# **Evolutionary computation in high-energy physics**

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#### Abstract

Evolutionary computation is a branch of computer science with which, traditionally, high-energy physics has fewer connections. Its methods were investigated in this field, mainly for data analysis tasks. These methods and studies are, however, less known in the high-energy physics community and this motivated us to prepare this lecture. The lecture presents a general overview of the main types of algorithms based on evolutionary computation, as well as a review of their applications in high-energy physics.

#### **1** Introduction

Evolutionary Computation is a branch of computer science which aims to develop efficient computer algorithms for solving complex problems by modelling the natural evolution.

Natural evolution, in this context, is defined as the optimisation process which aims to increase the ability of individuals to survive and reproduce in a specific environment. This ability is quantitatively measured by the evolutionary fitness of the individuals. The unique characteristics of each individual are represented in its chromosomes. Through the natural selection process the fitter chromosomes will mate more often creating offspring with similar or better fitness. The goal of the natural evolution process is to create a population of increasing fitness.

The algorithms based on Evolutionary Computation, called Evolutionary Algorithms, use simulation of natural evolution on a computer. The candidate solution of the problem to be solved by the algorithm represents an individual which is encoded in a form understood by the computer and called a chromosome. A chromosome can be divided into one or more constituent parts called genes. The quality of the candidate solution is evaluated with an objective function called the fitness function. The reproduction process of the individuals is simulated by applying on them a set of operators, called genetic operators, creating genetic variation. The selection of the individuals for reproduction is, usually, proportional to their fitness (the value of the fitness function for the individual). Through an iterative process, the algorithm improves the quality of the solution until an optimal solution is found.

Evolutionary Algorithms (EA) refer, traditionally, to four main types of algorithms: Genetic Algorithms (GA) [1], Genetic Programming (GP) [2], Evolutionary Strategies (ES) [3] and Evolutionary Programming (EP) [4]. More recent developments, such as Gene Expression Programming (GEP) [5], combine some characteristics of the previous versions.

In high-energy physics, EA were successfully tested but not largely used, mainly due to their high computational needs. GA were applied mainly to problems such as discrimination and parameter optimisation in both experimental and theoretical studies (for example, see [6–9]). GP was recently applied to event selection type problems [10–12]. ES were tested for optimisation of event selection criteria [13]. The first application of GEP to a high-energy physics problem was presented in [14]. Comparative studies of event selection with GEP and with commonly used methods in high-energy physics were presented in [15].

This lecture introduces the basics of EA, presents the main classes of such algorithms and summarises their applications in high-energy physics. Mode detailed presentations of EA can be found in textbooks such as [16], [17], [18], [19].

# 2 Evolutionary algorithms

#### 2.1 Basic structure of an evolutionary algorithm

The first steps, and the most difficult ones, of the application of any EA are the problem definition, the encoding of the candidate solution and the definition of the fitness function. The encoding and the fitness functions are specific to each problem. Adequate choices are crucial for the success of the algorithm. In making these choices knowledge about the problem and about the expected solution should be used.

The next step is the application of the algorithm itself. A basic representation of an EA is presented in Fig. 1.

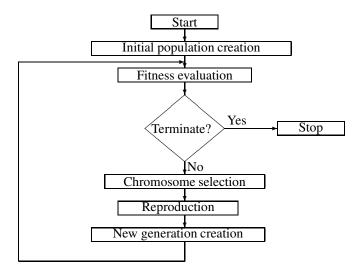


Fig. 1: Basic EA algorithm

The actual running of the algorithm starts with the random creation of an initial population of chromosomes. The fitness function is then evaluated for each chromosome determining the chromosome's fitness. Using this fitness, a termination criterion is evaluated indicating if a solution of the desired quality was found or a certain number of iterations was run. If the termination criterion is not met, some of the chromosomes are selected and reproduced, resulting in offspring. The new chromosomes will replace the old ones producing a new generation. The process continues until the termination criterion is met. The fittest chromosome is then decoded, producing the optimal solution of the problem as it was developed by the algorithm.

## 2.2 Solution representation

A candidate solution of the problem at hand is represented by a chromosome. In this respect, a chromosome represents a point in the search space.

Choosing an adequate chromosome representation is very important for the success of the algorithm as it will influence the efficiency and the complexity of the searching process.

Different types of EA use different solution representation schemes. Commonly used are schemes based on fixed or variable-length strings (GA, EA and EP), or on trees (GP). Binary strings with each bit representing a boolean value, an integer or a discretised real number (GA), or strings of real-valued variables (ES, EP) can be used. A combination of the string and tree representations is used by GEP. In this case the chromosome containing the genetic material (information from which the candidate solution is built) is represented by a string and mapped into a tree which represents the actual candidate solution.

# 2.3 Fitness function

The fitness function maps the chromosome representation into a scalar value. It describes how good a candidate solution is for the problem at hand. For this reason, it is one of the most important component of an evolutionary algorithm.

The fitness function has to contain all the criteria which need to be optimised in the searching process, and to reflect the constrains of the problem. Its value (fitness value) is used in the selection of the chromosome for reproduction, as well as in defining the probabilities with which the genetic operators are applied.

# 2.4 Initial population

The most common way of generating the initial population is by generating random values for each gene of the chromosomes from the allowed set of values. In this way, a uniform representation of the search space is ensured.

If *a priori* knowledge about the solution exists, the initial population can be biased towards potentially good solutions. This involves, however, a certain risk for a premature convergence to a local optimum.

The size of the initial population is chosen by the user. The size of the population will influence the time complexity per generation and the number of generations needed to reach the convergence of the algorithm. Small generations imply low time complexity per generation but more generations are needed for reaching convergence.

# 2.5 Selection operators

Selection operators are used to select individuals for applying genetic operators and for creating the new generation. Various selection methods exists. There is no clear evidence of any method being superior.

A few common selection methods are:

- random selection individuals are selected randomly, without any reference to fitness;
- proportional selection the probability to select an individual is proportional to the fitness value;
   when the fitness value is normalised to the maximum fitness, the method is known as the roulette wheel method;
- *rank-based selection* the probability to select an individual is proportional to the rank order of the fitness value, rather than to the fitness value itself.

# 2.6 Reproduction operators

Reproduction or genetic operators are applied on the selected individuals in order to create offspring which will constitute the next generation. Typical genetic operators are:

- cross-over combines genetic material of two parents, producing two new individuals;
- *mutation* randomly changes the values of genes in the chromosome, introducing new genetic material; in order not to disturb the good genetic material, this operator has to be applied with low probability;
- *elitism or cloning* copies the best individuals in the next generation, without any modification.

The exact structure of the genetic operators is specific to each chromosome representation, and hence to each type of EA. Examples will be given in the next sections.

## **3** Genetic algorithms

## 3.1 algorithm

Genetic Algorithms were proposed by J.H. Holland in 1975 [1]. The classical version of the algorithm uses a chromosome representation based on a binary string of fixed length. A chromosome consists of a set of variables encoded as a binary string. These variables could be binary variables (each variable encoded as a bit), nominal-valued discrete variables (each nominal value encoded as a bit string) or countinous-valued variables (each variable mapped to a bit string with a certain algorithm). Alternative chromosome representations were subsequently proposed such as integer or real-valued representations, order-based representations, chromosomes of variables length and many more [20].

Reproduction is traditionally made with the cross-over and mutation operators.

The cross-over operator is applied on a pair of chromosomes by exchanging genetic material between them and creating two new chromosomes. The operator is applied with a certain probability called the cross-over rate. Two common versions of the operator are one-point and two-point cross-over. One-point cross-over exchanges the genetic material between one randomly chosen point in the chromosomes and their ends. Two-point cross-over exchanges the genetic material between two points randomly chosen in the chromosomes. An example of how the two operators work is shown in Fig. 2.

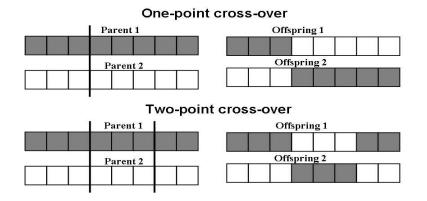


Fig. 2: One-point and two-point cross-over operators in GA

Mutation operator changes the value of randomly chosen genes in the chromosome. It is applied with a small probability, called mutation rate, in order to avoid a massive destruction of the good genetic material in the population. An example of how the mutation operator works in GA is shown in Fig. 3.

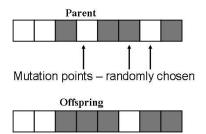


Fig. 3: Mutation operator in GA

#### 3.2 Applications in high-energy physics

In high-energy physics, GA were investigated for large-scale parameter optimisation and fitting problems in both experimental and phenomenological physics.

In experimental high-energy physics problems like cut value optimisation for event selection [21], trigger optimisation [8] or neural-network parameter optimisation for event selection [22] with GA were studied.

In [21], for example, a software implementation of GA adapted for the optimisation of the cut values of event variables was presented. Tests on simulated data showed improved optimised cut values produced by the algorithm. The effective gain, comparative to a manual optimisation, depends on the chracteristics of the data and of the physics analysis performed.

In phenomenological high-energy physics GA were used for optimising various parameters of the theoretical models as, for example, in isobar models for  $p(\gamma K^*)\Lambda$  reaction [6], SUSY model discrimination [7] or lattice calculations [9].

In [7], for example, GA was used to address the problem of discriminating SUSY breaking models by evaluating the accuracy on measurements required to distinguish two models. Three SUSY breaking scenarious were used in this study considering mass as the relevant observable. The fitness function was defined as a "relative distance" which describe the relative difference between two mass spectra. The procedure indicated values of the "relative distance" of the order of 1% which means the rough accuracy required for the sparticle mass measurements should be of this order for allowing the discrimination of the theoretical models.

## 4 Evolutionary strategies

## 4.1 Algorithm

Evolutionary Strategies were proposed by I. Rechenberg in 1973 [23] and developed further by H-P. Schwefel in 1975 [24]. They use the concept of evolution of evolution. Evolution is considered a process which optimises itself as the result of the interaction with the environment.

In order to implement this concept, an individual is represented by its genetic material and a so called strategy parameter which models the behavior of the individual in the environment:

$$C_{g,i} = (G_{g,i}, \sigma_{g,i}),\tag{1}$$

where  $C_{g,i}$  is the individual *i* of the generation *g*,  $G_{g,i}$  is the genetic material of the individual and  $\sigma_{g,i}$  is its strategy parameter.

The genetic material is represented by floating-point variables. The strategy parameter is, usually, the standard deviation of a normal distribution associated with each individual or with each variable of the individual.

The evolution process evolves both the genetic material and the strategy parameter.

The initial version of ES used only mutation in the reproduction process. Other versions were subsequently developed using both cross-over and mutation ( for a short description and more references, see [16]).

The cross-over operator is implemented as a local operator (randomly selected material from two parents is selected and recombined to form a new chromosome) or as a global operator (randomly selected material from the entire generation is selected and recombined to form a new chromosome). Two types of recombinations are commonly used: discrete recombination in which the gene value of the off-spring is the gene value from the parent, and intermediate recombination in which the midpoint between the gene value of the parents gives the gene value of the offspring.

Mutation operator has a special implementation in ES. It will mutate both the strategy parameter

 $\sigma_{g,i}$  and the genetic material  $G_{g,i}$  by modifying them with the following relations:

$$\sigma_{g+1,i} = \sigma_{g,i} e^{\tau \zeta_{\tau}}, \tag{2}$$

$$G_{g+1,i} = G_{g,i} + \sigma_{g+1,i}\zeta, \tag{3}$$

where  $\tau = \sqrt{I}$ , I being the chromosome dimension (number of genetic variables),  $\zeta_{\tau}$  and  $\zeta \sim N(0, 1)$ .

In ES and in other EA the offspring resulting from mutation is accepted only if it is fitter.

# 4.2 Applications in high-energy physics

To the best knowledge of the author of this lecture, there is only one study of the ES applicability to high-energy physics problems [13] in which the algorithm was tested for optimisation of event selection cuts and for parameter minimisation in a Dalitz plot analysis.

Using the squared signal significance  $(S^2/(S+2B), S - \text{number of signal events}, B$ - number of background events) as a fitness function and four input variables (momentum of the reconstructed system -  $D_s$  in this study, the width of the mass window around the reconstructed system, the probability of the vertex fit and the helicity angle) an ES algorithm was used to optimise the values of the cuts applied on these four variables such that the signal significance is maximised. The procedure was applied for the event selection corresponding to the following decay processes studied in the BaBar experiments [25]:  $D_s \rightarrow \phi \pi$ ,  $D_s \rightarrow \overline{K}^{*0}K^+$  and  $D_s \rightarrow \overline{K}^0K$ . Starting with values optimised manually, the algorithm found cut values which improved the squared signal significance for the three processes by 19.4%, 45% and 16%, respectively.

For the Dalitz plot analysis, ES was used to optimise the weights of the MC events such that the difference between the MC and data events in the Dalitz plot for the reaction  $p\gamma \rightarrow \pi^0 \eta$  (studied by the CB/ELSA collaboration [26]) was minimised. In this study 16 parameters were optimised. The resulting MC Dalitz plot was in good agreement with the experimental data.

#### **5** Genetic programming

### 5.1 Algorithm

Genetic programming was proposed by J.R. Koza in 1992 [2]. In contrast with the previously discussed EA, GP searches for the computer program which solves the problem at hand rather than for the solution to the problem. While the initial intentions and hopes were GP to be developed for generating computer programs in any computer language, it was only used for generating computer programs as S-expressions in LISP which are graphically translated as trees, as shown in Fig. 4. In this figure a,b,c are variables or constants and are called terminals. They are used together with mathematical functions in forming the S-expressions or the GP trees.

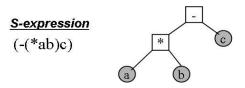


Fig. 4: An S-expression and its corresponding GP tree

In GP the chromosome is represented as a tree of variable length. The variable length gives more flexibility to the algorithm. There are, instead, syntax constraints which need to be satisfied. The unprotected evolution generates many invalid trees which need to be eliminated, resulting in waste of CPU resources.

Reproduction is performed in GP mainly with the cross-over and mutation operators. They have specific implementations, adapted to the tree representation.

The cross-over operator exchanges parts of two parent trees resulting in two new trees. An example is shown in Fig. 5 which displays the parent and the offspring trees, as well as the corresponding S-expressions and mathematical expressions.

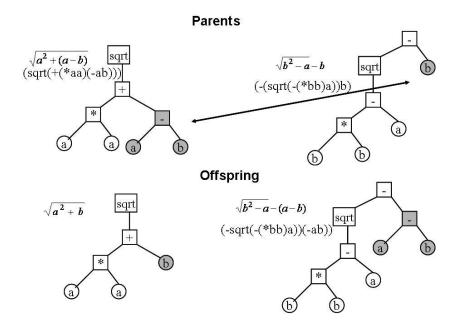


Fig. 5: Cross-over operator in GP

The mutation operator changes a function of the tree into another function, or a terminal into another terminal. An example is shown in Fig. 6 which displays the parent and the offspring trees, with the corresponding S-expressions and mathematical expressions, for the two types of mutation.

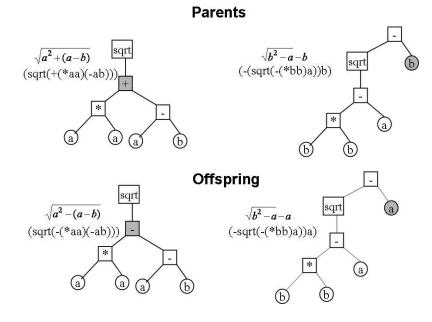


Fig. 6: Mutation operator in GP

In order to deal with the syntax constraints, various versions of GP were developed by imposing certain grammar checks in the evolution process.

#### 5.2 Applications in high-energy physics

GP was only recently tested for data analysis tasks in high-energy physics. The FOCUS experiment [27] developed a methodology for event selection with GP and applied it to the analysis of its experimental data for the following processes:  $D^+ \rightarrow K^+\pi^+\pi^-$ ,  $\Lambda_c \rightarrow pK^+\pi^-$  and  $D_s^+ \rightarrow K^+K^+\pi^-$  [11], [12]. A similar study for Higgs searches in ATLAS experiment was presented in [10] using Monte Carlo simulated data.

As an example, the procedure developed by the FOCUS collaboration is shortly summarised here.

The chromosome is built from candidate cuts for separating the signal events from background events for the desired physics process. It is represented by a tree built from a set of functions (common mathematical functions and operators, and boolean operators), a set of event variables (vertexing, kinematics and particle identification variables) and constants created by the algorithm in the range (-2.0,+2.0) for real constants and (-10,+10) for integer constants.

The following fitness function was minimised by the algorithm:

$$\frac{S+B}{S^2} \times 10000 \times (1+0.05 \times n),$$
(4)

where S and B represents the number of signal and background events, respectively, and n is the number of nodes in the GP tree.

The term proportional to n was introduced in order to control the number of nodes in the tree such that the big trees would have a high chance to survive in the evolution process only if they make a significant contribution to the background reduction or to the signal increase.

The basic procedure of the analysis was:

- an initial generation of chromosomes was almost randomly created,
- for all events in the sample the fitness value of each chromosome was calculated. Only the events for which the tree is evaluated to give a positive value were kept. For the surviving events, the invariant mass distribution of the studied system was fit with adequate functions and the number of signal and background events was determined.
- the chromosomes were selected, modified with genetic operators and a new generation created,
- the process was repeated for the desired number of generations.

The best chromosome developed at the end of the process represented the final selection criteria to be applied on the data for selecting the desired physics events. It had the shape of a quite complex tree, with 38 nodes.

The procedure was validated by comparing the results, in terms of events yield, with those obtained with a standard analysis, based on rectangular cuts applied on the event variables. Similar results were obtained in the two analyses.

# 6 Gene expression programming

## 6.1 Algorithm

Gene Expression Programming was proposed by C. Ferreira in 2001 [5]. The main difference between GEP and the other EA discussed here is the separation of the solution representation into two parts: the chromosome which encodes the information used in building the solution, and the expression tree (ET) which represents the candidate solution itself. Such separation, using different representations, was

proposed before as, for example, in Developmental Genetic Programming (DGP) [17] with which GEP has important similarities.

The GEP chromosome is a list of functions and terminals (variables and constants) organised in one or more genes of equal length. The functions and variables are input information while the constants are created by the algorithm in a range chosen by the user. Each gene is divided into a head composed of terminals and functions, and a tail composed only of terminals. The length of the head (h) is an input parameter of the algorithm while the length of the tail (t) is given by:

$$t = h(n-1) + 1, (5)$$

where n is the largest arity of the functions used in the gene's head.

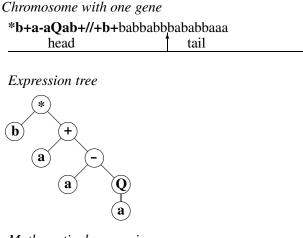
This head-tail partition of the gene ensures that every function of the gene has the required number of arguments available, making the chromosome correspond to a syntactically correct expression.

Each gene of a chromosome is translated (decoded) into an ET with the following rules:

- the first element of the gene is placed on the first line of the ET and constitutes its root,
- on each next line of the ET a number of elements equal to the number of arguments of the functions located on the previous line is placed,
- the process is repeated until a line containing only terminals is formed.

The reverse process, the encoding of the ET into a gene, implies reading the ET from left to right and from top to bottom.

An example of a chromosome with the head length equal to 15 made of five functions, Q, \*, /, + and -, (Q being the square root function) and two terminals, a and b, is shown in Fig. 7, together with its decoded ET and the corresponding mathematical expression.



Mathematical expression  $b * (a + (a - \sqrt{a})) = b * (2a - \sqrt{a})$ 

Fig. 7: Unigenic chromosome, the decoded ET and its corresponding mathematical expression

In the case of multigenic chromosomes, the ETs corresponding to each gene are connected with a linking function defined by the user. The mathematical expression associated with these combined ETs is the candidate solution to the problem.

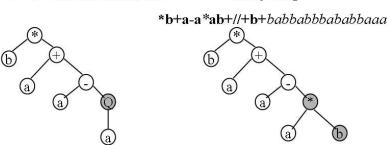
The reproduction process takes place by applying genetic operators on the chromosome (not on ET, as in GP). GEP uses four types of genetic operators:

- *elitism* the fittest chromosome is replicated unchanged into the next generation, preserving the best material from one generation to another.
- cross-over exchanges parts of a pair of randomly chosen chromosomes. In addition of the onepoint and two-point cross-over, as in GA, GEP uses gene cross-over in which entire genes are exchanged between two parent chromosomes, forming two new chromosomes containing genes from both parents.
- *mutation* randomly changes an element of a chromosome into another element, preserving the rule that the tails contain only terminals. In the head of the gene a function can be changed into another function or terminal and *vice versa*. In the tail a terminal can only be changed into another terminal.
- *transposition* randomly moves a part of the chromosome to another location in the same chromosome.

An example of how such an operator (mutation, for example) works in GEP is shown in Fig. 8.

# Parent

\*b+a-aQab+//+b+babbabbbababbaaa



Offspring

Fig. 8: Mutation operator in GEP

#### 6.2 Applications in high-energy physics

The author of this lecture performed the first study of the applicability of GEP to an event selection problem in high-energy physics. The selection of  $K_S$  particle produced in  $e^+e^-$  interaction at 10GeV and reconstructed in the decay mode  $K_S \rightarrow \pi^+\pi^-$  was used as an example application [14], [15]. The purpose of the study was the evaluation of the potential of the algorithm for solving such a problem rather than the extraction of particular physics results.

In this study a supervised statistical learning approach was followed. The algorithm was used to extract selection criteria for the signal/background classification from training data samples for which it was known to which class the event belonged. The generalisation power of the selection criteria were tested on independent data samples. Monte Carlo simulated data from BaBar experiment [25] was used in this study.

The input information of the algorithm was a set of event variables commonly used in a standard cut-based analysis for the process studied: doca (distance of closest approach between the two  $\pi$ daughters of  $K_S$ ), Rxy and |Rz| (dimensions of the cylinder which defines the  $e^+e^-$  interaction region)  $|cos(\theta_{hel})|$  (absolute value of the cosine of the  $K_S$  helicity angle), SFL ( $K_S$  signed flight length), Fsig(statistical significance of the  $K_S$  flight length), Pchi ( $\chi^2$  probability of  $K_S$  vertex) and Mass ( $K_S$  reconstructed mass). These variables, together with common mathematical functions and with floating point constants created by the algorithm were used to construct the GEP chromosomes.

The fitness function was the number of events correctly classified as signal or background. The GEP performance in solving the problem was evaluated in terms of classification accuracy defined as the ratio of the number of events correctly classified as signal or background to the total number of events in the data sample.

The GEP algorithm, using as input information only a list of logical functions and the event variables, developed selection criteria similar to those used in a standard cut-based analysis, proving the algorithm works correctly:

$$Fsiq > 4.10, Rxy < 0.20cm, Pchi > 0, SFL > 0.20cm, doca > 0cm, Rxy \le Mass.$$
 (6)

These selection criteria provided a classification accuracy of over 95% for both training and test data samples. The last two listed selection criteria do not have influence on the quality of the event selection as the inequalities are always satisfied. They are redundant information developed early in the evolution process.

The analysis was repeated using as input functions a combination of logical and common mathematical functions. Similar classification accuracy was obtained. Also, no significant change of the classification accuracy was obtained by increasing the number of events in the data sample or by applying a parsimony pressure to the fitness function. It was also observed that the GEP method does not suffer from overtraining on larger data samples or on those with a larger number of event variables. These initial results suggest GEP as a potential powerful alternative method for events selection.

#### 7 Conclusions

Evolutionary Algorithms are, in principle, quite easy to understand computer algorithms. They attempt to simulate the natural evolution of species providing, however, a quite simplistic version of this very complex process. These algorithms were successfully applied for solving complex real-world problems in various fields of science and engineering. Their main advantage is the parallel investigation of the solution landscape and the ability to avoid trapping in local minima. As they are not based on a rigorous theory, there is no way, however, to demonstrate the solutions found are indeed the best solutions. Their solutions are good as long as they are optimal for the problem studied.

Only a limited investigation of these algorithms has been performed in high-energy physics so far. The applications discussed in this lecture are almost everything existing in the literature (with the exception of GA for which not all available studies were included). The results of these applications are positive and justify further exploration. The main drawback of EA, the high computational needs, is expected to be alleviated by the increased computer power available these days, as well as by the development of new, more effcients versions of these algorithms.

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