

Emergence, Complexity and Computation ECC

Hendrik Richter  
Andries P. Engelbrecht *Editors*

# Recent Advances in the Theory and Application of Fitness Landscapes

 Springer

# Emergence, Complexity and Computation

## Volume 6

### *Series Editors*

Ivan Zelinka, Technical University of Ostrava, Czech Republic

Guanrong Chen, City University of Hong Kong, Hong Kong

Andrew Adamatzky, University of the West of England, Bristol, United Kingdom

### **Editorial Board**

Otto RöSSLer, Institute of Physical and Theoretical Chemistry, Tübingen, Germany

Edward Ott, University of Maryland, USA

Ajith Abraham, MirLabs, USA

Vaclav Snašel, Technical University of Ostrava, Czech Republic

Jouni Lampinen, University of Vaasa, Finland

Emilio Corchado, University of Salamanca, Spain

Hendrik Richter, HTWK Leipzig University of Applied Sciences, Germany

Martin Middendorf, University of Leipzig, Germany

Mohammed Chadli, University of Jules Verne, France

Juan C. Burguillo, University of Vigo, Spain

Sergej Čelikovský, Academy of Sciences of the Czech Republic, Czech Republic

Donald Davendra, Technical University of Ostrava, Czech Republic

Juan A. Rodríguez-Aguilar, IIIA-CSIC, Spain

Ana Lucia C. Bazzan, Universidade Federal do Rio Grande do Sul, Porto Alegre RS Brasil

Gheorghe Păun, Romanian Academy, Bucharest, Romania

Linqiang Pan, Huazhong University of Science and Technology, Wuhan, China

Ivo Vondrák, Technical University of Ostrava, Czech Republic

Andrew Ilachinski, Center for Naval Analyses, USA

For further volumes:

<http://www.springer.com/series/10624>

## *About this Series*

“The Emergence, Complexity and Computation (ECC) series publishes new developments, advancements and selected topics in the fields of complexity, computation and emergence. The series focuses on all aspects of reality-based computation approaches from an interdisciplinary point of view especially from applied sciences, biology, physics, or Chemistry. It presents new ideas and interdisciplinary insight on the mutual intersection of subareas of computation, complexity and emergence and its impact and limits to any computing based on physical limits (thermodynamic and quantum limits, Bremermann’s limit, Seth Lloyd limits...) as well as algorithmic limits (Gödel’s proof and its impact on calculation, algorithmic complexity, the Chaitin’s Omega number and Kolmogorov complexity, non-traditional calculations like Turing machine process and its consequences,...) and limitations arising in artificial intelligence field. The topics are (but not limited to) membrane computing, DNA computing, immune computing, quantum computing, swarm computing, analogic computing, chaos computing and computing on the edge of chaos, computational aspects of dynamics of complex systems (systems with self-organization, multiagent systems, cellular automata, artificial life,...), emergence of complex systems and its computational aspects, and agent based computation. The main aim of this series it to discuss the above mentioned topics from an interdisciplinary point of view and present new ideas coming from mutual intersection of classical as well as modern methods of computation. Within the scope of the series are monographs, lecture notes, selected contributions from specialized conferences and workshops, special contribution from international experts, as well as selected PhD theses.”

Hendrik Richter · Andries P. Engelbrecht  
Editors

# Recent Advances in the Theory and Application of Fitness Landscapes

 Springer

*Editors*

Hendrik Richter  
HTWK Leipzig University of Applied  
Sciences  
Faculty of Electrical Engineering  
and Information Technology  
Leipzig  
Germany

Andries P. Engelbrecht  
Department of Computer Science  
University of Pretoria  
Pretoria  
South Africa

ISSN 2194-7287

ISBN 978-3-642-41887-7

DOI 10.1007/978-3-642-41888-4

Springer Heidelberg New York Dordrecht London

ISSN 2194-7295 (electronic)

ISBN 978-3-642-41888-4 (eBook)

© Springer-Verlag Berlin Heidelberg 2014

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed. Exempted from this legal reservation are brief excerpts in connection with reviews or scholarly analysis or material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work. Duplication of this publication or parts thereof is permitted only under the provisions of the Copyright Law of the Publisher's location, in its current version, and permission for use must always be obtained from Springer. Permissions for use may be obtained through RightsLink at the Copyright Clearance Center. Violations are liable to prosecution under the respective Copyright Law.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

While the advice and information in this book are believed to be true and accurate at the date of publication, neither the authors nor the editors nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Printed on acid-free paper

Springer is part of Springer Science+Business Media ([www.springer.com](http://www.springer.com))

*To my daughter Malena Charlotte, who was  
conceived, carried, and born while this book  
was being prepared – Hendrik Richter*

*To Anneli Carien, who came to this world  
while the book was being prepared – Andries  
Engelbrecht*

# Foreword: Statable and Non–prestatable Fitness Landscapes

Stuart Kauffman

It is an honor to be asked to write a foreword for this fine book on recent advances in the theory and application of fitness landscapes. The topic is vast, the book a superb review of much of its current status. My task is not to present a précis of the book itself, but, I hope, to place its topics in an even wider context as I, with my own limited biases, see that context.

## *Topic 1*

The first context is that of this book. We are confronted, typically, with a well formulated continuous or discrete complex combinatorial optimization problem of a fixed fitness landscape and seek a search algorithm to find good optima or even the global optima. Here the landscape constitutes a fixed “potential function” whose peaks or valleys are the desired solutions. Derived from this, as discussed so well in this book, are co-evolutionary problems in which two or more landscapes are coupled, agents on each landscape making adaptive moves and thereby deforming the other landscape. Such systems are general dynamical systems and known to exhibit, as discussed in this book, two modes of behavior, one in which the agents reach mutually consistent local optima and the system stops changing. In the other, as agents move, their landscapes deform even more rapidly, resulting in chaotic behavior, sometimes called the Red Queen effect. Between these two regimes lies a “critical” phase transition. In general, these models are a subset of game theory in which each agent can, typically, only change to neighboring strategies in a genetically encoded strategy space. The mutually consistent local peak solution is the generalization of pure strategy Nash equilibria from games where any move can be made in strategy space, to those in which only neighboring moves can be made. Past work by this author has given initial results that optimal solutions are at least sometimes found at the critical phase transition [1]. Landscapes can occur without and with neutrality. The statistical structure of such landscapes is a major topic of concern, and with it, use of measures of that statistical structure, such as landscape

correlation lengths, Stadler et al.'s "reachability topology" (as discussed in Chapter 6 of this book) and others, to attempt to predict how hard learning or adaptation may be on fixed, or, harder, co-evolving landscapes. Beyond this, in this book are efforts to consider time varying landscapes that may vary in stochastic or non-stochastic ways. This latter topic will become of major concern below in this foreword. The well known no free lunch theorem suggests that averaged over all landscapes, no search algorithm outperforms any other algorithm. This book contains efforts noted above to study the structure of a given landscape to choose algorithms that may be better than average or even very good on a given landscape. The problem is stated to be insoluble in general, but sometimes good algorithms can be found.

## *Topic 2*

A second fundamental issue, which is outside the scope of this book, is the kinds of problems, the kinds of systems we or, say evolution, seeks to optimize, to generate what kinds of landscapes? Here little work, to my knowledge has been done. But it is of fundamental importance. I present a brief conjecture that some problems are not solvable by any local search algorithm in less than exponential time. Consider the shortest algorithm to produce a given output on a universal computer. Let its (unprovable) length be  $N$ . Gregory Chaitin has shown on the  $N$  dimensional Boolean hypercube there is on order of a single vertex that constitutes this program, where the binary string at that vertex is the program for the computer. Chaitin then shows that if one considers programs of length  $N, N + 1, N + 2, \dots, N + C$ , there are in the order of  $1, 2, 4, \dots, 2^C$  vertices on the hypercube that satisfy the requirement to be a program of that length that solves the problem. Now my conjecture, perhaps able to become a theorem: Take a fixed length input string and choose the single correct vertex on the  $N$  dimensional Boolean hypercube where only that single vertex yields the proper output on that input. Run the randomly chosen input string on the "correct" vertex and observe the output string taken as the proper solution. Now choose the  $N$  "one mutant neighboring points" to the "correct" vertex, and run the input string on each of these to obtain an output string. Use normalized compression distance to compare the correct output string and the output string of a given 1 mutant neighbor of the correct vertex. Normalized compression distance,  $NCD$ , a universal measure of, essentially, the mutual information between these two strings. Use  $1 - NCD$  as a measure of the "fitness" of the program at that one mutant neighbor of the correct vertex. Do this for all vertices on the  $N$  dimensional hypercube to obtain a "fitness landscape" of the fitness of each program, encoded at each vertex, to generate an output similar or dissimilar to the correct output. My bet is that for the minimal length program, length  $N$ , the resulting fitness landscape is *random*. That is, I bet, to be proven, that the fitness at neighboring vertices are random in value. It is known that such landscapes have on the order of  $\frac{2^N}{N+1}$  local optima. Thus finding the global optimum with the correct minimal program is NP hard, requiring search of the entire space or at least, as the space is exponential in  $N$ , a fixed fraction of this exponentially large space; hence, for large  $N$ , not solvable in less than exponential



time. My further guess is that if one started with a redundant program, longer than  $N$ , i.e.  $N + C$ , due to that redundancy, the fitness landscape on the  $N + C$  Boolean hypercube, it would be a correlated landscape whose correlation length increases as  $C$  increases. My further bet is that no procedure can start with an  $N + C$  landscape and evolve to ever smaller  $C$  approaching  $C = 0$  to achieve the minimal program, because as  $C$  decreases, the landscape becomes less correlated then uncorrelated. My guess is that as  $C$  decreases, correlations on the landscape may be related such that the evolving system is led into a region of the  $N$  dimensional space close to the correct vertex, but on the  $C = 0$  random landscape, no local search algorithm is likely to find the nearby correct solution before wandering off on the random landscape away from the correct solution. “Likely” may be quantifiable.

### ***Topic 3***

This discussion suffices to relate some problems, here finding the shortest algorithm to solve a problem and the structure of the induced fitness landscape. More it relates to the next issue, for the above problem, in my conjecture, cannot be solved by mutation and selection alone, and perhaps not by recombination, mutation and selection together, for recombination does not work on random landscapes [2]. If so, no evolutionary process in biology can evolve the shortest program. All this needs to become a set of theorems, relating to the issue of what problems induce what landscapes and why.

1. Do biological and economic and other evolutionary processes “tune” the very structure of the fitness landscapes upon which they evolve? This book does not address this topic. In [1], I had a first try at the problem, and believe I showed a model in which, with no group selection, “organisms” co-evolving on landscapes and invading one another’s niches could evolve the structure of the fitness landscapes upon which they evolved. In this model, an invading species, if successful in a new niche, carried with it the ruggedness of its own landscape. Thus landscape ruggedness itself becomes an evolving feature of the total evolving system, and landscape ruggedness itself can evolve. In this model, the system evolves from Red Queen, and from the stationary Nash equilibrium regime to the critical phase transition between the two, and, on average, the life time of species increases and their fitness increases. These results suggest that an evolutionary process can, in fact, evolve the very structure and couplings among co-evolving agents to the long term benefit of all the currently evolving agents. This topic remains very unexplored but is likely to be of major importance. It suggests that biological and economic evolution are “tuning” the statistical structure of the very problems and thus fitness landscapes over which they evolve to become more “evolvable” and “solvable”. Much remains to be learned.
2. Adaptive evolution in the biosphere and economy and elsewhere is probably not only occurring on time deforming and stochastically time deforming landscapes, it is far worse: Not only can we not characterize the stochastic process by which landscapes change, we cannot even prestate the possibility space, that is

the ever changing phase space of these evolutionary processes, hence we can neither mathematize actual evolution of the biosphere, biosphere and ecology, or the economy or culture or law. And even if we could write down laws of motion for this evolution, we would lack foreknowledge of the “niche” boundary conditions and so could not integrate the equations we do not have anyway. In short, if what I say with my colleagues, Giuseppe Longo, Mael Montevil, and myself [4, 5], is correct after careful examination, *no laws* entail the evolution of the biosphere or, a fortiori the economy or probably many aspects of life. Not only do we not know what *will* happen, we do not even know what *can* happen. Thus we cannot formulate a probability distribution over what “can happen” for we do not know the sample space beforehand. Therefore we cannot formulate a stochastic model of changing landscapes for, as we will see next, we cannot prestate the variables that will become relevant, so we do not know the space over which to formulate a fitness landscape.

## Topic 4

I discuss the fourth topic in several sections below.

### 1. The Non Ergodic Universe Above the Level of Atoms

Has the universe created in its 13.7 billion years all known atoms? Yes. But now consider proteins made of 20 kinds of amino acids strung together in a linear sequence by peptide bonds. A typical biological protein has a length of 300 amino acids. Consider, then, all possible proteins length 20 amino acids. There are  $20^{200}$  or about  $10^{260}$  such possible proteins. Now the universe has about  $10^{80}$  particles. Its fastest time scale is the Planck time scale of  $10^{-43}$  seconds. Ignoring space-like separation, if all the universe were doing in the past 13.7 billion years was constructing, in parallel, different proteins of length 200, it would require the current age of the universe raised to the 37th power to construct all possible proteins of length 200 just *once*. This has physical meaning. At levels above the atom in complexity, the universe is on a unique trajectory that cannot become ergodic in the lifetimes of many universes. Thus, most complex things will never exist, so those complex things that get to exist have a special status.

### 2. Kantian Wholes

Kant said that in an “organized being the parts exist for and by means of the parts”, that is, the whole exists by means of the parts and the parts exist by means of the whole. He was thinking of organisms.

### 3. Collectively Autocatalytic Peptide Sets as Minimal Kantian Wholes

Gonen Ashkenasy [6] at the Ben Gurion University, has a set of 9 peptides, each of which catalyzes the formation of the next peptide by ligating two fragments of that peptide, around a 9 peptide circle of peptides. The set as a *whole* is collectively autocatalytic. Note that no peptide catalyzes its own formation; the set as a whole collectively catalyses its own formation. As a side comment, Ashkenasy’s results demonstrate conclusively that molecular reproduction does not depend

upon DNA- or RNA-like template replication. Now, calling catalysis of a reaction a “catalytic task”, the 9 peptide collectively autocatalytic set achieves a *task closure*. All the reactions that must be catalyzed from within the set, are catalyzed from within the set. The system is also an open thermodynamic one deriving food from the two fragments of each peptide maintained at constant concentration.

Now note that a collectively autocatalytic set is a minimal model of a Kantian Whole, the parts, peptides, exist for and by means of the whole *task closure*, and the whole exists by means of the peptide parts. Note next, as an essential side point, that given the collectively autocatalytic set, we can define the *function* of a part by its causal consequences that serve to maintain the collectively autocatalytic whole; that is, catalyzing the appropriate next ligation reaction, not wiggling water in the petri plate. So functions that are real in the universe are a *subset* of the causal consequences of the parts. So Kantian wholes have parts with some causal consequences as functions and other causal consequences as irrelevant side effects in that environment.

#### 4. Task Closure in an Evolving Reproducing Bacterium

A reproducing bacterium achieves a *task closure* that is much wider than mere catalysis. Membranes are formed, DNA replicated, chemiosmotic pumps built and vectored to proper membrane locations, receptors are constructed and located in membranes all for the bacterium to reproduce.

#### 5. The Uses or Functions of a Screw Driver *Cannot be Algorithmically Enumerated*

I now jump to a seemingly strange topic. Can you list all the uses of a screw driver? Screw in a screw, open a paint can, wedge open or closed a door, stab an assailant, prop up a piece of cardboard.... The uses of a screw driver are *indefinite in number*. Next, the integers are orderable, 1, 2, 3, 4, ..., but are the uses of a screw driver orderable? Say beyond its “first use” to screw in screws? *No*. But this means that there is *no effective procedure, or algorithm, to list all the uses of a screw driver*. This is the famous unsolved *frame* problem of computer science.

#### 6. Evolution *Find Unprestatable Uses of Molecular Screw Drivers in Evolving cells, Then Selected at the Level of the Kantian Whole Cells*

In an evolving bacterium in, say a new environment, all that has to happen is that someone or more molecular or cellular component screw drivers *find a use* that enhances the fitness of the evolving cell. Then if there is heritable variation for that new or improved use, it will be grafted into evolution by Natural Selection. But we cannot list, hence cannot prestate the new use of the molecular screw driver selected at the level of the Kantian whole cell. Thus, we cannot prestate the way the very phase space, the space of possibilities, of evolution changes. (Note that this *is* the arrival of the fittest, never solved by the NeoDarwinian synthesis.)

## 7. The Evolution of the Biosphere is Not Mathematizable as Integrable Laws of Motion

Since we cannot prestate the new functionality of the cellular or molecular screw driver, we cannot prestate the way the evolving phase space of evolution changes. Hence we *cannot write down equations of motion for this evolution. Nor, since we lack prestatement of niche boundary conditions, could we integrate those equations of motion, even if we were to have them!*

*This implies that the evolution of the biosphere is entailed by no law. If correct, reductionism end at the watershed of the evolution of life. In turn this implies that we cannot prestate the space of possibilities that constitute the space over which there is a prestatable fitness landscape. Further, because we cannot prestate that ever changing phase space, we do not know its sample space, so we cannot construct a probability measure. In turn, this implies that we cannot formulate stochastic processes for the changes in the fitness landscape.*

## 8. The Evolving Biosphere, Without Selection “Acting to Achieve It”, Persistently Creates Its Own Future Possibilities

The last point I wish to make is beyond the subject of fitness landscapes themselves, but one which I find to be stunning. If true, as what I shall say appears to be, it changes our view of the reality we live in in the evolving living world. I need to define Darwinian Preadaptations. Were we to ask Darwin the function of the human heart, he would respond that it is to pump blood. But we might say hearts make heart sounds and jiggle water in the pericardial sac. Why are these causal consequences of the heart not its function? Darwin would answer that we have hearts because their pumping blood was of selective significance in our ancestors. Note that therefore, as with the peptide collectively autocatalytic set above, the function of the heart is a subset of its causal consequences. More Darwin is also implicitly answering the question of why a complex organ, the heart, exists in the non-ergodic universe: Because it plays a role in sustaining Kantian Whole organisms in existence in the non-ergodic universe.

Next, Darwin noted that a causal consequence of the heart, or other organ, of no selective significance in the current environment, might have selective significance in a new environment and be selected for that new functional significance. A new function might arise. These are called Darwinian preadaptations, or by Gould, exaptations.

I give but one example: Some fish have an organ called a swim bladder. The ratio of air and water in the bladder-sac determines neutral buoyancy in the water column. Paleontologists believe that the swim bladder evolved from the lungs of lung fish. Water got into some lung(s), now there were sacs partly filled with air and water, poised to evolve into swim bladders. Let’s assume the paleontologists are right.

I now ask three questions: First, did a new function come to exist in the biosphere? Yes, neutral buoyancy in the water column. Note that evolution here solves the *frame* problem which algorithmic computer science cannot solve. In my understanding, the *frame* problem is that, e.g. for a robot in a room, one

provides a finite list of “affordances” for objects in the room, e.g. corner of the room, floor electric plug, where the affordance finite list is of “is a”, “does a”, “uses a”, “needs a”, etc. Then anything that can be deduced from this *finite* list is within the *frame* yielded by the finite list of affordances. *But uses*, as in the screw driver uses, cannot be captured by any finite list in the sense that no effective procedure can do so. *We* solve the frame problem as humans all the time. We find new uses for object and processes. An example: Engineers, the story/fact says, were trying to invent the tractor. They needed a huge engine block, got one, mounted it on a series of ever bigger chassis, all of which broke. Finally an engineer said, “You know, the *engine block itself* is so big and *rigid*, that we can use the engine block itself *as* the chassis, and hang everything else off the engine block.” And that was the invention of the tractor and how they are made. So too were formula racing cars. This use of the engine block’s rigidity for a new function, is a technological Darwinian preadaptation and could not, in general be predated. This *is* the solving of the frame problem. As I said we do it all the time, Turing machines cannot, hence I believe human mind is not algorithmic, see my speculative paper, Answering Descartes: Beyond Turing [3]. So too, I think the swim bladder solves the frame problem.

Second, did the swim bladder, once it exists, alter the future evolution of the biosphere? Yes, new species evolved with swim bladders, new proteins evolved. And particularly important, once the swim bladder exists, a worm or bacterium or both might evolve to live in swim bladders, so the existing swim bladder is what I’ll call an “Empty Adjacent Possible Niche”. Thus the swim bladder, once it exists, changes the future possible evolution of the biosphere. I return to this for it is the main point of this last section. Third, now that you know what preadaptations are, can you name all possible Darwinian preadaptations, just for human evolution in the next 4 million years? We all say *NO*. Why? Well, how would we name all possible selective environments? Now that we had listed all those environments? How would we list all the features of one or several organisms that might constitute preadaptations? We cannot. And the reason was given above, “the uses” of a screw driver are indefinite in number and unorderable, so no algorithm can be an effective procedure to list them all. And if we take one use of a screw driver, say to open a can of paint, the number of other objects/processes that can open a can of paint is indefinite and unorderable, so again, no effective procedure or algorithm can list them. Hence our *no* above. Hence we not only do not know what *will* happen, we do not even know what *can* happen.

Now return to the existing swim bladder as an “Empty Adjacent Possible Niche” that changes the future possible evolution of the biosphere. Do we think that natural selection acted on a population of lung fish to “craft” a well functioning swim bladder? Yes, of course. The swim bladder is a selected preadaptation, “achieved” by natural selection. But do we think that natural selection “acted” in any sense of “act” to “achieve” the swim bladder as a new Adjacent Possible Empty Niche? *NO!* Selection was involved in achieving a functioning swim bladder. But selection was not evolved in creating that swim bladder *AS* a new Adjacent Possible Empty Niche. Yet once that niche exists, it alters the future

possible evolution of the biosphere, for the worm or bacterium really might come to evolve to live in the swim bladder.

But this means something profound: Without selection “acting” to do so, the biosphere is persistently creating its own future possibilities! The biosphere, beyond selection, persistently creates what it may become. If the above two sections are right, reductionism fails for the evolution of life and we are beyond Newton and Schrödinger. If the last section is right, we are beyond even Darwin.

May this fine book add to the growing discussion of all these topics.

**Acknowledgements.** This work is partially supported by the TEKES FOUNDATION for my position as a Finland Distinguished Professor.

## References

- [1] Kauffman, S.: *At Home in the Universe*. Oxford University Press, New York (1995)
- [2] Kauffman, S.: *The Origins of Order: Self-organization and Selection in Evolution*. Oxford University Press, New York (1993)
- [3] Kauffman, S.: *Answering Descartes: Beyond Turing*. In: Barry Cooper, S., Hodges, A. (eds.) *The Once and Future Turing: Computing the World*. Cambridge University Press, Cambridge (in press, 2013),  
<http://mitpress.mit.edu/sites/default/files/titles/alife/0262297140chap4.pdf>
- [4] Longo, G., Montevil, M., Kauffman, S.: No entailing laws, but enablement in the evolution of the biosphere (2012), <http://arxiv.org/abs/1201.2069>
- [5] Longo, G., Montevil, M., Kauffman, S.: No entailing laws, but enablement in the evolution of the biosphere. In: Soule, T., Moore, J.H. (eds.) *Proc. GECCO Companion*, pp. 1379–1392. ACM, New York (2012)
- [6] Wagner, N., Ashkenasy, G.: Symmetry and order in systems chemistry. *The Journal of Chemical Physics* 130, 164907–164911 (2009)

Santa Fe, N.M. USA, March 6, 2013

Stuart Kauffman

# Preface

Observing life on Earth, it is hard to ignore its overwhelming abundance, diversity and beauty, its finely-tuned structures and forms, and its imaginative as well as purposeful behaviors and functions. First and foremost this applies to all forms of natural life, meaning the molecular, carbon- and protein-based forms of life found on our planet. Clearly on a smaller scale but nevertheless, also instances and examples of artificial life forms created in digital computers can exhibit properties that surprise us in their beauty and complexity. For both cases, arguable for the former even more so than for the latter, it is as obvious as interesting to ask why life is as it is and how it came (or comes or will come) into being. It is scientific consensus and hence tempting to give a rather simple and in some ways self-explaining answer: by the mechanism of Darwinian evolution. This certainly is true but simply poses other questions. How is evolution working? How does it enable the development of life forms? Are evolutionary developments in some ways directed, or even forced and can be predicted within certain bounds? Or is evolution directionless, open-ended and indeterminate with respect to possible outcomes? What role does chance and randomness play in evolution in general? What can be realistically expected to be the outcome of a certain period of evolutionary development? What is a meaningful mathematization of evolutionary dynamics? What requirements and preconditions must be fulfilled for the emergence of complex biological forms and behaviors, may they be natural or artificial?

Admittedly, answering all these questions conclusively is far beyond the scope of this book; in fact, it is beyond the current understanding in the sciences in general. Nevertheless, we believe that the foundation for answering these questions is an understanding of evolution as a dynamical process. This goes along with (and is unthinkable without) describing the driving forces that enable evolutionary dynamics. Addressing the dynamics of evolution is the main scope of this book, and the approach we use is the framework of fitness landscapes.

Fitness landscapes are an abstract way for describing the relationship between the genetically possible (genotype), the actually realized (phenotype) and the survival/reproduction success (fitness). Differences in the fitness over genotypic space together with the Darwinian imperative to move into the direction of increasing

fitness (codified by the notion of natural and sexual selection) results into the driving forces that are behind evolutionary processes. Undeniably, evolution is a defining feature of natural life. However, we take the view that evolutionary processes are much more general than biology. In particular, the dynamical processes in evolutionary computation are in their core and essence as much a manifestation of evolution as the processes observed in biological systems. For using evolutionary search algorithms to solve optimization problems, we are interested in basically the same questions as above. What algorithmic performance can be expected for a given evolutionary search algorithm and optimization problem (that is a given genotype-to-fitness map)? How will performance scale if either the algorithm's parameters or the setting of the optimization problem, or both, were to change? Also, answering these questions requires understanding the underlying evolutionary dynamics and can hence be approached by fitness landscape methods.

In theoretical biology, recent experimental and numerical works involving mutational evolution of molecular functions revealed far-reaching implications on possible evolutionary paths, which have renewed the interest in fitness landscapes. In computer science, studies of artificial evolution in the form of artificial life and evolutionary computation increasingly used fitness landscape methods to describe evolutionary dynamics. Using these methods is particularly aimed at increasing our knowledge about the working principles of the algorithm, its expected behavior as well as some aspects of performance. Both fields, theoretical biology and evolutionary computation, to a certain degree experienced a renaissance in using landscape methods with a significant number of recent works. However, the recent progress can be found in the literature only in a very decentralized manner. Hence, the motivation to write and edit this book came from two observations: the recent advances in understanding fitness landscapes in both theoretical biology and computer science and the lack of a book covering it. We have invited some of the leading researchers that drove the recent advances in the field to provide their views on various aspects of fitness landscapes.

One main aspect of the book is that research in fitness landscapes has been separated into many distinct fields and would benefit from some kind of unification. This is also to promote communication between the fields and cross-fertilization of ideas. Consequently, we have encouraged the authors to put emphasis not only on specific questions and methodological details, but also on fundamental questions as to what is the inner sense and meaning of the approach, what is the background and the underlying principles, how is it related to research around it, and where is it going to (or could it go to). Of course, we were not aiming at compiling a tutorial or textbook, but we advocated the chapters (in difference to usual journal or proceedings papers) to be able to stand alone and to be understandable in itself by scientists of roughly related fields not yet working on fitness landscapes. In other words, if it appeared necessary to compromise between a certain degree of redundancy between chapters and the stand-alone ability of a chapter, we promoted the former over the latter.

The book has in total 20 chapters and a foreword. The chapters are not ordered by theory and application, as the book title might suggest, but by five groups of



themes. Almost all chapters address both theoretical and application aspects. We have divided the chapters that follow into five parts:

- Part I: Principles and perspectives
- Part II: Topology, measures and problem hardness
- Part III: Coevolution and dynamics
- Part IV: Visualization and characterization
- Part V: Outlook and afterthoughts

### ***Part I: Principles and Perspectives***

In this part, we intend to set out basic principles of and different perspectives to fitness landscapes. Chapter 1 by Hendrik Richter gives an introduction to the book and an overview of concepts, notions and mathematical descriptions of fitness landscapes. The chapter discusses major motivations to use landscape paradigms and considers how topological features of the landscape give rise to evolutionary dynamics. It further introduces examples of computational and empirical landscapes. Herschel Rabitz, Re-Bing Wu, Tak-San Ho, Katharine Moore Tibbetts and Xiao-jiang Feng review in Chapter 2 recent developments in considering the landscape's input variables as controls. The chapter further specifies three assumptions whose satisfaction permits a general analysis of the landscape topology and demonstrates that control landscapes may be devoid of suboptimal critical point traps. The chapter applies this analysis to control landscapes that arise in quantum mechanics, chemical and material science, and in natural and directed evolution. Takuyo Aita and Yuzuru Husimi study in Chapter 3 evolutionary processes using the concept of the information gaining process. As the evolutionary process can be modeled as a walk on a fitness landscape, the evolving entity collects biomolecular information. Using this information gaining approach the chapter draws a link between evolutionary dynamics and thermodynamics, introduces the concept of "free fitness" which is analogous to free energy, and proposes that evolution is driven in the direction in which the free fitness increases.

### ***Part II: Topology, Measures and Problem Hardness***

Non-trivial fitness landscapes originate from differences in fitness over genotypic space. These differences in fitness cast the landscape's topological features, which in turn shape possible evolutionary paths. This part is devoted to the relationships between the landscape's topology and the hardness of locating evolutionary paths. Crucial links between topology and problem hardness are formed by landscape measures which quantify the effects the topology has on search paths. Chapter 4 by Katherine M. Malan and Andries P. Engelbrecht considers metaheuristic search algorithms and their optimization performance. It focuses on the feasibility of predicting algorithm performance on unknown real-valued problems based on fitness landscape features. The chapter proposes normalized metrics for quantifying algorithm performance on known problems and shows that fitness landscape

techniques are useful as a part–predictor of algorithm performance. A related but slightly different aspect is discussed in Chapter 5 by Guanzhou Lu, Jinlong Li and Xin Yao, which also deals with problem hardness and evolutionary search algorithms. A problem hardness measure is presented in this chapter which is derived from a theoretical difficulty measure widely used in complexity theory. It is shown how the measure can be incorporated with a machine learning algorithm for parameter tuning and hence contributes to the goal of constructing better suited algorithms for solving problems. In Chapter 6 by Konstantin Klemm, Jing Qin and Peter F. Stadler another fundamental issue is addressed with considering geometric notions for describing the structure of landscapes as well as the dynamics of local search on them. Focusing on discrete, combinatorial landscapes and emphasizing the complications arising from local degeneracies, the authors introduce combinatorial vector fields as a mathematical tool for understanding landscape features. Also the coarse graining of landscapes is studied from two perspectives. Chapter 7 by Kristina Crona resumes with a geometrically oriented study of landscapes and concentrates on graphs and polytopes. It introduces fitness graphs for describing coarse properties of landscapes such as mutational trajectories and the number of peaks. Triangulations of polytopes give raise to shapes that can replace the well established concepts of positive and negative epistasis for two mutations. Yoshiaki Katada deals in Chapter 8 with two important topological features of landscapes: ruggedness and neutrality. As the evolutionary dynamics on a fitness landscape with neutrality shows special characteristics, ruggedness alone might be insufficient. In the chapter, a neutrality measure called standard genetic distance is introduced, which originates from population genetics, for measuring neutrality of fitness landscapes. Numerical experiments are reported and demonstrate that genetic distance is a reliable method for estimating the degree of neutrality of real-world problems. Chapter 9 by Gabriela Ochoa, Sébastien Verel, Fabio Daolio and Marco Tomassini gives an overview of local optima networks (LON) which are a recently introduced network–based model of combinatorial landscapes. The model compresses the information given by the whole search space into a smaller mathematical object and yields a new set of metrics to characterize the structure of combinatorial landscapes. The approach is applied to two well–known combinatorial optimization problems and the experimental results show that the network features correlate with and even predict the performance of heuristic search algorithms operating on these problems.

### ***Part III: Coevolution and Dynamics***

Traditionally, the structure and topology of fitness landscapes are considered to be static. This part brings together chapters that consider different approaches dealing with dynamic landscapes, particularly dynamics that is environmental or occurs in and is caused by coevolution. Chapter 10 by Hendrik Richter gives an overview of landscapes whose fitness values change with time. The chapter studies these time–dependent landscapes in two contexts. One is evolutionary processes that take place in dynamic environments and result in dynamic fitness landscapes. Another is

coevolutionary processes where the fitness of a given individual depends on the fitness and the genotype of other individuals in a temporal or spatial fashion and results in codynamic landscapes. The chapter gives an overview of issues in and problems of time-dependent fitness landscapes and particularly highlights several types of mathematical descriptions and their properties. Ricard V. Solé and Josep Sardanyés focus in Chapter 11 on coevolutionary dynamics. The chapter introduces the Red Queen hypothesis of evolution and comments on some theoretical aspects and empirical evidence. It further reviews key issues of evolution on simple and rugged fitness landscapes and presents modeling examples of coevolution on different fitness landscapes at different scales using examples from RNA viruses to complex ecosystems and macroevolution. Chapter 12 by Richard A. Watson and Marc Ebner treats another aspect of dynamic landscapes with the interactions of evolutionary and ecological dynamics. To understand these interactions as coupled processes leads to eco-evolutionary dynamics that can be modeled by deformable fitness landscapes. The chapter reports numerical experiments and observes that the model of deformable landscapes can exhibit either of the two behavioral modes: evolutionary stasis or continued evolutionary change (also known as Red Queen dynamics). Wim Hordijk present an overview of a statistical analysis to measure and express the correlation structure of fitness landscapes in Chapter 13. The correlation analysis is applied to both static and coupled fitness landscapes. The experimental results presented show that the correlation analysis gives a direct and useful link to the actual search performance of evolutionary algorithms that use a coevolutionary approach. Chapter 14 by Krzysztof Trojanowski concludes this part with a discussion about dynamic real-valued landscapes and methods of evaluating the efficiency of (meta-)heuristic optimization algorithms operating on these landscapes. The chapter introduces measures for dynamic performance evaluation and associated measurement methods, gives dynamic benchmarks and different types for implementing changes, and considers the role of time and uncertainty originating from the measurement method.

#### ***Part IV: Visualization and Characterization***

As the structure and topology of a fitness landscape offers to gain insight into evolutionary dynamics, it is vital to have methods and tools for visualizing and characterizing landscape's properties. The chapters in this part discuss such questions. Chapter 15 by Ivan Zelinka, Oldrich Zmeskal and Petr Saloun is devoted to fitness landscapes with fractal characteristics. The main topic of this chapter is to use elements from fractal geometry to measure attributes of fractal landscapes. These attributes are taken to characterize fractal properties of basic artificial test functions as well as cost functions of real application problems that appear in experimental chaos control and synchronization. Daniel Ashlock, Justin Schonfeld, Wendy Ashlock and Colin Lee describe in Chapter 16 three important tools that were recently suggested to explore fitness landscapes: agent-case embeddings, fitness morphs, and nonlinear projection. These techniques are examined using fitness landscapes for a variety of

discrete problems including finding self avoiding walks, finding features for DNA sequence classification, the Tartarus AI test problem, locating cellular automata rules, and a novel real optimization problem connected with the Mandelbrot set. The results show that the techniques discussed transform information about discrete fitness into real-valued spaces enabling both analysis and visualization. Another approach to visualize fitness landscapes is presented in Chapter 17 by Sebastian Volke, Simon Bin, Dirk Zeckzer, Martin Middendorf and Gerik Scheuermann. This approach is applied to the question of how and why changes in the design of a particle swarm optimization (PSO) algorithm influence its optimization behavior. The visual approach discussed in the chapter combines a terrain representation of the fitness landscape topology with configuration-local, time-dependent statistical measures of PSO runs and is implemented in a visualization tool called dPSO-Vis. It is demonstrated how dPSO-Vis can be used to analyze and compare the optimization behavior of PSO algorithms designed for solving the RNA folding problem. Bjørn Østman and Christoph Adami finally give in Chapter 18 a concise overview of the relationship between visualization of fitness landscapes and potential predictability of evolutionary dynamics. To know whether evolution is predominantly taking paths that move upwards in fitness and along neutral ridges, or else entails a significant number of valley crossings, there is the need to visualize these landscapes. For instance it must be determined whether there are peaks in the landscape, where these peaks are located with respect to one another, and whether evolutionary paths can connect them. The chapter focuses on the predictability of evolution on rugged genetic fitness landscapes and presents numerical results to answer the question of whether evolutionary trajectories towards the highest peak in the landscape can be achieved via a series of valley crossings.

### ***Part V: Outlook and Afterthoughts***

The final part of this book contains two shorter chapters devoted to the prospects of fitness landscape research. Possible future issues are discussed in Chapter 19 by Hendrik Richter. The chapter addresses challenges to fitness landscape approaches that result from recent experimental and theoretical findings about the information transfer in biological systems. It further sets out opportunities these results may open up and speculates about directions that landscape research may take. Chapter 20 by Edward D. Weinberger concludes the book with afterthoughts and discusses the past, the present and the future of the topic. In a personal reminiscence fueled by his involvement in fitness landscape research for over 20 years, he particularly highlights the need to rethink our concepts of fitness, the relevance of coevolutionary effects and the importance of information used by biological systems. The chapter also concludes that a main topic to be addressed by future research is to advance our understanding of biological evolution as a dynamical process. Landscape methods, if extended and adapted, have the potential to achieve this.

It is often said that there are more contributors to a book who should be acknowledged than the people whose names appear on the cover page. This literally applies to this book. So, our foremost thank goes to the in total 42 authors of the chapters who entrusted their contributions to this book. We are also very thankful for both the foreword and the afterthoughts. Stuart Kauffman, who moved the topic of fitness landscapes significantly beyond the scope of evolutionary biology with his seminal works in the late 1980s, provided a foreword that is rich in substance, even controversial and discusses limitations of current fitness landscape research as well as points at possible directions of further development. We are equally grateful that Edward Weinberger, who similarly and partly collaborating with Stuart Kauffman significantly extended the scope of fitness landscapes 20 years ago, provided afterthoughts.

To edit and write a publication collaboratively seems to be possible even over large distances nowadays due to communication devices such as email and chat. This book is also proof of that. Nonetheless, we also noted that some discussion is much more fruitful and efficient face to face by visiting each other. So, we thank the HTWK Leipzig University of Applied Sciences for providing a travel grant and the University of Pretoria for cordial hospitality that enabled this visit. Special thanks go to Dr. Thomas Ditzinger of Springer-Verlag for his support during the preparation of this book and to Prof. Ivan Zelinka, the series editor for the Springer Series Emergence, Complexity and Computation (ECC), for inviting the book to this series. Also thanks to all the reviewers who have provided very valuable inputs to improve the quality of the chapters within this book.

Last in order but clearly not in importance, our most heartfelt thanks goes to our families and friends for their support, love, encouragement and patience.

Leipzig, Germany  
Pretoria, South Africa

Hendrik Richter  
Andries P. Engelbrecht

# List of Contributors

Christoph Adami

Department Microbiology and Molecular Genetics & BEACON Center for the Study of Evolution in Action, Michigan State University,  
East Lansing, MI 48824, U.S.A.

e-mail: [adami@msu.edu](mailto:adami@msu.edu)

Takuyo Aita

Graduate School of Science and Engineering,  
Saitama University, Saitama 338-8570, Japan.

e-mail: [taita@mail.saitama-u.ac.jp](mailto:taita@mail.saitama-u.ac.jp)

Daniel Ashlock

Department of Mathematics and Statistics, University of Guelph,  
50 Stone Rd. E, Guelph, Ontario, N1G 2R4, Canada.

e-mail: [dashlock@uoguelph.ca](mailto:dashlock@uoguelph.ca)

Wendy Ashlock

Department of Computer Science and Engineering,  
York University, 4700 Keele Street, Toronto, Ontario, M3J 1P3, Canada.

e-mail: [washlock@sympatico.ca](mailto:washlock@sympatico.ca)

Simon Bin

Department of Computer Science, University of Leipzig,  
Augustusplatz 10, 04109 Leipzig, Germany.

e-mail: [sbin@informatik.uni-leipzig.de](mailto:sbin@informatik.uni-leipzig.de)

Kristina Crona

University of California at Merced, 5200 Lake Road, Merced, CA 95343, U.S.A.

e-mail: [kcrona@ucmerced.edu](mailto:kcrona@ucmerced.edu)

Fabio Daolio

Department of Information Systems, University of Lausanne,  
1015 Lausanne, Switzerland.

e-mail: [fabio.daolio@unil.ch](mailto:fabio.daolio@unil.ch)

Marc Ebner

Ernst Moritz Arndt Universität Greifswald, Institut für Mathematik und Informatik,  
Walther-Rathenau-Strasse 47, 17487 Greifswald, Germany.

e-mail: marc.ebner@uni-greifswald.de

Andries P. Engelbrecht

Department of Computer Science, University of Pretoria, Pretoria 0002,  
South Africa.

e-mail: engel@cs.up.ac.za

Xiaojiang Feng

Kadmon Corporation, 450 East 29th Street, New York, NY 10016, U.S.A.

e-mail: fengxiaojiang@yahoo.com

Tak-San Ho

Department of Chemistry, Princeton University, Washington Road,  
Princeton, NJ 08544, U.S.A.

e-mail: tsho@princeton.edu

Wim Hordijk

SmartAnalytiX.com, Lausanne, Switzerland.

e-mail: wim@WorldWideWanderings.net

Yuzuru Husimi

Innovative Research Organization, Saitama University, Saitama 338-8570, Japan.

e-mail: husimi. @mail.saitama-u.ac.jp

Yoshiaki Katada

Department of Electrical and Electronic Engineering, Setsunan University,  
17-8 Ikeda-nakamachi, Neyagawa, Osaka 572-8508, Japan.

e-mail: katada@ele.setsunan.ac.jp

Stuart Kauffman

University of Vermont, 85 South Prospect Street, Burlington, VT 05405, U.S.A.

University of Pennsylvania, 3451 Walnut St, Philadelphia, PA 19104, U.S.A.

Santa Fe Institute, 1399 Hyde Park Rd., Santa Fe, NM87501, U.S.A.

e-mail: stukauffman@gmail.com

Konstantin Klemm

Bioinformatics Group, Department of Computer Science, and Interdisciplinary  
Center for Bioinformatics, University of Leipzig, Härtelstrasse 16-18, 04107  
Leipzig, Germany.

e-mail: klemm@bioinf.uni-leipzig.de

Colin Lee

Department of Mathematics and Statistics, University of Guelph,  
50 Stone Rd. E, Guelph, Ontario, N1G 2R4, Canada.

e-mail: clee04@uoguelph.ca

Jinlong Li

Joint USTC-Birmingham Research Institute in Intelligent Computation  
and Its Applications

The Nature Inspired Computation and Applications Laboratory (NICAL), School  
of Computer Science and Technology, University of Science and Technology of  
China, Hefei, 230027, China.

e-mail: jlli@ustc.edu.cn

Guanzhou Lu

Joint USTC-Birmingham Research Institute in Intelligent Computation  
and Its Applications

The Centre of Excellence for Research in Computational Intelligence and  
Applications (CERCIA), School of Computer Science, University of Birmingham,  
Edgbaston, Birmingham, B15 2TT, UK

e-mail: g.lu@cs.bham.ac.uk

Katherine M. Malan

Department of Computer Science, University of Pretoria,  
Pretoria 0002, South Africa.

e-mail: kmalan@cs.up.ac.za

Martin Middendorf

Department of Computer Science, University of Leipzig,  
Augustusplatz 10, 04109 Leipzig, Germany.

e-mail: middendorf@informatik.uni-leipzig.de

Gabriela Ochoa

Department of Computing Science and Mathematics, School of Natural Sciences,  
University of Stirling, Stirling, FK9 4LA, Scotland, UK.

e-mail: gabriela.ochoa@cs.stir.ac.uk

Bjørn Østman

Department Microbiology and Molecular Genetics & BEACON Center for the  
Study of Evolution in Action, Michigan State University,  
East Lansing, MI 48824, U.S.A.

e-mail: ostman@msu.edu

Jing Qin

Max Planck Institute for Mathematics in the Sciences,  
Inselstraße 22, 04103 Leipzig, Germany.

e-mail: qin@bioinf.uni-leipzig.de

Herschel Rabitz

Department of Chemistry, Princeton University, Washington Road,  
Princeton, NJ 08544, U.S.A.

e-mail: hrabitz@princeton.edu



Hendrik Richter

HTWK Leipzig University of Applied Sciences, Faculty of Electrical Engineering and Information Technology, D-04251 Leipzig, Germany.

e-mail: richter@eit.htwk-leipzig.de

Petr Saloun

VSb-TUO, Faculty of Electrical Engineering and Computer Science,  
17. listopadu 15, 708 33 Ostrava-Poruba, Czech Republic.

e-mail: petr.saloun@vsb.cz

Josep Sardanyés

ICREA-Complex Systems Lab, Universitat Pompeu Fabra, Parc de Recerca Biomèdica de Barcelona (PRBB), Dr. Aiguader 88, 08003 Barcelona, Spain.

Institut de Biologia Evolutiva (CSIC-Universitat Pompeu Fabra), Passeig Marítim de la Barceloneta 37, 08003 Barcelona, Spain.

e-mail: josep.sardanes@upf.edu

Gerik Scheuermann

Department of Computer Science, University of Leipzig,  
Augustusplatz 10, 04109 Leipzig, Germany.

e-mail: scheuermann@informatik.uni-leipzig.de

Justin Schonfeld

Department of Integrative Biology and Biodiversity Institute of Ontario,  
University of Guelph, 50 Stone Rd. E, Guelph, Ontario, N1G 2R4, Canada.

e-mail: jschonfe@uoguelph.ca

Ricard V. Solé

ICREA-Complex Systems Lab, Universitat Pompeu Fabra, Parc de Recerca Biomèdica de Barcelona (PRBB), Dr. Aiguader 88, 08003 Barcelona, Spain.

Institut de Biologia Evolutiva (CSIC-Universitat Pompeu Fabra), Passeig Marítim de la Barceloneta 37, 08003 Barcelona, Spain.

Santa Fe Institute, 1399 Hyde Park Road, Santa Fe NM 87501, U.S.A.

e-mail: ricard.sole@upf.edu

Peter F. Stadler

Bioinformatics Group, Department of Computer Science, and Interdisciplinary Center for Bioinformatics, University of Leipzig, Härtelstrasse 16-18, 04107 Leipzig, Germany.

Max Planck Institute for Mathematics in the Sciences, Inselstraße 22, 04103 Leipzig, Germany.

Fraunhofer Institut for Cell Therapy and Immunology, Perlickstraße 1, 04103 Leipzig, Germany.

Institute for Theoretical Chemistry, University of Vienna, Währingerstrasse 17, A-1090 Vienna, Austria.

Santa Fe Institute, 1399 Hyde Park Rd., Santa Fe, NM87501, U.S.A.

e-mail: studla@bioinf.uni-leipzig.de

Katharine Moore Tibbetts

Department of Chemistry, Temple University, 1901 N. 13th St.,  
Philadelphia, PA 19122, U.S.A.

e-mail: [katharine.moore@temple.edu](mailto:katharine.moore@temple.edu)

Marco Tomassini

Department of Information Systems, University of Lausanne, 1015 Lausanne,  
Switzerland.

e-mail: [marco.tomassini@unil.ch](mailto:marco.tomassini@unil.ch)

Krzysztof Trojanowski

Institute of Computer Science, Polish Academy of Sciences, Jana Kazimierza 5,  
01-248 Warsaw, Poland.

Cardinal Stefan Wyszyński University, Faculty of Mathematics and Natural  
Sciences, Wóycickiego 1/3, 01-938 Warsaw, Poland.

e-mail: [trojanow@ipipan.waw.pl](mailto:trojanow@ipipan.waw.pl)

Sébastien Verel

INRIA Lille - Nord Europe and University of Nice Sophia-Antipolis,  
06903 Sophia Antipolis Cedex, France.

e-mail: [verel@3s.unice.fr](mailto:verel@3s.unice.fr)

Sebastian Volke

Department of Computer Science, University of Leipzig,  
Augustusplatz 10, 04109 Leipzig, Germany.

e-mail: [volke@informatik.uni-leipzig.de](mailto:volke@informatik.uni-leipzig.de)

Richard A. Watson

University of Southampton, School of Electronics and Computer Science, Institute  
for Life Sciences, Institute for Complex Systems Simulation, Agents Interaction  
and Complexity, Highfield, Southampton, SO17 1BJ, UK.

e-mail: [raw@ecs.soton.ac.uk](mailto:raw@ecs.soton.ac.uk)

Edward D. Weinberger

Weinberger Post-Quantitative, Inc., 370 Central Park West,  
#110, New York, NY 10025, U.S.A.

Department of Finance and Risk Engineering,  
Polytechnic Institute of New York University,  
6 Metrotech Center, Brooklyn, NY 12201, U.S.A.

e-mail: [edw@wpq-inc.com](mailto:edw@wpq-inc.com)

Re-Bing Wu

Department of Automation, Tsinghua University and Center for Quantum  
Information Science and Technology, TNLIST,  
Beijing, 100084, China.

e-mail: [rbwu@tsinghua.edu.cn](mailto:rbwu@tsinghua.edu.cn)

Xin Yao

Joint USTC-Birmingham Research Institute in Intelligent Computation and Its Applications

The Centre of Excellence for Research in Computational Intelligence and Applications (CERCIA), School of Computer Science, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK.

e-mail: x.yao@cs.bham.ac.uk

Dirk Zeckzer

Department of Computer Science, University of Kaiserslautern, Postfach 3049, 67653 Kaiserslautern, Germany.

e-mail: zeckzer@informatik.uni-kl.de

Ivan Zelinka

VSB-TUO, Faculty of Electrical Engineering and Computer Science, 17. listopadu 15, 708 33 Ostrava-Poruba, Czech Republic.

e-mail: ivan.zelinka@vsb.cz

Oldrich Zmeskal

Faculty of Chemistry, Brno University of Technology, Purkyňova 118, 612 00 Brno, Czech Republic.

e-mail: zmeskal@fch.vutbr.cz

# Contents

**Foreword: Statable and Non-prestable Fitness Landscapes . . . . .** VII

*Stuart Kauffman*

References . . . . . XIV

## Part I: Principles and Perspectives

**1 Fitness Landscapes: From Evolutionary Biology to Evolutionary Computation . . . . .** 3

*Hendrik Richter*

1.1 Introduction . . . . . 3  
    1.1.1 Motivation . . . . . 4  
    1.1.2 Historical Background . . . . . 7  
    1.1.3 Life, Evolution, and Fitness . . . . . 10  
1.2 Fitness and Fitness Landscapes . . . . . 12  
1.3 Fitness Landscapes in Evolutionary Biology . . . . . 15  
    1.3.1 Topological Features of Fitness Landscapes . . . . . 15  
    1.3.2 Computational and Empirical Landscapes . . . . . 20  
1.4 Concluding Remarks . . . . . 24  
References . . . . . 25

**2 Fundamental Principles of Control Landscapes with Applications to Quantum Mechanics, Chemistry and Evolution . . . . .** 33

*Herschel Rabitz, Re-Bing Wu, Tak-San Ho, Katharine Moore Tibbetts, Xiaojiang Feng*

2.1 Introduction . . . . . 34  
2.2 Basic Foundations of OptiSci . . . . . 35  
    2.2.1 Classical and Quantum Control Landscapes . . . . . 35  
    2.2.2 General Features of Control Landscapes . . . . . 36  
    2.2.3 Landscape Mapping . . . . . 38  
    2.2.4 Requirements for the Existence of Trap-Free Landscapes . . . . . 39

2.3	Optimal Control of Quantum Dynamics (OptiQ) . . . . .	39
2.3.1	Background . . . . .	39
2.3.2	Basic Assumptions Regarding Quantum Control Landscapes . . . . .	40
2.3.3	Quantum Control Landscape Theory . . . . .	42
2.3.4	Simulated Excursions over Quantum Control Landscapes . . . . .	44
2.3.5	Experimental Excursions over Quantum Control Landscapes . . . . .	45
2.3.6	Perspective . . . . .	46
2.4	Optimal Control of Chemical Synthesis and Properties (OptiChem) . . . . .	48
2.4.1	Introduction . . . . .	48
2.4.2	OptiChem Theory . . . . .	49
2.4.3	Predictions of OptiChem Theory . . . . .	51
2.4.4	Illustrations . . . . .	52
2.4.5	Perspective . . . . .	55
2.5	Biological Fitness Landscapes (OptiEvo) . . . . .	57
2.5.1	Background . . . . .	57
2.5.2	Physical Foundation of OptiEvo Theory . . . . .	58
2.5.3	Evolutionary Fitness Landscape Analysis . . . . .	59
2.5.4	Predictions and Empirical Assessments of OptiEvo Theory in Natural Evolution . . . . .	60
2.5.5	Application of OptiEvo Theory to Directed Evolution . . . . .	62
2.5.6	Perspective . . . . .	65
2.6	Conclusion . . . . .	65
	References . . . . .	67
<b>3</b>	<b>Biomolecular Information Gained through <i>In Vitro</i> Evolution on a Fitness Landscape in Sequence Space . . . . .</b>	<b>71</b>
	<i>Takuyo Aita, Yuzuru Husimi</i>	
3.1	Introduction . . . . .	72
3.1.1	Outline of In Vitro Molecular Evolution . . . . .	72
3.1.2	In Vitro Evolution as an Information Gaining Process . . . . .	73
3.1.3	Basis of Thermodynamic Concepts . . . . .	74
3.1.4	Outline of This Chapter . . . . .	75
3.2	Model of In Vitro Evolution . . . . .	76
3.2.1	Natural Selection-Type Model . . . . .	76
3.2.2	Artificial Selection-Type Model . . . . .	76
3.3	Analogy between Evolution and Thermodynamics . . . . .	78
3.3.1	Overview . . . . .	78
3.3.2	Quasi-species . . . . .	80

- 3.3.3 Attractor of Fitness in the Artificial Selection-Type Model . . . . . 82
- 3.3.4 Evolutionary Boltzmann Constant and Evolutionary Temperature . . . . . 83
- 3.3.5 Evolutionary Potential, Free Fitness and Evolutionary Force . . . . . 84
- 3.3.6 Fitness Flux and Einstein’s Relation-Like Formula . . . . . 85
- 3.4 Information Gained through In Vitro Evolution . . . . . 87
  - 3.4.1 Fitness Fluctuation and Energy Fluctuation . . . . . 87
  - 3.4.2 Biomolecular Information . . . . . 89
  - 3.4.3 Information-Gain Formula . . . . . 90
  - 3.4.4 Extent and Content of Information . . . . . 92
  - 3.4.5 Fitness Information . . . . . 93
  - 3.4.6 Pragmatic Information . . . . . 94
- 3.5 Conclusion . . . . . 96
- References . . . . . 97

**Part II: Topology, Measures and Problem Hardness**

- 4 Fitness Landscape Analysis for Metaheuristic Performance Prediction . . . . . 103**  
*Katherine M. Malan, Andries P. Engelbrecht*
  - 4.1 Introduction . . . . . 103
  - 4.2 The Algorithm Selection Problem . . . . . 106
  - 4.3 Performance Metrics . . . . . 107
    - 4.3.1 Existing Approaches to Measuring Performance . . . . . 108
    - 4.3.2 Proposed Performance Metrics . . . . . 109
    - 4.3.3 Performance Metrics for PSO . . . . . 113
  - 4.4 Feature Extraction for Continuous Optimisation Problems . . . . . 115
    - 4.4.1 What Makes an Optimisation Problem Hard? . . . . . 116
    - 4.4.2 Possible Techniques for Feature Extraction . . . . . 118
    - 4.4.3 Features and Algorithm Performance . . . . . 120
    - 4.4.4 Discussion . . . . . 127
  - 4.5 Conclusion . . . . . 128
  - References . . . . . 129
- 5 Fitness Landscapes and Problem Difficulty in Evolutionary Algorithms: From Theory to Applications . . . . . 133**  
*Guanzhou Lu, Jinlong Li, Xin Yao*
  - 5.1 Introduction . . . . . 134
  - 5.2 Background . . . . . 135
  - 5.3 Escape Probability versus Expected Runtime Time . . . . . 135
    - 5.3.1 Preliminaries . . . . . 136
    - 5.3.2 Derivation of the Mathematical Equation between Escape Probability and Expected Running Time . . . . . 136