Mathematical Analysis of Evolution, Information, and Complexity

Edited by
Wolfgang Arendt and Wolfgang P. Schleich

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Contents

Traveller, there are no paths.
Paths are made by walking.
Antonio Machado (1875–1939)

Preface

The present book is devoted to the mathematical analysis of evolution, information and complexity. The time evolution of systems or processes is a central question in science and covers a broad range of problems including diffusion processes, neural networks, quantum theory and cosmology. Analysis of information is needed in data compression, channel encoding, cryptography and often in the analysis of information processing in the computer or in the brain. Finally, the analysis of complexity is important for computer science, in particular algorithms, but more generally also for the investigation of complex and chaotic systems.

Since 2004 the University of Ulm has operated a graduate school dedicated to the field of *Mathematical Analysis of Evolution, Information and Complexity*. This program brings together scientists from the disciplines of mathematics, electrical engineering, computer science and physics. Our rather unique school addresses topics that need a unified and highly interdisciplinary approach. The common thread of these problems is mathematical analysis demonstrating once more the newly emerging notion of mathematics as technology.

Our book highlights some of the scientific achievements of our school and therefore bears its name *Mathematical Analysis of Evolution, Information and Complexity*. In order to introduce the reader to the subject we give elementary and thus accessible introductions to timely themes taken from different parts of science and technology such as information theory, neuro-informatics and mathematical physics.

Each article in the book was prepared by a team in which at least two different disciplines were represented. In this way mathematicians have collaborated on a chapter with physicists, or physicists have worked with electrical engineers and so on. Moreover, we have installed the rule that with every senior scientist there would be a graduate student working on this article. We hope that this rule has led to easily understandable contributions.

Mathematical Analysis of Evolution, Information and Complexity does not only represent the program of our school and has become the title of the book but has also served as the guiding principle for its organization. Indeed, we have chosen the three pillars "evolution", "information" and "complexity" of the school as titles for the three parts of the book. For each one we have identified one or two major themes as shown in Table 0.1.

Table 0.1 Organization of the book outlining its three pillars with their themes. The number above each topic indicates the chapter.

Evolution		**Information**		**Complexity**
Spectral analysis	**Networks**	**Pattern recognition**	**Signal analysis**	**Algorithms**
1 Weyl's law	4 biological neural networks	7 speech recognition: remote access	12 Shannon's theorem	15 Shor algorithm
2 differential equations	5 gene regulation	8 speech recognition: machine learning	13 codes	16 quantum and classical algorithms
3 cosmology	6 quantum graphs	9 cluster analysis in genomics	14 signal processing in the brain	17 sorting algorithms
		10 image analysis in computer science and cosmology		
		11 data analysis and learning		

We have taken the liberty to assign each article to one of these themes. However, in many instances the contributions could have also been attributed to another theme. This feature is certainly a trade mark of an interdisciplinary article. These articles form the individual chapters of the book.

The topics addressed in each pillar range from quantum physics via bioinformatics to computer science and electrical engineering. The common element linking all chapters is mathematical analysis. To quote Galileo Galilei:

> *"Egli [il libro che è l'universo] è scritto in lingua matematica."*
> *("The book which is the universe is written in mathematical language.")*

In order to bring out most clearly the interconnections between the chapters of the book, we now briefly summarize the essential ideas of each contribution. We start with the pillar "evolution" consisting of the two themes of spectral analysis and networks.

Weyl's law describes the asymptotic distribution of the eigenvalues of the Laplacian. It has played an important role in the development of quantum theory. Chapter 1 gives a comprehensive summary of the history of Weyl's law, its generalization based on trace formulae, its application in quantum chaos, as well as a modern proof. A review and comparison of different methods of solving systems of linear ordinary differential equations is the topic of Chapter 2. Applications and extensions to partial differential equations such as the heat equation or the Schrödinger equation are given. The theme on evolution concludes in Chapter 3 with an introduction into general relativity with an alternative approach based on the scalar-tensor theory and the Higgs potential.

The theme of evolution in networks addresses biological neural networks, gene regulation and quantum graphs. For example, Chapter 4 provides an overview over models describing biological and computational neural networks. Here the central topic is the specific model developed in Ulm using neural populations as associative memories. Another example of a network of signalling compounds within the kernel of a cell is summarized in Chapter 5. The mathematical model of Boolean networks describes the gene regulation in living organisms. Quantum graphs, the topic of Chapter 6, represent yet another network. They are a toy model for a Schrödinger operator on a thin, quasi-one-dimensional network. The article studies the symmetries that emerge in such quantum networks.

A major portion of the book is dedicated to the mathematical analysis of information. Here the topics range from speech recognition via cluster analysis to signal processing in the brain. Usually speech recognition is implemented on powerful computers. In Chapter 7 tools are developed which allow remote access, for example, using cellular phones. Here, the Ulm technology of associative memories plays an important role. Spoken language dialogue systems are interactive, voice-based interfaces between humans and computers. They allow humans to carry out tasks of diverse complexity such as the reservation of tickets or the performance of bank transactions. Chapter 8 describes different appproaches for the categorization of caller utterances in the framescope of a technical support dialog system, with special focus on categorizers using small amounts of labeled examples. Functional genomics aim to provide links between genomic information and biological functions. One example is the connection between gene patterns and tumor status. Cluster analysis generates a structure of data solely exploring distances or similarities. A special feature of Chapter 9 is the demonstration that already sparse additional information leads to stable structures which are less susceptible to minor changes. Image analysis tries to detect complex structures in high-dimensional data. Chapter 10 compares and contrasts approaches developed in computer vision and cosmology. We conclude the theme of pattern recognition by discussing in Chapter 11 the fundamental method of classification in data analysis. Unfortunately, the true concept of classification is often not known. A method of combining several such concepts, called boosting, which leads to highly accurate classifiers, is described here.

Another important theme in the part on information is represented by signal analysis covering the topics of Shannon's sampling theorem, codes and signal processing in the brain. The sampling theorem shows how a signal can be reproduced by a finite number of measurements. Chapter 12 gives a historical overview and provides two proofs. Coding theory tells us how, by adding redundancy and correcting errors, information can be transmitted accurately. An overview of codes with emphasis on algebraic geometric codes is given in Chapter 13. This section concludes with Chapter 14 describing a model of how the human cortex processes its sensor signals. Mathematically this model consists of a system of coupled nonlinear ordinary differential equations whose long time behavior is discussed.

The last part addresses the topic of complexity focusing on classical as well as quantum algorithms. A central task in computer science is to find efficient algorithms. Chapter 15 lays the foundation of this chapter by explaining the famous Shor algorithm to factor numbers from a physics point of view. In the same vein Chapter 16 describes the state of the art of two famous problems, integer factorization and the graph isomorphism problem. It points out similarities and differences between these two problems when approached by classical or quantum computing. The QuickSort algorithm is a most efficient sorting method. It relies on dividing the sequence into parts of smaller lengths. In Chapter 17 the complexity of the method is studied with a special emphasis on varying the random source which governs the division.

We would like to take the opportunity to thank the authors for their contributions, enthusiasm and reliability in producing this volume. Moreover, we are most grateful to Robin Nittka for his competent help in putting this book together. Finally, we appreciate the support of the Ministerium für Wissenschaft, Forschung und Kunst, Baden-Württemberg in the framework of the Promotionskolleg *Mathematical Analysis of Evolution, Information and Complexity*.

Ulm, August 2008

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Prologue

Milestones of Evolution, Information and Complexity

Wolfgang Arendt, Delio Mugnolo and Wolfgang Schleich

> *The modern world, our world of triumphant rationality, began on November 10, 1619, with a revelation and a nightmare. On that day, in a room in the small Bavarian village of Ulm, René Descartes, a Frenchman, twenty-three years old, crawled into a wall stove and, when he was well-warmed, had a vision. It was not a vision of God, or of the mother of God, or of the celestial chariots, or of the New Jerusalem. It was a vision of the unification of all science.*
>
> Philip J. Davis and Reuben Hersh, *Descartes' Dream*, Penguin, London 1986

René Descartes laid the foundation of modern science not only by his natural philosophy, but also by his mathematical contributions. For example, he addressed the tangent problem, which was only solved in its entirety 50 years later by Leibniz and Newton. For this purpose both of them invented mathematical calculus. In 1637 Descartes in his essay *Discours de la méthode* brought to light the physics of diffraction. He was the first to explain the most beautiful spectral phenomenon, the rainbow.

Δ Δ Δ

Since then, spectral analysis has come a long way. It has developed into one of the most fruitful concepts in natural sciences and technology. The overtones of an instrument, such as a tambourine or an organ pipe, and even the bodywork of a Mercedes limousine, exhibit a spectrum. Also in the microscopic world the concept of spectrum is useful. For example, the energy levels of the electron in a hydrogen atom form a spectrum. This fact turned out to be a crucial stepping stone for the development of quantum theory (Chapter 1).

Cosmic microwave background radiation was discovered in 1965 by Arno Penzias and Robert Wilson. In accordance with the Big Bang Theory, it fills the whole universe and is currently considered to be the major evidence for an expanding universe. For this discovery, Penzias and Wilson received the Nobel Prize in Physics in 1978 (Chapter 10). Such a microwave radiation possesses a spectrum which is characteristic of a so-called *black body*. Black bodies have been first considered by Gustav Kirchhoff in 1859 when he laid the foundation of the theory of thermal radiation. Fourteen years earlier he had already introduced two famous laws describing the time evolution of voltages and currents in electric circuits. In this way Kirchhoff single-handedly established modern electrical engineering.

Black bodies have also played a central role in the creation of quantum mechanics. Indeed, motivated by the problem of designing efficient lightbulbs, Max Planck in 1900 discovered that the energy of oscillators is quantized. Building on Planck's insights, Albert Einstein, born in Ulm in 1879, could explain the photoelectric effect. This explanation together with his discovery of the momentum of the light quantum opened the door to the development of quantum mechanics. For these achievements he was awarded the Nobel Prize in 1921. Moreover, his groundbreaking work on relativity, deeply rooted in Riemann's geometric theory, completely changed our understanding of the time evolution of the universe and marked the birth of modern cosmology (Chapter 3).

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To a large degree today's electrical engineering lives off the spectral analysis of signals, for example, making cell phones work. It was Claude Shannon who in 1949 discovered that a finite number of samples suffices to capture a wave (Chapter 12). Here he could build on the concept of the Fourier transform, which was introduced by Joseph Fourier in 1822 in his *Théorie analytique de la chaleur*. Shannon's sampling theorem provides the basis for the technology of digitalising and eventually perfectly reconstructing a signal. Moreover, in the very same paper entitled *Communication theory of secrecy systems*, Shannon laid the mathematical foundation of cryptography.

Still, signal processing faces a major theoretical limitation: The shorter a pulse in time, the less well defined the frequency. Bounds of this kind are intimately related to Shannon's investigations collected in his seminal paper *A mathematical theory of communication* from 1948. In this article he introduced the concept of *information entropy*, a measure of the information contained in a random message. Today this article is commonly considered to have initiated information theory.

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Also at the end of the 1940s, Donald Hebb was completing his most influential study, *The organization of behavior*. Therein he proposed a quantitative approach to the process of learning, thus giving birth to modern neuropsychology. Hebb was the first to analytically investigate the dual nature of the brain – biological tissue as well as source of perception – combining traditional behavioral studies and modern electrophysiology. His theory of learning suggested that synaptic connections are strengthened or weakened in order to achieve more efficient apprehension. Hebb's work introduced the notion of *synaptic plasticity* and paved the road for the interpretation of the brain as an ever-changing computing system.

Shortly before, in 1943, the first artificial *neural networks* had been introduced by Warren McCulloch and Walter Pitts in their article entitled *A logical calculus of the ideas immanent in nervous activity*. It soon became clear that boolean logic could be implemented in these theoretical devices, thereby enabling them to perform complex computations. Unfortunately, the early neural networks lacked any form of adaptation or learning features. It was Hebb's research that filled this gap. Even today Hebb's laws in their mathematical formulation are among the favorite theoretical tools when setting up and tuning an artificial neural network (Chapters 4, 7 and 14). They allow one to translate learning phenomena into the time evolution of a system of differential or difference equations (Chapter 2).

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The spectrum of a wave can be viewed as a band of eigenfrequencies determined by the Helmholtz equation. This distribution of eigenvalues provides us with a deeper insight into the behaviour of light and matter and is described by Weyl's law, proven by Hermann Weyl in 1911. Surprisingly, there is a close analogue in number theory. The prime numbers are intimately related to Riemann's ζ-function whose non-trivial zeros look very much like a spectrum encountered in atomic physics. In this context Marcus de Sautoy talks about *the music of primes*, which is the title of his book on the Riemann ζ-function. Much is known about the distribution of the primes but the related Riemann's hypothesis on the zeros of the ζ-function is still a mystery. First formulated by Bernhard Riemann in 1859, it is probably the biggest open problem in mathematics today – in fact, it has been dubbed a Millennium Problem, whose solution would be rewarded with a \$1 000 000 prize by the Clay Mathematics Institute (Chapter 1).

Prime numbers and their distribution have fascinated mathematicians for generations. Today they serve us as a mathematical technology in cryptography. A modern life necessity is to transmit secret data, for example, for online banking purposes. It is counterintuitive that encryption can be made safer and more efficient by the use of public keys. In fact, cryptographic keys had to be kept strictly secret until the 1970s. However, even codes based on secret keys are not secure. The most prominent example is the Enigma code used by the Germany military in World War II and broken by Alan Turing in 1943. *Public keys* constituted a breakthrough and a radical change of the paradigm of secrecy. They were first proposed in 1976 in a famous paper by Whitfield Diffie and Martin Hellman entitled *New directions in cryptography*. In Diffie's and Hellman's words, "each user of the network can, therefore, place his enciphering key in a public directory. This enables any user of the system to send a message to any other user in such a way that only the intended receiver is able to decipher it." The actual realization of their project is due to Ronald Rivest, Adi Shamir, and Leonard Adleman, who in 1978 developed the RSA cryptographic system. This work won them the Turing Award in 2002. It is surprising that the long awaited solution of the most famous and originally thought to be useless problem, the proof of Fermat's Last Theorem by Andrew Wiles in the 1990s, also provided us with new tools for cryptography such as *elliptic curves*. In fact, their use for enciphering and deciphering was already implicitly contained in the work of Diffie and Hellman (Chapter 16).

Efficient cryptography is just one problem of modern signal theory. Another one is to find a language which permits error-free transmission of information in a process called coding/encoding. And it is again number theory, but also Fourier analysis, that gives us the right tools to perform this task with enormous efficiency (Chapter 13). Again, Shannon's sampling theorem plays a decisive role in this context.

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Quantum theory, even though formulated in a quite abstract mathematical language, has reached a state of broad technological applications. In 1965, Richard Feynman received the Nobel Prize in Physics for his work on quantum electrodynamics. Seventeen years later he was one of the first to recognize the potential of a *quantum computer*. In all digital computers, starting from the Zuse Z3 and the ENIAC of the early 1940s to modern miniaturised devices, the logic is based on memory devices which store either a 0 or a 1, forming a bit of information. In a quantum computer this on/off dichotomy is replaced by the possibility of a *quantum bit* being in a superposition state. Abecedarian forms of such a quantum device exist to date in research labs only. Nevertheless, they have already been studied extensively at a theoretical level.

Once available, a quantum computer would substantially simplify large data analysis. Applications known today include, but are not limited to, the determination of shortest paths in networks or even the factorization of large numbers, for instance, by means of the algorithm discovered by Peter Shor in 1994 (Chapter 15). For this work he was awarded the Gödel Prize in 1999. It is remarkable that Shor's algorithm, implemented on a reasonably large quantum computer, could easily break common cryptographic techniques, including both RSA and methods based on elliptic curves. Possible remedies are random number generators based on Riemann's ζ-function. A fascinating relation between elliptic curves and the ζ-function is suggested by the Birch and Swinnerton–Dyer conjecture, formulated in the 1960s. It is still open and represents another of the Millennium Problems named by the Clay Institute.

However, not even quantum computers have an infinite potential. They may be exponentially faster when confronted with certain tasks, but they are not inherently more powerful than today's computers. Whenever we have to solve a problem with the help of a machine, even an ideal one such as a *universal Turing machine*, we have to use an algorithm which should be optimized. To quantify the intrinsic efficiency of algorithms to be implemented on computers is the goal of *algorithmic complexity theory*, founded by Juris Hartmanis and Richard Stearns in 1965. Their paper *On the computational complexity of algorithms* earned them the Turing Award in 1993.

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Obviously, to *determine* the explicit solution of a problem in a short time, such as factoring of a large number, or to *check* whether given data indeed solve the problem, for example whether the product of a given set of primes yields the original large number, represent two different tasks. The problems which are solvable by a fast algorithm constitute the class P, whereas NP consists of those problems which allow for a fast algorithm that is able to check whether a given possible answer is indeed a solution of the problem. Here an algorithm is called *fast* if it can be performed in a time which grows at most polynomially with the input size.

While algorithms for finding prime numbers were already known to the ancient Greek, checking whether a given number is actually a prime seems to be demanding. Nevertheless, it is only a P-problem as shown by Manindra Agrawal in 2002 after his post-doc stay at the University of Ulm. This stunning discovery won him the Clay Research Award in the same year and the Gödel Prize (together with his coauthors) in 2006. Another example of the P vs. NP question is the prime factorization of large numbers (Chapters 15 and 16). Today most of the cryptography devices rely upon the belief that factorization into primes, which is clearly an NP problem, is not a P problem. Still, all attempts to prove this hypothesis have remained unsuccessful. In 1956, Gödel conjectured in a letter to von Neumann that, in general, it should be possible to replace trial and error approaches by efficient algorithms – as for example done for various problems in number theory – thus implicitly suggesting that $P = NP$. Still, more than fifty years later we do not yet know the answer to the P vs. NP problem.

While it is clear that each P problem is also NP, most computer scientists firmly believe that the converse is not true, that is $P \neq NP$. This question represents a major research field of theoretical computer science and is also one of the seven Millennium Problems of the Clay Institute.

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Consider the task of coloring a geographical map under the constraint that no two adjacent countries can have the same color. To decide for a given map whether it is possible to complete this task using only three different colors is at least as difficult as any NP problem, whereas it is a P problem to find a four-coloring of the map. The latter task is closely related to the four-color-theorem, stating that each map can in fact be colored with a maximum of four colors. This theorem was first proposed as a conjecture in 1852 and proven only in 1976 by Kenneth Appel and Wolfgang Haken. Their proof is the first one ever to rely in an essential way upon computer aid, rather than human thought, and has therefore started an everlasting debate in the philosophy of science. The four-color-theorem represents the zenith of the interplay between mathematics, logic and theoretical computer science. In contrast, Kurt Gödel's incompleteness theorem from 1931 was this interplay's nadir. It was a great enlightment to the scientific community to learn from Gödel that no automatic, computer-based mathematics will ever be possible.

Coloring problems belong to *graph theory*, a field studying properties of discrete structures. Also based on graph theoretical objects is a recent proof of the long standing Horn conjecture on the distribution of eigenvalues of a sum of matrices. This question was addressed by Weyl in 1912 but was not proven until the 1990s.

One of the key elements of the proof are surprising connections between ideas from discrete and continuous mathematics as well as from quantum mechanics. For his contributions to the solution of the Horn conjecture, the Clay Research Award was assigned to Terence Tao in 2003. He was also awarded the Fields Medal in 2006 for his results in the arithmetic of prime numbers. It is remarkable that the once abstract graph theory has also found useful applications in algorithmic computer science, especially in data clustering (Chapters 8 and 9), sequencing (Chapter 5), classification (Chapter 11), and sorting (Chapter 17).

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In spite of its limitations in large data analysis, the most efficient system for information processing and computing is still a natural one – the brain. Hermann von Helmholtz was the first to suggest and eventually prove in 1852 that thoughts – or rather neural transmissions – have a finite speed, in fact as slow as 30 m/s. In the year of von Helmholtz's discovery Santiago Ramón y Cajal, the father of modern neurobiology, was born. To him we owe the insight that the nervous system is a fine network consisting of neurons which communicate by means of synapses. For this work, based on a biochemical technique developed by Camillo Golgi, both Golgi and Ramón y Cajal were awarded the Nobel Prize in Medicine in 1906. In 1952 Alan Hodgkin and Andrew Huxley proposed a mathematical model for the propagation of electrical pulses inside individual neurons. They were able to show that the neural transmission happens by means of an ionic current, which can also be modeled as a diffusion process and propagates as a wave. Their model won them the Nobel Prize in Medicine in 1963 (Chapter 4).

The theory of diffusion was originated in 1822 by Fourier in his studies on heat conduction. Eventually, thirty-three years later Adolf Fick formulated the law of diffusion as a partial differential equation involving time as a variable. Such laws are called *evolution equations*. Already Fick recognized that his model was not limited to thermodynamics but had many more fields of application ranging from chemistry to finance. In fact, Fick's law also agrees up to nonlinear correction terms with Hodgkin's and Huxley's differential equations. Moreover, the signalling across synapses is a chemical phenomenon that is partially based on diffusion. Further Nobel Prizes in Medicine have been awarded for related discoveries in 1936, 1963, and 1970, in a *crescendo* that was made possible by the development of electron microscopy. A hundred years after Ramón y Cajal, diffusion processes still belong to the core of computational neuroscience – in a braid of chance, linear determinism, and chaos.

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In 1887, Henri Poincaré won a contest sponsored by the King of Sweden asking for the solution of the famous *three-body problem* in celestial mechanics. In fact, Poincaré did not present the solution, but rather indicated a major problem in the mainstream approach to celestial mechanics itself. He pointed out that even a perfect deterministic theory would not yield a useful result, since usually the initial