TÉCNICO LISBOA

# Optimization in Architecture

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# Contributions

The development of this thesis resulted in several scientific contributions exploring different perspectives of optimization problems:

1. Caetano, I., Ilunga, G., **Belém, C.**, Aguiar, R., Feist, S., Bastos, F., and Leitão, A. (2018). Case Studies on the Integration of Algorithmic Design Processes in Traditional Design Workflows. Proceedings of the 23rd International Conference of the Association for CAADRIA, 1(Giedion 1941), 111–120.

2. **Belém, C.**, and Leitão, A. (2018). From Design to Optimized Design An algorithmic-based approach. Proceedings of the 36th eCAADe Conference - Volume 2, Lodz University of Technology, Poland, 549-558

3. Martinho, H., Leitão, A, **Belém, C.**, Loonen, R, and Gomes, M. G. (2019). Algorithmic Design and Performance Analysis of Adaptive Façades. Proceedings of the 24th Annual Conference of the Association for CAADRIA, Welligton.

4. **Belém, C.**, and Leitão, A. (2019). Conflicting Goals in Architecture: A study on Multi-Objective Optimization. Proceedings of the 24th Annual Conference of the Association for CAADRIA, Welligton.

5. **Belém, C.**, Santos, L. S., and Leitão, A. (2019). On the Impact of Machine Learning: Architecture without Architects?. 18th International Conference CAAD Futures 2019, Korea (Submitted).

# Abstract


# Keywords

Algorithmic Design; Algorithmic Analysis; Algorithmic Optimization; Derivative-Free Optimization; Machine Learning; Surrogate-based Modeling

# Resumo

# Palavras Chave

Design Algorítmico; Otimização livre de derivadas; Aprendizagem Máquina; Modelos baseados em aproximações.

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# Listings

# Acronyms

| | |
|---|---|
| **AD** | Algorithmic Design |
| **AA** | Algorithmic Analysis |
| **BIM** | Building Information Modelling |
| **BPO** | Building Performance Optimization |
| **BPS** | Building Performance Simulation |
| **CAD** | Computer-Aided Design |
| **CRS** | Controlled Random Search |
| **DIRECT** | DIviding RECTangles |
| **ER** | Error Ratio |
| **ES** | Evolution Strategy |
| **GA** | Genetic Algorithm |
| **GD** | Generational Distance |
| **GUI** | Graphical User Interface |
| **HJ** | Hooke-Jeeves |
| **HV** | Hypervolume |
| **HVAC** | Heating, Ventilation, and Air Conditioning |
| **HypE** | Hypervolume Estimation Algorithm for Multi-Objective Optimization (MOO) |
| **IGD** | Inverted Generational Distance |
| **ML** | Machine Learning |

| | |
|---|---|
| **MOEA** | Multi-Objective Evolutionary Algorithm |
| **MPFE** | Maximum Pareto Front Error |
| **MOO** | Multi-Objective Optimization |
| **MOOA** | Multi-Objective Optimization Algorithm |
| **NFLT** | No Free Lunch Theorem |
| **NMS** | Nelder-Mead Simplex |
| **NN** | Neural Network |
| **NSGA-II** | Non-dominated Sorting Genetic Algorithm II |
| **ONVG** | Overall Non-dominated Vector Generation |
| **ONVGR** | Overall Non-dominated Vector Generation (ONVG) Ratio |
| **PSO** | Particle-Swarm Optimization |
| **RBF** | Radial Basis Function |
| **RF** | Random Forest |
| **SPEA2** | Strength Pareto Evolutionary Algorithm 2 |
| **SOO** | Single-Objective Optimization |
| **SVM** | Support Vector Machine |

# 1 Introduction

## Contents

The act of making something as fully perfect, functional or effective as possible is a behavior that is constantly sought by us, Humans, in a process known as optimization [Webster, 2018]. Intuitively, through optimization one aims to improve a system in terms of different quantitative measurable aspects. Although usually striving to fully optimize these systems, i.e., to obtain *perfect* systems, it is often the case that finding a better one or a near-optimal system suffices.

Generally, optimization processes are composed of two main parts: (1) the model of the system to be optimized and (2) the algorithm responsible for finding the optima. Conceptually, the model is a description of the system that is comprised of (a) variables or unknowns, i.e., representations of the system's characteristics, (b) objectives or criteria, i.e., quantitative measures of the system's performance and that are usually functions of the system's variables, and, optionally, (c) constraints, i.e., system's conditions that have to be satisfied to guarantee the system's feasibility [Nocedal and Wright, 2011]. Subsequent to model definition, we reach the second part of optimization processes, that is, to search among the set of possible solutions for the optimal ones. The strategy used to search the solution space is the responsibility of optimization algorithms, which enclose a detailed description of the steps necessary to attain optimal solutions. The optimal solutions depend on the values of the model's objectives, and the search directions depend on whether they should be maximized or minimized.

In the mathematical sense of optimization, these processes can be classified differently depending on the numerous alternatives for representing models or on the strategy underlying the search for optimal solutions. Concretely, models representations may differ in the variables' type, the presence of absence or constraints, the number and nature of objective functions, among others, whereas search strategies might explore vaster or narrower regions of the solution space. Although we introduce four of these classifications, we refer the interested reader to [Nocedal and Wright, 2011, Nemhauser and Wolsey, 1988] for a more comprehensive treatments of these subjects. We selected four classifications due to their relevance and their ubiquitous in optimization problems.

The first classification differentiates continuous and discrete optimization problems depending on the variables' types. Continuous optimization refers to problems defined uniquely by continuous variables and, therefore, characterized by an infinite solution space, whereas discrete optimization refers to problems for which some or all their variables are discrete, hence yielding a finite solution space. In continuous optimization, the smoothness of functions make it possible to reason about the behavior of all points close to $x$ and, consequently, to solve these problems more easily, whilst the commonly present irregularities of discrete optimization functions do not, in general, allow to draw any information about the behavior of points close to $x$. Moreover, the discrete classification encloses finer classes, such as integer optimization or combinatorial optimization [Nemhauser and Wolsey, 1988].

The second classification is related to the absence or presence of constraints on the variables. Unconstrained optimization problems result from many practical applications and have no restrictions on the values of the variables. Contrastingly, constrained optimization problems usually emerge from systems for which constraints are crucial (e.g., economy problem, imposing cargo constraints) and, therefore, incorporate such constraints into the problem's definition [Nocedal and Wright, 2011]. Variables can be conditioned using hard or soft constraints. The former sets conditions for the variables that must be satisfied, i.e., to vary within simple bounds (e.g.: $-1 < x < 1$) and to relate to other variables in certain ways (e.g.: $\sum_i x_i$), whereas the latter sets penalties for the variables whose value violates the condition. Constrained optimization are often converted to unconstrained optimization problems by replacing hard constraints by soft constraints, i.e., by adding penalization terms in the objective function to discourage the violation of constraints.

The third classification distinguishes optimization problems in terms of the aim of the search, particularly, whether it is a global or a local search. In local optimization, the search process strives to find a solution that is locally optimal, i.e., for which its value is better than all other points in its vicinity. The points that satisfy the previous property are known as local optima. On the other hand, global optimization problems strive to find the globally optimal solutions, i.e., the best of all the local optima.

The fourth, and final, dichotomy herein discussed is with respect to the number of objectives to optimize, which are distinguished in single-objective and multi-objective optimization. Indeed, optimization is frequently required to address problems involving more than one objective. For example, people often face decisions involving two or more conflicting objectives, either to effectively manage resources, or just to ponder several factors associated with certain decisions (e.g.: purchase a house). As opposed to simpler single-objective optimization problems, which focus on the optimization of one objective, these processes are examples of Multi-Objective Optimization (MOO) problems, as they attempt to simultaneously optimize multiple conflicting objectives.

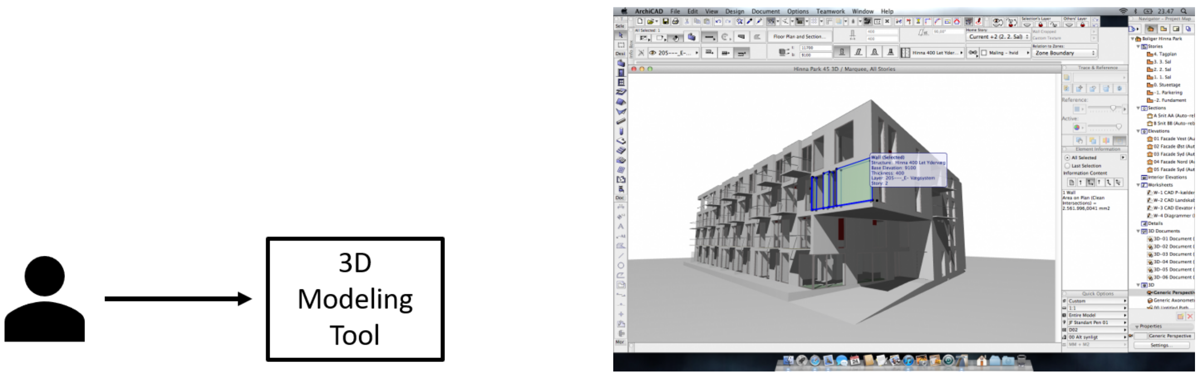
The application of optimization goes beyond day-to-day life decisions, also having a paramount impact on decisions involved in fields like economy, science, engineering, among others. As a case in point, optimization yields a great potential to architectural practices, for it directly impacts the building industry: optimization enables the reduction of the economic and ecological footprint of the building sector through the finding of more efficient building variants, prior to their construction. Given its importance to the world's sustainability and economy, this thesis focus on the application of optimization processes to enhance the architectural practice. The following sections provide an overview of the involvement and the evolution of these processes in the architectural field. We end this chapter by highlighting our research goals and by outlining this thesis structure.

## 1.1 From Design to Optimized Design

The usefulness of optimization goes beyond architectural design applications, benefiting other engineering fields, like Mechanics and Electronics, through the optimization of components and circuits designs.

In the architectural practice, optimization has been gaining relevance for the past few years [Cichocka et al., 2017a], especially due to the impact of building construction and building maintenance in the economy and environment. For this reason, designers are shifting from a pure aesthetically-based to performance-based design, where buildings are being optimized to achieve the best possible values regarding different aspects of their design, such as thermal comfort, energy consumption, lighting comfort, structural behavior, cost, among others.

This has only been possible due to the technological improvements in the architectural practice over the last few decades. The adoption of computer science techniques was responsible for the dissemination of digital modelling tools, which allowed for more accurate and efficient design of highly complex buildings. These tools enabled a shift from traditional paper-based approaches to more computerized ones, such as Computer-Aided Design (CAD) and Building Information Modelling (BIM) applications, where changes to designs are trivial and do not require manually erasing and redrawing parts of the original design [Ferreira and Leitão, 2015]. Figure 1.1 illustrates the general view of this computer-aided design process, as well as an example of a 3D modeling tool. The architect interacts directly with these modeling tools to incrementally realize his design ideas.




**(a)** **(b)**

**Figure 1.1:** (a) Simplification of a computer-aided design workflow (b) Building design example in a 3D modeling tool. Image retrieved from [Jared Banks, 2012]

Shortly after, the development of computer-based simulation tools enabled designers to simulate the behavior of building designs regarding specific criteria, i.e., to get a measurement of its performance [Malkawi and Kolarevic, 2005]. Through this process, called Building Performance Simulation (BPS), designers could easily validate whether their building's performance satisfied the efficiency requirements and, ultimately, optimize their design by iteratively generating multiple variations of the same design, assessing their performance, and selecting the better ones. Albeit being very primitive, architects now had the elementary mechanisms required for optimizing their building's designs, which spurred a new performance-based approach.

### 1.1.1 Building Performance Optimization

Building Performance Optimization (BPO), a simulation-based optimization approach, treats the results produced by the simulation tool as the functions to optimize. Although invariably suffering from some degree of imprecision and inaccuracy, using these simulations it becomes possible to estimate the performance of complex designs. Particularly, these estimates are beneficial in designs for which analytical solutions are often very difficult or even impossible to derive [Kolda et al., 2003]. In these cases, the objective function, i.e., the function to optimize, is derived from the simulations' results. These functions have a domain which corresponds to the range of acceptable designs, as specified by the architect.

A known drawback of simulation-based approaches is the time required to achieve reasonable results for complex systems [Law and Kelton, 1991] which is associated with different aspects of the problem, namely: (1) its **domain** which, depending on the nature of the problem, might use different methodologies to produce the corresponding estimates (e.g., thermal *versus* structural); (2) its **intrinsic structure** which, depending on the attributes and relations of the system, might lead either to simpler or to more complicated computations (e.g., skyscraper *versus* a small house); and (3) its **analytical model**, which has the essential properties of the system we are trying to simulate and that will be used as input to the simulation tool. Generally, the domain and structure do not change for the same problem, albeit there are numerous ways to produce multiple analytical models. Depending on the level of detail of the analytical model (e.g., using a single plane *versus* a mesh to represent a non-planar surface), both the computational time and the result of the simulation might change.

In architecture, the generation of each analytical model is a time-consuming and complex task. On the one hand, it is often necessary to generate multiple models of the same design because of the simulation tools' specificity, i.e., in order to evaluate a design, each simulation tool requires a specialized model of the same design. On the other hand, simulation tools often yield time-consuming processes, where a single simulation can take up to seconds, minutes, hours, days, or even weeks to complete.

In addition to the simulations' specificity and complexity, architectural designs are inherently complex, thus leading to less predictable objective functions, for which mathematical forms are difficult to formulate [Machairas et al., 2014]. For this reason, information about the derivatives of such functions cannot be extracted, and methods depending on function derivatives cannot be used to address architectural optimization problems. Particularly, classical gradient-based optimization methods cannot be used because they exploit the function's derivatives. Instead, other methods that do not rely on the existence of an explicit mathematical form should be used, i.e., methods that treat the optimization functions as black-boxes, relying uniquely on the outputs of numerical simulations.

Despite the flexibility provided by CAD and BIM tools, architects often face difficulties when modeling complex geometry. A BPO methodology requires the experimentation of different design variations, which implies spending a large amount of time to manually make changes to the design. Since an optimization process requires evaluating several variations of the same design, the manual execution of the required changes implies a lot of effort, hence making the whole optimization process unviable.

### 1.1.2 Algorithmic Design

An approach capable of creating forms through algorithms is crucial for overcoming the aforementioned limitations. An example of such approach is Algorithmic Design (AD) [Branco and Leitão, 2017] and Figure 1.2 illustrates a simplified view of its application in a design workflow. In this approach, the architect entails an algorithmic description of the intended design. After elaborating the algorithm, executing it will automatically generate the corresponding 3D model in a CAD or BIM tool. Algorithmic approaches are inherently parametric, thus enabling the generation of different variations of the same design by making simple modifications to the values of the parameters [Leitão et al., 2014].

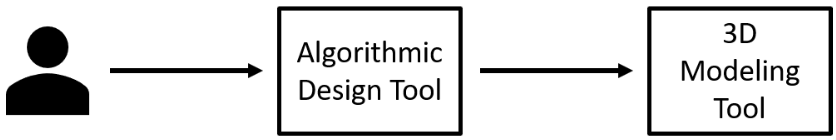
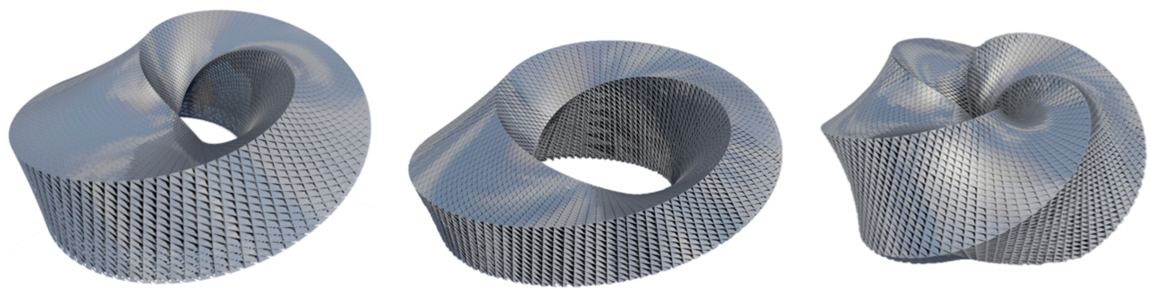



**Figure 1.2:** Algorithmic-based design workflow

As an example, consider the algorithmic design of Astana's National Library from the Bjarke Ingels Group (BIG) architects, illustrated in Figure 1.3(a). Initially, the architect selects an AD tool providing the necessary design primitives. Then, he uses those primitives to create a computational program enclosing the relative relations among the different design elements, so that when a modification occurs in one element, that same modification is propagated throughout that element's dependencies. In the end, the architect creates a procedure responsible for creating the whole design, which when executed will produce the corresponding Astana 3D model. Because the Astana's design resembles a *möbius* strip, define the procedure in terms of two parameters: the radius, defining the whole width of the design, and the number of twists of the strip. Now, he is able to easily generate different variations of the Astana by invoking the procedure with different values for these parameters. Figure 1.3 illustrates the original design, two design variations, where the radius and the number of turns in the design are increased, respectively.

Only recently has the algorithmic paradigm begun to settle in the architectural practice. The requirement for programming knowledge is often an obstacle to the adoption of these approaches, since it



**(a)** **(b)** **(c)**

**Figure 1.3:** Astana's National Library Design variations: (a) Original (b) Larger diameter (c) Two *möbius* twists

requires larger initial investments for architects to learn how to program. Despite these investments, the benefits obtained with algorithmic approaches surpass the ones obtained when using CAD or BIM tools directly for the design of complex buildings. Particularly, initial investments can be quickly recovered when the need for the incorporation of changes arises or when it becomes necessary to experiment different design variations [Leitão et al., 2014]. This is especially important when facing design processes characterized by continuously changing constraints and requirements of the design. In these scenarios, a manual-based approach requires to constantly change the design by hand, thus incurring in a dreadful and tiresome process, whereas an algorithmic approach enables the effortlessly generation of a broader range of design solutions, as well as the easy modification of the algorithmic model to comply with new requirements. As a result, with algorithmic approaches, architects are able to explore larger regions of the design solution space, as well as to explore innovative solutions which were not previous considered due to their time and effort complexity [Leitão et al., 2014].

Another benefit of the AD approach is the ease of maintenance of the models involved in building design. In fact, since AD usually requires a single model of the design, the algorithmic model, it is easier to maintain in scenarios where changes are frequent. On the other hand, manual-based-approaches often involve the creation and maintenance of multiple models of the same design (e.g., analytical models, 3D models), which quickly becomes hard and tiresome to maintain.

The appearance of AD was crucial for the automation of optimization processes as it enables the automated generation of multiple designs by simply changing the values of the design's algorithmic model. However, to optimize such designs, it is necessary to create the analytical models, which can be very dissimilar to the 3D models produced by the AD tool. Therefore, to evaluate the 3D models produced by the AD tool, the architect must manually generate the corresponding analytical models. Particularly, for complex buildings, this task requires large time and effort investments, which makes most optimization processes impracticable.

### 1.1.3 Algorithmic Analysis

Faster and broader design space exploration prompted the creation of increasingly complex building designs, which became less predictable with respect to different aspects [Branco and Leitão, 2017], such as thermal, lighting, acoustics, among others. Moreover, recent requirements for efficient and sustainable buildings led to the demand for buildings that not only are well-designed, but also exhibit a good performance at those aspects.

Nowadays, most of the available simulation-based analysis tools are single-domain toolsets, each analysing different parameters within their domain [Malkawi and Kolarevic, 2005], i.e., while a lighting analysis tool measures daylight and glare coefficients, an energy simulation tool measures other coefficients related to thermal, energy consumption, and Heating, Ventilation, and Air Conditioning (HVAC) systems. Unfortunately, this often implies the production of different analytical models for the corresponding simulation tools. Moreover, the 3D models produced by 3D modeling tools are generally dissimilar to the specialized models required by each analytical tool. To evaluate the design performance on different domains (e.g., lighting, energetic, structural), the corresponding analytical models have to be produced either by hand, or through translation processes that convert generic 3D models into specialized models required for analysis.

Currently available techniques for the production of analytical models exhibit a few limitations, including: (1) hand-made analytical models, which might be a more faithful representation of the original model but they require a considerable amount of effort to create; (2) despite the existence of tools that attempt to convert a 3D model into the corresponding analytical model, this conversion is frequently fragile and can cause errors or loss of information; (3) ideally, the results of the analysis would be used to guide changes in the original design, but these changes require additional time and effort to implement, as does redoing the analysis to confirm the improvements. For this reason performance analyses are typically postponed to later stages of the design process, only to verify the fulfillment of the performance requirements.

To overcome the time and effort limitations associated with the production of analytical models, one can exploit the ideas of algorithmic approaches to automatically generate the necessary analytical models from an algorithmic description. Algorithmic Analysis (AA) is an extension to the AD approach that besides enabling the automatic generation of analytical models from a design's algorithmic model, also automates the setup of the analysis tool and the collection of its results [Aguiar et al., 2017]. Following this approach, in an AD tool, the architect creates the algorithmic model that describes his design's intents and then changes its configurations as to reflect the analysis tool to use, for example, by changing the values of the configuration parameters. Figure 1.4 illustrates the AD and AA design workflow, as well as examples of the Astana's National Library models produced for each tool. Note that, even though the abstract description of the design is the same for 3D and analytical models, the produced models can be very different, e.g., a truss is represented as a graph of nodes and edges when submitted for structural analysis, whereas for lighting analysis the truss is represented by its surfaces, and, in the 3D model, the truss is represented by a set of masses representing its bars and nodes.

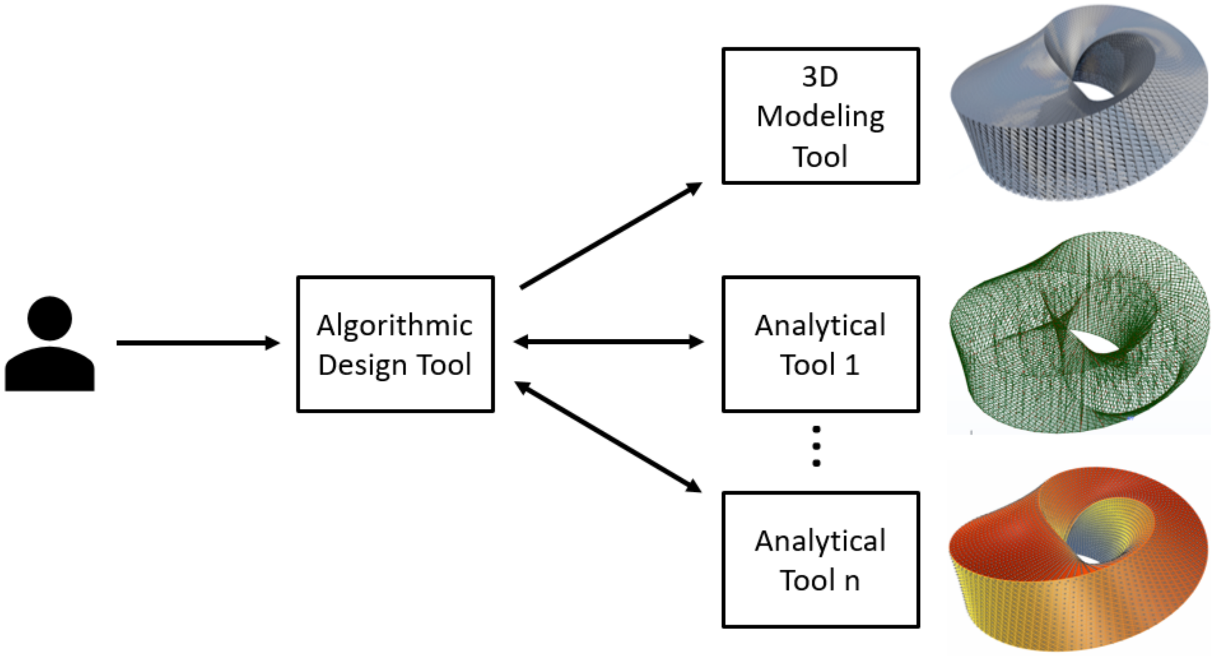



**Figure 1.4:** Algorithmic Design and Analysis design workflow with examples of the Astana's National Library design and analytical models: (top) 3D model; (center) Robot's structural analysis model; (bottom) Radiance's pos-radiation analysis model.

The AA approach is able to enhance performance-based design approaches, as it provides means to effortlessly perform analysis throughout the whole design process, instead of just at final stages. Depending on the performance requirements, architects might need to use different analysis tools: (1) for daylight analysis, Daysim and Radiance are very popular among the community, (2) for energy simulations, EnergyPlus, TRNSYS and DOE-2 are widely used [Nguyen et al., 2014], (3) for structural analysis, Robot Structural analysis is a well-known reputed tool, and (4) Olive Tree Lab and Pachyderm Acoustical Simulation are examples of good acoustic analysis tools.

The AA approach was also very important to allow the automation of optimization processes, as it abstracted the production of the analytical model, removing the need for direct human intervention and reducing the errors and information loss. Additionally, together with AD, it provides the mechanisms to quickly update a design, to generate the corresponding analytical model, to automatically evaluate the design in an analytical tool, and, finally, to collect the results and use them to guide the search for optimal solutions. Despite being possible to automate optimization processes, in order to do so, the architect must define a script entailing an optimization algorithm every time he intends to attain better designs. Besides lacking enough knowledge or expertise about optimization algorithms themselves, in order to entail one, architects would have to either create their own algorithm, or they would have to use one available in some optimization framework. Moreover, because of the efforts associated with the implementation of the optimization algorithm, architects are tempted to adopt the same algorithm to optimize every design, thus instilling performance impacts in the overall optimization time. Among other obstacles, the large time and investment efforts, as well as the lack of knowledge, are often main setbacks to the application of optimization processes in architectural design contexts.

Despite all the obstacles, optimization prevailed and different approaches have spawned into the architectural practice. During this time, multiple surveys have identified the difficulties and the advantages of each approach, which enabled the development of optimization tools more targeted to architects needs. In the following section, we briefly mention some of these approaches and we emphasize the key points of optimization processes in architecture.

### 1.1.4 Architectural Optimization Workflow

In architecture, design optimization might be approached differently. In the past, most optimization processes were comprised of different frameworks, which often had to be integrated with each other. Architects often attempted to integrate existing mathematical optimization and visualization frameworks within their workflow. Due to the tools' specificity, their integration was often an obstacle to the optimization process itself. More recently, the emergence of visual parametric approaches, such as Grasshopper, Dynamo [David G. Rutten, 2007, Ian Keough, 2011], among others, coupled with the growing consciousness of both the limitations and the benefits of optimization in building design, have led to the development of ready-to-use optimization toolsets (e.g., Galapagos, Goat, Octopus, Opossum). However, despite enabling the optimization of several designs, visual parametric tools are known to scale poorly with the complexity of the design [Heijden et al., 2015], thus diminishing and restricting its optimization capabilities.

On the other hand, textual algorithmic approaches are known to scale well with designs' complexity. In addition to its scalability benefits, its growing popularity among building design practitioners [De Kestelier and Peters, 2013], its models' flexibility, as well as its capacity to automate optimization processes allow the development of more robust and complete optimization tools. To successfully take advantage of such a tool, an AD-based design workflow optimization methodology must be followed. In this approach, the architect idealizes a design which he ought to produce in the corresponding AD tool. For this purpose, he creates the computational program, defining the parameters that represent the degrees of freedom in the design, i.e., the parameters which he is willing to manipulate in order to achieve more efficient designs. After the conception of the design's algorithmic model and, provided the values for the parameters, the AD tool generates 3D or analytical models for visualization and performance analysis purposes, respectively. Optionally, the architect may decide to optimize his design according to some particular aspects, potentially leading to the exploration of design solutions that were not previously considered. In that case, the optimization algorithm explores different design candidates, using the results produced by simulation tools as the functions to optimize. The execution of the optimization algorithm then yields optimal (or near optimal) design solutions.

Considering the previous view of an algorithmic-based design workflow, we identify four key dimensions in an optimization process:

1. **Analytical models**: when the optimization algorithm specifies a candidate design, i.e., a concrete configuration for the parameters of the model, analytical models are automatically generated by the AD tool. These models are then used as input for the corresponding analytical tools. These models can be improved, either through simplification of the analytical models, or by enriching them with context information. The former enables the simplification of the analysis itself and potentially reduces the simulation time, by providing an equivalent but simpler model to the tool, whilst the latter enables the attainment of a more detailed and realistic simulation, which is not always possible due to limitations in the AD tool.

2. **Optimization algorithms**: the algorithms that explore the design space in the quest for optimal (or near optimal) solutions. These algorithms use the results obtained from performance analysis of different design variations as the functions to optimize, i.e., as objective functions. Generally, the algorithm uses these inferred functions to guide the search for optimal solutions. The time complexity of the algorithm is typically dependent on the number of function evaluations. In architectural design, these functions entail time-intensive simulations, thus instilling optimization processes that may take minutes, hours, days, or even weeks to complete.

3. **Intelligibility of Results**: Cichocka et al. identify the need for intelligibility of the optimization processes within the architectural community [Cichocka et al., 2017a]. Having access to an explanation, regarding the quality of a design solution, allows architects to make more informed decisions. With these explanations, the architect can not only provide valuable arguments for its implementation, but also, depending on the quality of the explanations, learn with the process, thus fostering more efficient and faster future designs.

4. **Interactivity and Visualization**: interactive and visual aspects are highly important features in the context of optimization processes [Ashour, 2015]. On the one hand, an interactive optimization process enables its user to transfer knowledge about the problem at hand, for instance, by adding or removing constraints or by exploring different, yet unexplored regions of the design space, hence potentially increasing this process' performance. On the other hand, optimization processes providing better visualizations and representations of their own evolution can present their users with better feedback about the course of the search. This feedback is important, as it also allows

the comparison of variable-objective correlations and the making of more informed decisions about the optimization process itself, e.g., whether the evaluations made so far suffice or if the algorithm is converging to non-conventional designs that he refuses to accept.

## 1.2 Goals

The interest in design optimization is evident within the architectural community. However, the currently existing tools are often fragile or limited, frequently compromising the application of optimization in architecture. This thesis focus on optimization processes within the architectural domain, providing a framework for optimizing both single and multi-objective problems. The implementation of such framework requires the definition of: (1) a modeling language to support the specification of optimization problems, (2) a wide variety of optimization algorithms to solve optimization problems, and (3) a visual presentation of the obtained results to provide a more comprehensive feedback over the optimization results.

To achieve the goals that we propose, we reviewed different mathematical optimization modeling languages and optimization frameworks, pondering the benefits and obstacles of each one. Based on these languages and frameworks, we established the base requirements for the implementation of a simpler framework and its seamless application within the architectural practice.

## 1.3 Organization of the Document

The next chapters of this thesis are organized as follows:

**Chapter** 2 presents an overview of the current optimization practices in architecture and makes a balance of the benefits and drawbacks associated to each one.

**Chapter** 3 describes the architecture of the implemented framework and enumerates important design decisions that were made during its implementation.

**Chapter** 4 evaluates both quantitative and qualitative aspects of the proposed solution, evaluating its performance in the context of three real-world case studies.

**Chapter** 5 emphasizes the importance of optimization in architecture and draws some conclusions about the final work and how it can effectively influence the architectural practice. Finally, we reflect over future improvements for the proposed frameworks.

# 2

# Background

## Contents

The development of an algorithmic-based framework for optimization, applicable to architectural domains, requires a careful review over the current literature on BPO practices and limitations.

Firstly, the *ad-hoc* nature of the functions used for performance assessment in BPO motivates the application of a special class of optimization algorithms, the derivative-free algorithms. Within this class, different categories emerge, emphasizing the algorithms' different properties and search strategies. Applying the adequate algorithm to a certain problem may potentially increase the efficiency of an optimization process.

Secondly, there are multiple approaches to optimization that might be considered. Generally, BPO practices include the simultaneous optimization of multiple aspects. However, they often opt for simpler specifications, often disregarding all but one of the initially considered aspects.

Finally, currently available architectural design optimization tools explore the parametric models produced in visual programming environments, such as Grasshopper and Dynamo. These visual programming environments are implemented as plug-ins, which are tightly integrated with CAD and BIM tools, respectively. As a result, the connection between optimization tools and visual design workflows becomes seamless and friendlier. Additionally, these optimization tools usually expose a *ready-to-run* interface, which is very appealing to most BPO practitioners [Cichocka et al., 2017a].

The proceeding sections go into detail about these three views of BPO practices.

## 2.1 Derivative-Free Optimization

Different optimization algorithms can solve, more or less efficiently, specific optimization problems, depending on their characteristics. Particularly, for optimization problems explicitly defined through mathematical formulations, algorithms that explore the information from the derivatives of such formulations to guide the search for optimal solutions are very efficient. These algorithms are referred to as classical gradient-based algorithms. However, when neither the mathematical form, nor the information about the derivatives is easily available, it becomes necessary to explore other classes of algorithms. Fortunately, derivative-free algorithms are remarkably suitable for addressing these problems, as they do not use information about the objective functions' derivatives to find optimal solutions, instead, they treat the objective functions as *black-boxes* and guide the search based on the result of previously evaluated solutions [Rios and Sahinidis, 2013].

In architecture, it is often impossible to attain a mathematical formulation for the objective functions, especially for complex designs. Alternatively, architects frequently use simulation tools as means to replace the closed-form mathematical expressions relating design's parameters to the objective functions [Wortmann and Nannicini, 2016]. As a consequence, information about the objective functions becomes difficult to attain, often requiring excessive amounts of resources. This lack of information prompts the need for algorithms that treat these functions as *black-boxes*. A simple approach is to systematically experiment with different parameter values until the best solutions are found, whereas a second, and more complex, approach is to use derivative-free optimization algorithms, also commonly referred to as black-box optimization algorithms within the architectural community [Wortmann and Nannicini, 2016].

Derivative-free algorithms allow to overcome the difficulty of deriving analytical forms that has has been rising with the increase of building design's complexity. [Machairas et al., 2014]. For this reason, derivative-free algorithms are sought as useful tools to optimize designs, having been applied extensively to optimize building designs' manifold aspects. Among the numerous studies that apply derivative-free optimization algorithms to optimize building designs, we refer to the distinct works of Wortmann [Wortmann and Nannicini, 2016, Wortmann et al., 2015, Wortmann et al., 2017, Wortmann, 2017b], Evins [Evins and Vaidyanathan, 2011, Evins et al., 2012, Evins, 2013], and Waibel [Waibel et al., 2018] which cover the optimization of various aspects, including, among others, structural, lighting, thermal, energy consumption, and carbon-emissions.

For the past decades, the constant development and improvement of derivative-free optimization algorithms led to a diversified tools' gamut, each with its own characteristics and limitations. While the main ideas behind each algorithm's category seem to be more or less recognized throughout the architectural community, the lack of standards make it difficult to decide which definitions to convey [Rios and Sahinidis, 2013, Wortmann and Nannicini, 2017]. The currently most relevant classifications are: (1) the one presented by [Rios and Sahinidis, 2013] that, based on the functions being used to guide the search process, classifies the algorithms into direct search or model-based algorithms; and (2) the classification provided by [Wortmann and Nannicini, 2017], which first subdivides the algorithms in two groups according to the number of solutions generated in each iteration, namely metaheuristics and iterative algorithms, and only then proceeds to classify iterative algorithms as direct search or model-based algorithms, depending on the function that is used during the search.

This thesis will consider an approach similar to the one proposed by Wortmann [Wortmann and Nannicini, 2017] by exploring the concepts of metaheuristics, direct-search, and model-based algorithms. Albeit the apparent chasm between these classifications, some algorithms draw ideas from distinct classes, thus emphasizing not only the blurred lines of such categorizations, but also the difficulties that lie with the definition of more standardized classifications.

The following sections describe each class and its intrinsic characteristics, proceeded by a brief comparison among them in light of the architectural design practice.

### 2.1.1 Direct Search Algorithms

Although there seems to be no precise definition for direct search algorithms [Kolda et al., 2003], these are often identified as algorithms that iteratively [Kolda et al., 2003, Wortmann and Nannicini, 2016]: (1) evaluate a finite sequence of candidate solutions, proposed by a simple deterministic strategy; and (2) select the best solution obtained up to that time. They are sought as valuable tools to address complex optimization problems, not only because most of them were proved to rely on solid mathematical principles, but also due to their good performance at initial stages of the search process [Rios and Sahinidis, 2013, Wortmann and Nannicini, 2016].

The main limitations of the algorithms in this class is their performance deterioration with the increase on the number of input variables, and their slow asymptotic convergence rates as they become closer to the optimal solution [Kolda et al., 2003].

Some examples of relevant direct-search algorithms include Hooke-Jeeves (HJ) [Hooke and Jeeves, 1961], Nelder-Mead Simplex (NMS) method [Nelder and Mead, 1964], SUBPLEX [Rowan, 1990], DIviding RECTangles (DIRECT) [Jones et al., 1993], among others.

### 2.1.2 Metaheuristics Algorithms

In the original definition [Glover and Kochenberger, 2003], these algorithms were solely based in the interaction between local improvement procedures, called heuristics, and higher-level strategies, called metaheuristics. On the one hand, heuristics are techniques that locate good solutions, but not necessarily the optimal, nor the correct solution, and that often consider the trade-off between precision and quality, and computational effort. On the other hand, a metaheuristic is an algorithmic framework that can be applied to different problems, with a few modifications to add problem-specific knowledge [Glover and Kochenberger, 2003], if so is desired. Moreover, a metaheuristic is a higher-level strategy that extends the capabilities of heuristics by combining one or more heuristic methods (referred to as procedures), while being agnostic to each heuristic. The "'meta" classification of these algorithms results from the fact that they control the heuristics applied in the process.

Throughout time, this class has grown to include any algorithm that includes simple heuristics to locate good solutions in complex design spaces, while considering the trade-off between precision, quality, and computational effort of the solutions. These algorithms often rely on randomization, and biological or physical analogies, to perform robust searches and to escape local optima [Glover and Kochenberger, 2003, Wortmann and Nannicini, 2016]. Additionally, their non-deterministic and inexact nature confers them the ability to effortlessly handle complex and irregular objective functions [Wortmann et al., 2017], as well as, to easily adapt to MOO contexts, or even to provide domain-specific knowledge through the heuristics [Wortmann et al., 2017].

Metaheuristics are efficient optimization algorithms when provided with sufficient amount of time to do the necessary objective function evaluations [Conn et al., 2009]. However, advantages can quickly become disadvantageous by simply changing the application context. This is the case of BPO in the architectural practice, where each evaluation is a time-consuming task and the execution of thousands of evaluations rapidly becomes an infeasible scenario. Due to their stochastic nature, limiting the number of evaluations has severe repercussions, both on the convergence and performance guarantees [Hasançebi et al., 2009].

In the architectural design context, some of the most relevant metaheuristics algorithms include the Particle-Swarm Optimization (PSO) algorithms, some evolutionary algorithms, such as Genetic Algorithm (GA), Evolution Strategies (ESs), and even local search algorithms like tabu search and simulated annealing. We refer the interested reader to [Blum and Roli, 2003, Glover and Kochenberger, 2003] for more details about these metaheuristics algorithms.

### 2.1.3 Model-based Algorithms

Model-based algorithms are effective handlers for time-consuming problems, where sensitive information is expensive to collect [Forrester and Keane, 2009, Wortmann and Nannicini, 2016]. These problems are characterized by the large time complexity associated with the computation of the values of the objective function, and by the absence of previous knowledge about the objective function. Model-based algorithms are able to provide instant estimates of a design's performance, by supplementing or replacing the original objective function by its approximation [Wortmann and Nannicini, 2016]. This approximation, called the surrogate, is generated from a set of known objective function values, and is then used to determine the promising candidate solutions to evaluate next. These candidate solutions are then used to improve the surrogate and this process is repeated until a stopping condition is satisfied [Koziel and Yang, 2011].

Despite having a well-defined analytical form, which makes computations on the surrogate model more efficient than on the original objective function, the surrogate is only an approximate representation of the original function, and, therefore, must be constantly updated to guarantee a reasonable locally accurate representation [Koziel and Yang, 2011]. Figure 2.1 illustrates a surrogate that is accurate near the initial solutions. However, as we analyse solutions far from the initial ones, the accuracy of the surrogate model worsens.

Nowadays, the existing plethora of techniques applicable to the generation of surrogate models range from trust region methods to Machine Learning (ML) techniques. These techniques can be used to create (1) local surrogates, i.e., models where the approximation to the objective function is built around a certain point, and (2) global surrogates, i.e, models where the approximation is generated from all the obtained points. Whilst the former relies on the construction of simple, partial models of the objective

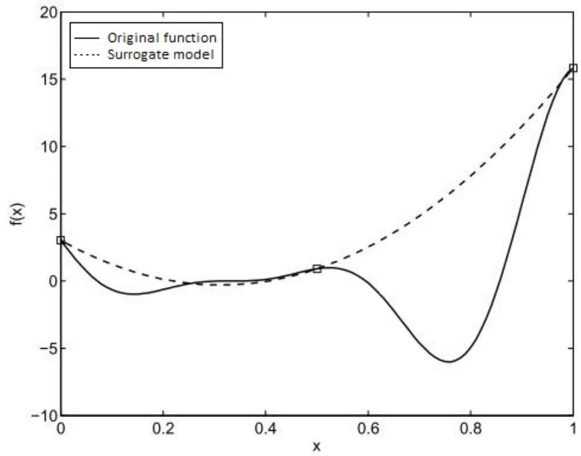



**Figure 2.1:** Original function and corresponding surrogate model, created based on three initial solutions (squares). This image was retrieved from [Koziel and Yang, 2011].

function, the latter relies on the creation of a full model. The creation of the full model, requires balancing the need for improving the accuracy of the model by exploring broader regions in the solution space, with the need for improving the value of the objective function by exploiting promising regions [Koziel and Yang, 2011]. This balance is determined by a strategy that selects the next promising solution to evaluate.

Undoubtedly, the best feature of model-based algorithms is the reduction in the total optimization time. This is particularly relevant in the context of BPO, where each simulation may take seconds, minutes, hours, days, or even weeks to complete. However, the lower availability and the lack of necessary technical knowledge to implement or incorporate these algorithms into optimization processes are still obstacles to a broader adoption of this approach. Notwithstanding the existence of different studies involving ML techniques for the creation of full surrogate models [Koziel and Yang, 2011, Forrester and Keane, 2009], such as Neural Networks (NNs), Support Vector Machines (SVMs), Radial Basis Functions (RBFs), and Random Forests (RFs), among others, only a few have actually been applied in the context of architecture. This scenario is even more self-evident when we shift from the single- to multi-objective optimization context.

### 2.1.4 Comparison

This section considers the applicability of different classes of derivative-free optimization algorithms for architectural design. The multidisciplinary aspect of building design raises distinct problems, ranging from well-behaved problems with simple, unimodal, convex functions to more ill-behaved problems with irregular, multimodal objective functions [Wortmann and Nannicini, 2017]. In addition to problem's diversity, the time complexity associated to function evaluations also becomes an important factor to consider, when pondering each category's impact on BPO problems.

The problems' plethora within performance-based design is vast: a specific optimization algorithm may perform well for some problems and have a terrible performance in other problems [Wortmann et al., 2017, Fang, 2017]. This idea resembles the ones captured in Wolpert's No Free Lunch Theorems (NFLTs) for optimization, which state that any algorithm's worse performance over some classes of problems offsets its better performance in other classes. Because of the distinct nature of architectural design problems, the arguments applied in architecture are not necessarily applicable to the other fields, like science and engineering.

Inevitably, the same building design description might yield different problem descriptions according to the performance aspects being considered. Some algorithms might explore certain descriptions more effectively than others, e.g., because the objective functions describing the lighting and structural behavior of a certain design may have completely different properties. In an attempt to exploit this property, BPO practitioners often dedicate a small amount of their total time budget to test various algorithms and different setup parameters, before finally settling for an optimization algorithm [Hamdy et al., 2016].

Regarding the different algorithms' categories, it is interesting to see the metaheuristics' popularity among researchers and practitioners. The main reasons behind the idolization of the metaheuristics are their (1) inherent simplicity, (2) ease of implementation, and (3) wide applicability to different domains [Wortmann and Nannicini, 2017]. Unfortunately, other categories do not benefit from such properties, which is a limitation towards their application in architectural domains. Moreover, the lack of easy-to-use tools involving algorithms from other categories are also limiting their application in architectural contexts. Firstly, the existing non-metaheuristic tools are usually available as programming libraries, instead of being integrated in architectural design workflows. As a result, to use the optimization algorithms, architects often need some programming knowledge to create the scripts to integrate the algorithms into the design workflow. However, since architects typically lack the required knowledge, they tend to struggle with the scripts' production and, eventually, opt for using friendlier metaheuristics ready-to-use tools. Given this facts, it is not surprising that most of the existing building design optimization literature ends up focusing on the application of algorithms from the metaheuristics category [Hamdy et al., 2016, Nguyen et al., 2014, Evins, 2013].

However, in the light of the NFLTs, the need for more short-term efficient optimization approaches fostered the development of tools exposing algorithms with different properties. Particularly, plug-ins like Goat [Simon Flöry, 2019] and Opossum [Wortmann, 2017b] enable the usage of algorithms from both direct search and model-based classes. These tools expose optimization algorithms from the NLopt [Steven G. Johnson, 2010] and RBFOpt [Costa and Nannicini, 2014] frameworks, respectively, providing friendly, ready-to-use interfaces within Grasshopper [David G. Rutten, 2007], a visual programming environment that enables the parametric design and performance evaluation of building designs for different values of the parameters. For the past few years, few works have compared different algorithms using these tools with the ones available in other metaheuristics tools (e.g., Galapagos [David G. Rutten, 2010], Octopus [Vierlinger, 2013], Optimo [Zarrinmehr and Yan, 2015], Silvereye [Cichocka et al., 2017b]).

Although the results may vary, in general, direct search and surrogate-based algorithms seem to be more effective than the metaheuristics ones in initial stages of the optimization process [Wortmann, 2017a, Wortmann and Nannicini, 2016, Wortmann et al., 2017]. Even some metaheuristics algorithms can be very effective approaches for some optimization problems [Waibel et al., 2018]. One can explore these performance fluctuations to find the most effective optimization algorithm for a specific problem. This performance gain can be determining in the overall optimization time, especially when complex and time-consuming simulations are involved. Indeed, several authors [Wortmann and Nannicini, 2016, Hamdy et al., 2016] suggest that the selection of the optimization algorithm should be based on the results of several tests with different methods for a fixed number of evaluations or a fixed amount of time.

Optimization is a useful tool to address both single and multi-objective problems. In architecture, most optimization applications focus on single-objective problems and cover the three different derivative-free algorithms classes. However, the same does not happen with multi-objective problems, with only one of the classes being extensively applied to MOO building design: the metaheuristics [Hamdy et al., 2016]. The main reason behind metaheuristics popularity is their broader adaptability to both varying degrees of complexity and to different problem domains [Blum and Roli, 2003].

Recent developments in multiple surrogate-assisted Multi-Objective Evolutionary Algorithms (MOEAs) in the fields of science and engineering [Zapotecas-Martínez and Coello, 2016, Hussein and Deb, 2016] made it possible to decrease the number of expensive evaluations in MOO problems. Generally, these techniques combine metaheuristics methods, which find more than one solution within a single execution, with surrogate models, which are approximations of the original objective functions. Diaz-Manriquez et al. [Díaz-Manríquez et al., 2016] provide a comprehensive overview of surrogate-assisted techniques for MOO from the engineering perspective.

The following sections focus on the current BPO practices both for Single-Objective Optimization (SOO) and MOO, the currently available tools, and the advantages and disadvantages of each approach.

## 2.2 Single-Objective Optimization

SOO processes aim to find the best solution with respect to a unique objective function. This function is described in terms of the values of the problem's parameters. Equation (2.1) illustrates an example of a mathematical unconstrained minimization SOO problem, where $f$ represents the single objective function and $x$ represents the vector of parameters.

$$\min f(x) \tag{2.1}$$

Generally, the computational complexity of optimization processes is exponential on the number of objectives and, consequently, the more objectives, the more expensive these processes are. In particular, SOO processes rely exclusively on a single objective function and, therefore, are usually less time-consuming than MOO processes. The gains in computational resources become particularly relevant when considering simulation-based objective functions. For instance, in the case of building design, most problems include simulation-based objective functions. As a result, architects commonly opt for SOO processes [Wortmann, 2017b]: either by simply considering a single objective, or, in the case of problems involving multiple conflicting objectives, by combining them in a unique function as it will be further explained in section 2.3.2.

A literature review over the architectural practice will evidence the prevalence of SOO algorithms. Firstly, single-objective problems are easier to model. Secondly, plug-ins, like Galapagos and Goat, allow to easily address single objective building design problems, hence enabling to solve simpler optimization problems and reducing the total complexity of optimization processes. Finally, these plug-ins expose different derivative-free optimization algorithms, enabling the selection of the best algorithm to specific problems and potentially improving the optimization processes' complexity [Wortmann and Nannicini, 2016].

Despite its lower optimization time, these processes are also usually less informative than the ones for multi-objective problems. Particularly, in the architectural practice, building design often involves different conflicting aspects, such as thermal, energy consumption, lighting, among others. In such situations, one is interested in obtaining a view over the compromises between conflicting aspects in order to make an informed decision.

## 2.3 Multi-Objective Optimization

MOO belongs to the set of problems concerned with the optimization of more than one objective simultaneously. The addition of other, potentially conflicting, objectives to the optimization process requires the re-definition of *optimality*.

While in SOO problems we expect the optimal solution to be the set of parameters that achieve the best[1] objective value possible, in multi-objective the best possible configuration for one of the objectives is rarely the best possible configuration for all other objectives as well, which results from the fact that these objectives are often contradictory. In order to be able to compare different multi-objective solutions,

[1] For simplification purposes, we simply refer to the optimal solution as being the best. When dealing with a minimization problem, the best solution is the one that achieves the lowest value of the objective function, whereas in maximization problems, the best solution is the one achieving the highest value of the objective function.

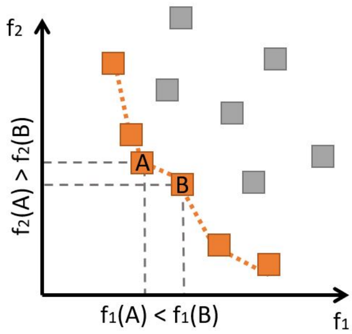



**Figure 2.2:** Representation of the set of non-dominated (orange squares) and dominated (gray squares) solutions for a two-objective minimization problem. The Pareto front is composed of all the non-dominated solutions.

these problems are often addressed considering the Pareto optimality (or Pareto efficiency) concept. This concept, named after the economist Vilfredo Pareto, defines an optimal solution as being a solution for which it is impossible to improve an objective value without deteriorating others. Such a solution is also said to be non-dominated or noninferior, and the set of non-dominated solutions is called the Pareto Front. An example of a bi-objective minimization problem is illustrated in Figure 2.2. The two objectives are $f_1$ and $f_2$ and the solutions shown in orange are non-dominated. The goal of optimization algorithms is to find, in the search space, design solutions that lie on the Pareto Front.

Building design is a complex task that frequently involves dealing with multiple conflicting objectives, such as maximum lighting comfort *versus* maximum thermal comfort, or minimum energy consumption *versus* maximum thermal comfort. The architect might follow different approaches depending on his knowledge and on his level of expertise. The following three sections describe the benefits and limitations of each approach.

### 2.3.1 Design of Experiments

The experimental or design of experiments approach is widely used in research and in practice to address both single and multi-objective problems [Fang, 2017]. Besides being intuitive and flexible, it can achieve a potentially better solution without having to deal with complex optimization algorithms. This approach evaluates designs generated with different combinations of design parameters. These combinations can be obtained through sampling methods, such as Full-factorial, Monte Carlo Sampling, and Latin Hypercube Sampling [Giunta et al., 2003], which generate different combinations of design to be evaluated. This approach returns multiple design solutions instead of just one, leaving the final choice in the hands of the architect.

Unfortunately, this approach does not guarantee that good solutions will be found. In fact, in most cases, new solutions are generated without taking advantage of the information obtained from previously evaluated designs. Consequently, the old information is not used to guide the search towards the most efficient designs and useless candidate designs can sometimes be evaluated.

On the other hand, given its simplicity and flexibility, this approach allows architects to easily combine different processes in order to direct the search towards better design solutions. For example, the architect can choose a sampling method to generate different design variations, which are then evaluated. After analyzing the results of the evaluations, the architect may wish to explore regions of the design space near the most promising design solutions. In that case, he might constrain the design variations to lie within the promising regions, by updating the problem's definition. The redefined problem is then subsequently sampled and redefined until the architect is satisfied with the quality of the obtained solutions.

Despite the constant need for manual intervention, the previous technique can be adapted to automatically extract information about the design problem itself, for example, to study the impact of design parameters in the performance. This process, commonly known as *sensitivity analysis* [Saltelli et al., 2007], has already been applied in the context of building design optimization [Tian, 2013], not only to achieve better solutions, but also to enhance the performance of existing optimization algorithms, e.g., by dropping irrelevant parameters.

Overall, while it does not provide guarantees about the solutions' optimality, this approach is simple, easy to use, and it is available in numerous tools. Moreover, although this process is not intelligent *per si*, since the decisions are always made by the architect, it enables a more intelligent and informed design process, as it presents all the design variations generated and their associated performance.

### 2.3.2 *A Priori* Articulation of Preferences

This approach allows combining multiple objectives according to one's preferences, using what is called a utility function [Marler and Arora, 2004], i.e., a function which ranks alternatives according to their utility for global performance. Among all the possible utility functions, the most commonly used is the weighted sum or linear scalarization [Wortmann, 2017b]. This function reduces multi-objective problems to single-objective ones by defining the objective function as the weighted sum of multiple objectives. The weights represent the relative importance of each objective to the architect and must be defined before the optimization. The final objective function is then provided to a SOO algorithm, which tries to find an optimal (or a near optimal) solution. Equation (2.2) represents an unconstrained example of the mathematical definition of such approach, where $w_i$ is the weight associated to the objective $f_i$, and $n$ is the total number of objectives of the problem.

$$\min_{x \in X} \sum_{i=1}^{n} w_i f_i(x) \tag{2.2}$$

One important consideration to have when following this approach is its sensitivity to the chosen weights, as different weights can yield potentially distinct results. Architects often use their experience or knowledge about the problem itself to set these weights properly, thus ensuring they obtain an optimal (or near optimal) solution.

Virtues of this approach, in architecture, include the ease of use, the availability, the heterogeneity of ready-to-use SOO tools (e.g., Opossum, Goat, Galapagos, Silvereye), and the time required.

Overall, this approach enables a more intelligent design process because the algorithm uses knowledge about previously evaluated solutions to guide the search towards optimal regions of the design space. However, since the algorithms used are usually autonomous, architects are often removed from the optimization loop, thus losing control over the design optimization process. Moreover, most of these algorithms retrieve a single optimum and provide no other design options. This is a major drawback [Cichocka et al., 2017a], as the architect either complies to the retrieved solution or he must rerun the optimization with another articulation of preferences. Either way, this optimization approach no longer provides enough information to make informed decisions.

### 2.3.3 Pareto-based Optimization

A more informative approach consists in the retrieval of a diverse and potentially heterogeneous set of Pareto-optimal solutions. When confronted with this set of optimal solutions, architects can compare different design options, according to different performance criteria, and make informed decisions about the compromises taken. Equation (2.3) is an example of a mathematical unconstrained minimization Pareto-based MOO problem, where $F(x)$ represents the vector of $k$ objectives, and $f_i$ represent the objective function $i$.

$$\min \{F(x) = [f_1(x), f_2(x), ..., f_k(x)]\} \tag{2.3}$$

On the other hand, in this approach, (1) the number of function evaluations is larger due to the need to find a set of optimal solutions instead of focusing on a single one, (2) the visual representation of the solutions' objectives values becomes problematic when the number of objectives is greater than three, and (3) the way the optimization problem is modeled has a direct impact on the quality of the solutions.

Notwithstanding the considerations above, a few studies concerning Pareto-based optimization emerged in the past years, evidencing its utility [Evins, 2013, Hamdy et al., 2016]. Moreover, recent works show that even though approaches based on the *a priori* definition of preferences are less time-consuming, they are not as desirable as Pareto-based approaches, as they return a single solution instead of multiple alternative solutions [Attia et al., 2013, Hamdy et al., 2016, Cichocka et al., 2017a]. In fact, Pareto-based approaches support the decision making process, providing a clear trade-off between the different objectives involved. Moreover, these multiple compromises represent different articulation of preferences from which the architect selects one. This approach is also called *a posteriori* articulation of preferences.

Despite the growing trend of Pareto optimization approaches [Evins, 2013, Hamdy et al., 2016], the lack of relevant benchmarks comparing the performance of different Multi-Objective Optimization Algorithms (MOOAs) in architecture is evident.

## 2.4 Performance Indicators

Despite the large interest in MOO, the question of how to quantitatively compare the performance of different algorithms still remains unanswered. Firstly, in multi-objective problems, the number of objectives is greater than the number of objectives in single-objective problems: the former considers a collection of vectors representing the Pareto-optimal solutions, whereas the latter considers real numbers. Secondly, it is often the case that the application of exact methods to MOO contexts is impracticable due to the complexity introduced by underlying applications (e.g., simulation tools, physical experiments). In these cases, the generation of the true Pareto-optimal set is often infeasible, requiring vast computational resources to be generated. Thirdly, despite the availability of alternatives to exact methods, such as metaheuristics algorithms (e.g., evolutionary algorithms, particle swarm), these are not guaranteed to identify optimal trade-offs, instead yielding good approximations [Zitzler et al., 2003]. Finally, we are interested in knowing which of the non-exact algorithms yields better approximations for a given problem, hence prompting the need for assessing the performance of MOOAs.

The notion of performance includes not only the quality of the results, but also of the computational resources needed to generate such results. While the latter aspect is usually identical for both SOO and MOO, which either typically consider the number of expensive evaluations or the overall run-time on a particular computer, the quality aspect is considerably different. Because SOOs consider real-valued objective spaces, the quality is defined in terms of the objective function: the smaller (or larger) the value, the better the solution. However, MOOs consider vector-valued objective spaces, thus requiring another concepts like Pareto dominance. Unfortunately, when considering the Pareto dominance concept a few issues may arise, namely the possibility of two solutions being incomparable, i.e., when neither dominates the other, or having solutions in one set that either dominate or are incomparable to those in the other set of solutions and vice versa.

Literature review evidences the existing struggle to define the meaning of quality with respect to approximation of Pareto-optimal sets [Knowles and Corne, 2002, Riquelme et al., 2015]. However, the quality of Pareto sets is usually evaluated in terms of three aspects: (1) cardinality, meaning larger sets of solutions, (2) diversity, meaning that solutions should be as uniformly distributed as possible, so as to obtain a representative set of solutions covering to larger extents the different trade-offs, and (3) accuracy, meaning that solutions should be as close as possible to the true Pareto-optimal set or Pareto Front.

For the past decades, several indicators have been proposed to measure the quality of Pareto sets, ranging from unary quality measures, which assign each approximation set a number that reflects a certain quality aspect, to binary quality measures, which assign numbers to pairs of approximation sets, among others. This thesis considers a small but representative set of quantitative indicators to measure the quality of MOOAs' results with respect to the three aspects: cardinality, diversity, and accuracy.

Literature review reveals the existence of dozens of indicators that consider either one of the mentioned aspects or a combination of them. In the following definitions we use the term *approximation set* to denote the Pareto Front returned by an optimization algorithm, and we use the term *reference set* to denote the true Pareto Front or, whenever that is not possible, an estimate of the true Pareto front. In this section, we list some of the most used indicators for assessing the performance of evolutionary MOOs [Riquelme et al., 2015].

### 2.4.1 Unary Indicators

With regards to the cardinality aspect, there are essentially two indicators:

- **Overall Non-dominated Vector Generation (ONVG)** computes the number of non-dominated solutions in the approximation set [Veldhuizen, 1999].
- **ONVG Ratio (ONVGR)** computes the ratio of non-dominated solutions in the approximation set with regards to a reference set [Veldhuizen, 1999].

Cardinality indicators are based on the intuition that a good approximation set would have many optimal solutions. However, these indicators alone do not suffice to provide an accurate measure, as they privilege quantity over quality of solutions [Veldhuizen, 1999], i.e., they often qualify approximation sets having dozens or hundreds of dominated solutions as being better than sets that provide fewer non-dominated solutions. This completely distorts the initial idea of finding the best Pareto front, i.e., set of non-dominated solutions.

To complement cardinality indicators, it is often advisable to consider the diversity aspect of approximation sets as well. A few well known diversity-based indicators are:

- **Spacing** (or Set Spacing) computes the variance of the Manhattan distances between each non-dominated solution and its closest neighbor. It measures how well-spaced the solutions from the approximation set are. A value of zero represents equally spaced non-dominated solutions.
- **Spread** (or $\Delta$) is similar to Spacing. However, it calculates the normalized variance and uses the Euclidean distance instead.

- **Maximum Spread** (or $M_3^*$) computes the Euclidean distance between the bounds of each objective dimension. It measures the extent of the objective space in each dimension by calculating the distance between the maximum and minimum of each objective. A greater value indicates larger coverage of the objective space.
- **Entropy** uses the Shannon's entropy concept to measure the uniformity of the approximation set distribution. This indicator makes the assumption that each solution provides some information about its vicinities, thus modeling each solution with Gaussian distributions. These distributions add up to form a density function capable of identifying peaks and valleys in the objective space, corresponding to dense and sparse zones, respectively.
- **Diversity Metric** is similar to the Entropy indicator. However, it projects the solutions of both the approximation set and the reference set to an hyperplane which is subdivided uniformly. It assigns each interval two numbers: one number marking whether that interval contains at least one optimal solution in the reference set, and the second number marking whether the interval in addition to the optimal solution in the reference set, also contained at least one solution in the approximation set. Then, the diversity measure is the sum of the score of each interval, which are assigned using a sliding window technique (considering one interval and its immediate neighbors) based on the value of the marks[2]. So, the diversity of the reference set considers the value of the first marks, whereas the diversity of the approximation set considers the values of the second marks. In the end, the diversity metric is given by the relative difference between the diversity of the approximation set and the diversity of the reference set. The best diversity possible is achieved if all intervals enclose at least one point [Deb and Jain, 2002].

While these indicators are more robust, considering these indicators alone will not necessarily identify sets having Pareto optimal solutions, as they prioritize sets where solutions are spaced evenly apart or that cover broader regions of the objective space [Veldhuizen, 1999]. Moreover, because most of them assume that the Pareto front will be continuous, they may behave erroneously when facing problems with disconnected Pareto fronts. The diversity metric attempts to alleviate these limitations by comparing the non-dominated solutions of the approximation set with those of the reference set [Deb and Jain, 2002].

Previous metrics are not good indicators of how close the approximation sets really are to the reference set. To obtain a measure of the convergence of the results, one should consider accuracy indicators, such as:

- **Error Ratio (ER)** computes the proportion of false-positives in the approximation set, i.e., the ratio of optimal solutions in the approximation set that are not optimal in a given reference set [Veldhuizen, 1999]. Lower values of ER, represent better approximation sets.

[2] The scoring function considers the distribution of the marks in three consecutive grids. The function's proper definition can be found in [Deb and Jain, 2002].

- **Maximum Pareto Front Error (MPFE)** computes, for each solution in the approximation set, the minimum Euclidean distance to the closest solution in a given reference set, returning the maximum of those distances [Veldhuizen, 1999]. In other words, it returns the maximum error of the approximated Pareto Front. Lower values of MPFE imply better approximation sets.

- **Generational Distance (GD)** computes the average distance of an approximation set to a given reference set by computing the distance of the solutions in the approximation set to the nearest points in a given reference set averaged on the number of solutions in the approximation set [Veldhuizen, 1999]. A value of $0$ indicates that all the solutions in the approximation set are in the reference set. Different authors [Zitzler et al., 2000] refer to this metric as $M_1^*$.

Accuracy indicators, like the previous indicators, can also produce misleading results and, therefore, should be considered together with other metrics. In general, all these three indicators have flaws, for instance, ER focus on errors instead of focusing on the optimal solutions. As a result, it penalizes larger approximation sets that, despite having a more representative set of the real optimal solutions, have made more errors than other approximation sets with fewer solutions and, potentially, less errors. On the other hand, MPFE focus on the maximum error of an optimal solution in the approximation set, when compared to the reference set. As a result, approximation sets, whose points are closer to the Pareto front but that have an outlier, will have higher values of MPFE than other approximation sets, whose points are further away from the reference set but at a smaller distance than the outlier is from the reference set. At last, GD has also been shown to behave erroneously, especially due to its dependency on the cardinality of the approximation set [Ishibuchi et al., 2005].

The final set of indicators considers the accuracy and diversity aspects simultaneously:

- **Hypervolume (HV)** (or Lebesgue measure or S-metric) measures the size of the objective space covered by an approximation set, i.e., it measures the volume of the dominated space. It provides the unique and desirable properties of (i) Pareto *compliance*, i.e., an approximation set which completely dominates another, will necessarily have a greater volume than the latter, and (ii) convergence guarantees, i.e., any approximation set that achieves the maximum possible volume is guaranteed to contain all Pareto-optimal solutions.

- **Inverted Generational Distance (IGD)** is the opposite of GD, instead computing the average distance between a given reference set and the approximation set. IGD computes the distances between each solution in the reference set and its closest solution in the approximation front, averaged over the size of the reference set. When the solutions in the reference set are well distributed, smaller values of IGD suggest better and well-distributed approximation sets. Previous works have referred to this metric as $D1_R$ [Ishibuchi et al., 2005].

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Despite considering the diversity and accuracy aspects of Pareto fronts, IGD is still Pareto non-compliant and has been shown to behave erroneously under certain conditions [Ishibuchi et al., 2005]. Conversely, HV is the only metric that exhibits the Pareto-compliance property. However, its usage is often impractical in problems, where the number of objectives is greater than ten, due to the its exponential grow with the number of objectives [Ishibuchi et al., 2005].

### 2.4.2 Binary Indicators

In situations where the original Pareto-optimal set is not available, the binary indicators provide a way to compare approximation sets with respect to all the aspects. Among the most frequently used indicators, we emphasize:

- **Two set coverage** (or $C$) yields the number of solutions in one approximation set that are dominated by at least one of the solutions of the other approximation set. A value of $1$ suggests that the second approximation set is completely dominated by some solutions in the first one, whereas a value of $0$ represents the situation when none of the solutions of the second approximation set is covered by the first approximation set.
- **Epsilon Indicators** ($\epsilon$) that gives a factor by which an approximation set is worse than another considering all objectives, i.e., given two approximation sets $A$ and $B$, it computes the smallest amount $\epsilon$ by which $A$ must be translated, so that every solution in $B$ is dominated by at least one solution in $A$.
- **R-metrics** consider a family of indicators where the quality of each approximation set is defined according to a set of utility functions, and the larger the utility value of some set, the better the quality. R-metrics declare that the best approximation set will be the one that is better with regards to most utility functions:
  - $R1$ determines whether the an approximation set is better, equal, or worse than the other.
  - $R2$ computes the expected mean difference in the utilities of both approximation sets.
  - $R3$ computes the expected mean relative difference in the utilities of both approximation sets.

When comparing the usefulness of binary indicators, these usually aim at comparing different approximation sets and not necessarily the quality of the sets. This is the case of the two set coverage indicator, which allows to compare the existing Pareto-dominance relation between two sets, but does not allow to infer any other information (e.g., how worse one set is regarding the other). Moreover, this indicator becomes erroneous when the two sets are incomparable, i.e., neither dominates the other [Zitzler et al., 2003]. In contrast to the two set coverage indicator, the epsilon family indicators enable more

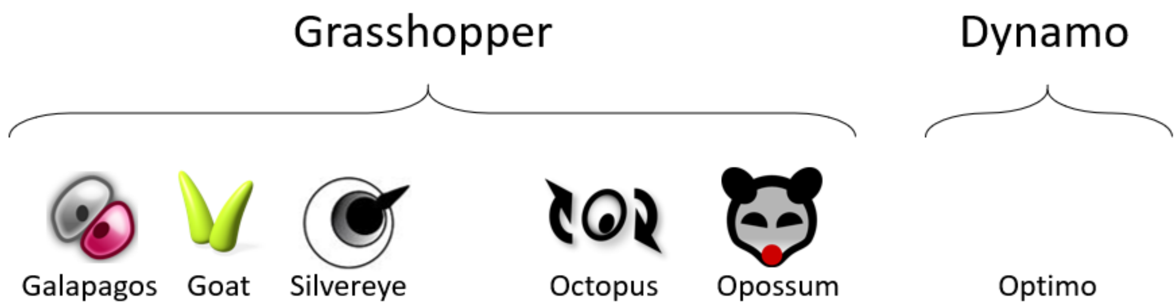


**Figure 2.3:** Optimization frameworks currently used in architectural practices.

informed comparison among two different approximation sets, as it provides a measure of the relative difference between the two sets. Finally, because the R-metrics incorporate utility functions, the user is able to introduce a preference over the objectives, thus influencing the optimality of each set.

## 2.5 Optimization Tools in Architecture

For years, multiple derivative-free optimization libraries have been developed (e.g., NLopt, RBOpt, Platypus, DEAP, Pyomo, PISA, jMetal, MOEAFramework). However, in order to use them within architectural practices, architects had to code the integration scripts to connect the simulation models for different variations of the parametric models and the optimization libraries [Attia et al., 2013]. Moreover, these frameworks often lacked post-processing and visual features, which antagonized the readability and comprehension of the results [Attia et al., 2013, Nguyen et al., 2014].

Several plug-ins have been developed in an attempt to reduce the limitations associated to the coupling of simulation tools and mathematical optimization frameworks, thus providing a seamless connection between the parametric models produced in computational design tools, like CAD and BIM tools, the simulation or analytical models, and the optimization frameworks. Given the visual nature of architects, these plug-ins provide friendly, ready-to-use optimization interfaces, which are usually coupled with a few post-processing and visual features to enhance the intelligibility of optimization results.

Currently, existing optimization plug-ins are implemented on top of the visual parametric tools: Grasshopper [David G. Rutten, 2007] and Dynamo [Ian Keough, 2011]. In Figure 2.3, we represent the most relevant optimization plug-ins among BPO practitioners: Galapagos, Goat, Octopus, Opossum, and Silvereye implemented on top of Grasshopper, and Optimo implemented on top of Dynamo. In the following sections we briefly discuss each plug-in.

### 2.5.1 Galapagos

Galapagos [David G. Rutten, 2010] is a generic plug-in, implemented on top of Grasshopper, designed to allow the application of metaheuristics algorithms by non-programmers to solve a wide variety of problems.

Particularly popular amongst architects [Wortmann and Nannicini, 2017] for its GA, Galapagos also provides other global metaheuristic solver, called simulated annealing (see ).

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To use one of the solvers, architects must first define a script in using Grasshopper's components, such as sliders, values lists, area, distance, among others. This script should be organized in three distinct parts: (1) the Input, where they specify the design's parameters; (2) the Generation, where they create the design's algorithmic model that when instantiated with the parameters' values will generate the 3D model; and (3) the Analysis, where they define the analysis or objective function which they ought to optimize.

After creating the program script, the architect must drag the Galapagos' component to the script and connect it to the design parameters and to the objective function. Note, however, that Galapagos require the variables to be defined in terms of sliders components, interpreting their numerical range as the variables' lower and upper bounds, and the objective function to be output to a number component. The Galapagos' component refers to the variables as genome and to the objective function as fitness.

Galapagos' Graphical User Interface (GUI) is displayed upon double-clicking the Galapagos' component (see Figure 2.4(a)). The interface is simple, friendly, intuitive, and well-organized. Moreover, all options are filled by default, thus promoting a ready-to-use (or click-and-run) interaction, which makes it particularly easy to use by users with no experience or expertise in the field. Unfortunately, more experienced users might feel frustrated using this plug-in, as they are only able to modify a few parameters of the solver, thus lacking a finer control over the process.

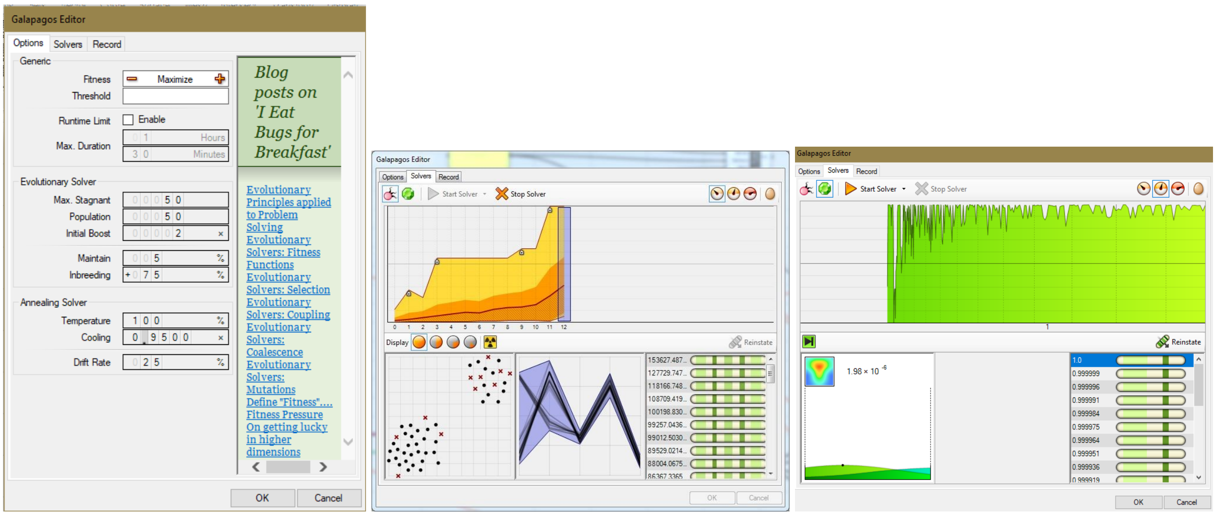
In addition to not requiring any integration efforts or any programming-related knowledge to setup and use its capabilities, Galapagos also provides a visually rich experience, by providing different run-time graphical views of the optimization process. Galapagos supports different views depending on the optimization solver being used (see Figure 2.4(b) and Figure 2.4(c)):

- fitness graph that either represents the distribution of fitness values in the population discriminated by generations. Exhibited for both solvers;
- similarity representation graph that represents solutions that are genetically similar close to each other, and marks solutions that contribute to the creation of the next generation with black dots, whilst non-contributors are marked with a red cross. Exhibited for the GA solver;
- vertical parallel coordinates graph, where each vertical line corresponds to a parameter, and solutions are represented as line segments connecting different parameters values. Exhibited for the

GA solver;

- ranked list of the best solutions found. Exhibited for both solvers;
- temperature graph, representing the temperature decrease rate of the simulated annealing process with each time step. Exhibited for the simulated annealing solver.

Overall, these views provide a visual feedback about the course of the optimization run and highlight the best solutions found up to that generation. In the end, the user is able to navigate through generations and re-instantiate these solutions in the corresponding CAD tool, and, consequently to better understand the obtained results. Moreover, the ranked list of the results allow the user to select the one he appraises the most the amongst multiple optimal solutions found by the solver. Unfortunately, Galapagos lacks logging mechanisms which causes the information about the optimization enclosed within these views to be lost as soon as the GUI is closed.




**(a)** **(b)** **(c)**

**Figure 2.4:** Three views of the Galapagos' GUI: (a) Solvers configuration menu (b) Graphical views for the GA solver (c) Graphical views for the simulated annealing solver

### 2.5.2 Goat

Goat [Simon Flöry, 2019] is a generic optimization plug-in, implemented on top of Grasshopper, designed to enable non-programmers to solve numerous problems.

Unlike Galapagos, Goat interfaces the NLopt mathematical optimization library [Steven G. Johnson, 2010] to provide single-objective algorithms from all the derivative-free classes mentioned earlier (see section 2.1), including one global direct search (DIRECT), one local direct search (Subplex), one global metaheuristic (CRS2), and two local model-based algorithms (COBYLA and BOBYQA).

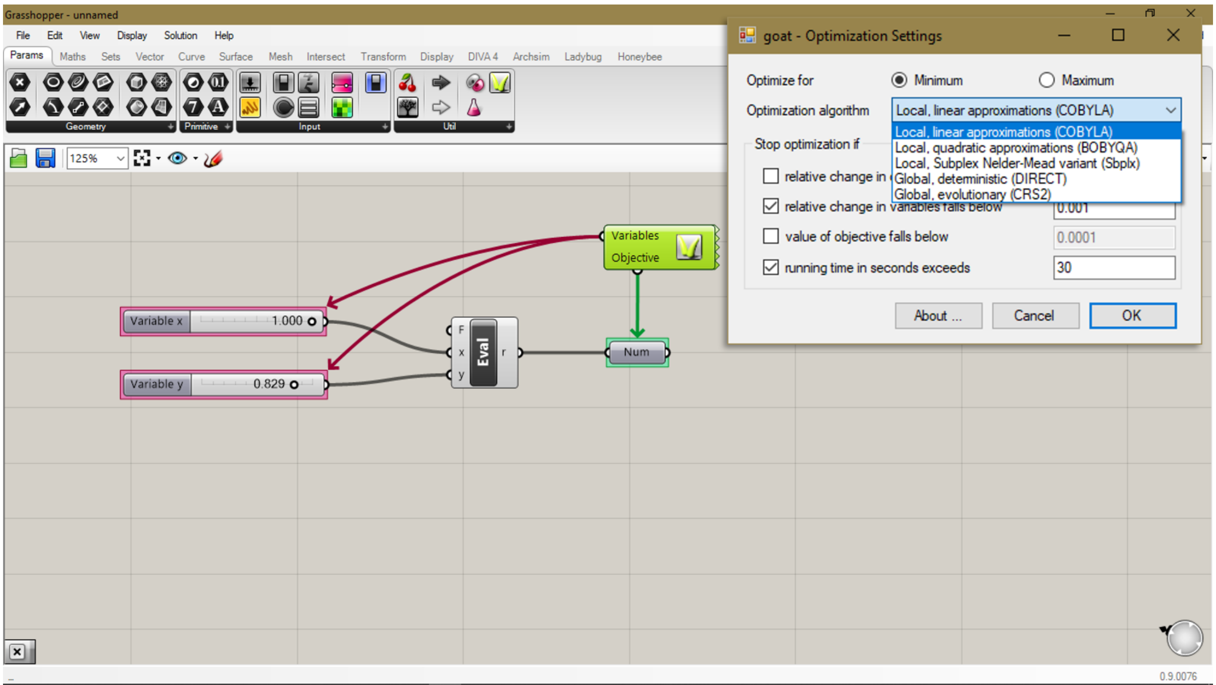



**Figure 2.5:** Simple view of the Grasshopper's script with the problem definition and the Goat component. On the foreground, the GUI exhibits the list of available algorithms within Goat

Goat is strongly influenced by Galapagos, also requiring a script in Grasshopper entailing the definition of the problem. In this script, the user drags the Goat's component to the script connecting it to the design parameters and the objective function, which, like Galapagos, must be sliders and number components, respectively (see Figure 2.5).

Goat's GUI is displayed after double-clicking the Goat's component (see Figure 2.5). This interface comprises a single menu, which is simple and straightforward to use. Like Galapagos, Goat is also distributed in a ready-to-use format with all the extra configuration parameters' values filled by default. As a result, non-programmers can easily explore this tool to address complex problems. Unfortunately, Goat provides no options for a more experienced user to configure the algorithms, except to configure the initial point of the search.

Despite requiring no additional efforts to use Goat's optimization capabilities, the absence of visual and interactive mechanisms severely hinders the reputation of Goat. Firstly, it provides no visual feedback (e.g., solution lists, plots) about the course of the optimization run. Secondly, it also does not create log files to monitor the optimization process. Thirdly, the user is not able to interact with the optimization process. Finally, it returns a single optimal solution, whose values are represented in the sliders and number components. All these reasons contribute to a non-informed and non-traceable optimization process that inspires no confidence it the attained results.

### 2.5.3 Silvereye

Silvereye [Cichocka et al., 2017b] is a generic optimization plug-in, implemented on top of Grasshopper, developed under the same design principles as Galapagos to enable non-experts to solve complex optimization problems.

Silvereye interfaces a C# implementation of a global single-objective PSO algorithm.

Similarly to the previous tools, Silvereye also requires the definition of the problem in a Grasshopper script, and that the variables and the objective function value are represented by sliders and number components, respectively. Thus, it does not require any additional effort in order to be used.

Likewise Galapagos, the user must double-click Silvereye's component in Grasshopper to visualize its GUI (see Figure 2.6). Even though Besides being very simple and intuitive to use, Silvereye also allows less experienced users to start using the tool immediately by providing default values to the extra configuration parameters. As the users gain more experience, they might decide to change some configurations associated with the solver. One other difference to Galapagos is the ability to save the solver's configurations so that it can be used in subsequent runs.

Regarding its visual capabilities, Silvereye is resemblant of Goat, providing no graphical views of the optimization run's state. However, Silvereye does present a list that is updated in real-time with the value of the best fitness value per iteration, which can be exported to a file and then used to create fitness graphs (see Figure 2.6(b)). Unfortunately, since this file merely contains the fitness values, the user is not able to trace them back to the values of the design parameters which originated them. Moreover, despite the existence of a functionality in the first menu (Figure 2.6(a)) to create a log file, this file only contains information about the temporal behavior of each evaluation. While this information is useful to monitor and identify irregularities during the optimization run, it does not provide enough information to traceback the error.

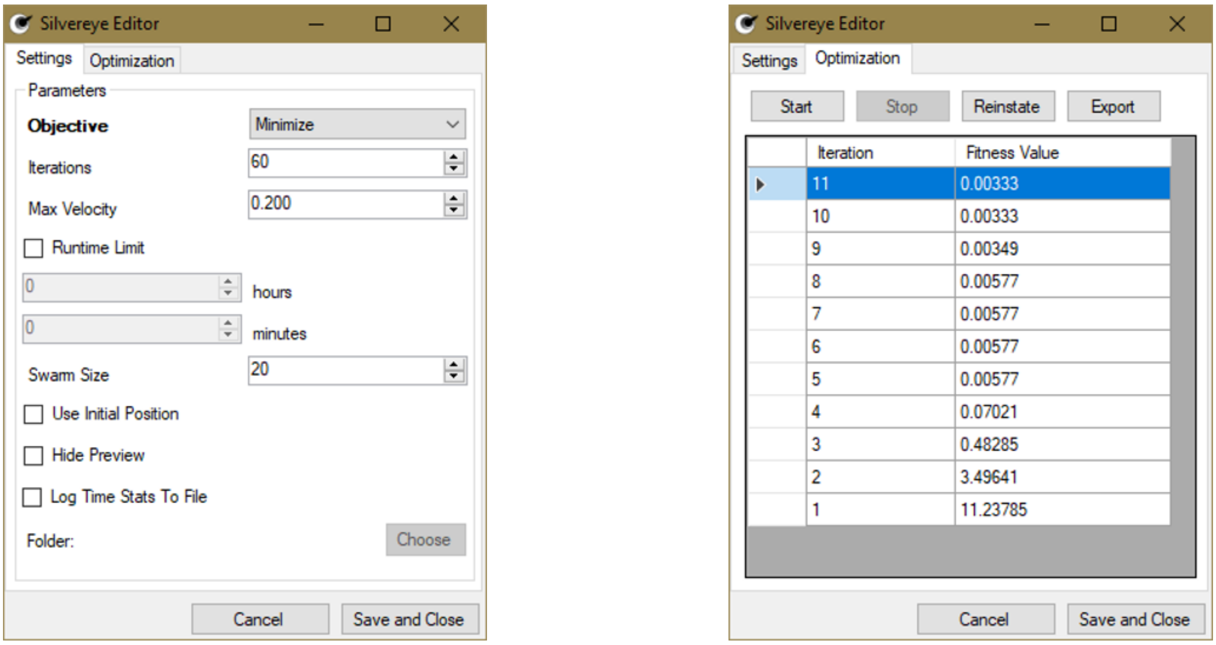
Overall, the lack of visual feedback in the form of graphs hinders the comprehension of and confidence on the results. The ranked list helps filling this gap, as long as there are multiple solutions and the user is able to visualize them in a CAD tool.

### 2.5.4 Opossum

Opossum (OPtimizatiOn Systems with SUrrogate Models) [Wortmann, 2017b] is a generic plug-in, developed on top of Grasshopper, that explores Galapagos ideas to confer non-programmers an easy way to tackle a wide variety of problems.

Opossum interfaces that the model-based RBFOpt library [Costa and Nannicini, 2014], exposing two single-objective variants of the global RBF algorithm.

In terms of usability, Opossum also resembles Galapagos, only requiring the definition of the problem




(a) (b)

**Figure 2.6:** Two views of Silvereye's GUI: (a) Solvers configuration menu (b) Optimization control and results menu

in a Grasshopper script. To use the Opossum's solvers, the user must drag the Opossum's component to the Grasshopper script and connect it with the variables and the objective function components.

Opossum's GUI is simple, friendly, intuitive, and well-organized (see Figure 2.7). In contrast to other plug-ins, Opossum presents different menus tailored for different levels of expertise. On the one hand, Opossum promotes a ready-to-use format, in order to ensure that less experienced users are able to use Opossum's capabilities. Therefore, Opossum provides two top-level configurations menus for which the values are already filled by default. On the other hand, Opossum provides more experienced users with the ability to create a finer configuration for the optimization solvers and, thus, achieve potentially more efficient optimization processes.

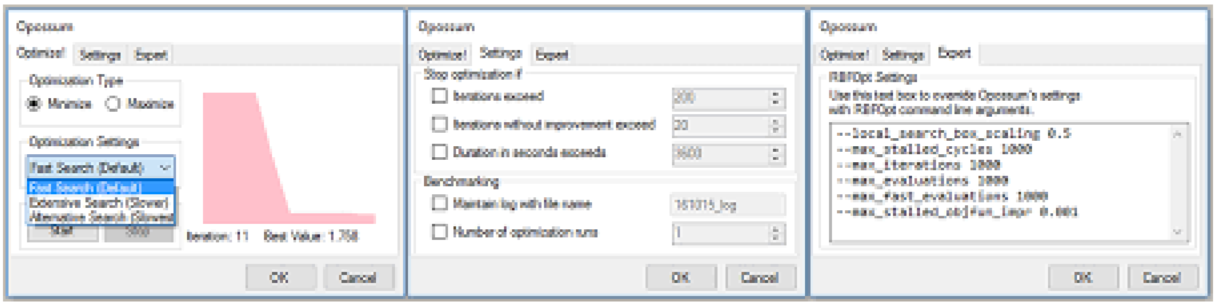



**Figure 2.7:** The three views of Opossum's GUI. Image retrieved from [Wortmann, 2017b]

The main deception of this plug-in lies in its visualization features. Although Opossum presents a fitness graph that is very useful for obtaining immediate feedback about the course of optimization, it does not provide an overview of the extent of the design space that is being explored, nor about the distribution of the designs that are being evaluated. Moreover, Opossum supports the creation of a log file that records all the solutions evaluated during the optimization run. Using other post-processing tools, the user can then either produce more insightful visualizations of the data, or re-use this information to create more accurate surrogate models, for example, for sensitivity analysis.

One other disadvantage of this plug-in is the fact that the result of the optimization run is a single solution, instead of multiple ones. As a result, the intelligibility of results and the confidence on the process is greatly hindered, especially, due to its low visual support.

### 2.5.5 Octopus

Octopus [Vierlinger, 2013] is a generic plug-in, developed on top of Grasshopper, that allows non-programmers to address a wide variety of MOO problems.

Octopus exposes two global metaheuristics algorithms, that explore evolutionary principles to search for Pareto-optimal solutions: Strength Pareto Evolutionary Algorithm 2 (SPEA2) and Hypervolume Estimation Algorithm for MOO (HypE) algorithms. These algorithms have been reported to yield promising results on numerous MOO test problems [Zitzler et al., 2001, Bader and Zitzler, 2011].

Even though Octopus was originally designed exclusively for optimization purposes, more recently, it focus has grown to include other ML utilities, like supervised and clustering mechanisms. In fact, the first difference to the Galapagos-based plug-ins is related to this features' multiplicity, i.e., whereas previous Galapagos-based plug-ins focussed exclusively on optimization, Octopus covers multiple functionalities. This extra functionality is implemented as Grasshopper's components that are made available during Octopus' installation process under a tab that is created within Grasshopper (see Figure 2.8(a)).

The second difference affects the Grasshopper script. Like Galapagos, Octopus does require the definition of a Grasshopper script defining the variables and the objective functions. However, since Octopus focusses on MOO, the user has to ensure that all the results of the objective functions are aggregated in single number component and then connected to the Octopus component. Additionally, because Octopus only performs minimizations, the problem definition must be modified to guarantee that all objectives are being minimized. One other important difference is that Octopus is able to tackle constrained problems. In this case, the hard constraints must be represented by a boolean component, and then connected to the Octopus component.

After creating the Grasshopper script, Octopus GUI can be accessed by double-clicking the Octopus component (see Figure 2.8(b)). Despite its simplicity and friendliness, the GUI is poorly organized and overloaded with information, hence making it difficult for a non-experienced user to locate any functionality in the interface. Although Octopus is distributed in a ready-to-use format, this plug-in exposes mechanisms to fine-tune a few parameters of the solvers. Even more surprising is the ability to change some of these parameters (e.g., elitism, mutation probability, crossover rate, mutation type) during run-time, thus increasing the user interactivity, and allowing the user to influence the optimization process.

Octopus provides good support in terms of graphical feedback, providing three distinct views of the optimization problem (see views 1, 8, and 10 in Figure 2.8(b)), namely:

- Solutions' Objective Space graph, which illustrates the distribution in the objective space of the solutions obtained during the optimization run. This graph also exhibits the approximated Pareto front that is currently known by the algorithm;
- Horizontal parallel coordinates graph, which serve the same purpose of the vertical parallel coordinates graph and that provide a view over the different design solutions that have been tested;
- Objective convergence graphs (one for each objective dimension), showing the upper- and lower-bounds of the Pareto front (dark gray) and the elite (light gray) of the number of history generations.

Even though Octopus is capable of solving problems with up to five objective dimensions[3], the readability of these graphs becomes strongly damaged after the three dimensions. Besides the strong visual mechanisms, Octopus provides mechanisms to interact and instantiate each one of the solutions in the corresponding CAD tool, which not only gives confidence to the user about the results, but also allows him to understand them better. Optionally, Octopus makes it possible to disable the real-time visualization of the optimization process with the aim of reducing the associated time penalizations.

One other important feature of Octopus is the ability to create logs with the information about the evaluated solutions discriminated by generation. The only setback is that it does not allow to create a single file simultaneously containing the information about the design parameters and the objectives.

### 2.5.6 Optimo

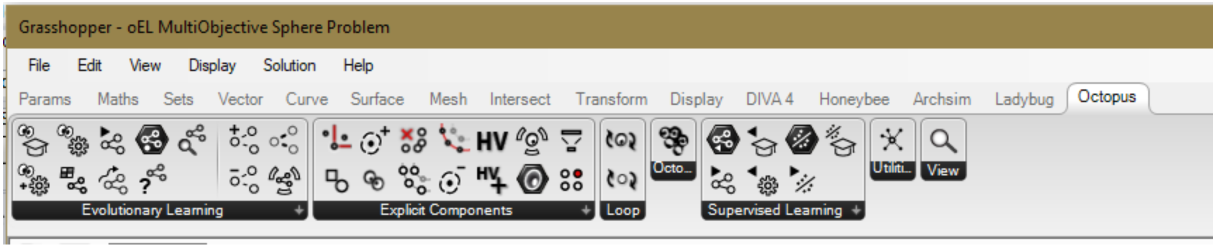
Optimo [Zarrinmehr and Yan, 2015] is a generic plug-in, implemented on top of Dynamo, that allows non-programmers to address a wide variety of MOO problems in the context of a BIM tool.

Optimo interfaces the MOO metaheuristics library, jMetal.NET and its current version merely supports the Non-dominated Sorting Genetic Algorithm II (NSGA-II) algorithm [Deb et al., 2002].

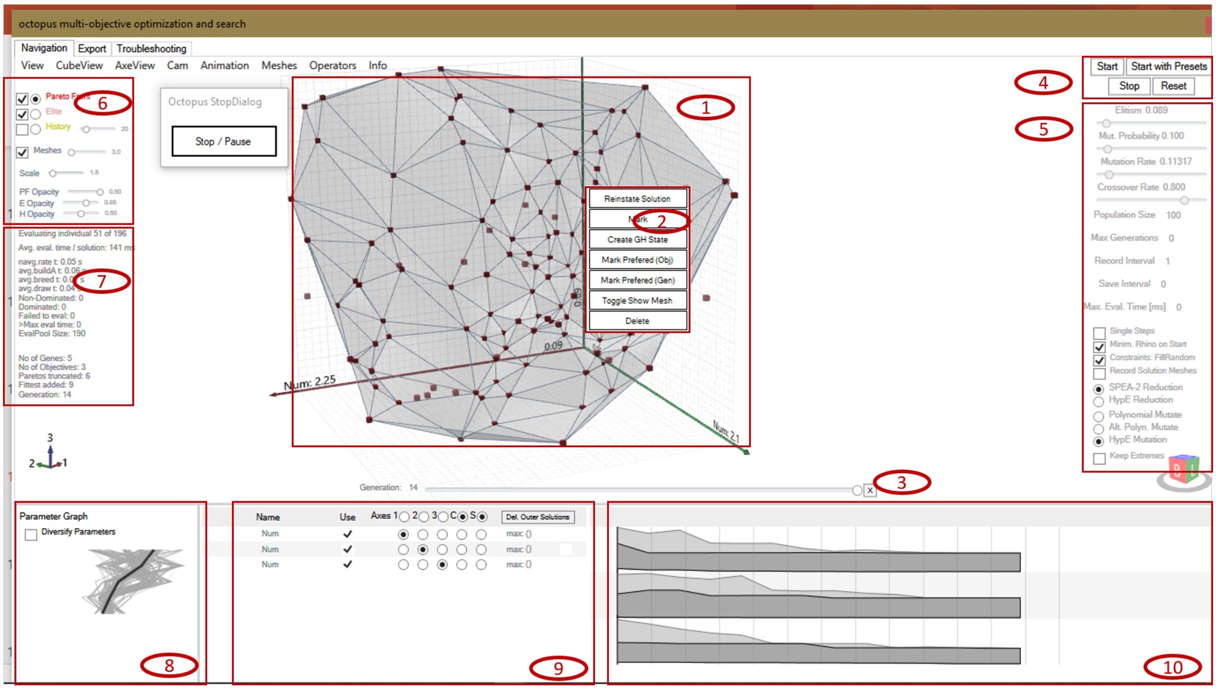
To use the solver, users must create the Dynamo script that encodes the problem definition, but also encode the optimization algorithm. To create the latter, Optimo provides four Dynamo nodes:

- Initial Solution list, which generates the initial set of random design configurations within a provided range and with the specified size of population;

[3]Octopus uses the three spatial dimensions, color, and size to represent the five objective dimensions.




**(a)**




**(b)**

**Figure 2.8:** Octopus's GUI: (a) Octopus menu in Grasshopper (b) Octopus optimization menu: (1) Solutions' Objective Space, (2) Solution's context menu, (3) Generation's history slider, (4) Process control options, (5) Algorithm Settings, (6) Display Settings, (7) Statistics, (8) Parallel Coordinates Graph, (9) List of Objectives (10) Convergence graphs per Objective

- Assign Fitness Function Results, which evaluates and assigns the objective values to each configuration;
- Generation Algorithm, which takes the parent population and generates the children population;
- Sorting, which uses the Pareto Front sorting to sort the solutions

When compared to the previous plug-ins, Optimo demands larger initial investments for the production of the script. As a result, whereas less experienced users might find it more difficult to use, more experienced ones might adjust the algorithm to their needs, which directly results from the finer-grain control of Optimo. Moreover, instead of providing a default template, Optimo foster the constant arrangement of the algorithm's nodes everytime a new optimization process is to be applied, which can quickly become monotonous and tiresome. Moreover, Optimo does not have a explicit GUI editor, instead being directly integrated in the Dynamo environment in the form of nodes.

Regarding the visual mechanisms, it does not support feedback mechanisms during the optimization run, only presenting a small side-by-side view of the initial design variation and the optimal designs, thus allowing the user to visualize and compare the results of the optimization process. Finally, we were not able to conclude whether Optimo enabled the creation of log files or not.

### 2.5.7 Comparison

Table 2.1 shows a comparison between the optimization plug-ins analysed in this chapter at the light of four aspects: (1) the optimization algorithms; (2) the interaction and visualization mechanisms; (3) the comprehension of results; and (4) the user experience.

Taking into account the first aspect, we can observe that most optimization tools focus on single-objective and global optimization. Regarding the diversity of the algorithms most plug-ins provide either one or two options with the exception of Goat which provides five different algorithms from different derivative-free classes. Apart from Goat and Opossum, all other plug-ins support exclusively meta-heuristics algorithms.

When considering the interactivity and visualization mechanisms of the explored tools, all plug-ins but Goat yield multiple solutions and allow the user to interact with it and re-instantiate these solutions directly in the corresponding CAD or BIM tool. Surprisingly, only Galapagos, Opossum, and Octopus present graphical feedback mechanisms. Particularly, Galapagos and Octopus provide not only mechanisms about the state of the optimization (e.g., parameters values being explored, current fitness values), but also provide an overall ranking of the best solutions. On the other hand, none of the plug-ins except for Octopus enable the user to influence and interact with the optimization process during its execution. Even the interactions supported by Octopus are very limited consisting of the modification in runtime of the values of the elitism, mutation, and crossover operators. Regarding the traceability feature (e.g.

| | | Galapagos | Goat | Silvereye | Opossum | Octopus | Optimo |
|---|---|---|---|---|---|---|---|
| Optimization Algorithms | Objectives | S | S | S | S | M | M |
| | Search | G | GL | G | G | G | G |
| | Classes | Meta | ALL | Meta | Model | Meta | Meta |
| | Algorithms | 2 | 5 | 1 | 2 | 2 | 1 |
| Interactivity and Visualization | Results | M | S | M | S | M | M |
| | Graphical Feedback | +++ | - | - | + | +++ | - |
| | Real-time Interactivity | - | - | - | - | + | - |
| | Traceability (e.g., logs) | + | - | + | ++ | ++ | ? |
| Intelligibility of Results | | + | - | - | - | + | + |
| GUI Experience | Ease of Use | +++ | +++ | +++ | +++ | ++ | - |
| | Intuitive/Organized | ++ | +++ | +++ | +++ | + | + |
| | Flexible (e.g., fine-tune) | + | - | + | +++ | ++ | ++ |

**Table 2.1:** A comparison between the analysed optimization plug-ins. S - single, M - multi, G - Global, L - Local.

creation of logs, solutions' lists), it is poorly supported. While Goat has no traceability, both Galapagos and Silvereye provide a "semi-traceable" list with the fitness values of the best attained solutions. At last, both Opossum and Octopus support, in a way, the creation of logs describing the state of the whole optimization process, i.e., information about the evaluated design variations with their parameters and corresponding objectives values.

Regarding the third aspect, there are no mechanism explicitly designed to enhance the comprehension of the optimization results in any of the analysed tools. However, the existence of visualization mechanisms like Galapagos and Octopus, do enable a better understanding of the the results. This understanding can be further improved by enabling the direct materialization of such solutions in the corresponding 3D model, so that the user may draw conclusions by comparing different solutions. Despite the absence of visual mechanisms in Octopus, Octopus exhibits the best solutions next to the initial solution, thus allowing the user to compare them and better understand them.

Finally, regarding the user experience, all plug-ins are straightforward to use, except for Octopus and Optimo. Both plug-ins require the user to elaborate the program in order to be run, but they differ, however the former requires a single component to be added, whereas the latter requires the definition of the solver using the provided nodes.

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## 2.6 Problems to Address

Despite the existence of both optimization (e.g., DEAP, MOEAFramework, NLopt, RBFOpt), and visualization (e.g. Matplotlib, Plotly, Seaborn) libraries, architects often lack the programming skills necessary to integrate them into an optimization process.

Several optimization tools integrated in the architectural design workflow have been proposed throughout the years (see section 2.5). In general, these tools are easy to learn and use, which also results from the fact that they make use of visual programming languages. However, the visual programming paradigm often leads to scalability and program's legibility issues, hence impacting the way users interact with these optimization tools.

On the other hand, the textual paradigm does not face from these scalability issues. Currently existing AD tools (e.g., Khepri) do not support optimization, but already provide the primitive mechanisms to create automated optimization processes. Moreover, AD tools usually offer portability of their programs, thus allowing architects to visualize and analyze their models in different 3D modeling and analysis tools, without the need to change the program.

In contrast to the multi-objective view of most BPO problems, where architects aim to optimize multiple aspects simultaneously, most of these tools focus on SOO. The usage of these tools often requires the simplification of the corresponding MOO problem either by relaxing the objectives or by assigning preferences to each objective (see section 2.3.2).

Most tools only provide global optimization support. While global optimization algorithms are good for obtaining close to optimal solutions, these often fail to provide more exact solutions. Particularly, not only are local optimization algorithms able to find more exact solutions but they also do so faster, especially if provided with useful initial information, such as the starting point.

Also, in terms of the optimization algorithms, most tools adopt metaheuristics algorithms. While these algorithms are flexible and applicable to nearly almost domain, they lack convergence guarantees, often requiring hundreds or thousands of evaluations to reach good results. Especially for simulation-based problems with time-consuming evaluations, these numbers are a main obstacle for the application of optimization. The situation becomes even more complicated in the MOO context, as the number of evaluations raises exponentially with the number of objectives. This problem can be partially reduced by using model-based algorithms, where a secondary and faster model is used for evaluation.

Regarding the visualization, most plug-ins do not provide enough visual information about the optimization state and the results themselves. Inclusively, most of them generate poorly formatted files with insufficient information, thus impeding to trace back the process and even hindering the comprehension of the results (e.g., associate the design parameters' configurations with the corresponding performance values). Even if users use external tools to produce visualization mechanisms based on the information exported from the optimization plug-ins, these are often only available in the end of the optimization run. As a result, the computer or the system crashes during the optimization run (e.g., energy failure), no log file will be produced and all the information collected by the plug-in will be lost.

At last, most tools do not offer the possibility for interacting with them, nor do they provide means to pause and resume optimization runs. This is an inconvenience because it impedes users to add the knowledge they have learned, i.e., during the optimization run users would ideally extract information from good visualization mechanisms, that they could add to the process to make it more efficient.

Taking all the *pros* and *cons* of the analyzed tools into consideration, our solution enables the user to use a derivative-free optimization tool to address not only SOO but also MOO problems. The solution also provides integrated visualization mechanisms that aim to complement and enrich the information extracted during an optimization run.

Additionally, our solution is flexible enough to allow the user to select between a set of algorithms with different properties [Wolpert and Macready, 1997], including algorithms that handle time-consuming evaluations. By providing algorithms from different classes, our solution potentiates the efficiency of optimization processes. In order to help in the choice of the algorithms, our solution also adds support to easily run benchmarks with multiple algorithms, providing a quantitative measure of their performance.

Our solution also values the traceability of results especially for enhancing user comprehension. To improve existing mechanisms, our solution produces files involving all the necessary information about the configurations (e.g., algorithm parameters) and the solutions evaluated during the optimization process. Using these files, we are able not only to input them to other post-processing tools (e.g., visualization, statistics), but also to hot start and pause/resume optimization processes.

At the light of the architectural practice, our solution makes use of the textual programming paradigm and, consequently, has a special affinity with textual AD tools (e.g., Khepri). As a result, when coupled with these AD tools, our solution also benefits from their portability and scalability properties. We aim at reducing the abnormal time-complexity of BPO by providing model-based algorithms.

Finally, we consider the complexity of our solution. Unlike the analyzed tools, our solution does not benefit from the visual paradigm, which means that it should be simple to use and intuitive, even for non-programmers. As a result, we hide the complexity of the integration of optimization libraries under an abstraction layer, providing a clean and succinct set of primitives. These primitives draw inspiration from simple optimization mathematical models and should be rather intuitive and easy to use.

In the next chapter, we describe the architecture of our solution and explain how each component achieves the features highlighted in this section.

## 2.7 TROUBLEMAKERS

- GALAPAGOS Galapagos provides two metaheuristics algorithms, namely, the genetic algorithm, inspired by biological evolution processes, and the simulated annealing, motivated by the metallurgical process of annealing [Brownlee, 2011]. Although both algorithms are the basis for a large variety of extensions and/or specializations, supporting different heuristics, we will not provide a full description of such extensions, instead referring the interested reader to proper literature throughout this section.

As evolutionary algorithms, genetic algorithms explore Darwinian natural selection concepts, such as heredity, reproduction, and natural selection, and genetics concepts and mechanisms, including genes, chromosomes, recombination, crossover, and mutation, in order to search for better solutions in the solution space. More concretely, genetic algorithms generate an initial random set of solutions, called population, which is then iteratively evolved, creating new generations. The evolution process is comprised of four main phases: (1) adaptability, where individuals of the population are assigned a suitability or fitness value; (2) selection, where pairs of individuals are selected for reproduction, based on a probabilistic function which is proportional to each individual's fitness value; (3) crossover, where the genotypes of the selected individuals are recombined to produce new individuals; and (4) mutation, where new individuals are subjected to random copying errors with a certain probability. While earlier generations are usually diverse, final generations are often very similar to the fittest individuals, i.e., we observe an intensification of the traits of the most suitable individuals, thus emulating the mechanism of natural selection, described by Darwin [Brownlee, 2011]. Besides genetic algorithms [Golberg, 1989, Holland, 1992], evolutionary algorithms encompass other algorithms such as Genetic Programming [Koza, 1992], Evolution Strategies [Schwefel, 1981], Differential Evolution [Storn and Price, 1997], among others.

Besides genetic algorithms, Galapagos also provides a metaheuristics global optimization physical algorithm, the simulated annealing. Resemblant of hill climbing algorithms, where new candidate solutions are randomly sampled, this algorithm iteratively re-samples the solution space aiming at finding an optimal solution. During the search, the algorithm is propitious to accept the re-sampled solutions with lower performance, according to a probabilistic function that becomes more discerning of the quality of the samples over the execution of the algorithm, thus resembling the natural annealing process [Brownlee, 2011].

- GOAT ———————————————————————— One of the key differences between Goat and Galapagos is the number and diversity of the algorithms available. Whilst Galapagos supports two global metaheuristics algorithms, Goat supports five distinct algorithms: one metaheuristic, two direct-search, and two model-based algorithms, called CRS2, DIRECT, SUBPLEX, COBYLA, and BOBYQA, respectively. Due to space constraints, a full description of these algorithms will not be provided, instead we refer the interested reader to the relevant literature.

The CRS2 algorithm is a variant of the Controlled Random Search (CRS) algorithm for global optimization [Price, 1983]. A CRS algorithm is a population-based random search algorithm that creates an initial set of points, the population, which are then randomly evolved by means of heuristic rules. In the original CRS algorithms, heuristic rules modify a point at a time, replacing the worst point with a better one (called trial point), using a technique resemblant of the NMS algorithm [Nelder and Mead, 1964]. Similarly to NMS, CRS algorithms use a simplex, i.e., a generalized triangle in N dimensions, to envelope a region described by a random subset of points in the population. The worst point of the population is replaced with the reflection of the worst point in the simplex [Kaelo and Ali, 2006]. The CRS2 variant differs from the original in that it assumes that the worst population point will always be a part of the simplex. The actual version that is made available by Goat is a modified version of the CRS2 algorithm that introduces a local mutation component in an attempt to overcome situations where heuristic rules constantly fail to find a trial points that actually improve the worst point. Fundamentally, this local mutation generates a second trial point that results from the exploitation of the region around the best point in the population [Kaelo and Ali, 2006].

Vantagens e desvantagens ? Lack sound convergence properties, robustness and performance are highly problem dependent ler Kaelo

The second algorithm is a global deterministic direct search algorithm that relies on the division of rectangles, as explained in [Jones et al., 1993]. DIRECT, the DIviding RECTangles algorithm, recursively subdivides the design space into smaller multidimensional hyper-rectangles, estimating the quality value of each rectangle. DIRECT uses these values to focus the search on more promising regions of the design space and to further subdivide those in smaller hyper-rectangles. The SUBPLEX algorithm is an unconstrained local optimization algorithm [Rowan, 1990]. As a generalization of the NMS algorithm, SUBPLEX subdivides the design space in low-dimensional subspaces and then applies the NMS algorithm to a set of these subspaces, in order to seek for a better solution. In contrast to NMS, which has difficulties in high-dimensional problems, SUBPLEX reduces the limitations through the decomposition of the problem in low-dimensional subspaces which are more efficiently optimized by NMS.

Besides metaheuristics and direct-search algorithms, Goat also provides two local model-based implementations, namely the COBYLA (or Constrained Optimization BY Linear Approximation) algorithm [Powell, 1994], and the BOBYQA (or Bound Optimization BY Quadratic Approximation) algorithm [Powell, 2009], that rely on the construction of simple, partial models of the objective function [Koziel and Yang, 2011]. The former uses the concept of simplex to iteratively generate linear approximations of the objective function, whereas the latter generates quadratic approximations instead.

One of the main advantages of Goat is the algorithms' diversity. By providing algorithms with different characteristics and strategies, architects can test the suitability of each algorithm to their problem and, thus, select the most effective. The right choice may result in large optimization gains, especially when complex and time-consuming simulations are necessary [Wortmann and Nannicini, 2016]. For this reason, and due to the uniqueness of each BPO, several authors suggest that the selection of the optimization algorithm should be based on the results of several tests with different algorithms for a fixed number of evaluations or a fixed amount of time [Hamdy et al., 2016, Wortmann and Nannicini, 2016]. Moreover, the distinction between global and optimal algorithms is also critical when striving for accurate and precise optimal solutions. Most global optimization algorithms invest most of their effort searching for the truly optimal solution across large regions of the search space and rarely focusing on promising regions. Consequently, they might return a not so precise global optimum. To overcome this lack of precision and accuracy, one should apply a local optimization algorithm and provide the globally imprecise optimum as input.

- Silvereye The PSO algorithm is a global metaheuristic algorithm inspired by biological systems, such as the collective behavior of flocking birds and schooling fish, which interact and learn from one another to solve problems [Brownlee, 2011]. In PSO, the intelligence is decentralized, self-organized, and distributed throughout the participating particles, also known as swarm. These particles maintain information about their velocity, their current and personal best positions, and also the global best position known to the swarm. At each time step, the position and velocity of each particle are updated according to the best swarm or close neighbor position [Brownlee, 2011].

- Opossum ———————————————————————— Opossum is a model-based optimization tool for Grasshopper that uses the RBF machine learning technique to create global approximations of the objective function [Forrester and Keane, 2009]. These approximations are simply the weighted sum of other, simpler, real-valued functions, the radial functions. These functions are defined on the Euclidean space $\mathbb{R}^n$ and their value depends on the distance to a center $c$, so that $\phi(x, c) = \phi(\|x - c\|)$. In a RBFs technique, the weights are estimated based on the interpolation of data. A comprehensive detailed explanation of the RBF's estimation process is provided in [Forrester and Keane, 2009].

Since its invention, multiple implementations of RBF have been proposed. RBFOpt implements two well-known versions, namely, the Gutmann's [Gutmann, 2001] and the Regis and Shoemaker's [Regis and Shoemaker, 2007], commonly known as MSRSM. These techniques differ in the search strategy for the next candidate solution to be evaluated using the original objective function. The former uses the solution, which is likely to yield the largest improvement in the surrogate's accuracy, whereas the latter tries to balance the surrogate's accuracy amelioration with the exploitation of promising solutions, using other search strategies, such as genetic algorithms, sampling algorithms, or other mathematical solvers [Wortmann, 2017b]. Moreover, RBFOpt provides five different types of radial basis function: linear, multi-quadratic, cubic, thin plate spline, and automatic selection, which are also provided in the Opossum interface.

- Octopus ————————————————————————

Similarly to evolutionary algorithms, MOEAs adopt the evolutionary principles discussed in section 2.5.1 but, generally, have an additional archive to store the non-dominated solutions found [Zitzler et al., 2001]. The archive technique is incorporated to prevent losing current non-dominated solutions due to random mutations or recombinations. Most MOEAs differ in the selection and reproduction operators used to iteratively evolve populations. These differences are usually related to the very own goals of approximating the Pareto Front: (1) maximize the accuracy of the approximation (by minimizing the distance to the optimal front) and (2) maximize the diversity of the solutions within the front. While the first goal is related to the search strategy and how to assign fitness values in such a way that the individuals selected for offspring production will be closer to the Pareto-optimal front, the second goal is related to the time and storage constrains of the evolution process and which individuals to keep in each generation [Zitzler et al., 2001]. Although a thorough description of different MOEAs and their mechanisms is not herein presented, we refer the interested reader to [Zhou et al., 2011].

Most modern MOEAs realize the accuracy and diversity ideas through some implementation of the following mechanisms [Zitzler et al., 2001]:

- Selection (or environmental selection): Besides the population, most MOEAs maintain an archive with the non-dominated front among all the solutions that were evaluated. The archive preserves individuals during several generations, only removing them if (1) a new solution is found to dominate them, or (2) if the archive size is exceeded and they happen to be in crowded regions of the front.

- Reproduction (or mating selection): At each generation, individuals are evaluated in two stages. The first stage compares them regarding the relation of Pareto dominance, using this information to define a ranking among these individuals. The second stage refines these rankings through the incorporation of density information, i.e., if the individuals lie in crowded regions.

These mechanisms can be completely indifferent from one another, e.g., the first one applying a Pareto-based criteria and the second one applying weighting approach. However, many MOEAs implement both concepts similarly. In the particular case of SPEA2, the algorithm explores two independent sets of individuals: the population and the archive. In this algorithm, the archive size is fixed and, therefore, whenever the number of non-dominated individuals is less than its size, some dominated individuals are added to the archive. At each iteration, the algorithm computes each individual's fitness value (a *strength* value, defined as terms of the number of solutions it dominates, the *raw fitness* value, defined in terms of the strength of its dominators, and a density estimate, defined as the inverse of the distance to the $k^{th}$ to the nearest neighbor) and copies the non-dominated individuals from the population to the archive, removing any individual that is dominated, whose objective values are duplicated, or that, when the size of the updated archive is exceeded, lies in crowded regions of the non-dominated front. After filling the archive, pairs of individuals are chosen from the archive to reproduce and produce the offspring through recombination and mutation operators that will make the population of the next generation [Zitzler et al., 2001].

Unfortunately, algorithms incorporating the Pareto dominance relation and diversity measures appear to have difficulties in optimization scenarios with more than two objectives, which spurred the development of algorithms using other quality measures, including quality indicators. To overcome the objective limitation and provide the user with the flexibility to use a more efficient algorithm, Octopus provides the option to use HypE, an algorithm that explores the HV indicator to rank individuals. Particularly, to minimize time penalties associated with the computation of the HV, in scenarios with more than three objectives, HypE uses Monte Carlo simulations to estimate the HV value of each individual [Bader and Zitzler, 2011].

As a MOEA, NSGA-II attempts to achieve an approximation to the Pareto front that is both accurate and diverse. In this particular algorithm, both the selection and reproduction mechanisms rely on the same basis criteria: Pareto dominance relations and a crowding measure. To define the order among the individuals, the pool of individuals is split into different Pareto fronts and ranked accordingly, i.e., the first non-dominated front is assigned the highest rank, the second front is assigned the second highest rank, and so on. Each individual in each rank is ordered according to a crowding measure, represented in terms of the sum of distances to the two closest individuals along each objective. The archive and the generation's population are combined, deleting the worst 50%. Afterwards, binary tournaments are carried out on the remaining individuals (the archive members) in order to generate the next offspring population.

# 3

# Solution

**Contents**

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## 3.1 Architecture Overview

## 3.2 Architecture Design Requirements

### 3.2.1 Problem Modelling

### 3.2.2 Simple Solver

### 3.2.3 Meta Solver

## 3.3 Architecture Design Implementation

### 3.3.1 Problem Modelling

### 3.3.2 Simple Solver

### 3.3.3 Meta Solver

# 4

# Evaluation

## Contents

- Relembrar o objectivo do trabalho e dizer como o vamos avaliar de um modo geral introduzindo os proximos subcapitulos.

## 4.1 Qualitative Evaluation

- Number and Heterogeneity of Available algorithms - Differences / Benefits / Disadvantages when compared to Grasshopper's frameworks

## 4.2 Quantitative of Applications

- Dizer que de um modo geral começámos de forma incremental por considerar problemas single-objective, nomeadamente a casa da ericeira, que remonta a primeira publicação. Depois evoluimos para a avaliação bi-objetivo de dois casos de estudo reais - Pavilhão Preto para exposições e de uma arc-shaped space frame.

- Comentar a facilidade c/ que alguém que já tem um programa AD consegue acopolar optimização a AD.

### 4.2.1 Ericeira House: Solarium

### 4.2.2 Black Pavilion: Arts Exhibit

#### 4.2.2.A Skylights Optimization

#### 4.2.2.B Arc-shaped Space Frame Optimization

# 5

# Conclusion

## Contents

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Rui Cruz
You should always start a Chapter with an introductory text

## 5.1 Conclusions

## 5.2 System Limitations and Future Work

### 5.2.1 Optimization Algorithms

### 5.2.2 ML models

### 5.2.3 Constrained Optimization

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