover) Flipover or problem specific

Genetic algorithms Replacement

Delete all

 Remove the whole population and replace it by the offspring

Steady-state

- Delet n old members and replace them with offspring members
- Best, parents,...

Steady-state no duplicates

Better coverage at a computational cost

Genetic algorithms other topics

Hybridization

- Combing GA with other technique, e.g. local search
 - Produce stronger results
 - Memetic algorithms
- Repair, initialisation, case based memory, heuristics

Applications: ample

 Machine scheduling, electrical power systems, sports scheduling, nuclear power plants, airline scheduling

Genetic algorithms: tricks

- Off the shelf
- Software package (GA-LIB)
- Representation
 - (bit-representation <-> complex data structures)
- Minimum: evaluation function
 - Problem specific data (intelligent crossover operators, heuristic initial population)
- Hybridize

Genetic algorithms: parameters

- Population size
- Mutation probability
- Crossover probability
 - --> Experiments (use statistics and ev. experimental design)
 - --> consider dynamic parameter settings (in fact introduces extra parameters)
 - -> Go to the literature

Some examples

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- Electrostatic potential

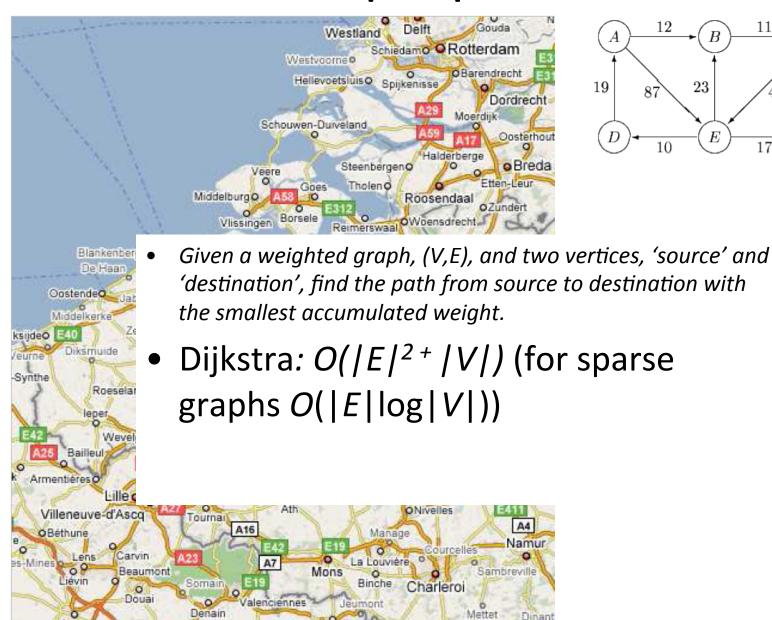
METAPHORS

Tabu Search: background

- Search space / landscape
- Heuristic moves through the landscape
- Hill climber
 - tries moves in the direction of (the fastest/some) improvement
- local optimum
 - Hill climber and has no way of escaping it
- 1983: simulated annealing (Kirkpatrick et al.)
 - 1986 tabu search (Glover), 1992 ant systems (Dorigo),
 1975 genetic algorithms (Holland)
 - > field of metaheuristics (Glover)

Example problem

B



Optimising what?

Bargiekaai 1, 9000 Gent naar Etienne Sabbelaan 53, 8500 Kortrijk - ...

http://maps.google.be/maps?f=d&hl=nl&geocode=&saddr=bargiekaa...



Beginpunt Bargiekaai 1 9000 Gent Eindpunt Etienne Sabbelaan 53 8500 Kortrijk Rei 48.9 km - ca 34 min.



Met de auto: 48.9 km - ca. 34 min.

	 Vertrek in noordoostelijke richting op d Bargiekaai 	e 67 m
+	2. Sla linksaf om op de Bargiekaai te blijv	en 58 m
+	3. Sla linksaf bij Noordstraat	30 m
→	4. Flauwe bocht naar rechts bij Waldamka	aai 0.1 km
	5. Ga verder op Coupure Rechts	0.6 km 2 min.
→	6. Sla rechtsaf bij Papegaaistraat	50 m
+	7. Sla linksaf bij Coupure Links	1.0 km 2 min.
+	8. Sla linksaf bij Nederkouter	0.1 km

Overzicht



Beginpunt



Stock cutting

X 10000

Ir

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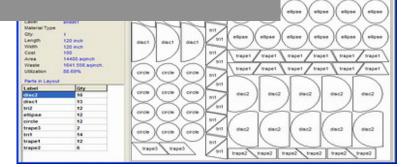
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How to

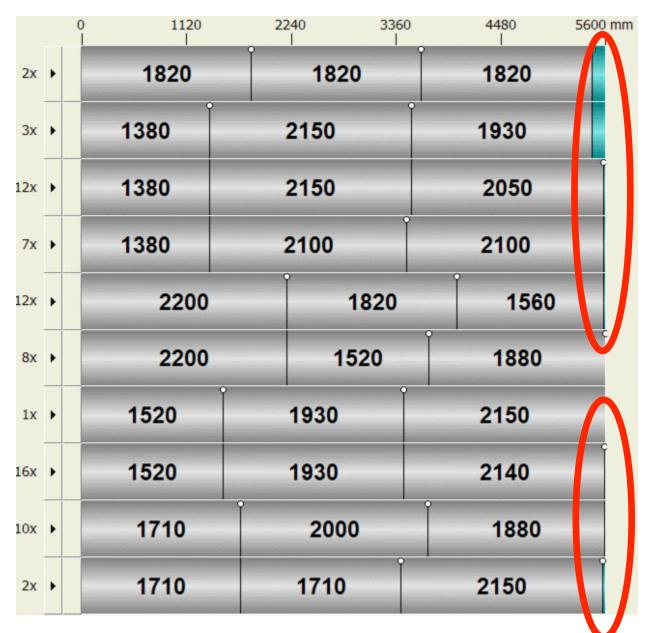
NP-complete, even in one dimension (pipe-cutting)

Integer programming, branch and bound, dynamic programming,...

Heuristics apply
 (E.K.Burke, G.Kendall and G.Whitwell, A New
 Placement Heuristic ..., Operations Research Volume 52
 Number 4, 2004)



Optimising what?



Optimising what?

- Goal function: measure of optimality
 - -> (only) guide through the space
- Shortest path problem
 - Find the path between source and destination of minimum total weight
- Stock cutting problem
 - Find the layouts that minimise the waste produced

Another example

- The Employee Timetabling Problem (ETP)
 - An ETP consists of assignments of employees to working shifts while satisfying all constraints
 - Constraints:
 - Shifts have start times and end times
 - Employees have a qualification
 - A required capacity per shift is given per qualification
 - Employees can work subject to specific regulations

• ...

Shift	1	2	3	4	5	7	1	2	3	C
Pjotr	Α	Α	Α			С	Τ	Т	F	1
Ludwig	С	С			R	R	Т	Т	Т	0
Clara	Т	Т	С		R	R	F	Т	Т	1
Hildegard			Α	Α	Α		Т	Т	Т	0
Johann			С	С			Т	Т	F	1
Wolfgang		С	Т	Т	С		Т	Т	Т	0
Guiseppe	R	R			Α	Α	F	Т	Т	1
Antonio	R	R			C	С	F	Т	Т	1
Arranger	2	2	2	1	0	0				
Tonesetter	1	2	1	1	0	0				
Composer	1	1	1	1	2	0				
Reader	3	1	1	1	2	0				

ETP: Optimise what?

- Just solve the problem (CP)
- (Weighed) number of constraints violated
- Weighted number of constraints violated
- Amount under assignment
- Amount over assignment
- This may lead to the definition of a goal function (representing a lot of domain information)

Shift	1	2	3	4	5	7	1	2	3	A
Pjotr	Α	Α	Α			С	Т	Т	Y	1
Ludwig	С	С			R	F	Т	Т	J	0
Clara	Т	Т	С		R	Fk	F	Т	-	1
Hildegard			Α	Α	Α		Т	Т	-	0
Johann			С	С			Т	Т	F	1
Wolfgang		С	Т	Т	С		Т	Т	7	0
Guiseppe	R	R			Α	A	F	Т	J	1
Antonio	R	R			С	C	F	Т		1
										V
Arranger	2	2	2	1	0	0				
Tonesetter	1	2	1	1	0	0				
Composer	1	1	1	1	2	0				
Reader	3	1	1	1	2	0				
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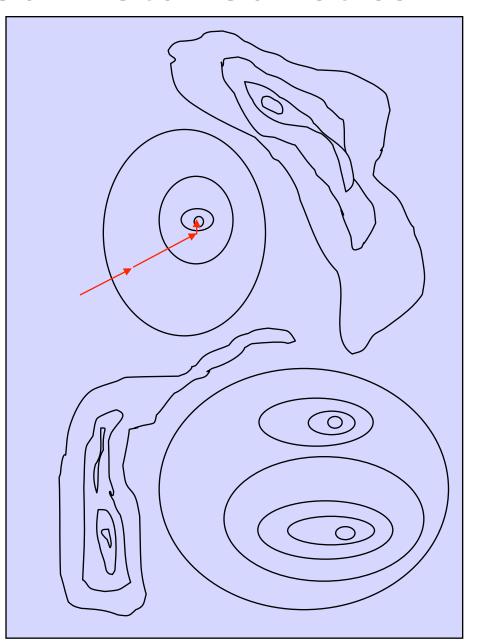
Heuristics for ETP

- One can easily think of
 - Swaps
 - Removals
 - Insertions
 - 'Large Swaps'
- These 'easy' options do depend on the domain
- They define 'steps' in a 'solution space' with an associated change in the goal function.
- One obvious heuristic is a hill-climber based on a selection of these possible steps.

		l	i	l						
Shift	1	2	3	4	5	7	1	2	3	C
Pjotr	Α	Α	Α			С	Т	Т	F	1
Ludwig	С	С			R	R	Т	Т	Т	0
Clara	Т	Т	С		R	R	F	Т	Т	1
Hildegard			Α	Α	Α		Т	Т	Т	0
Johann			С	С			Т	Т	F	1
Wolfgang		С	Т	Т	С		Т	Т	Т	0
Guiseppe	R	R			Α	Α	F	Т	Т	1
Antonio	R	R			С	С	F	Т	Т	1
Arranger	2	2	2	1	0	0				
Tonesetter	1	2	1	1	0	0				
Composer	1	1	1	1	2	0				
Reader	3	1	1	1	2	0				

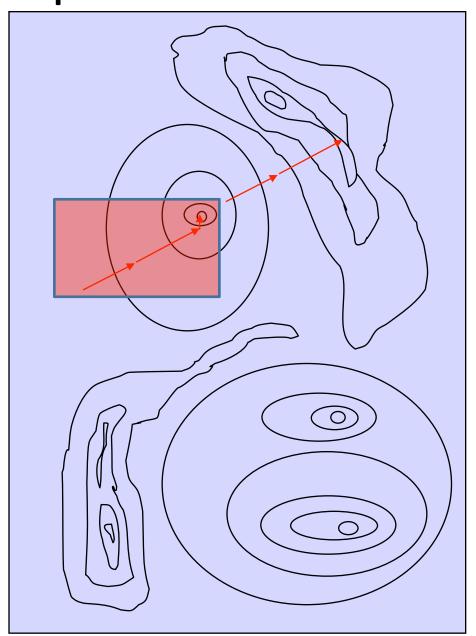
Local search based metaheuristics

- Hill-climbing allows to introduce domain specific elements through
 - The goal function
 - The selection of the steps
- It describes a procedure to use these elements in a procedure that eventually produces an answer
- It does not guarantee optimality
- This is a local search heuristic



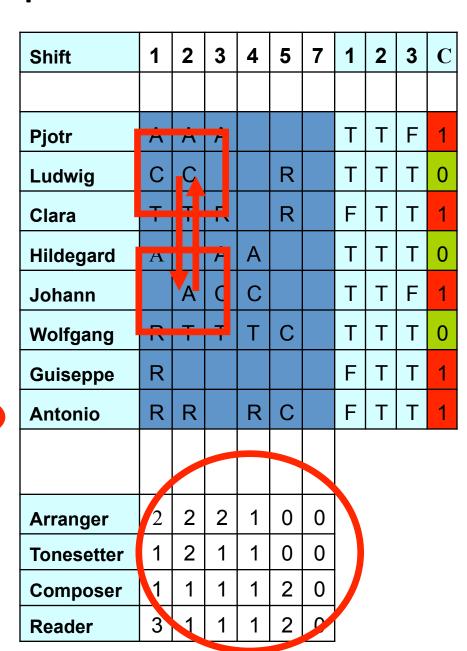
How to escape: Tabu

- While moving through the space, regions become forbidden
- This allows to escape from the local
- After a while, we may revisit
- Tabu supports diversification of the search
- Local search intensifies
- These phases alternate



Example ETP

- Initialise to satisfy the required amounts
- Allow only vertical swaps (neighbourhood)
- If a swap has influenced a certain region of the timetable, do not allow any other swap to influence this region for a specified number of moves (Tabu list, Tabu attributes)
 - The search has now been parametrised



Tabu search: tricks

- We introduced a number of parameters
- -> tuning
 - Neighbourhoods
 - List size
 - Aspectratio
 - Diversification/intensification
- Tabu search allows to introduce domain information through
 - the solution approach
 - the steps
 - the neighborhoods
 - the Tabu attributes

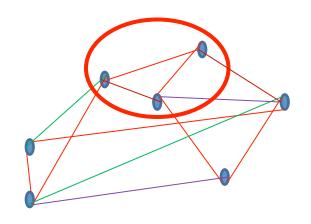
benchmarks

Important
sector
requiring a lot
of effort

Examples

- Nurse rostering
- Multimodal transportation
- Data mining
- Clustering
- Gene prioritisation
- Tourist guide

Another example: another neighborhood: 2-change in TSP



- (n-1)! or (n-1)!/2 Routes
- 2-change connects them all
 - -> connectedness of search space
- Lin, Lin and Kernighan: k-opt

Some examples

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- Simulated annealing
- Great deluge
- Hyperheuristics

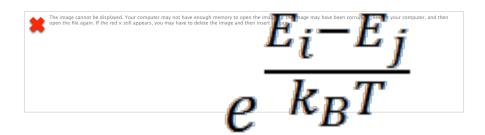
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METAPHORS

Annealing

- Solid state physics
 - Increase the temperature above melting point
 - Decrease carefully the temperature until the particles arrange in the gound state
- Ground state: minimal energy
- **1953** (Metropolis)
 - Simulate annealing in materials by Monte Carlo techniques

- Use **perturbation** to generate a new state j (energy E_j) from an existing state I (energy E_i)
- If $E_i E_i < 0$ accept state j
- If $E_i E_i > 0$ accept state j with probability
- (T is the temparature, k_B is the Boltzmann constant)



- If the temperature decreases sufficiently slowly, the solid reaches *Thermal equilibrium* at each temperature.
- The Metropolis algorithm generates a large number of transitions at a given temperature.
- Thermal equilibrium:

$$P_T[X = i] = \frac{\exp(-E_i/k_B T)}{\sum_j \exp(-E_j/k_B T)}$$

- Solutions combinatorial optimisation problem
 - <-> states of the physical system
- Cost of a solution
 - <-> energy of a state
- Control parameter c
 - <-> temperature * Boltzmann constant
- -> basic simulated annealing algorithm (Kirkpatrick 1983)

Simulated annealing algorithm

- Initialize (i_{start}, c₀,L₀)
- Let k = 0, $i = i_{start}$
- Repeat until stopcriterion is met
 - For l=1 to L_k do
 - Generate (j from S_i)
 - If f(j) < f(i) then i = j
 - Else if exp(f(i)-f(j)/ck) > random[0,1) then i =j
 - k = k + 1
 - Compute length (L_k) , control (c_k)

Simulated annealing Theorem (Aarts, Korst)

- S, f is an instance of an optimisation problem (S is the solution space, f is the goal function)
- A sufficiently large number of transitions in the SA algorithm leads to the probability of state i in S:

$$P_T[X=i] = \frac{\exp(-f(i)/c)}{N_0(c)} \qquad P_T[X=i] \equiv q(i)$$

$$N_0(c) = \sum_{j \text{ in } S} \exp(-\frac{f(i)}{c})$$

Simulated annealing Corollary(Aarts, Korst)

• It is not hard to prove that from the theorem follows: (S^*) is the set of globally optimal solutions in S, X_A is the characteristic function on the set A)

$$\lim_{c\to 0} q_i(c) = \frac{1}{|S^*|} \chi_{S^*}(i)$$

- Is open to statistical (theoretical) analysis
- Works well for graph partitioning problems
- Produces competitive results for quadratic assignment, scheduling and graph colouring at a computational cost
- Underperforms with respect to tailored solutions for TSP, number partitioning, ...

Simulated annealing and the real world

- VLSI, image processing, assembly
 - > no tailored algorithms are available, goal function is messy
- Better than time-equivalent iterative improvement. More substantial for larger problems.
- Depends on skill and effort! (neighborhood, Cooling,..)

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METAPHORS

Variable neighborhood search (Mladenovic and Hanssen 1997)

Fact 1

A local minimum with respect to one neighborhood structure is not necessarily so for another

Fact 2

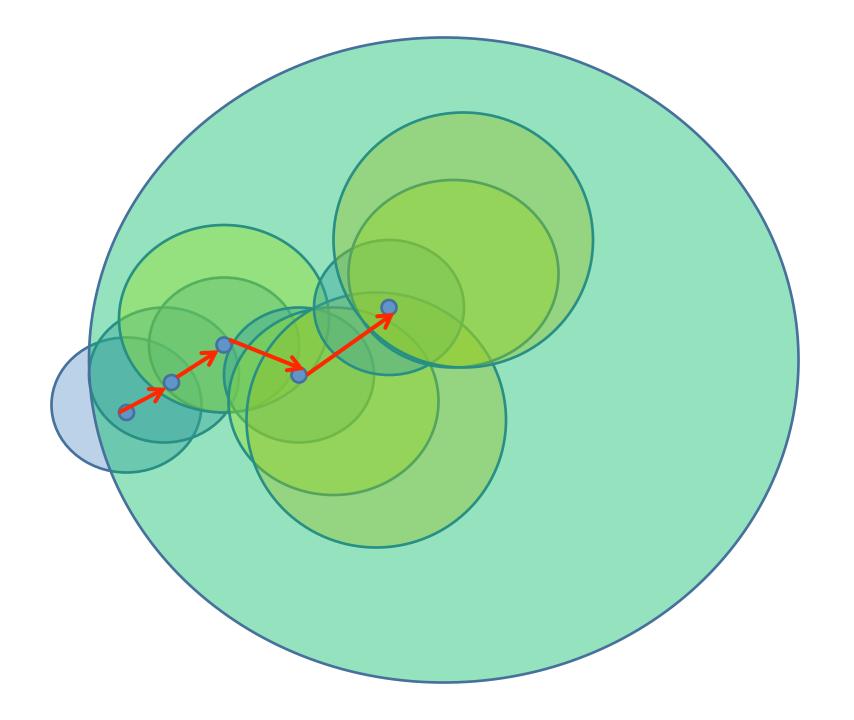
A global minimum is a local minimum with respect to all neighborhood structures

Fact 3

For many problems local minima with respect to one or several neighbourhoods are relatively close to each other

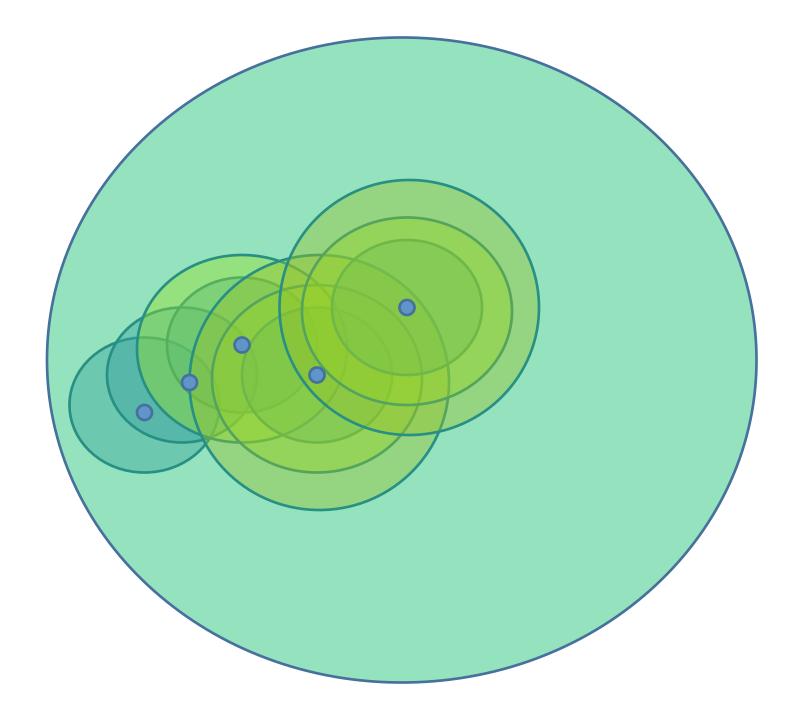
Variable neighbourhood search Descent

- Select a set of neighbourhood structures N_{l} (l = 1 to l_{max}) Find an initial solution x
- Set I = 1, repeat until I = I_{max}
 - Exploration:
 - find the best neighbour x' of x in $N_1(x)$
 - Acceptance
 - If the solution x' is better than x, let x = x', I = 1
 - else let | = |+1



Variable neighbourhood search Reduced

- Select a set of neighbourhood structures N_{l} (l = 1 to l_{max}) Find an initial solution x; choose a stoping condition
- Repeat until the stopping condition is met
- Let I = 1; repeat until I = I_{max}
 - Shake:
 - Generate a random neighbor x' of x in N_I(x)
 - Acceptance
 - If the solution x' is better than x, let x = x', l = 1
 - else let | = |+1

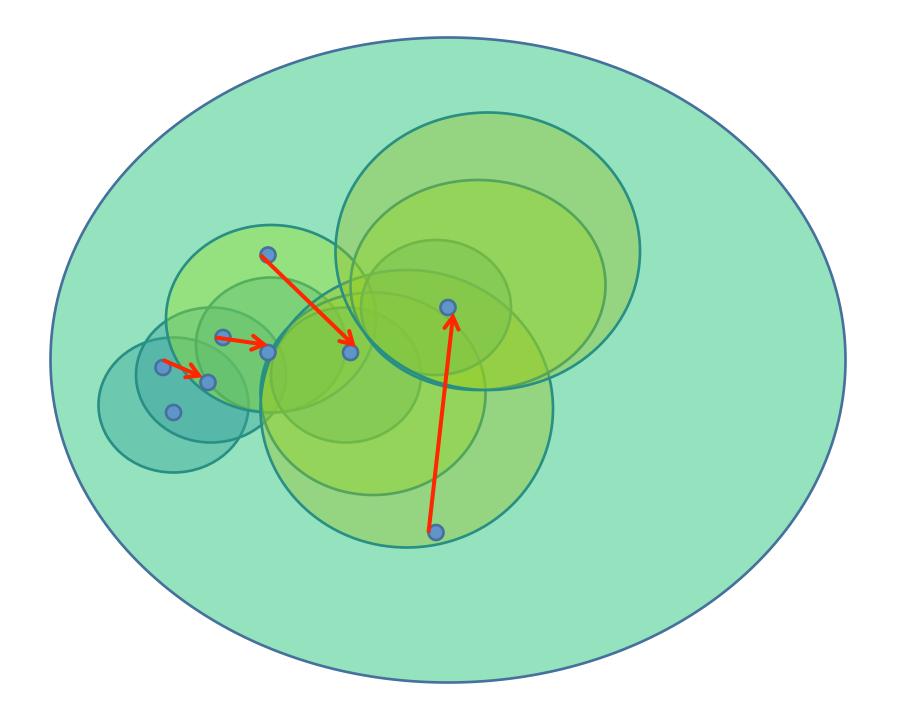


Variable neighbourhood reduced

- Neighbourhoods are often nested here, and in any case, lower I neighbourhoods should be smaller
- Results in an intensification/diversification behaviour of the algorithm
- This bears on Fact 3 (closeness of local optima) and Fact 2 (once we make it to the last (largest) neighbourhood we may be in a global optimum

Variable neighbourhood Basic

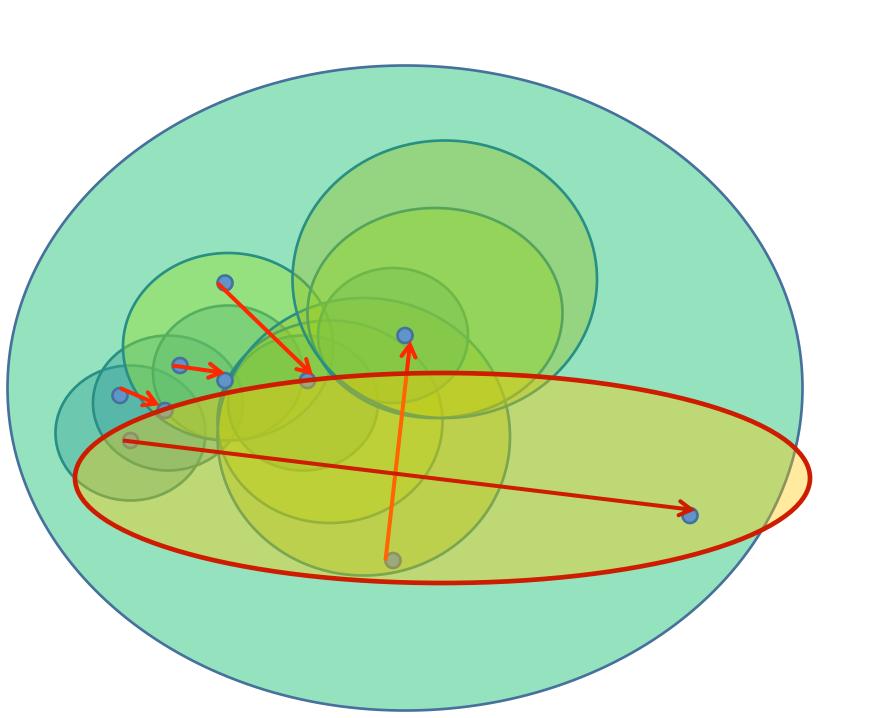
- Select a set of neighbourhood structures $N_l(l = 1 \text{ to } l_{max})$ Find an initial solution x; choose a stoping condition
- Repeat until the stopping condition is met
- Let I = 1; repeat until I = I_{max}
 - Shake:
 - find a random neighbour x' of x in $N_1(x)$
 - Local search
 - Local search with x' as initial solution to find x"
 - Acceptance
 - If the solution x" is better than x, let x = x", l = 1
 - else let l = l+1



Variable neighbourhood search General

~RVNS

- Select a set of neighbourhood structures N_k (k = 1 to k_{max}) for shaking, N_l (l = 1 to l_{max}) for local search. Find an initial solution x and improve it by RVNS; choose a stoping condition
- Repeat until the stopping condition is met
- Let k = 1
- Repeat until k = k_{max}
 - Shake:
 - find a random neighbour x' of x in N_k(x)
 - Let I = 1; repeat until $I = I_{max}$
 - Explore:
 - find the best neighbour x'' of x' in $N_l(x')$
 - Acceptance
 - If x" is better than x', let x' = x", l = 1, else let l = l+1
 - Acceptance
 - If the local minimumb x" is better than x, let x = x", k = 1
 - else let k = k+1



Applications

- Graph theory
- Plant location
- Timetabling
- ETP
- ...

Shift	1	2	3	4	5	7	1	2	3	C
Pjotr	Α	Α	Α			С	Т	Т	F	1
Ludwig	C	C			R	R	Т	Т	Т	0
Clara	Т	Т	С		R	R	F	Т	Т	1
Hildegard			Α	Α	Α		Т	Т	Т	0
Johann			C	С			Т	Т	F	1
Wolfgang		С	Т	Т	С		Т	Т	Т	0
Guiseppe	R	R			Α	Α	F	Т	Т	1
Antonio	R	R			С	С	F	Т	Т	1
Arranger	2	2	2	1	0	0				
Tonesetter	1	2	1	1	0	0				
Composer	1	1	1	1	2	0				
Reader	ധ	1	1	1	2	0				

(Variable neighbourhood) Tricks,...

- Familiarization
- Read
- Test instances
- Data structure
- Initial solution
- Objective value calculation
- Shaking
- Local search

- First-Best improvement
- Reduce neighborhood
- Intensify shaking
- Neighborhood structures
- Parameter setting
 - 1 parameter in VNS: the number of neighborhoods

General important properties for metaheuristics

- Simplicity (clear principle)
- Precision (mathematical)
- Coherence (principle)
- Efficiency (near optimal)
- Effectiveness (computing time)
- Robustness (variety of instances)
- User friendliness (parameters)
- Innovation (new applications)

Some examples

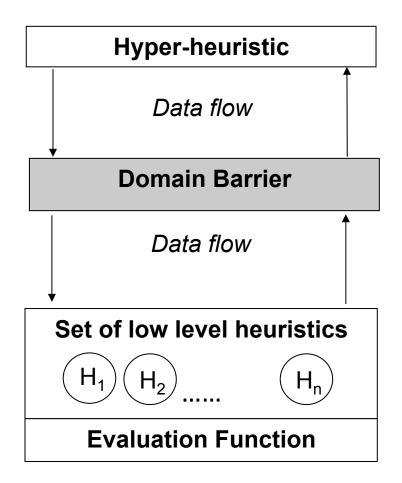
- Genetic algorithms
- Evolutionary algorithms
- Tabu search
- Simulated annealing
- Great deluge
- Hyperheuristics

- Variable neighbourhood search
- Late acceptance
- Extreme optimisation
- Neural networks
- Electrostatic potential

METAPHORS

- Simple Idea: Heuristics to choose heuristics
- Operates on a search space of heuristics rather than directly on a search space of solutions

- Metaheuristics tackle specific problems
- Are often tailored
- Can we increase the level of generality?
- Good enough, cheap enough, fast enough?



- No 'Superalgorithms' (No Free Lunch)
- Intelligent schemes that function well on a number of problems
- Give the developer extra handles to bring in his domain expertise without requiring him to study the details of an advanced optimisation strategy

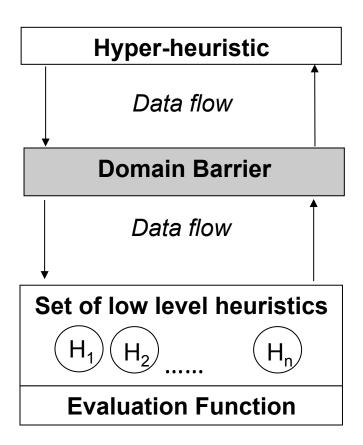
Hyperheuristics Example

- Choice Function
- f1 + f2 + f3
- How well has each heuristic done +
- How well have pairs of heuristics done +
- Time since last called
- Applied to sales summit scheduling,
- nurse rostering, exam timetabling

- Sales Summit Scheduling
- Low level heuristics are based on three types of neighborhood moves:
 - Add / Remove one delegate to / from the current solution
 - Add / remove a meeting to / from the current solution (random, 1st improving, best improving, etc)
 - Remove excess of meetings from an overloaded delegate

- Nurse Rostering, Exam timetabling
 - Competitive with other results in the literature
 - Same algorithm worked across a range of problems

- Above the domain barrier
 - Genetic algorithm
 - Genetic programming
 - Tabusearch
 - Simple random
- Room for machine learning
 - Learn the weights of the low level heuristics
 - Relate them to solution space features (> expert?!)
 - Reduce the number of parameters
- Hyper heuristic competition



Conclusions

- Combinatorial problems often require heuristic approaches
- Metaheuristics offer a framework to express domain knowledge
- Hyperheuristics separate domain expertise from heuristics expertise
- No single best one fits all solution
- Often a lot of tailoring is required

Heuristics and Learning

- Machine learning may help to reduce the number of parameters
- What should we look at
 - What are solution space features
 - How to recognise phases in the search
 - E.g. diversification/intensification
 - What does the heuristic really need to see?
 - Hyperheuristics going on performance alone (improvement, time taken,...)

Heuristics and learning

- Online/Offline learning
- Features
 - Expert specified
 - Automatically detected
 - Generically generated
- -> An example, off line, from nurse rostering