DM811
Heuristics for Combinatorial Optimization

Lecture 14
Stochastic Local Search and Metaheuristics (2/2)

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Course Overview

1. Combinatorial Optimization, Methods and Models
2. General overview
3. Solver System and Working Environment
4. Construction Heuristics
5. Local Search: Components, Basic Algorithms
6. Local Search: Neighborhoods and Search Landscape
7. Efficient Local Search: Incremental Updates and Neighborhood Pruning
8. Stochastic Local Search & Metaheuristics
9. Methods for the Analysis of Experimental Results
10. Configuration Tools: F-race
11. Very Large Scale Neighborhoods

Examples: GCP, CSP, TSP, SAT, MaxIndSet, SMTWP, Steiner Tree

SLS Methods and Metaheuristics

Trajectory based:

- Stochastic Local Search
- Simulated Annealing
- Iterated Local Search
- Tabu Search
- Variable Neighborhood Search
- Guided Local Search

Poplation based:

- Evolutionary Algorithms
- (Ant Colony Optimization)
- (Particle Swarm Optimization)
- (Scatter Search and Path Relinking)
- (Cross Entropy Method / Estimation of Distribution Algorithms)

Outline

1. Population Based Metaheuristics
    Evolutionary Algorithms

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1. Population Based Metaheuristics
    - Evolutionary Algorithms

Evolutionary Algorithms

Key idea (Inspired by Darwinian model of biological evolution): Maintain a population of individuals that compete for survival, and generate new individuals, which in turn again compete for survival

Iteratively apply genetic operators mutation, recombination, selection to a population of candidate solutions.

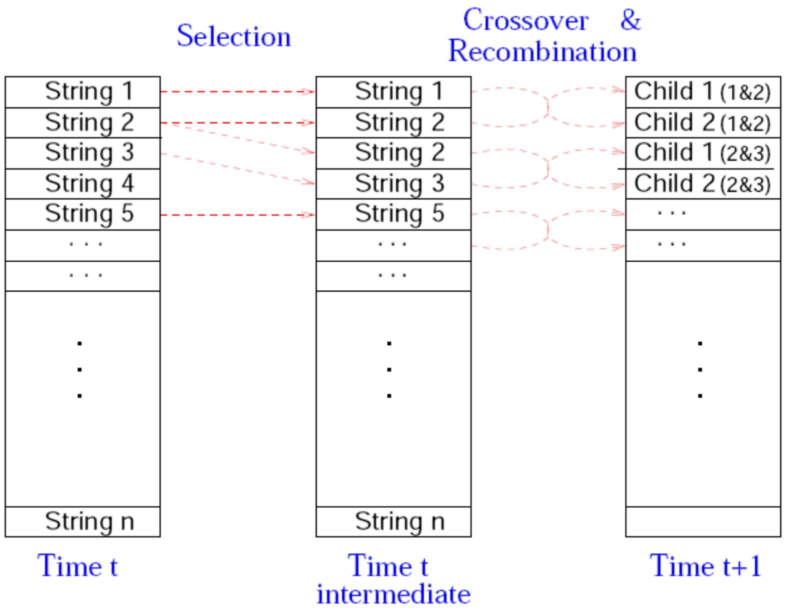
- Mutation introduces random variation in the genetic material of individuals (unary operator)
- Recombination of genetic material during reproduction produces offspring that combines features inherited from both parents (N-ary operator)
- Differences in evolutionary fitness lead selection of genetic traits ('survival of the fittest').

```
Evolutionary Algorithm (EA):
determine initial population sp

while termination criterion is not satisfied: do
    generate set spr of new candidate solutions
      by recombination

    generate set spm of new candidate solutions
      from spr and sp by mutation

    select new population sp from
      candidate solutions in sp, spr, and spm
```



Original Streams

- Evolutionary Programming [Fogel et al. 1966]:
  - mainly used in continuous optimization
  - typically does not make use of recombination and uses stochastic selection based on tournament mechanisms.
  - often seeks to adapt the program to the problem rather than the solutions

- Evolution Strategies [Rechenberg, 1973; Schwefel, 1981]:
  - similar to Evolution Programming (developed independently)
  - originally developed for (continuous) numerical optimization problems;
  - operate on more natural representations of candidate solutions;
  - use self-adaptation of perturbation strength achieved by mutation;
  - typically use elitist deterministic selection.

- Genetic Algorithms (GAs) [Holland, 1975; Goldberg, 1989]:
  - mostly for discrete optimization;
  - often encode candidate solutions as bit strings of fixed length, (which is now known to be disadvantageous for combinatorial problems such as the TSP).

Problem: Pure evolutionary algorithms often lack capability of sufficient search intensification.

Solution: Apply subsidiary local search after initialization, mutation and recombination.

Memetic Algorithms [Dawkins, 1997, Moscato, 1989]

- transmission of memes, mimicking cultural evolution which is supposed to be direct and Lamarckian
- (aka Genetic/Evolutionary Local Search, or Hybrid Evolutionary Algorithms if more involved local search including other metaheuristics, eg, tabu search)

Memetic Algorithm (MA):

```
determine initial population sp
perform subsidiary local search on sp
while termination criterion is not satisfied: do
    generate set spr of new candidate solutions
        by recombination
    perform subsidiary local search on spr
    generate set spm of new candidate solutions
        from spr and sp by mutation
    perform subsidiary local search on spm
    select new population sp from
        candidate solutions in sp, spr, and spm
```

Terminology

Individual	$\Longleftrightarrow$	Solution to a problem
Genotype space	$\Longleftrightarrow$	Set of all possible individuals determined by the solution encoding
Phenotype space	$\Longleftrightarrow$	Set of all possible individuals determined by the genotypes (ie, the variable–value themselves)
Population	$\Longleftrightarrow$	Set of candidate solutions
Chromosome	$\Longleftrightarrow$	Representation for a solution in the population
Gene and Allele	$\Longleftrightarrow$	Part and value of the representation of a solution (*e.g.*, parameter or degree of freedom)
Fitness	$\Longleftrightarrow$	Quality of a solution
Crossover Mutation	$\Longleftrightarrow$	Search Operators
Natural Selection	$\Longleftrightarrow$	Promoting the reuse of good solutions

Solution representation

Separation between solution encode/representation (genotype) from actual solution (phenotype)

Let $\mathcal{X}$ be the search space of a problem

- genotype set made of strings of length l whose elements are symbols from an alphabet $\mathcal{A}$ $\rightsquigarrow$ set of all individuals is $\mathcal{A}^l$
  - the elements of strings are the genes
  - the values that each element can take are the alleles
- the search space is $\mathcal{S} \subseteq \mathcal{A}^l$ (set of feasible solutions)
- if the strings are member of a population they are called chromosomes and their recombination crossover
- an expression maps individual to solutions (phenotypes) $c : \mathcal{A}^l \to \mathcal{X}$ (example, unrelated parallel machine and Steiner tree)
- strings are evaluated by $f(c(s)) = g(s)$ which gives them a fitness

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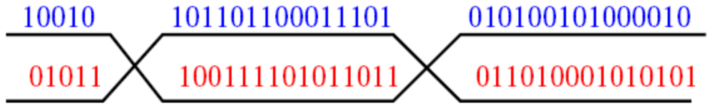
Example

1001010 1101100 0111010 1010010 1000010

0101110 0111101 0110110 1101000 1010101



Which Produces the Offspring

01011101101100011101011010001010101

10010100111101011011010100101000010

Note: binary representation is appealing but not always good (in constrained problems binary crossovers might not be good)

Conjectures on the goodness of EA

schema: subset of $\mathcal{A}^l$ where strings have a set of variables fixed.
Ex.: $S = 1 * * 1$

1. exploit intrinsic parallelism of schemata (but epistasis)
2. Schema Theorem:

$$E[N(S, t+1)] \geq \frac{F(S,t)}{\bar{F}(t)} N(s,t)[1 - \epsilon(S,t)]$$

$\bar{F}(t)$ av. fitness of population, $F(S,t)$ fitness schema, $\epsilon(S,t)$ destroy effect of operators

- a method for solving all problems $\Rightarrow$ disproved by No Free Lunch Theorems: no metaheuristic is better than rnadom search; success comes from adapting the method to the problem at hand
- building block hypothesis

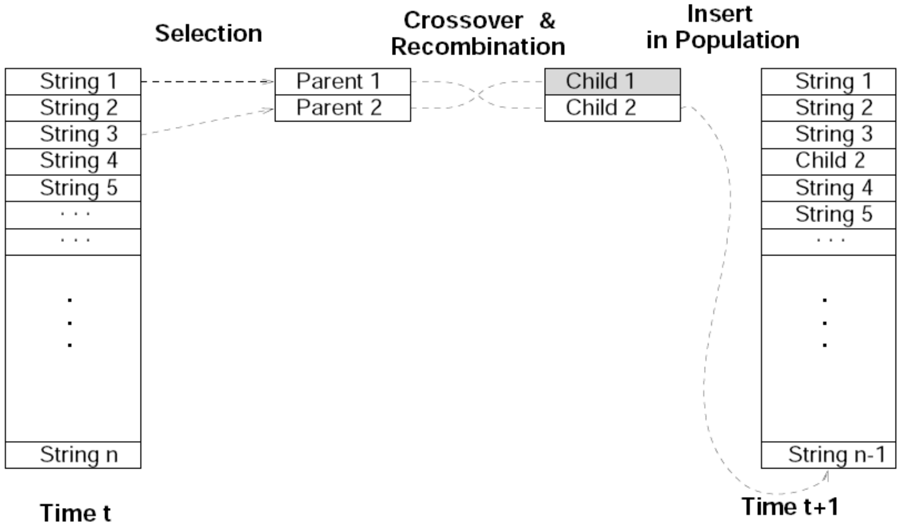
Initial Population

- Generation: often, independent, uninformed random picking from given search space.
- Which size? Trade-off
- Minimum size: connectivity by recombination is achieved if at least one instance of every allele is guaranteed to be present at each gene.
  Eg: binary repr. and uniform sampling with replacement:

$$\Pr\{\text{presence of allele in M strings of length } l\} = (1 - (0.5)^{M-1})^l$$

  for $l = 50$, it is sufficient $M = 17$ to guarantee $P_2^* > 99.9\%$.
- Attempt to cover at best the search space, eg, Latin hypercube, Quasi-random (low-discrepancy) methods (Quasi-Monte Carlo method).
- But: can also use multiple runs of randomized construction heuristic.

Selection



Selection

Main idea: selection should be related to fitness

- Fitness proportionate selection (roulette-wheel method)

$$p_i = \frac{f_i}{\sum_j f_j}$$

- Tournament selection: a set of chromosomes is chosen and compared and the best chromosomes chosen.
- Rank based and selection pressure
- Fitness sharing (aka niching): probability of selection proportional to the number of other individuals in the same region of the search space.

Selection pressure:
$p_k = \alpha + \beta k$ probability for individual k

$$\begin{cases} \sum_{k=1}^{M}(\alpha + \beta k) = 1 \\ \phi = \frac{\Pr[\text{selecting the best}]}{\Pr[\text{selecting the median}]} \end{cases} \qquad \text{selection pressure}$$

$\Pr[\text{selecting the best}] = \alpha + \beta M$; $\Pr[\text{selecting the median}] = \alpha + \beta(\frac{M+1}{2})$
Solving the system of equations

$$\alpha = \frac{2M - \phi(M+1)}{M(M-1)} \qquad \beta = \frac{2(\phi - 1)}{M(M-1)} \qquad 1 \leq \phi \leq 2$$

Then for a pseudo-random number the selected individual k from the cumulative probability is found in $O(1)$ solving the quadratic equation:

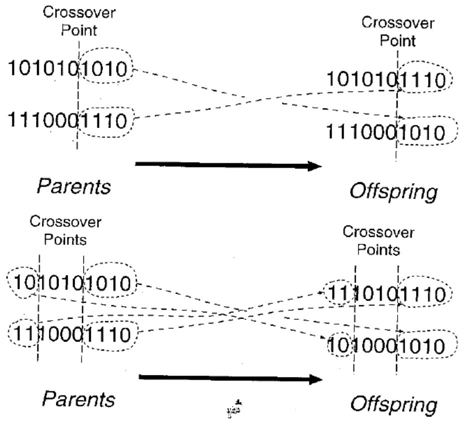
$$\sum_{i=1}^{k} \alpha + \sum_{i=1}^{k} \beta i = \alpha k + \beta \frac{(k+1)k}{2} = r$$

Crossovers

Recombination operator (Crossover)

- Binary or assignment representations
  - one-point, two-point, m-point (preference to positional bias w.r.t. distributional bias)
  - uniform cross over (through a mask controlled by a Bernoulli parameter p)
- Permutations
  - Partially mapped crossover (PMX)
  - Mask based crossover
  - Order crossover (OX)
  - Cycle crossover (CX)
- Sets
  - greedy partition crossover (GPX)
- Real vectors
  - arithmetic crossovers
  - k-point crossover

Example: crossovers for binary representations



Uniform (mask):

s1: 1010101010
s2: 1110001110

mask: 1101011110

o1: 1010001010
o2: 1110101110

Permutations: relations of interest: adjacency, relative position, absolute position
Partially mapped crossover: defines interchanges

s1: 16 345 2
s2: 43 126 5

o1: __ 126 _
o2: __ 345 _

o1: 35 126 4
o2: 21 345 6

Order crossovers:
One point crossover: $q \in \{1..n\}$ at random

$$\begin{array}{ll} \pi^{o_1}_\lambda := \pi^{s_2}_\lambda & \lambda = 1..q \\ \pi^{o_1}_\lambda := \pi^{s_1}_k & k \text{ smallest with } \pi^{s_1}_k \notin \{\pi^{o_1}_1 .. \pi^{o_1}_\lambda\} \end{array}$$

s1: 7132 58469
s2: 1426 39875

o1: 1426 73589
o2: 7132 46985

preserves relative positions

Order crossovers:
Two point crossover: $q_1, q_2 \in \{1..n\}$, $q_1 < q_2$ at random

$$\begin{array}{lll} \pi^{o_1}_\lambda := \pi^{s_2}_\lambda & & \lambda = 1..q \\ \pi^{o_1}_\lambda := \pi^{s_1}_k & & k \text{ smallest with } \pi^{s_1}_k \notin \{\pi^{o_1}_1..\pi^{o_1}_\lambda\} \end{array}$$

```
s1:   71 3258 469
s2:   14 2639 875

o1:   71 ____ 469
o2:   14 ____ 875

o1:   71 2385 469
o2:   14 ____ 875
```

preserves relative positions

Order crossovers:
Uniform crossover: $\lambda = \{1..n\}$, $\xi_\lambda \in \{0,1\}$

$$\begin{array}{llll} if \xi_\lambda = 1 & \pi^{o_1}_\lambda := \pi^{s_2}_k & & k \text{ smallest with } \pi^{s_2}_k \notin \{\pi^{o_1}_1..\pi^{o_1}_\lambda\} \\ if \xi_\lambda = 0 & \pi^{o_1}_\lambda := \pi^{s_1}_k & & k \text{ smallest with } \pi^{s_1}_k \notin \{\pi^{o_1}_1..\pi^{o_1}_\lambda\} \end{array}$$

Cycle crossover:

- divide elements into cycles
- select randomly cycles from parents

Positions:	1	2	3	4	5	6	7	8	9	10	11	12
Parent 1:	A	B	C	D	E	F	G	H	I	J	K	L
Parent 2:	h	k	c	e	f	d	b	l	a	i	g	j
Cycle label:	1	2	3	4	4	4	2	1	1	1	2	1
Offspring:	A	k	C	e	f	d	b	H	I	J	g	L

Partitions:
Greedy partitioning crossover

```
s1={{1,2,3,4}{5,6,7}{8,9,10}}
s2={{4,6,7,8},{1,2,10},{3,5,9}}
```

choose the largest set left alternating parent selection

```
s1={{ , , , }{5, , }{ , ,  }}
s2={{ , , , },{ , ,  },{ ,5, }}
```

```
o1={{1,2,3,4},{6,7,8},{9,10}}
```

reassign randomly left elements

```
o1={{1,2,3,4},{6,7,8,5},{9,10}}
```

- Crossovers appear to be a crucial feature of success
- Therefore, more commonly: ad hoc crossovers
- Two off-springs are generally generated
- Crossover rate controls the application of the crossover. May be adaptive: high at the start and low when convergence

Mutation

- Goal: Introduce relatively small perturbations in candidate solutions in current population + offsprings obtained from recombination
- Typically, perturbations are applied stochastically and independently to each candidate solution
- Mutation rate controls the application of bit-wise mutations.
  It may be adaptive: low at the start and high when convergence
- Possible implementation through Poisson variable which determines the m genes which are likely to change allele.
- Can also use subsidiary selection function to determine subset of candidate solutions to which mutation is applied.
- With real vector representation: Gaussian mutation

Subsidiary local search

- Often useful and necessary for obtaining high-quality candidate solutions.
- Typically consists of selecting some or all individuals in the given population and applying an iterative improvement procedure to each element of this set independently.

New Population

- Determines population for next cycle (generation) of the algorithm by selecting individual candidate solutions from
  - current population +
  - new candidate solutions from recombination, mutation (and subsidiary local search).
- Generational Replacement (λ, μ): $\lambda \leftarrow \mu$
- Elitist strategy $(\lambda + \mu)$ the best candidates are always selected
- Steady state (most common) only a small number of least fit individuals is replaced
- Goal: Obtain population of high-quality solutions while maintaining population diversity.

  Survival of the fittest and maintenance of diversity (duplicates avoided)

Example

A memetic algorithm for TSP

- **Search space:** set of Hamiltonian cycles
  Tours represented as permutations of vertex indexes.
- **Initialization:** by randomized greedy heuristic (partial tour of $n/4$ vertices constructed randomly before completing with greedy).
- **Recombination:** greedy recombination operator GX applied to $n/2$ pairs of tours chosen randomly:
  1) copy common edges (param. p_e)
  2) add new short edges (param. p_n)
  3) copy edges from parents ordered by increasing length (param. p_c)
  4) complete using randomized greedy.
- **Subsidiary local search:** LK variant.
- **Mutation:** apply double-bridge to tours chosen uniformly at random.
- **Selection:** Selects the μ best tours from current population of $\mu + \lambda$ tours (=simple elitist selection mechanism).
- **Restart operator:** whenever average bond distance in the population falls below 10.

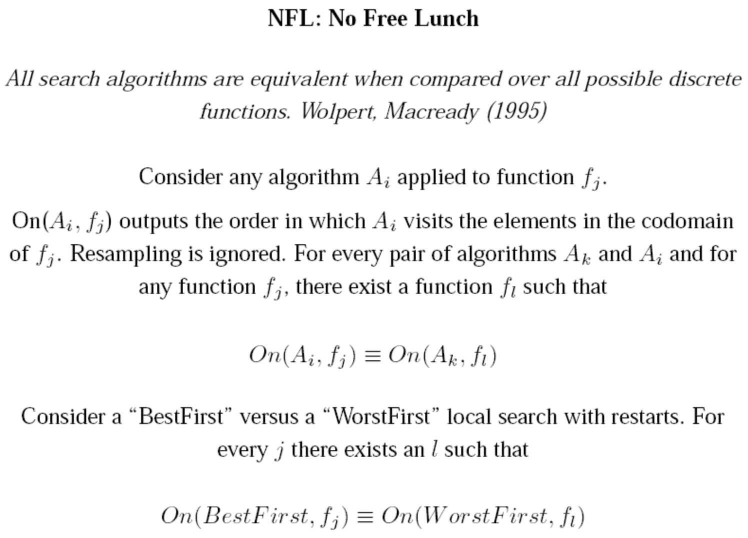
Theoretical studies

- Through Markov chains modelling some versions of evolutionary algorithms can be made to converge with probability 1 to the best possible solutions in the limit [Fogel, 1992; Rudolph, 1994].
- Convergence rates on mathematically tractable functions or with local approximations [Bäck and Hoffmeister, 2004; Beyer, 2001].
- "No Free Lunch Theorem" [Wolpert and Macready, 1997]. On average, within some assumptions, blind random search is as good at finding the minimum of all functions as is hill climbing.

However:

- These theoretical findings are not very practical.
- EAs are made to produce useful solutions rather than perfect solutions.

No Free Lunch Theorem



NFL: No Free Lunch

All search algorithms are equivalent when compared over all possible discrete functions. Wolpert, Macready (1995)

Consider any algorithm A_i applied to function f_j.

On(A_i, f_j) outputs the order in which A_i visits the elements in the codomain of f_j. Resampling is ignored. For every pair of algorithms A_k and A_i and for any function f_j, there exist a function f_l such that

$$On(A_i, f_j) \equiv On(A_k, f_l)$$

Consider a “BestFirst” versus a “WorstFirst” local search with restarts. For every j there exists an l such that

$$On(BestFirst, f_j) \equiv On(WorstFirst, f_l)$$

Research Goals

- Analyzing classes of optimization problems and determining experimentally the best components for evolutionary algorithms.

- Applying evolutionary algorithms to problems that are dynamically changing.

- Gaining theoretical insights for the choice of components.

- Prove bounds on the runtime that such algorithms have in order to obtain optimal or nearly optimal solutions.
  (Bio-inspired algorithms are
  - general-purpose algorithms
  - randomized algorithms = stochastic search algorithms

  computational complexity analysis is achieved by bounding the expected runtime to achieve good solutions for a certain problem

References

Moraglio A. and Poli R. (2011). **Topological crossover for the permutation representation**. *Intelligenza Artificiale*, 5(1), pp. 49–70.

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Reeves C. (2002). **Genetic algorithms**. In *Handbook of Metaheuristics*, edited by F. Glover and G. Kochenberger, vol. 57 of **International Series in Operations Research & Management Science**, pp. 55–82. Kluwer Academic Publishers, Norwell, MA, USA.