CRANFIELD UNIVERSITY

MATTIA PADULO

Computational Engineering Design under uncertainty

An aircraft conceptual design perspective

SCHOOL OF ENGINEERING
Department of Aerospace Engineering

PhD THESIS
Academic Year 2008-09

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This thesis is submitted in fulfillment of the requirements for the degree of
Doctor of Philosophy

“What science can there be in a matter in which, as in all practical matters, nothing can be defined and everything depends on innumerable conditions, the significance of which is determined at a particular moment which arrives no one knows when?”

L. Tolstoy, *War and Peace*

Abstract

Presented in this thesis is a novel methodology for aircraft design optimization in the presence of uncertainty, with emphasis on the conceptual design stage.

In the initial part of the thesis, the uncertainty typologies of interest for aircraft design are identified within a broader epistemological framework. The main implications for non-deterministic computational design are also outlined.

The focus is then restricted to uncertainties that can be modeled by probability theory. In this context, a methodology is developed to enhance robust design optimization (RDO). Firstly, the problem is formulated in order to relax, when required, the common RDO assumption about the normality of objectives and constraints. Secondly, starting from engineering considerations about the risk related with design unfeasibility, suitable estimates of tail conditional expectation are introduced in the set of robustness metrics.

The proposed formulation requires the estimation of mean and variance of objectives and constraints. To calculate such moments, a novel uncertainty propagation technique is proposed, which achieves a favorable trade-off between the accuracy of the estimates and the required computational cost. Peculiar features of the propagation technique are exploited to couple the propagation and the optimization phases for the classes of gradient-based methods and the derivative-free pattern search methods. Also analyzed are the possible advantages achievable when the two types of algorithms are hybridized.

The usefulness of the proposed methodology for conceptual design optimization is demonstrated with the aid of two engineering design problems, concerning the sizing of passenger aircraft and the design of transonic airfoils.

Acknowledgements

I am indebted to my supervisor, Prof. M. Guenov, for his patient support and guidance through these three years at Cranfield. I would also like to express my gratitude to Dr. S. Campobasso for his help and advice, and to Dr. S. Forth for his availability and kindness during our collaboration.

Thanks to my colleagues and friends: Paolo, Libish, Jeremy, Yves, Marco N. and Vis. Thanks to the musicians I had the pleasure to play with, and especially Dario, Pierre, Ben, Greg, Javi, Kostas, Luismi. These have been unforgettable years, and also because of them. Thanks to Sue for the support in setting up the Music Society.

Elena, Stefano, Guido S., Guido M., Frank and Marco B.: thank you, for many reasons.

Thanks to Alessandro, Gianni, Fabrizio, Antonio, Piero, Serena e Daniela. Thanks to Nuria. Thanks to my family.

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Abbreviations

AD	Automatic Differentiation
CDF	Cumulative Distribution Function
CFD	Computational Fluid Dynamics
CVaR	Conditional Value at Risk
CVM	Complex Variable Method
EA	Evolutionary Algorithm
FD	Finite Difference
FORM	First Order Reliability Method
GQ	Gaussian Quadrature
GSS	Generating Set Search method
I MM	First order Taylor-based Method of Moments
II MM	Second order Taylor-based Method of Moments
III MM	Third order Taylor-based Method of Moments
LTB	Larger-The-Better
MCS	Monte Carlo Simulation
MDAO	Multidisciplinary Design Analysis and Optimization
MPP	Most Probable Point
NTB	Nominal-The-Better
PCE	Polynomial Chaos Expansion
PDF	Probability Density Function
PMA	Performance Measure Approach
PS	Pattern Search method
QN	Quasi-Newton method
RBDO	Reliability-Based Design Optimization
RDO	Robust Design Optimization
RIA	Reliability Index Approach

SA	Stochastic Approximation
SC	Stochastic Collocation
SE	Stochastic Expansion
SORM	Second Order Reliability Method
STB	Smaller-The-Better
TCE	Tail Conditional Expectation
URQ	Univariate Reduced Quadrature
VaR	Value at Risk
VGK	Viscous Garabedian-Korn CFD code

Chapter 1

Introduction

1.1 Problem area

During the last decades, the striving for increased performance and reduced cost within the aerospace industry has emphasized the importance of accounting for the interactions between disciplines such as aerodynamics, propulsion, structures and control since the first phases of the design process. The methods under the subject of Multidisciplinary Design Analysis and Optimization (MDAO) follow such paradigm by integrating the computational tools that model the various aspects of the product under development and by coupling them with an appropriate optimization algorithm to systematically explore the design space. Such approach is expected to reduce the time needed to assess the outcome of a specific design choice, giving the designer the freedom needed to experiment with new solutions.

However, from the outset, the product development process is usually affected by severe uncertainty, for example, the complete problem frame might be only approximately known, the adopted computer models have low fidelity and assumptions based on previous experience have to be largely used. Such variety of nondeterministic aspects ought to be taken into account by MDAO for it to be of practical usefulness, especially in the knowledge that during conceptual and preliminary phases the design decisions commit up to about 75% of the total cost of the development program.

1.2 Research aim and objectives

This thesis aims at developing a methodology to appropriately tackle the problem outlined above in the context of conceptual aircraft design. Such purpose is achieved by fulfilling the following objectives: the identification and understanding of typologies of uncertainty in engineering design and their theoretical representation; the development of suitable numerical techniques to improve current uncertainty-based methods for engineering computational design; the incorporation of additional metrics of system performance under uncertainty to widen the currently available scope of design choices.

1.3 Thesis overview

The initial part of the research, presented in Chapter 2, is devoted to grounding the study in a broader epistemological framework, in which the importance of uncertainty analysis is acknowledged not only as a necessity, but also as a powerful cognitive opportunity. Such framework allows to identify the uncertainty typologies of interest for aircraft design, together with their mathematical modeling options, and highlights a number of key implications for computational design in the presence of uncertainty.

The focus is then restricted on uncertainties that can be modeled by probability theory. The state of the art regarding the optimization of designs affected by such kind of uncertainty is reviewed in Chapter 3, with an emphasis on the special case of robust design optimization (RDO).

In this context, a methodology is presented in Chapter 4 to enhance the current approach to RDO. Firstly, the problem is formulated in order to relax, when required, the common RDO assumption regarding the normality of objectives and constraints. Secondly, starting from engineering considerations about the risk related with design unfeasibility, suitable estimates of tail conditional expectation are introduced in the set of robustness metrics. In the third place, a novel uncertainty propagation technique is proposed to estimate the required robustness metrics for objective and constraints, with the intent of achieving a favorable trade-off between the accuracy of the estimates and the required computational cost. Furthermore, peculiar features of the propagation technique are exploited to intimately couple the propagation and the optimization phases. This is achieved for two classes of algorithms, namely gradient-based methods and the derivative-free pattern search methods. Also analyzed are the possible advantages achievable when the two types of algorithms are hybridized.

The proposed methodology is tested on two engineering design problems, concerning aircraft sizing and airfoil design, in Chapter 5 and 6, respectively. This allows discussing the advantages and the limitations of the methodology within the scope of the thesis. The conclusions are presented in Chapter 7, together with the vision on future work.

Chapter 2

Background

2.1 Introduction

This chapter constitutes a reflection on the problem of uncertainty in design, with the aim of identifying the scope of the research.

In the first instance, we realize that the concept of managing uncertainty, which is recurrent in the literature, is elusive for three fundamental reasons: firstly, it is not clear what kind of actions such managerial approach should incorporate; secondly, it is not clear what its purposes are; and thirdly, the subject matter - uncertainty - is obscure.

Such challenges are typical of a problem that stands, by definition, at the limits of knowledge. Identifying and overcoming such limits requires a “meta-perspective” [144] through which engineering rationality could examine itself.

We root such “meta-perspective” in the current philosophical discussion concerning engineering knowledge, which is introduced in Section 2.2. Section 2.3 focuses more specifically on the design activity, to outline the cognitive and behavioral aspects required by our discussion. Section 2.4 collects the elements presented throughout the chapter to provide a working definition of uncertainty in engineering design and highlights some key implications for computational design. The result is a holistic outlook, which helps to define the scope of the present study, hence serving as foundation for the rest of the thesis.

2.2 The need for an epistemology of engineering

We could trace the origins of the uncertainty management approach back to Descartes, who identified four rules which could lead to certainty [48]:

> "The first of these was to accept nothing as true which I did not clearly recognize to be so: that is to say, carefully to avoid precipitation and prejudice in judgements, and to accept in them nothing more than what was presented to my mind so clearly and distinctly that I could have no occasion to doubt it. The second was to divide up each of the difficulties which I examined into as many parts as possible, and as seemed requisite in order that it might be resolved in the best manner possible. The third was to carry on my reflections in due order, commencing with objects that were the most simple and easy to understand, in order to rise little by little, or by degrees, to knowledge of the most complex, assuming an order, even if a fictitious one, among those which do not follow a natural sequence relatively to one another. The last was in all cases to make enumerations so complete and reviews so general that I should be certain to have omitted nothing".

The first principle has kept its validity through the centuries, but has to face, in practice, the pressure imposed by time and budget constraints. The second and the third principles express, respectively, the principles of separation and reduction [74], which are employed by human rationality to handle otherwise unmanageable problems, but overlook the interactions of disciplines and components of a complex system such as an aircraft, which are key to the advancement of design [114, 182]. The fourth principle is also ultimately untenable when applied to uncertainty management, since it is impossible to imagine and enumerate a priori all the categories of the unknown [194].

We can partially solve the contradictions arising from the principles above if we understand that the failure of Descartes' programmatic rules does not stand in their specific content, but in their nature. In fact, they were conceived in absolute terms, and are nowadays outdated, in the light of the foundational crisis which has permeated into the fields of philosophy, science and mathematics during the 20^{th} century [144, 194].

An updated version of such principles might be, instead, a set of *provisional* strategies to explore uncertainty and, at the same time, maintain awareness of the uncertainty related with the exploration, in a recursive, never-ending confrontation between knowledge and its limitations, between an aspiration to complexity and holism and a need for simplicity and reduction [144]. Applying such renovated uncertainty management approach to engineering design requires understanding engineering "as a practice and form of reasoning" [70], endowed with an autonomous body of knowledge [206].

Such task has been carried out over the last thirty years by the increasing community of philosophers and engineers, who have advocated the need for a philosophy of engineering in the context of philosophy of technology [52, 70, 110, 120, 206], in sharp contrast with the view of engineering as applied science suggested by Bunge [23]. To understand the epistemological repercussion of overcoming such restrictive definition, we start from a definition of engineering, as proposed by Vincenti [206] (as a readaptation from Rogers [177]):

> "Engineering refers to the practice of bringing into being the design, production and operation of any artifice which transforms the world around us to meet some recognized need."

The teleological specification concluding the above definition marks the first difference between engineers, who work towards the achievement of practical objectives, and scientists, who pursue a more general understanding of the world. Such finalistic qualification presupposes a volitional character of engineering: while science develops with the purpose of adapting knowledge to the facts, by contrast, engineering aims at modifying the facts to match value preferences [53].

Not surprisingly, both scientific and engineering knowledge are outcomes of epistemic reduction processes. They are both made of conventional truths, inscribed in closed (and consequentially incomplete) precincts, which are continually renegotiated. However, the rules to which such reduction obey are completely different: science "pragmatically ignores considerations of practical value" [78], which are, in turn, fundamental to engineering. This marks the difference between the contingent character of engineering rationality, as opposed to the scientific way of thinking based on necessity [70]. While the former is uncertain, particular, closely dependent on context, value and time, the latter is certain, universal, independent from contexts and values, and timeless [70]. An instance of this difference can be found in the idealizations and approximations typically adopted for computational purposes, both in engineering and scientific contexts. In the latter case, in fact, the formally correct statement that idealizations and approximations introduce falsity in the performed calculations would formally protect from falsification any inference based on the results. For the engineer such formal correctness would have no value, since what matters is the practical usability of the results [120]. Such differences are justifiable by the fact that science seeks a description of natural reality, while engineering is action-oriented.

This brief exposition suggests that pragmatical methodologies for managing uncertainty intrinsically belong to engineering, which has to acknowledge the unknown and cannot refuse the challenges it poses. Our objective becomes then to gain a “meta-perspective” on engineering knowledge to understand that uncertainty analysis is not only required, but also represents a powerful cognitive opportunity if guided by the appropriate epistemological awareness. The next section will narrow the scope of the engineering activity as made of design, production and operation, down to the design phase only, which is the focus of this work.

2.3 Design and design knowledge

An interpretation of engineering design, which stems from the work of Simon [189] and is still accepted at large by the research community [209], describes it as a problem solving activity. However, the problem to be solved does not have an unique nor predetermined solution, and this gives design its strongly creative connotation and much of its epistemological complexity [39].

The process is initiated by a set of requirements issued by the customer or identified within the company to respond to an opportunity in the market. Such requirements have to be translated into a problem formulation which allows to devise a technical strategy for working towards their satisfaction. This includes one or more identified criteria of excellence, together with constraints such as date of completion, standards and codes of practice to be adopted [66].

For the case of aircraft design, a hierarchical articulation of the activity would subdivide the overall design, whose purpose is to achieve a suitable layout to meet the specifications, into major component design such as wing, fuselage, empennage. The problem of designing such components would then be partitioned by disciplinary, functional or operational decomposition.

Such subdivisions take place while the project advances along the project timeline, which is usually made of three main stages: conceptual, preliminary and detailed design. In the conceptual design, the focus is on the design rationale: designers compare alternative solutions looking for a configuration which is in some sense optimal in meeting the requirements. Heuristics and low-fidelity models are used at this stage to predict the aircraft mass, performance and cost. This phase presents the opportunity for substantial improvements and, at the same time, significant program risks. It is in fact usually the shortest of the design phases, and determines nearly the 75% of the costs allocated for the whole cycle of product development. At the end of such phase, one or few configurations are downselected to proceed to the following stage, during which they are developed in much greater detail, subject to the constraints issued by the conceptual design in form of mass, performance and cost targets. Such constraints, and their successive refinement, imply that there is a great deal of feedback from the preliminary to the conceptual phase. At the end of such iterations, the best concept amongst the ones considered at the preliminary design level is retained. Finally, detailed design prepares the aircraft to production by deciding on a very large number of elements such as bolts.

Such design phases involve in various ways the work of discipline specialists, or groups of specialists. The related decentralization of design tasks puts considerable importance on communication and organization issues, which may result in nugatory design iterations or non-optimal design “fixes”, or may hinder the design for innovative configurations [114]. Furthermore, the evaluation of the proposed design solution might be difficult, since the criteria depend on the designer’s level and domain of expertise, and have to be often negotiated.

Due to the complexity of the problem, the hypothesis of the so-called decision-based design, which puts forward that design can be interpreted by axiomatic rules of rational choice [81] are often untenable. In fact, design decisions are usually not taken once all the facts concerning the relevant downstream stages of design [208] are mastered, but rather on the basis of previous knowledge, contingent value judgements [70] and heuristics [110], by resorting to successive decompositions and refinements, similarly to what described by the model of opportunistic planning [80, 207]. For example, early decisions are made by considering only simplified information about the identified alternatives, for which a limited range of outcomes is taken into account. This is a consequence of the bounded nature of human rationality [190], which has limited computational resources, a given time horizon, and cannot deterministically predict the environment. This is fundamental to understanding how limits on cognitive action at a point in time can determine the overlooking or underweighing of factors whose overall effect on the design can be significant. It also helps to explain the reason why the ideal overall hierarchical organization of the design process is hence often compromised or limited to "local" episodes [207]: sometimes the upper level determines the lower level, while sometimes the opposite happens [208].

Eventually, acquiring further knowledge in response to problems occurring during the design initiates a process of discovery at the end of which the initial problem is reformulated. The following subsections will suggest a model to explain how such knowledge acquisition takes place in aerospace design.

2.3.1 The cognitive adjustment

Knowledge is the result of a continuous, successive cognitive adjustment of rationality with respect to the phenomenological world in which it is situated and in which it operates [144]. A number of contextual relationships have been found to trigger such adjustment in the design activity, by making designers aware of their lack of adequate knowledge. Following Vincenti [206], who starts from considerations from Laudan [129], we can identify them as follows:

- failure of current technological solutions (also highlighted by [18, 164]); an example from aeronautical history is given by the two accidents involving the De Havilland Comet in 1954 (BOAC Flight 781 and South African Airways Flight 201), due to metal fatigue stress concentration, which was at the time not accounted for; it is worth underlying that this category does not represent only catastrophic failures, but any functional failure;
- issues descending from extrapolation from past technological success; an example of this category is the Convair F-102 Delta Dagger, which was designed in response to a 1950 USAF request for proposal for a Mach 2 interceptor. Convair was confident of meeting the requirement by suitably ex-

trapolating from the Convair XF-92 design. However, the increased ambitions of the new design had a dramatic set back during the first test flights, when higher than expected transonic drag levels hindered the achievement of sonic speed. The subsequent redesign of the plane managed to reach the performance targets by taking into account the recently discovered area rule;

- potential technological failures or opportunities; they may be perceived internally in the design team, or externally (causing for example a change in demand from the customer). An example of (potential) opportunity is the case of the Boeing B2707, which was heavily subsidized by the US government since 1963 with the purpose of catching up with the development of the Concorde in Europe, at a time when the supersonic liners were thought to be the future of civil aviation. In such effort, the requirements for the US program were unrealistically increased with respect to the Concorde. This led to substantial design problems and delay in the program, which finally ended in 1971 due to funding cuts;

- issues related to the unequal development of the elements of a system, at a given time; an example are the difficulties faced by the the Avro Vulcan's designers when the Rolls-Royce Avon engines fitted on the first prototypes were substituted with the newly developed Olympus engines. To fully exploit the potential flight envelope of the vehicle, it became clear that the problematic behaviour of the straight delta wing at high angles of incidence and high speed had to be addressed. This lead, in steps, to the development of the ogee delta wing, a concept that was later reused and refined for the Concorde design;

- internal needs of design; we subsume under this category different instances of inadequate knowledge, which span from the need for accurate data, obtained either experimentally or numerically, to the lack of clarity in specifications, to the absence of appropriate regulations for the task at hand. An example of the last case is the Hawker Siddeley Harrier, the first generation of the Harrier series, for which there were no normative regulation concerning vertical take-off and landing operations. The designers had to compile suitable requirements themselves to define the control of the sideslip while translating from hover to horizontal flight. Uncertainty reduction plays then as a drive for knowledge growth, and not just as one of its possible consequence [206];

- external influences, coming from corporate, economic, military, political social, cultural or user contexts [44, 141]. The heteronomy and heterogeneity of those contexts make their influence on the design unpredictable. A famous example of this category is given by the BAC TSR-2, which was canceled in 1965, after seven years' development, due to a change in military and political priorities and to its very high cost.

2.3.2 Growth of knowledge

Growth of knowledge is a result of the effort invested in answering to such problems. Several authors have interpreted such growth by analogy with biological evolution in response to environmental challenges [24,26,222]. For the purposes of our discussion, we could consider adequate the model proposed by Vincenti [206], which adapts Campbell's model [26] of knowledge growth to the context of aeronautical design. Such model describes the growth of knowledge in terms of "blind variation and selective retention" and could be decomposed into two successive stages:

- blind variation: is a variation from the current state of knowledge, whose effect cannot be foreseen nor predicted, hence its blindness;
- selective retention: choice of the cognitive solution which improves the quality of future engineering practice; hence the main criterion to retention is the utility for design of the new piece of knowledge discovered by variation. Such utility is assessed by means of theoretical tools, numerical simulation and direct test.

The importance of this model for us here is to identify how uncertainty affects the process of knowledge growth. As knowledge advances, in fact, variation mechanisms are modified and improved, which in turn results in a change in blindness, and in a change on the field of variation which is considered to be relevant. The first effect decreases uncertainty *in degree*, while the second increases uncertainty *in kind*. This has significant repercussion on the way computational tools for uncertainty analysis should be managed, due for example to the paralleling increase in computational power and specialized codes complexity. In the second phase, the satisfaction of the retention criteria - which would be based on the usefulness of the acquired knowledge, interpreted in the light of the current system of values and on the perceived possibilities - is not certain. While the sharpening of surrogate means of analysis such as theoretical and simulations tools can reduce the uncertainty with respect to a particular criterion, it is clear that increased awareness and knowledge also lead to questioning the acceptability of the criterion, and call for the inclusion of new criteria which were previously deemed irrelevant.

2.3.3 Knowledge organization

The knowledge that results from the described process is a highly specialized form of knowledge which eclectically adopts various theoretical tools and ways of thinking. A useful characterization can be drawn by building again on Vincenti's work [206] on aeronautical design knowledge. The knowledge concerning designs which evolves by successive refinements (as opposed to revolutionary design), which we may call “adaptive design” following Pahl and Beitz [158], is then constituted by:

- fundamental design concepts (also called primary generators, kernel ideas, central concepts, primary positions, guiding themes and early solution conjectures, see [209]), which constitute a framework for adaptive design and have been acquired by the engineering community through experience; they may cause “premature commitment” [209] towards a solution;
- criteria and specifications to translate qualitative needs into quantitative specifications;
- theoretical tools, such as:
    1. intellectual concepts for thinking about design, embracing physics, mathematics and engineering practice;
    2. mathematical methods and theories to make design calculations, which enclose again physical and mathematical models of various fidelity, quantitative assumptions, but also methods and tools developed specifically for engineering design, such as CAD software, optimization codes or numerical techniques for uncertainty analysis;

- quantitative data: descriptive knowledge of physical constants, chemical-physical, mechanical and technological properties of materials, operational conditions or ergonomic information; they might be subject to various degrees of incompleteness, inconsistency and error;

- practical considerations, which take the form of more or less conscious heuristics, and may include elements of operation and production knowledge;

- design instrumentalities:

    1. routines, procedures and practices such as problem decomposition, optimization and satisfaction of feasibility;

    2. ways of thinking, which employ the above mentioned intellectual concepts; they enable to understand the operation of a device and to perform mental simulation [10] of the effect of alterations in its design. One of such processes is analogy, through which knowledge coming from previous experiences, or from a non-directly related field is reused. Visual thinking, in terms of sketches, drawings and presentations plays an important role within this category;

    3. judgmental skills, which are required to make decisions and find solutions within the contingencies given by funding priorities, time pressures, conflicting biases, personal and institutional politics etc. The process of evaluating the proposed solutions runs in parallel with their elaboration, and shape the whole problem-solving process by judging the adequacy of any proposed solution element, and the reformulation of the considered constraints in due course [19]. Such skills are acquired through experience of technical successes and failures; they might suffer from biases such as representativeness, anchoring, confirmation and landmark biases [78, 99, 164];

    4. practical skills, which are required to put the above mentioned tools into use, within the specific, constrained context of design. They may depend on experience, and include organizational and managerial skills. Their importance is clearly recognized in technology, but not in science [40].

2.4 Modeling design uncertainty

Expanding on the examples from literature [1], we can proceed to cataloguing the instances of uncertainty in design that we have met in the previous sections, and which we could summarize here as follows:

- design has a contingent nature; it is immersed in a context on which it depends, and which involves political, social, military and other aspects and shows an uncertain behavior;
- the difficulties in framing the problem are intrinsic in design, due to its open-ended nature, especially but not exclusively in innovative design. They may involve disagreement on what is to be decided, or the impossibility of conjuring up all the possible design options;
- predicting the outcome of a design choice suffers from the cognitive limitations implicitly or explicitly incorporated into the adopted methods and models; it involves the mentioned trade-off between cost and accuracy of methods and/or models; it may rely on the judgment of experts, who may disagree, or be difficult to identify. The existence of expert could be problematic for very innovative problems;
- the values motivating the ordering of preference amongst of the outcomes might be subject to evolution and negotiation;
- knowledge growth cannot be considered certain a priori. In fact, it is sought for only when it is judged to be likely within the given resource constraints. It proceeds, as we have seen, by blind variation and selective retention; the degree of blindness and the kind of variation to be explored change unpredictably along the process; here too, the values establishing the concept retention are subject to evolution and negotiation;
- the opportunistic character for design cognitive action may compromise optimal choices. In particular, the decompositions operated to simplify the problem may hinder the adequate accounting for interactions across the subproblems;

[1] A review of the most relevant uncertainty categorizations appeared in literature during the last thirty years, spanning the fields of mathematics [106, 108], philosophy [77, 144, 194, 195], psychology [88, 99], risk analysis [143, 152, 153, 180], engineering [5, 6, 15, 44, 46, 92, 113, 119, 138, 139, 148, 151, 193, 203, 211] and applied sciences [97, 175] is presented in Appendix A.

- quantitative data can be distorted (either inaccurate or imprecise) or incomplete.

2.4.1 A classification of engineering design uncertainty

From the discussion above it emerges that, in an engineering design context, the recursive knowledge acquisition process dialectically involves two levels, which we may call the problem formulation and the problem solution levels.

At the first level, a correspondence is sought between rationality and the outer world. Firstly, in the light of the current values, the need at the origin of the design process is tentatively formalized. The problem is then framed by simplifications and reductions, which give it a determinate horizon, decompose it into manageable subproblems and apply assumptions to facilitate its solution. For example, in computational design, models which are deemed relevant may be selected for the conceptual study of the aircraft, and a computational workflow may be set up around them. This may include the formulation of an optimization problem which depends on selected variables and parameters.

At the second level, a problem solution is sought which coherently descends from the given formulation. In the computational design example, this corresponds to solving the optimization problem.

These levels form the two main categories of a novel taxonomy of uncertainty in engineering design, presented in Figure 2.1. Such categories, which we call uncertainty *about the problem* and *within the problem*, are then populated with the instances of uncertainty presented in the previous section, whose definitions are explained in Table 2.1. The learning process, for which uncertainty is both a cause and a consequence, takes place as we move iteratively from one level to the other, as depicted in Figure 2.1. Moves from left to right in the scheme reduce the complexity of the problem to make it handleable. Moves from right to left increase such complexity, and occur when the inadequacy of the current problem frame becomes evident. For example, recognized deficiencies in the solution of the design optimization problem may lead to the problem reformulation. Such taxonomy, coherently with the reasoning made in Section 2.2, is considered as provisional, and is hence subject to future updates and amendments. However, it constitutes a useful way to define the current understanding of uncertainty in de-

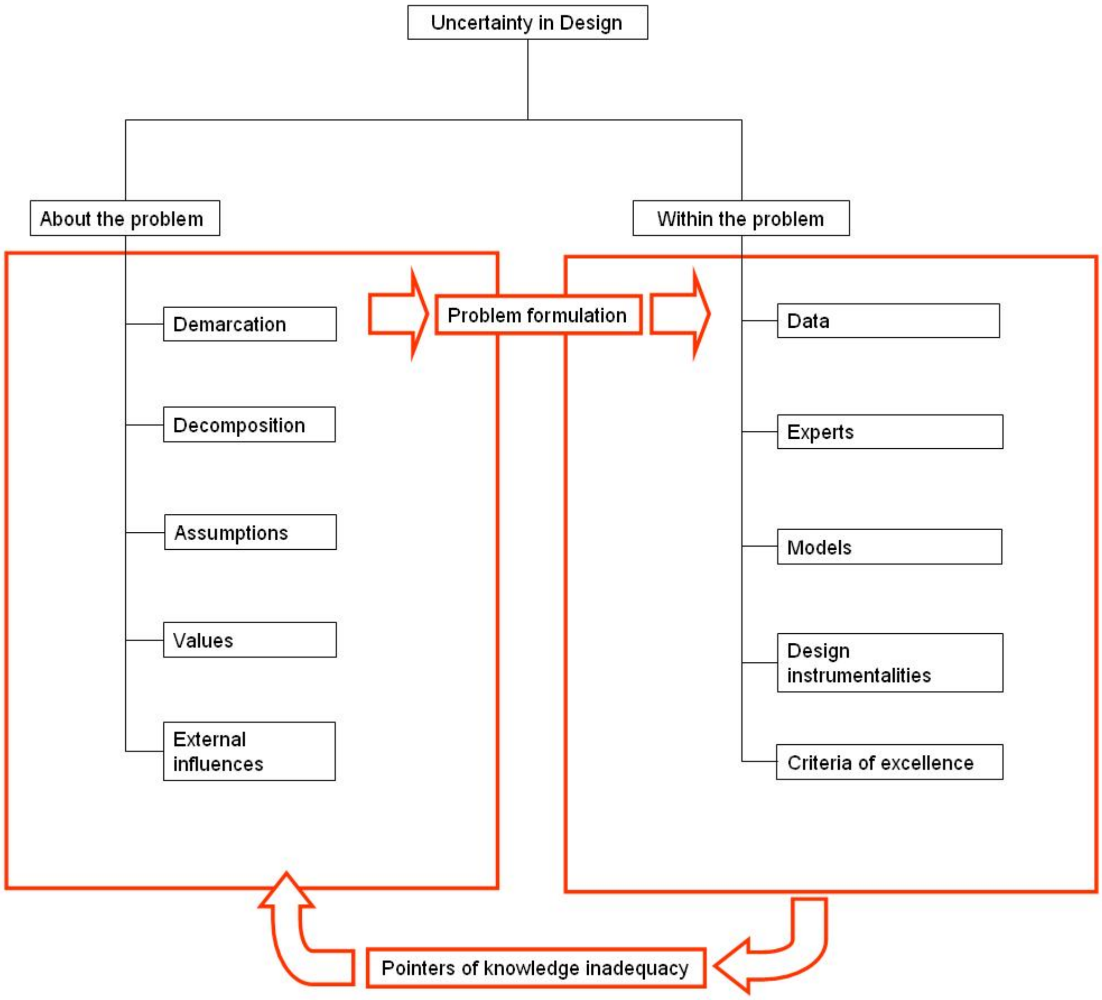


Figure 2.1: A classification of uncertainty in Engineering Design.

sign: it implicitly embeds, in simple terms, the epistemological theory presented above.

In the process of giving the problem its frame, also the involved uncertainties may be given a tentative model. Several possible approaches to perform such a task are very briefly reviewed in the next section.

2.4.2 Mathematical theories of uncertainty

Probability theory currently constitutes the most commonly used theoretical tool to model uncertainty. Since the 1960s, however, new normative attempts have been made to broaden the field of non-deterministic theories. During the last

Kind of Uncertainty	Definition
Demarcation	refers to the uncertainty about the problem horizon and the considered options (see A.2.3).
Decomposition	concerns the uncertainty introduced when simplifying the problem into a set of subproblems with negligible interactions.
Assumptions	is introduced by the assumption whose traceability is uncertain.
Value	arises from the fact that values are subject to evolution and negotiation.
External influences	is caused by heteronomous and heterogeneous factors acting in the context in which the design is situated.
Data	is due to the distorted or incomplete nature of data used for the problem solution.
Experts	concerns the dubious reliability of the experts or their disagreement.
Models	regards various aspects of modeling uncertainty, including model structure, parameters, boundary and accuracy.
Design instrumentalities	regards the use of tools and tacit knowledge for solving the problem, and their associated uncertainties.
Criteria of excellence	concerns the uncertainty in translating the values and the need into comprehensive criteria.

Table 2.1: Uncertainty definitions for the classification in Figure 2.1.

twenty years, encouraged by the success encountered in the applications (predominantly in control theory) significant theoretical efforts have been made in consolidating and attempting to understand those theories as a whole. The research aiming at generalizing the classical probability-based Information Theory, founded by Shannon, has arrived in 1991 to the formulation, due to Klir [107], of the so-called Generalized Information Theory (GIT). This theory gives an interpretation of the mathematical theories of uncertainty as descending from the combined outcome of Fuzzy Set theory and the theory of monotone measures.

Fuzzy set theory was first proposed by Zadeh [220] in the mid sixties. Its first purpose was answering to the objection that nature is not "crisp", i.e. it is not forcedly true that an element either belongs to one set, or it is excluded from it. This difficulty was tackled by the introduction of a membership function that belongs to the interval $[0, 1]$, instead of being binary, thus allowing to express gradual transitions.

On the other hand, the monotone measure theory enables to model super- and sub-additivity, which generalize the probabilistic feature of additivity. In simple terms, it means that it allows modeling cases for which the uncertainty related with two mutually exclusive events is not forcedly equal to the sum of the uncertainties associated with each of them.

Beside the mentioned Fuzzy Set theory, among the available theories in the GIT framework to be cited are: Evidence theory [188], Info-gap theory [12, 13], P-Boxes [96] and Rough Sets [162]. Is worth noting that there is no general agreement in the scientific community about such theories. Experts' orientations range from the negation of the existence of any non-probabilistic theory of uncertainty, to the pragmatic attitude of using the newly available mathematical tools in conjunction with the classical ones [28, 29, 104, 112, 221].

The spectrum of uncertainty typologies which can be modeled by GIT is supposed to be wider than the original concept of uncertainty intended as randomness, by including for example ambiguity and vagueness (see Appendix A). Hence the interest for design. In particular, applications of GIT theories to engineering design include Fuzzy sets [145, 213, 214], imprecise probabilities [4], Evidence theory [2, 9, 63, 96, 205, 213, 214] and Info-gap theory [12, 13]. Such applications entail an increased computational complexity which often makes them unsuitable for industrial problems.

2.4.3 Implications for computational design in the presence of uncertainty

Three main implications to the way computational engineering design should handle non-deterministic aspects derive from the above exposition:

- design qualities which are deemed as desirable responses to uncertainty have to be identified. In fact, there are several qualities that could be of interest beyond the insensitiveness to variability, which is usually considered. A partial list [43] includes concepts such as versatility, flexibility, evolvability and interoperability. Such qualities should be translated into a set of suitable mathematical metrics, based on one of more of the theories presented above;

- to enable the learning process sketched in terms of horizontal moves in Figure 2.1, the adopted computational methods have to be efficient. This feature gives the designer the time needed to see the outcomes of one or another hypothesis or design choice, and the freedom to experiment with new solutions, thus indirectly increasing innovation;

- the designer has to be made aware of the limitations and the uncertainty embedded in the analysis method in use, which is also inevitably affected by hypotheses and assumptions, has limited accuracy and is valid within a specific context. The assumptions and simplifications done when formulating the problem have to be clearly stated, and need to be checked. GIT uncertainty theories require less assumptions on the input uncertainty models than probability theory, and this might be of advantage for engineering design, if the other conditions hold.

Such considerations are valid for any of the non-deterministic models presented in the previous section. In a first step towards their recognition in computational design, we restrict the focus of attention to probability theory, which is the least complex and the most established of the uncertainty theories.

2.5 Summary and conclusions

This chapter has introduced the foundational framework for the thesis. An uncertainty management approach to design has been presented as an integral part of engineering practice and rationality. Such approach takes the form of *provisional* strategies constantly updated by accounting for the state of the available knowledge and its inherent limitations. The adopted epistemological interpretation has allowed to grasp the powerful cognitive opportunities intrinsically related to uncertainty, and has resulted in a classification of uncertainty in engineering design. Possible approaches to modeling uncertainty have also been identified within the context of Generalized Information Theory, in which also probability theory finds its place as the least complex and the most established theory to handle uncertainty.

The exposition allows to contextualize the methods for computational design under uncertainty and outline some of their key features related to:

1. the assumptions underlying the design problem formulation and solution;
2. the existence of additional metrics to extend the current practice of design under probabilistic uncertainty;
3. the accuracy of the uncertainty methods in use, in a system approach that aims at ensuring that the methods are efficient enough to be readily applied in the industrial practice.

With the aim of developing the research in such direction, the state of the art regarding the methods and practices for design optimization under probabilistic uncertainty is reviewed in the next chapter.

Chapter 3

Literature review

3.1 Introduction

This Chapter reviews the state of the art within the area of engineering design optimization affected by probabilistic uncertainties. Section 3.2 identifies the common structure underlying the main current approaches to the problem. Its building blocks such as objectives formulations (Section 3.3), moment propagation methods (Section 3.4) and constraints formulations (Section 3.5) are then analyzed in detail. Finally, Sections 3.6 and 3.7 present some approaches to using optimization methods and surrogate models with particular pertinence to the problem of design under uncertainty.

3.2 Design optimization under uncertainty

Let's assume that the design analyses are performed by functions $f(\mathbf{x}, \mathbf{p})$ and $g_i(\mathbf{x}, \mathbf{p})$, $i = 1, 2, \ldots I$, where $\mathbf{x} \in \mathrm{R}^n$ is the vector of design variables and $\mathbf{p}$ is a vector of parameters. The deterministic design optimization problem is hence formulated as follows:

$$
\begin{aligned}
&\text{Find } \mathbf{x} \in \mathbb{R}^n \text{ to minimize } f(\mathbf{x}, \mathbf{p}), \\
&\text{subject to: } g_i(\mathbf{x}, \mathbf{p}) \leqslant 0, i = 1, 2, \ldots, I, \\
&\text{ and: } \mathbf{x}_L \leqslant \mathbf{x} \leqslant \mathbf{x}_U.
\end{aligned}
\tag{3.1}
$$

The identification and quantification of uncertainties affecting the input variables and/or parameters by means of probabilistic models renders Problem (3.1) stochastic. The resulting *design optimization problem under uncertainty* can be written, generically enough, as follows:

$$\begin{aligned} &\text{Find } \mu_{\mathbf{x}} \in \mathbb{R}^n \text{ to minimize } F\left[f(\mathbf{x}, \mathbf{p})\right], \\ &\text{subject to: } P(g_i(\mathbf{x}, \mathbf{p}) \leqslant 0) \geqslant P_{0_i},\ i = 1, 2, \ldots, I, \\ &\text{ and: } P(\mathbf{x}_L \leqslant \mu_{\mathbf{x}} \leqslant \mathbf{x}_U) \geqslant P_{\mathbf{x}}, \end{aligned} \tag{3.2}$$

where:

- $\mathbf{x}$ and $\mathbf{p}$ are now random variables; $\mathbf{x}$ has mean $\mu_{\mathbf{x}}$;
- F is a suitable function of the deterministic objective and the uncertain variables;
- P_{0i} and $P_{\mathbf{x}}$ are the desired probability of satisfying the ith constraint and the input bounds, respectively.

The specific formulation of objectives and constraints is key to classifying the approaches to engineering design optimization into two main branches, Robust Design Optimization (RDO) [159] and Reliability-based Design Optimization (RDBO) [1, 171]. The origins of RDO can be traced back to Taguchi [165, 200], whose fundamental intuition was to understand that *quality*, interpreted as a minimization of the statistical variation of performance, has to be designed into the product, and not sought after only during the production phase. His methodology, termed Robust Design, was based on direct experimentation. It was later extended to simulation-based design, and gradually improved to exploit nonlinear constrained optimization techniques [159]. RBDO originated from quality control requirements [184], but evolved through a completely different path. As can be seen in Figure 3.1, the difference between the two approaches concerns primarily the considered design scenario [91]:

- RDO tries to minimize the sensitivity of the optimum with respect to everyday fluctuations degrading the performance of the designed system;
- RDBO is instead concerned with rare events, which have to be limited by a suitable probability of occurrence since they lead to system failure.

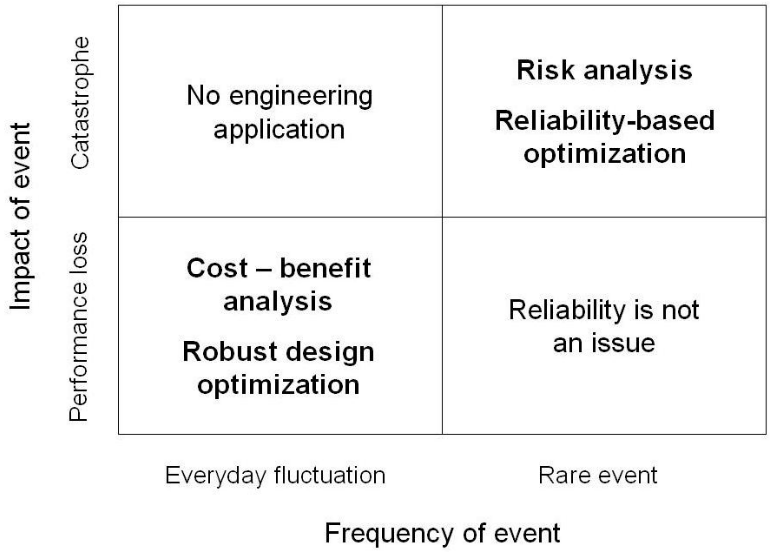


Figure 3.1: Approaches for design under uncertainty [91].

Such considerations result in algorithmic differences in the implementation of the two methods that will be highlighted in the following sections. However, both strategies can be thought of as made up of three main parts [101]:

1. identifying, qualifying and quantifying the sources of uncertainty associated with the design input and the analysis modules;

2. propagating the uncertainty through the analysis system, to obtain adequate metrics modeling the non-deterministic behavior of the objective functions and constraints;

3. optimization of such metrics by means of an appropriate algorithm.

The quantification of input uncertainties is usually performed upstream of the design optimization process. It builds on the identification of sources of uncertainty affecting the system under study, and makes use of one or more non-deterministic mathematical theories presented in Section 2.4.2. The mathematical model is chosen to match as close as possible the uncertain knowledge about the design under study, which is either based on sufficiently significant statistical data or relies on expert opinion, or a combination of both. It is well known that a correct quantification of the input uncertainty is paramount for the success of the optimization results. However, an extensive analysis of the subject falls beyond the scope of this review. We refer the reader to [5, 105] for an introduction on experts selection, elicitation and opinion aggregation, and to [85] for a review of the available methods to deal with the issue when the uncertainty is described by crisp stochastic models.

The next subsections will hence focus on points two and three of the list above. For simplicity of notation, $\mathbf{x}$ will indicate the vector of random variables.

3.3 Objectives formulations

The objective function F in Problem (3.2) depends, in general, on the probability density function (PDF) of the deterministic objective p_f induced by the multivariate distribution $p_{\mathbf{x}}$. In RDO, this dependence is usually expressed in terms of the expectation and variance of the deterministic objective, and thus $F = F(\mu_f, \sigma_f^2)$. In this setting, the optimization of the expectation over the input distributions guarantees on-target design performance, while variance minimization reduces the sensitivity of the solution to undesired change in the input variables. In the literature, the interplay of performance and robustness has been commonly aggregated in a single response function by using loss or utility functions [146]. A notable example are Box and Jones' squared loss functions [21] and their derivatives, such as [121]:

- Nominal-the-best (NTB) type:

$$F = w_1 \left(\frac{\mu_f - f_{target}}{\mu_{f_0} - f_{target}} \right)^2 + w_2 \left(\frac{\sigma_f}{\sigma_{f0}} \right)^2 ; \tag{3.3}$$

- Smaller-the-better (STB) type:

$$F = w_1 \mathrm{sign}(\mu_f) \left(\frac{\mu_f}{\mu_{f_0}} \right)^2 + w_2 \left(\frac{\sigma_f}{\sigma_{f0}} \right)^2 ; \tag{3.4}$$

- Larger-the-better (LTB) type:

$$F = w_1 \mathrm{sign}(\mu_f) \left(\frac{\mu_{f0}}{\mu_f} \right)^2 + w_2 \left(\frac{\sigma_f}{\sigma_{f0}} \right)^2 , \tag{3.5}$$

where μ_{f_0} and f_{target} are the mean at the starting point and the target nominal value respectively, and w_1 and w_2 are suitable weights to be decided by the designer. Similar approaches in terms of mean and standard deviation can be found in literature [159]. For example, in the STB case we would obtain:

$$F = \mu_f + k_f \sigma_f, \tag{3.6}$$

where $k_f = \frac{w_2 \mu_{f0}}{w_1 \sigma_{f0} \mathrm{sign}(\mu_{f0})}$. Analogous expressions could be found for the LTB and the NTB cases. In fact, the use of the weights highlights that the two statistical moments are thought of as representing two conflicting objectives. A better approach to the problem might hence require the deployment of a multi-objective optimization strategy to handle the robust counterpart of a single objective deterministic optimization problem [30, 41]. Several approaches have been developed to adequately accommodate this issue, ranging from the weighted sum method to physical programming [32, 94, 140, 159]. Alternatively, one among expectation and variance can be optimized, and the other constrained [45, 142]. When the considered deterministic problem is multi-objective, multiple system performance metrics have to be traded-off. A more complex robust design strategy may then be required to adequately account for objectives correlation structure [146].

3.4 Moment propagation methods

If all variables are continuous, the mean and variance of $f(\mathbf{x})$ are given by:

$$\mu_f = E\left[f(\mathbf{x})\right] = \int_{-\infty}^{+\infty} f(\mathbf{x}) p_{\mathbf{x}}(\mathbf{x}) d\mathbf{x}, \tag{3.7}$$

$$\sigma_f^2 = E\left[(f(\mathbf{x}) - \mu_f)^2\right] = \int_{-\infty}^{+\infty} [f(\mathbf{x}) - \mu_f]^2 p_{\mathbf{x}}(\mathbf{x}) d\mathbf{x}, \tag{3.8}$$

in which $p_{\mathbf{x}}$ is the joint probability distribution function corresponding to the input variables. Unfortunately, a closed-form expression for these integrals exists for few cases of practical interest. Their numerical approximation involves a fundamental trade-off between computational cost and accuracy of the estimated statistical moments. Existing approaches to performing such a task, also termed *uncertainty propagation*, include Monte Carlo simulation (MCS) methods, Taylor-based method of moments (MM), Gaussian quadrature (GQ) techniques and Stochastic Expansion (SE). Such methods are reviewed in the following subsections.

3.4.1 Monte Carlo methods

Several techniques, collected here under the name of Monte Carlo simulation (MCS) methods, originate from the stochastic interpretation of the integrals in Eqs. (3.7) and (3.8). Probability distributions over the outputs of a process induced by the probability distribution over the inputs are obtained by performing m repetitions of the process, each of which corresponds to a sampling point $\mathbf{x}_i$ drawn from the input space. For the simplest case, that of random sampling, unbiased estimators for the integrals in Eq. (3.7) and Eq. (3.8) are given by the following formulas:

$$\mu_{f_{\text{MCS}}} = \frac{1}{m} \sum_{i=1}^{m} f(\mathbf{x}_i); \tag{3.9}$$

$$\sigma^2_{f_{\text{MCS}}} = \frac{1}{m-1} \sum_{i=1}^{m} \left[f(\mathbf{x}_i) - \mu_{f_{\text{MCS}}} \right]^2 . \tag{3.10}$$

Both $\mu_{f_{\text{MCS}}}$ and $\sigma^2_{f_{\text{MCS}}}$ converge to their expected value with an error which is $\mathcal{O}(m^{-\frac{1}{2}})$, and thus the number of required runs depends on the desired relative accuracy for the output distribution, but is independent of the number of inputs n. Variance reduction techniques [76] such as control variates, antithetic variables, importance, stratified, Latin Hypercube [82] and descriptive sampling [202] have been developed to achieve faster convergence for MCS methods. An improved rate of convergence can be obtained, for problems with low to medium dimensionality, also by using the so called quasi-Monte Carlo methods, which substitute computer generated pseudo-random numbers with low-discrepancy sequences [25]. MCS methods are a simple and robust solution for multidimensional integration. However, the number of function evaluations required suggests to adopt, if possible, alternative methods for design optimization applications, particularly in the case of computationally demanding analysis codes. Finally, the RDO problem formulated by using MCS estimates is not deterministic and requires appropriate algorithms able to handle noisy functions.

3.4.2 Taylor - based moment propagation

When the system response is differentiable a sufficient number of times with respect to the uncertain variables $\mathbf{x}$, its statistical moments can be calculated through a Taylor series expansion around the mean of the input variables. This is also called method of moments (MM), and classified following the level of approximation and the number of moments considered. By averaging the Taylor series expansion truncated to the fourth order:

$$
\begin{aligned}
y = f(\mu_{\mathbf{x}}) + \sum_{p=1}^{n} \left(\frac{\partial f}{\partial x_p}\right) dx_p + \frac{1}{2} \sum_{p=1}^{n}\sum_{q=1}^{n} \left(\frac{\partial^2 f}{\partial x_p \partial x_q}\right) dx_p dx_q + \\
+ \frac{1}{6} \sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n} \left(\frac{\partial^3 f}{\partial x_p \partial x_q \partial x_r}\right) dx_p dx_q dx_r + \\
+ \frac{1}{24} \sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n} \left(\frac{\partial^4 f}{\partial x_p \partial x_q \partial x_r \partial x_s}\right) dx_p dx_q dx_r dx_s + \mathcal{O}(d\mathbf{x}^5),
\end{aligned}
\tag{3.11}
$$

the following expressions are obtained for mean and variance for the case of independent input variables:

$$
\begin{aligned}
\mu_{f_{\text{MM}}} = \overbrace{f(\mu_{\mathbf{x}})}^{M_1} + \overbrace{\frac{1}{2} \sum_{p=1}^{n} \left(\frac{\partial^2 f}{\partial x_p^2}\right) \sigma_{x_p}^2}^{M_2} + \overbrace{\frac{1}{6} \sum_{p=1}^{n} \left(\frac{\partial^3 f}{\partial x_p^3}\right) \gamma_p \sigma_{x_p}^3}^{M_3} + \\
+ \overbrace{\frac{1}{24} \sum_{p=1}^{n} \left(\frac{\partial^4 f}{\partial x_p^4}\right) \Gamma_p \sigma_{x_p}^4}^{M_4} + \overbrace{\frac{1}{8} \sum_{p=1}^{n} \sum_{\substack{q=1 \\ q \neq p}}^{n} \left(\frac{\partial^4 f}{\partial x_p^2 \partial x_q^2}\right) \sigma_{x_p}^2 \sigma_{x_q}^2}^{M_5} \; + \; \mathcal{O}(\sigma_x^5),
\end{aligned}
\tag{3.12}
$$

$$
\begin{aligned}
\sigma_{f_{\text{MM}}}^2 = \overbrace{\sum_{p=1}^{n} \left(\frac{\partial f}{\partial x_p}\right)^2 \sigma_{x_p}^2}^{V_1} + \overbrace{\sum_{p=1}^{n} \left(\frac{\partial^2 f}{\partial x_p^2}\right) \left(\frac{\partial f}{\partial x_p}\right) \gamma_p \sigma_{x_p}^3}^{V_2} + \\
+ \overbrace{\sum_{p=1}^{n} \sum_{\substack{q=1 \\ q \neq p}}^{n} \left(\frac{\partial^3 f}{\partial x_p^2 \partial x_q}\right) \left(\frac{\partial f}{\partial x_q}\right) \sigma_{x_p}^2 \sigma_{x_q}^2}^{V_3} + \overbrace{\frac{1}{2} \sum_{p=1}^{n} \sum_{\substack{q=1 \\ q \neq p}}^{n} \left(\frac{\partial^2 f}{\partial x_p \partial x_q}\right)^2 \sigma_{x_p}^2 \sigma_{x_q}^2}^{V_4} + \\
+ \overbrace{\frac{1}{3} \sum_{p=1}^{n} \left(\frac{\partial^3 f}{\partial x_p^3}\right) \left(\frac{\partial f}{\partial x_p}\right) \Gamma_p \sigma_{x_p}^4}^{V_5} + \overbrace{\frac{1}{4} \sum_{p=1}^{n} \left(\frac{\partial^2 f}{\partial x_p^2}\right)^2 (\Gamma_p - 1) \sigma_{x_p}^4}^{V_6} + \; \mathcal{O}(\sigma_x^5),
\end{aligned}
\tag{3.13}
$$

where the skewness γ_p and the kurtosis Γ_p for the pth variable x_p are defined as follows:

$$
\gamma_p = \frac{E(x_p - \mu_{\mathbf{x}})^3}{\sigma_{\mathbf{x}}^3}; \tag{3.14}
$$

$$\Gamma_p = \frac{E(x_p - \mu_{\mathbf{x}})^4}{\sigma_{\mathbf{x}}^4}. \tag{3.15}$$

First order MM is often used in literature (see for example [51, 125, 160, 169]). However, even for reduced spread of the input variables, the accuracy of the method may be severely spoiled by non-linearities in the system response. A natural improvement of those methods would be to consider higher order Taylor series expansions, for example retaining second order terms [71, 125]. However, while those terms guarantee a better accuracy with respect to linearization in the case of the mean approximation (by considering the term M_2 in Eq. (3.12)), this is not always true for variance approximation. Let's look at Eq. (3.13), considering the case of symmetric input variables, for which the term V_2 is zero. A variance estimate of order σ_x^4, which improves the accuracy of linearization, can be obtained only by retaining, together with the terms V_4 and V_6, the terms V_3 and V_5. However, this would imply the calculation of the third derivatives contained in V_3 and V_5.

The principal advantage of this method is a great computational efficiency, in a degree that depends on the available methods for calculating derivatives. In particular, it profits from the spread of advanced techniques, such as Automatic Differentiation (AD) [11, 72, 73, 198], which allows to obtain exact derivatives of the function of interest, up to machine accuracy, at a low cost, or the Complex Variable Method (CVM) [136].

3.4.3 Gaussian quadrature

Gaussian quadrature (GQ) formulas give the approximation of the integral of a function $f(\mathbf{x})$ on a domain $D \subseteq \mathbb{R}^n$ by a properly weighted sum of particular values $f(\mathbf{x}_i)$, $i = 1, ...N$, where the $\mathbf{x}_i$ are N suitably selected points in D, also called nodes. For the case of scalar x, such formulas require the fewest evaluations to obtain a given degree of accuracy, and are largely used in practice. The straightforward approach to multivariate integration is called a product rule, which consists in applying such formulas to each of the n dimensions of D. More precisely, assume that $D = D_1 \times D_2 \times \ldots \times D_n$, where $\times$ denotes the Cartesian product, and $D_i \subseteq \mathbb{R}$, for $i = 1 \ldots n$. If we apply the same one dimensional integration rule with N nodes and given weights W_i to each D_i, the integrals in

Eqs. (3.7) and (3.8) can be approximated as follows:

$$\mu_{f_{\mathrm{GQ}}} = \sum_{i1}^{N} W_{i1} \left(\sum_{i2}^{N} W_{i2} \left(\ldots \sum_{in}^{N} W_{in} f(\mathbf{x}_{i1,i2,\ldots,in}) \right) \right); \tag{3.16}$$

$$\sigma^2_{f_{\mathrm{GQ}}} = \sum_{i1}^{N} W_{i1} \left(\sum_{i2}^{N} W_{i2} \left(\ldots \sum_{in}^{N} W_{in} \left[f(\mathbf{x}_{i1,i2,\ldots,in}) - \mu_{f_{\mathrm{GQ}}} \right]^2 \right) \right). \tag{3.17}$$

Three nodes formulas (N=3) are usually adopted to obtain a sufficient accuracy. The arrays of uncertain variables in Eqs. (3.16) and (3.17) are distributed at the vertices of a hypergrid of dimension 3^n. The vector associated with $i1 = i2 = \ldots = in = 2$ corresponds to the mean of the input variables $\mu_{\mathbf{x}}$. Denoting suitable scalars by h^+ and h^-, the states with one or more subscript ip equal to 1 have the corresponding components perturbed by $h^- \sigma_{x_{ip}}$ with respect to their mean, whereas the states with one or more subscript ip equal to 3 have the corresponding components perturbed by $h^+ \sigma_{x_{ip}}$. Three values for weights W_i and the values for h^+ and h^- then have to be determined.

In the field of statistical tolerance design, for the case of independent Gaussian variables, Taguchi [199] proposed a solution for which equal weights $W_i = \frac{1}{3}$, and $h^+ = -h^- = h_{\mathrm{GQ}} = \frac{\sqrt{3}}{2}$ were used. D'Errico and Zaino [47] modified this approach suggesting the adoption of $h_{\mathrm{GQ}} = \sqrt{3}$ and distinctive weights $W_i = \{\frac{1}{6}, \frac{2}{3}, \frac{1}{6}\}$. Seo and Kwak [187] generalized this approach to consider non-Gaussian distributions. However, methods adopting full factorial designs, despite attaining an accuracy of $\mathcal{O}(\sigma_x^6)$, have limited applications in computational robust design [89], since the number of function evaluations required is $N = 3^n$. Evans [60] proposed an improved integration technique for which the approximated mean and variance can be obtained from the weighted sum of $2n^2 + 1$ function evaluations, corresponding to suitable sampling points in the input space. Evans shown as well that the error of his formula is $\mathcal{O}(\sigma_x^5)$ in the general case, and $\mathcal{O}(\sigma_x^6)$ in the case where all the input distributions are symmetric. Other techniques based on the same idea were developed in Control Theory and go under the name of Sigma-Point methods [33, 98, 149, 155]. They require $2n + 1$ function evaluations and have an accuracy of $\mathcal{O}(\sigma_x^3)$ in the general case, and $\mathcal{O}(\sigma_x^4)$ in the case where all the input distributions are symmetric. A general framework for reduced order quadrature formulas is provided by the recently introduced Generalized Dimension-Reduction method [217], which we may think of as embracing both Evans method and SP-methods as bivariate and univariate formulas, respectively. In particular, the univariate method [172] had a certain resonance in recent literature [90, 121–123, 219].

3.4.4 Stochastic expansion

Polynomial chaos expansion (PCE) [67] and stochastic collocation (SC) [137] are two related techniques which expand f in series of random variables - hence the name of stochastic expansion (SE). Given such expansion, the required moments can be calculated analytically.

PCE and SC were originally developed to solve stochastic partial differential equations. Here the focus is on the so-called non-intrusive versions of these methods, which consider the deterministic function f as a black-box.

Supposing that f is square integrable, its PCE can be written as:

$$f = a_0 H_0 + \sum_{i1=1}^{\infty} a_{i1} H_1(u_{i1}) + \sum_{i1=1}^{\infty}\sum_{i2=1}^{i1} a_{i1,i2} H_2(u_{i1}, u_{i1}) + \\ + \sum_{i1=1}^{\infty}\sum_{i2=1}^{i1}\sum_{i3=1}^{i2} a_{i1,i2,i3} H_3(u_{i1}, u_{i2}, u_{i3}) + ... \quad (3.18)$$

where $\mathbf{u}$ is a vector of standard normal variables (which can be derived from $\mathbf{x}$ by resorting to a transformation, see 3.5.3), H_q is a qth order multidimensional Hermite Polynomial and the a_i are suitable coefficients. The expansion can also be performed as function of other kinds of random variables (also of mixed type), if other suitable polynomials belonging to the Askey scheme are chosen instead of the Hermite polynomials [216]. For example, Legendre, Jacobi and Laguerre polynomials correspond to uniform, beta and exponential distribution, respectively. If we truncate the expansion at the order N_t, we can adopt the following shortened notation:

$$f \approx \sum_{q=0}^{N_t} b_q \chi_q(\mathbf{u}), \quad (3.19)$$

where b_q corresponds to $a_{i1,i2,...in}$ and χ_q to $H_n(u_{i1}, u_{i2}, ..., u_{in})$. There are several ways to obtain the coefficients b_q. For example, by projecting the response f against the basis function χ_q, the so called spectral projection can be performed:

$$b_q = \frac{E\left[f\chi_q(\mathbf{u})\right]}{E\left[\chi_q^2(\mathbf{u})\right]}, \tag{3.20}$$

where the denominator can be calculated analytically, and the numerator by any quadrature technique, including the ones mentioned in this review, such as MCS and Gaussian quadrature. The coefficients can also be found by linear regression (also known as point collocation or stochastic response surface) over the vector of responses $\mathbf{f}$, which is obtained as result of a design of experiments:

$$\boldsymbol{\chi}_q \mathbf{b} = \mathbf{f}. \tag{3.21}$$

In a similar way to PCE, SC writes f as:

$$f \approx \sum_{q=0}^{N_t} L_q(\mathbf{x}) f(\mathbf{x}_q); \tag{3.22}$$

where $L_q(\mathbf{x})$ derives from the application of the tensor-product rule [55] to the single dimensional Lagrange interpolation polynomial, given by the following expression:

$$L_q(x) = \prod_{\substack{p=1 \\ p \neq q}}^{N} \frac{x - x_p}{x_q - x_p}. \tag{3.23}$$

The optimal choice of the $\mathbf{x}_q$ are the so-called Gauss points, i.e. the roots of the orthogonal polynomial belonging to the Askey scheme. The major difference between PCE and SC is hence that PCE has to find the coefficients b_q given that a polynomial basis is known, whereas SC gets the coefficients from functional values corresponding to the Gauss points and has to find an interpolant polynomial [55]. It is found in practice that, if the same set of collocation points is considered, SC can require less function evaluations than PCE in achieving the desired accuracy. However, SC is less flexible than PCE, which can evaluate the function of interest on other points than the Gauss points alone, thus increasing simulation fault tolerance [55]. The interest in SE methods for design applications is quite recent [57, 123, 131]. However, when only the first moments are of interest, there is no clear advantage in employing SE instead of Gaussian quadrature techniques [123].

3.5 Constraint formulations

In Problem (3.1), the constraints $g_i(\mathbf{x})$ identify crisp boundaries for the feasible region. In contrast, a probabilistic definition of feasibility is required when dealing with engineering design under aleatory uncertainty. Given the distinction made between RDO and RBDO, it is then clear that the latter requires a more accurate estimation of events located on the tail of the probability distribution of the output function of interest, compared to RDO, which seeks a less critical 'feasibility robustness'. In general, a probabilistic feasibility formulation can be expressed as follows:

$$P[g_i(\mathbf{x}) \leqslant 0] \geqslant P_{0i},\ i = 1, \dots I. \tag{3.24}$$

If the joint probability distribution of $\mathbf{x}$ is known, the probability of feasibility in Eq. (3.24) is given by the following integral:

$$P[g_i(\mathbf{x}) \leqslant 0] = \Psi(\mathbf{x}) = \int_{g_i(\mathbf{x})\leqslant 0} p_{\mathbf{x}}(\mathbf{x}) d\mathbf{x}, \tag{3.25}$$

where $\Psi(\mathbf{x})$ is the cumulative distribution function (CDF) for the constraint satisfaction determined by $\mathbf{x}$; it is important to stress that in general $\Psi(\mathbf{x}) \neq \Phi(\mathbf{x})$, where $\Phi(\mathbf{x})$ is the CDF for the normal distribution. The calculation of the integral in Eq. (3.25) is obtained in an approximate fashion for most cases of interest. The method adopted for such an approximation affects both the accuracy and the computational cost of the overall optimization. For this reason, some relevant techniques which can be applied to estimate feasibility robustness are reviewed in the following subsections.

3.5.1 Monte Carlo approach

As for the integrals defining the moments, stochastic quadrature can be employed to estimate the integral in Eq. (3.25). In the case of random sampling, this is done by using the following formula:

$$P[g_i(\mathbf{x}) \leqslant 0] \approx \hat{P} = \frac{1}{m} \sum_{j=1}^{m} I\left[g_i(\mathbf{x}_j)\right], \tag{3.26}$$

where I is the indicator function, which takes value 1 in the feasible zone, and 0 otherwise. However, to obtain a suitable confidence level for demanding constraint satisfaction targets a large number of samples would be required, even by using variance reduction techniques.

3.5.2 Moment-based formulation

Assuming $g_i(\mathbf{x})$ to be normally distributed, Eq. (3.24) can be written as [160]:

$$\mu_{g_i} + k\sigma_{g_i} \leqslant 0, \tag{3.27}$$

where $k = \Phi^{-1}(P_{0i})$. μ_{g_i} and σ_{g_i} are usually estimated by method of moments. Moment-based constraint-handling strategies can only give approximate results when the output function is not normally distributed. Such Normal distribution is theoretically achieved if the number of random input variables is large. However, as mentioned in the previous section, in such a case other estimation strategies such as MCS would be adopted. More often, the choice of the moment-based formulation can be justified when the inputs are normally distributed and the considered functions are linear or approximatively linear, since any linear function of a normally distributed random variable is also normally distributed. Such an approach is often adopted in robust design literature [159,174,201] since the estimation of the first moment of the constraints is less computationally demanding than the calculation of the CDF, but is deemed unacceptable for accuracy and the probability levels usually required by reliability-based design, where it is known under the name of Mean Value (MV) approach [54].

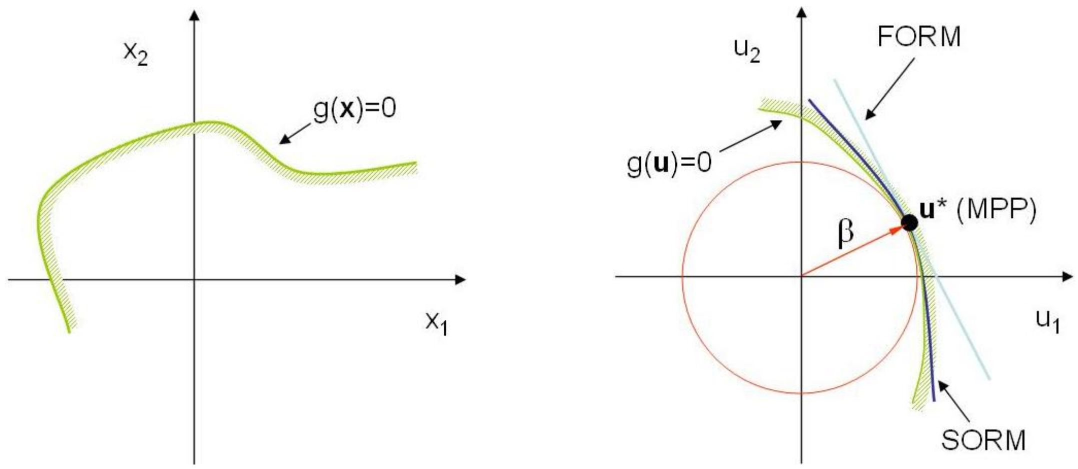
3.5.3 Reliability-based approaches

We collect under this definition a number of approaches that have been developed to perform reliability calculations efficiently, by coupling nonlinear optimization methods and integration techniques. It is usually considered convenient to simplify the study (although this is not always the case [54]) to first transform the input variables $\mathbf{x}$ into standard, uncorrelated normal variables $\mathbf{u}$, via the Rosenblatt or the Nataf transformation [49,179]. Hence the constraints take the form $g_i(\mathbf{u}) \leqslant 0$. If the limit state function $g_i(\mathbf{u})$ is affine in the transformed space, i.e.

$g_i(\mathbf{u}) = \mathbf{r}^T\mathbf{u} + q$, then the exact solution of Eq. (3.25) is:

$$P[g_i(\mathbf{x}) \leqslant 0] = \Phi(\frac{q}{\parallel \mathbf{r} \parallel}). \tag{3.28}$$

This can be understood from basic geometric considerations in the case of 2 variables (Fig. 3.2).



(a) Limit state in the original design space.

(b) After the transformation, **u** space.

Figure 3.2: FORM and SORM formulations for a bidimensional design space [1].

In the transformed space, the circumference with radius $\beta = \frac{q}{\|\mathbf{r}\|}$ defines the points with probability $\Phi(\beta)$. Since the limit state function is affine, then also $\Psi(\mathbf{x}) = \Phi(\mathbf{x})$, and hence the result in Eq. (3.28). If $g_i(\mathbf{u}) \approx \mathbf{r}^T\mathbf{u} + q$ with $q = -\mathbf{r}^T\mathbf{u}^*$, where $\mathbf{u}^*$ is the solution of the following optimization problem:

$$\begin{gathered} \min \parallel \mathbf{u} \parallel \\ \text{subject to } g_i(\mathbf{u}) = 0, \end{gathered} \tag{3.29}$$

then Eq. (3.28) gives the estimate for the first order reliability method (FORM) of the probability of failure. The solution point $\mathbf{u}^*$ is the so called most probable point (MPP) (of constraint activation). A variety of algorithms can be adopted to linearize the constraint while searching for the MPP, encompassing the Advanced Mean Value (AMV) and the iterative AMV (known as AMV$^+$) [54, 218]. An alternative to FORM is the second order reliability method (SORM), which calculates Eq. (3.25) via a quadratic approximation of the limit state function at the MPP, by using the following formula:

$$P[g_i(\mathbf{x}) \leqslant 0] = 1 - \phi(-\beta) \prod_{i=1}^{n-1} \left(1 - \frac{\phi(\beta)}{\Phi(-\beta)} k_i\right)^{-1/2},$$

where k_i are the principal curvatures of $g_i(\mathbf{u})$, taken positive for convex limit states. The integration phase can also be performed by coupling the MPP search with variance reduction techniques such as importance sampling [50] or control variables [7], which succeeds in speeding up MCS reliability calculation. Problem (3.29) specifies the limit state and seeks the corresponding reliability index β, for which it is also known as Reliability Index Approach (RIA). RIA yields a singularity if the design has zero failure probability [1]. To overcome this difficulty, the Perfomance Measure Approach (PMA) can be adopted [1]. PMA consists of an inverse reliability strategy which seeks the maximal constraint value within a certain probability of satisfaction. Mathematically, it is formulated as follows:

$$\begin{aligned} &\max g_i(\mathbf{u}), \\ &\text{subject to } \ \| \mathbf{u} \| \leqslant \beta_{reqd}. \end{aligned} \tag{3.30}$$

The RIA and the PMA problems, for which several optimization algorithms are available, ranging from specialized algorithms such as the Hasofer-Lind Rackwitz-Fissler [75] to standard sequential quadratic programming, yield the same result if the constraint g_i is active at the optimum. However, in the general case, RIA yields a more conservative solution and is less computationally effective [1].

Local MPP-search based methods rely on the assumption of monotonicity of the constraint function over the interval spanned, with a specific probability, by the input distributions [215]. In case the function is not monotonic, and the constraint function crosses the limit state multiple times [102], the equation linking the reliability constraint to the safety factor β_{reqd} is not guaranteed to be true:

$$P_{0i} \lesseqgtr \Phi(\beta_{reqd}).$$

In such case, the efforts have to be focused on finding the global MPP, and the resulting accuracy has to be checked, for example by using MCS approaches.

Reliability-based constraints have been already considered in a unified approach together with robust objectives (see for example [50] and [145]). The computational cost of such a strategy is clearly increased with respect to the moment matching formulation, and the achievable improvement is not usually considered worth the effort required, in applications for which reliability is not an issue.

3.5.4 VaR and CVaR

Value at Risk (VaR) is a concept developed in financial engineering [95] to quantify the risk of a monetary loss. $\mathrm{VaR}_{1-P_{0i}}(g_i(\mathbf{x}))$ is given by the smallest $g_i(\mathbf{x})$ which is exceeded with probability not larger than $1 - P_{0i}$. VaR is hence the $P_{0i}-$quantile of $g_i(\mathbf{x})$, and constraining VaR is equivalent to applying a PMA reliability approach. Given the similarity of the two concepts, some of the recent developments in the financial engineering field which have stemmed from recognizing the limitations of the VaR approach - such as the fact that it pays no attention to what happens once the VaR is exceeded [37] - could be relevant for engineering design under uncertainty. The metrics of risk developed in the financial sector as an alternative to VaR include the conditional value at risk (CVaR) and related metrics such as Mean Expected Loss, Mean Shortfall, Tail VaR and Tail conditional expectation. CVaR is defined as follows:

$$\mathrm{CVaR}_{1-P_{0i}}(g_i) = E\left[g_i | g_i \geq \mathrm{VaR}_{1-P_{0i}}(g_i)\right] = \frac{1}{1-P_{0i}} \int_{\Omega} g_i(\mathbf{x}) p_{\mathbf{x}}(\mathbf{x}) d\mathbf{x}, \quad (3.31)$$

where $\Omega = \{\mathbf{x} : g_i(\mathbf{x}) \geqslant \mathrm{VaR}_{1-P_{0i}}(g_i(\mathbf{x}))\}$. Thus CVaR represent the expectation of the constraint function $g_i(\mathbf{x})$ once VaR is exceeded, and is never smaller than VaR, i.e. $\mathrm{CVaR}_{1-P_{0i}} \geqslant \mathrm{VaR}_{1-P_{0i}}$. Instead of finding VaR and then solving the integral in Eq. (3.31), CVaR can be found by minimizing a suitable function $F_{1-P_{0i}}(\mathbf{x}, \nu)$ with respect to the auxiliary variable ν:

$$\mathrm{CVaR}_{1-P_{0i}}\left(g_i(\mathbf{x})\right) = \min_{\nu} F_{1-P_{0i}}\left(g_i(\mathbf{x}), \nu\right), \quad (3.32)$$

where $F_{1-P_{0i}}$ is defined as follows:

$$F_{1-P_{0i}}(g_i(\mathbf{x}), \nu) = \nu + \frac{1}{1-P_{0i}} \int [g_i(\mathbf{x}) - \nu]^+ p_{\mathbf{x}}(\mathbf{x}) d\mathbf{x}, \quad (3.33)$$

where $[t]^+ = t$ when $t > 0$ and $[t]^+ = 0$ when $t \leqslant 0$.

Since $F_{1-P_{0i}}(g_i(\mathbf{x}), \nu) \geqslant \mathrm{CVaR}_{1-P_{0i}}(g_i(\mathbf{x}))$ for any $\mathbf{x}$, $F_{1-P_{0i}}(\mathbf{x}, \nu)$ can be constrained instead of $\mathrm{CVaR}_{1-P_{0i}}(g_i(\mathbf{x}))$ by imposing:

$$F_{1-P_{0i}}(g_i(\mathbf{x}), \nu) \leqslant \mathrm{CVaR}_{reqd}. \tag{3.34}$$

If such a constraint is active, then $\nu = \mathrm{VaR}_{1-P_{0i}}(g_i(\mathbf{x}))$. It is worth underlying that conditional expectation is not well defined when conditioning on probability zero events [167]. Hence CVaR approach would not give a meaningful result in cases of designs with zero probability of failure, just as the RIA approach.

CVaR and the related metrics have not received significant attention in the field of design under uncertainty. Two main features have then to be investigated to assess their suitability for probabilistic design. The first one is related with the engineering meaning of such metrics, whereas the second one regards the availability of more efficient algorithms for the case of continuous variables than the sampling-based strategy presented above.

3.6 Optimization methods for design under uncertainty

In this section the principal algorithmic approaches for optimization under uncertainty are reviewed. Following Giunta *et al.* [68], it is useful to draw a distinction between the considered methods and the field of stochastic programming [17]. The latter, which has also been applied to engineering problems [14,183], usually relies on a specific mathematical structure of the problem, such as linearity of objective and constraint functions. The double-edged implications of such reliance are that identifying such structure constitutes a significant effort in the stochastic programming strategy, but is fundamental to guarantee polynomial runtime. We will favour here optimization strategies which can be applied to generic non-linear constrained problems, with the additional burden of including aleatory variables and parameters. Such uncertain elements are translated into the objectives and constraints with one or more of the strategies presented in Sections 3.4 and 3.5. The choice of a particular propagation method impacts on the selection of a suitable optimization strategy because of the mathematical properties induced on the objectives and constraints. If f is deterministic, non-deterministic objectives and constraints are obtained, for example, by using a randomized propagation approach. Hence optimization strategies developed to handle noisy functions are the option of choice, such as:

- Evolutionary algorithms (EA) [8, 100], including Genetic algorithms, Genetic programming, Evolutionary programming, Evolution strategies and Simulated annealing. They are characterized by a stochastic search of the optimal solution, which is driven by specific kinds of evolutionary strategies;

- Stochastic approximation (SA) algorithms originated from the work of Robbins and Monro [176]. Further evolutions of the strategy include the adoption of quasi-gradients [58] or simultaneous stochastic perturbation [181];

- Generating Set Search methods (GSS) [111], including Pattern Search methods [127]: they are a class of direct search methods which rely on crypto-gradient information, obtained through patterns of points sampled in the input space.

On the other hand, Gaussian quadrature, stochastic expansion (if no randomization is involved in the obtention of the coefficients) or Taylor-based method of moments would supply noise-free robust objectives and constraints, which could be handled by classical gradient-based deterministic optimization methods [64]. If applicable, such methods might be preferred over the direct search methods because of their better convergence properties. The impact of the chosen propagation method on the adoption of a specific optimization strategy is summarized in Figure 3.3. A generic theoretical comparison of such search methods is not

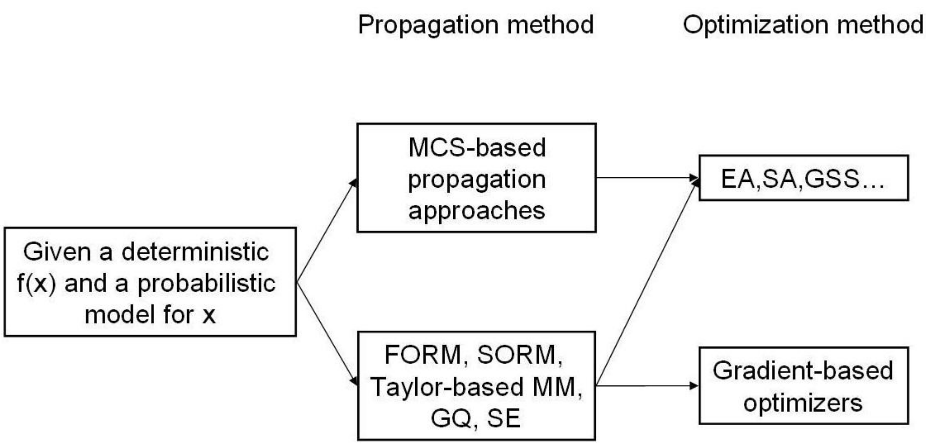


Figure 3.3: Impact of the propagation method on the optimization strategy.

possible, as known from the “No Free Lunch” theorems [212]: if all possible problems are considered, the expected performance of any pair of optimization algorithms over the space of all possible problems is identical. The choice of a specific algorithm is hence intrinsically problem dependent. Noisiness of objectives and constraints may be one of the basic criteria for such choice. Other criteria may involve the capability of obtaining accurate and possibly cheap gradients, some available knowledge about the functions under study, or the possibility to exploit the working principle of the adopted propagation technique.

3.7 Using surrogate models

Surrogate models, also known as metamodels, are used to approximate the response of simulation models over the entire design space, or over specific regions within such domain. They come useful in engineering design when the original models or the simulation and optimization procedures evaluating them are computationally expensive.

There are many surrogate modeling techniques available for engineering design optimization [191, 192]. Such richness stems from the combination of four related aspects of the problem, for which more than one variant strategy could be applied:

1. the choice of points in the design space where the original function is evaluated [69];
2. the particular model to be adopted, such as polynomial, splines, radial-basis function, etc.;
3. the fitting strategy, such as least-squares regression, maximum likelihood estimation etc.;
4. global or local approach: the surrogate can be created before the optimization, and cover the entire design space, or during the optimization, by approximating local regions.

When polynomial models (usually linear or quadratic) are adopted, the surrogate models are also known as Response Surface Model (RSM). Other popular metamodels include Kriging and Radial Basis Functions [170]. Various approaches are possible for the use of surrogate models in optimization under uncertainty: at the uncertainty quantification level, at the optimization level, or at both [56]. However, there are problematic aspects specifically related to the application of metamodels for optimization under uncertainty:

1. the significant computational time required in some case to build or update the surrogate model may offset the appealing feature of working with a model that is cheap to evaluate;
2. the higher the dimension of the input space is, the more function evaluations are required to build a satisfactory model. Such undesirable feature is worsened in case of optimization under uncertainty, since uncertainty analyses require the integration of the original deterministic function over the entire range of the uncertain variables. This implies a large number of runs for a surrogate model to be validated for RDO or RBDO [3]. In fact, it has been noted [69] that undersampled surrogates might have lower estimation accuracy than equally expensive direct sampling techniques. This issue might be partially accounted for by resorting to Bayesian approaches [3, 16, 116];
3. if optimization under uncertainty is to be performed on the surrogate models, MCS strategies, called sometimes Decoupled MCS [178], can be readily used, with the disadvantage of adding sampling error to the approximation error; on the other hand, since the formulation of the model is analytic, it is possible to obtain the analytic formulation for the integrals of interest [31].

3.8 Summary and conclusions

This chapter has been devoted to the review of the state of the art regarding engineering design optimization in the presence of probabilistic uncertainty. The review has concerned the available problem formulations, the numerical methods to achieve a probabilistic description of objectives and constraints, together with the possible options to perform their optimization. It has been shown that these three aspects are interrelated and ultimately imply, given the problem at hand, a trade-off between the achievable accuracy and the effectiveness of the solution.

In particular, MCS approaches are a simple and robust propagation option. In principle, they can estimate the moments required by the design problem formulation with an arbitrary accuracy, by using a sufficient number of samples m. Such number does not depend on the dimension of the input space n, but is usually large for the accuracy typically required by the applications of interest here. This implies that, at the conceptual stage, where a small to moderate number of uncertain variables are considered, quadrature based methods, stochastic expansions and Taylor-based method of moments are more efficient than MCS. Amongst them, first-order Taylor-based method of moments is the cheapest available option, and is largely used for this reason. However, relying on objectives' and constraints' linearization might lead to poorly accurate moments estimates.

The contrast between the randomized and non-randomized approach to uncertainty propagation is exacerbated when it comes to estimating the probability of feasibility. For a small probability of unfeasibility, MCS becomes very expensive, and usually more efficient techniques, which we have grouped under the name of reliability-based approaches, could be deployed. In the least expensive way, the probability of feasibility might be described as function of the constraint moments, as commonly done in RDO, under the hypothesis that the constraint distribution is normal. However, the poor accuracy of the estimates and the questionable normality assumption may render this option unreliable.

Hence identified are three gaps in the current knowledge which need to be addressed:

1. the lack of accurate methods which can be efficiently applied in robust optimization at the conceptual stage without incurring the additional issues related with surrogate models;

2. the shortage of intermediate options between accurate but expensive formulations of the probabilistic constraints and cheap but potentially unreliable moment based formulations;

3. the assessment of metrics such as the tail conditional expectation, which may contribute, in analogy to recent developments in the financial engineering field, to extend the set of available robustness metrics.

The next chapter builds upon such considerations to propose an enhancement to the currently adopted design optimization strategies under uncertainty.

Chapter 4

Methodology

4.1 Introduction

In the previous chapter, Robust Design Optimization (RDO) was presented as a numerical strategy to cope with some of the challenges deriving from the uncertain nature of engineering design. With the aim of overcoming some of its current limitations, we propose in the present chapter an enhanced RDO methodology.

First of all, the problem is formulated in order to relax, when required, the assumption of normality of objectives and constraints, which often underlies RDO. Such formulation, presented in Section 4.2, extends the validity of robust design and does not impact on its cost, since objectives and constraints are still formulated by means of their first two moments. Furthermore, taking into account engineering considerations concerning the risk of design unfeasibility, suitable estimates of tail conditional expectations are introduced in the set of robustness metrics; they are also expressed in terms of the first two moments of the function constraints.

A novel uncertainty propagation technique, introduced in Section 4.3, is proposed to estimate the above mentioned moments. The aim is to achieve a favorable trade-off between the accuracy of the estimates and the required computational cost. This is done by employing a novel reduced quadrature method, which can handle a fairly generic class of input distributions having known and finite first four moments, also in presence of correlation. By means of mathematical analyses and simple numerical examples it is demonstrated that the proposed approach improves the accuracy of the estimation with respect to methods of comparable computational cost.

In addition, peculiar features of the propagation phase and the problem formulation are exploited to intimately couple the propagation and the optimization phases. As shown in Section 4.4, this is achieved for two classes of algorithms, namely gradient-based methods and the derivative-free pattern search methods. In the first case, we propose a way of estimating the propagation error, with respect to third order Taylor-based method of moments, at each step of the optimization. In the second case, we show how first order information gathered by the propagation phase can be exploited as a heuristic to increases the efficiency of the pattern search. We also analyze the possible advantages achievable when the two types of algorithms are hybridized.

4.2 Problem formulation

The objective of this section is to identify a strong case for the adoption of a moment-based problem formulation. Consider, as an example, an instance of the weighted sum smaller-the-better (STB) problem, as presented in Section 3.3 (an analogous reasoning can be applied to the other two cases):

$$\begin{aligned}
&\text{Find } \mu_{\mathbf{x}} \in \mathbb{R}^n \text{ to minimize } F = \mu_{\mathbf{f}} + k_f \sigma_{\mathbf{f}} \\
&\text{subject to: } G_i = \mu_{g_i} + k_{g_i}\sigma_{g_i} \leqslant 0, i = 1, 2, \ldots, I, \\
&\text{ and: } \mathbf{x}_L + k_{\mathbf{x}}\sigma_{\mathbf{x}} \leqslant \mu_{\mathbf{x}} \leqslant \mathbf{x}_U - k_{\mathbf{x}}\sigma_{\mathbf{x}}.
\end{aligned} \tag{4.1}$$

The key to our approach lies in the formulation of the coefficients k_f, k_{g_i}, $k_{\mathbf{x}}$, which departs from the assumption - which is fairly common in design optimization - that the distributions of objectives, constraints and input variables are normal.

While this might be true in the case of the input variables, since the distributions may be chosen to be normal, or transformed into standard normal variables (e.g. via the Rosenblatt transformation [49, 179]), the same cannot be said about the objectives and constraints, since the underlying functions are not known a priori. In fact, the assumption of normality can be supported in two ways [160]:

- if $\mathbf{x}$ is normally distributed and the output function can be assumed to be approximately linear in $\mathbf{x}$, then the output function is approximately normal;

- if the dimension of $\mathbf{x}$ is large, regardless of the distribution of $\mathbf{x}$, the output function distribution tends to normality, under the central limit theorem.

In many applications of interest, however, these conditions do not apply. Hence the normality assumption might be unjustified, and negatively impact on the result of the optimization. If the distributional assumptions are completely removed, however, the knowledge of the first two moments of the output probability distribution functions p_f and p_{g_i} would provide only a loose probability bound, which is given, for the generic function y, by the Chebyshev inequality [168]:

$$P(|y(\mathbf{x}) - \mu_y|) \geqslant k\sigma_y) \leqslant \frac{1}{k^2}, \tag{4.2}$$

where k is a real number, $\mu_y < \infty$ and $\sigma_y \neq 0$ are mean and standard deviation of y. A one-sided version of this inequality, also known as Cantelli inequality, is given by the following formula:

$$P(y(\mathbf{x}) - \mu_y \geqslant k\sigma_y) \leqslant \frac{1}{1+k^2}. \tag{4.3}$$

Such probability bound might be too conservative to be of practical use for design optimization. For example, the probability of satisfying a single constraint, imposed by shrinking the design space through a factor $k = 2$ would be just $1 - \frac{1}{1+k^2} = 0.8$, versus the value of 0.977 given by the normal assumption.

Our aim is to find an intermediate approach which relaxes the normality assumption on the output distributions and can still supply meaningful bounds for the moment problem. For such purpose, we consider some known mathematical results in the following subsection.

4.2.1 Probability bounds under distributional assumptions

We may start by restricting Eq. (4.2) to symmetric distributions. We would then improve the bound given by Eq. (4.3) as follows [166]:

$$P(y(\mathbf{x}) - \mu_y \geqslant k\sigma_y) \leqslant \begin{cases} \frac{1}{2k^2}, & \text{if } k \geq 1; \\ \frac{1}{2}, & \text{if } k \leq 1. \end{cases} \tag{4.4}$$

A second possible assumption is related to unimodality, which denotes distributions characterized by a CDF which is convex until the mode, and concave thereafter. We are then considering a broader class of output distribution which includes, beside the normal, other common distributions such as the triangular, Student, chi-squared, and uniform distribution. The Gauss inequality is useful in this direction. It holds for symmetric unimodal distributions and is given by the following formulas [186]:

$$P(|y(\mathbf{x}) - \mu_y| \geqslant k\sigma_y) \leqslant \begin{cases} \frac{4}{9k^2}, & \text{if } k \geq \sqrt{\frac{4}{3}}; \\ 1 - \frac{k}{\sqrt{3}}, & \text{if } k \leq \sqrt{\frac{4}{3}}. \end{cases} \tag{4.5}$$

A one-sided version of this inequality can be expressed as follows [166]:

$$P(y(\mathbf{x}) - \mu_y \geqslant k\sigma_y) \leqslant \begin{cases} \frac{2}{9k^2}, & \text{if } k \geq \frac{2}{3}; \\ \frac{1}{2}, & \text{if } k \leq \frac{2}{3}. \end{cases} \tag{4.6}$$

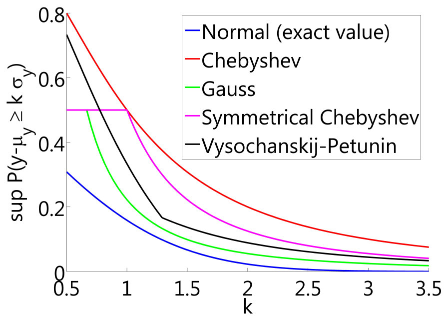
Gauss inequality has been generalized by Vysochanskij and Petunin to the case of asymmetric unimodal variables [168]:

$$P(|y(\mathbf{x}) - \mu_y| \geqslant k\sigma_y) \leqslant \begin{cases} \frac{4}{9k^2}, & \text{if } k \geq \sqrt{\frac{8}{3}}; \\ \frac{4}{3k^2} - \frac{1}{3}, & \text{if } k \leq \sqrt{\frac{8}{3}}. \end{cases} \tag{4.7}$$

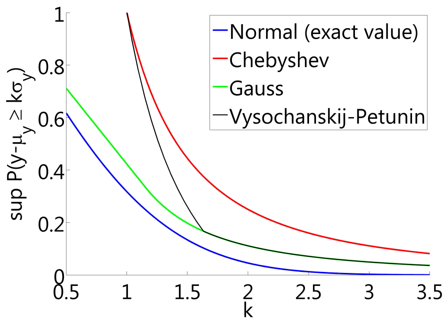
The one-sided Vysochanskij-Petunin inequality is given instead by the following relationship [210]:

$$P(y(\mathbf{x}) - \mu_y \geqslant k\sigma_y) \leqslant \begin{cases} \frac{4}{9(1+k^2)}, & \text{if } k \geq \sqrt{\frac{5}{3}}; \\ 1 - \frac{4}{3}\frac{k^2}{1+k^2}, & \text{if } k \leq \sqrt{\frac{5}{3}}. \end{cases} \tag{4.8}$$

The impact of the different distributional assumptions can be appreciated in Figure 4.1, in which the probability bounds for the three cases above are shown, together with the exact value given by the normal distribution. From Figure 4.1(b), note that the two tailed Vysochanskij-Petunin bounds coincide with the Gauss bounds for $k \geq \sqrt{\frac{8}{3}}$, despite relaxing the symmetric assumption, and with Chebyshev bounds for $k \leq 1$, for which both results are not usable. Furthermore, we see in Figure 4.1(a) that for $k > \sqrt{\frac{3}{5}}$ the assumption of symmetry is less informative, in terms of probability of satisfaction, compared with the unimodality assumption. The situation is reversed for $k < \sqrt{\frac{3}{5}}$. In the range commonly used



(a) One tailed.



(b) Two tailed.

Figure 4.1: The effect of k on the probability bounds.

in conceptual design, i.e. for k roughly between 1.5 and 3, we now have at our disposal several theoretical tools that can be used to ground the formulation of objectives and constraints.

4.2.2 Objectives and constraints formulation

The probability bounds presented in the previous section translate into the constraint formulation as follows: chosen the relevant constraint assumption for the constraint g_i, for which one of the inequalities above holds, and identified the corresponding required probability of satisfaction P_{0i}, we can write:

$$P(g_i(\mathbf{x}) \geqslant \mu_{g_i} + k_{g_i}\sigma_{g_i}) \leqslant 1 - P_{0i}, \tag{4.9}$$

where the coefficient k_{g_i} is chosen so that $1 - P_{0i}$ equals the right hand side of relevant inequality among those in Eqs. (4.3),(4.4),(4.6) and (4.8) (the relationships $k_{g_i} = k_{g_i}(P_{0i})$ for the various distributional assumptions are summarized in Table 4.1). Hence by formulating the robust constraint as

$$G_i = \mu_{g_i} + k_{g_i}\sigma_{g_i} \leq 0, \tag{4.10}$$

we impose, as required, that:

$$P(g_i(\mathbf{x}) \leqslant 0) \geqslant P_{0i} \iff g_{i,P_{0i}} \leq 0, \tag{4.11}$$

where $g_{i,P_{0i}}$ is the P_{0i}−quantile of $g_i(\mathbf{x})$, defined for continuous random variables as the value such that $P(g_i(\mathbf{x}) \leqslant g_{i,P_{0i}}) = P_{0i}$.

The objective formulation is also affected by such assumptions. Though seldom interpreted in this way, the minimization of a weighted sum $\mu_f + k_f\sigma_f$ corresponds to searching the smallest threshold which is exceeded by f with a probability not greater than the given probability $1 - P_{0f}$, which depends on k_f through the relevant equation among those shown in Table 4.1. For example, suppose that

	Distributional assumption	$k_{g_i}(P_{0i})$	**Validity**
I	None	$k_{g_i} = \sqrt{\frac{P_{0i}}{1-P_{0i}}}$	$0 \leq P_{0i} \leq 1$
II	Symmetry	$k_{g_i} = \frac{1}{\sqrt{2(1-P_{0i})}}$	$P_{0i} \geq \frac{1}{2}$
III	Unimodality	$k_{g_i} = \sqrt{\frac{9P_{0i}-5}{9(1-P_{0i})}}$	$P_{0i} \geq \frac{5}{6}$
		$k_{g_i} = \sqrt{\frac{3P_{0i}}{(3P_{0i}-2)}}$	$P_{0i} \leq \frac{5}{6}$
IV	Symmetry + unimodality	$k_{g_i} = \sqrt{\frac{2}{9(1-P_{0i})}}$	$P_{0i} \geq \frac{1}{2}$

Table 4.1: Coefficient k_{g_i} as function of the probability of feasibility.

the underlying (unknown) distribution of f is a $\Gamma(2, 2)$ distribution as shown in Figure 4.2. If we assume that such distribution is unimodal, to ensure that at least the 90% of the designs lie below the robust objective $F = \mu_f + k_f\sigma_f$ we would adopt from Table 4.1, case III, a value of $k_f = 1.856$. Hence by minimizing F, we minimize the worst case 0.9-quantile threshold for f, under a specified distributional assumption. This view allows to deal with the familiar mean and variance weighted sum as a justifiable single objective, without having to interpret it as the simplistic formulation of a multiobjective problem (for a detailed analysis of the difficulties that such formulation would involve, see [42]).

The problem, formulated as above, allows to increase the generality of robust design optimization by relaxing the assumptions on the output distributions. The fact that such assumptions are often implicit and overlooked is crucial to understand the importance of the reinterpretation of the RDO problem in terms of moments.

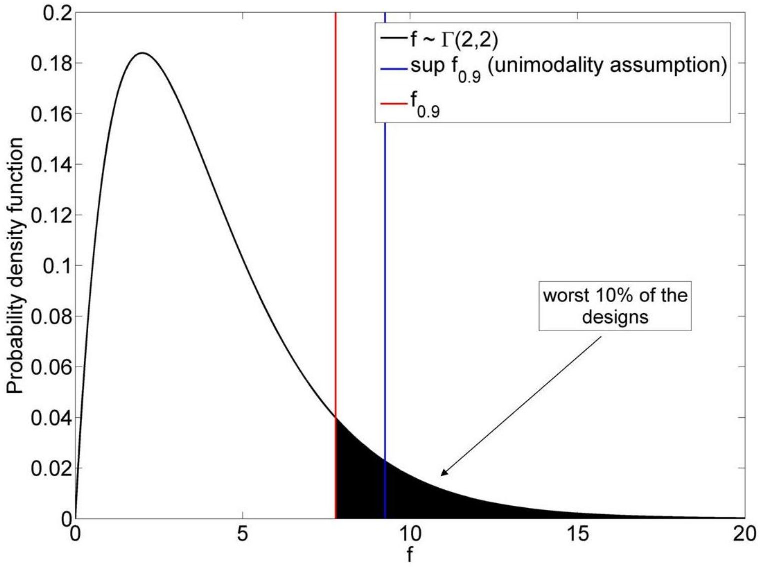


Figure 4.2: The robust objective as a worst-case threshold. The true 0.9-quantile of the underlying (unknown) distribution is shown in red, while its unimodal bound is in blue. The area in black identifies the worst 10% of the designs.

4.2.3 Extension to the tail conditional expectation

In this subsection we propose a possible extension of the RDO formulation, which is based on the idea that the criteria driving the robust optimization cannot overlook the behavior of the system response once the identified constraints' limits are exceeded.

This might be relevant, in particular, for conceptual robust designs for which unfeasibility probabilities of about 10% might be deemed acceptable. Assessing such designs in terms of a probability $1 - P_{i0}$ for which a prescribed limit $g_i = 0$ does not have to be violated, as in Eq. 4.11, may not enable the exercise of engineering judgment on a significant portion of the distribution tails. In fact, nothing is said about the extent of such constraint violation, and hence we are not able to discern designs which are on average closer to the bound from designs which lie further away.

A possible solution is the adoption of a metric such as the tail conditional expectation (TCE), which for continuous distributions is equivalent to the CVaR reviewed in Section 3.5.4. Such expectation, given a probability of constraint satisfaction P_{0i}, is defined as follows:

$$\mathrm{TCE}_{1-P_{0i}}(g_i) = E\left[g_i | g_i \geq g_{i,P_{0i}}\right] = \frac{1}{1-P_{0i}} \int_{\Omega} g_i(\mathbf{x}) p_X(\mathbf{x}) d\mathbf{x}, \tag{4.12}$$

where $\Omega = \{\mathbf{x} : g_i(\mathbf{x}) \geqslant g_{i,P_{0i}}\}$ is the unfeasible region. Hence TCE quantifies the expected functional value once the probabilistically defined feasible bounds are exceeded. For example, suppose that the true (but unknown in general) model for the random behavior of $g(\mathbf{x})$ is, in correspondence of a certain point $\mathbf{x}$ of the design space, a $\Gamma(2, 2)$ distribution, and that a probability of feasibility $P_0 = 0.92$ is of interest. As shown in Figure 4.3, while the quantile $g_{0.92}$ identifies the specific design which can occur with probability 0.08, $\mathrm{TCE}_{0.08}(g)$ takes into account all the designs in the worst 8% range, by calculating their expected value. This entails a number of consequences for engineering design. The most

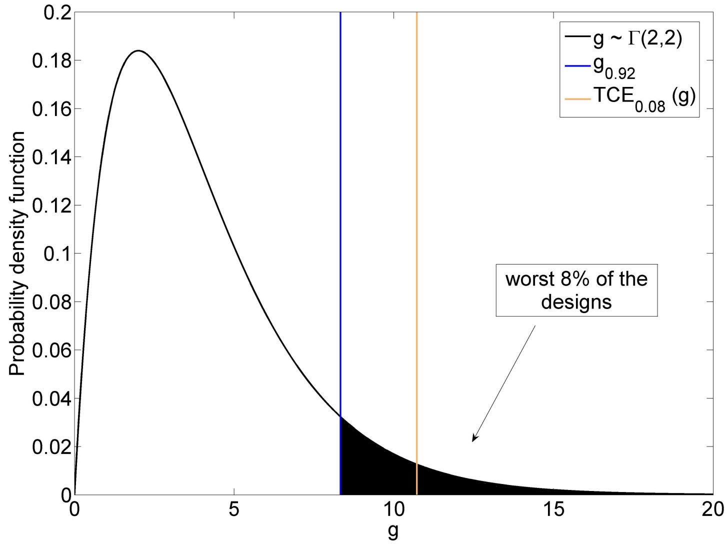


Figure 4.3: Comparison between TCE and quantile constraints.

important is probably the consideration that the conditional expectation couples an information about the possible losses deriving from exceeding the constraints with the probability of such an event to happen. It may then be interpreted as quantifying the risk [1] associated with getting into the unfeasible region or, in short, the risk of unfeasibility. Such quantification can be useful for establishing

[1]The concept of risk is closely related to the concept of uncertainty. Lipshitz and Strauss [130] collected a sample of definitions in the decision-making literature between 1960 and 1990, that shows how the two definitions have been often confused and misused. This is probably due to the large impact of the first formal distinction between risk and uncertainty, dating back to the work of Frank Knight [109], which defined unknown outcomes as risky if it is possible to

suitable margins on design feasibility. Alternatively, it can be interpreted within a probabilistic fail-safe perspective, which seeks to minimize the (expected) losses one would incur if the constraint are violated.

As we have seen, the quantile type of constraints are formulated by imposing a probability of satisfaction P_{i0} and a limit value $g_i = 0$. In the TCE case, instead, the designer has to specify a percentage $1-P_{i0}$ identifying the worst designs whose performance has to be monitored, and a threshold for $\mathrm{TCE}_{1-P_{i0}}(g_i)$, which is in general larger than $g_i = 0$. However, in a conservative option, $g_i = 0$ could be chosen for such a purpose.

Fortunately, TCE metrics can be included within our framework without weighing on the computational cost of the optimization. Under assumptions similar to the presented above,in fact, we can obtain tractable mathematical expressions for $\mathrm{TCE}_{1-P_{i0}}(g_i)$ in terms of the first two moments of g_i.

For the normal case, by truncating the distribution at $g_i = \mu_{g_i} + \Phi^{-1}(P_{0i})\sigma_{g_i}$ and taking the right tail expectation, we obtain the following exact result:

$$\mathrm{TCE}_{1-P_{0i}}(g_i) = \mu_{g_i} + \frac{\phi(\Phi^{-1}(P_{0i}))}{1-P_{0i}}\sigma_{g_i}, \tag{4.13}$$

where ϕ and Φ are, respectively, the density and cumulative density of the standard Gaussian variable. Expressions of the same form have been presented in [118] for elliptical distributions. However, it might be useful to retrieve a more general expression, which is an inequality of the Chebyshev type applied to the conditional expectation [27, 134, 166]:

$$\mathrm{TCE}_{1-P_{0i}}(g_i) \leq \mu_{g_i} + \sqrt{\frac{P_{0i}}{1-P_{0i}}}\sigma_{g_i}. \tag{4.14}$$

In the case where symmetry can be assumed for the output distribution, the

assign them probability distributions (based on observable frequencies), and uncertain if their probability distribution is not known. This distinction was abandoned in 1950's thanks to Savage's [185] concept of subjective probability and the corresponding theory of decision under uncertainty, for which the problem of assigning probability distributions becomes epistemic (i.e. associated with the agent's state of knowledge, see Appendix A) and no more ontological (it is not of interest to know wether or not those probabilities exist in the world). The concept of risk we agree upon is instead *the uncertainty regarding a negative event coupled with its impact* (i. e. on safety, on performance, etc.). Nasa PRA Guide [197] equals this definition to the question: "*What can go wrong? How likely is it? What are the consequences?*".

following formulation can be obtained for $\mathrm{TCE}_{1-P_{0i}}(g_i)$ [27]:

$$\mathrm{TCE}_{1-P_{0i}}(g_i) \leqslant \begin{cases} \mu_{g_i} + \frac{\sigma_{g_i}}{\sqrt{2(1-P_{0i})}}, \text{ if } P_{0i} \geq \frac{1}{2}; \\ \mu_{g_i} + \frac{\sigma_{g_i}}{(1-P_{0i})}\sqrt{\frac{P_{0i}}{2}}, \text{ if } P_{0i} \leq \frac{1}{2}. \end{cases} \tag{4.15}$$

An interesting property of the TCE bounds appears from considering the quantile constraint formulation presented in the previous section:

$$g_{i,P_{0i}} \leq \mu_{g_i} + k_{g_i}\sigma_{g_i} \leq 0. \tag{4.16}$$

When k_{g_i} is taken from the distributional assumptions I or II (for $P_{0i} > 1/2$) in Table 4.1, such inequality gives the same bounds of Eq. (4.14) and Eq. (4.15), respectively. Therefore, since $\mathrm{TCE}_{1-P_{0i}}(g_i) \geq g_{i,P_{0i}}$ by definition, the following inequalities hold:

$$g_{i,P_{0i}} \leq \mathrm{TCE}_{1-P_{0i}}(g_i) \leq \mu_{g_i} + k_{g_i}\sigma_{g_i} \leq 0. \tag{4.17}$$

This means that the TCE bound is tighter than the quantile bound, and in case no assumption can be made on the output distribution, or in case such distribution is assumed symmetric, we would be less conservative in substituting a quantile constraint with a TCE constraint. An example of this property can be shown by resorting again to the case shown in Figure 4.3. Hence suppose again that the underlying model for the random behavior of $g(\mathbf{x})$ is a $\Gamma(2,2)$ distribution, and that a probability of feasibility $P_0 = 0.92$ is of interest. The Chebyshev bounds for the 0.92-quantile $g_{0.92}$ and for the TCE, calculated by using Eq. (4.3) and Eq. (4.14), respectively, coincide and are approximately equal to 13.59. However, the true values for the quantile and the TCE, which could be obtained if distribution were known, are 8.33 and 10.72, respectively. This means that adopting the TCE bound to constrain $g(\mathbf{x})$ would result in a drastic reduction (45%) of the overconservativeness yielded by considering the corresponding quantile bound. It is important to stress that such improvement is achieved with no additional assumption nor further calculation. Instead, it is based on the reinterpretation of the feasibility bounds in terms of thresholds delimiting the average performance of a selected worst percentage of designs.

Note that the TCE formulation is not limited to the constraints g_i, but can be extended also to the objective f, in analogy with the reasoning in Section 4.2.2. In fact, it allows interpreting the weighted sum objective as a bound on the

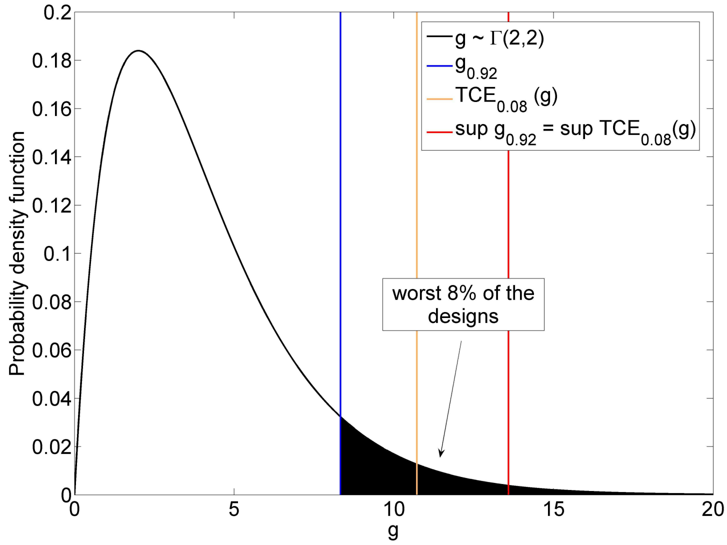


Figure 4.4: TCE bounds are tighter than quantile bounds in the Chebyshev (shown) and symmetric cases.

expectation over the worst selected percentage of designs.

The expressions presented in this section require the estimate of mean and variance to be as accurate as possible, through the phase of uncertainty propagation. A novel technique to accomplish such task is presented in the next section.

4.3 Proposed propagation method

The proposed propagation method is central to the RDO strategy presented in the thesis. It is based on a quadrature approach that we may term univariate reduced quadrature (URQ hereafter) to be consistent with the nomenclature introduced in [172]. Starting from the Sigma-Points methods [155] and Evans' statistical tolerancing method [60], with the aim of obtaining an univariate integration method for generic non-symmetric distributions, the following formulas to estimate mean and variance are obtained (see Appendix B):

$$\mu_f = W_0 f(\mu_{\mathbf{x}}) + \sum_{p=1}^{n} W_p \left[\frac{f(\mathbf{x}_{p+})}{h_p^+} - \frac{f(\mathbf{x}_{p-})}{h_p^-} \right]; \tag{4.18}$$

$$\sigma_f^2 = \sum_{p=1}^{n} \left\{ W_p^+ \left[\frac{f(\mathbf{x}_{p_+}) - f(\mu_\mathbf{x})}{h_p^+} \right]^2 + W_p^- \left[\frac{f(x_{p_-}) - f(\mu_\mathbf{x})}{h_p^-} \right]^2 + \right.$$
$$\left. + W_p^\pm \frac{\left[f(\mathbf{x}_{p_+}) - f(\mu_\mathbf{x})\right]\left[f(x_{p_-}) - f(\mu_\mathbf{x})\right]}{h_p^+ h_p^-} \right\}. \quad (4.19)$$

The sampling points are found as follows:

$$\mathbf{x}_{p_\pm} = \mu_\mathbf{x} + h_p^\pm \sigma_{\mathbf{x}_p} \mathbf{e}_p, \quad (4.20)$$

where $\mathbf{e}_p$ is the p^{th} vector of the identity matrix of size n and $h_p^\pm$ are given as follows:

$$h_p^\pm = \frac{\gamma_p}{2} \pm \sqrt{\Gamma_p - \frac{3\gamma_p^2}{4}}. \quad (4.21)$$

γ_p and Γ_p represent, respectively, skewness and kurtosis of the input distribution of the p^{th} variable, and are given by Eqs. (3.14) and (3.15). Following the inequality $\Gamma_p \geqslant \gamma_p^2 + 1$, due to Pearson [103, 163], which holds for any non-degenerate distribution with finite fourth moment, and noting that $\gamma_p^2 + 1 > \frac{3\gamma_p^2}{4}$, the inequality $\Gamma_p > \frac{3\gamma_p^2}{4}$ holds. Hence the quantities $h_p^\pm$ defined in Eq. (4.21) are always real numbers for our cases of interest (i.e. input distributions having finite first four moments). The weights have to be chosen as:

$W_0 = 1 + \sum_{p=1}^{n} \frac{1}{h_p^+ h_p^-}$;

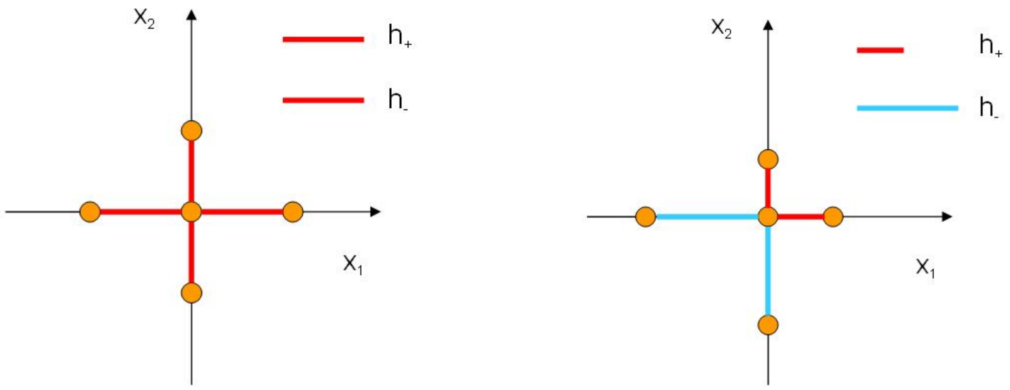
$W_p = \frac{1}{h_p^+ - h_p^-}$;

$W_p^+ = \frac{(h_p^+)^2 - h_p^+ h_p^- - 1}{(h_p^+ - h_p^-)^2}$;

$W_p^- = \frac{(h_p^-)^2 - h_p^+ h_p^- - 1}{(h_p^+ - h_p^-)^2}$;

$W_p^\pm = \frac{2}{(h_p^+ - h_p^-)^2}$.

In Figure 4.5 we show the effect of skewness on the selection of the nodes, for the bivariate case. The proposed method requires $2n + 1$ function evaluations, and is hence comparable to linearization, when the derivatives are obtained through finite differences.



(a) Symmetric bivariate distribution. (b) Left-skewed distributions.

Figure 4.5: Propagation stencil for symmetric and non-symmetric bivariate case with $\mu_{\mathbf{x}} = 0$, $\sigma_{\mathbf{x}} = 1$.

4.3.1 Error analysis for generic distributions

The accuracy of the adopted quadrature rule is guaranteed by matching the appropriate terms yielded by the Taylor approximation of the first two statistical moments. Expanding $f(\mathbf{x}_{\mathbf{p}\pm})$ in Eqs. (4.18) and (4.19), respectively, into fourth order Taylor series centered in $f(\mu_{\mathbf{x}})$, as in Eq. (3.11), and subtracting the results from Eqs. (3.12) and (3.13), the following expressions are obtained (see Appendix B for a complete demonstration):

$$\varepsilon_{\mu_y} = M_5 + \text{terms of order} > \sigma_x^4, \tag{4.22}$$

$$\varepsilon_{\sigma_y} = V_3 + V_4 + \text{terms of order} > \sigma_x^4. \tag{4.23}$$

These errors coincide with the ones obtained for one of Sigma-Points methods, the Divided Difference Filter [150], in the symmetric case [155], but are smaller in the general, non-symmetric case, since the such method cannot model the term $V_2 \propto \sigma_x^3$. Now compare it with I MM, which just considers the terms M_1 and V_1 for mean and variance estimate, respectively. The mean estimate is always more accurate for the proposed method with respect to I MM. The accuracy of the variance estimate is comparable with the one given by I MM in case of considering only symmetric distributions (with $\gamma_x = 0$) for functions showing non-negligible cross-interactions between input variables. In all the other cases, the variance estimate yielded by the presented method is more accurate than the linearization-based one. Our method matches the accuracy yielded by the Univariate Reduction Method, as presented in [122], and has a higher efficiency in the nonsymmetric case, since it requires $2n+1$ versus $3n$ function evaluations.

4.3.2 Requirements on input variables

The importance of a correct quantification of input uncertainties was introduced in Section 4.2. In principle, the more information that can be included into the input probabilistic model, the better, as long as it is deemed to be necessary and/or sufficient for the chosen design strategy, and can be handled by the adopted propagation technique. For example, a precise modeling of input distribution tails would be usually of secondary importance for robust design, which focuses on variations around the mean. Moreover, a popular propagation method such as first-order Taylor based method of moments would make no use of more information than the first two moments of input variables.

A key requirement of the presented propagation approach is that the first four moments are available for each uncertain variable. Typically, such knowledge can arise from three situations:

1. independent input variables: the input marginal distributions, each identifying weights and nodes for the quadrature rule, are known. The joint PDF is in this case given as the product of all the marginal PDFs;
2. dependence of input variables modeled through correlation: if the marginal distributions (which do not have to be identical) are known, it is always possible to transform the original set of variables to a new, uncorrelated set of variables, for example by means of the spectral decomposition [93], for which:

$$\Sigma_{xx} = VDV^{-1}, \tag{4.24}$$

where:

$$\Sigma_{xx} = \begin{bmatrix} \sigma_{x_1}^2 & \rho_{1,2}\sigma_{x_1}\sigma_{x_2} & \cdots & \rho_{1,n}\sigma_{x_1}\sigma_{x_n} \\ \rho_{1,2}\sigma_{x_1}\sigma_{x_2} & \sigma_{x_2}^2 & \cdots & \rho_{2,n}\sigma_{x_2}\sigma_{x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{n,1}\sigma_{x_n}\sigma_{x_1} & \rho_{n,2}\sigma_{x_n}\sigma_{x_2} & \cdots & \sigma_{x_n}^2 \end{bmatrix}$$

is the input covariance matrix, and $\rho_{i,j} = \frac{cov(x_i,x_i)}{\sigma_{x_i}\sigma_{x_j}}$ is the Pearson product-moment correlation coefficient;

V is the eigenvector matrix, giving the principal axis of the input distribution and hence the new coordinate system $\mathbf{x}'$;

D is the diagonal eigenvalue matrix, with each eigenvalue $\lambda_{ii} = \sigma^2_{x'_i}$.

The interesting feature of such decomposition is that it allows correlation to be included in a straightforward way into the propagation phase, by choosing the new points as:

$$\mathbf{x}_{p\pm} = \mu_{\mathbf{x}} + V\sqrt{D}h_p^{\pm}\mathbf{e}_p. \tag{4.25}$$

Geometrically, this corresponds to a rotation of the input variable sampling stencil, as shown in Figure 4.6, where the bivariate normal distribution is shown by means of the ellipsoids corresponding to unitary variance. The

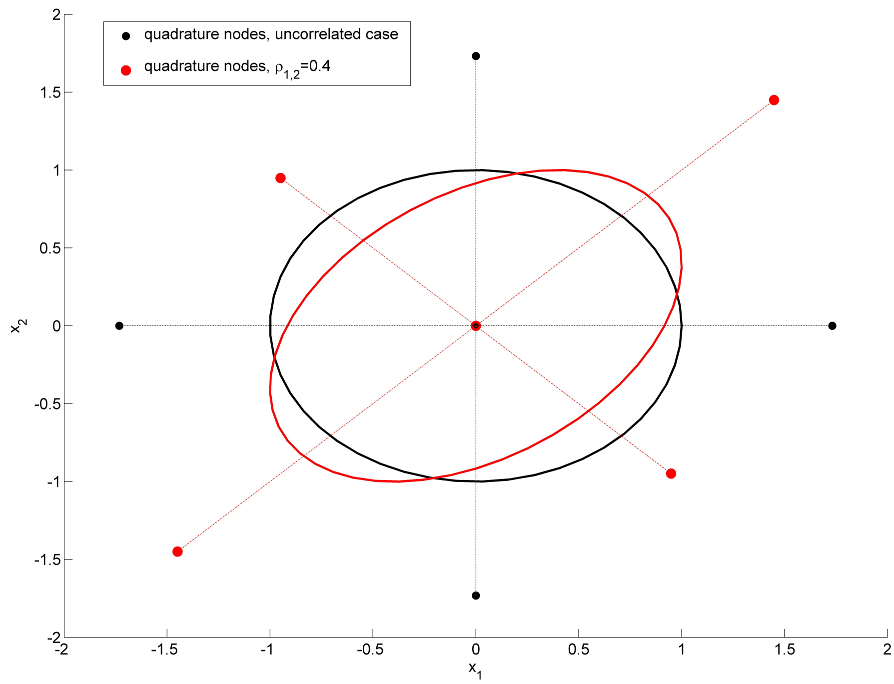


Figure 4.6: The effect of correlation ($\rho_{1,2} = 0.4$) on a standard bivariate normal distribution.

spectral decomposition, also known as Karhunen-Loève expansion, Principal component analysis, Proper orthogonal decomposition, or the Hotelling transform, can be applied to a larger class of distribution than the multivariate Gaussian distribution. In this particular case, the computationally cheaper Cholesky decomposition [93] may be adopted, which gives the covariance matrix as $\Sigma_{xx} = CC^T$, where C^T is a lower triangular matrix.

3. the joint distribution is known; this is quite rare, beyond the textbook case of multivariate normal distribution. Copulas [34, 147] could be adopted to model the dependence between the variables. We would then resort to a Rosenblatt transformation [49, 179] to reduce the input space to a standard Gaussian space, and then perform the propagation.

4.3.3 Analytical examples

The presented theoretical results can be demonstrated with some simple but meaningful analytical examples. With the aim of including non-linearities and interaction effects, and being able to visualize the results, the following test functions have been considered:

1. $f(\mathbf{x}) = \sin(x_1 - 0.21)\sin(x_2 - 0.21)$;
2. $f(\mathbf{x}) = 0.5x_1^2 - 1.5x_1 + 0.7x_2^2 - 1.2x_2 + 1$;
3. $f(\mathbf{x}) = x_1^2 - 0.5x_1 + 2x_2^2 - 0.5x_2 + 0.5x_1^2x_2 + 0.05x_1^2x_2^2 + 0.3$;
4. $f(\mathbf{x}) = 1.7x_1^3 + (1.3 + 0.4x_2)x_1^2 + (0.8 - 2x_2^2)x_1 + 0.1x_2 - 2.8x_2^2 - 0.5x_2^3$.

The results are presented by comparison with first, second and third order Taylor-based method of moments, as percentage errors calculated with respect to the solution of a Monte Carlo simulation with 10^6 samples. The mean of the input variables is fixed at $\mu_{\mathbf{x}} = (1, 1)$. The different estimation accuracies of the considered methods are stressed by gradually increasing the input standard deviation. Tables 4.2 and 4.3 show the results of mean and variance estimation corresponding to bivariate normal input variables, while Tables 4.4 and 4.5 reports the results for the case of uniform input distribution. Tables 4.6 and 4.7 deal instead with an instance of non-symmetric input variables, which have been modeled by triangular distributions with skewness $\gamma = 0.5$ and unitary mean. With regard to the mean estimation, URQ approximates the function behavior better than linearization, reducing the error for all the three cases by two orders

Case	$\sigma_{\mathbf{x}}$	**I MM**	**II MM** **III MM**	**URQ**
1	0.05	0.2499	-0.0007	-0.0005
	0.175	3.1108	-0.0469	-0.0228
	0.3	9.4277	-0.4208	-0.2012
2	0.05	0.6037	0.0000	0.0000
	0.175	7.9334	0.0000	0.0000
	0.3	27.5502	0.0000	0.0000
3	0.05	-0.3145	0.0003	0.00030
	0.175	-3.7290	-0.0048	-0.00480
	0.3	-10.2086	-0.0007	-0.00070
4	0.05	0.0449	0.0002	0.0002
	0.175	0.5505	-0.0002	-0.0002
	0.3	1.6431	0.0071	0.0071

Table 4.2: Uncertainty propagation results: mean estimation for Gaussian bivariate input distribution, expressed as percentage error with respect to the solution of a Monte Carlo simulation with 10^6 samples.

Case	$\sigma_{\mathbf{x}}$	**I MM**	**II MM**	**III MM**	**URQ**
1	0.05	0.0888	0.3391	-0.1614	-0.0361
	0.175	3.1590	6.3183	-0.0002	1.5938
	0.3	9.2925	19.1288	-0.5438	4.5048
2	0.05	-1.1411	0.1202	0.1202	0.1202
	0.175	-13.5546	-0.0438	-0.0438	-0.0438
	0.3	-31.1837	0.4244	0.4244	0.4244
3	0.05	0.0652	0.2207	0.2784	0.2054
	0.175	-2.7316	-0.8801	-0.1926	-1.0621
	0.3	-6.6947	-1.4752	0.4630	-1.9882
4	0.05	0.0988	0.2384	0.1689	0.0257
	0.175	-0.8573	0.8352	-0.0071	-1.7393
	0.3	-2.3703	2.5277	0.0901	-4.8851

Table 4.3: Uncertainty propagation results: variance estimation for Gaussian bivariate input distribution, expressed as percentage error with respect to the solution of a Monte Carlo simulation with 10^6 samples.

of magnitude. In the asymmetric case (Table 4.6), it is even better than II MM, which uses second order derivatives. This is due to the modeling of the term M_3 in Eq. 3.12, which includes third derivatives. In the symmetric cases, II MM and III MM coincide. With regard to the variance estimation, in the symmetric case

Case	$\sigma_{\mathbf{x}}$	**I MM**	**II MM III MM**	**URQ**
1	0.05	0.2424	-0.0082	-0.0080
	0.175	3.1117	-0.0461	-0.0316
	0.3	9.4596	-0.3918	-0.2595
2	0.05	0.6117	0.0080	0.0080
	0.175	7.9582	0.0233	0.0233
	0.3	27.5452	-0.0045	-0.0045
3	0.05	-0.3053	0.0095	0.0095
	0.175	-3.7606	-0.0377	-0.0377
	0.3	-10.1703	0.0419	0.0419
4	0.05	0.0419	-0.0028	-0.0028
	0.175	0.5474	-0.0033	-0.0033
	0.3	1.6140	-0.0215	-0.0215

Table 4.4: Uncertainty propagation results: mean estimation for uniform bivariate input distribution, expressed as percentage error with respect to the solution of a Monte Carlo simulation with 10^6 samples.

Case	$\sigma_{\mathbf{x}}$	**I MM**	**II MM**	**III MM**	**URQ**
1	0.05	0.3373	0.5128	0.1115	0.2370
	0.175	2.8366	5.0412	0.0022	1.5849
	0.3	8.3978	15.227	-0.3824	4.5684
2	0.05	-0.3640	0.1385	0.1385	0.1385
	0.175	-6.0386	-0.1644	-0.1644	-0.1644
	0.3	-15.6775	-0.1854	-0.1854	-0.1854
3	0.05	0.0806	0.1520	0.2098	0.1367
	0.175	-1.6569	-0.7976	-0.1025	-0.9816
	0.3	-4.4695	-2.0167	-0.0324	-2.5420
4	0.05	0.1363	0.2550	0.2288	0.0854
	0.175	-0.8628	0.5769	0.2586	-1.4778
	0.3	-3.4234	0.6986	-0.2128	-5.1706

Table 4.5: Uncertainty propagation results: variance estimation for uniform bivariate input distribution, expressed as percentage error with respect to the solution of a Monte Carlo simulation with 10^6 samples.

URQ has the same accuracy of linearization. Case 2 is an exception for which URQ performs better, since $f(\mathbf{x})$ does not have cross-derivative terms (V_3 and V_4 in Eq. 3.13). If such terms are present but negligible, the URQ estimates approach the results given by III MM. In such cases, the URQ is more accurate

Case	$\sigma_{\mathbf{x}}$	I MM	II MM	III MM	URQ
1	0.05	0.2498	-0.0007	0.0013	0.0015
	0.175	2.9153	-0.2364	-0.1445	-0.1259
	0.3	8.9753	-0.8324	-0.3421	-0.1769
2	0.05	0.5914	-0.0121	-0.0121	-0.0121
	0.175	7.8807	-0.0486	-0.0486	-0.0486
	0.3	27.6018	0.0398	0.0398	0.0398
3	0.05	-0.3252	-0.0105	-0.0105	-0.0105
	0.175	-3.8214	-0.1008	-0.1008	-0.1008
	0.3	-10.1094	0.1097	0.1097	0.1097
4	0.05	0.0460	0.0018	0.0015	0.0015
	0.175	0.5276	-0.0230	-0.0112	-0.0112
	0.3	1.5892	-0.0459	0.0142	0.0142

Table 4.6: Uncertainty propagation results: mean estimation for triangular (skewed) bivariate input distribution, expressed as percentage error with respect to the solution of a Monte Carlo simulation with 10^6 samples.

Case	$\sigma_{\mathbf{x}}$	I MM	II MM	III MM	URQ
1	0.05	-2.2014	0.4514	0.0113	0.1277
	0.175	-5.5858	5.1331	-0.0714	1.1410
	0.3	-5.6223	15.754	0.4650	3.5958
2	0.05	-2.2784	0.4476	0.4476	0.4476
	0.175	-14.6292	0.3777	0.3777	0.3777
	0.3	-30.4001	-0.1026	-0.1026	-0.1026
3	0.05	2.4408	-0.1453	-0.0862	-0.1610
	0.175	8.0689	-0.4081	0.3558	-0.6103
	0.3	11.3720	-1.7104	0.6031	-2.3227
4	0.05	-0.8087	0.1636	0.1162	-0.0268
	0.175	-3.9408	0.4391	-0.1232	-1.8457
	0.3	-7.3529	1.6809	0.0872	-4.8560

Table 4.7: Uncertainty propagation results: variance estimation for triangular (skewed) bivariate input distribution, expressed as percentage error with respect to the solution of a Monte Carlo simulation with 10^6 samples.

than II MM for variance estimation. The opposite would happen, however, for quadratic functions with significant interactions (see Section 3.4.2). In the asymmetric case, URQ has a better accuracy than linearization, by incorporating the term V_2 in Eq. 3.13. This can be seen from Table 4.6, in particular from case

3. Cases 1 and 4 show the same behavior for $\sigma_{\mathbf{x}} = 0.05$. When the input standard deviation increases, the effect of the interactions between variables becomes significant, which reduces the accuracy of URQ.

4.4 Integration with optimization methods

The proposed propagation gives deterministic estimates of μ_f, σ_f, μ_{g_i} and σ_{g_i}, which are then suitably combined to form the robust objectives and constraints. Despite its underlying probabilistic formulation, the problem is then deterministic and can be solved by any of the algorithms presented in Section 3.6. The working principle of the propagation method, however, make us prefer some specific algorithms, which are detailed in the following subsections.

4.4.1 Gradient-based optimization

When the function performing the system analysis is differentiable, the proposed propagation technique can be efficiently used in gradient-based optimization: since the robust objective is not built using derivatives, its gradient is obtained through a combination of the deterministic gradients calculated at the sampling points determined through Eq. (4.20). Mean and variance design sensitivities are then the following ones:

$$\frac{\partial \mu_f}{\partial \mu_{x_q}} = W_0 \frac{\partial f}{\partial x_q}\Big|_{\mu_{\mathbf{x}}} + W_p \sum_{p=1}^{n} \left(\frac{1}{h_p^+} \frac{\partial f}{\partial x_q}\Big|_{x_p^+} - \frac{1}{h_p^-} \frac{\partial f}{\partial x_q}\Big|_{x_p^-} \right), \tag{4.26}$$

$$\frac{\partial \sigma_f^2}{\partial \mu_{x_q}} = \sum_{p=1}^{n} \left(A_p \frac{\partial f}{\partial x_q}\Big|_{x_p^+} + B_p \frac{\partial f}{\partial x_q}\Big|_{x_p^-} - (A_p + B_p) \frac{\partial f}{\partial x_q}\Big|_{\mu_{\mathbf{x}}} \right), \tag{4.27}$$

where:

$$A_p = \tfrac{2W_p^+}{h_p^+} \left[f(x_p^+) - f(\mu_x) \right] + \tfrac{W_p^\pm}{h_p^+ h_p^-} \left[f(x_p^-) - f(\mu_x) \right];$$

$$B_p = \tfrac{2W_p^-}{h_p^-} \left[f(x_p^-) - f(\mu_x) \right] + \tfrac{W_p^\pm}{h_p^+ h_p^-} \left[f(x_p^+) - f(\mu_x) \right].$$

Requiring a single level of differentiation directly benefits gradient-based methods, the performance of which heavily depends on the accuracy of the supplied derivatives. To understand why, we consider three possible cases, depending on the adopted method for obtaining derivatives:

1. finite differences (FD): derivative accuracy, which suffers in this case from truncation and round-off error, may be significantly spoiled by a double level of differentiation, such as the one required for I MM [156]; this is worsened in quasi-Newton methods, for which the Hessian updates based on gradient evaluations might be corrupted because of such inaccuracies;

2. automatic differentiation (AD): currently the most computationally convenient adjoint differentiation is available just for gradient calculation; calculating the Hessian, as required to calculate the gradient of I MM objectives and constraints, would require the adoption of forward AD;

3. complex variable method (CVM): this method can obtain gradients with no round-off error; a second level of differentiation would reintroduce differences and hence round-off [117].

In any of those cases, there is no significant cost increase for each optimization step with respect to the case where I MM is used for the propagation phase. Considering a scalar function $y = f(\mathbf{x})$, in the most expensive case, when finite differences are used to obtain the derivatives, such cost is $\propto n^2$, and it reduces to $\propto n$ in the best case, in which adjoint techniques are used for the first level of differentiation.

In case terms V_3 and V_4 in Eq. 3.13 are negligible, for example when input variables have weak cross interactions, the URQ would have, at the same price of I MM (which uses just first order derivatives) the accuracy of the III MM (which includes second and third order derivatives). In the general case, however, it would be useful to estimate this error during the optimization, to keep under control the accuracy of the adopted propagation method.

In the context of gradient-based optimization, for the case in which the uncertain variables are a subset of the design variables, this can be achieved at no extra cost by using the derivatives calculated by the optimizer at each major optimization step. The missing terms are then calculated by finite differences of gradient values, which results in the following formulas:

$$V_3 \backsimeq \sum_{p=1}^{n} \sum_{\substack{q=1 \\ q\neq p}}^{n} \frac{\frac{\partial f}{\partial x_q}\big|_{\mathbf{x}_p^+} + \frac{\partial f}{\partial x_q}\big|_{\mathbf{x}_p^-} - 2\frac{\partial f}{\partial x_q}\big|_{\mu_{\mathbf{x}}}}{(h_p^+ - h_p^-)^2} \frac{\partial f}{\partial x_q}\Big|_{\mu_{\mathbf{x}}} \sigma_{x_q}^2, \tag{4.28}$$

$$V_4 \backsimeq \frac{1}{8} \sum_{p=1}^{n} \sum_{\substack{q=1 \\ q\neq p}}^{n} \left[\frac{\frac{\partial f}{\partial x_q}\big|_{\mathbf{x}_p^+} - \frac{\partial f}{\partial x_q}\big|_{\mathbf{x}_p^+}}{(h_p^+ - h_p^-)\sigma_{\mathbf{x}_p}} + \frac{\frac{\partial f}{\partial x_p}\big|_{\mathbf{x}_q^+} - \frac{\partial f}{\partial x_p}\big|_{\mathbf{x}_q^+}}{(h_q^+ - h_q^-)\sigma_{\mathbf{x}_q}} \right]^2 \sigma_{x_p}^2 \sigma_{x_q}^2. \tag{4.29}$$

Being able to estimate the accuracy of the propagation phase constitutes a significant enhancement with respect to current practices based on method of moments, for which the accuracy of probabilistic estimates is checked, if at all, only in correspondence to the optimal design point.

4.4.2 Pattern Search methods

Pattern Search (PS) methods are a class of derivative-free methods which may be deployed when accurate derivatives are either not available or too expensive to obtain. They provide a robust exploratory tool that can be coupled with more refined methods (such as Quasi-Newton methods), for which they can provide a good initial guess [204]. This aspect will be investigated in Section 4.4.3.

The central concept to the method is a set of vectors, the pattern P, which indicates the allowed exploration directions in the design space. Starting from the point $\mathbf{x}$, having defined a positive scalar parameter Δ_k with initial value Δ_0, the algorithm for unconstrained optimization (which also constitutes the core of the constrained optimization approach) is fully defined by the following loop, to be repeated until convergence:

1. find a step $\mathbf{s}_k$ using the possible moves defined by P_k and Δ_k (termed "exploratory moves" in [128]);
2. if $f(\mathbf{x}_k + \mathbf{s}_k) < f(\mathbf{x}_k)$, then $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$, otherwise $\mathbf{x}_{k+1} = \mathbf{x}_k$;
3. update Δ_k,P_k.

The exploratory moves are critical for the algorithm, together with the way the updates are performed. There are few rules that have to be maintained to guarantee the convergence of the algorithm, as demonstrated in [128]:

1. the step has to belong to the pattern: $\mathbf{s}_k \in \Delta_k P_k$;

2. any step satisfying $f(\mathbf{x}_k + \mathbf{s}_k) < f(\mathbf{x}_k)$ is acceptable;

3. the pattern must contain at least $n+1$ vectors, and a maximum of $2n$, to guarantee a direction of descent and prevent from premature convergence to a nonstationary point; a maximal positive basis (constituted by $2n$ vectors) must be adopted in the bound constrained case [126];

4. reduce the step if no step satisfies the simple decrease condition.

As noted in [20], the results on convergence allow for a great deal of flexibility in the choice of the exploratory heuristic, which defines the order in which the algorithm searches the points in the stencil given at a particular iteration.

The importance of such heuristic on the efficiency of the optimization can be illustrated by a simple bidimensional example. Consider Figure 4.7. If a straightforward coordinate search is adopted, the algorithm visits, in consecutive order, x_A, x_B, x_C and x_D. In the best case, x_A satisfies the simple decrease condition, and the iteration requires just one function evaluation. The point x_A hence becomes the center of the new pattern, and the poll phase can start again. In the worst case, all the points would need to be explored, either because x_D satisfies the simple decrease condition, or because no point can satisfy it. This would require 4 function evaluations.

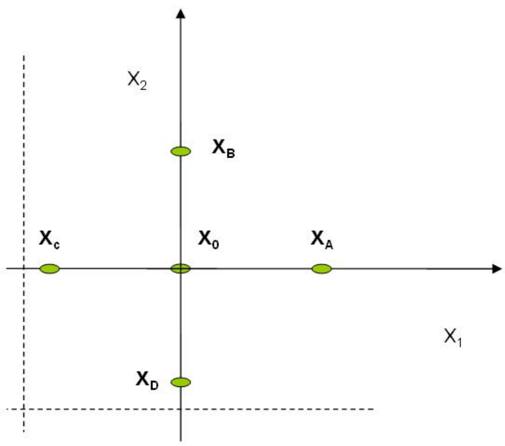


Figure 4.7: A basic instance of pattern for a pattern search method.

Other polling strategies different than the consecutive one may be put in place, with the aim of finding the suitable descent direction with as few as possible function evaluations. Such strategies range from a random search among the stencil points, to the use of surrogates (the latter case was developed in [20]). The method presented here might be considered as a particular case of optimization using surrogates, where a surrogate is intended in the general sense of function approximation. It builds on the analogy between the stencils required by both propagation method and PS algorithm, in the case for which the design variables are a subset of the uncertain variables. In fact, as shown intuitively in Figure 4.8, the search directions can be chosen to coincide with the propagation sampling directions, which constitute a maximal positive basis. The information collected at the sampling locations can therefore be used to prioritize the exploratory directions. One of the possible ways to achieve such approximate information is to simplify Eqs. (4.26) and (4.27) supposing that first order cross derivatives of the deterministic objectives and constraints are zero. This gives the following equations (similar expressions were found, for other purposes, in [122]):

$$\frac{\partial \mu_f}{\partial \mu_{x_q}} \backsimeq \frac{\partial f}{\partial x_q}\Big|_{\mu_{\mathbf{x}}}, \tag{4.30}$$

$$\frac{\partial \sigma_f^2}{\partial \mu_{x_q}} \backsimeq 2\frac{\partial f}{\partial x_q}\Big|_{\mu_{\mathbf{x}}}\frac{\partial^2 f}{\partial x_q^2}\Big|_{\mu_{\mathbf{x}}}\sigma_{x_q}^2. \tag{4.31}$$

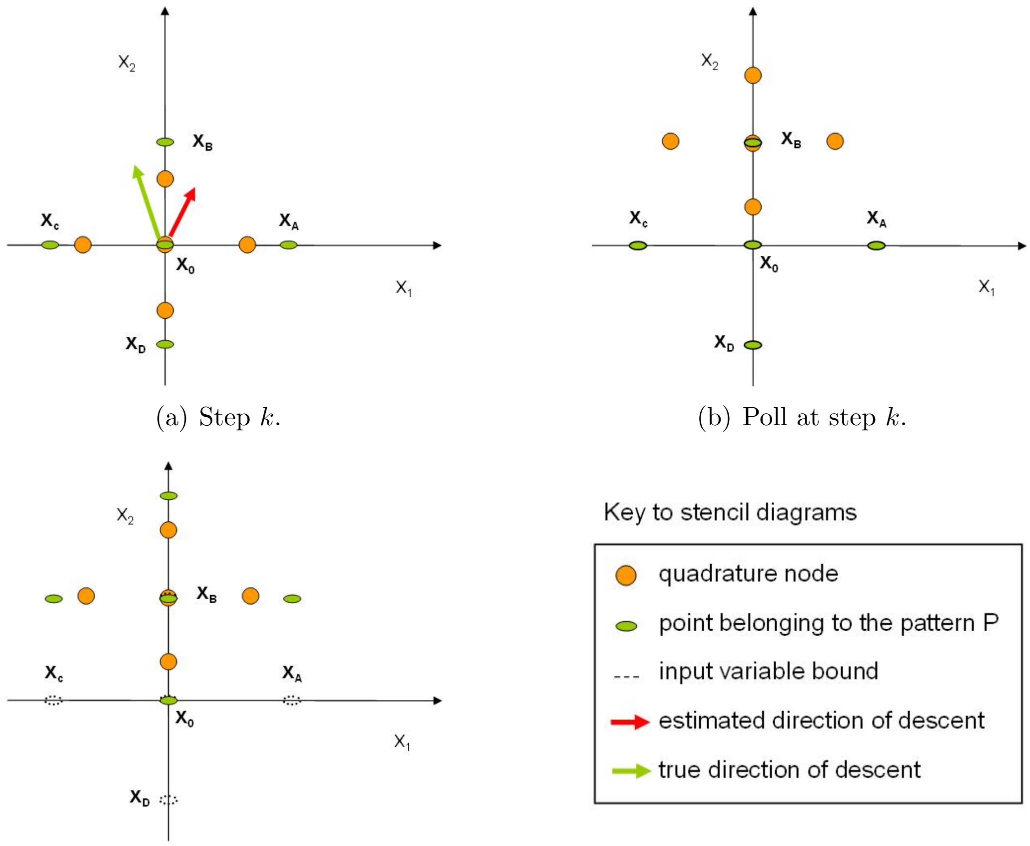
Eqs. (4.30) and (4.31) can be estimated by finite difference by using the function evaluation at the quadrature nodes, as shown in the following formulas:

$$\frac{\partial \mu_f}{\partial \mu_{x_q}} \backsimeq \frac{f(\mathbf{x}_{q+}) - f(\mathbf{x}_{q-})}{h_q^+ - h_q^-}, \tag{4.32}$$

$$\frac{\partial \sigma_f^2}{\partial \mu_{x_q}} \backsimeq 4\frac{f(\mathbf{x}_{q+}) + f(\mathbf{x}_{q-}) - 2f(\mu_{\mathbf{x}})}{(h_q^+ - h_q^-)^2}. \tag{4.33}$$

Hence they do not require additional function evaluations. Despite their accuracy could turn out to be unsatisfactory for their adoption in gradient-based methods, such approximate sensitivities supply the PS algorithm with a useful heuristic which may serve to accelerate the algorithm by exploiting first order knowledge about the statistics of the considered objectives and constraints probability density functions. To understand the way the integrated PS-URQ algorithm works, consider for simplicity the case of unconstrained optimization shown in

Figure 4.8. At the step k, in Figure 4.8(a), x_0 is the center of the PS pattern given by the points x_A, x_B, x_C and x_D, in green in the picture. This implies that the robust objective has been evaluated on a URQ stencil centered in x_0 at the step $k-1$ (the quadrature nodes composing the stencil are displayed in orange). Through the sensitivities in Eq. (4.32) and Eq. (4.33), an approximation of the



(a) Step k.

(b) Poll at step k.

(c) Step $k+1$.

Figure 4.8: Use of the URQ approximate sensitivities as exploratory heuristic on an iteration of the PS algorithm.

direction of descent, shown in red in the picture, is then available. Depending on the impact of the approximations, such direction may differ from the true direction of descent (shown in green). However, since the PS algorithm is only allowed to try points along the search directions x_1 and x_2, the approximate information given by the red vector is sufficient to suggest the evaluation of the point x_B first. Such evaluation is illustrated in Figure 4.8(b), where the center of the URQ stencil is moved from x_0 to x_B. If $F(x_B) < F(x_0)$, then the pattern at the step $k+1$ is centered in x_B (Figure 4.8(b)). If the simple decrease condition is not satisfied, the other points of the pattern at the step k would have to be visited. In that case, the heuristic would suggest the order x_A, x_C and x_D.

Since our method complies with the above mentioned conditions to guarantee convergence, the results presented in [126, 127] still hold and do not need to be demonstrated. In particular, the general case of constrained optimization can also be tackled by using augmented Lagrangian approaches [35] or Lagrangian barrier methods [36], as shown in [127].

4.4.3 Hybrid methods

PS methods, introduced in the previous section, can generally locate the region of a stationary point from any starting point $\mathbf{x}_0$ [204]. However, they exhibit slow local convergence rates, since they do not exploit second order information about the function, as gradient-based methods do. This facts naturally suggest the coupling between the two class of algorithms in the framework of an integrated optimization strategy which can build on the strengths of both, and exploit the features of the propagation phase, as shown. At the inception of the optimization, a fast rate of reduction of the objective function is thus attained by the PS, which is carried out in such a way to exploit the information available by the design of experiment performed by the URQ method in the propagation stage. Appropriate termination criteria are then developed, depending on the problem at hand, to switch the optimization algorithm to a quasi-Newton method, which performs the final phase of the convergence. This is demonstrated with a practical example in Chapter 6.

4.5 Summary and conclusions

This chapter has presented the methodological aspects of the thesis. In Section 4.2, we have reformulated the usual RDO problem in the light of a set of possible assumptions which are less stringent than the usually adopted normality assumption for the output probability distributions. This provides a stronger justification for the adoption of weighted sums of mean and standard deviation to form the robust objectives and constraints, which is based on the interpretation of the robust optimization as a worst-case quantile minimization under a specific distributional assumption. Guidelines for the choice of the relative weights have also been provided.

In addition, we have incorporated the metric of tail conditional expectation in the design formulation, with the aim of quantifying the risk of design unfeasibility. Bounds for the TCE of the objectives and constraints are also obtainable through weighted sum of mean and standard deviation. This has two main implications: firstly, TCE bounds enable the interpretation of the robust optimization process in terms of worst-case TCE minimization, under a specific distributional assumption. Secondly, TCE bounds expressed in function of mean and standard deviation of objectives and constraints are tighter than quantile bounds. This allows to reduce the overconservativeness exhibited by the worst-case quantile formulation.

In Section 4.3, we have proposed a novel propagation technique to obtain the moments required by such formulations. We have shown by means of theoretical analysis and by using simple analytical test functions that the propagation technique has enhanced accuracy with respect to the currently available methods of comparable cost. Such cost is linear in the number of function evaluations required, which makes the method well suited for problems with a small to moderate number of variables, such as those encountered during the conceptual and the preliminary phases. In Section 4.4 we have investigated the integration of the proposed method with two class of optimization algorithms. In the case of gradient-based methods, the propagation error at each step of the optimization can be used if the uncertain variables are a subset of the design variables. In the case of Pattern Search methods, when the design variables are a subset of the uncertain variable, first-order information harvested during the propagation phase can be reused to guide the optimizer poll. Finally, we have suggested how to exploit the advantages of both kinds of algorithms via their hybridization. Next chapters will apply the methodology to test cases of industrial relevance, to demonstrate its advantages and discuss its limitations.

Chapter 5

Aircraft sizing

5.1 Introduction

Presented in this chapter is the application of the proposed methodology to an industrial aircraft sizing test case. The test case is presented in detail in Section 5.2, together with the initial deterministic problem formulation. In Section 5.3, the problem is rendered stochastic by introducing symmetrical input variables distributions. In Section 5.4, we consider the case of asymmetrical distributions. In Section 5.5, the methodology is applied to the robust counterpart of a deterministic multiobjective optimization problem. Section 5.6 discusses the main implications of the obtained results, while Section 5.7 summarizes the chapter.

5.2 The test case

The adopted conceptual design model is derived from a proprietary tool of one of the industrial partners of our research. It determines performance and sizing of a short-to-medium range commercial passenger aircraft and makes use of 96 sub-models and 126 variables.

The original deterministic optimization problem is the following:

Objective: Minimize Maximum Take-Off Weight $f = MTOW(\mathbf{x})$ with respect to the design variables $\mathbf{x}$.

Constraints:

1. Approach speed: $v_{app} < 120$ Kts $\Rightarrow g_1 = v_{app} - 120$;
2. Take-off field length: $TOFL < 2000$ m $\Rightarrow g_2 = TOFL - 2000$;
3. Percentage of total fuel stored in wing tanks: $K_F > 0.75 \Rightarrow g_3 = 0.75 - K_F$;
4. Percentage of sea-level thrust available in cruise: $K_T < 1 \Rightarrow g_4 = K_T - 1$;
5. Climb speed: $v_{zclimb} > 500$ ft/min $\Rightarrow g_5 = 500 - v_{zclimb}$;
6. Range: $RA > 5800$ Km $\Rightarrow g_6 = 5800 - RA$.

Table 5.1 provides descriptions of the design variables with their permitted ranges. The problem's fixed parameters are given in Table 5.2.

Design variable	**Definition [units]**	**Bounds $[\mathbf{x}_L,\ \mathbf{x}_U]$**
S	Wing area [m^2]	[140, 180]
BPR	Engine bypass ratio [ ]	[5, 9]
b	Wing span [m]	[30, 40]
Λ	Wing sweep [deg]	[20, 30]
t/c	Wing thickness to chord ratio [ ]	[0.07, 0.12]
$T_{e_{SL}}$	Engine sea level thrust [kN]	[100, 150]
FW	Fuel weight [Kg]	[12000, 20000]

Table 5.1: Considered design variables, aircraft sizing test case.

Parameter	**Value**
Number of passengers	150
Number of engines	2
Cruise Mach number	0.75
Altitude [ft]	31000

Table 5.2: Fixed parameters.

5.3 RDO with symmetric input distributions

Consider the case for which the design variables are affected by uncertainty. The resulting instance of design under uncertainty is termed sometimes "type

II robust design" [30]. Randomizing the design variables is the first step of a strategy which aims at rendering the optimal conceptual design insensitive to variations that are likely to occur downstream in the development process, with the purpose of avoiding nugatory iterations between design phases.

We model the design variables by means of normal distributions truncated to the range $[\mu_{\mathbf{x}} - 3\sigma_{\mathbf{x}}, \mu_{\mathbf{x}} + 3\sigma_{\mathbf{x}}]$. The standard deviation $\sigma_{\mathbf{x}}$ is chosen to introduce a coefficient of variation of 0.07 in correspondence to the central point of the design space.

The mathematical problem to be solved is hence formulated as in Problem (4.1), where the adopted coefficients are: $k_f = k_{g_i} = 1.3$, for $i = 1 \ldots 6$, and $k_{\mathbf{x}} = 1$. It results in the following formulation:

$$\begin{aligned} &\text{Find } \mu_{\mathbf{x}} \in \mathbb{R}^n \text{ to minimize } F(\mathbf{x}) = \mu_{MTOW} + 1.3\sigma_{MTOW} \\ &\text{subject to: } G_i(\mathbf{x}) = \mu_{g_i} + 1.3\sigma_{g_i} \leqslant 0, i = 1, 2, \ldots, 6, \\ &\text{ and: } \mathbf{x}_L + \sigma_{\mathbf{x}} \leqslant \mu_{\mathbf{x}} \leqslant \mathbf{x}_U - \sigma_{\mathbf{x}}. \end{aligned} \tag{5.1}$$

The first set of numerical experiments that we have performed regards the comparison of two gradient-based optimizations, in which the robust objective and constraints are built with URQ and I MM, respectively. The starting point considered for the optimizations is the result of the optimization of the deterministic problem, which is summarized in Table 5.3. The two robust optimizations differ only in their calculations of mean and variance, the first making use of I MM and the second the URQ method. Both optimization problems are solved using Matlab's gradient-based constrained optimizer `fmincon`. To exploit accurate derivative information where possible, we make use in this experiment of the automatic differentiation software MAD [65], some extension of which were demonstrated by the author in [156] with the aid of this test case.

In the I MM optimization, MAD is used to calculate the first derivatives of the deterministic objective and constraints (required to estimate the variance by Eq. (3.13)), and their second derivatives to form the gradient of the robust objective and constraints. In the URQ-based optimizations, MAD is used to calculate the robust gradients, as given by Eq. (4.26) and Eq. (4.27). Table 5.4 presents the results of the two optimizations. The nominal MTOW for the two optimal values is 84.3 tonnes and 84.5 tonnes, respectively. Therefore, both robust op-

Input variables		Obj./Constr.	
S [m^2]	140.00	$MTOW$ [Kg]	77560.62
BPR [ ]	9.00	g_1 [Kts]	0.00
b [m]	40.00	g_2 [m]	-80.00
Λ [deg]	20.00	g_3 [ ]	0.00
t/c [ ]	0.081	g_4 [ ]	-0.12
$T_{e_{SL}}$ [kN]	101.60	g_5 [ft/min]	0.00
FW [Kg]	14817.13	g_6 [Km]	0.00

Table 5.3: Optimal deterministic design which serves as starting point for RDO.

Input variables	I MM	URQ
S [m^2]	165.18	166.02
BPR [ ]	8.51	8.51
b [m]	37.55	37.55
Λ [deg]	21.75	21.75
t/c [ ]	0.085	0.085
$T_{e_{SL}}$ [kN]	125.30	126.09
FW [Kg]	18267.04	18363.38
Obj./Constr.	**I MM**	**URQ**
F [Kg]	86453.81	86662.39
G_1 [Kts]	0.00	0.00
G_2 [m]	-200.10	-196.14
G_3 [ ]	0.00	0.00
G_4 [ ]	-11.30	-0.10
G_5 [ft/min]	0.00	0.000
G_6 [Km]	0.00	0.000

Table 5.4: Results of the robust optimizations.

tima are almost the 10% heavier than the original deterministic optimum shown in Table 5.3. The required fuel is about 3.5 tons more than for the deterministic optimum and the required thrust and wing area are significantly increased, to keep the wing loading and the thrust-weight ratio almost unvaried. This is an example of the margins that robust optimization procedures build into the design. Such margins may be substantial, and hence each of the steps leading to their estimation has to be justified. It can also be noted that the solution found by adopting the URQ is slightly more conservative with respect to the one given by the I MM. More articulated considerations concerning such result are detailed in the next subsections.

5.3.1 Probabilistic analysis

A probabilistic post-optimal analysis is performed by using MCS (Latin Hypercube with 10^5 samples) to validate Table 5.4's results with respect to the accuracy of the estimates and the probability of feasibility. Two simulations are performed, by choosing a truncated multivariate normal distribution with the mean corresponding to the optimal $\mathbf{x}$ given by the two optimization processes, while the variance corresponds to the one adopted for the input random variables during the optimization. First, we can compare the accuracy of the URQ and I MM propagation methods in estimating the moments.

	Mean estimation		**Variance estimation**	
Obj./Constr.	$x_{opt,IMM}$	$x_{opt,URQ}$	$x_{opt,IMM}$	$x_{opt,URQ}$
$MTOW$	$-0.35 \cdot 10^{-4}$	$0.26 \cdot 10^{-5}$	$0.11 \cdot 10^{-1}$	$0.11 \cdot 10^{-1}$
v_{app}	$-0.15 \cdot 10^{-2}$	$0.82 \cdot 10^{-6}$	$0.18 \cdot 10^{-1}$	$0.13 \cdot 10^{-2}$
$TOFL$	$-0.87 \cdot 10^{-2}$	$0.34 \cdot 10^{-4}$	$0.60 \cdot 10^{-1}$	$0.18 \cdot 10^{-1}$
K_F	$-0.82 \cdot 10^{-2}$	$0.10 \cdot 10^{-3}$	$0.11 \cdot 10^{-1}$	$0.26 \cdot 10^{-1}$
K_T	$-0.87 \cdot 10^{-2}$	$0.65 \cdot 10^{-4}$	$0.51 \cdot 10^{-1}$	$0.23 \cdot 10^{-1}$
V_{zclimb}	$-0.13 \cdot 10^{-1}$	$0.69 \cdot 10^{-4}$	$0.90 \cdot 10^{-2}$	$0.14 \cdot 10^{-1}$
RA	$-0.24 \cdot 10^{-2}$	$-0.55 \cdot 10^{-5}$	$0.15 \cdot 10^{-2}$	$0.14 \cdot 10^{-2}$

Table 5.5: Post-optimality analysis: relative error on mean and variance estimation of objective and constraints with respect to MCS.

As shown in Table 5.5, the URQ method can attain an increased mean accuracy - at least one order of magnitude better - with respect to linearization. Variance estimates show instead the same accuracy for the two methods.

We can use such results also to understand the implications of a correct probabilistic formulation of constraints and objectives, and its extension to include the tail conditional expectation, as discussed in Chapter 4.

With this respect, we need to elaborate further the reason why we have adopted $k_f = k_{g_i} = 1.3$, for $i = 1 \dots 6$, and $k_{\mathbf{x}} = 1$ for the described optimizations. The coefficient $k_{\mathbf{x}} = 1$ implies that, for each of the variables, either the upper or lower bound cannot be exceeded with a probability of about 84.3%, which can be easily calculated as a function of the normal CDF by discarding the truncated tails.

However, since the distributions of objectives and constraints are not known at the time of setting the problem, the right choice of k_f and k_{g_i} could be a matter

Active constraint	**I MM**	**URQ**
$P(v_{app} < 120\ Kts)$	0.8893	0.9011
$P(K_F > 0.75)$	0.9235	0.9136
$P(v_{zclimb} > 500\ ft/min)$	0.8949	0.8990
$P(RA > 5800\ Km)$	0.8988	0.9064

Table 5.6: Probabilities of feasibility verified by MCS.

of debate. If we analyze retrospectively the probability of satisfaction of the active constraints (which for both optimizations are the constraints 1, 3, 5 and 6) we find the probabilities shown in Table 5.6. Such results can be interpreted as a combination of two main levels of approximations. The first one regards the estimation of the moments, and has been discussed and assessed above. The second regards the assumption that the probability of feasibility can be estimated satisfactorily by using only two moments, by supposing that the output functions can be modeled by known distributions. The relative magnitude of such errors is the key to understand the suitability of the proposed RDO methodology to conceptual design problems.

For example, if we had assumed normal behavior for the constraints, aiming at a probability of feasibility of $\Phi(1.3) = 0.9032$, we would have slightly missed our probability target for 5 of the 8 constraints.

The discrepancy is larger for the I MM, because of the worse mean accuracy. In particular, we verify that the optimal I MM point is considered unfeasible by an URQ analysis, and this is the reason why the URQ optimization chooses another, more conservative, optimal location.

However, also the solution found by the URQ, despite increasing the design margin on the MTOW by $84.5 - 84.3 = 0.2$ tonnes with respect to the I MM solution, turns out to be slightly unfeasible to a MCS analysis. This happens not because of the moment estimation this time, but because of the normality assumption. Such finding shows the importance of a system approach to the problem of design optimization under uncertainty. In fact, it is not sufficient to improve one of the aspects of the problem - in this case the accuracy of the moments' estimates - to obtain an improved solution.

We could have also interpreted the coefficients k_f and k_{g_i} as deriving from the probability bounds described in Chapter 4, which allow relaxing the normality assumption. Of course, considering such bounds, which correspond to the worst case quantiles within a set of distributions (e.g., the set of symmetric distributions) is more conservative than assuming normal behavior for objective and constraints. For example, the probability of feasibility satisfied by all the unimodal distributions for $k_{g_i} = 1.3$ would have been 0.8348 (Table 4.1, case III), while the one given by the unimodal symmetric assumption would have been 0.8685 (Table 4.1, case IV). By comparison with the results in Table 5.6, for the URQ case, such overconservativeness is quantified to be around 8% and the 4% for the unimodal and unimodal symmetric assumption, respectively.

Finally, we can analyze the possible consequences of substituting a quantile constraint with a TCE type of constraint. As explained in Chapter 4, such bounds impose a limit on the acceptable average performance for the worst chosen percentage of designs which descend from the nominal design due to the uncertainties within the problem. We have reported three possible choices to formulate such constraint: the Chebyshev bound, the symmetric bound and the normal TCE value.

Had we preferred to avoid any assumption on the output distribution, we would have used a Chebyshev TCE bound. Hence $k_{g_i} = 1.3$ would have identified the upper bound for the average over the worst 37% of the designs via Eq. (4.14). We would then have imposed such bound to be smaller than the original deterministic limit. For example, in the case of v_{app}, the upper bound on TCE, i.e. $\sup[\mathrm{TCE}_{0.37}(v_{app})]$, would have been imposed to be smaller than 120 Kts, and we would have formulated the constraint again as:

$$G_1 = \sup[\mathrm{TCE}_{0.37}(v_{app})] - 120 = \mu_{g_1} + 1.3\sigma_{g_1} \leqslant 0. \tag{5.2}$$

Since the constraint is active, $\sup[\mathrm{TCE}_{0.37}(v_{app})] = 120$. A validation of the TCE approach on the MCS results, shows that the average v_{app} on the worst 37% of the samples is $\mathrm{TCE}_{0.37}(v_{app}) = 119.28$ Kts. Such result is still conservative, but physically very close to the estimated 120 Kts. With respect to imposing a quantile constraint, this is a sharp improvement. Without any assumption on v_{app} PDF, in fact, the corresponding Chebyshev quantile bound would have guaranteed only that $P(v_{app} < 120) > 62.82\%$, while it is verified via MCS that $P(v_{app} < 120) = 90.11\%$, as reported in Table 5.6.

5.3.2 The impact of derivatives

Another potential advantage of the URQ over I MM is the fact that the URQ is derivative-free. This feature is especially desirable when accurate derivatives are not obtainable, or when just one level of accurate derivatives is available.

To such purpose, the two mentioned robust optimization problems were solved again by using finite differences (FD) in place of AD. By comparing the two approaches in terms of number of optimization iterations, as shown in Table 5.7, we see that when accurate derivatives are not available, a single level of differentiation is less prone to generate inaccuracies, which cause the optimizer to wander and sometimes hinder its convergence to a feasible point. In addition, as we highlighted in [156], AD is able to drastically reduce the time required to obtain the derivatives, and hence turns out to be particularly beneficial for I MM. However, this also depends on the specific implementation of the test case, because of the time required for MAD function overloading.

	I MM, AD Iterations	**I MM, FD Iterations**	**URQ Iterations**
Robust gradients by AD	12	12	12
Robust gradients by FD	12	39	12

Table 5.7: The negative impact of a double level of finite differentiation.

5.4 RDO with asymmetric input distributions

The uncertainty affecting the input variables might also be modeled by asymmetric probability distributions. In this case, it is important that such differences in input are respectfully considered in the optimization.

We consider an application for which the input variables have been modeled by triangular distributions with means and standard deviations equal to the previous case, but with a skewness of -0.5 for all the variables. We adopt the same coefficients $k_f = k_{g_i} = 1.3$, for $i = 1 \dots 6$, and $k_{\mathbf{x}} = 1$ used for the symmetric case. Due to the skewness of the input distributions, the choice of $k_{\mathbf{x}} = 1$ implies a different upper and lower probabilistic bound for the design variables, i.e. about 82.7% and 81.5% respectively. Such difference does not necessarily have an engineering justification and could be eliminated by choosing two suitable $k_{\mathbf{x}}$ for the two bounds. We prefer however to keep $k_{\mathbf{x}} = 1$ to facilitate the comparison of this case with the symmetric one.

5.4.1 Optimization with III MM

If we perform an optimization where I MM is used for the propagation, we would obtain the same result as for the case of the truncated normal distribution described in Section 5.3, since the propagation phase can only exploit the information regarding mean and variance of the input, and neglects the skewness.

In contrast, such information can be readily exploited by the URQ method, as we can show by comparing a URQ and a III MM robust optimization.

III MM is a propagation method with higher accuracy than I MM and URQ (see Section 3.4.2). It requires the obtention of third derivatives to estimate the robust objectives and constraints, and a fourth level of derivation if the gradients of such objectives and constraints are needed by the optimizer. Such computational effort is clearly unaffordable for most practical applications. For this reason, such method is used here only as a benchmark, within an auxiliary optimization study in which objectives and constraints are modeled through III MM, and the required derivatives are obtained through MAD. Table 5.8 presents the results of the two optimizations. We can see that the optimal points for URQ and III MM have changed with respect to the case of symmetric input variables, to account for the new models of uncertainty introduced in the problem. This allows establishing a more realistic correspondence between the optimization process and the mathematical modeling of the problem at hand. On the other side, it presupposes that more detailed information about the input uncertainty than the sole mean and variance is available. Furthermore, the design points designated as optimal by the two methods are very close, since at each step of the optimization the two propagation methods supply very marginally different information to the optimizer. However, since in the general case the URQ variance estimate might differ from the one obtained by III MM, it is desirable to quantify such eventual discrepancy. For this reason, we have presented in Section 4.4.1 a method to estimate the error produced by the URQ propagation phase at each step of the optimization, when gradient-based methods are adopted. In this case, such method predicts that the variance error with respect to III MM is approximately

Input variable	**URQ**	**III MM**
S [m^2]	166.41	166.39
BPR [ ]	8.51	8.51
b [m]	37.55	37.55
Λ [deg]	21.75	21.75
t/c [ ]	0.095	0.095
$T_{e_{SL}}$ [kN]	126.35	126.35
FW [Kg]	18400.59	18398.94
Obj./Constr.	**URQ**	**III MM**
F [Kg]	86745.21	86742.78
G_1 [Kts]	0.00	-1.09
G_2 [m]	-195.73	-200.03
G_3 [ ]	0.00	0.00
G_4 [ ]	-1.06	-1.08
G_5 [ft/min]	0.00	-2.78
G_6 [Km]	0.00	-5.76

Table 5.8: Results of the robust optimizations, asymmetric case.

$3 \cdot 10^{-4}$ for all the optimization steps, which has then a negligible impact on the total variance estimate for the case at hand.

5.4.2 Probabilistic analysis

The results have been validated by means of Monte Carlo simulation (random sampling with $2 \cdot 10^5$ samples). The analysis in Table 5.9 shows that the URQ can achieve a very good approximation of the first two moments when compared with III MM.

	Mean estimation		**Variance estimation**	
Obj./Constr.	$x_{opt,URQ}$	$x_{opt,IIIMM}$	$x_{opt,URQ}$	$x_{opt,IIIMM}$
$MTOW$	$-0.35 \cdot 10^-5$	$0.26 \cdot 10^-5$	$0.37 \cdot 10^-2$	$-0.23 \cdot 10^-2$
v_{app}	$-0.37 \cdot 10^-4$	$0.85 \cdot 10^-4$	$0.46 \cdot 10^-2$	$0.14 \cdot 10^-2$
$TOFL$	$-0.13 \cdot 10^-3$	$0.23 \cdot 10^-4$	$0.15 \cdot 10^-1$	$0.18 \cdot 10^-1$
K_F	$-0.29 \cdot 10^-2$	$-0.28 \cdot 10^-3$	$0.29 \cdot 10^-1$	$0.24 \cdot 10^-1$
K_T	$-0.68 \cdot 10^-4$	$0.21 \cdot 10^-4$	$0.13 \cdot 10^-1$	$0.13 \cdot 10^-1$
V_{zclimb}	$-0.42 \cdot 10^-4$	$-0.11 \cdot 10^-3$	$0.39 \cdot 10^-2$	$0.39 \cdot 10^-2$
RA	$-0.25 \cdot 10^-3$	$0.14 \cdot 10^-3$	$0.16 \cdot 10^-2$	$0.17 \cdot 10^-2$

Table 5.9: Post-optimality analysis: relative error on mean and variance estimation of objective and constraints with respect to MCS.

The probabilities of satisfaction of the active constraints (which for both optimizations are the constraints 1, 3, 5 and 6) have also been quantified on the MCS samples, and the results are shown in Table 5.10. From such results, and

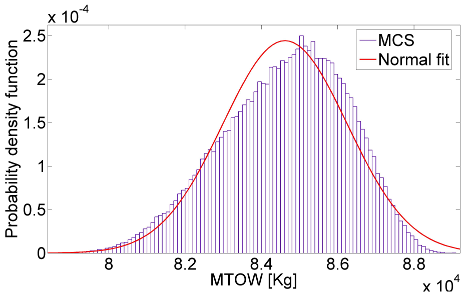
Active constraint	URQ	III MM
$P(v_{app} < 120$ Kts$)$	0.8746	0.8739
$P(K_F > 0.75)$	0.9024	0.9026
$P(v_{zclimb} > 500$ ft/min$)$	0.8819	0.8825
$P(RA > 5800$ Km$)$	0.8902	0.8901

Table 5.10: Probability of feasibility verified by MCS, asymmetric case.

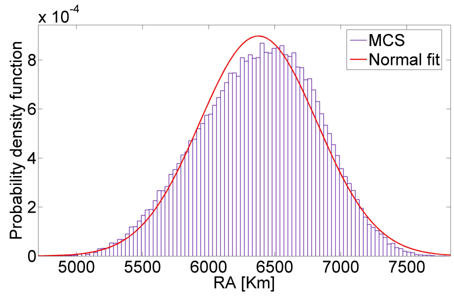
from Figure 5.1, where the MCS data regarding the URQ solution are shown together with their normal fits, it is clear that this time the normal assumption is unsatisfactory. Furthermore, the mismatch between the normal assumption and the probabilistic distributions of objectives and constraints does not occur in correspondence of the optimum alone, but can be observed throughout the optimization process. Hence the result is not optimal in the sense sought by a formulation which makes use of the normal assumption.

As an alternative, we could have resorted to the Vysochanskij-Petunin inequality in Eq. (4.8). In this case, relying on the unimodality of the probability distributions of the constraints, the optimal solution would have guaranteed, for $k_{g_i} = 1.3$, a probability of feasibility of at least 0.8348. Analogously, $k_f = 1.3$ would have guaranteed that at least the 83.48% of the designs have $MTOW$ below the threshold given by F in Table 5.8. Hence the solution can be interpreted as optimal in a worst-case sense, for a given probability, under the unimodality assumption of objective and constraints.

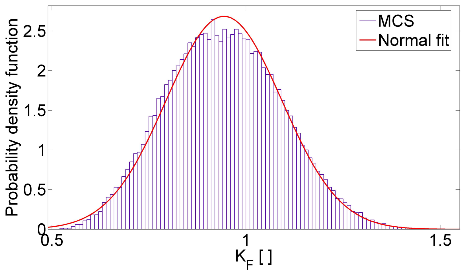
Removing all the distributional assumptions, we may have used the TCE Chebyshev inequality in Eq. (4.14) to formulate the objective and the constraints. For $k_{g_i} = 1.3$, as mentioned above, such constraints would have put a bound on the average value for the worst 37% of the designs. The comparison between the prediction through such a bound and the average taken on the sample, presented in Table 5.11, shows that the estimates are conservative, but much closer to the predicted value than what would be achievable through quantile bounds. This makes TCE bounds a useful tool for design optimization when the problem is described in terms of mean and variance.



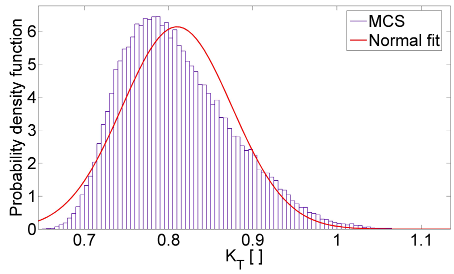
(a) $MTOW$.



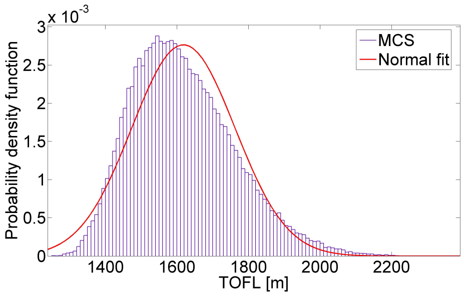
(b) RA.



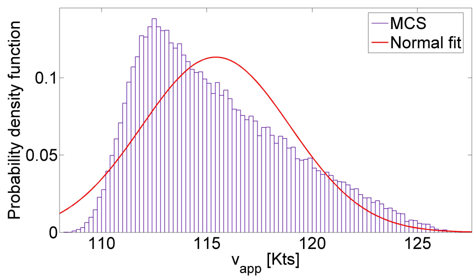
(c) K_F.



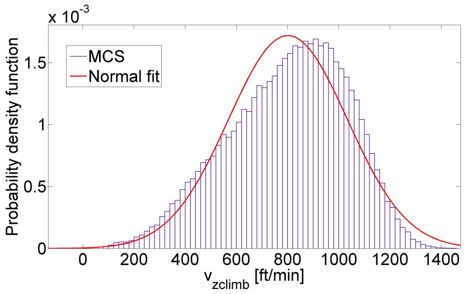
(d) K_T.



(e) $TOFL$.



(f) v_{app}.



(g) v_{zclimb}.

Figure 5.1: MCS validation of optimal results.

Obj./Constr.	$\mu_{y,URQ} + 1.3\sigma_{y,URQ}$	$\text{TCE}_{0.37,MCS}(y)$
$MTOW$ [Kg]	86745.21	86259.9
v_{app} [Kts]	120.00	119.26
$TOFL$ [m]	1804.30	1769.36
K_F [ ]	0.75	0.79
K_T [ ]	0.89	0.88
v_{zclimb} [ft/min]	500.00	553.37
RA [Km]	5800.00	5910.53

Table 5.11: MCS validation of the TCE bounds corresponding to the optimal URQ solution. The bounds are based on the Chebyshev inequality for $k = 1.3$.

5.5 Multi-objective optimization

The test case has been also employed to study the case in which multiple physical objectives are of interest for the designer. In this case, the deterministic problem is set as follows:

Objective: Minimize Maximum Take-Off Weight $f_1 = MTOW(\mathbf{x})$ and maximize Range $f_2 = RA(\mathbf{x})$ with respect to the design variables $\mathbf{x}$.
Constraints:

1. Approach speed: $v_{app} < 120$ Kts $\Rightarrow g_1 = v_{app} - 120$;
2. Take-off field length: $TOFL < 2000$ m $\Rightarrow g_2 = TOFL - 2000$;
3. Percentage of total fuel stored in wing tanks: $K_F > 0.75 \Rightarrow g_3 = 0.75 - K_F$;
4. Percentage of sea-level thrust available in cruise: $K_T < 1 \Rightarrow g_4 = K_T - 1$;
5. Climb speed: $v_{zclimb} > 500$ ft/min $\Rightarrow g_5 = 500 - v_{zclimb}$.

The solution of this multi-objective problem is a set of design points which are Pareto optimal, i.e. they represent optimal compromises for which is not possible to improve one objective without worsening another.

To attack the robust counterpart of the optimization problem, a choice has been made in this case to consider mean and standard deviation of $MTOW$ and RA as two separate objectives, without any assumption on relative weights k_{f_1} and k_{f_2}. The problem to be solved is then a 4 objective optimization. Constraints are still considered in the weighted sum formulation, but the weighting coefficients are this time $k_{g_i} = 1$, for $i = 1 \dots 5$ and $k_{\mathbf{x}} = 1$. The assumed uncertainties of input variables, in terms of standard deviation, are shown in Table 5.12, together with considered ranges. The URQ propagation method has been adopted to obtain mean and variance of objectives and constraints. The DHCBI software, developed by Fantini [61] within our research center, has been used to set the multi-objective optimization problem. The obtained robust Pareto front is

Design variable	**Definition [units]**	**Bounds $[\mathbf{x}_L, \mathbf{x}_U]$**	$\sigma_{\mathbf{x}}$
S	Wing area [m^2]	[152, 158]	2
BPR	Bypass ratio [ ]	[5, 8.5]	0.5
b	Wing span [m]	[30, 38]	0.5
Λ	Wing sweep [deg]	[28, 32]	1
t/c	Thickness to chord ratio [ ]	[0.07, 0.10]	0.002
T_{esL}	Engine sea level thrust [kN]	[125, 130]	20
FW	Fuel weight [Kg]	[17000, 18000]	50

Table 5.12: Design variables stardard deviations and ranges of variation.

presented in Figure 5.2. It is useful to compare it with the deterministic results

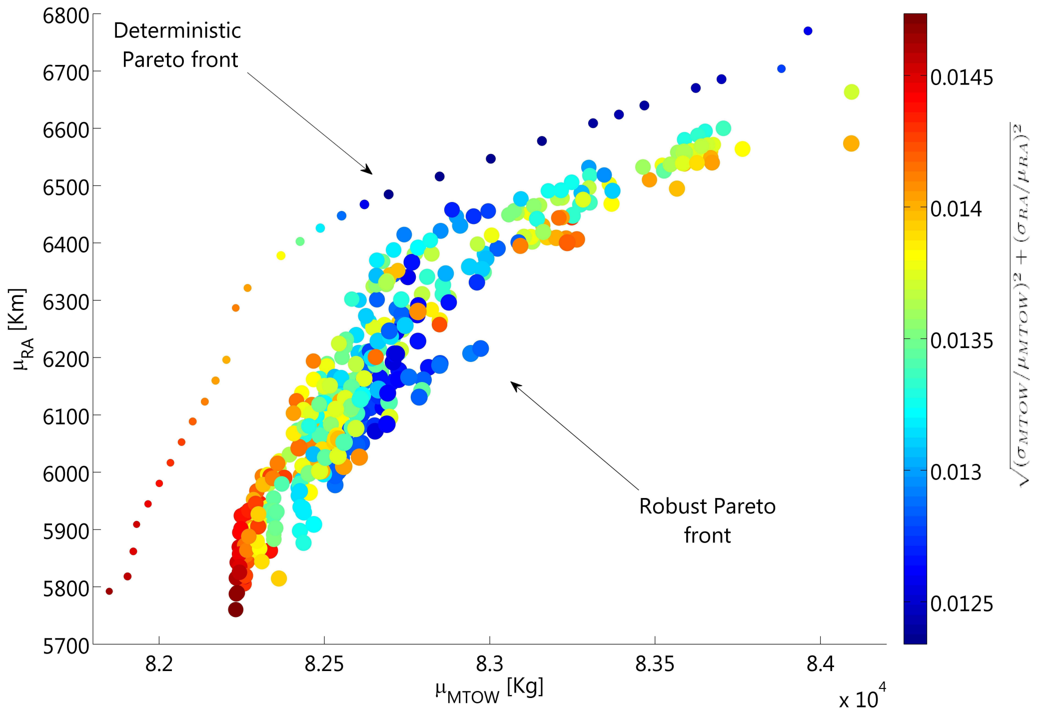


Figure 5.2: Comparison between the deterministic and the robust Pareto fronts.

obtained by Fantini [61], by performing an URQ *a posteriori* uncertainty analysis on the deterministic Pareto points to obtain for each of them mean and variance of objectives and constraints. The uncertainty attached to each solution is represented through the color and the size of the Pareto points. The color is scaled with the Euclidean lenght of the coefficients of variation of the two objectives, while the size is linearly dependent on the probability of feasibility. Is therefore evident that the robust optimal solutions differ from the deterministic optima mainly due to the imposed stricter constraint. To ensure their satisfaction, the robust Pareto points turn out to be dominated by the deterministic ones in terms of mean values.

5.6 Discussion of the results

We have shown with the aid of the aircraft sizing test case that the URQ method is well suited to enhance RDO. It has an increased accuracy with respect to linearization, and this has a positive impact on the identification of robust solutions. Furthermore, it can account for non-symmetric input distributions, for which it improves the accuracy of linearization for both mean and variance. However, this also implies the availability of the third and the fourth moments, which might not be the case in practice. It has been shown that the departure from III MM accuracy can be kept under control during the optimization phase; however, this feature is exploited at present only as a warning. Future work may investigate the deployment of higher order quadratures in correspondence of the points for which the error exceeds the prescribed tolerances. The derivative-free nature of the URQ benefits gradient-based optimization, since the optimizer requires a single level of optimization; even in the worst case, for which only finite differences can be deployed, the optimization is reliable and can locate the optimum without significant additional effort. This might not be true for I MM, which may suffer from numerically corrupted finite difference hessians. For the cases of interest, in which a small to moderate number of variables is of interest, the normality assumption of objectives and constraints might be disappointingly inaccurate in case the input distribution functions are not normal or the uncertainty in input is sufficiently large that the linear approximation of the considered output function is not acceptable; such feature impacts the meaning of the optimization process, which should be rather interpreted on the basis of the formulation proposed in Chapter 4. Under that point of view, the moment-based RDO is seen as an optimization of the worst-case within a chosen distributional assumption; the disadvantage of such formulation is that, since it minimizes a worst-case distribution statistics, it may be overconservative for the majority of the cases of interest. Quantile constraints and objectives can be advantageously substituted by tail conditional expectations. This has a double repercussion: on the one hand, it allows interpreting the robust optimization as a minimization of a threshold of acceptable average performance amongst the worst selected percentage of designs; on the other hand, it enables a less conservative approach than the worst case formulation in terms of quantiles, in the Chebyshev and symmetric cases. The first feature is not valid only in the context of moment-based optimization, but could also be extended, for example, to the field of reliability-based methods. Such extension may be subject of future work. Finally, the proposed propagation method can be adopted with advantage also in a multiobjective framework, in which an optimal compromise is sought between means and variances of the original physical objectives.

5.7 Summary and conclusions

In this chapter, the proposed methodology has been applied to an industrial test case constituted by a Matlab code which performs aircraft sizing at the conceptual stage. This has allowed to demonstrate the usefulness of the proposed methodology, and to highlight some of its potential improvements to the current state of the art:

1. a rigorous formulation of the robust optimization problem in terms of its first two moments, through worst-case quantile and TCE bounds;
2. an improved accuracy in the estimation of such moments with respect to methods of comparable cost;
3. the enhanced numerical robustness of the gradient-based RDO process due to the derivative-free nature of the propagation phase.

The presented examples include robust optimizations with symmetric and asymmetric input distributions, single and multi-objective. Their discussion has highlighted some current limitations of the methodology, which will be the scope of future work. The following chapter focuses on the application of the proposed methodology to an airfoil test case.

Chapter 6

Airfoil design

6.1 Introduction

This chapter applies the proposed methodology to the case of airfoil design under transonic flight conditions. Such test case is considered because it complements the aircraft sizing example, and brings additional computational complexity to the optimization problem in terms of noise and nonlinearities. In Section 6.2 the test case is presented in detail, together with the starting deterministic problem formulation. In Section 5.3, the problem is rendered stochastic by modeling the design variables by means of symmetrical input variables distributions. The robust optimization based on the URQ moments estimates is therefore compared with the one adopting the first-order method of moments. In Section 6.4 the robust optimization problem is solved by a Pattern Search algorithm, which is successively hybridized with a gradient-based method. Section 6.5 discusses the results presented in the chapter, while Section 6.6 concludes.

6.2 The test case

This test case concerns the optimization of an airfoil shape for transonic flight conditions. Three main components need to be combined for the study:

- a geometry generation module, which generates the airfoil profile using a set of geometric design parameters;

- a CFD code, which calculates the aerodynamic characteristics of the airfoil at hand;
- an optimization algorithm, which selects suitable values for the independent variables at each step of the optimization.

In the present study, these three modules have been wrapped in a Matlab environment. The geometry parameterization and the CFD code are briefly described in the following subsections.

6.2.1 Geometry generation

A variety of shape representation methods have been used in optimization studies, which include B-splines [38, 124], Hicks-Henne functions [86], Wagner functions [173], PARSEC-11 [196] and CST [115]. The choice of a particular technique is based on the technique's suitability for the application at hand. In the present work, we make use of the PARSEC-11 parameterization because of its intuitive airfoil description and its reduced number of parameters. This method, developed by H. Sobieczky [196] has found a good number of applications in the field of airfoil and wing optimization. It makes use of a fractional order polynomial to describe the (l, h) coordinates of the upper and lower surface of an airfoil:

$$h = \sum_{n=1}^{6} a_n(\mathbf{x}) l^{n-1/2}, \tag{6.1}$$

where l varies between 0 and 1. The coefficients a_i of the polynomial are real and depend on the design vector $\mathbf{x}$ through simple mathematical relations. $\mathbf{x}$ is composed of 11 geometric parameters such as radius of curvature, max crest value and max crest location, as illustrated in Figure 6.1. The parameters are described in Table 6.1, where their bounds for the deterministic problem are also given. We have listed some issues related with using Parsec in [157]. In particular, we have shown that PARSEC-11 is prone to failures which may hinder the propagation and the optimization phases. To solve such problem, we proposed a methodology to achieve a robust parameterization within the design space, based on self-organizing maps. All the results presented here are obtained within a parametric space which has been preliminarily rendered robust through such methodology.

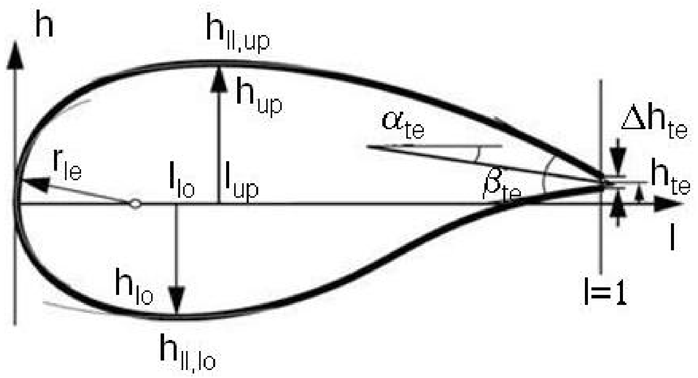


Figure 6.1: Parsec geometry parameterization.

Design variable	Definition [units]	Bounds $[\mathbf{x}_L,\ \mathbf{x}_U]$
r_{le}	Leading edge radius [ ]	[0.005, 0.009]
l_{up}	Upper surface maximum crest location [ ]	[0.360, 0.450]
l_{lo}	Lower surface maximum crest location [ ]	[0.300, 0.560]
h_{up}	Upper surface maximum crest [ ]	[0.045, 0.057]
h_{lo}	Lower surface maximum crest [ ]	[−0.058, −0.040]
$h_{ll,up}$	Upper surface curvature at l_{up} [ ]	[−0.555, −0.260]
$h_{ll,lo}$	Lower surface curvature at l_{lo} [ ]	[0.280, 1.100]
h_{te}	Trailing edge position [ ]	[−0.020, −0.009]
Δh_{te}	Trailing edge thickness [ ]	[0.005, 0.008]
β_{te}	Trailing edge aperture angle [deg]	[0.100, 0.290]
α_{te}	Angle of trailing edge bisector [deg]	[−0.130, −0.080]

Table 6.1: Considered design variables, airfoil test case.

6.2.2 CFD code

The CFD code used for this study is VGK (Viscous Garabedian-Korn), developed by DERA and made available to ESDU subscribers [59]. It can predict the aerodynamic characteristics of airfoils in subsonic free-stream by coupling the full potential equations governing the inviscid flow region and the integral equations representing the viscous flow region. The method can also account for mild shocks by using an approximate form of the Rankine-Hugoniot equations. The VGK code has good accuracy for flows with attached boundary layer, weak shock waves with Mach number before the shock smaller than 1.3. The CFD code is used by assigning a target lift, and varying the angle of attack accordingly. The retained viscous drag coefficient is based on far-field momentum thickness, applying the

Cooke implementation of the Squire and Young approximation, while the wave drag contribution is calculated by Lock's second order method.

VGK was originally conceived to work under direct control of the user. Its inclusion within the design optimization framework has required an interface to the Matlab environment, in which appropriate pre- and post-processing modules are created. In particular, the post-processing modules include appropriate checks to verify VGK results' reliability, and "help" the code converging for particularly difficult airfoils or flow conditions, by automating the instructions given in the user manual [59]. No check is implemented to automatically verify the quality of the grid. The details of the implementation can be found in [132, 133].

6.2.3 Problem formulation

The deterministic problem of interest is the minimization of the drag coefficient c_d with respect to the vector $\mathbf{x}$ specifying the PARSEC-11 parameters. The lift coefficient is fixed and the angle of attack is changed accordingly within the VGK. Two of the considered constraints regard the pitching moment coefficient c_m; the third and the fourth consider the thickness at the 12% and the 60% of the chord l, where the main spars are assumed to be located. The problem can be formulated as follows:

Objective: Minimize drag coefficient c_d with respect to the design variables $\mathbf{x}$.
Constraints:

1. Pitching moment: $c_m > -0.10 \Rightarrow g_1 = -c_m - 0.10$;

2. Pitching moment: $c_m < -0.04 \Rightarrow g_2 = c_m + 0.04$;

3. Thickness at 12% l: $thickness_{12\%} > 0.076 \Rightarrow g_3 = -thickness_{12\%} + 0.076$;

4. Thickness at 60% l: $thickness_{60\%} > 0.072 \Rightarrow g_3 = -thickness_{60\%} + 0.072$.

The flight conditions considered are shown in Table 6.2.

Parameter	**Value**
Mach	0.72
Re	$21.1 \cdot 10^6$
Transition location, upper surface	1% chord
Transition location, lower surface	1% chord
Lift coefficient c_l	0.707

Table 6.2: Flight conditions and VGK settings.

6.3 Gradient-based robust shape optimization

We focus our interest on the optimization of the airfoil shape subject to uncertainties in the geometric parameters. The robust problem is hence set up by assigning a probability distribution to the 11 input variables, which is propagated in the probabilistic distributions for the objective and the constraints.

The input variables are described by independent Gaussian variables, with standard deviation equal to the 3% of the input variable range. Such coefficient of variation for $\mathbf{x}$ corresponds to a coefficient of variation of 7% for both the maximum thickness and the camber, which can be considered as appropriate for the conceptual phase of the airfoil definition. In analogy with Problem (4.1), the optimization problem is hence formulated as follows:

$$\begin{aligned}
&\text{Find } \mu_{\mathbf{x}} \in \mathbb{R}^n \text{ to minimize } F(\mathbf{x}) = \mu_{c_d} + k_f \sigma_{c_d} \\
&\text{subject to: } G_i(\mathbf{x}) = \mu_{g_i} + k_{g_i}\sigma_{g_i} \leqslant 0, i = 1, 2, \ldots, 4, \\
&\text{ and: } \mathbf{x}_L + k_{\mathbf{x}}\sigma_{\mathbf{x}} \leqslant \mu_{\mathbf{x}} \leqslant \mathbf{x}_U - k_{\mathbf{x}}\sigma_{\mathbf{x}}.
\end{aligned} \tag{6.2}$$

The adopted coefficients are: $k_f = \sqrt{2}$, $k_{\mathbf{x}} = 1$ and $k_{g_i} = 1.22$, for $i = 1 \ldots 4$. The starting point is derived from previous studies considering different flight conditions. The first application of interest is the comparison, within the context of gradient-based optimization, of the novel propagation method URQ with the commonly adopted first-order method of moments. Such comparison is performed by carrying out two different optimizations, the first using I MM and the second the URQ technique. This is done to prove that the URQ method can more effectively deal with noisy function than I MM based on finite differences. To separate the impact of the propagation phase from other numerical effects, the other conditions influencing the optimizations have to be the same for the two experiments. In particular, the derivatives required by the optimizer have to be obtained as accurately as possible. The way this is achieved is explained in the next section.

6.3.1 Obtaining the derivatives

VGK exhibits a noisy behavior, i.e. there are oscillations in the returned function values, which are ascribable to difference in convergence within its iterative routines. In such cases, the obtention of accurate derivatives by finite differences (FD) is problematic.

FD derivatives are obtained by the following well known formulas:

$$\begin{aligned}
\frac{df}{dx} &= \frac{f(x+h_{FD})-f(x)}{h_{FD}} + O(h_{FD}) \quad \text{in the forward difference scheme,} \\
\frac{df}{dx} &= \frac{f(x+h_{FD})-f(x-h_{FD})}{2h_{FD}} + O(h_{FD}^2) \quad \text{in the central difference scheme.}
\end{aligned}$$

Such an approximation is then affected by two different errors. The first one is the truncation error, given by $O(h_{FD})$ and $O(h_{FD}^2)$ in the equations above, which is reduced with the reduction of the step; the second is the round-off, which is due to subtractive cancellation, and increases as the differentiation step is reduced. Hence a preliminary study to find a step which finds an optimal compromise between the two errors is usually performed before approximating the derivatives in this way. Such search is complicated by the existence of noise. In fact, the accuracy of derivatives obtained in this way is dubious when the scale of change induced by the FD perturbation is the same of the scale of the noise.

An alternative to FD, and to the technique of automatic differentiation presented in the previous Chapter, is the obtention of derivatives through the complex variable method (CVM) [136]. Such method approximates the first derivative as follows:

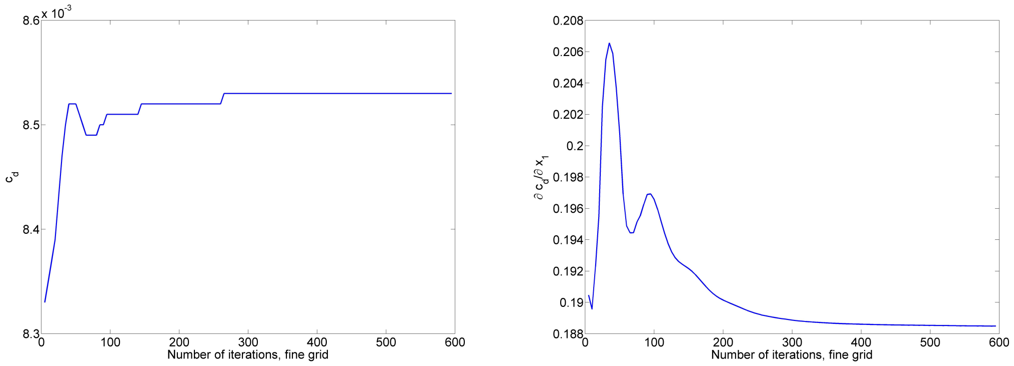
$$\frac{df}{dx} = \frac{Imag\left(f(x+ih_{CVM})\right)}{h_{CVM}} + O(h_{CVM}^2).$$

Since there is no subtraction involved, there is no round-off error in the CVM first derivative, and hence the step h_{CVM} can be chosen to be as small as possible within machine accuracy, which drastically reduces the truncation error. The CVM method is therefore a valid alternative to AD for the calculation of gradients, and is used in this chapter to estimate the derivatives required by the optimizer. This is aimed at performing the two optimization experiments under the same conditions, exception made for the propagation phase, which is carried out by using I MM in one case and URQ for the other. Having the same, accurate derivatives for both cases will allow to ascribe the discrepancies between the two optimization processes and results entirely to the adopted propagation methods.

There are a few key points that need to be stressed regarding the implementation of the CVM method. First of all, the code of interest has to be composed of real functions. Some of the routines in VGK, however, use complex numbers. Hence the first operation on the code requires splitting such complex routines into their real and imaginary parts. Once the code has been made real, it has to be "complexified" in its totality, i.e. the real variables have to be made complex, and functions which are not originally conceived for complex operations have to be transformed to accept and return complex variables. This is achieved by performing real operations, separately, on the real and imaginary part of such variables. Very useful work in this direction has been published by Martins *et al.* [136]; Martins has also made available on his webpage [135] a Fortran module which helps in this operation.

To practically obtain the derivatives, it is then sufficient to interrogate the function with a complex input $x + ih_{CVM}$, where x is the (real) value of interest and h_{CVM} is an arbitrarily small step. As a consequence, the value returned as output is complex. Its real part gives the original function output, while the imaginary part, divided by the step chosen, gives the code's derivative.

The computational cost of obtaining the derivatives in this way is higher than for finite differences, because more expensive complex arithmetic is involved. Furthermore, the iterative behavior of VGK is reflected into its derivatives, which requires for convergence around 200 iterations more than the function value. Such behavior, which can be observed in Figure 6.2, agrees with the observations in [136]. The validation of the CVM derivatives has been possible only by comparison with finite differences. Centered finite differences have been employed, and the step h_{FD} has been varied in the range $[10^{-5}, 10^{-1}] \cdot \mathrm{abs}(\mathbf{x})$. In Figure 6.3, as an example, the CVM and FD derivatives of VGK with respect to $x_9 = \Delta h_{te}$ are shown. We can see that the FD derivative is strongly varying around the value yielded by the CVM. The validation study also gives a value of reference for the FD step used in the I MM estimate.



(a) Calculated drag coefficient. (b) CVM derivative $\partial c_d/\partial x_1$.

Figure 6.2: Convergence of the VGK output and its CVM derivative.

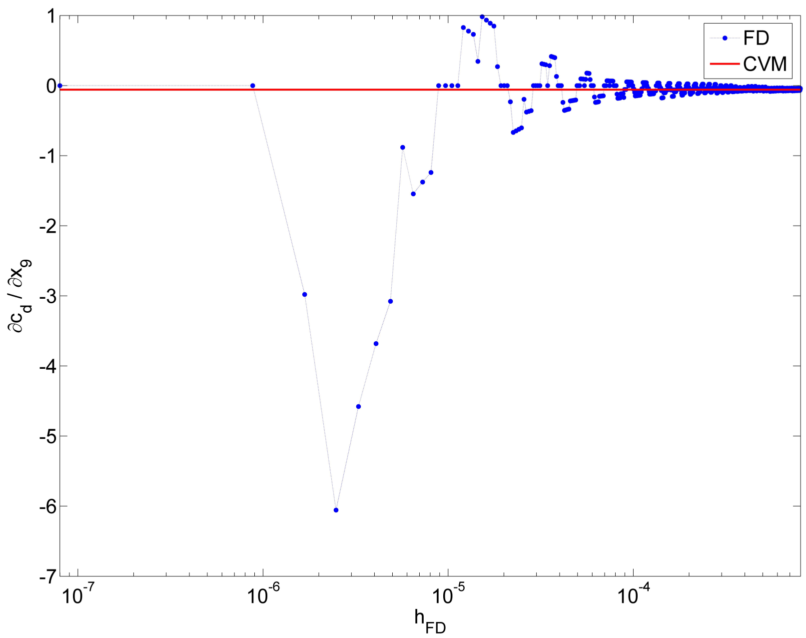


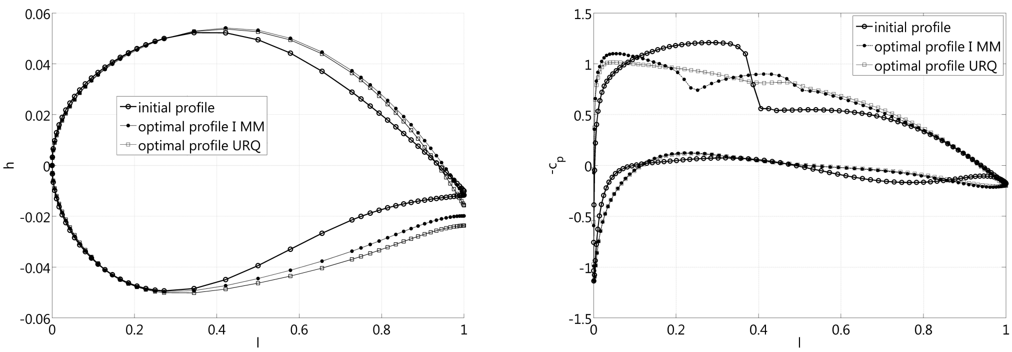
Figure 6.3: CVM and FD derivatives for $\partial c_d/\partial x_9$.

6.3.2 Comparison between I MM and URQ

The complexification of the adopted CFD code enables the comparison of I MM and URQ by means of two optimizations, for both of which CVM gradients are available. The gradients required by the I MM propagation phase are instead obtained through finite differences. From such optimizations two different optimal profiles are obtained, whose nominal features are shown in Table 6.3, together with the features of the initial profile.

Parameter	Initial profile	I MM	URQ
c_d	0.00852	0.00797	0.007839
c_l	0.70697	0.70702	0.70704
c_m	-0.06263	-0.09371	-0.09488
$thickness_{12\%}$	0.07769	0.07688	0.07683
$thickness_{60\%}$	0.07361	0.08909	0.09083
angle of attack α [deg]	1.860	1.191	0.954

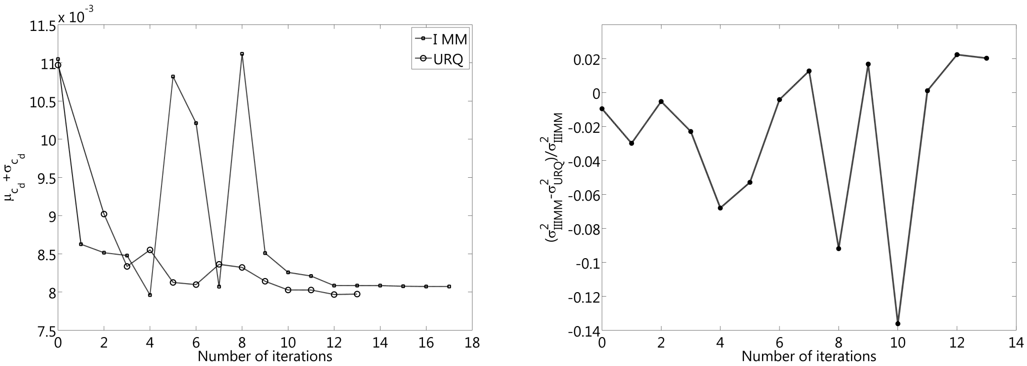
Table 6.3: Nominal features of the RDO solutions and the initial profile.



(a) Airfoil geometry. (b) Pressure distribution.

Figure 6.4: Robust optimizations solutions compared with the initial profile.

The nominal solution given by the URQ optimization has lower drag than the one found when the I MM is employed. This is due to the more effective reduction of the shock located on the upper surface of the initial airfoil at approximately $l = 0.35$ (Figure 6.4(b)). As can be seen in Figure 6.4(a), the main geometrical differences between the two robust optima regard the trailing edge (in particular the variables h_{te} and β_{te}) and the lower and upper surfaces curvatures $h_{ll,lo}$ and $h_{ll,up}$. It can be seen from Figure 6.5(a)that when the URQ is adopted for the propagation phase, the optimizer (which is the Matlab nonlinear constrained optimizer `fmincon`) converges to the solution in a reduced number of iterations, and without the strong oscillations observed in the I MM case. This behavior is due to the better handling of the numerical noise by an integral approach, such as the one performed by the URQ, with respect to the differential approach given by the I MM (when the derivatives are obtained by finite differences). The larger "sampling" step, which in the case of URQ is dependent on the input moments through Eq. (4.20) is hence able to smooth out the noise hindering the reliability of FD estimates. Figure 6.5(b) shows how the estimation error with respect to third-order method of moments, obtained by means of Eqs. (4.28) and (4.29), varies during the optimization. In this case, the error is still considered acceptable even if it occasionally exceeds 10%. During the various optimizations performed, however, we have noticed that the error indicated by such formula may be higher than 100%. In that case, suitable higher order quadrature may be deployed to obtain accurate mean and variance. To validate the results,



(a) Convergence of the two optimizations. (b) URQ variance error during the optimization.

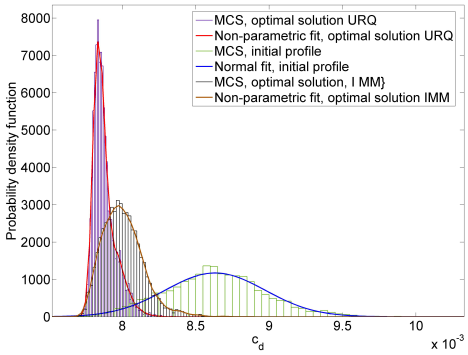
Figure 6.5: I MM and URQ optimization.

and analyze the features of the two optimal solutions, a post-optimal analysis is performed through a MCS (Latin Hypercube with 6000 samples). $\mathbf{x}_{opt}$ is represented as a Gaussian random variable centered at the values of the input variables resulting from the two optimizations. The variance of $\mathbf{x}$ is the same as the one used throughout the optimizations. The improved accuracy in estimating the moments yielded by the URQ method can be checked from Table 6.4.

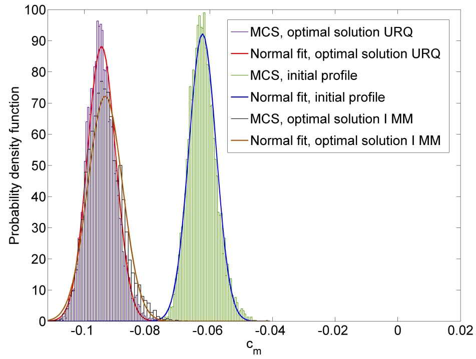
	Mean estimation		**Variance estimation**	
Obj./Constr.	$x_{opt,IMM}$	$x_{opt,URQ}$	$x_{opt,IMM}$	$x_{opt,URQ}$
c_d	$0.43 \cdot 10^{-2}$	$-0.15 \cdot 10^{-3}$	0.72	-0.14
c_m	$-0.38 \cdot 10^{-2}$	$-0.18 \cdot 10^{-3}$	0.20	$0.18 \cdot 10^{-1}$
$thickness_{12\%}$	$0.18 \cdot 10^{-4}$	$0.24 \cdot 10^{-5}$	$0.10 \cdot 10^{-1}$	$-0.02 \cdot 10^{-2}$
$thickness_{60\%}$	$-0.62 \cdot 10^{-4}$	$0.69 \cdot 10^{-5}$	$0.71 \cdot 10^{-1}$	$-0.86 \cdot 10^{-2}$

Table 6.4: Post-optimality analysis: relative error on mean and variance estimation of objective and constraints with respect to MCS.

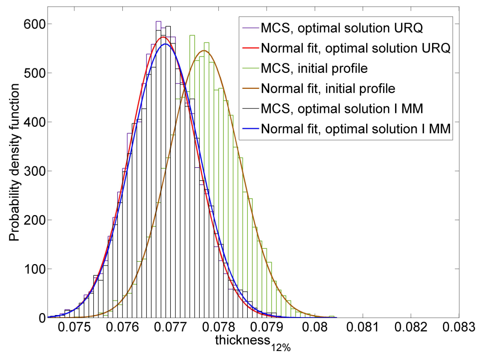
From Figure 6.6(a), it can be seen that the URQ optimal solution outperforms the I MM solution in terms of drag estimate, yielding a lower mean and a lower standard deviation.



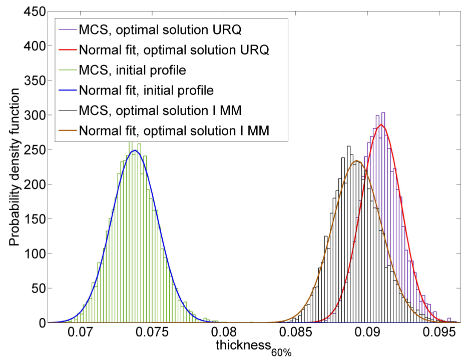
(a) Objective: drag coefficient.



(b) Constraint: pitching moment coefficient.



(c) Constraint: thickness at 12% chord.



(d) Constraint: thickness at 60% chord.

Figure 6.6: MCS validation of optimal results.

6.4 Adopting Pattern Search methods

As mentioned in Section 3.6, Pattern Search methods can be advantageously adopted for problems such as Problem (6.2) when objectives and constraints are noisy as in our VGK application.

Our interest here is, in the first instance, to evaluate the ability of the URQ to supply a valid heuristic to the poll phase of the optimization algorithm. It is not our purpose to demonstrate that such heuristic is superior to the existing ones. Such a demonstration would be, in general terms, a daunting task, since it depends on many features of the function under study which are not known

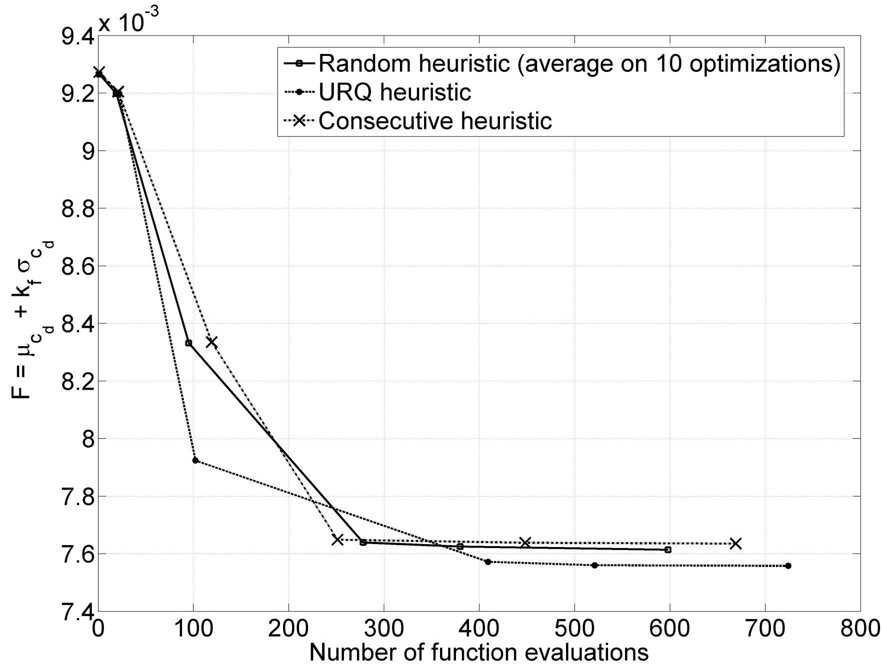


Figure 6.7: Comparison of the optimization performance yielded by the different heuristics.

a priori, and on many optimization parameters which usually require tuning. However, we have found frequent cases in which such application is convenient, such as the one shown in Figure 6.7, obtained for the coefficients $k_f = \sqrt{2}$, $k_{\mathbf{x}} = 1$ and $k_{g_i} = 1.22$, for $i = 1 \ldots 4$, having modeled the design variables as normal variables truncated to the range $[\mu_{\mathbf{x}} - 3\sigma_{\mathbf{x}}, \mu_{\mathbf{x}} + 3\sigma_{\mathbf{x}}]$ with a standard deviation $\sigma_{\mathbf{x}}$ chosen to be the 3% of the input variable range. The results yielded by the algorithm employing such heuristic are compared with two others implemented in the Matlab optimizer `patternsearch`, which are:

- the consecutive poll, which checks for improvement along x_1, then x_2 and so on;
- the random poll, which chooses at random the direction on the stencil where to start interrogating the function at each iteration.

For the airfoil test case, an effective decrease can be achieved by our method in the first phases of the optimization. Later on, despite attaining the lowest c_d value, the algorithm employing the URQ heuristic requires the largest number of function evaluations to converge. Such result mainly depends on the size of initial pattern, which is one of the parameter which has to be tuned when performing PS optimization. In this case, in fact, the initial pattern is chosen to have comparable size with the URQ stencil. When the pattern size decreases, as the optimizer moves towards convergence, the approximate derivative information harvested on the URQ stencil belongs to a larger scale of variation and ceases to be useful. A possible implication of this observation is that the adoption of the URQ heuristic may suggest a choice of the initial pattern. Furthermore, the ratio between the scale of the pattern and the scale of the URQ stencil can be exploited as a criterion to switch to another optimization algorithm, thus realizing an hybridization. In fact, it is known that PS can quickly identify an area of smaller function values in the design space. However, the deployment of QN methods might be beneficial in the final stages of the optimization because of their second order convergence capabilities. To exploit the advantages of both kinds of algorithm, we hence proceed to their hybridization, which needs a criterion to switch from the Pattern Search to the gradient based method. Such criterion is chosen to be dependent on the mesh size contraction ratio, which is limited to 100. We solve again Problem (6.2), using the coefficients $k_f = 1$, $k_{\mathbf{x}} = 1$ and $k_{g_i} = 1$, for $i = 1 \ldots 4$, and having modeled the design variables as normal variables with a standard deviation $\sigma_{\mathbf{x}}$ chosen to be the 3% of the input variable range. It can be seen from Figure 6.8 that the resulting hybrid algorithm

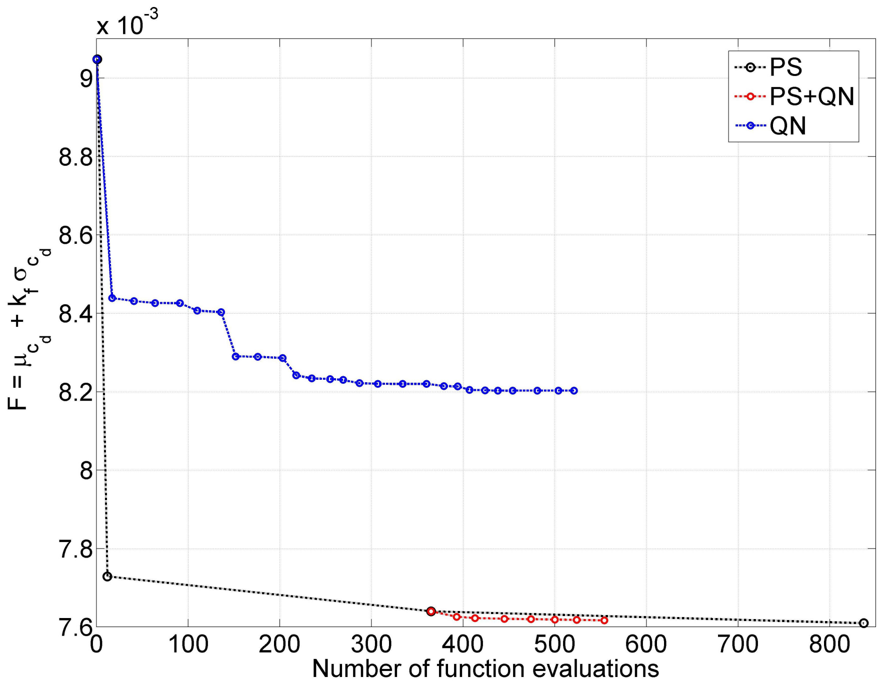
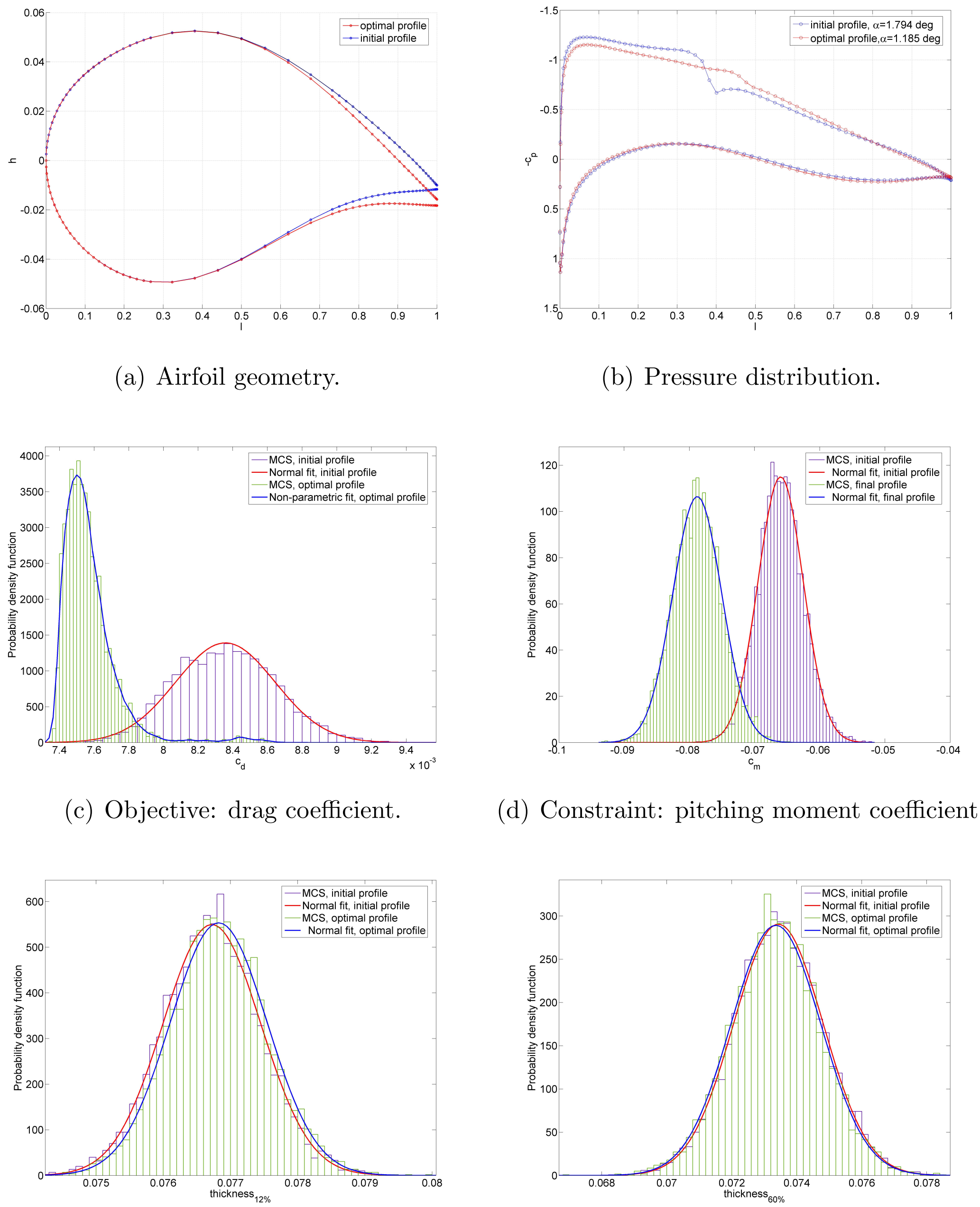


Figure 6.8: Convergence history of the hybrid optimization algorithm.

requires a smaller number of iterations to locate a robust solution, compared to the PS method alone, and is more effective than the QN in minimizing the drag. The initial airfoil and the one obtained by hybrid optimization are presented, with their pressure distributions, in Figure 6.9(a) and Figure 6.9(b).



(a) Airfoil geometry. (b) Pressure distribution.

(c) Objective: drag coefficient. (d) Constraint: pitching moment coefficient.

(e) Constraint: thickness at 12% chord. (f) Constraint: thickness at 12% chord.

Figure 6.9: MCS validation of optimal results.

Geometrically, the main differences are noticeable at the trailing edge. Under the aerodynamic point of view, the optimization locates a good area in the design space by identifying the critical variables to be tuned to soften the shock located on the upper surface of the initial airfoil at approximately $l = 0.34$. A MCS analysis carried out by using Latin Hypercube with 6000 samples has been used to validate the URQ technique, in correspondence of the initial and the optimal airfoils. The relative error of the URQ estimates for mean and standard deviation with respect to the MCS estimates are limited to 0.3% and 4%, respectively. Such *a posteriori* analysis can also demonstrate the successful reduction of the objective in mean and variance, as it is shown in Figure 6.9(c), in which for the sake of presentation the data from the simulation has been fitted with a normal and a non-parametric distributions. From Figures 6.9(d), 6.9(e), 6.9(f) it can be appreciated that normal distributions fit the MCS data well. The visual assessment of the goodness of the fits with respect to the simulation data may be sufficient to justify the adoption of the normality assumption for the constraint. At the same time, it would suggest either assuming the unimodality of the objective, and hence taking into account the Vysochanskij-Petunin inequality (Eq.(4.8)), or the Chebyshev TCE bound (Eq. (4.14)).

6.5 Discussion of the results

The transonic airfoil design test case has confirmed the benefits for design optimization relating to the increased accuracy of the URQ with respect to linearization. Furthermore, it has been shown that the URQ is more robust than I MM in dealing with functions which are affected by noise due, for example, to incomplete convergence. This is due to the integral approach at the basis of the URQ method. In addition, such method is simpler to implement than propagation methods relying on finite differences, since it does not require any preliminary study aimed at finding the optimal step h_{FD} which minimizes truncation and round-off errors.

A single level of accurate derivatives of the system analysis code can be obtained by the Complex Variable Method, at the price of an increased computational cost. In such case, it has been shown that the effectiveness of gradient-based RDO can be significantly enhanced by adopting the derivative-free URQ method instead of the I MM to build the robust objectives and constraints.

If no accurate derivative is available, the class of direct search methods constituted by the Pattern Search methods could be the option of choice. In fact, by coupling a Pattern Search algorithm with the URQ propagation method, a robust design optimization method is built which does not require any explicit derivative information. Such method has been applied to the airfoil test case and the use of objective's and constraints' URQ approximate sensitivities as an heuristic for the PS has been assessed. Despite the test has been successful in showing that it is possible in this way to increase the effectiveness of the RDO process, we cannot claim that such improvement is achievable in all the cases of interest. There are two important limitations that have to be noted with this regard:

- the hypothesis that quickly identifying a direction of descent within a poll leads to quicker overall optimizations is not always verified and depends on the structure of the underlying function;
- nothing can be said about the possibility of converging towards a lower minimum than the one found by the other heuristics.

Nevertheless, such limitations affect also to the other available heuristic. Pattern Search algorithms can also succeed in identifying promising design regions, at the outset of the optimization, which are then explored by means of gradient based methods. On this basis, the hybridization of the two algorithms has been evaluated. The results on the test case exhibit improvements on the robustness of the optimal design and the efficiency of the optimization.

6.6 Summary and conclusions

In this chapter, the proposed methodology has been applied to the process of shape optimization at the conceptual design stage. The considered test case makes use of the CFD code VGK, the geometry parameterization technique PARSEC-11, and is wrapped in Matlab. We have shown:

1. the benefits yielded by an integral uncertainty propagation approach such as the URQ when dealing with noisy functions, in contrast with the differential approach represented by Taylor-based method of moments;

2. the possibility of applying the URQ method within a gradient-based approach, when a single level of accurate derivative is available; in this respect, the analysis concerning the use of the complex variable method complements the study on the adoption of AD techniques in the RDO context presented in Chapter 5;

3. the application of a completely derivative-free robust optimization algorithm which couples Pattern Search algorithms and the URQ method and can be very effective when the functions of interest are noisy;

4. the possibility of improving Pattern Search algorithm performance by adopting the poll heuristic based on the URQ propagation, and via the hybridization with gradient-based methods.

The following chapter resumes the advantages of the proposed methodology, and discusses its limitations, within the scope of this research.

Chapter 7

Conclusions

7.1 Introduction

This Chapter presents the conclusions of the thesis. In Section 7.2, the achievement of the research objectives is assessed. In Section 7.3, the thesis contributions are summarized. In Section 7.4, the current limitations are examined, while the vision on future work is presented in Section 7.5.

7.2 Summary of research

The presented research stems from the recognized need that computational design tools have to account for the uncertain facets of design to benefit engineering practice. A first research objective has been, therefore, *to identify and understand the typologies of uncertainty in engineering design and their theoretical representation* (Obj. 1). Such objective has been achieved by framing the problem in an epistemological domain which is specific to engineering. Engineering, in fact, adopts a pragmatic and contingent form of rationality which also shapes the tools required to handle uncertainty in design. Within such framework, uncertainty analysis turns out to be not only a necessity, but also a powerful cognitive opportunity, in a never-ending dialectic confrontation between known and unknown. Hence the fundamental understanding that the ways we are given to deal with uncertainty are doomed to be provisional, at the upper level, at which the computational design problem is formulated, and at the lower level, at which it is solved. Within such levels, significant challenges to computational design emerge, regarding the relevance of the assumptions made when formulating the problem, the identification of desirable design qualities when the uncertainty is considered, the accuracy and the efficiency achievable in solving the problem. Hence the two complementary research objectives: (Obj. 2) *the development of suitable numerical techniques to improve current uncertainty-based methods for engineering computational design* and (Obj. 3) *the incorporation of additional metrics of system performance under uncertainty to widen the currently available scope of design choices.* The state of the art regarding such aspects for the case of probabilistic uncertainties has been reviewed in Chapter 3, and has helped identifying specific knowledge gaps:

1. the lack of accurate methods which can be efficiently applied in robust optimization at the conceptual stage;

2. the shortage of intermediate options between accurate, but expensive formulations of the probabilistic constraints and cheap, but potentially unreliable moment based formulations;

3. the assessment of metrics such as the tail conditional expectation, which may contribute, in analogy to recent developments in the financial engineering field, to extending the set of available robustness metrics.

The methodology presented in Chapter 4 has been proposed to overcome such difficulties. Firstly, the problem has been formulated in order to relax, when required, the common RDO assumption regarding the normality of objectives and constraints, which might be inaccurate and negatively impact on the meaning of the optimization process. The proposed formulation extends the validity of robust design and does not impact on its cost, since objectives and constraints are still formulated, as in the usual RDO practice, by means of their first two moments. Secondly, starting from engineering considerations about the risk related with design unfeasibility, suitable estimates of tail conditional expectation (TCE) have been introduced in the set of robustness metrics. We have proposed the adoption of TCE type of metrics in RDO for two purposes. On the one hand, to allow the designer to specify the preference as a threshold on the expected value of a given worst percentage of the considered designs. On the other, when they are expressed in terms of mean and variance, to relax the unverified distributional assumptions on the output, while obtaining a tighter estimate than the corresponding quantile bounds. In the third place, a novel uncertainty propagation technique has been proposed to estimate the first two moments of objective and constraints, required by the formulation above. In this respect, a favorable trade-off between the accuracy of the estimates and the required computational cost has been achieved, by employing an improved reduced quadrature method, which can handle a fairly generic class of input distributions identified by their first four moments (assumed finite), also in the presence of correlation. By means of mathematical analyses and simple numerical examples we have demonstrated that the proposed approach improves the accuracy of the estimation with respect to methods of comparable computational cost. Furthermore, we have shown how to exploit peculiar features of the propagation technique to intimately couple the propagation and the optimization phases for two classes of algorithms, namely gradient-based methods and the derivative-free pattern search methods. We have also analyzed the possible advantages achievable when the two types of algorithms are hybridized. The capability of the proposed methodology to achieve objectives Obj.2 and Obj.3 has been tested on two engineering design problems, concerning aircraft sizing and airfoil design, in Chapter 5 and 6, respectively. Such assessment have highlighted the advantages yielded by the adoption of the proposed methodology and shown some of its limitations, which form the scope for future work.

7.3 Contributions to knowledge

The main contributions of the thesis in achieving the objectives can be summarized as follows:

1. a schematic representation of the design process involving computational tools. It enables to frame the relevant uncertainty types and to contextualize the methods for computational design under uncertainty;

2. the formulation of the robust design optimization problem as a worst-case optimization within a given distributional assumption. The proposed formulation extends the validity of robust design and does not impact on its

cost, since objectives and constraints are still formulated, as in the usual RDO practice, by means of their first two moments;

3. the introduction of suitable estimates of tail conditional expectation to extend the set of the currently available robustness metrics. Such metrics allow the designer to specify objectives and constraints as thresholds on the expected value of a given worst percentage of the considered designs. Furthermore, when they are expressed in terms of mean and variance, they help in relaxing an unverified distributional assumption on the output, while obtaining a tighter estimate than the corresponding quantile bounds;

4. a novel uncertainty propagation technique to estimate the first two moments of the output response. It employs an univariate reduced quadrature method, which can handle a fairly generic class of input distributions identified by their first four moments (assumed finite), also in the presence of correlation. Such approach improves the accuracy of the estimation with respect to methods of comparable computational cost, and exhibits peculiar features which can be exploited to advantageously couple the propagation and the optimization phases.

7.4 Limitations

There are a number of limitations associated with the proposed methodology. First of all, the problem formulation through quantile and tail expectation bounds is always conservative and might be judged to be overconservative for many of the cases of interest. However, such judgment depends on a trade-off between the accuracy of constraint evaluation and its computational cost. If very narrow margins are of interest, approaches such as MCS or reliability-based constraints should be adopted, alone or together with the bounds formulation. Furthermore, the current formulation does not take into account skewness and kurtosis of the output distributions. By adopting higher order quadrature schemes, however, such moments also could be estimated with sufficient accuracy. Tighter inequality bounds could then be formulated as function of the first four moments.

The higher accuracy which can be achieved by adopting the URQ (and higher quadrature schemes) rests on the availability of the third and the fourth moments, which in practice might not be available or not known with sufficient accuracy.

In such case, the adoption of the method is questionable and other less precise uncertainties models for the input variables and parameters should be adopted.

The URQ obtains mean and variance as weighted sums of functional values evaluated in correspondence of a number of *fixed* nodes in the input space. However, its predictions may be prejudiced if, for any of such nodes, the code at hand fails to give a reliable output or crashes.

7.5 Future work

Future work could focus on the extension of the proposed methodological framework. The objective might be formulated to exploit the information of correlation for objectives and constraints, which can be obtained through the URQ propagation method. Multidimensional inequalities could be explored to take into account the joint probability of constraint feasibility, instead of relying on single constraints formulation. With regard to the TCE, obtaining such metrics by means of reliability-based and MCS algorithms could allow extending the use of TCE to other fields of design under uncertainty. Furthermore, TCE bounds could be formalized for other assumptions such as the unimodality of the output probability density function. We have shown that the departure from III MM accuracy can be kept under control during the optimization phase; however, this feature is exploited at present only as a warning. Future work may investigate the deployment of higher order quadratures in correspondence of the points for which the error exceeds the prescribed tolerances.

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Appendix A

Uncertainty taxonomies in literature

One of the common strategies identified in literature to handle uncertainty is the formulation of uncertainty taxonomies. Many of those have appeared in literature during the years with the purpose of ordering and simplifying the field of uncertainty analysis each time it was expanded by a new theoretical breakthrough. A significant research effort has therefore concerned their review, which is presented in this Appendix with the aim of complementing the theoretical discourse in Chapter 2. We start the review with the distinction about two recurrent classes of uncertainty (Section A.1), and then we move on to more articulated classifications: in Section A.2 classifications concerning the nature of uncertainty, which often imply a relationship of the categories with formalized mathematical theories, are presented; Section A.3 shows instead categorizations identifying sources of uncertainty.

A.1 Some recurrent dualistic classifications

Very often, uncertainty is classified from a dualistic point of view. One of the most common distinctions is related to the concepts of aleatory and epistemic uncertainty. Aleatory uncertainty is a synonymous for randomness, and is said to embrace phenomena that are predictable, in principle, but are treated as random for simplicity, and phenomena which are intrinsically unpredictable. Epistemic uncertainty, instead, represents subjective uncertainty about propositions, due to lack of knowledge or information. It is clear that the problematic nature of this categorization stands in the impossibility to conclusively demonstrate that there is a complexity in the world that is independent from cognitive limitations or, on the other side, that such complexity is due to those limitations. This separation recalls the old issue of the duality between objective and subjective probability, and for this reason turns out to be an issue for Bayesians. They usually refuse this conjectural distinction, denying to it any solid foundational basis, nevertheless, they think that it is useful for eliciting, propagating and analyzing, to distinguish between those two kinds of uncertainties (see for example [62,87,161,223]). Other similar taxonomies occur in literature, where epistemic is sometimes substituted by *reducible*, *subjective*, *cognitive*, *secondary* or *internal* uncertainty, in opposition to *irreducible*, *objective*, *stochastic*, *primary* or *external* uncertainty. However, not all those kinds of binary divisions are equivalent, as supposed for example in [153] or [51], at least not in all their interpretations. For example, while it is clear that reducible uncertainty forms a separate entity from irreducible uncertainty, epistemic and aleatory uncertainty are not disjoint [148]. In fact, complete ignorance about the nature of a quantity (i.e., epistemic uncertainty) can reveal, after careful enquiry, an intrinsic aleatory nature. Besides, Oberkampf and his coauthors [153] judge such division useful to distinguish between what probability can deal with (aleatory uncertainty) and what would better be treated with evidence theory (see Section 2.4.2). This implicitly means admitting that aleatory uncertainty is a particular case of epistemic uncertainty, as probability is a particular case of evidence theory. Pragmatically, it could be said that we may want to know which is the uncertainty reducible by acquiring more information, or appropriate knowledge, but *at the time of action and with the available resources*, and what kind of uncertainty we should consider at that time as irreducible.

A.2 Classification by nature

A.2.1 Klir and Folger, 1988

G. Klir is the author of a huge and path breaking literature in the field of uncertainty. In this 1988 book [106], coauthored by T. Folger, the foundations of what

Kind of Uncertainty	**Definition**
Vagueness	is peculiar to a domain that cannot be limited by sharp boundaries.
Ambiguity	is associated with one-to-many relations.
Nonspecificity in evidence	is connected with the size of the subsets that are designated by a fuzzy measure as prospective locations of the element in question.
Dissonance in evidence	arises when disjoint subsets of a same set are designated by the given fuzzy measure as prospective locations of the element of concern.
Confusion in evidence	is associated with the number of subsets of a same set that are designated as prospective location of the element under consideration and that do not overlap, or overlap only partially.

Table A.1: Uncertainty definitions for Klir and Folger [106].

will be later call Generalized Information Theory (see Section 2.4.2) were laid. Within GIT, the uncertainty affecting a specific problem represents the total amount of information potentially available about it. It may be caused by different kinds of information deficiency, which were described in [106] as summarized in Figure A.1 and defined in Table A.1.

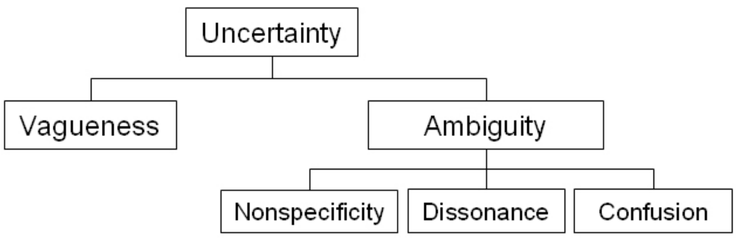

Figure A.1: Uncertainty classification following Klir and Folger [106].

A.2.2 Smithson, 1989

With the aim of finding a working definition of ignorance, Smithson [194] points out that common language distinguishes between *ignoring* and *being ignorant*, the first meaning "deliberate inattention to something", and the second a kind of "distorted or incomplete knowledge". As we can see from Figure A.2, for

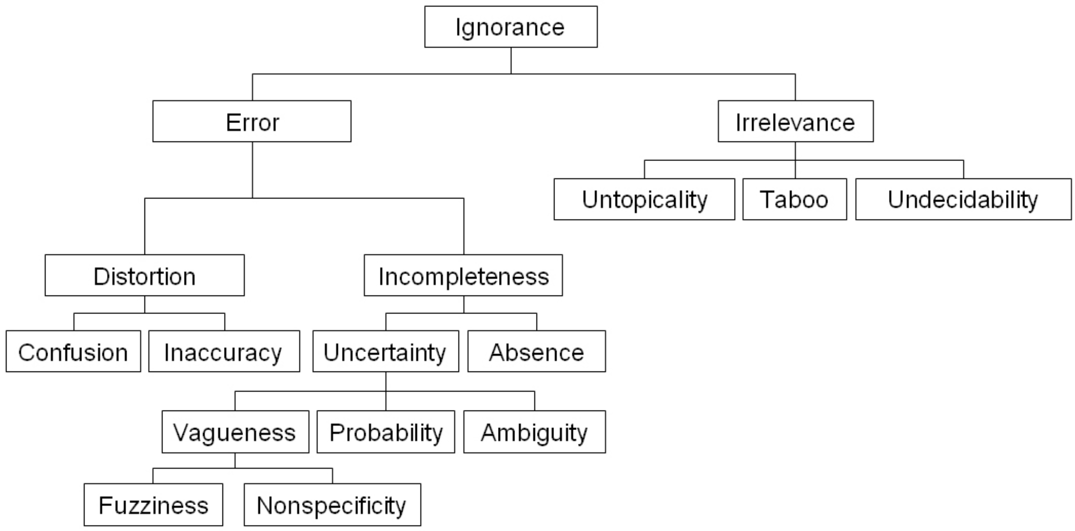

Figure A.2: Ignorance classification following Smithson [194].

Kind of Uncertainty	**Definition**
Probability	refers to the likelihood that an event will happen.
Ambiguity	refers to two or more distinct possible states for a single concept or event.
Vagueness	refers to a range of possible values on a continuum.
Fuzziness	characteristic of event or categories that have blurry edges.
Nonspecificity	characteristic of imprecise fuzzy events.

Table A.2: Uncertainty definition following Smithson [195].

representing such duality in his taxonomy, he separates ignorance into *irrelevance* and *error*. One type of error is *distortion*, which involves either the degree of a considered entity (which is termed *inaccuracy*), or its kind (which is called *confusion*). Error can also be generated from *incompleteness*, in turn separated into *absence* (incompleteness of kind) and *uncertainty* (incompleteness in degree), whose detailed definition is provided in Table A.2, taken from [195]. On the other side, irrelevance is divided into *untopicality*, which concerns something that can be declared out of context, *taboo*, if the limits for the investigation are enforced either by social rules or intellectual dogmas, and finally *undecidability*, which refers to matters that are considered insoluble, or whose “validity or verifiability is not pertinent”.

A.2.3 Hansson, 1996

With the purpose of identifying possible strategies to cope with uncertainty affecting real life problems, in particular environmental issues, Hansson proposed in 1996 [77] a very interesting categorization of "great uncertainty". As shown in Figure A.3, four main components are distinguished:

1. *uncertainty of demarcation*: there is no agreement on what the decision is about, or what the options are;
2. *uncertainty of consequences*: very little is known about the possible decision outcomes, and their probability of occurrence;
3. *uncertainty of reliance*: refers to the impossibility of relying on expert judgement;
4. *uncertainty of values*: concerns the doubtful quantification of decision consequences into comparable values.

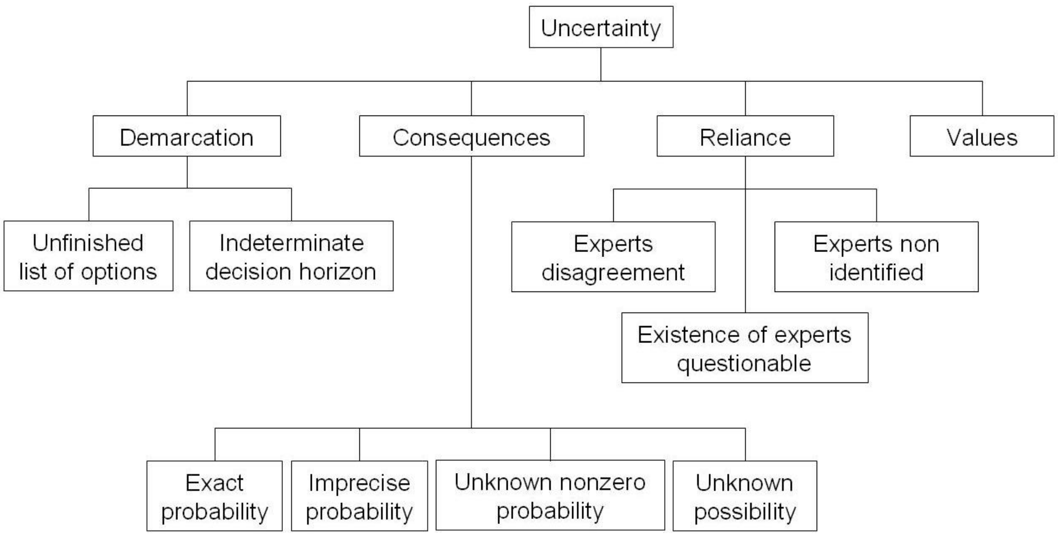

Figure A.3: Categories of great uncertainty, from Hansson [77].

A.2.4 Oberkampf *et al.*, 1999

Oberkampf and his research group, based at Sandia National Laboratories, have obtained several results on uncertainty analysis during last years (see for example [83, 84, 152–154]). In [152], they presented their ideas about the so-called *total uncertainty* in computer simulation, which they split in three categories, as shown in Figure A.4. The first of those categories is *Variability*, defined as "the inherent variation associated with the physical system or the environment under consideration". *Uncertainty* is defined as a "potential deficiency in any phase or activity of the modeling process due to lack of knowledge or incomplete information". Such double nature of uncertainty reflects one of the distinctions pointed out already by Smithson [194] between what he called *informational* and *epistemological* ignorance: it seems to be a very subtle distinction, but is useful to distinguish an erroneous knowledge about factual manners (the information), and about the ability to process them (the knowledge). In [153], Oberkampf terms the latter category *epistemic* [1] uncertainty, while variability becomes *aleatory* uncertainty, thus assuming the popular distinction among the uncertainty community. Uncertainty is hence subclassified into three further categories, which are summarized in table A.3, and resemble in some aspects the classification made by Klir and Folger [106], not considering *confusion*.

The last category of this classification, *error*, is described as a "recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge", and then subclassified into *acknowledged* error, such as finite precision arithmetic, model simplifications or PDE discretization, or *unacknowledged* error like programming mistakes. Qualifying this deficiency as "recognizable" presupposes, on the one hand, the existence and the knowledge of a condition that is universally considered to be true; on the other, it stresses that unrecognizable errors, due for example to some unknown limits of the theory in use, are not captured by this taxonomy, which only accounts for first-order uncertainty.

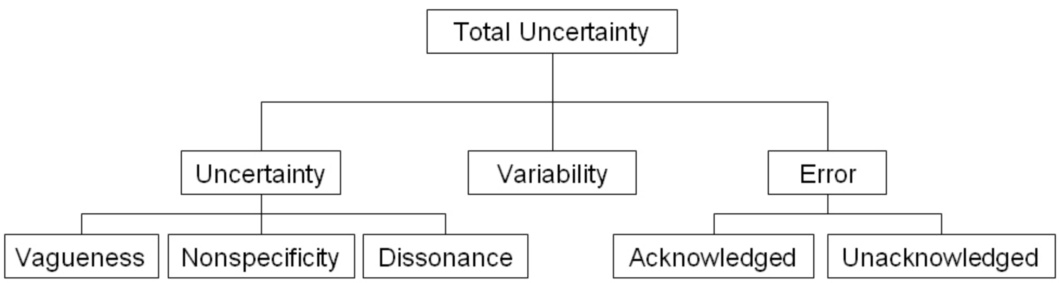

Figure A.4: Total uncertainty in computer simulation [152].

[1] The term "epistemic" indicates something pertaining to knowing or knowledge, while "epistemological" defines something pertaining to the study of knowledge.

Kind of Uncertainty	**Definition**
Vagueness	refers to information that is imprecisely defined, unclear, or indistinct.
Nonspecificity	reflects the variety of alternatives in a given situation that are all possible, i.e. non specified.
Dissonance	refers to the existence of totally or partially conflicting evidence.

Table A.3: Uncertainty definitions in computer simulation [152].

A.2.5 Ayyub, 2001

Undoubtedly influenced by Smithson's work, Ayyub [5] proposed the taxonomy of ignorance presented in Figure A.5 and in Table A.4.

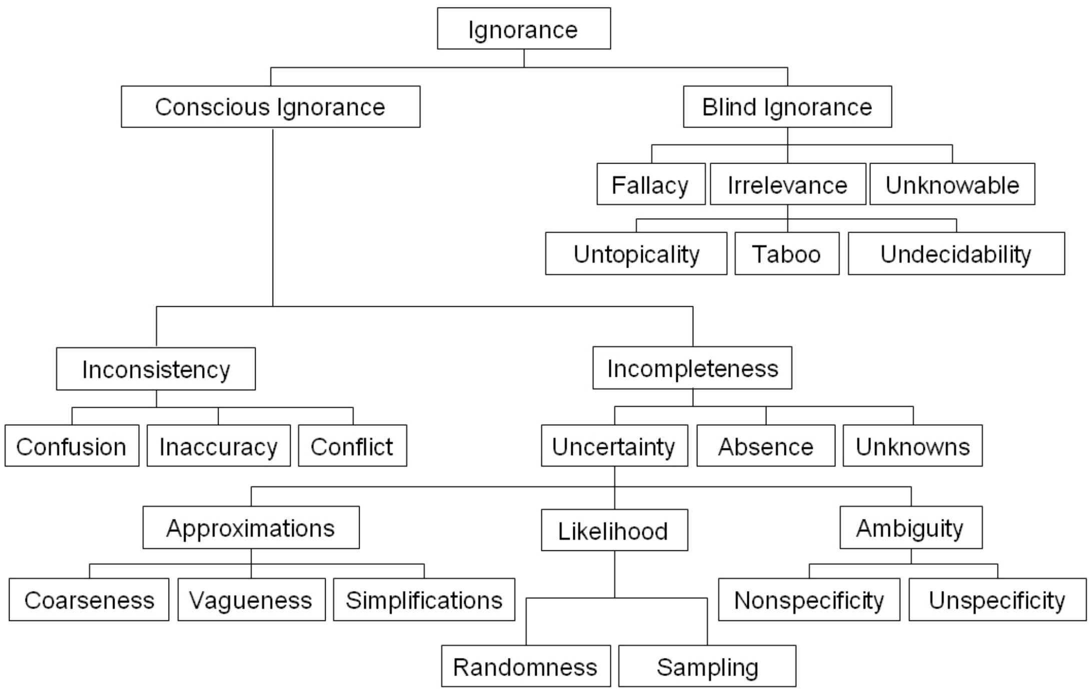

Figure A.5: Taxonomy of ignorance following Ayyub [5].

The distinction between *conscious ignorance* and *blind ignorance*, already mentioned in [194], is used in an equivocal way. First of all, blind ignorance contains Smithson's category of *irrelevance*, which was defined as deliberate (i.e. conscious) inattention; besides, a second order ignorance, or meta-ignorance, as blind ignorance is, should not be included in a first-order taxonomy. *Likelihood* category contains *randomness* and *sampling*, as to distinguish an inherent randomness in nature, from an uncertainty coming from a statistical interpretation of phenomena. *Vagueness* is thought to be a subcategory of *approximation*, while *nonspecificity* is included in *ambiguity*, following Klir, though the category of *conflict* is considered a special kind of *inconsistency*.

Kind of Uncertainty	**Definition**
Uncertainty	knowledge incompleteness due to inherent deficiencies with acquired knowledge.
Ambiguity	the possibility of having multi-outcomes for processes or systems.
Unspecificity	outcomes or assignments that are not completely defined.
Nonspecificity	outcomes or assignments that are improperly defined.
Approximations	a process that involves the use of vague semantics in language, approximate reasoning, and dealing with complexity by emphasizing relevance.
Vagueness	noncrispness of belonging and nonbelonging of elements to a set or a notion of interest.
Coarseness	approximating a crisp set by subsets of an underlying partition of the sets universe that would bound the set of interest.
Simplifications	assumptions needed to make problems and solutions tractable.
Likelihood	defined by its components of randomness, statistical and modeling.
Randomness	nonpredictability of outcomes.
Sampling	derives from considering samples to account for the underlying populations.

Table A.4: Uncertainty definitions following Ayyub [5].

A.2.6 Regan *et al.*, 2002

Regan and coauthors [175] focus their attention on uncertainty taxonomy in the field of ecology and conservation biology. They distinguish between *epistemic* and *linguistic* uncertainty, which are associated, respectively, with knowledge in the state of a system, and communication. This distinction views uncertainty as a social and cultural product rather than a sole property of the natural environment, as noted by Smithson, who argued: "people have interest in and motivation for creating and maintaining uncertainty and even ignorance, and any overview that does not take this into account will fail to be comprehensive" [195]. Epistemic uncertainty is divided into six main types, which are heavily inspired by the work of Morgan and Henrion [143]:

1. *measurement error*: results from imperfections in measuring equipment and observational techniques, and includes operator error and instrument error;
2. *systematic error*: due to measurement or theoretical biases;
3. *natural variation*: refers to unpredictable change;
4. *inherent randomness*: occurs because the system is irreducible to a deterministic one;
5. *model uncertainty*: arises because of the interpretation and representation, by the use of mathematical abstractions and approximations, of physical systems;
6. *subjective judgement*: occurs as a result of interpretation of data.

It is worth noting that in this case natural variation, or inherent randomness, that were elsewhere considered to be features of the world in itself, are ascribed to cognitive limitations. The category "model uncertainty" could be also called *interpretation* uncertainty (due to the rationalization of a phenomenon) or *abstraction* uncertainty (that arises every time a theory is called to describe the reality). However, some of the mentioned causes of uncertainty, such as surrogate-modeling errors, distinguish uncertainty by source, rather than by nature. At this regard, the authors stress the importance of validation studies to cope with model uncertainty.

The classification of linguistic uncertainty indicates the following types:

1. *vagueness*: as per the standard usage;
2. *ambiguity*: as per the standard usage;
3. *underspecificity*: occurs when the statement in question does not provide the degree of specificity we desire, causing unwanted generality;

4. *context dependency*: arises from a failure to specify the context in which a proposition is to be understood;

5. *indeterminacy of theoretical terms*: caused by the fact that the future usage of theoretical terms is not completely fixed by past usage and, for example, a term that is not ambiguous at the moment can have the potential for ambiguity.

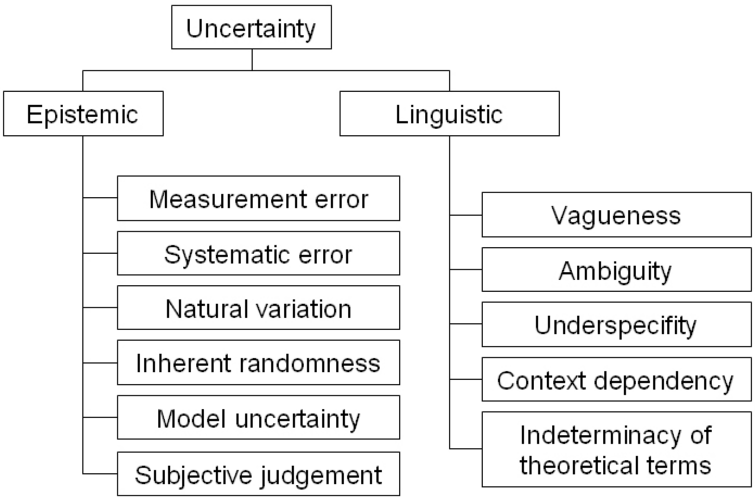

Figure A.6: Uncertainty in ecology and conservation biology [175].

A.2.7 Thunnissen, 2005

On the basis of an extensive literature review, Thunnissen proposed in his Ph.D. thesis [203], a taxonomy for the design of complex systems, which is shown in Figure A.7.

Thunnissen defines uncertainty as "the condition of not knowing", which thus overlaps with the concept of ignorance formalized by Smithson. Such interpretation is common in literature, and may be thought as originating by the implicit use of an irrelevance rule. The author'effort is aimed at finding a synthetic taxonomy that could take into account more types of uncertainty than usually done in the field of design. The first level of classification considers a sort of distinction by nature, dividing uncertainty in *ambiguity*, *epistemic*, *aleatory*, and *interaction* uncertainty, where ambiguity stands for linguistic uncertainty.

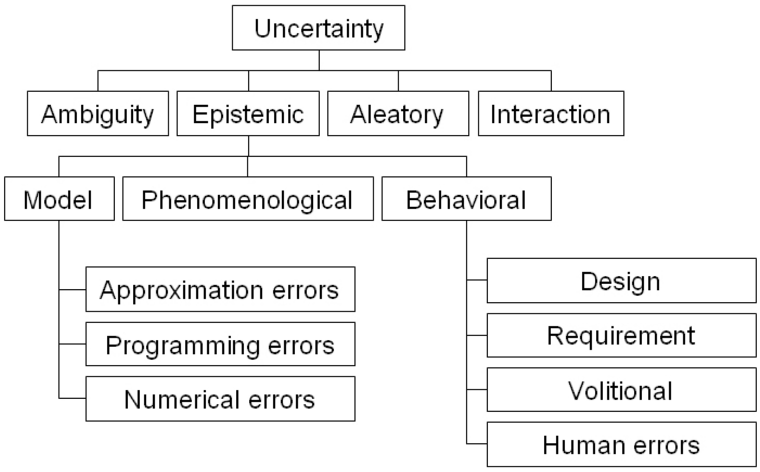

Figure A.7: Uncertainty in the design of complex systems (from [203]).

At the second level, when describing in detail epistemic uncertainty, the classification shows some similarities with classifications by source. Epistemic uncertainty is then divided into *model*, *phenomenological* and *behavioral* uncertainty. It is noteworthy to stress the difference with Oberkampf's distinction between error and epistemic uncertainty (which includes error in this taxonomy). Phenomenological and model uncertainty resemble Melchers' definitions (see Section A.3.2); the latter is further subdivided into *approximation*, *numerical* and *programming* error. Behavioral uncertainty, related to how individuals and organizations act, is subdivided into *design*, *requirement*, *volitional* uncertainty and *human error*. A design uncertainty occurs if any of the design decisions has not been made yet, while requirement uncertainty refers to changes in specifications. Volitional uncertainty reflects the not complete predictability of human will, while human mistakes are due to blunders.

A.3 Classification by source

A.3.1 Rowe, 1994

Rowe [180] ascribed the cause of uncertainty to the absence of information, and proposed a multilevel, multidimensional framework which is more than a taxonomy by source. A first decomposition regards four classes of uncertainty:

1. *Temporal*: related to future or past states;

2. *Structural*: due to complexity;

3. *Metrical*: due to measurement;

4. *Translational*: due to communication.

All these classes are affected by *variability*, which counts among its sources *underlying variants* (like apparent inherent randomness of nature, inconsistent human behavior or nonlinear dynamic systems), *collective/individual membership* (characteristic of stochasticity) and *value diversity* (due to varying perspectives and value system among people). Uncertainty ascribable to those classes can be originated by different sources, as shown in Figure A.8. We would notice

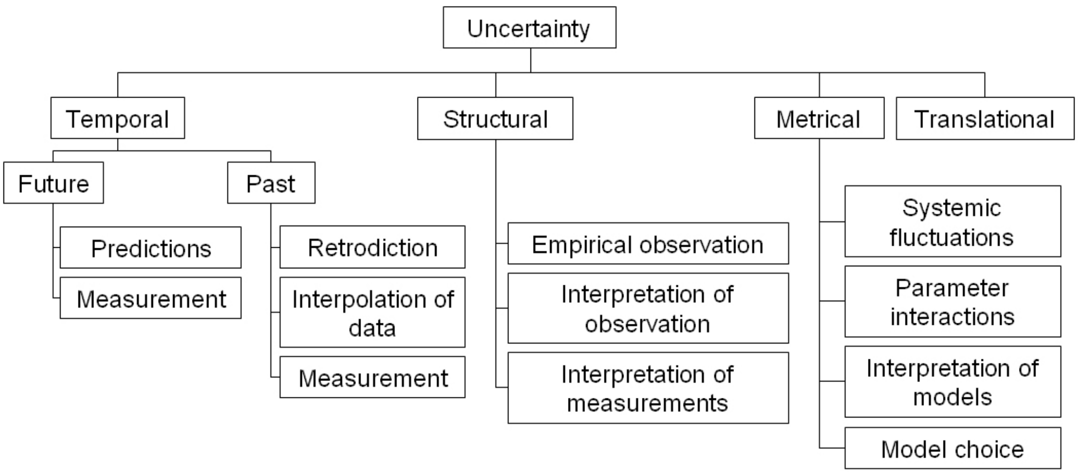

Figure A.8: Uncertainty categorization following Rowe [180].

that temporal uncertainty is mainly made of what is elsewhere called statistical uncertainty, while structural uncertainty, coupled with the categories of model choice and interpretation could be assimilated to a strict subjective uncertainty.

A.3.2 Melchers, 1999

Melchers' categories of uncertainty [139], whose definitions are reported in Table A.5, are shown in Figure A.9; we reproduce the original illustration here, to take into account interactions between categories, as probably in Melchers' intentions. This categorization shows all the limitations that are common to

Kind of Uncertainty	**Definition**
Phenomenological	arises whenever the form of construction or the design technique generates uncertainty about any aspect of the possible behavior of the structure under construction, service, and extreme conditions.
Decision	arises in connection with the decision as to whether a particular phenomenon has occurred.
Modeling	is associated with the use of one (or more) simplified relationships between the basic variables to represent the "real" relationship or phenomenon of interest.
Prediction	is associated with the prediction of some future state of affairs.
Physical	is related with the inherent random nature of a basic variable.
Statistical	arises in the associated parameters when a simplified probability density function is implemented.
Human factors	
Human error	is due to natural variation in task performance and gross errors.
Human intervention	is associated with the intervention in the process of design, documentation and construction and, to some extent, also in the use of a structure.

Table A.5: Uncertainty definitions in structural reliability assessment [139].

classifications by source: since an attempt to exhaustively enumerate all possible sources of uncertainty would be doomed to failure, the field of application is often restricted. So, more than a complete taxonomy, it appears to be a description of some interacting kinds of uncertainty that are common in structural reliability assessment. This classification has inspired, in part, several posterior taxonomies (see for example Sections A.2.7 and A.3.7).

Melchers recognizes the importance of *phenomenological* uncertainty, related with outcomes that is not possible to expect, because of the novelty of the design, for example, or a never before used technique. He also stresses the peculiarity of *human factors*, which are seen as a particular case of *modeling* uncertainty: despite understanding their importance (is it known that human error is at the root of most of the surveyed structural failures, for example), their complex and multifaceted nature does not allow a satisfactory modeling, resulting in the need of a quality assurance and hazard management programs.

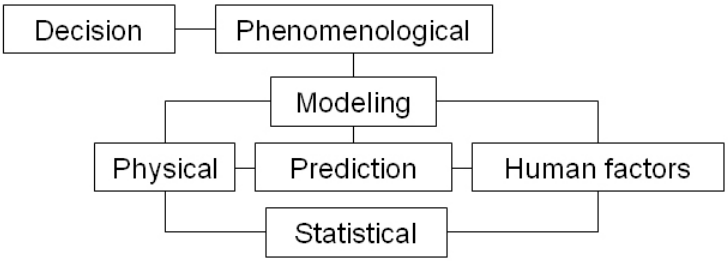

Figure A.9: Uncertainty classification for structural reliability assessment [139].

A.3.3 Isukapalli, 1999

In his Ph.D. Thesis [92], Isukapalli suggests a classification of uncertainty for transport-transformation models in chemical engineering, that has been schematized in Figure A.10. *Natural* uncertainty is due to the inherent randomness of the considered phenomena and its mathematical representation. It is also possible that a stochastic representation is chosen for practical matters also for variables that are not naturally random, but would need a difficult precise determination. *Variability* refers instead to heterogeneity across space, time or members of a population, while *model* uncertainty can be found in the own formulation of the model (*structural* uncertainty), or in its application (*data/parametric* uncertainty). Isukapalli also presents a wide-ranging enumeration of possible subcases for those uncertainties.

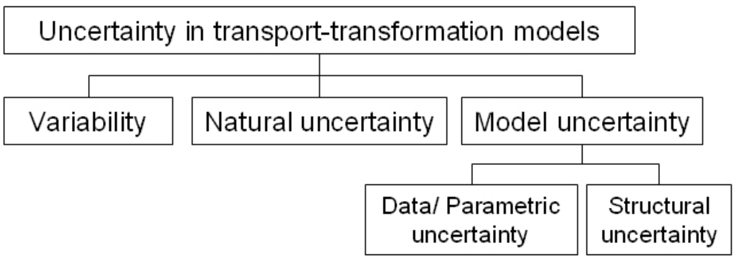

Figure A.10: Uncertainty in transport-transformation models (extrapolated from [92]).

A.3.4 DeLaurentis and Mavris, 2000

DeLaurentis and Mavris indicated in [46] several sources of uncertainties which can cause model-based predictions to differ from reality, as resumed in Table A.6 and in Figure A.11. Ambiguity of requirements is taken into account

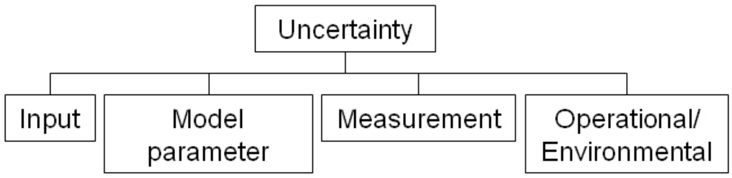

Figure A.11: Uncertainty in aerospace multidisciplinary analysis and synthesis [46].

Source of Uncertainty	**Definition**
Input	arises when the requirements that define a design problem are imprecise, ambiguous, or not defined.
Model parameter	refers to error present in all mathematical models that attempt to represent a physical system.
Measurement	occurs when the response of interest is not directly computable from the mathematical problem (i.e. it must be inferred indirectly from other measurements).
Operational/environmental	due to unknown/uncontrollable external disturbances.

Table A.6: Uncertainty in aerospace multidisciplinary analysis and synthesis [46].

as a major source of *input uncertainty*; the need for methodologies to suitably handle this kind of uncertainties is stressed. It should be noted that the category of *model parameter* uncertainty represents alone the issues related with model uncertainty, i.e. no category is proposed to account for related aspects such as the wrong choice of the model.

A.3.5 Oberkampf *et al.*, 2001

As a complement to the mentioned classification by nature, in a more recent publication [153], Oberkampf and his coauthors also give a classification of uncertainty by source, which is schematized in Figure A.12. *Parametric* uncertainty concerns parameters contained in the mathematical model of a system while *physico-chemical modeling* uncertainty is caused by limited knowledge of a phenomenon that has to be modeled. *Scenario abstraction* uncertainty, on the other side, is due to the difficult task of identifying all possible physical events that may affect the system under study, which could result in not including or not imagining scenarios that are possible.

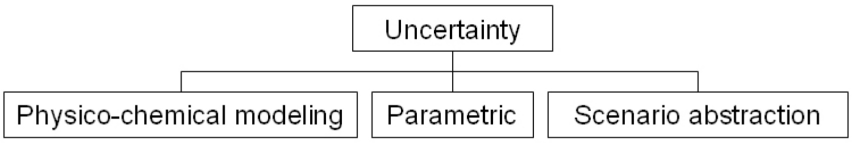

Figure A.12: Sources of uncertainty in computer simulation [153].

A.3.6 Walton, 2002

A classification aimed at incorporating uncertainty into conceptual design of space systems architectures was given by Walton in his Ph. D. thesis [211].

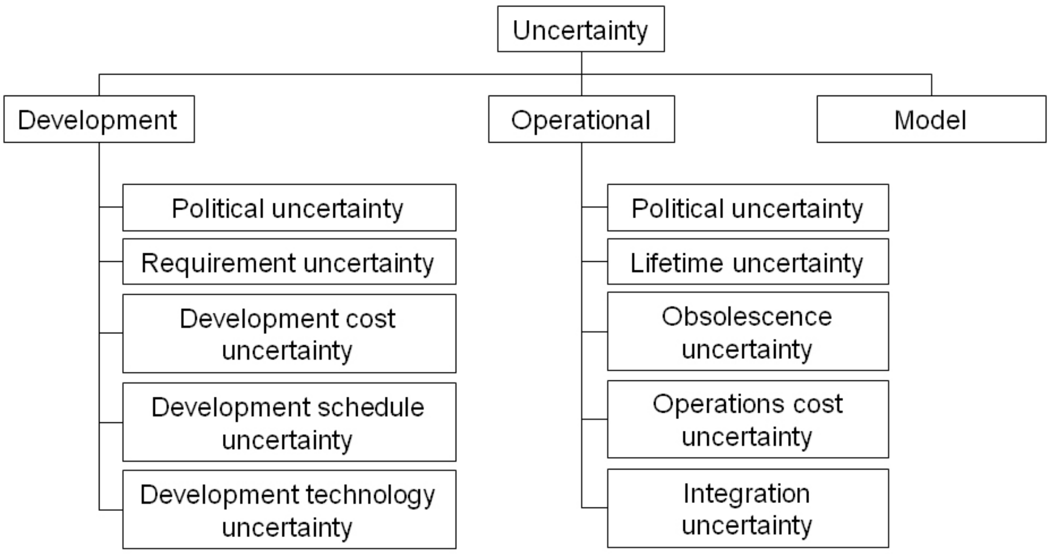

Figure A.13: Sources of uncertainty in the design of space system architectures [211].

He defines uncertainty as the "inability to deterministically predict an outcome". As shown in Figure A.13, he proposes three categories, called *development*, *op-*

Source of Uncertainty	Definition
Political	regards development/operational funding instability.
Requirements	regards requirements stability.
Development Cost/Schedule	occurs when developing within a given budget/schedule profile.
Development technology	caused by the uncertain contribution of technology to performance.
Lifetime/Obsolescence	regards the satisfaction of requirements/evolving expectations in a given lifetime.
Integration	refers to the uncertainty of operating within other necessary systems.
Operations cost	defined as the uncertainty of meeting operations cost targets.
Market uncertainty	encountered in meeting the demands of an unknown market.

Table A.7: Sources of uncertainty in the design of space system architectures (from [211]).

erational and *model* uncertainty, which are further classified as summarized in Table A.7. The relevance of this taxonomy consists in its extension to the entire life cycle, where both risks and opportunities might be hidden.

A.3.7 Nikolaidis, 2005

In an attempt to synthesize older taxonomies in the context of decision-based design, Nikolaidis [148] defines uncertainty as the gap between certainty (in decision theory, the condition in which the decision maker knows everything needed to chose the action with the most desirable outcome) and the present decision maker's knowledge.

An action of the decision maker is temporally articulated in three moments: the framing of the decision, the predictions of outcomes and finally their evaluation. As shown in Figure A.14, uncertainty might be encountered in each of such phases. During the first one, uncertainty is due to wrong or unclear problem statement, or to unexplored available actions. During the second phase, uncertainty can be *aleatory*, *epistemic* (reflecting Oberkampf's definition [153]) or characterized by *human error*. Aleatory uncertainty is caused by *variabil-*

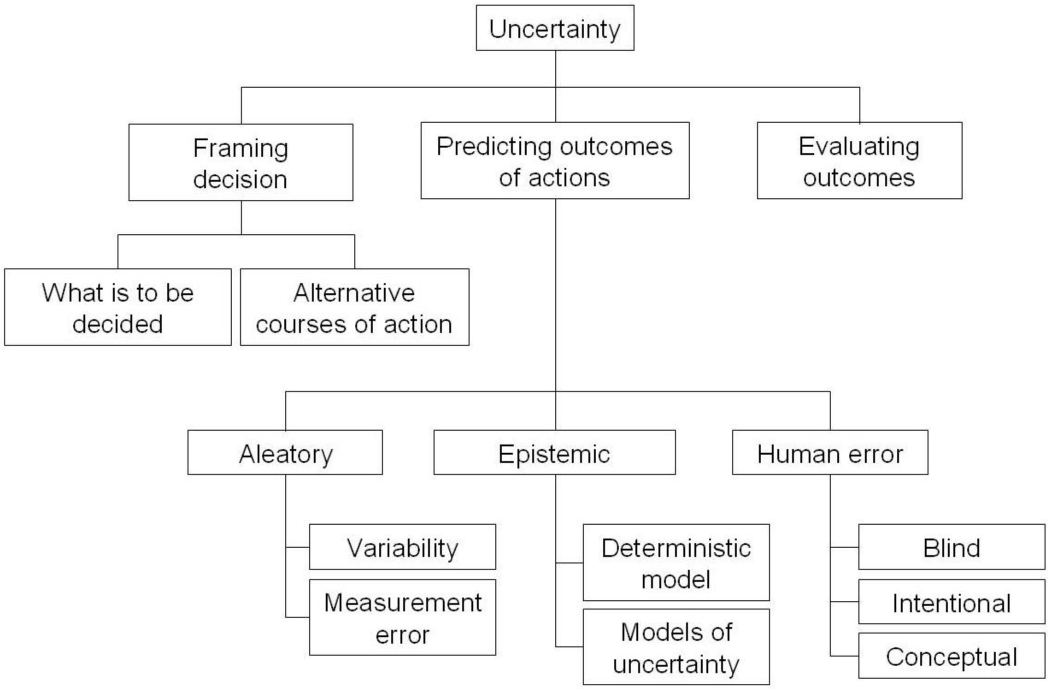

Figure A.14: Types of uncertainty in design decision making (taken from [148]).

ity and *measurement error*, while epistemic uncertainty is caused by the use of partially wrong model forms or missing variables, or by the use of an incorrect model of uncertainty. Nikolaidis argues that epistemic and aleatory uncertainty are not disjoint categories, individuating an intersection of the two species, that could happen if some of the missing variables in the model are also random variables (Nikolaidis acknowledges the work of Haukass [79] for this distinction). Finally, human error is defined as a departure from accepted procedures, and is divided into *execution*, *intentional* and *conceptual* errors, following Nowak and Collins [151]. The last category of uncertainty is identifiable with *decision* uncertainty, which derives from the mentioned work by Melchers [139] and was already defined in Table A.5.

Appendix B

Accuracy of the URQ propagation method

Presented in this Appendix are the reasons underlying the choice of the formulas in Eq. (4.18) and Eq. (4.19). This also serves to demonstrate the accuracy of the URQ propagation method.

The basic idea is to provide an integration formula which solves Eq. (3.7) and Eq. (3.8) by matching the highest number of terms of the mean and variance expressions derived from a third order Taylor series expansion, as detailed in Eq. (3.12) and Eq. (3.13), respectively.

In analogy with Gauss-type quadrature formulas [22], our formulas can be written as weighted sums of functional values. By considering 2 nodes for each dimension of the input space D, with $D \subseteq \mathcal{R}^n$, plus a central point corresponding to the mean $\mu_{\mathbf{x}}$, we can write the following expressions:

$$\mu_f = W_0 f(\mu_{\mathbf{x}}) + \sum_{p=1}^{n} \left[W_A f(\mathbf{x}_{p_+}) + W_B f(\mathbf{x}_{p_-}) \right] ; \tag{B.1}$$

$$\sigma_f^2 = \sum_{p=1}^{n} \Bigg\{ W_a \left[f(\mathbf{x}_{p_+}) - f(\mu_{\mathbf{x}}) \right]^2 + W_b \left[f(\mathbf{x}_{p_+}) - f(\mu_{\mathbf{x}}) \right]^2 + \\ + W_c \left[f(\mathbf{x}_{p_+}) - f(\mu_{\mathbf{x}}) \right] \left[f(x_{p_-}) - f(\mu_{\mathbf{x}}) \right] \Bigg\}. \tag{B.2}$$

The sampling points are given as follows:

$$\mathbf{x}_{p\pm} = \mu_{\mathbf{x}} + h_p^{\pm}\sigma_{\mathbf{x}_p}\mathbf{e}_p, \tag{B.3}$$

We consider in the following $\sigma_{\mathbf{x}_p} = 1$ for easiness of notation. Suppose that f is analytic on the range $[\mathbf{x}_{p-}, \mathbf{x}_{p+}]$. Therefore the functional values $f(\mathbf{x}_{p+})$ and $f(\mathbf{x}_{p-})$ can be written by means of a Taylor series expansion centered in $\mu_{\mathbf{x}}$, as given by the following equations:

$$f(\mathbf{x}_{p+}) = f(\mu_{\mathbf{x}}) + \sum_{i=0}^{\infty} \frac{\partial^i f}{\partial x_p^i} \frac{(h_p^+)^i}{i!}; \tag{B.4}$$

$$f(\mathbf{x}_{p-}) = f(\mu_{\mathbf{x}}) + \sum_{i=0}^{\infty} \frac{\partial^i f}{\partial x_p^i} \frac{(h_p^-)^i}{i!}. \tag{B.5}$$

By substituting Eq. (B.4) and Eq. (B.5) into Eq. (B.1) and Eq. (B.2), the following equations are obtained:

$$\mu_f = W_0 f(\mu_{\mathbf{x}}) + \sum_{p=1}^{n} \left(f(\mu_{\mathbf{x}})(W_A + W_B) + \sum_{i=0}^{\infty} \frac{\partial^i f}{\partial x_p^i} \frac{W_A (h_p^+)^i + W_B (h_p^-)^i}{i!} \right); \tag{B.6}$$

$$\sigma_f^2 = \sum_{p=1}^{n} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{\partial^i f}{\partial x_p^i} \frac{\partial^j f}{\partial x_p^j} \frac{W_a (h_p^+)^{i+j} + W_b (h_p^-)^{i+j} + W_c (h_p^+)^i (h_p^-)^j}{i!j!}. \tag{B.7}$$

These equations are the approximations for mean and variance given by the URQ. Their accuracy depends on the value chosen for the weights W_0,W_A,W_B,W_a,W_b and W_c and for the sampling locations identified by h_p^+ and h_p^-.

To find the best values for such parameters, we need 8 conditions, that we can obtain by equalling Eq. (B.6) and Eq. (B.7) to Eq. (3.12) and Eq. (3.13), respectively. In particular, we recognize that we can match the terms $M1$, $M2$, $M3$, $M4$ in Eq. (3.12) and the terms $V1$, $V2$, $V5$, $V6$ in Eq. (3.13), but not the terms $M5$, $V3$ and $V4$, since Eq. (B.6) and Eq. (B.7) do not show cross-derivative terms.

Those conditions correspond to the following system of equations:

$$
\begin{cases}
1: & W_0 + \sum_{p=1}(W_A + W_B) = 1; \\
2: & W_A h_p^+ + W_B h_p^- = 0; \\
3: & W_A (h_p^+)^2 + W_B (h_p^-)^2 = 0; \\
4: & W_A (h_p^+)^3 + W_B (h_p^-)^3 = \gamma_p; \\
5: & W_A (h_p^+)^4 + W_B (h_p^-)^4 = \Gamma_p; \\
6: & W_a (h_p^+)^2 + W_b (h_p^-)^2 + W_c h_p^+ h_p^- = 1; \\
7: & W_a (h_p^+)^3 + W_b (h_p^-)^3 + \frac{W_c}{2}\left[(h_p^+)^2 h_p^- + h_p^+ (h_p^-)^2\right] = \gamma_p; \\
8: & W_a (h_p^+)^4 + W_b (h_p^-)^4 + \frac{W_c}{2}\left[(h_p^+)^3 h_p^- + h_p^+ (h_p^-)^3\right] = \Gamma_p; \\
9: & W_a (h_p^+)^4 + W_b (h_p^-)^4 + W_c (h_p^+)^2 (h_p^-)^2 = \Gamma_p - 1.
\end{cases}
\tag{B.8}
$$

One amongst 6,7 and 8 can be expressed as function of the other two. Hence by removing the dependent equation, we are left with 8 independent equations which uniquely determine the 8 parameters identifying the weights and the sampling locations. By solving the system, we obtain:

$$
h_p^{\pm} = \frac{\gamma_p}{2} \pm \sqrt{\Gamma_p - \frac{3\gamma_p^2}{4}}, \tag{B.9}
$$

and

$$W_0 = 1 + \textstyle\sum_{p=1}^{n} \frac{h_p^+ + h_p^-}{h_p^+ h_p^-};$$

$$W_A = \frac{1}{h_p^+\left(h_p^+ - h_p^-\right)};$$

$$W_B = \frac{1}{h_p^-\left(h_p^+ - h_p^-\right)};$$

$$W_a = \frac{(h_p^+)^2 - h_p^+ h_p^- - 1}{(h_p^+)^2 (h_p^+ - h_p^-)^2};$$

$$W_b = \frac{(h_p^-)^2 - h_p^+ h_p^- - 1}{(h_p^-)^2 (h_p^+ - h_p^-)^2};$$

$$W_c = \frac{2}{h_p^+ h_p^- (h_p^+ - h_p^-)^2}.$$

After some simple algebraic manipulation on the weights, we can rewrite Eqs. (B.1) and (B.7) as in Chapter 4:

$$
\mu_f = W_0 f(\mu_{\mathbf{x}}) + \sum_{p=1}^{n} W_p \left[\frac{f(\mathbf{x}_{p_+})}{h_p^+} - \frac{f(\mathbf{x}_{p_-})}{h_p^-}\right]; \tag{B.10}
$$

$$\sigma_f^2 = \sum_{p=1}^{n} \left\{ W_p^+ \left[\frac{f(\mathbf{x}_{p_+}) - f(\mu_{\mathbf{x}})}{h_p^+} \right]^2 + W_p^- \left[\frac{f(x_{p_-}) - f(\mu_{\mathbf{x}})}{h_p^-} \right]^2 + \right.$$
$$\left. + W_p^{\pm} \frac{\left[f(\mathbf{x}_{p_+}) - f(\mu_{\mathbf{x}})\right] \left[f(x_{p_-}) - f(\mu_{\mathbf{x}})\right]}{h_p^+ h_p^-} \right\}, \quad \text{(B.11)}$$

for which the weights are defined as follows:

$W_0 = 1 + \sum_{p=1}^{n} \frac{1}{h_p^+ h_p^-}$;

$W_p = \frac{1}{h_p^+ - h_p^-}$;

$W_p^+ = \frac{(h_p^+)^2 - h_p^+ h_p^- - 1}{(h_p^+ - h_p^-)^2}$;

$W_p^- = \frac{(h_p^-)^2 - h_p^+ h_p^- - 1}{(h_p^+ - h_p^-)^2}$;

$W_p^{\pm} = \frac{2}{(h_p^+ - h_p^-)^2}$.