



Preface to the Special Issue on "Control, Optimization, and Mathematical Modeling of Complex Systems"

Mikhail Posypkin *^D, Andrey Gorshenin *^D and Vladimir Titarev *^D

Federal Research Center "Computer Science and Control" of the Russian Academy of Sciences, 119333 Moscow, Russia

* Correspondence: mposypkin@frccsc.ru (M.P.); agorshenin@frccsc.ru (A.G.); vladimir.titarev@frccsc.ru (V.T.)

1. Aims, Scope, and Statistics of the Special Issue

Complex systems have long been an integral part of modern life and can be encountered everywhere. A comprehensive study of such systems is a challenging problem, the solution of which is impossible without the use of contemporary mathematical modeling techniques. Mathematical models form the basis for optimal design and control of complex systems.

This Special Issue is focused on recent theoretical and computational studies of complex systems modeling, control, and optimization. Topics include, but are not limited to, the following themes:

- Numerical simulation in physical, social, and life sciences [1–4];
- Modeling and analysis of complex systems based on mathematical methods and AI/ML approaches [5,6];
- Control problems in robotics [3,7–12];
- Design optimization of complex systems [13];
- Modeling in economics and social sciences [4,14];
- Stochastic models in physics and engineering [1,15–18];
- Mathematical models in material science [19];
- High-performance computing for mathematical modeling [20].

Cross-border modeling and numerical simulation in Physics and Engineering are particularly welcome in this Special Issue.

In total, 31 manuscripts were submitted, and 20 papers by 49 authors were successfully published. Authors come from the following 11 countries:

- China [4,7,18];
- Czech Republic [8];
- Great Britain [11];
- Hungary [10];
- Pakistan [4];
- Russia [1,2,5,6,8,10,13,15–17,19];
- Saudi Arabia [4];
- Spain [3,9,12,20];
- Taiwan [4];
- Tunisia [20];
- Vietnam [8,14].

A rose diagram of the number of unique authors from different countries is shown in Figure 1.



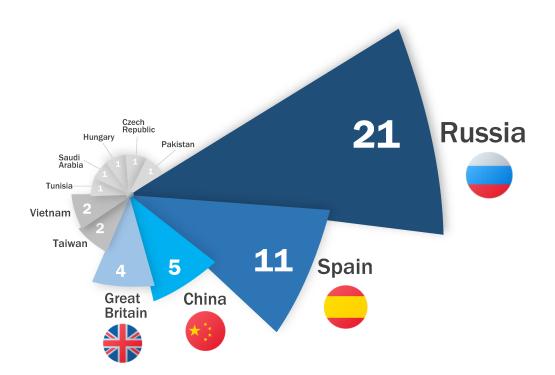
Citation: Posypkin, M.; Gorshenin, A.; Titarev, V. Preface to the Special Issue on "Control, Optimization, and Mathematical Modeling of Complex Systems". *Mathematics* 2022, *10*, 2182. https://doi.org/10.3390/ math10132182

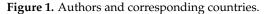
Received: 16 June 2022 Accepted: 20 June 2022 Published: 23 June 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/).





2. Papers of the Special Issue

Zeifman et al. [1] consider the computation of the (limiting) time-dependent performance characteristics of one-dimensional continuous-time Markov chains with discrete state space and time-varying intensities. Numerical solution techniques can benefit from methods providing ergodicity bounds because the latter can indicate how to choose the position and the length of the "distant time interval" (in the periodic case) on which the solution has to be computed. They can also be helpful whenever the state space truncation is required. In this paper, one such analytic method—the logarithmic norm method—is reviewed. Its applicability is shown within the context of the queuing theory with three examples: the classical time-varying M/M/2 queue; the time-varying singleserver Markovian system with bulk arrivals, queue-skipping policy, and catastrophes; and the time-varying Markovian bulk-arrival and bulk-service system with state-dependent control. In each case, it is shown whether and how the bounds on the rate of convergence can be obtained. Numerical examples are provided.

Ilyin [2] considers the development of the two-dimensional discrete velocity Boltzmann model on a nine-velocity lattice. Compared with the conventional lattice Boltzmann approach for the present model, the collision rules for the interacting particles are formulated explicitly. The collisions are tailored in such a way that mass, momentum, and energy are conserved, and the H-theorem is fulfilled. By applying the Chapman–Enskog expansion, the author shows that the model recovers quasi-incompressible hydrodynamic equations for a small Mach number limit, and he then derives the closed expression for the viscosity, depending on the collision cross-sections. In addition, the numerical implementation of the model with the on-lattice streaming and local collision step is proposed. As test problems, the shear wave decay and Taylor–Green vortex are considered, and a comparison of the numerical simulations with the analytical solutions is presented.

Nagua et al. [3] design and simulate a soft joint to perform as a robotic joint with two degrees of freedom (DOF) (inclination and orientation). The joint actuation is based on a cable-driven parallel mechanism (CDPM). To study its performance in more detail, a test platform is developed using components that can be manufactured in a 3D printer using a flexible polymer. The mathematical model of the kinematics of the soft joint is developed, which includes a blocking mechanism and the morphology workspace. The model is validated using finite element analysis (FEA) software. Experimental tests are performed to validate the inverse kinematic model and to show the potential use of the prototype in robotic platforms such as manipulators and humanoid robots.

Masood et al. [4] analyze the designed fractional-order Stuxnet, the virus model, to investigate the spread of the virus in the regime of isolated industrial networks environment by bridging the air gap between the traditional and critical control network infrastructures. Removable storage devices are commonly used to exploit the vulnerability of individual nodes, as well as the associated networks, by transferring data and viruses in the isolated industrial control system. A mathematical model of an arbitrary order system is constructed and analyzed numerically to depict the control mechanism. Local and global stability analysis of the system is performed on the equilibrium points derived for the value of $\alpha = 1$. To understand the depth of fractional model behavior, numerical simulations are carried out for the distinct order of the fractional derivative system, and the results show that fractional-order models provide rich dynamics by means of fast transient and super-slow evolution of the model's steady-state behavior, which are seldom perceived in integer-order counterparts.

Gorshenin and Kuzmin [5] present a feature construction approach called statistical feature construction (SFC) for time-series prediction. The creation of new features is based on statistical characteristics of analyzed data series. First, the initial data are transformed into an array of short pseudo-stationary windows. For each window, a statistical model is created, and the characteristics of these models are later used as additional features for a single window or as time-dependent features for the entire time series. To demonstrate the effect of SFC, five plasma physics and six oceanographic time series are analyzed. For each window, unknown distribution parameters are estimated with the method of moving separation of finite normal mixtures. First, four statistical moments of these mixtures for initial data and increments are used as additional data features. Multilayer recurrent neural networks are trained to create short- and medium-term forecasts with a single window as input data; additional features are used to initialize the hidden state of recurrent layers. A hyperparameter grid search is performed to compare fully optimized neural networks for original and enriched data. A significant decrease in the RMSE metric is observed, with a median of 11.4%. There is no increase in the RMSE metric in any of the analyzed time series. The experimental results show that SFC can be a valuable method for forecasting accuracy improvement.

The paper by Diveev et al. [6] is devoted to an emerging trend in control—a machine learning control. Despite the popularity of the idea of machine learning, there are various interpretations of this concept, and there is an urgent need for its strict mathematical formalization. An attempt to formalize the concept of machine learning is presented in this paper. The concepts of an unknown function, work area, and training set are introduced, and a mathematical formulation of the machine learning problem is presented. Based on the presented formulation, the idea of machine learning control is considered. One of the problems of machine learning control is the general synthesis of control. It implies finding a control function that depends on the state of the object, which ensures the achievement of the control goal with the optimal value of the quality criterion from any initial state of some admissible region. Supervised and unsupervised approaches to solving a problem based on symbolic regression methods are considered. As a computational example, a problem of general synthesis of optimal control for a spacecraft landing on the surface of the Moon is considered as a supervised machine learning control, using a training set.

Li and Zhou [7] propose a novel control strategy to address the precise trajectory tracking control problem of a ship towing system. First, the kinematics and dynamics models of a ship towing system are established by introducing a passive steering angle and using its structure relationship. Then, by using the motion law derived from its nonholonomic constraints, the relative curvature of the target trajectory curve is used to design a dynamical tracking target. By applying the sliding mode control and inverse dynamic adaptive control methods, two appropriate robust torque controllers are designed via the dynamical tracking target, so that both the tugboat and the towed ship are able to

track the desired path precisely. As the authors show, the proposed strategy provides an excellent agreement with the numerical simulation results.

Diveev et al. [8] present a numerical method based on the Pontryagin maximum principle for solving an optimal control problem with static and dynamic phase constraints for a group of objects. Dynamic phase constraints are introduced to avoid collisions between objects. Phase constraints are included in the functional in the form of smooth penalty functions. Additional parameters for special control modes and the terminal time of the control process are also introduced. The search for additional parameters and the initial conditions for the conjugate variables is carried out using the modified self-organizing migrating algorithm. An example of using this approach to solve the optimal control problem for the oncoming movement of two mobile robots is given. Simulation and comparison with the direct approach show that the problem is multimodal. The application of the evolutionary algorithm for its solution is presented.

Mena et al. [9] propose a modular robot with an origami structure. The idea is based on a self-scalable and modular link made of soft parts. The kinematics of single and multiple interconnected links is studied and validated. In addition, the link is prototyped, identified, and controlled in position. The experimental data show that the system meets the scalability requirements, and that its response is totally reliable and robust.

Diveev et al. [10] present a new formulation of the optimal control problem with uncertainty, in which an additive bounded function is considered as uncertainty. The purpose of the control is to ensure the achievement of terminal conditions with the optimal value of the quality functional, while the uncertainty has a limited impact on the change in the value of the functional. This article introduces the concept of feasibility of the mathematical model of the object, which is associated with the contraction property of mappings if we consider the model of the object as a one-parameter mapping. It is shown that this property is sufficient for the development of stable practical systems. To find a solution to the stated problem that would ensure the feasibility of the system, the synthesized optimal control method is proposed. This article formulates the theoretical foundations of the synthesized optimal control. The method consists of making the control object stable relative to some point in the state space and controlling the object by changing the position of the equilibrium points. The article provides evidence that this approach is insensitive to the uncertainties of the mathematical model of the object. An example of the application of this method for optimal control of a group of robots is given. A comparison of the synthesized optimal control method with the direct method on the model with and without disturbances is also presented.

Kuang et al. [11] investigate visual navigation, which is an essential part of planetary rover autonomy. Rock segmentation emerged as an important interdisciplinary topic in image processing, robotics, and mathematical modeling. It is a challenging topic for rover autonomy because of the high computational consumption, real-time requirement, and annotation difficulty. This research proposes a rock segmentation framework and a rock segmentation network (NI-U-Net++) to aid with the visual navigation of rovers. The framework consists of two stages: the pretraining process and the transfer-training process. The pretraining process applies the synthetic algorithm to generate the synthetic images; then, it uses the generated images to pretrain NI-U-Net++. The synthetic algorithm increases the size of the image dataset and provides pixel-level masks—both of which are challenges with machine learning tasks. The pretraining process accomplishes the state of the art, compared with the related studies, which achieved an accuracy, intersection over union (IoU), Dice score, and root-mean-squared error (RMSE) of 99.41%, 0.8991, 0.9459, and 0.0775, respectively. The transfer-training process fine-tunes the pretrained NI-U-Net++ using the real-life images, which achieved an accuracy, IoU, Dice score, and RMSE values of 99.58%, 0.7476, 0.8556, and 0.0557, respectively. Finally, the transfer-trained NI-U-Net++ is integrated into a planetary rover navigation vision and achieves a real-time performance of 32.57 frames per second (or the inference time is 0.0307 s per frame). The framework only manually annotates about 8% (183 images) of the 2250 images in the navigation vision, which is a labor-saving solution for rock segmentation tasks. The proposed rock segmentation

framework and NI-U-Net++ improve the performance of the state-of-the-art models. The synthetic algorithm improves the process of creating valid data for the challenge of rock segmentation. All source codes, datasets, and trained models of this research are openly available in Cranfield Online Research Data (CORD).

The paper by Quevedo et al. [12] is devoted to soft robotics, which is becoming an emerging solution to many of the problems in robotics, such as weight, cost, and human interaction. In order to overcome such problems, bio-inspired designs have introduced new actuators, links, and architectures. However, the complexity of the required models for control has increased dramatically, and geometrical model approaches, widely used to model rigid dynamics, are not enough to model these new hardware types. In this paper, different linear and nonlinear models are used to model a soft neck consisting of a central soft link actuated by three motor-driven tendons. By combining the force on the different tendons, the neck is able to perform a motion similar to that of a human neck. In order to simplify the modeling, first a system input–output redefinition is proposed, considering the neck pitch and roll angles as outputs and the tendon lengths as inputs. Later, two identification strategies are selected and adapted to the case in hand: set membership, a data-driven, nonlinear, and nonparametric identification strategy that needs no input redefinition; and recursive least-squares (RLS), a widely recognized identification technique. The first method offers the possibility of modeling complex dynamics without specific knowledge of its mathematical representation. This method is selected considering its possible extension to more complex dynamics and the fact that its impact on soft robotics is yet to be studied according to the current literature. On the other hand, RLS shows the implication of using a parametric and linear identification in a nonlinear plant and also helps to evaluate the degree of nonlinearity of the system by comparing the different performances. In addition to these methods, neural network identification is used for comparison purposes. The obtained results validate the modeling approaches proposed.

Posypkin and Khamisov [13] investigate the problem of reliable bounding of a function's range, which is essential for deterministic global optimization, approximation, locating roots of nonlinear equations, and several other computational mathematics areas. Despite years of extensive research in this direction, there is still room for improvement. The traditional and compelling approach to this problem is interval analysis. They show that accounting convexity/concavity can significantly tighten the bounds computed by interval analysis. To make the approach applicable to a broad range of functions, the authors also develop techniques for handling nondifferentiable composite functions. Traditional ways to ensure convexity fail in such cases. Experimental evaluation shows the remarkable potential of the proposed methods.

Nguyen [14] investigates the logistics industry, which can be considered the economic lifeline of each country because of its role in connecting the production and business activities of enterprises and promoting socio-economic development between regions and countries. However, the COVID-19 pandemic, which began at the end of 2019, has seriously affected the global supply chain, causing heavy impacts on the logistics service sector. In this study, the authors use the Malmquist productivity index to assess the impact of the pandemic on logistics businesses in Vietnam. Moreover, the authors employ a super-slack-based model to find strategic alliance partners for enterprises. The authors also utilize the Grey forecasting model to forecast the business situation for enterprises during the period 2021–2024, in order to provide the leaders of these enterprises with a complete picture of their partners as a solid basis for making decisions to implement alliances that will help logistics enterprises in Vietnam to develop sustainably. The results show that the alliance between LO₇ and L₁₀ is the most optimal, as this alliance can exploit freight in the opposite direction and reduce logistics costs, creating better competitiveness for businesses.

Popkov [15] has formulated the problem of randomized maximum entropy estimation for the probability density function of random model parameters with real data and measurement noises. This estimation procedure maximizes an information entropy functional on a set of integral equalities depending on the real dataset. The Gâteaux derivative technique is developed to solve this problem in analytical form. The probability density function estimates depend on Lagrange multipliers, which are obtained by balancing the model's output with real data. A global theorem for the implicit dependence of these Lagrange multipliers on the data sample's length is established using the rotation of homotopic vector fields. A theorem for the asymptotic efficiency of randomized maximum entropy estimate in terms of stationary Lagrange multipliers is formulated and proved. The proposed method is illustrated in the problem of forecasting the evolution of the thermokarst lake area in western Siberia.

Borisov [16] presents the guaranteeing estimation of parameters in uncertain stochastic nonlinear regression. The loss function is the conditional mean square of the estimation error given the available observations. The distribution of regression parameters is partially unknown, and the uncertainty is described by a subset of probability distributions with a known compact domain. The essential feature is the usage of some additional constraints describing the conformity of the uncertain distribution to the realized observation sample. The paper contains various examples of the conformity indices. The estimation task is formulated as the minimax optimization problem, which, in turn, is solved in terms of saddle points. The paper presents the characterization of both the optimal estimator and the set of least favorable distributions. The saddle points are found via the solution to a dual finite-dimensional optimization problem, which is simpler than the initial minimax problem. The paper proposes a numerical solution procedure to the dual optimization problem. The interconnection between the least favorable distributions under the conformity constraint, and their Pareto efficiency in the sense of a vector criterion is also indicated. The influence of various conformity constraints on the estimation performance is demonstrated by illustrative numerical examples.

Tsitsiashvili [17] develops a method for detecting synergistic effects of the interaction of elements in multielement stochastic systems of separate redundancy, multiserver queuing, and statistical estimates of nonlinear recurrent relations parameters. The detected effects are relatively strong and manifest themselves even with rough estimates. This allows their analysis with relatively simple mathematical methods and thereby helps expand the set of possible applications. The new methods are based on special techniques of the structural analysis of multielement stochastic models in combination with majorant asymptotic estimates of their performance indicators. They allow moving to more accurate and rather economical numerical calculations, as they indicate in which direction it is most convenient to perform these calculations.

A review of Ge [18] is devoted to the latest progress in the controllability of stochastic linear systems and some unsolved problems. Firstly, the exact controllability of stochastic linear systems in finite-dimensional spaces is discussed. Secondly, the exact, exact null, approximate, approximate null, and partial approximate controllability of stochastic linear systems in infinite-dimensional spaces are considered. Thirdly, the exact, exact null, and impulse controllability of stochastic singular linear systems in finite-dimensional spaces are investigated. Fourthly, the exact and approximate controllability of stochastic singular linear systems in infinite-dimensional spaces are studied. Lastly, the controllability and observability for a type of time-varying stochastic singular, linear system are studied using stochastic GE-evolution operator in the sense of mild solution in Banach spaces; some necessary and sufficient conditions are obtained, and the dual principle is proven to be true. An example is given to illustrate the validity of the theoretical results obtained in this part, and a problem to be solved is introduced. The main purpose of this paper is to facilitate readers to fully understand the latest research results concerning the controllability of stochastic linear systems and the problems that need to be further studied, thus prompting more scholars to engage in this research.

Morozov et al. [19] are concerned with the issues of modeling dynamic systems with interval parameters. In previous works, the authors proposed an adaptive interpolation algorithm for solving interval problems. The essence of the algorithm is the dynamic construction of a piecewise, polynomial function that interpolates the solution of the problem with a given accuracy. The main problem of applying the algorithm is related to the curse of dimension, i.e., exponential complexity relative to the number of interval uncertainties in parameters. The main objective of this work is to apply the previously proposed adaptive interpolation algorithm to dynamic systems with a large number of interval parameters. In order to reduce the computational complexity of the algorithm, the authors propose using adaptive sparse grids. This article introduces a novel approach to applying sparse grids to problems with interval uncertainties. The efficiency of the proposed approach has been demonstrated on representative interval problems of nonlinear dynamics and computational materials science.

Derbeli et al. [20] investigate a proton exchange membrane (PEM) fuel cell. This problem has recently gained widespread attention from many researchers due to its cleanliness, high efficiency, and soundless operation. The high-performance output characteristics are required to overcome the market restrictions of PEMFC technologies. Therefore, the main aim of this work is to maintain the system operating point at an adequate and efficient power stage with high-performance tracking. To this end, a model predictive control (MPC) based on a global minimum cost function for a two-step horizon is designed and implemented in a boost converter integrated with a fuel cell system. An experimental comparative study is carried out between the MPC and a PI controller to reveal the merits of the proposed technique. Comparative results indicate that a reduction of 15.65% and 86.9%, respectively, in the overshoot and response time can be achieved using the suggested control structure.

Author Contributions: Conceptualization, A.G.; formal analysis, A.G., V.T., M.P.; project administration, M.P.; supervision, M.P.; visualization, A.G., V.T.; writing—original draft, A.G., V.T., M.P.; writing—review and editing, A.G., V.T., M.P. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Acknowledgments: The authors are grateful to Dinara Yambaeva (Moscow, Russia) for helping to create the rose diagram and https://icons8.com/ for their icons of the countries.

Conflicts of Interest: The authors declare no conflict of interest.

References

- Zeifman, A.; Satin, Y.; Kovalev, I.; Razumchik, R.; Korolev, V. Facilitating Numerical Solutions of Inhomogeneous Continuous Time Markov Chains Using Ergodicity Bounds Obtained with Logarithmic Norm Method. *Mathematics* 2021, 9, 42. [CrossRef]
- 2. Ilyin, O. Discrete Velocity Boltzmann Model for Quasi-Incompressible Hydrodynamics. Mathematics 2021, 9, 993. [CrossRef]
- 3. Nagua, L.; Relaño, C.; Monje, C.; Balaguer, C. A New Approach of Soft Joint Based on a Cable-Driven Parallel Mechanism for Robotic Applications. *Mathematics* **2021**, *9*, 1468. [CrossRef]
- Masood, Z.; Raja, M.; Chaudhary, N.; Cheema, K.; Milyani, A. Fractional Dynamics of Stuxnet Virus Propagation in Industrial Control Systems. *Mathematics* 2021, 9, 2160. [CrossRef]
- Gorshenin, A.; Kuzmin, V. Statistical Feature Construction for Forecasting Accuracy Increase and Its Applications in Neural Network Based Analysis. *Mathematics* 2022, 10, 589. [CrossRef]
- Diveev, A.; Konstantinov, S.; Shmalko, E.; Dong, G. Machine Learning Control Based on Approximation of Optimal Trajectories. *Mathematics* 2021, 9, 265. [CrossRef]
- Li, O.; Zhou, Y. Precise Trajectory Tracking Control of Ship Towing Systems via a Dynamical Tracking Target. *Mathematics* 2021, 9,974. [CrossRef]
- 8. Diveev, A.; Sofronova, E.; Zelinka, I. Optimal Control Problem Solution with Phase Constraints for Group of Robots by Pontryagin Maximum Principle and Evolutionary Algorithm. *Mathematics* **2020**, *8*, 2105. [CrossRef]
- 9. Mena, L.; Muñoz, J.; Monje, C.; Balaguer, C. Modular and Self-Scalable Origami Robot: A First Approach. *Mathematics* 2021, 9, 1324. [CrossRef]
- 10. Diveev, A.; Shmalko, E.; Serebrenny, V.; Zentay, P. Fundamentals of Synthesized Optimal Control. *Mathematics* 2021, 9, 21. [CrossRef]
- 11. Kuang, B.; Wisniewski, M.; Rana, Z.; Zhao, Y. Rock Segmentation in the Navigation Vision of the Planetary Rovers. *Mathematics* **2021**, *9*, 3048. [CrossRef]
- 12. Quevedo, F.; Muñoz, J.; Castano Pena, J.; Monje, C. 3D Model Identification of a Soft Robotic Neck. *Mathematics* 2021, *9*, 1652. [CrossRef]

- 13. Posypkin, M.; Khamisov, O. Automatic Convexity Deduction for Efficient Function's Range Bounding. *Mathematics* **2021**, *9*, 134. [CrossRef]
- 14. Nguyen, H. Application of Mathematical Models to Assess the Impact of the COVID-19 Pandemic on Logistics Businesses and Recovery Solutions for Sustainable Development. *Mathematics* **2021**, *9*, 1977. [CrossRef]
- 15. Popkov, Y. Qualitative Properties of Randomized Maximum Entropy Estimates of Probability Density Functions. *Mathematics* **2021**, *9*, 548. [CrossRef]
- 16. Borisov, A. Minimax Estimation in Regression under Sample Conformity Constraints. Mathematics 2021, 9, [CrossRef]
- 17. Tsitsiashvili, G. Study of Synergistic Effects in Complex Stochastic Systems. Mathematics 2021, 9, 1396. [CrossRef]
- Ge, Z. Review of the Latest Progress in Controllability of Stochastic Linear Systems and Stochastic GE-Evolution Operator. Mathematics 2021, 9, 3240. [CrossRef]
- 19. Morozov, A.; Zhuravlev, A.; Reviznikov, D. Sparse Grid Adaptive Interpolation in Problems of Modeling Dynamic Systems with Interval Parameters. *Mathematics* **2021**, *9*, 298. [CrossRef]
- Derbeli, M.; Charaabi, A.; Barambones, O.; Napole, C. High-Performance Tracking for Proton Exchange Membrane Fuel Cell System PEMFC Using Model Predictive Control. *Mathematics* 2021, 9, 1158. [CrossRef]