Quality-Diversity Optimization: a novel branch of stochastic optimization

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Traditional optimization algorithms search for a single global optimum that maximizes (or minimizes) the objective function. Multi-modal optimization algorithms search for the highest peaks in the search space that can be more than one. Quality-Diversity algorithms are a recent addition to the evolutionary computation toolbox that do not only search for a single set of local optima, but instead try to illuminate the search space. In effect, they provide a holistic view of how high-performing solutions are distributed throughout a search space.

1 Introduction

Optimization has countless uses in engineering, from designing mechanical parts [71] to controlling robots [26, 52]. In an ideal situation, the user of an optimization algorithm would write the cost function that corresponds to the problem at hand, select the right optimization algorithm, and get the perfect solution.

Unfortunately, many real-world optimization problems are not easily captured by a simple cost function, which is why it is often required to add new terms to the cost functions and/or tune the parameters until the optimization algorithm finally reaches an acceptable solution.

Consequently, optimization in engineering is often an iterative process that requires many runs of the optimizers and many changes of the cost function.

Moreover, even after fine-tuning the cost function, the optimized solution is rarely used as the final, optimal solution. In practice, optimization is most often used at the beginning of the design process to explore various options and examine the trade-offs that are inherent to the domain [6]. This calls for algorithms that are designed as exploration tools more than as pure optimization tools.

Quality-Diversity (QD) optimization algorithms address this challenge: instead of searching for the optimum of the cost function, they provide a large set of high-performing solutions (typically a few thousands) that differ according to a few user-defined features of interest. The user can then pick the high-performing solutions that they deem as the most interesting according to their own knowledge, like aesthetics or easiness of manufacturing. He/she can also use the resulting set to better understand how features of solutions influence performance.

For instance, if the feature descriptors are discretized, the outcome of a QD algorithm can be a table. See Table 1 for an example:

One of the features might have no influence on the cost function, or another one might need to be below a given threshold to attain acceptable performance.

For instance, QD algorithms have been used to find gait parameters for a 6-legged robot [10, 16, 23]. In that task, instead of finding parameters to go forward, a QD algorithm can find in a single run parameters so that the robot can reach any point in its vicinity (e.g., walking forward, backward, left, etc.). For each direction, the algorithm will find a different set of high-performing parameters; however, close directions are likely to have similar solutions, which means that it may be more efficient to optimize for all the directions simultaneously. In particular, if a set of parameters is tested and makes the robot turn right, it will be useless to go forward, but will be a promising solution to turn right.

In addition, these parameters may be good “stepping stones” to go forward (or backward, or left, etc.), that is, a useful intermediate step in the optimization process.

Numerous QD algorithms have been proposed during recent years, which are mostly based on the principles of evolutionary algorithms. This chapter gives an overview of these algorithms and introduce several recent ideas to increase the data-efficiency, scale to high-dimensional spaces. Application examples are discussed all along the chapter.

2 Problem Formulation

We assume that the objective function returns both the fitness value \( f_\theta \) and a behavioral descriptor (or a feature vector) \( b_\theta \) [55]:

\[
f_\theta, b_\theta \leftarrow f(\theta)
\]

The behavioral descriptor (BD) typically describes how the solution solves the problem, while the fitness value \( f_\theta \) quantifies how well it solves it. For example, the BD can be the curvature of a 3D design, its volume, or the trajectory of a robot, while the fitness values would be the aerodynamic drag, the energy consumption, or the distance to the target state.

Without loss of generality, we assume hereafter that the fitness function is maximized. Let us define by \( B \) the feature space, the goal in QD optimization is to find for each point \( b \in B \) the parameters, \( \theta^* \), with the maximum fitness value:

\[
\forall b \in B \quad \theta^* = \arg \max_\theta f_\theta
\]

s.t. \( b = b_\theta \) (2)

For instance, if the feature descriptors are discretized, the outcome of a QD algorithm can be a table. See Table 1 for an example:

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When the BD is 2-dimensional, this result is usually displayed as a colored image or heatmap.

At first sight, QD algorithms look like multitask optimization [55], that is, solving an optimization problem for each combination of features. However, first BD can be continuous, which would mean an infinite number of problems; second, we do not know the BD before calling the fitness function, which explains why the QD problem can be viewed as a set of optimizations constrained by each BD.

The central hypothesis of QD algorithms is that solving this set of problems is likely to be faster if they are all solved together than by independent constrained optimizations. Intuitively, it is indeed likely that high-performing solutions for close feature descriptors will be close, therefore sharing information between the optimizations can be beneficial. In addition, independent constrained optimization would be especially wasteful in a black-box optimization context because a candidate solution that has not the right features would be discarded, whereas it could be useful for a different feature combination.

### 2.1 Collections of Solutions

The outcome of QD optimization is a set of solutions. This set of solutions, also called “collection”, “archive”, or “map”, is expanded, improved, and refined during the optimization process. Each point in this collection represents a different “solution type” or “species”. In practice, two solutions with similar behavioral descriptor will be considered to be of the same solution type and will compete together to be maintained in the collection. Necessarily, the notion of similarity is defined by using a hyper-parameter that sets the tolerance used to determine when two descriptors are different or similar. This hyper-parameter defines a sort of “resolution” in the behavioral descriptor space: only one solution will occupy a certain region of the space.

The simplest way to implement this segmentation of the BD space is by discretizing it into a grid, in which each cell of the grid corresponds to one type of solution (i.e., to one BD location). This approach is used by the MAP-Elites algorithm [54], one of the most used QD algorithm. In this case, the collection is a grid (or multidimensional array) and the goal of the algorithm is to fill every cell of that grid with the best possible solution. However, it is possible to avoid this discretization and replace it with distance thresholds or local density estimates (section 3).

### 2.2 How do we measure the performance of a QD algorithm?

The overall performance of a QD algorithm is defined by the quality of the produced collection of solutions according to two criteria:

1. the performance of the solution found for each type of solutions (how much we have optimized);
2. the coverage of the behavior space (how much of the feature space is covered).

The first criterion (performance) is obvious to compute: depending on the application or use-case, we can compute the mean, median or the sum of the individual fitness values in the collection. The second criteria (coverage) can be more challenging to evaluate when the behavior/feature space is not discretized. If we are in low-dimensional spaces, we can discretize the behavior space arbitrarily and compute the percentage of the bins filled by the algorithms [66]. Alternatively, if we are operating in a high-dimensional space, we can resort to density metrics, like the average distance of the k-nearest neighbors. A third option is to define a distance threshold between behavioral descriptions, and then compute a similar filling percentage as in the low-dimensional space case.

### 3 Optimizing a collection of solutions

In this section, we begin with the introduction of Multidimensional Archive of Phenotypic Elites (MAP-Elites) [54], and then present a modern categorization of QD algorithms [15] that makes it to define many variants of QD algorithms, including more advanced algorithms.

#### 3.1 MAP-Elites

MAP-Elites takes inspiration from evolutionary algorithms: at each iteration, MAP-Elites alters copies of solutions that are already in the grid to form new solutions (see Algo. 1). The alterations are done with mutation and cross-over operators like in traditional evolutionary algorithms. The new solutions are evaluated and then potentially added to the cell corresponding to their BD. If the cell is empty, the solution is added to the grid. Otherwise, only the best solution is kept in the cell.

| BD | fitness | Parameter values |
|----|---------|------------------|
| 23 | 16      | -85 27 -58 -44 54 |
| 39 | 10      | -86 -23 -59 -20 -86 |
| : | :       | :                |
| -7 | 2       | 45 -49 89 82 62  |

Table 1. An example of discretized feature descriptor.
to generate images that resemble natural objects [57]; and 3-D-printable objects by leveraging feedback from neural networks trained on 2-D images [48].

The main strength of MAP-Elites is its simplicity to understand and to implement. However, depending on the domain, it is sometimes difficult to discretize the feature/behavior space (for instance, in high dimensions or when the bounds are highly irregular). It is also possible to bias the selection in different ways: the uniform selection among the elites of the original gives surprisingly good results but several ideas have been investigated to select parents in other ways that can make the convergence faster.

In the following section, we present a modern categorization of QD algorithms that make it possible to describe most QD algorithms within the same algorithmic framework.

### 3.2 A Unified Framework

Cully and Demiris [15] proposed a unified formulation of QD algorithms that see all QD algorithms as an instantiation of a single high-level algorithm (Alg. 2). In this formulation, the main axes of variation of all QD algorithms are: (1) the type of container, that is, how the data are gathered and ordered into a collection, (2) the type of the selection operator, that is, how the solutions are selected to be altered in the next generation, and (3) the type of scores that are being computed in order for the container and the selection operator to work.

In particular, after a random initialization, the execution of a QD-algorithm based on this framework follows four steps that are repeated:

- the selection operator produces a new set of individuals that will be altered in order to form the new batch of evaluations,
- the individuals are evaluated and their performance and BD are recorded,
- each of these individuals is then potentially added to the container, according to the solutions already in the collection,
- finally, several scores, like the novelty, the local competition, or the curiosity score, are updated.

These four steps repeat until a stopping criterion is reached (typically, a maximum number of iterations) and the algorithm outputs the collection stored in the container. In the following sections, we will detail different variants of the containers, the selection operators, and of the most widely used scores.

#### 3.2.1 Containers

The main purpose of a container is to gather all the solutions found so far into an ordered collection, in which only the best and most diverse solutions are kept.

One of the most popular container types in the literature is the N-dimensional grid structure, which is the one that MAP-Elites is using. In this container, we simply discretize the behavior space in a grid, where each cell of the grid corresponds to one type of solution. Originally, the MAP-Elites grid was built with only one solution per cell. Of course, one can imagine having more individuals per cell (e.g., [66] uses two individuals) in order to perform more complicated computations (e.g., for multi-objective optimization or noisy optimization [27, 39]).

In high-dimensional behavior spaces, it is possible to use a Centroidal Voronoi Tessellation to define cells of identical volume regardless of the dimension (see Sec. 5.2).

An alternative container type is the *distanced-based archive*. In this type of containers, the solutions are kept in an unstructured array by using their behavior descriptor and the Euclidean distance. In essence, the user specifies a threshold parameter and a new individual is added to the archive (a) if it is “far away” from all other solutions in the archive (its Euclidean distance greater than the user-defined threshold), or (b) if it is better than its closest(s) neighbor(s). In contrast with the grid container presented previously, the descriptor space here is not discretized and the structure of the collection autonomously emerges from the encountered solutions. However, in practice this container type requires a slightly more sophisticated maintenance mechanism to avoid the “erosion effect” that may progressively remove solutions that are far from the rest of the collection in favor of solutions that are slightly closer but with a higher value, slowing down the overall optimization process.

#### 3.2.2 Selection Operators

One of the keys for the success of QD algorithms, but also evolutionary algorithms in general, is the selection operators. The selection operators aim at answering the following question: given the current collection (or population), how do we sample or generate new individuals to be evaluated?

The most naive way of generating solutions is by randomly sampling the parameter space, that is, by not using the current collection. This is unlikely to be effective as it makes the QD algorithms identical to random search.

The original MAP-Elites implementation randomly samples solutions from the ones already in the container. This is a very simple strategy to implement and very computational efficient. However, one of its main drawbacks is that the selection pressure decreases as the number of solutions in the collection increases (the chance for a solution to be selected being inversely proportional to the number of solutions in the collection), which is likely to be ineffective with large collections.

Another interesting way of selecting new individuals is adopting a score-based weighting for the random sampling. In this way, we can insert more weight on more “interesting” individuals based on a specific score, and bias the selection pressure towards desired behaviors or more “interesting” individuals. In QD optimization, we aim at devising scores that will improve the collection, that is, to either discover new behaviors or optimize the already discovered ones (see Sec. 3.2.3).

So far, all the defined selection operators are operating on the stored container. In this case, the population of the QD algorithm is the container itself that evolves and improves over time. One can imagine having multiple populations that evolve in parallel. For example, Novelty Search with Local Competition (NSLC) [47] uses two distinct populations, one as a container storing information about novelty (they call it novelty archive) and one more traditional population storing information about performance and using it to perform the selection operation.

#### 3.2.3 Population Scores

Traditionally, evolutionary algorithms consider only the fitness value (quality) to take decisions. Most of these approaches will struggle to identify diverse solutions, and might even fail at finding the global optimum. On the contrary, QD algorithms consider
is a promising selection heuristic. These results showcase that relying on individuals with a high-
to-learn behavior repertoires for a six-legged robot to walk in
variants [15]. In particular, this type of algorithms were able
algorithms with the curiosity score both in distance-based and
Sec. 3.2.3) in a QD algorithm seems to be an effective way of
Results from [15] indicate that the usage of curiosity score (see
authors practically implement this idea by introducing a score that
can potentially lead to novel regions of the search space. The
implementation of the curiosity score (see Algo. 2) is to begin
offsprings that will be added to the container. One practical
do this by modelling the probability of an individual to generate
or replace already occupied cells. The variation (Pparents)
individuals that will most likely produce new cells in the container
or replace already occupied cells. The curiosity score attempts
to do this by modelling the probability of an individual to generate
offsprings that will be added to the container. One practical
implementation of the curiosity score (see Algo. 2) is to begin
with zero curiosity score for all individuals, and then each time
that one of their offsprings gets added to the container, their
curiosity score increases, whereas it decreases each time their
offsprings do not enter the container.

Finally, Go-Explore [24, 25] introduced the concept of attempting
to expand the frontier of the search by promoting the selection
of newly discovered individuals. The intuition is that a newly
discovered individual will most likely contain an interesting behavior
that can potentially lead to novel regions of the search space. The
authors practically implement this idea by introducing a score that
is based on visit and selection counters.

3.3 Considerations of Quality-Diversity
Optimization

Results from [15] indicate that the usage of curiosity score (see
Sec. 3.2.3) in a QD algorithm seems to be an effective way of
keep exploring interesting regions of the behavior space while
also locally optimizing the solutions. The performance of QD
algorithms with the curiosity score both in distance-based and
grid-based containers was consistently better than many other
variants [15]. In particular, this type of algorithms were able
to learn behavior repertoires for a six-legged robot to walk in
any direction or walk in a straight line in many different ways.
These results showcase that relying on individuals with a high-
propensity to generate individuals that are added to the collection
is a promising selection heuristic.

Another quite interesting takeaway is the fact that using the uniform random selection operator (over the container), MAP-Elites’ selection operator, is very effective both when used in distance-based and grid-based containers (the original MAP-Elites implementation) [15, 17, 54]. This showcases the strength of selecting candidates to reproduce from the elites (contained in the archive), rather than randomly generating new ones.

Additionally, Novelty-Search with Local Competition [47] is less effective than curiosity-based QD instances and QD instances with the MAP-Elites’ selection operator [15]. This finding advocates that evolving the whole collection of solutions is more effective than splitting it in multiple populations with different characteristics and functionalities.

Finally, the distance-based containers produce containers with smaller numbers of individuals. This of course depends on the choice of the threshold for the distance comparisons, but also highlights the need for better structure of the containers as it is often not very easy to tune these parameters. In Sec. 5.2, we discuss different types of containers to handle some of these limitations.

4 Origins and Related Work

4.1 Searching for Diverse Behaviors

Quality-Diversity algorithms mainly originate from the desire to evolve multiple and diverse behaviors in the evolutionary robotics community [46, 47, 53]. In particular, they build on top of Novelty Search (NS) [46], and Novelty-Search with Local Competition (NSLC) [47] algorithms, which propose to search for novel solutions instead of high-performing ones. This proved to be particularly interesting to escape from deceptive regions in the search space (local optima) and reach eventually high-performing solutions [53]. Searching for novel solutions is done by rewarding solutions that are different from the previously encountered ones thanks to the novelty score (described in section 3.2.3). This score is implemented in practice by maintaining an archive, called the novelty archive, of the previously encountered solutions, which is then used to compute the average distance in the BD space between the contained solutions and any newly generated one. The archive is mainly used as a tool to compute the novelty score, while the actual outcome of the algorithms is their final population (like most evolutionary algorithms). It is also important to note that the archive was designed to quantify the coverage of the
of the earliest attempts, was the (Fig. 1B).

issues, by employing various diversity maintenance techniques, problems\[45,70\]). Multimodal optimization (MMO) algorithms
algorithm to return all local optima in order to choose between
divergent, which might cause even sophisticated gradient-free
often the case, however, that (1) the objective function is highly
ally optimal solution of the objective function (Fig. 1A). It is

4.2 Connections to Multimodal Optimization

Traditionally, the focus of optimization was to find a single, globally
optimal solution of the objective function (Fig. 1A). It is
often the case, however, that (1) the objective function is highly
nonlinear, which might cause even sophisticated gradient-free
algorithms, such as evolution strategies, to converge to local op-
tima \[67\], and (2) the user would like from the optimization
algorithm to return all local optima in order to choose between
them (for example, this could be the case in engineering or design
problems \[45,70\]). Multimodal optimization (MMO) algorithms
(e.g., see \[18, 33, 35, 51, 62, 63, 68, 72, 80\]) seek to address these
issues, by employing various diversity maintenance techniques,
also known as niching methods, with the aim to return multi-
ple solutions that correspond to the peaks of the search space
(Fig. 1B).

Niching has a long history in evolutionary computation. One of
the earliest attempts, was the preselection method \[9\] in which
an offspring replaces its least fit parent, if it has higher fitness.
Crowding \[19\] was the first to propose the use of distances (to the
best of our knowledge). Fitness sharing \[33\] assumes that fitness
is a precious resource that is shared among neighboring indi-
viduals, therefore, it reduces the fitness of individuals in densely
populated areas. Clearing \[62\] is a technique that has the
same inspiration as sharing, but rather than lowering the fitness,
removes less fit individuals from the neighborhoods. In re-
stricted tournament selection \[35\] an offspring competes with its
closest individual in a randomly selected sample of the popu-
lation. Clustering \[80\] and multi-objective optimization \[21\] were
also proposed (among others) as a way to maintain diversity.
In addition, niching techniques have been proposed for various
nature-inspired optimization algorithms, such as particle swarm
optimization \[3\]. A comprehensive survey is outside the scope
of this chapter, however, the interested reader can refer to \[18, 63\].

In order to better highlight the similarities and differences be-
tween global and multimodal optimization (assuming maximiza-
ton) let us formally define their objectives. Global optimization
can be written as:

$$
\theta^*_{g} = \arg \max_{\theta \in \Theta} f(\theta)
$$

or in set-builder notation:

$$
\{ \theta^*_{g} \in \Theta : f(\theta^*_{g}) > f(\theta), \forall \theta \in \Theta \}
$$

where $\Theta$ is the parameter space. In other words, global opti-
mization algorithms aim to return a set that contains a single
solution which is the globally optimal one. MMO can typically
be expressed as:

$$
\{ \theta^*_{q} \in \Theta : f(\theta^*_{q}) > f(\theta), \forall \theta \in \Theta, d(\theta, \theta^*_{q}) < \epsilon, \epsilon > 0 \}
$$

where $d$ is a distance function; in other words, MMO aims to
return the set of all locally optimal solutions, typically in parameter
space.

Quality-Diversity optimization on the other hand aims at opti-
mizing a different objective function that returns both a fitness
value and a behavior descriptor (see Sec. 2 and Eq. 1, 2). Alter-
natively, it can be expressed as:

$$
\{ \theta^*_{qO} \in \Theta : f(\theta^*_{qO}) > f(\theta), \forall \theta \in \Theta, d(b(\theta), b(\theta^*_{qO})) < \epsilon, \epsilon > 0 \}
$$

where $f : \Theta \rightarrow \mathbb{R}$, and $b : \Theta \rightarrow \mathcal{B}$. Observing Eq. 6, we can
easily identify that the main difference of QD from multimodal
optimization is in the focus on finding the optimal parameters for
each point in the behavior space, as well as returning many more
points than optima (Fig. 1C).

It is clear by now that QD algorithms attempt to solve a dif-
f erent problem than more traditional optimization techniques. It
should also be obvious that it might be possible to use off-the-
shelf (local or global) optimizers with restart procedures (or in
parallel) to solve the multimodal optimization problem, however,
not the QD problem. For example, if we instantiate parallel hill
climbers from uniformly-distributed random initial points, they might
return the optima, however (1) some of them might return the
same solution, and (2) the whole set of solutions will most prob-
lably not be as diverse as the one returned by QD optimization
algorithms. Two questions arise now: (1) can we use multimodal
optimization algorithms to solve the QD problem? (2) can we use
QD algorithms to solve the multimodal optimization problem?

Although there are not many works in the literature that inves-
tigate these questions, it has been shown that some multimodal
optimization algorithms can perform as well as QD algorithms
if set to compare distances in behavior space \[76\], while oth-
ers fail at doing so. In particular, the clearing method \[62\] was
able to solve QD problems, whereas Restricted Tournament Se-
lection \[35\] was not able to do so, mainly because of its strong
focus on performance (rather than diversity) which makes it even
lose certain local optima (Fig. 1B). This showcases the need for
algorithms that attempt to solve the specific QD problem, and that
the QD problem cannot be generically solved by other types of
optimization methods. There are, however, a lot of intuitions to
be taken from the multimodal optimization literature to improve
QD algorithms.

Additionally, it is shown that QD algorithms can also work in
high-dimensional parameter space \[77, 78\], and thus QD algo-
rithms can be used to solve multimodal optimization problems.
Typically, QD algorithms return many more solutions than the
optima of the underlying search space, therefore, finding the optima
in the returned set of solutions could potentially be done using
some filtering technique (such as the nearest better clustering
heuristic \[64\]).

4.3 Connections to Multi-task Optimization

As introduced in section 2, QD algorithms assume that the fitness
function $f(\theta)$ returns both the fitness value $f_{\theta}$ and a behavioral
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the traditionnal approach is to learn an algorithm, if not for all the optimization algorithms. In such cases, parallelizing on large clusters and multicore computers.

minutes or even hours: in these engineering problems, calling the many interesting engineering problems, for example aerodynamics with 36 parameters that define the gait [10, 17]. Unfortunately, MAP-Elites is typically given a budget of 20 million evaluations to find about 15,000 effective gaits for a 6-legged robot, which represents the uncertainty here. Intuitively, the optima of the UCB function are regions that are predicted as having a high predicted value (μ(θ)) and a high uncertainty (σ(θ)). β tunes the exploration-exploitation trade-offs (a large β will favor candidates that have a high uncertainty, a small β the candidates that have the highest predictions).

In Bayesian optimization, the algorithm would optimize the UCB according to the model and evaluate the optimum solution on the true objective function. However, in QD algorithms there is no single, most promising solution. Instead, Gaier et al. used Bayesian optimization — trying candidates in uncertain regions — and exploitation — trying candidates that are in the most promising regions according to the approximate model. In essence, Bayesian optimization loops over three steps: (1) finding the optimum of the acquisition function, which is a non-convex optimization problem with a “cheap” objective function, (2) evaluating the selected solution on the expensive function, and (3) updating the model with the new point. The model is usually initialized with a few candidates that are randomly chosen and evaluated on the expensive function.

The concepts of Bayesian optimization are easy to transfer to QD algorithms: the same models and the same model/optimization loop can be used. The only difference lies in the acquisition function (and how it is optimized), since the algorithm is not trying to find the optimum of a function anymore.

In the first experiments with surrogate-based QD algorithms, Gaier et al. [29, 30, 31] took inspiration from the Upper Confidence Bound (UCB) [12, 73], which is a simple but successful acquisition function in Bayesian optimization [7, 69]:

\[
\text{UCB}(\theta) = \mu(\theta) + \beta \sigma(\theta)
\]

where \(\mu(\theta)\) is the mean prediction according to the Gaussian processes (the surrogate model), \(\sigma(\theta)\) is the prediction of the variance (which represents the uncertainty here). Intuitively, the optima of the UCB function are regions that are predicted as having a high predicted value (\(\mu(\theta)\)) and a high uncertainty (\(\sigma(\theta)\)). β tunes the exploration-exploitation trade-offs (a large β will favor candidates that have a high uncertainty, a small β the candidates that have the highest predictions).

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descriptor \(b_\theta\):

\[
f_0, b_\theta \leftarrow f(\theta)
\]

By contrast, multitask optimization considers a fitness function that is parameterized by a task descriptor \(\tau\) and returns the fitness value:

\[
f_{0,\tau} \leftarrow f(\theta, \tau)
\]

The task descriptor might describe, for example, the morphology of a robot or the features of a game level; it is typically a vector of numbers that describes the parameters of the task.

The overall objective is to find, for each task \(\tau\), the solution \(\theta^*_\tau\) with the maximum fitness:

\[
\forall \tau \in T, \theta^*_\tau = \arg\max_{\theta} (f(\theta, \tau))
\]

To our knowledge, only a few algorithms have been proposed for multitask optimization, mainly in the framework of Bayesian optimization [61]. However, the MAP-Elites algorithm was recently extended to solve multitask optimization problems [55]. The general idea is to select the task \(\tau\) in the neighborhood of the parents, selected using the standard MAP-Elites procedure (uniform selection from the archive). The results show that Multi-task-MAP-Elites can outperform independent optimizations with the same model/optimization loops over three steps: (1) finding the optimum of the acquisition function, which is a non-convex optimization problem with a “cheap” objective function, (2) evaluating the selected solution on the expensive function, and (3) updating the model with the new point. The model is usually initialized with a few candidates that are randomly chosen and evaluated on the expensive function.

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![Fig. 1. Difference between global, multimodal and QD optimization.](image-url)

QD optimization algorithms, such as MAP-Elites (C), discover significantly more solutions, each one being the highest-performing of a local neighborhood defined in some feature space of interest. For finding the solutions of the function illustrated, we used (A) Covariance Matrix Adaptation Evolution Strategies [34], (B) Restricted Tournament Selection [35], and (C) MAP-Elites [54]. Figure adapted from [78].

5 Current Topics

5.1 Expensive Objective Functions

QD algorithms are designed for non-convex, black-box functions with many peaks. As such, they typically assume that the objective function can be queried millions of times. For instance, MAP-Elites is typically given a budget of 20 million evaluations to find about 15,000 effective gaits for a 6-legged robot, with 36 parameters that define the gait [10, 17]. Unfortunately, many interesting engineering problems, for example aerodynamics optimization, require simulating each candidate solution for minutes or even hours: in these engineering problems, calling the objective function millions of times is not possible, even when parallelizing on large clusters and multicore computers.

This challenge is common for all black-box optimization algorithms, if not for all the optimization algorithms. In such cases, the traditional approach is to learn a surrogate model of the objective function [4, 59], that is a data-driven approximation of the objective function that can be used in lieu of the objective function.

The most popular theoretical framework for surrogate-based optimization is currently “Bayesian optimization” [7, 69]. Most instantiations model the objective function with Gaussian processes [79] because (1) they are designed to give uncertainty estimates and (2) their explicit smoothness assumption allows them to make accurate predictions when little data is available. Once the model is defined, an acquisition function is used to select the next solution to evaluate on the expensive objective function; this function typically uses the uncertainty estimates to balance exploration — trying candidates in uncertain regions — and exploitation — trying candidates that are in the most promising regions according to the approximate model. In essence, Bayesian optimization loops over three steps: (1) finding the optimum of the acquisition function, which is a non-convex optimization problem with a “cheap” objective function, (2) evaluating the selected solution on the expensive function, and (3) updating the model with the new point. The model is usually initialized with a few candidates that are randomly chosen and evaluated on the expensive function.

The concepts of Bayesian optimization are easy to transfer to QD algorithms: the same models and the same model/optimization loop can be used. The only difference lies in the acquisition function (and how it is optimized), since the algorithm is not trying to find the optimum of a function anymore.

In the first experiments with surrogate-based QD algorithms, Gaier et al. [29, 30, 31] took inspiration from the Upper Confidence Bound (UCB) [12, 73], which is a simple but successful acquisition function in Bayesian optimization [7, 69]:

\[
\text{UCB}(\theta) = \mu(\theta) + \beta \sigma(\theta)
\]

where \(\mu(\theta)\) is the mean prediction according to the Gaussian processes (the surrogate model), \(\sigma(\theta)\) is the prediction of the variance (which represents the uncertainty here). Intuitively, the optima of the UCB function are regions that are predicted as having a high predicted value (\(\mu(\theta)\)) and a high uncertainty (\(\sigma(\theta)\)). β tunes the exploration-exploitation trade-offs (a large β will favor candidates that have a high uncertainty, a small β the candidates that have the highest predictions).

In Bayesian optimization, the algorithm would optimize the UCB according to the model and evaluate the optimum solution on the true objective function. However, in QD algorithms there is no single, most promising solution. Instead, Gaier et al. used MAP-Elites with the UCB as the objective function. This gives a “acquisition map” instead of a maximum of an acquisition
function, that is, MAP-Elites outputs the candidate with best UCB value for each bin. In the spirit of MAP-Elites, and because no bin is considered more important than the others, Gaier et al. select candidates to be evaluated on the expensive function uniformly from this “acquisition map”.

The resulting algorithm, called Surrogate-Assisted Illumination (SAIL), has been evaluated on the optimization of airfoils (minimizing drags for a given lift) [29, 30, 31]. The results show that with the same number of evaluations required by CMA-ES to find a near-optimal solution in a single bin (without a surrogate), SAIL finds solutions of similar quality in every bin (625 bins in these experiments); in addition, when CMA-ES is used with a new surrogate for each bin, it requires an order of magnitude more evaluations than SAIL. Gaier et al. also showed promising results in a more complex 3-dimensional aerodynamic optimization in [31]. In these experiments, the authors assumed that the bin was known from the values of a candidate solution (which is true in the design problem that they explored), but they suggest that the mean prediction of a second GP can be used to compute the coordinate sof the bin when creating the acquisition map (the variance of this prediction would be ignored).

In recent work, Kent and Branke proposed a different acquisition function that captures in a single value the expected improvement to the whole map, called the Expected Joint Improvement of Elites (EJIE) [41]. Their starting point is the Expected Improvement (EI) acquisition function, which is another popular acquisition function in Bayesian optimization [37]. However, the expected improvement is defined relative to the best known value, which does not make sense in a QD algorithm. Instead, Kent and Branke propose to compute the expected improvement for each niche, then sum all the values, so that the acquisition function is maximum for points that are likely to provide large improvements to the objective value of one or more niches. In addition, they note that it is usually not possible to know the cell from the values of the candidate solution (an hypothesis that was made in the experiments with the SAIL algorithm): a second Gaussian process is needed to predict the bin for each candidate. This second process is integrated in the Expected Joint Improvement of Elites (EJIE) by weighting the expected improvement by the probability for a candidate to be in a given cell:

\[ \text{EJIE}(\theta) = \sum_{i=1}^{C} P(\theta \in c_i) EI_{c_i}(\theta) \]  

where \( i \) is the bin index, \( P(\theta \in c_i) \) is the probability of \( \theta \) to be in bin \( c_i \) (computed with a Gaussian process that models the features) and \( EI_{c_i}(\theta) \) is the expected improvement for the bin \( c_i \) (computed with a Gaussian process that models the objective function). For now, the EJIE acquisition gave promising results for a 1-dimensional benchmark problem [41] and more work is needed to compare it to SAIL.

An interesting side-effect of modeling the objective function with a surrogate model is that it becomes easy to increase the resolution of the map by running a QD algorithm using only the models, which can usually be achieved in minutes.

### 5.2 High-Dimensional Feature Space

The grid-based container approach of MAP-Elites has various benefits, such as conceptual simplicity, easy implementation, and it can form the basis for both quantitative QD metrics (e.g., number of filled bins, or the QD score [65]), as well as qualitative evaluation (by visual inspection of a 2D map). For creating the grid, the user needs to provide a number of discretization intervals per feature dimension. This, however, has the drawback of not scaling to high-dimensional feature spaces, as the number of bins increases exponentially with the feature dimensions. For instance, for a 50-dimensional space and 2 discretizations per dimension, MAP-Elites would create an empty matrix of \( 1.13 \times 10^{15} \) cells that requires 4 petabytes of memory (assuming 4 bytes for the pointer of each cell). This motivates the question whether grid-based containers can be used in high-dimensional feature spaces.

Vassiliades et al. [78] proposed an extension of MAP-Elites that addresses its dimensionality limitation using a tool from computational geometry known as a Centroidal Voronoi Tessellation (CVT) [22]. The key insight is that MAP-Elites defines the feature space using a bounding box that contains well-spread rectangular regions (Fig. 2 left). A similar partitioning can be achieved using a CVT with the important difference that the number of regions is explicitly controlled, while the resulting regions have a convex polygonal shape (Fig. 2 right).

The resulting CVT-MAP-Elites algorithm [78], requires a first, offline step (before QD optimization) to compute an approximate CVT based on a user-provided number \( k \) which defines the capacity of the container. The approximate CVT computation typically involves creating a dataset of \( K \gg k \) uniformly-distributed random points in the bounded feature space, and using the \( k \)-means clustering algorithm [50] on this dataset to find \( k \) centroids (Algo. 3). If \( K \) is large enough, the \( k \) centroids become well-spread in the bounding volume. Typically as the number of dimensions increases so should \( K \), however, the approximate nature of the algorithm, as well as the large number of solutions requested \( (k) \) by QD algorithms makes the algorithm perform well. For instance, for finding 10,000 effective gaits for a 6-legged robot, Vassiliades et al. [78] used as feature space, subsets of the 36 parameters that define the gait [17] (i.e., 12, 24 and 36), and demonstrated that CVT-MAP-Elites has the same performance irrespective of the dimensionality, in contrast to MAP-Elites.

**Algorithm 3 CVT approximation**

1. \[ \text{procedure CVT}(k, K) \]
2. \[ D \leftarrow \text{sample_points}(K) \text{ \quad K \ random \ samples} \]
3. \[ C \leftarrow \text{kmeans}(D, k) \text{ \quad cluster \ dataset \ D \ using \ k \ centroids} \]
4. \[ \text{return centroids } C \]

It is important to note that special care needs to be taken when the high-dimensional feature space is defined by sequences. Vassiliades et al. [78] report experiments with a simulated maze-

![Fig. 2. MAP-Elites (left) partitions the feature space using a number of bins (25 in this example), \( k \), that is computed by the number of discretization intervals per dimension requested by the user (i.e., \( k = \prod_{i=1}^{D} n_i \), where \( d \) is the dimensionality of the feature space and \( n_i \) is the discretization interval of dimension \( i \). CVT-MAP-Elites (right) has explicit control over the number of bins (7 in this example) irrespective of the dimensionality of the feature space. Figure taken from [78].](image-url)
navigating mobile robot, and feature spaces of up-to 1000 dimensions composed by trajectories of the robot’s (x, y) location. In order for CVT-MAP-Elites to work, it needs representative centroids, and sampling from a uniform distribution (Algo. 3 line 2) would not work, as it assumes that the various dimensions are independent. For these experiments, the authors [78] used knowledge about the robot’s physical constraints (i.e., it can move at most 2 units and it cannot exceed the bounds of the maze) in order to effectively sample random trajectories that cover the space well.

Another related issue (that can also apply to lower dimensional feature spaces) is when the bounds of the various feature space dimensions are not known a priori. If wrong values are used, the performance of (CVT-)MAP-Elites might deteriorate as it will not be able to fill the grid (the size of the bins would either be too small or too big). A natural way of dealing with this issue is to let the feature descriptors of the sampled solutions define these bounds. Variants of MAP-Elites and CVT-MAP-Elites have explored this direction [77] and allow for the expansion of the bounding box that defines the feature space.

Archive-based containers can naturally be used when the feature space is high-dimensional, as they calculate distances between the sampled solutions. However, algorithms that use such containers, for example, NSLC [47], often come with various parameters that need to be tweaked for the task at hand. An approach called Cluster-Elites [77], that blends ideas from CVT-MAP-Elites and archive-based containers, allows the generation of centroids in non-convex spaces based on the sampled solutions.

5.3 Learning the Behavior Descriptor

Defining the behavioral descriptor space remains a challenging and crucial aspect in QD algorithms, as this decision determines the shape of the produced collections. It often requires a certain level of expertise or prior knowledge on the task at hand to know what are the features that the solutions can exhibit to define the corresponding behavioral descriptor space. However, in certain situations, this prior knowledge is not available or a user might target specific subsets of the possible solutions according to some conditions that are not easy to define in practice. Several pieces of work have proposed solutions to make easier and more automatic the definition of the behavioral descriptor using learning algorithms.

Sometimes the range of possible or desired types of solutions is known in advance, but there is no easy way to programmatically encode this knowledge into a low-dimensional BD definition. This is, for instance, the case when one wishes to generate solutions resembling a set of examples that has been obtained from a different process. A solution to address this problem is to collect all the possible features of each example into a dataset which is then used to train a dimensionality reduction algorithm, such as an auto-encoder or principal component analysis. The outcome of this training is a low-dimensional latent space that captures the relations and similarities of the different examples and that can serve as a behavioral descriptor space. The encoder in the case of the auto-encoder (or the projector for the PCA) algorithm can project any new solution in the descriptor space. With this learned behavioral descriptor space, a QD algorithm produces a collection of solution that covers the latent space and that maximize a fitness function. The fitness function can be totally unrelated to the dimensionality reduction algorithm, or it can be defined as the reconstruction error of the algorithm, to encourage the QD algorithm to generate solutions that look similar to the example set. A schematic illustration of this approach is provided in Figure 3-a.

For example, this approach has been used to teach a robot to execute trajectories that resemble handwritten digits. Finding a way to characterise an arbitrary trajectory into a low-dimensional behavioral descriptor capturing the diversity of handwritten digits is particularly challenging. To side-step this challenge, Cully and Demiris [14] employed an existing dataset of handwritten digits (the well-known MNIST dataset [44]) and train an auto-encoder to find a low-dimensional latent space that captures the most prominent features of the different digits. This latent space can then be used as the behavioral descriptor space and QD algorithms produce a collection of solutions that covers the space of the learned features. As a result, this enabled a robotic arm to learn how to draw digits without having to manually define what are the main features of the different digits.

Instead of using an existing dataset, an alternative is to directly use the solutions generated by the QD algorithm. In this case, the randomly generated samples used in the initialisation of the QD algorithm are used to train the dimensionality reduction algorithm. The corresponding latent space definition becomes the behavioral descriptor space for the execution of a few steps of the QD process. during these steps, the number of solutions in the collection grows, which has the direct effect of accumulating new samples that can be used to extend the training of the dimensionality reduction algorithm and thus change the definition of the latent space. The latent space is then redefined to better include the new solutions that have been discovered and redistribute them in the latent space according to their high-level features. This process can be repeated periodically to enable both the QD algorithm and the auto-encoder to converge simultaneously. A schematic illustration of this approach is provided in Figure 3-b.

The AURORA algorithm (AUtonomous RObots that Realise their Abilities, [13]) uses this approach to enable robots to discover large collections of diverse skills without any prior knowledge on the capabilities of the robots. After each solution evaluation, the trajectories of objects in the environment are recorded and collected for the training of the auto-encoder. This resulted in a collection of solutions to interact differently with objects in the robot’s environment. This concept has been extended in the TAXONS [60] algorithm by using raw images from cameras placed on top of the robot and to discover how to move or interact in the environment. A similar concept has also been used in the DeLeNoX algorithm [49] to evolve a diversity of spacecraft sprite for video games using the Novelty-Search algorithm.

5.4 Improving Variation Operators

The state-of-the-art black-box optimization algorithms exploit the distribution of the highest-performing candidate solutions [36]; most notably, CMA-ES [34] computes a covariance matrix to sample the next population in the most promising direction. By contrast, the first QD algorithms used simple Gaussian variation (mutation) to generate new solutions, because they were focused on the selective pressure. However, the success of modern black-box optimization algorithms suggest that there is much to be improved by exploiting the distribution of the best candidate solutions in the variation operators.

Vassiliades and Mouret investigated how the genotypes of the archives of MAP-Elites are distributed in several benchmark tasks [75]: while the elites are well spread in the feature space (by construction), they occupy a specific volume in the genotype space, that they called the “Elite Hypervolume”. This should not be surprising because high-performing solutions often share...
The training of the auto-encoder is then extended and the process can repeat until convergence of both the QD algorithm and the auto-encoder. Several QD steps are executed to generate new solutions in the latent space, which increase the amount of data available to train the auto-encoder. Starting from randomly generated solutions, the auto-encoder is trained and the produced latent space used as a behavioral descriptor. Then, the solutions filling this latent space. (a) A latent representation of the data. This latent space is then used as the behavioral descriptor space and a QD algorithm can build a collection of successful; instead, Gaier et al. [32] proposed to use a Variational Auto-Encoder (VAE) [42] that is learned from the genotype of the current archive of a QD algorithm. By learning the “latent space” of the data, the algorithm learns the non-linear “recipes” that define the high-performing solutions, so that more elites can be produced.

As a consequence, cross-over is surprisingly effective in QD algorithm, whereas its utility is more controversial in black-box optimization. For instance, evolutionary strategies like CMA-ES [34] do not use it all. Classic cross-over operators like SBX often work well [20], but Vassiliades and Mouret proposed a simplified cross-over that gives good results in many QD problems, called “directional variation”. Given two random elites \( \theta_i^{(t)} \) and \( \theta_j^{(t)} \), a new candidate solution \( \theta_i^{(t+1)} \) is generated by:

\[
\theta_i^{(t+1)} = \theta_i^{(t)} + \sigma_1 N(0, I) + \sigma_2 \left( \theta_j^{(t)} - \theta_i^{(t)} \right) N(0, 1)
\]

where \( \sigma_1 \) controls the variance of the isotropic Gaussian distribution and \( \sigma_2 \) controls the magnitude of the perturbation of \( \theta_i^{(t)} \) along the direction of correlation with \( \theta_j^{(t)} \).

During the same time, an independent study by Nordmoen et al. [58] investigated how static and dynamic mutation rates affect the exploration vs exploitation ability of MAP-Elites in a quadrupedal locomotion task. They tested three dynamic mutation schemes, the isotropic self-adaptation scheme of evolution strategies [5], one based on simulated annealing [43] and another based on the QD coverage metric and found them to have either similar or better QD performance than the static mutation rates. Interestingly, the study by Vassiliades and Mouret [75] also compared isotropic self-adaptation and found it to be less effective than their directional variation operator.

While crossover is a straightforward way to generate individuals that are likely to be in the elite hypervolume, it might sometimes be possible to fit a distribution so that we can directly sample from it. Since this volume can have any shape, modeling it with a simple Gaussian distribution is unlikely to be successful; instead, Gaier et al. [32] proposed to use a Variational Auto-Encoder (VAE) [42] that is learned from the genotype of the current archive of a QD algorithm. By learning the “latent space” of the data, the algorithm learns the non-linear “recipes” that define the high-performing solutions, so that more elites can be produced.

However, if the algorithm uses a Variational Auto-Encoder as a variation operator, it cannot generate candidates that are not in the current approximation of the hypervolume. In other words, when
the QD algorithm is running, it can apply the current “current recipe” but not discover a “better recipe” for elites. It is therefore important to balance exploration — trying candidates outside of the current distribution — and exploitation — learning and using the current recipe. To tackle this issue, Gaier et al. implemented a multi-armed bandit algorithm [2, 40] that tunes the probability of using the VAE and the probability of using other variation operators like Gaussian mutation and directional variation. As a result, the VAE is used only when it helps.

Gaier et al. tested this approach, called Data-Driven Encoding (DDE), in tasks up to 1000-dimensional [32]. The results show that the VAE allows MAP-Elites to be used these kind high-dimensional task, although more tasks need to be investigated in the future. Interestingly, the latent space that is learned by the VAE is a representation of the elite hypervolume that can be reused for future optimization of tasks from the same distribution. For instance, it can be leveraged to quickly recompute a higher-dimensional map by using the latent space as the genotype space, or to fine-tune for a specific bin using a black-box optimizer like CMA-ES.

The combination of the uniform selection operator with standard mutation and crossover operators, which is used for instance in MAP-Elites, is a simple, yet very effective mechanism to produce new solutions. One of its strengths is that it is not biased toward any specific aspect of the optimization process. However, as a direct consequence, the exploration of the search space might be slower than alternative approaches. In particular, we can note that the selective pressure (i.e., the probability of a solution to be selected) induced by this mechanism is inversely proportional to the number of solutions in the collection, which can make this approach less appropriate for the generation of large collections.

Instead of such an unbiased selection mechanism, Fontaine et al. [28] proposed in the Covariance Matrix Adaptation MAP-Elites (CMA-ME) algorithm, the concept of emitters that are independent processes in charge of the generation of new solutions. They defined three types of emitters, each based on the CMA-ES algorithm [34] to drive the exploration according to a specific intrinsic motivation. More precisely, they introduced the Optimizing emitters that use CMA-ES to sample solutions that with higher performance, the Random Direction emitters that favor solutions that are as far as possible along a randomly generated direction in the BD space, and the Improvement emitters that reward solutions that are added to the collection (similarly to the curiosity score detailed above). These different emitters enable the user to specialise the search process for instance to accelerate the coverage of the behavioural space, or searching the nearest local optimum.

5.5 Noisy Functions

One of the main current challenges in QD algorithm is noisy domains, in which the evaluation of the fitness and the behavioural descriptor values are subject to noise. This noise mainly perturbs the addition of solutions in the collection: a noisy BD measure might place a solution in a wrong cell (or region of the BD space), while a noisy fitness value might make the quality of the solution lead to its undeserved preservation in the collection. A simple approach to overcome this challenge is to replicate the evaluation of each solution multiple times (e.g., 100 times) to collect statistics, such as the median for the fitness and the geometric median for the BD, to ensure a robust optimization process. However, this severely deteriorates the data-efficiency of the algorithm. To mitigate this problem and offer a solution that is both robust the noise and more data-efficient, Justesen et al. [39] proposed to use the concept of adaptive sampling [8] to allocate the evaluation budget only on solutions that are promising while avoiding the re-evaluations of solutions that are unlikely to be competitive. The results show that this approach is particularly effective when only the fitness function is noisy, as the noise on the BD creates drifting elites (solutions that drifts to different cells and leaving behind them an empty cell). An alternative approach is proposed by Flageat et al. [27] with the Deep-Grid MAP-Elites (DG-MAP-Elites), in which the grid of MAP-Elites is extended to store multiple solutions per cell, up to a fixed number (e.g., 50). This sub-population of solutions in each cell can be seen as the depth of the grid. Additionally, the selection and addition mechanisms have been changed to select with a higher probability high-performing solutions within each subpopulation, while any new solution is added to the collection by replacing a randomly selected existing one. This avoids maintaining illegitimate solutions and forces the subpopulations to contain solutions that are likely to produce offspring that land in the same cell, thus improving the robustness of the BD.

6 Conclusion

Quality-Diversity Optimization is a novel branch of stochastic optimization that deals with a special kind of objective functions that return not only a fitness value, but also a behavior descriptor (or a feature vector). The goal of this type of optimization is to collect solutions in a container (or archive) so that they cover as much as possible the behavioral space, and they are locally optimized. We presented a short review of the history of QD optimization, and the main current topics under consideration in the community focusing more on the ones that we believe are the most promising directions to follow. Finally, we presented throughout the chapter many successful applications of QD algorithms on numerous fields, and gave an overview of the current limitations.

In particular, QD algorithms are very effective at (a) optimizing very sparse or non-convex functions, (b) illuminating the search space according to user-defined or learned features, and (c) producing locally optimized repertoires of behaviors (e.g., robots walking in every direction). We hope that readers of this chapter will now have an additional tool in their optimization toolkit, which will allow them to solve new problems or visualize their search spaces.

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