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Heuristics and Approximation Algorithms

Evolutionary Algorithms

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Outline

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 Evolutionary 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)

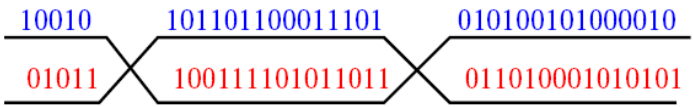
Let $\mathcal{X}$ be the search space of a problem

- 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

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

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 random search; success comes from adapting the method to the problem at hand
- building block hypothesis

Initial Population

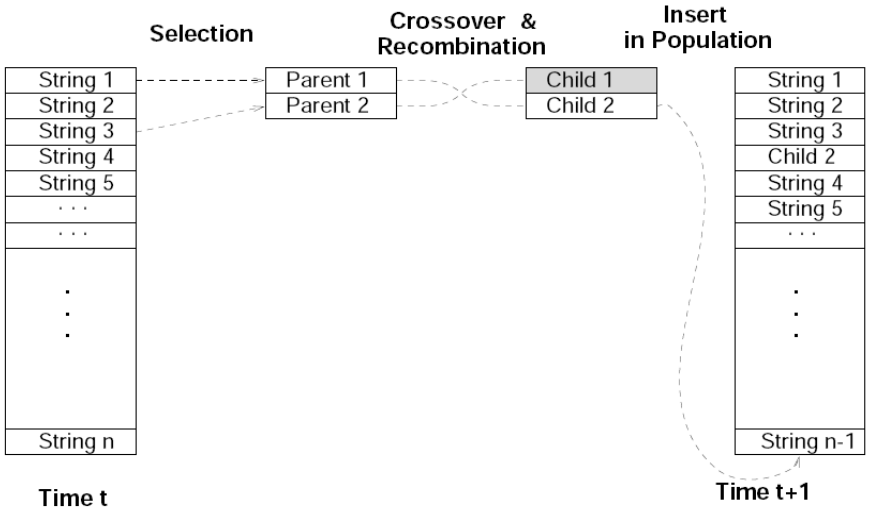
- Generation: often, independent, uninformed random picking from given search space.
- Which size? Trade-off
- Minimum size: connectivity by recombination is achieved if at least one instance of every allele is guaranteed to be present at each gene.
  Eg: binary repr. and uniform sampling with replacement:

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

  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
Crossover & Recombination
Insert in Population
String 1
String 2
String 3
String 4
String 5
String n
Parent 1
Parent 2
Child 1
Child 2
String 1
String 2
String 3
Child 2
String 4
String 5
String n-1
Time t
Time t+1

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 ranked kth (linear function)

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

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

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

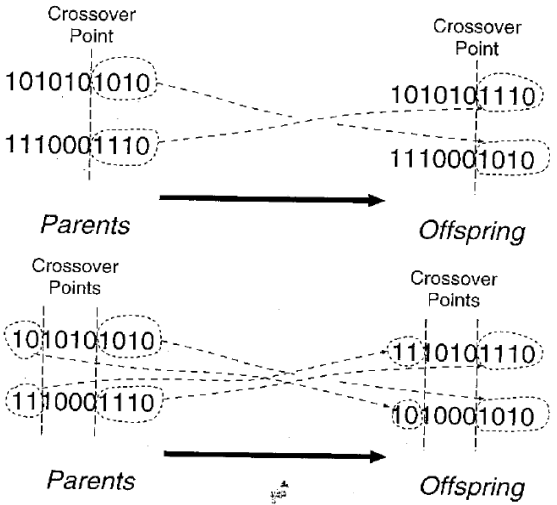
Crossovers

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

Assignments

Example: crossovers for binary representations



Assignments

Uniform (mask):

```
s1:   1010101010
s2:   1110001110

mask: 1101011110

o1:   1010001010
o2:   1110101110
```

Permutations

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
```

Permutations

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

$$\pi^{o_1}_{\lambda} := \pi^{s_2}_{\lambda} \qquad \lambda = 1..q$$
$$\pi^{o_1}_{\lambda} := \pi^{s_1}_{k} \qquad k \text{ smallest with } \pi^{s_1}_{k} \notin \{\pi^{o_1}_{1}..\pi^{o_1}_{\lambda}\}$$

```
s1:    7132 58469
s2:    1426 39875

o1:    1426 73589
o2:    7132 46985
```

preserves relative positions

Permutations

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

$$\pi_\lambda^{o_1} := \pi_\lambda^{s_2} \qquad \lambda = 1..q_1, q_2..k$$
$$\pi_\lambda^{o_1} := \pi_k^{s_1} \qquad k \text{ smallest with } \pi_k^{s_1} \notin \{\pi_1^{o_1}..\pi_\lambda^{o_1}\}$$

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

o1:   71 ____ 469
o2:   14 ____ 875

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

preserves relative positions

Permutations

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

$$
\begin{array}{lll}
if\, \xi_\lambda = 1 & \pi_\lambda^{o_1} := \pi_k^{s_2} & k \text{ smallest with } \pi_k^{s_2} \notin \{\pi_1^{o_1}..\pi_\lambda^{o_1}\} \\
if\, \xi_\lambda = 0 & \pi_\lambda^{o_1} := \pi_k^{s_1} & k \text{ smallest with } \pi_k^{s_1} \notin \{\pi_1^{o_1}..\pi_\lambda^{o_1}\}
\end{array}
$$

Permutations

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
```

Sets

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

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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.