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EVOLVE – A Bridge between Probability, Set Oriented Numerics, and Evolutionary Computation V

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Preface

This volume encloses a series of research articles and contributions that were presented at the EVOLVE 2014 International Conference in Beijing, China, July 1–4, 2014.

The aim of the EVOLVE (http://www.evolve-conference.org) conference series is to build a bridge between probability, statistics, set oriented numerics and evolutionary computing, as to identify new common and challenging research aspects. The event is intended to foster a growing interest for robust and efficient new methods with a sound theoretical background. Furthermore, EVOLVE aspires at unifying theory and applied cutting-edge techniques that ensure performance guarantee factors. The massive use and large applicability spectrum of evolutionary algorithms in real-life applications, as an example, determined a need for establishing solid theoretical grounds. In a similar way, one may consider mathematical objects that are sometimes difficult and/or costly to calculate, namely in the light of acknowledged new results which show that evolutionary algorithms can act in some cases as good and fast estimators. The handling of large quantities of data may require the use of distributed environments where the probability of failure and the stability of the algorithms may need to be addressed. And examples could continue. What this collection is in the end about and what common practice confirms in many cases is that theory-based and applied results have to be considered in a unified perspective. The volume is thus focused on challenging aspects arising at the passage from theory to new paradigms and practice, aiming to provide a unified view while, at the same time, raising questions related to reliability, performance guarantees and modeling. As a consequence of these aims and by gathering researchers with different backgrounds, e.g. computer science, mathematics, statistics and physics, a unified view and vocabulary can emerge where theoretical advancements may echo throughout different domains.

The volume gathers contributions that emerged from the conference tracks, ranging from probability to set oriented numerics and evolutionary computation; all complemented by the bridging purpose of the conference, e.g. *Complex Networks and Landscape Analysis*, or by the more application oriented perspective. The novelty of the volume, when considering the EVOLVE series, comes from targeting also the practitioner's view. This is supported by the *Machine Learning Applied to Networks* and *Practical Aspects of Evolutionary Algorithms* tracks, providing surveys on new (some of them unhandled) application areas, as in the networking area and useful insights in the development of evolutionary techniques, from a practitioner's perspective. Complementary to these directions, the conference tracks supporting the volume, follow on the individual advancements of the subareas constituting the scope of the conference, through the *Computational Game Theory*, *Local Search and Optimization*, *Genetic Programming*, *Evolutionary Multi-objective optimization* tracks.

As an ending thought, our gratitude goes out to all the invited speakers for accepting to give an outstanding presentation and an overview of their latest work during the event, to all the authors, for sharing their knowledge and expertise and, last but not least, to all the participants for their extraordinary support. We would also like to express our foremost appreciation to all the referees and members of the program committee which, through their considerate work, contributed to the creation of a bridge between the different fields covered by the event. The editors would furthermore like to thank Dr. Thomas Ditzinger and Professor Janusz Kacprzyck (Editor-In-Chief, Springer Studies in Computational Intelligence Series) for the extraordinary collboration, since the begining of the EVOLVE series and this during the entire editing process. Finally, we would like to gratefully thank the partner institutions and the sponsors of the event which all made EVOLVE 2014 possible and a great success.

Luxembourg, Merced, Beijing, Mexico City
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Part I

Set Oriented Numerics

Response Analysis of a Forced Duffing Oscillator with Fuzzy Uncertainty

Ling Hong[1,⋆], Jun Jiang[1], and Jian-Qiao Sun[2]

[1] State Key Lab for Strength and Vibration
Xi'an Jiaotong University
Xi'an 710049, China
`hongling@mail.xjtu.edu.cn`
[2] School of Engineering
University of California at Merced
Merced, CA 95344, USA

Abstract. The transient and steady-state membership distribution functions (MDFs) of fuzzy response of a forced Duffing oscillator with fuzzy uncertainty are studied by means of the Fuzzy Generalized Cell Mapping (FGCM) method. The FGCM method is first introduced. A rigorous mathematical foundation of the FGCM is established with a discrete representation of the fuzzy master equation for the possibility transition of continuous fuzzy processes. The FGCM offers a very effective approach for solutions to the fuzzy master equation based on the min-max operator of fuzzy logic. Fuzzy response is characterized by its topology in the state space and its possibility measure of MDFs. The response topology is obtained based on the qualitative analysis of the FGCM involving the Boolean operation of 0 and 1. The evolutionary process of transient and steady-state MDFs is determined by the quantitative analysis of the FGCM with the min-max calculations. It is found that the evolutionary orientation of MDFs is in accordance with invariant manifolds leading to invariant sets. In the evolutionary process of a steady-state fuzzy response with an increase of the intensity of fuzzy noise, a merging bifurcation is observed in a sudden change of the MDFs from two sharp peaks of most possibility to one peak band around unstable manifolds.

Keywords: Fuzzy Uncertainty, Possibility Measure, Fuzzy Response, Membership Distribution Function, Generalized Cell Mapping.

1 Introduction

Engineering systems are often subjected to uncertainties that are associated with the lack of precise knowledge of system parameters and operating conditions and that are originated from variability in manufacturing processes. The uncertainties can have significant influence on the dynamic response and the reliability of the system, and are often modeled as random variables or fuzzy sets. This paper proposes the FGCM method to analyze the response of nonlinear dynamical systems with fuzzy uncertainties. Specifically, we are interested in a nonlinear dynamical system whose response

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[⋆] Corresponding author.

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is a fuzzy process, and study the transient and steady-state membership distribution functions (MDFs) of fuzzy response.

For fuzzy nonlinear dynamical systems, a response process is difficult to analyze because the evolution of the MDFs of the fuzzy response process cannot be readily obtained analytically. Many studies dealt with fuzzy dynamical systems governed by linear ordinary differential equations [1–3]. Chaotic sequences of fuzzy nonlinear maps were studied [4]. A master equation was derived for the evolution of MDFs of fuzzy processes [5,6]. However, the solution to the fuzzy master equation is rare, particularly for nonlinear dynamical systems. The theory on the evolution of the MDFs of fuzzy processes is far less complete and mature compared to that for the probability density of stochastic processes [7]. The first attempt to describe the dynamics of fuzzy systems was done in 1973 by Nazaroff [8], who investigated fuzzy topological polysystems. From that time several approaches to describing fuzzy dynamics were proposed. For instance, Kloeden [9] defined and considered the extension of dynamical systems to fuzzy states. However, the notion of fuzzy velocity was not introduced there and an explicit differential equation for continuous evolution was not given. Another approach to fuzzy dynamics using differential inclusions was developed by Aubin and others [10]. The notion of fuzzy set of velocities was introduced and the standard equations of evolution were fuzzyfied. Since these equations were obtained outside fuzzy logic framework, the fuzzy differential inclusion leads to the problem that the restriction of the values of the MDFs to the interval [0,1] was not preserved by the evolution in general. For the same reason, similar problems occur in the solution of the Cauchy problem for fuzzy differential equation [11].

Fuzzy response is naturally global in the sense that it is represented by a fuzzy set of a finite possibility measure in the state space. It is computationally intensive and ineffective to study such a solution by using numerical simulations [12, 13]. The cell mapping method represents a major advancement in this regard. Chen and Tsao pioneered the work of fuzzy control design with the simple cell mapping method [14, 15]. Smith and his associates further extended the simple cell mapping method to fuzzy optimal control problems in higher dimensional state space [16, 17]. The generalized cell mapping (GCM) method offers a probabilistic tool for the global analysis of nonlinear dynamical systems [18]. Edwards and Choi proposed to impose the initial probability distribution in each cell that has the same form as a typical fuzzy membership function [19]. However, they did not apply Zadeh's extension principle to manipulate fuzzy sets. The resulting generalized cell mapping, however, is still a Markov chain. Sun and Hsu extended the generalized cell mapping to fuzzy systems by applying Zadeh's extension principle [20]. A variety of random vibration and stochastic optimal problems were studied by Sun, Hsu and their associates [21,22]. Crises in chaotic dynamical systems were investigated by Hong and Xu using the GCM with digraphs [23, 24]. More recently, the GCM method was applied to study bifurcations of fuzzy nonlinear dynamical systems [25, 26].

The remainder of the paper is outlined as follows. In Section 2, we introduce the FGCM method, and discuss its properties. In Section 3, we study the evolution of transient and steady-state MDFs of a forced Duffing oscillator with fuzzy noise. The paper concludes in Section 4.

2 Fuzzy Generalized Cell Mapping

2.1 Discrete Representation of the Fuzzy Master Equation

A rigorous mathematical foundation of the FGCM method can be established. Consider the fuzzy master equation for the possibility transition of continuous fuzzy processes [3, 5, 6],

$$p(\mathbf{x},t) = \sup_{\mathbf{x}_0 \in \mathbf{D}} \left[\min\{p(\mathbf{x},t|\mathbf{x}_0,t_0), p(\mathbf{x}_0,t_0)\} \right], \quad \mathbf{x} \in \mathbf{D} \tag{1}$$

where $\mathbf{x}$ is a fuzzy process, $p(\mathbf{x},t)$ is the membership distribution function of $\mathbf{x}$ at t, and $p(\mathbf{x},t|\mathbf{x}_0,t_0)$ is the transition possibility function, also known as a fuzzy relation [3]. $\mathbf{D}$ is a bounded domain of interest in the state space. A partial differential equation from Equation (1) for continuous time processes has been derived by Friedman and Sandler [5, 6]. This equation is analogous to the Fokker-Planck-Kolmogorov equation for the probability density function of stochastic processes [7]. The solution to this equation is in general very difficult to obtain analytically.

Next we show that FGCM can be introduced as a discrete representation of the fuzzy master equation (1). Consider a dynamical system with fuzzy uncertainty.

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x},t,S), \quad \mathbf{x} \in \mathbf{D}, \tag{2}$$

where $\mathbf{x}$ is the state vector, t the time variable, S a fuzzy set with a membership function $\mu_S(s) \in (0,1]$ where $s \in S$, and $\mathbf{f}$ is a vector-valued nonlinear function of its arguments. When the system parameter S is a fuzzy number. Equation (2) is a fuzzy differential equation.

The cell mapping method proposes to further discretize the time and state variables in searching for the global solution of the system [18]. In order to apply the cell mapping method, we also need to discretize the fuzzy set S. We divide S into M segments of appropriate length and sample a value $s_k \in S$ $(k = 1, \cdots, M)$ in the middle of each segment. The division of S is such that there is at least one s_k with membership grade equal to one.

The domain $\mathbf{D}$ is then discretized into N small cells. Each cell is identified by an integer ranging from 1 to N. For a cell, say cell j, N_p points are uniformly sampled from cell j. By applying the method of numerical simulation, we generate $M \times N_p$ fuzzy sample trajectories of one period T long. The length T is taken to be one mapping step. Each trajectory carries a membership grade determined by that of s_k's. We then find the cells in which the end points of the trajectories fall. Assume that cell i is one of the image cells of cell j, and that there are m $(0 < m \leqslant MN_p)$ trajectories falling in cell i. Define a quantity

$$p_{ij} = \max_{i_k}[\mu_S(s_{i_k})], \quad 0 < p_{ij} \leqslant 1, \tag{3}$$

where i_k $(k = 1, 2, ..., m)$ are referred to the trajectories falling in cell i, and $\mu_S(s_{i_k})$ are the membership grades of the corresponding trajectories. This procedure for computing p_{ij} is known as the sampling point method in the context of generalized cell mapping [18]. We should note that partition of the domain $\mathbf{D}$ and fuzzy set S need not be uniform.

Now, assume that the membership grade of the system being in cell j at the n^{th} mapping step is $p_j(n)$ $(0 < p_j(n) \leqslant 1)$. Cell j is mapped in one step to cell i with the membership grade given by

$$\max\left\{\min\left[\mu_S\left(s_{i_1}\right), p_j\left(n\right)\right], \min\left[\mu_S\left(s_{i_2}\right), p_j\left(n\right)\right], \cdots, \min\left[\mu_S\left(s_{i_m}\right), p_j\left(n\right)\right]\right\}$$
$$= \min[\max_{i_k}\left(\mu_S\left(s_{i_k}\right)\right), p_j\left(n\right)] = \min[p_{ij}, p_j\left(n\right)]. \tag{4}$$

Considering all possible pre-images of cell i, we have the membership grade of the system being in cell i at the $(n+1)^{th}$ step as

$$p_i\left(n+1\right) = \max_j \min\left[p_{ij}, p_j\left(n\right)\right]. \tag{5}$$

Let $\mathbf{p}\left(n\right)$ be a vector with components $p_i\left(n\right)$, and $\mathbf{P}$ a matrix with components p_{ij}. Equation (5) can be written in a compact matrix notation

$$\mathbf{p}\left(n+1\right) = \mathbf{P} \circ \mathbf{p}\left(n\right), \;\; \mathbf{p}\left(n\right) = \mathbf{P}^n \circ \mathbf{p}\left(0\right), \tag{6}$$

where $\mathbf{P}^{n+1} = \mathbf{P} \circ \mathbf{P}^n$ and $\mathbf{P}^0 = \mathbf{I}$. $\circ$ denotes the min-max operation. The matrix $\mathbf{P}$ denotes the one-step transition membership matrix. $\mathbf{P}^n$ denotes the n-step transition possibility matrix. The vector $\mathbf{p}\left(n\right)$ is called the n-step membership distribution vector, and $\mathbf{p}\left(0\right)$ the initial membership distribution vector. The $(i,j)^{th}$ element p_{ij} of the matrix $\mathbf{P}$ is called the one-step transition membership from cell j to cell i.

Equation (6) is called a fuzzy generalized cell mapping (FGCM) system, which describes the evolution of the fuzzy solution process $\mathbf{x}\left(t\right)$ and its MDFs $p(\mathbf{x}, t)$, and is a finite approximation to the fuzzy dynamical system (2) in $\mathbf{D}$.

Equation (5) of the FGCM can be viewed as a discrete representation of Equation (1). The FGCM offers a very effective method for solutions to this equation, particularly, for fuzzy nonlinear dynamical systems.

2.2 The Qualitative and Quantitative Properties of FGCM

Qualitative Properties. Recall that the min-max operation in Eq. (5) really represents the intersection (product) and union (summation) of fuzzy sets in the form of cells in $\mathbf{D}$. Hence, $\mathbf{P} \circ \mathbf{p}$ is an inner product of fuzzy sets. The topological matrix of $\mathbf{P}$, denoted by $[\overline{p}_{ij}]$, and the topological vector of $\mathbf{p}\left(n\right)$, denoted by $\{\overline{p}_i(n)\}$, are defined as

$$\overline{p}_{ij} = \begin{cases} 1, p_{ij} > 0 \\ 0, p_{ij} = 0 \end{cases}, \;\; \overline{p}_i(n) = \begin{cases} 1, p_i(n) > 0 \\ 0, p_i(n) = 0 \end{cases}, \; n \geq 0. \tag{7}$$

Topologically, Eq. (6) becomes

$$\overline{\mathbf{p}}\left(n+1\right) = \overline{\mathbf{P}} \circ \overline{\mathbf{p}}\left(n\right), \;\; \overline{\mathbf{p}}\left(n\right) = \overline{\mathbf{P}}^n \circ \overline{\mathbf{p}}\left(0\right), \tag{8}$$

where $\overline{\mathbf{P}}^{n+1} = \overline{\mathbf{P}} \circ \overline{\mathbf{P}}^{n}$ and $\overline{\mathbf{P}}^{0} = \mathbf{I}$. Note that the min-max operation is equivalent to the logic operations of multiplication $\wedge$ and addition $\vee$ of binary numbers: $0 \wedge 1 = 0$, $1 \wedge 0 = 0, 0 \wedge 0 = 0, 1 \wedge 1 = 1, 0 \vee 1 = 1, 1 \vee 0 = 1, 0 \vee 0 = 0$, and $1 \vee 1 = 1$. Hence, the min-max operation in Eq. (8) leads to the identical result to that of the topological matrix of the Markov chains. Hence, $\overline{\mathbf{P}}$ forms a digraph and can be partitioned to identify persistent groups of cells representing stable solutions and the transient cells including the unstable solutions [27].

Quantitative Properties. Under the min-max operation in Eq. (5), the membership function of the cells is non-increasing in the sense that,

$$||\mathbf{p}\,(n+1)\,|| \leq ||\mathbf{p}\,(n)\,||,\ \forall n \geq 0, \tag{9}$$

where the norm of the fuzzy membership vector is defined as

$$||\mathbf{p}\,(n)\,|| = \max_{i}\{p_i\,(n)\}. \tag{10}$$

Furthermore, the min-max operator does not introduce any new numbers that are not the entries of the matrix $\mathbf{P}$ or the vector $\mathbf{p}(0)$. This implies that $\mathbf{p}(n)$ can assume only finite number of possible values as $n \to \infty$. In the steady state, $\mathbf{p}(n)$ will either converge to a constant vector, or to a set of vectors which form a periodic group and repeat themselves as the iteration goes on. In either case, we consider the system to have converged to the steady state. Because there are only finite number of possible values for $\mathbf{p}(n)$, Eq. (5) will converge in finite number of iterations. This is a sharp contrast to Markov chains, which theoretically converge to steady state in infinite iterations.

The qualitative and quantitative properties lead to a dichotomy in the computation treatment of the FGCM, and ensure the accuracy and efficiency of the FGCM. Boolean operations are only used in the qualitative analysis of the FGCM, while the min-max operations are only involved in the quantitative analysis of FGCM. As a result, the transient and steady-state MDFs of a fuzzy response process can be effectively determined in a new way.

3 Response Analysis of a Forced Duffing Oscillator with Fuzzy Uncertainty

3.1 The Global Properties of Deterministic Forced Duffing Oscillator

Consider the forced Duffing oscillator.

$$\ddot{x} + \kappa\dot{x} + x^3 = B\cos t. \tag{11}$$

It is a mathematical model of various physical systems where the damping κ and forcing magnitude B are system parameters. The system has various types of steady state motions depending on system parameters (κ, B) as well as initial conditions. In the present work, we are interested in the region of periodic motions. In particular, we take (κ, B)=(0.2, 0.3) where the system has two coexistent period-one attractors $\mathbf{A}_1$ and $\mathbf{A}_2$.

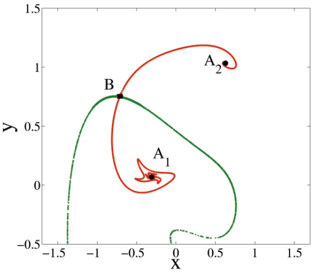

Fig. 1. Global phase portrait of the deterministic Duffing (11) with κ=0.2 and B=0.3. A_1 and A_2 denote two period-one attractors. On basin boundary lies the saddle denoted by B. The basin boundary denoted by a green line is the stable manifold of the saddle B. The unstable manifolds of the saddle B denoted by a red line are directed to A_1 and A_2 respectively.

In Fig. 1 is shown the global properties of the equation (11) by means of point mapping under cell reference (PMUCR), a two-scaled numerical global analysis method [28,29]. The basin boundary (a green line) is the stable manifolds of the unstable saddle B. The two branches (a red line) of the unstable manifolds of B are directed to the two fixed points A_1 and A_2 respectively. B is the unstable invariant set of the Duffing system (11). A_1 and A_2 the stable invariant sets.

In the following sections, we will study transient and steady-state MDFs of a fuzzy response for the forced Duffing oscillator with fuzzy uncertainty.

3.2 Fuzzy Response

Consider now the Duffing equation with fuzzy noise

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= -x^3 - 0.2y + S\cos t. \end{aligned} \tag{12}$$

where S is a fuzzy parameter of the forcing amplitude with a triangular membership function,

$$\mu_S(s) = \begin{cases} [s-(s_0-\varepsilon)]/\varepsilon, & s_0-\varepsilon \leqslant s < s_0 \\ -[s-(s_0+\varepsilon)]/\varepsilon, & s_0 \leqslant s < s_0+\varepsilon \\ 0, & \text{otherwise} \end{cases} \tag{13}$$

$\varepsilon > 0$ is a parameter characterizing the intensity of fuzziness of S and is called a fuzzy noise intensity. s_0 is the nominal value of S with membership grade $\mu_S(s_0) = 1$. In the computation, we take $s_0 = 0.301$.

The domain $\mathbf{D} = (-1.5 \leq x \leq 1.7) \times (-0.5 \leq y \leq 1.5)$ is discretized into 141×141 cells. The 5×5 sampling points are used within each cell. S is discretized into 401 segments. Hence, out of each cell, there are 10,025 trajectories with varying membership grades to determine the one-step transition possibility with the time length $\triangle T = T = 2\pi$. T is called one mapping step. The FGCM is used to analysis the transient and steady-state MDFs of the fuzzy response of the system (12).

Transient Analysis of MDFs. In this section, we take the intensity of fuzzy noise $\varepsilon = 0.07$. Figs. 2, 3, and 4 show the evolutionary process of transient MDFs of displacement x and velocity y with initial possibility distributions $p_{n_1}(0) = 1$ and $p_{n_2}(0) = 1$. n_1 and n_2 denote the persistent groups representing the two attractors A_1 and A_2.. In Fig. 2 is shown the time evolution of marginal MDFs for x and y respectively. In Figs. 3 and 4 are respectively shown the contour and 3D surface plots of joint MDFs of x and y. The evolutionary trend to follow in Figs. 3 and 4 is that as the time increases we move from (a) to (b) in (c) and (d), two peaks of possibility one of MDFs move respectively along the two branches of the unstable manifold of B and converge around A_1 and A_2.

Steady-State Analysis of MDFs. We study the evolutionary process of the steady-state fuzzy response of the noisy Duffing system (12) as the intensity of fuzzy noise

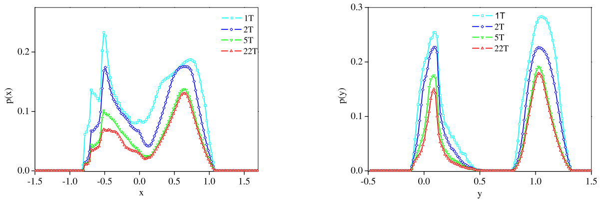

Fig. 2. Transient marginal MDFs of displacement x and velocity y for the fuzzy Duffing equation (12) with initial possibility distributions p_{n_1}(0)=1 and p_{n_2}(0)=1

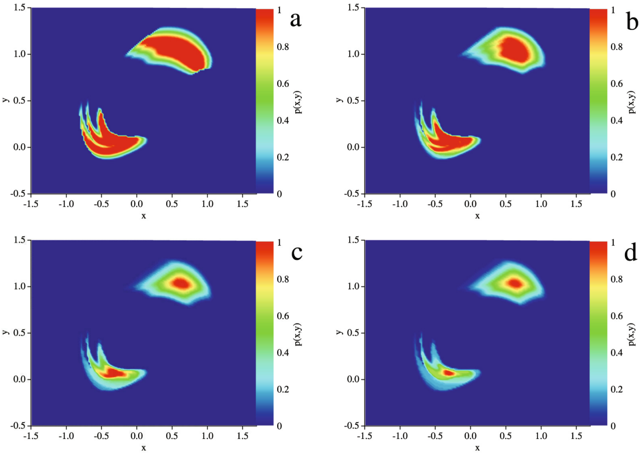

Fig. 3. Transient joint MDFs of displacement x and velocity y for the fuzzy Duffing equation (12) in contour plot at different times. (a) 1T, (b) 2T, (c) 5T, (d) 22T.

ε increases. Fig. 5 shows the evolution of the marginal steady-state MDFs for different intensities of fuzzy noise ε. In Figs. 6 and 7 is shown the evolution of the joint steady-state MDFs for different intensities in the plots of contour and 3D surface respectively. From these figures, it is found that the possibility distribution with two peaks becomes broader and extends toward to B along the unstable manifolds as the intensity of fuzzy noise increases. A merging bifurcation occurs when the possibility distribution merges in through B in the interval $\varepsilon \in (0.07, 0.071)$. The bifurcation results in a sudden change of MDFs from the two peaks of possibility one to one peak band around the unstable manifolds of B. The evolutionary trend of the steady-state MDFs is in accordance with the unstable manifolds expanding toward B as the intensity of fuzzy noise increases.

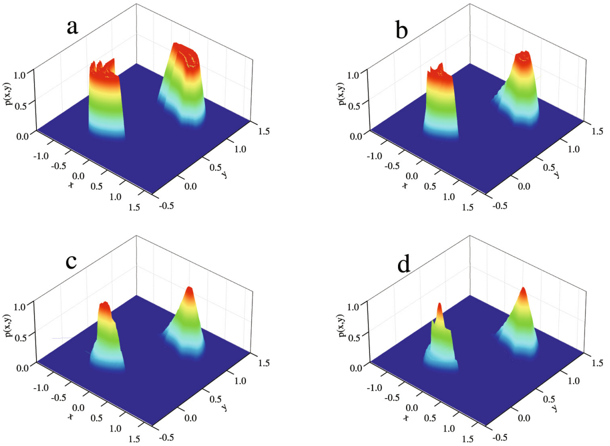

Fig. 4. Transient joint MDFs of displacement x and velocity y for the fuzzy Duffing equation (12) in surface plot at different times. (a) 1T, (b) 2T, (c) 5T, (d) 22T.

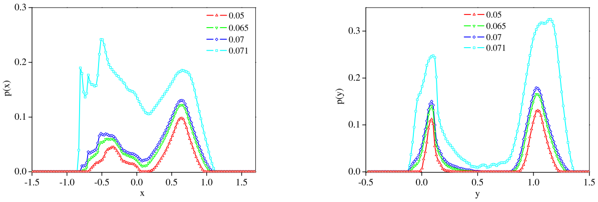

Fig. 5. Steady-state marginal MDFs of displacement x and velocity y for the fuzzy Duffing equation (12) with initial possibility distributions $p_{n_1}(0)$=1 and $p_{n_2}(0)$=1

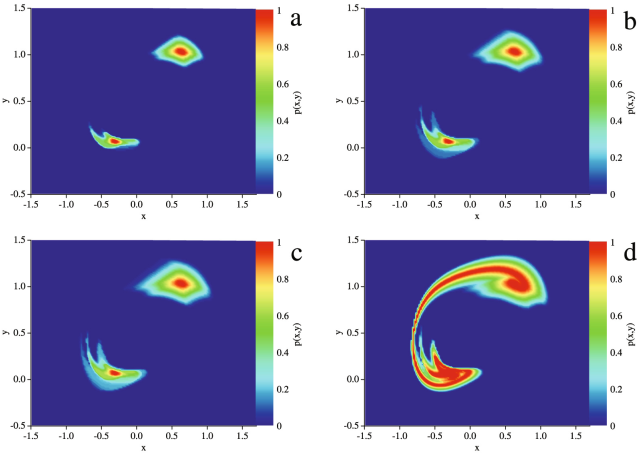

Fig. 6. Joint steady-state MDFs of the fuzzy Duffing system (12) for different intensity of fuzzy noise in contour plot. (a) ε=0.05, (b) ε=0.065, (c) ε=0.07, (d) ε=0.071.

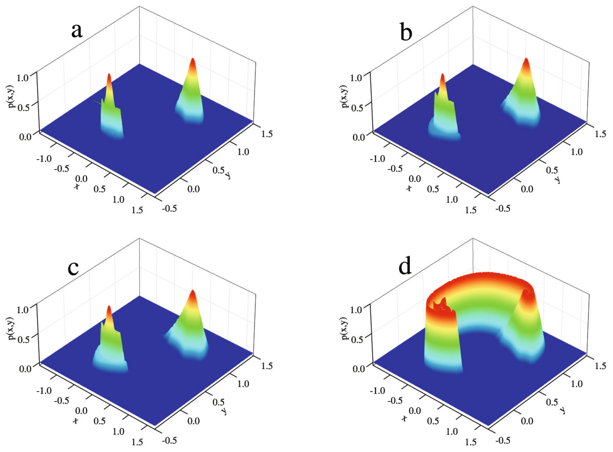

Fig. 7. Joint steady-state MDFs of the fuzzy Duffing system (12) for different intensity of fuzzy noise in 3D surface plot. (a) ε=0.05, (b) ε=0.065, (c) ε=0.07, (d) ε=0.071.

4 Concluding Remarks

The transient and steady-state membership distribution functions (MDFs) of fuzzy response of a forced Duffing oscillator with fuzzy uncertainty are studied by means of the Fuzzy Generalized Cell Mapping (FGCM) method. The FGCM method is first introduced. A rigorous mathematical foundation of the FGCM is established with a discrete representation of the fuzzy master equation for the possibility transition of continuous fuzzy processes. The FGCM offers a very effective approach for solutions to the fuzzy master equation based on the min-max operator of fuzzy logic. Fuzzy response is characterized by its topology in the state space and its possibility measure of MDFs. The response topology is obtained based on the qualitative analysis of the FGCM involving the Boolean operation of 0 and 1. The evolutionary process of transient and steady-state MDFs is determined by the quantitative analysis of the FGCM with the min-max calculations. It is found that the evolutionary orientation of MDFs is in accordance with invariant manifolds leading to invariant sets. In the evolutionary process of a steady-state fuzzy response with an increase of the intensity of fuzzy noise, a merging bifurcation is observed in a sudden change of the MDFs from two sharp peaks of most possibility to one peak band around unstable manifolds. The results obtained herein are of value to real engineering problems. Especially, the evolution of transient and long term steady state MDFs may be difficult to obtain by other conventional methods.

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Hypervolume Maximization via Set Based Newton's Method

Victor Adrián Sosa Hernández[1], Oliver Schütze[1], and Michael Emmerich[2]

[1] Computer Science Department, CINVESTAV-IPN, Av. IPN 2508, C.P. 07360,
Col. San Pedro Zacatenco, Mexico City, México
`msosa@computacion.cs.cinvestav.mx, schuetze@cs.cinvestav.mx`
[2] Multicriteria Optimization and Decision Analysis Group, LIACS, Leiden University,
Niels Bohrweg 1, 2333 CA Leiden, The Netherlands

Abstract. The hypervolume indicator is one of the most widely used tool to measure the performance in evolutionary multi-objective optimization. While derivative free methods such as specialized evolutionary algorithms received considerable attention in the past, the investigation of derivative based methods is still scarce. In this work, we aim to make a contribution to fill this gap.

Based on the hypervolume gradient that has recently been proposed for general unconstrained multi-objective optimization problems, we first investigate the behavior of the related hypervolume flow. Under this flow, populations evolve toward a final state (population) whose hypervolume indicator is locally maximal. Some insights obtained on selected test functions explain to a certain extend observations made in previous studies and give some possible insights into the application of mathematical programming techniques to this problem. Further, we apply a population-based version of the Newton Raphson method for the maximization of the hypervolume. Fast set-based convergence can be observed towards optimal populations, however, the results indicate that the success depends crucially on the choice of the initial population.

Keywords: multi-objective optimization, hypervolume indicator, set based optimization, multi-objective gradient, Newton Raphson method.

1 Introduction

The problem of finding a good approximation set to a Pareto front in multiobjective optimization can be recast as a single-objective optimization problem, where the elements of the search space are approximation sets, and the objective function is a unary performance indicator that measures how close the points in a set are converged to and distributed across the Pareto front [1, 2]. Ideally, the performance indicator must not take into account a-priori information of the true Pareto front. The hypervolume indicator [3] is a performance indicator that has these properties and solely requires as a parameter a reference point that bounds the Pareto front from above.

While stochastic, derivative free methods that maximize the hypervolume indicator received considerable attention in the last decade [4–8], research on using deterministic and derivative based methods is still in its infancy.

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Set-based hypervolume gradient ascent methods and relay-hybrids with evolutionary methods were proposed in [9] with a focus on the bi-objective case. A full analytical derivation of the hypervolume gradient for more than two objectives and its efficient computation was discussed in [10]. These first results showed that gradient based methods can locally improve accuracy of hypervolume maximal sets, but when started far away from the Pareto front tend to stagnate without reaching the optimum. A full explanation of this behavior is not yet available, nor are there any results on second order methods, such as the Newton Raphson method that promises superlinear or even quadratic convergence rates. A first gradient based memetic strategy to maximize the hypervolume can be found in [11].

The contributions of this paper are two-fold:

1. An investigation of the dynamics and potential problems of gradient based hypervolume maximization is provided by a detailed analysis of its gradient flow. To be more precise, for selected test problems hypervolume maximization will be considered as an initial value problem of the ODE $\dot{P} = \nabla H(P)$, where P denotes the current state of the population and H the hypervolume indicator.
2. A set-based Newton Raphson method for hypervolume maximization is formulated based on the hypervolume gradient and set based Hessian approximation and tested on Pareto fronts with different shapes. This will be the first study on using a second order optimization method for finding Pareto front approximation sets. The findings on this are related to the first study.

The remainder of this paper is organized as follows: In Section 2, we briefly state the background for the understanding of this work. In Section 3, we investigate the hypervolume gradient flow empirically on several test problems. In Section 4, we consider the population based Newton Raphson method for hypervolume maximization. Finally, we draw our conclusions in Section 5 and point out possible paths of future research.

2 Background and Related Work

In the following we consider unconstrained continuous MOPs

$$\min_{x \in \mathbb{R}^n} \{F(x)\}, \tag{MOP}$$

where F is defined as the vector of the objective functions $F : \mathbb{R}^n \to \mathbb{R}^k$, $F(x) = (f_1(x), \ldots, f_k(x))$, and where each objective $f_i : \mathbb{R}^n \to \mathbb{R}$ is (for simplicity) sufficiently smooth. The optimality of a MOP is defined by the concept of *dominance* ([12]): A vector $y \in \mathbb{R}^n$ is *dominated* by a vector $x \in \mathbb{R}^n$ ($x \prec y$) with respect to (MOP) if and only if $f_i(x) \leq f_i(y)$, $i = 1, \ldots, k$, and there exists an index j such that $f_j(x) < f_j(y)$, else y is non-dominated by x. A point $x \in \mathbb{R}^n$ is called *(Pareto) optimal* or a *Pareto point* if there is no $y \in \mathbb{R}^n$ which dominates x. The set of all Pareto optimal solutions is called the *Pareto set*, and is denoted by P. The image $F(P)$ of the Pareto set is called the *Pareto front*. Both sets typically form a ($k-1$)-dimensional object. The hypervolume of a population $H(P)$ is defined as

$$H(P) = \lambda(\cup_{x \in P}[F(x), r]), \tag{1}$$

where λ denotes the Lebesgue measure and r is a user-defined and constant reference point should be dominated by all elements in P [3,5]. By increasing the size of the space that is dominated by a population the hypervolume indicator increases. The hypervolume indicator is a Pareto compliant unary indicator [13]. As a consequence, excepting degenerate cases, maxima of the hypervolume indicator consists of only Pareto optimal elements. Moreover, approximation sets that maximize the hypervolume indicator distribute across the Pareto front with a density of points depending on the deviation of the local slope of the Pareto front from $-45°$ (see [14]). As discussed in [15], a population $\{\mathbf{x}^1, \ldots, \mathbf{x}^\mu\}$ can be expressed as a single vector

$$P := (x_1^{(1)}, \ldots, x_n^{(1)}, \ldots, x_1^{(\mu)}, \ldots, x_n^{(\mu)})^\top \in \mathbb{R}^{\mu \cdot n}. \tag{2}$$

As there are multiple mappings between a set and a population vector, we will consider the one where the μ points are ordered in ascending lexicographical order with respect to the values of F, i. e. a 2-D Pareto front the index of the points will grow from left (1) to right (μ). The hypervolume function on population vectors can now be viewed as a mapping $H : \mathbb{R}^{n\mu} \to \mathbb{R}$. For differentiable population vectors, the gradient field $\nabla H : \mathbb{R}^{n\mu} \to \mathbb{R}^{n\mu}$ and the Hessian $\nabla^2 H : \mathbb{R}^{n\mu} \to \mathbb{R}^{n\mu \times n\mu}$ are defined in the standard way. In [15] it was shown that H is differentiable for population vectors that stem from points sets without duplicate coordinates, with all points in the interior of the reference region $(-\infty, r]$, and with existing Jacobian of F in all points. For sets with duplicate coordinates one sided derivatives are to be taken in some cases. The gradient can be computed by means of the chain rule [15], whereas for the computation of the Hessian matrix so-far only numerical methods using finite differences are available. In the gradient for each point $\mathbf{x}^{(i)}$, $i = 1, \ldots, \mu$ a subgradient of dimension n can be isolated, comprising exactly the partial derivatives for the coordinates of the i-th subvector. It was shown in [15] that this is the gradient of the hypervolume contribution of the i-th point, i. e. $\nabla \mathit{\Delta} H(\mathbf{x}^{(i)})$ with $\mathit{\Delta} H(\mathbf{x}^{(i)}) = H(P) - H(P - \{\mathbf{x}^{(i)}\})$. Subgradients of non-dominated points are positive, unless a stationary point of $\mathit{\Delta} H$ is given, and subgradients of strictly dominated points are zero vectors.

3 Investigating the Hypervolume Flow

First we investigate the flow that is induced by the hypervolume gradient field. This is done in order to see properties to understand the success or failure of gradient based search algorithms applied to this problem. In particular, we will observe a certain 'creepiness' in the movement of some individuals compared to some others (the ones at the boundary and in relative steep/flat regions of the Pareto front). This has the consequence that certain individuals get 'lost' (dominated by other points) under iteration of these set-based algorithms.

Recall from the introduction that after a straightforward re-ordering of the variables we can state the hypervolume function H population-wise (i.e., the variables of H are individuals of a given population). Doing so, we can state the hypervolume flow starting with a given population as the following initial value problem:

$$\begin{aligned} P(0) &= P_0 \subset \mathbb{R}^n \quad \text{with} \quad |P_0| = \mu \\ \dot{P}(t) &= \nabla H(P(t)) \end{aligned} \tag{3}$$

By following this flow, we obtain for every initial population P_0 a final population whose hypervolume is locally optimal (this is due to the fact that the hypervolume gradient is zero at every end point of (3)). Thus, the geometry of such solution curves are of particular interest for the understanding of the success and failure of the related gradient-based numerical optimization techniques.

Within this study, we make our experiments on the following four bi-parameter bi-objective models: The generalized Schaffler problems (GSP) by Emmerich and Deutz ([16])

$$\begin{aligned} f_1 &= \frac{(\sum_{i=1}^n x_i^2)^\alpha}{(n^\alpha)} \\ f_2 &= \frac{(\sum_{i=1}^n (1-x_i)^2)^\alpha}{(n^\alpha)} \end{aligned} \tag{4}$$

The Pareto set of this problem family is given by the line segment connecting the points $(0,0)^T$ and $(1,1)^T$ (including the end points). The Pareto front is concave for $\alpha < 0.5$, linear for $\alpha = 0.5$, and convex for $\alpha > 0.5$. For $\alpha = 0.5$ the hypervolume indicator maximum is known to be an evenly spaced point set on the efficient set and Pareto front [16].

The next model is MOP CONV1 ([17])

$$\begin{aligned} f_1 &= (x_1-1)^4 + (x_2-1)^2 \\ f_2 &= (x_1+1)^2 + (x_2+1)^2 \end{aligned} \tag{5}$$

The Pareto set is a curve connecting the points $m_1 = (1,1)^T$ and $m_2 = (-1,-1)^T$ and its Pareto front is convex.

A variant of the above model is CONV2 ([18])

$$\begin{aligned} f_1 &= (x_1-1)^2 + (x_2-1)^2 \\ f_2 &= (x_1+1)^2 + (x_2+1)^2 \end{aligned} \tag{6}$$

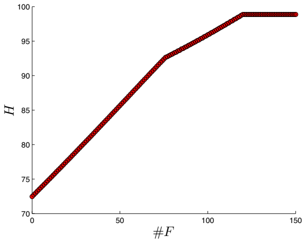
The Pareto set is a line segment connecting m_1 and m_2, and the Pareto front is convex. Finally, we will consider the MOP DENT ([19])

$$\begin{aligned} f_1 &= \frac{1}{2} \cdot (\sqrt{(1+(x_1+x_2)^2)} + \sqrt{(1+(x_1-x_2)^2)} + x_1 - x_2) + \lambda \cdot e^{(-1\cdot(x_1-x_2)^2)} \\ f_2 &= \frac{1}{2} \cdot (\sqrt{(1+(x_1+x_2)^2)} + \sqrt{(1+(x_1-x_2)^2)} - x_1 + x_2) + \lambda \cdot e^{(-1\cdot(x_1-x_2)^2)} \\ \lambda &= 0.85 \end{aligned} \tag{7}$$

For the domain $Q = [-4,4]^2$ the Pareto front is the line segment connecting the points $(4,-4)^T$ and $(-4,4)^T$ and its Pareto front is convex-concave.

(a) Parameter space

(b) Objective space



(c) Hypervolume

Fig. 1. Hypervolume flow on a 2-element population on MOP GSP for $\alpha = 0.5$

To examine the hypervolume flow we first consider MOP GSP for $\alpha = 0.5$ (see Figure 1). The optimal archive in this case are two Pareto optimal solutions near to the end points of the solution set. Starting with the 2-element archive $P_0 = \{x_1 = (-0.25, -2.5)^T, x_2 = (0, 2.5)^T\}$, we can observe that both individuals x_1 and x_2 directly move toward the nearest optimal solution. The flow hence yields the desired behavior.

As a second positive example we consider a 5-element population on MOP GSP for $\alpha = 1.25$, see Figure 2. Similarly to the above example, all individuals of the initial population perform a more or less direct movement (both in decision and objective space) toward the optimal 5-element HV archive for the reference point $r = (10, 10)^T$.

Next, we consider the same initial population as before, but consider the MOP GSP with $\alpha = 0.5$ (i.e., only the value of α in the model has been changed, the Pareto front is now linear). Instead of a convergent behavior we see in Figure 3 that the extreme solutions x_1 and x_5 (to be more precise, the solutions such that the images $F(x_i)$ are minimal according to f_1 and f_2, respectively) perform a movement toward the extreme points of the Pareto set/front. The other solutions also perform a movement toward the Pareto set, however, it is apparent that this is done with a much slower 'speed'. The reason for this 'creepiness' is certainly the huge difference in the norms of the subgradients: A discretization of (3) via the Euler method leads from a given population P_i to the new one

$$P_{i+1} = P_i + t_i \nabla H(P_i), \tag{8}$$