

Danylo Tavrov

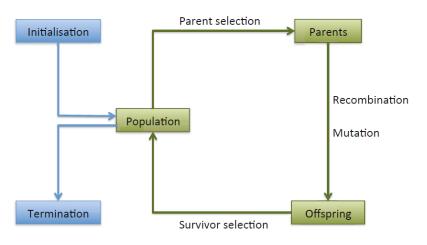
Outline

- Applying Genetic Algorithms to Real-Valued Optimization
- 2 Beyond Fitness-Proportionate Selection
- 3 Ideas for Multimodal Optimization
- 4 Beyond Binary Representations
- 5 Parameter Control in Evolutionary Algorithms
- Constraint Handling

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- 1 Applying Genetic Algorithms to Real-Valued Optimization
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General Scheme of an Evolutionary Algorithm



Eiben, A.E., Smith, J.E.: Introduction to Evolutionary Computing. Springer-Verlag, Berlin, Heidelberg (2015), Fig. 3.2

- To implement an evolutionary algorithm for a given problem, one needs to make a number of choices
- Representation and fitness function
- Type of crossover applicable to selected representation
- Type of mutation applicable to selected representation
- Population model
- Type of selection
- Initialization procedure
- Termination condition(s)
- Numerical parameters of variation operators (population size, offspring number crossover probability, mutation probability, etc.)

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- In this lecture, we will consider the problem of parameter optimization
- The task is to find a vector of parameters \mathbf{x} such that $g(\mathbf{x})$ is optimal (minimal or maximal, depending on the problem)
- To even begin solving such problems, one needs to answer two questions
- How to represent real numbers with binary chromosomes?
- How to connect a fitness function f and objective function q to each other

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 - On the other hands, objective functions can be negative and typically need to be minimized

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- One way to represent real numbers, which is native to GA, is using binary strings
- In a general case, we need to code n real parameters limited to interval [a; b]
- For each parameter we use l bits
- Then the binary string of all 0's is mapped onto a
- The binary string of all 1's is mapped onto b
- And all other numbers are linearly mapped onto values in between
- Clearly, l determines precision

$$precision = \frac{b-a}{2^l - 1}$$

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- For example, suppose we want to encode 3 parameters in [-1;2] and use l=5 bits for each of them
- Then we can have a chromosome

• Since $00000 \rightarrow -1$ and $11111 \rightarrow 2$, we compute

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• For minimization problems, we can use

$$f(\mathbf{x}) = \begin{cases} C_{\text{max}} - g(\mathbf{x}) , & g(\mathbf{x}) < C_{\text{max}} \\ 0 , & \text{otherwise} \end{cases}$$

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$$f(\mathbf{x}) = \begin{cases} g(\mathbf{x}) - C_{\min}, & g(\mathbf{x}) > C_{\min} \\ 0, & \text{otherwise} \end{cases}$$

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• n-point crossover:

- 1) Choose n random integers in [1; l-1]
- 2) Split the parents along these points
- 3) Glue parts, alternating between parents
- Has positional bias: genes located close to each other have tendency to be kept together

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Eiben, A.E., Smith, J.E.: Introduction to Evolutionary Computing. Springer-Verlag, Berlin, Heidelberg (2015), Fig. 4.2

- 1) Generate l random numbers in [0;1] (where l is the total length of the chromosome)
- 2) For each gene i, decide whether ith number is below 0.5
- 3) If yes, copy the gene from parent 1 to child 1, and from parent 2 to child 2
- Does *not* have positional bias
- Has distributional bias: has a tendency against transmitting a large number of coadapted genes from one parent to an offspring
- Choice of a crossover depends on a problem to be solved (and representation)

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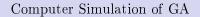
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 $Genetic\ Algorithm\ Jupyter\ Notebook,\ sections\ 1-2$

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- When we select parents to be mated using fitness-proportionate selection, we select them probabilistically given their relative fitness
- The main issue in algorithms of this kind is that once the probability distribution is computed, the expected number of copies of each parent is

$$e_i = p_i \cdot \mu$$
,

- Clearly, in practice, e_i has to be an integer, whereas $p_i \cdot \mu$ might not necessarily be so
- Therefore, different implementations can lead to different estimators of e_i , having different biases and variances
- An interesting approach² that is claimed to have lower mean-squared error that the regular fitness-proportionate selection is called stochastic remainder selection
- We represent each e_i as a sum of its integer part $[e_i]$ and its fractional part (remainder) $r_i = \{e_i\}$
- We select each individual $exactly |e_i|$ times
- Then we create another probability distribution as follows: $q_i = r_i / \sum_{i=1}^{\mu} r_i$

^{2.} Brindle, A.: Genetic Algorithms for Function Optimization. PhD thesis, University of Alberta (1981)

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where p_i is the fitness-proportionate probability

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- We represent each e_i as a sum of its integer part $[e_i]$ and its fractional part (remainder) $r_i = \{e_i\}$
- We select each individual exactly $[e_i]$ times

Then we create *until the probability* distribution as follows: $q_i = r_i / \sum_{i=1}^{r} r_i$.

We select remaining parents using those probabilities q_i .

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- When we select parents to be mated using fitness-proportionate selection, we select them probabilistically given their relative fitness
- The main issue in algorithms of this kind is that once the probability distribution is computed, the expected number of copies of each parent is

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- Then selection probabilities are allocated according to individuals' ranks
- Most commonly, a linear mapping is used
- One particular formula suggested in (Eiben and Smith, 2015) is as follows

$$p_i = \frac{2-s}{\mu} + \frac{2i(s-1)}{\mu(\mu-1)}, \quad 1 < s \le 2$$

 If stronger selection is required for fitter individuals, exponential mapping is used:

$$p_i = \frac{1-e^{-\epsilon}}{c}$$
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- where c is chosen so that all probabilities sum to 1
- Then, stochastic remainder selection can be used with these probabilities

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Tournament Selection

- This approach looks at relative rather than absolute fitness
- ullet To select an individual, we pick q members at random, and select the best one among them
- a is called tournament size
- This method relies only on ordering relation that can rank any two individuals
- The larger the tournament, the greater the chance that it will contain members of above-average fitness
- Thus, as q is increased, the probability of selecting a high-fitness member increases, and that of selecting a low fitness member decreases
- In other words, increasing q increases the selection pressure
- Even though this method exhibits some variance, it is perhaps the most widely used method, at least in some evolutionary algorithms

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Computer Simulation of GA

 ${\it Genetic~Algorithm~Jupyter~Notebook},~{\rm section}~3$

- ullet Up to this point, we discussed only generational population models, where all μ individuals are replaced with the new offspring
- In the steady-state population model, only $G \cdot \mu$ individuals are replaced
- G is called generation gap
- Individuals to be replaced can be chosen

 Arguments in favor of each approach are mixed, the final choice needs to be made according to each task being solved

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Computer Simulation of GA

 ${\it Genetic~Algorithm~Jupyter~Notebook},~{\rm section}~4$

Outline

- Applying Genetic Algorithms to Real-Valued Optimization
- 2 Beyond Fitness-Proportionate Selection
- 3 Ideas for Multimodal Optimization
- Beyond Binary Representations
- 5 Parameter Control in Evolutionary Algorithms
- Constraint Handling

• Many real-life problems have multimodal fitness landscapes

- One approach is to pick the right parameters to be able to escape local optima (including parameter control techniques discussed next)
- Another approach is to try to obtain several sets of solutions that correspond to different local optima, especially when they are very close to each other
- In practice, the finite population size usually leads to genetic drift, i.e. convergence to one optimum
- In nature, there are many cases that can be used as inspirations for developing advanced techniques in evolutionary computing
- E.g., speciation: different species adapt to occupy different environmental niches
- Or punctuated equilibria and local adaptation: periods of evolutionary stasis are interrupted by rapid growth when the main population is "invaded" by individuals from isolated groups from the same species
- In the latter case, the population is split into isolated subpopulations (demes) with only occasional migrations

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Implicit and Explicit Techniques

- \bullet Evolutionary approaches to solving multimodal problems can be classified into $^6\colon$
 - Implicit: a framework is used that permits, but does not guarantee, the preservation of diverse solutions
 - Explicit: specific operators are used to preserve diversity in the population

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- Multiple populations are run in parallel in some kind of communication structure (usually a ring or a torus)
- After a (usually fixed) number of generations (epoch), a number of individuals are selected from each population to be exchanged with others from neighboring populations (migration)
- The idea is that each subpopulation explores the search space around the fitter solutions that they contain (exploitation), and migration facilitates exploration
- In practice, however, there is no guarantee that different subpopulations are actually exploring different regions of the search space
- Some questions need to be addressed
- How often to migrate? Too frequently will lead to all subpopulations converging on the same solution, too infrequently will waste computational effort
- Which individuals to select for migration? First of all, it is generally better to migrate a small number (2-5) of individuals to prevent too rapid convergence.
 The individuals can be selected at random or based on fitness
- How to divide the population into subpopulations? Usually, more subpopulations give better results

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 The individuals can be selected at random or based on fitness
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- Multiple populations are run in parallel in some kind of communication structure (usually a ring or a torus)
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- In cellular (fine-grain parallel, diffusion model, distributed) evolutionary algorithms, one population is divided into demes⁷
- Each individual has its own neighborhood, which acts as a separate deme
- Evolution proceeds as follows
- For each individual, we select two parents from its deme
- We recombine and mutate the parents to obtain one offspring
- We replace the individual with the offspring

^{7.} Pettey, C.C.: Diffusion (Cellular) Models. In: Baeck, T., Fogel, D.B., Michalewicz, Z. (eds.) Evolutionary Computation 2. Advanced Algorithms and Operators, pp. 125-133. Institute of Physics Publishing, Bristol (2000)

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- E.g., in the tag-template scheme, each individual consists of three strings:

- The tag and template are initialized randomly
- They don't participate in fitness calculation, but they are subject to crossover
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- If q different optimal solutions are desired, the minimum template string length is [log_n q] + 1

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- Another explicit approach is called sharing⁹
- For each individual, we obtain a degree of sharing as the sum of sharing function values contributed by all other individuals, and then the fitness is derated:

$$f'(\mathbf{x}_i) = \frac{f(\mathbf{x}_i)}{\sum_{j=1}^{\mu} \operatorname{sh}(d(\mathbf{x}_i, \mathbf{x}_j))}$$

- Here d is the distance between two individuals (Hamming distance for binary strings, Euclidean distance for real vectors, etc.)
- The closer the individuals are to each other, the higher should be their sharing function values
- Thus, when many individuals are close to each other, they derate each other's fitness, and so the uncontrolled growth of particular species within population is limited.
- A common sharing function is

$$\operatorname{sh}(x) = \begin{cases} 1 - \left(\frac{x}{\sigma}\right)^{\alpha}, & x < \sigma \\ 0, & \text{otherwise} \end{cases}$$

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Computer Simulation of GA

 $Genetic\ Algorithm\ Jupyter\ Notebook,\ section\ 5$

Outline

- Applying Genetic Algorithms to Real-Valued Optimization
- ② Beyond Fitness-Proportionate Selection
- 3 Ideas for Multimodal Optimization
- 4 Beyond Binary Representations
- 5 Parameter Control in Evolutionary Algorithms
- Constraint Handling

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• Each chromosome is still a binary string

- But unlike conventional binary coding, we use Gray coding
- It is thought to be better in the sense that Hamming distance between consecutive integers is always one, hence mutations are more uniform
- We can convert a binary number $\mathbf{a} = (a_1, \dots, a_n)$ to a Gray coded number $\mathbf{b} = (b_1, \dots, b_n)$ as follows:

$$b_i = \begin{cases} a_i , & i = 1 \\ a_{i-1} \oplus a_i , & i > 1 \end{cases}$$

- Here \oplus stands for sum modulo 2
- Backward conversion is achieved by

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- Let us discuss the partially mapped crossover (PMX)¹⁰
- We choose two random integers $k_1, k_2 \in [1; l]$ (where l is the chromosome size)
- We copy the segment between appropriate alleles (matching section) from parent 1 to child 1
- Starting from k_1 , for each element i in the matching section of parent 2, we do the following steps:

- Fill the rest of child 1 using parent 2
- The whole process is then repeated, replacing parent 2 (1) with parent 1 (2) and child 1 with child 2

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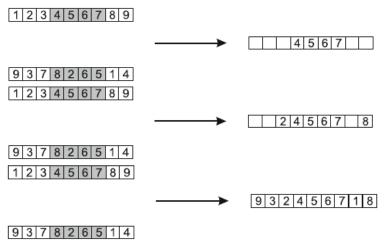
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Eiben, A.E., Smith, J.E.: Introduction to Evolutionary Computing. Springer-Verlag, Berlin, Heidelberg (2015), Fig. 4.12–4.14

- PMX is best suited for order-based problems
- Other similar algorithms are order crossover¹¹ and cycle crossover¹²
- For adjacency-based problems, a commonly used crossover is **edge crossover** ¹³
- We will not discuss these crossovers here but you can always look them up in appropriate sources

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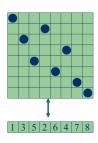
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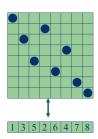
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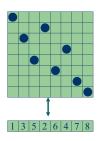
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- Consider the so-called Eight queens puzzle
- The goal is to place n queens on an $n \times n$ chessboard so that they cannot check each other
- Phenotype: a board configuration
- Genotype: a permutation of integers from 1 to n



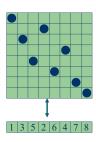
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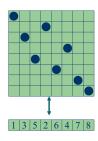
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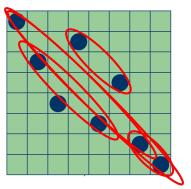
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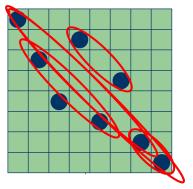


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- Then, fitness function can be defined as f(P) = 28 q(P)



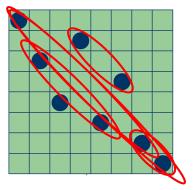
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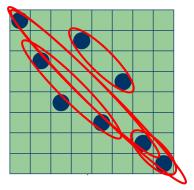
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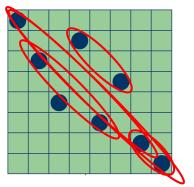
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- Given a set of cities with known distances between then, we need to find the order of visiting them so that the total distance covered in minimal
- Is known to be NP-hard
- Many heuristics specifically tailored for this problem exist
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- Let us have the following parameters:
- J the set of jobs
 Q the set of operations
- Let Able : $O \rightarrow M$ be the mapping defining which machine can perform which operation (for simplicity, each operation can be carried out only on one machine
- Let Pre ⊆ O × O be the relation defining which operation should precede which
 operations
- Let $d: O \times M \to \mathbb{R}$ be the function defining the duration of a particular operation on a particular machine
- Scheduling an operation means to assign a starting time to it on the machine that can perform it
- A schedule is a collection of such assignments containing each operation at most once

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- The goal is to find a schedule that is:
 - Complete: all jobs are scheduled
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 - Optimal: the total duration of the schedule is minimal
- The representation is the permutation of the set of possible operations (for each machine)
- The phenotype is a schedule created the following way:

- This mapping guarantees both the completeness and correctness of the scheduled
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Outline

- Applying Genetic Algorithms to Real-Valued Optimization
- ② Beyond Fitness-Proportionate Selection
- Ideas for Multimodal Optimization
- 4 Beyond Binary Representations
- **(5)** Parameter Control in Evolutionary Algorithms
- Constraint Handling

- To run any evolutionary algorithm, it is important to fully specify all of its parameters
- In particular, one has to choose population size μ , crossover probability p_c , mutation probability p_m , and selection parameters (e.g., tournament size q)
- Values of these parameters greatly influence the algorithm's ability to find a solution and the efficiency of the search
- There can be distinguished two major forms of setting parameter values

- Conceptually, parameter control should provide better results
- Indeed, the run of a GA is a dynamic and adaptive process, so different values of parameters might be better at different stages
- E.g., mutation probability can be large in the early generations to provide better exploration of the search space, and small in the late generations to facilitate exploitation

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- Parameter control techniques can be classified according to several criteria 15:
 - What is changed (population size, crossover probability, mutation probability selection parameters)
 - How the change is made (deterministic, adaptive, self-adaptive)
 - The evidence upon which the change is carried out (e.g., diversity of the population)
 - The scope of change (e.g., population-level, individual-level etc.)

^{15.} Eiben, A.E., Smith, J.E.: Introduction to Evolutionary Computing. Springer-Verlag, Berlin, Heidelberg (2015)

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- E.g., mutation probability can be time-varying ¹⁶:

$$p_m(t) = \sqrt{\frac{c_1}{c_2}} \cdot \frac{e^{-c_3 \frac{t}{2}}}{\mu \sqrt{l}}$$

where c_1, c_2, c_3 are user-defined constants, l is chromosome length, t is the generation number

• In general, deterministic schedules are of limited utility

^{16.} Hesser, J., Maenner, R.: Investigation of the m-Heuristic for Optimal Mutation Probabilities. In: Maenner, R., Manderick, B. (eds.) Parallel Problem Solving from Nature 2, pp. 115-124. North-Holland, Amsterdam (1992)

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$$p_m(t) = \sqrt{\frac{c_1}{c_2}} \cdot \frac{e^{-c_3 \frac{t}{2}}}{\mu \sqrt{l}}$$

where c_1, c_2, c_3 are user-defined constants, l is chromosome length, t is the generation number

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- Each individual is assigned some lifetime
- The idea is that on each new generation every individual becomes *older*: its age is increased by 1
- When an individual reaches maximum lifetime, it is removed from the population
- Authors of this approach proposed to perform parent selection absolutely at random
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- Mutation and crossover probabilities are also self-adapted: at the tail of every individual, 10 bits are added to code crossover probability, and then 10 bits are added to code mutation probability
- Crossover probability can range between 0 and 1, mutation probability can range between 0.001 and 0.250
- When performing mutation, first the 10 bits that encode mutation probability are mutated with the constant metamutation probability (provided by the user
- Then, the mutated 10 bits are decoded to obtain mutation probability for the given individual. The individual is mutated using these new probabilities (excep for 20 last bits)
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- Mutation and crossover probabilities are also self-adapted: at the tail of every individual, 10 bits are added to code crossover probability, and then 10 bits are added to code mutation probability
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Outline

- Applying Genetic Algorithms to Real-Valued Optimization
- 2 Beyond Fitness-Proportionate Selection
- 3 Ideas for Multimodal Optimization
- Beyond Binary Representations
- 5 Parameter Control in Evolutionary Algorithms
- Constraint Handling

- Up to this point, we considered only unconstrained optimization problems
- In reality, many problems are in fact constrained
- We need to optimize some function $f(\mathbf{x})$ of many arguments subject to certain constraints:

$$g_j(\mathbf{x}) \le 0 , \quad j = 1, \dots, q$$

 $h_j(\mathbf{x}) = 0 , \quad j = q + 1, \dots, m$

- Genetic algorithms need to be modified to take into account the constraints
- Constraint handling techniques can be classified into four broad categories

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- The idea is to change²⁰ the objective function from $f(\mathbf{x})$ to

$$f_p(\mathbf{x}) = f(\mathbf{x}) + p(d(\mathbf{x}, B))$$

- Here B is the feasible region
- d is some distance metric:

 \bullet p is the penalty function, which can be static, dynamic, or adaptive

^{20.} Smith, A.E., Coit, D.W.: Penalty Functions. In: Baeck, T., Fogel, D.B., Michalewicz, Z. (eds.) Evolutionary Computation 2. Advanced Algorithms and Operators, pp. 41-48. Institute of Physics Publishing, Bristol (2000)

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• Static penalty functions can look like

$$f_p(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^m C_i (d_i(\mathbf{x}))^k$$

Here

$$d_i(\mathbf{x}) = \begin{cases} \delta_i g_i(\mathbf{x}), & i = 1, \dots, q \\ |h_i(\mathbf{x})|, & i = q + 1, \dots, m \end{cases}$$

- Here δ_i is an indicator of whether ith constraint is violated, C_i are some weights
- Disadvantage: necessary to choose weights, which is not easy in most cases

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$$f_p(\mathbf{x},t) = f(\mathbf{x}) + \sum_{i=1}^m s_i(t) (d_i(\mathbf{x}))^k$$

- Here the only difference is that s_i is a monotonically non-decreasing function, and t is either the generation number or the number of objective function evaluations
- The severity of the penalty should be increased with time
- Then, highly infeasible solutions can survive early during the exploration phase but eventually the solution will be moved to the feasible region
- If s_i is too weak, we can get infeasible solutions; otherwise, the search may converge to non-optimal feasible solutions
- Therefore, tuning is needed for each problems
- One example is as follows

$$f_p(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{m} (C_i t)^{\alpha} (d_i(\mathbf{x}))^k$$
, $\alpha \in \{1, 2\}$

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- Here $\beta_1 > \beta_2 > 1$ are user-defined constants, N_f is the user-defined number of generations
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- Let us discuss a different way to handle constraints²¹
- The chromosome "gives instructions" to a **decoder** on how to build a feasible solution
- Stated formally, a decoder is a mapping from a representation space to the solution space
- It is important that several conditions are satisfied

- E.g., consider the **knapsack problem**: for a given set of weights w_i , profits p_i , and capacity C, find a binary vector \mathbf{x} such that $\sum_{i=1}^{n} x_i p_i$ is maximized subject to $\sum_{i=1}^{n} x_i w_i \leq C$
- Obviously, if we represent the solutions as binary strings where ith bit is 1 only
 when we select ith item to place in the knapsack, and 0 otherwise, many
 solutions will be infeasible
- We can apply the following decoder

- Then, any bit string will translate to a feasible solution
- 21. Michalewicz, Z.: Decoders. In: Baeck, T., Fogel, D.B., Michalewicz, Z. (eds.) Evolutionary Computation 2. Advanced Algorithms and Operators, pp. 49-55. Institute of Physics Publishing, Bristol (2000)

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Repair Algorithms

- For many combinatorial optimization problems (knapsack, traveling salesman, set covering, etc.), it is relatively easy to repair the solution²²
- The repaired solution can be:
- Usually, some mix is used, where the second option is applied with a certain probability
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- This approach is widely used in practice
- We already saw this idea when we were talking about crossovers and mutations for permutation representations
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 - A solution matrix is feasible if all the marginal sums equal the constraints
 - For instance, let us have the following constraints
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 - Destinations: (3, 5, 10, 7, 5)
 - Example of a feasible solution:

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0.0	0.0	5.0	0.0	3.0
0.0	4.0	0.0	0.0	0.0
0.0	0.0	5.0	7.0	0.0
3.0	1.0	0.0	0.0	2.0

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- We can devise at least two different mutation operators that would preserve the feasibility
- In the first one, we select a random submatrix, e.g. rows 1 and 3 and columns 1, 3, and 5 (bold on the previous slide)
- The values in this submatrix are changed to introduce as many zeros as possible leaving marginal totals unchanged
- We can get something like:

- In the second mutation, we do the same thing but introduce as few zeros as possible
- A crossover that can be used in this case is to create children (C_1, C_2) by averaging out the two parents (P_1, P_2) as follows:

$$C_1 = aP_1 + bP_2$$
$$C_2 = aP_2 + bP_3$$

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where $c_1 + c_2 = 1$, $c_1, c_2 > 0$

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0.0	4.0	0.0	0.0	0.0
0.0	0.0	2.0	7.0	3.0
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