THE CROATIAN ACADEMY OF SCIENCES AND ARTS
The Department of Biomedical Sciences in Rijeka

THE UNIVERSITY OF RIJEKA

COVID – 19 MESSAGES III

STEM FOR HUMAN SPECIES SURVIVAL

Rijeka, October 22, 2020

12,00 am

University Campus Rijeka, Faculty of Civil Engineering
Lecture hall G-003, Radmile Matejčić 3, Rijeka

Organizers

THE CROATIAN ACADEMY OF SCIENCES AND ARTS
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COVID-19 Messages Conference Program Committee

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Registration: online via registration form for online and onsite participants

Event address for ZOOM attendees will be sent to all registered participants by e-mail

Free admission for both registrations, but note that the capacity of the lecture hall is restricted. Once all spaces have been filled, no more onsite registrations will be permitted.

Refreshments are with no charge.

Parking is free and provided in the building of Student Center Rijeka
(Radmile Matejčić 5)

Information

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P R O G R A M

OPENING

(12,00 – 12,30)

INTRODUCTION

Snježana Prijić Samaržija, PhD., Professor, Rector, The University of Rijeka, Rijeka, Croatia

Daniel Rukavina, M.D., PhD., Professor Emeritus, Head of the Department of Biomedical Sciences in Rijeka, Croatian Academy of Sciences and Arts, Rijeka

Senka Maćešić, PhD., Professor, Vice-rector, The University of Rijeka, Rijeka

12,30 – 14,30 h

II. SURVIVAL CHALLENGES: THE BIG PICTURE

Chairmen: Senka Maćešić

Marin Karuza, PhD, Professor, Department of Physics, University of Rijeka, Rijeka, Croatia, and Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Tireste, Italy
Physics of space travel: prospects of humans as multi planet species

Neven Duić, PhD, Professor, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Zagreb, Croatia
COVID-19, climate change and energy transition

Edgar Roldan, PhD, Professor, International Center for Theoretical Physics, Trieste, Italy
Lecithin as a putative biodegradable inhibitor of SARS-CoV-2

Ivan Štajduhar, PhD, Professor, Faculty of Engineering, University of Rijeka, Rijeka, Croatia
BirdbrAIn genius – the reach and limitations of machine intelligence

Coffee break: 14,30 – 15,00

15,00 – 17,00 h

III. IT against COVID-19

Chairmen: Jonatan Lerga

Jan Stedul, Mislav Malenica, Mindsmiths, Zagreb, Croatia
Companion Healthcare - a new paradigm in treatment of chronic patients

Ana Meštrović, PhD, Professor, Department of Informatics, University of Rijeka, Rijeka, Croatia
A multilayer network approach for fake news detection during the COVID-19 crisis

Kristijan Lenac, PhD, Professor, Faculty of Engineering, University of Rijeka, Rijeka, Croatia
Blockchain solutions for postpandemic society

Goran Mauša, PhD, Professor, Faculty of Engineering, University of Rijeka, Rijeka, Croatia
Application of soft computing in peptide design

Coffee break: 17,00 – 17,30

17,30 – 18,30 h

III. KEYNOTE LECTURE

Chairman: Senka Maćešić

Igor Mezić, PhD, Professor, University of California, Santa Barbara, USA
Predictions and black swans

18,30 – 19,30 h

IV. ROUND TABLE DISCUSSION:

ARE WE EQUIPPED FOR OUR FUTURE?

Panelists: Mladen Pejković, Igor Mezić, Neven Duić, Mislav Malenica

ABSTRACTS

Predictions and black swans

Igor Mezić
University of California, Santa Barabara, USA

The problem of prediction of behavior of dynamical systems has undergone a paradigm shift in the second half of the 20th century with the discovery of the possibility of chaotic dynamics in simple, physical, dynamical systems for which the laws of evolution do not change in time. The essence of the paradigm is the long term exponential divergence of trajectories. However, that paradigm does not account for another type of unpredictability: the ``Black Swan'' event. It also does not account for the fact that short-term prediction is often possible even in systems with exponential divergence. In our framework, the Black Swan type dynamics occurs when an underlying dynamical system suddenly shifts between dynamics of different types. A learning and prediction system should be capable of recognizing the shift in behavior, exemplified by ``confidence loss''. In this paradigm, the predictive power is assessed dynamically, and confidence level is used to switch between long term prediction and local-in-time prediction. Here we explore the problem of prediction in systems that exhibit such behavior. The mathematical underpinnings of our theory and algorithms are based on an operator-theoretic approach in which the dynamics of the system are embedded into an infinite-dimensional space. As an outcome of global learning capability, our algorithms indicate an exponential global (in time) trend for the number of influenza cases worldwide, that has been present since at least 1997. We also show that the framework correctly identifies the 2009-2010 flu pandemic as a black swan event, that prevented machine learning-based algorithms (e.g. Google Flu) from showing subsequent good performance.

We discuss the prediction problem in other complex dynamics datasets, such as signature indices of geomagnetic substorms. In addition, fundamental limits on predictability that our theory implies are discussed. We have deployed the algorithm to assess the global and United States evolution of the COVID-19 pandemic. The results indicate that, despite the fact that the data on COVID-19 cases was at times inaccurately reported, causing ``black swan'' -like events, the prediction algorithm recognizes the deviations and adjusts to continue accurate prediction entirely from data, without any underlying models.

Key words: prediction algorithms, detection of black swan-like events

Physics of space travel: prospects of humans as multi planet species

Marin Karuza
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Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Trieste, Italy

The COVID-19 pandemic has shown the fragility of the human society. While in the short-term medicine, biotechnology, medical sciences and biomedicine can provide an answer to current challenges in the long term the occurrence of a catastrophic event that could cause extinction of human race cannot be excluded. Thus, survival of human species can be insured only by colonization of other planets. However, physics puts some stringent limits to space travel and consequently number of planets that could be reached. The current limits and the possibilities of overcoming them will be given. Furthermore, a brief overview of search for extrasolar planets and its techniques will be presented.

Key words: interferometry, space travel, extrasolar planets, propulsion, astronomy

COVID-19, climate change and energy transition

Neven Duić
University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture, Zagreb, Croatia

We know for more than a century that fossil fuels cause climate change, and we know for five decades that the climate change will bring upon us and habitats devasting effect during XXI century, but a joint endeavour of fossil fuel industry, financial institutions and involved governments have blocked mitigation. Fortunately, the World is divided on 200 sovereignties, so some of them saw interest in moving forward, by investing in learning curve of technologies needed for mitigation: renewables, energy efficiency, clean mobility. The process was slow due to lack of global effort, and intensive work of fossil fuel lobbies on blocking the effort on international, multilateral, and national levels, but by 2008 we had technologies able to compete and replace fossil fuels. Some of the sovereignties went forward, financial institution who suddenly saw profit in saving climate obliged, but relentless progress made the transition too slow to help against climate change reaching point of no return, even though it became clear that fossil fuel interests are losing the war on climate. The enemy will be defeated, but patient will eventually have to adapt to catastrophic 3-4 degrees higher temperature, which may spell the end of civilisation and the World as we know it.

What COVID-19 did was amazing. It brought short but relentless stop to travel and much non-essential economic activity, and with it fall of marginal energy use, which means mainly fossil fuels. It will not have per se lasting effect on climate change, since the rate of growth of carbon dioxide concentration in atmosphere will be only negligibly reduced, but it brought much more profound change, it has shown the fragility of fossil fuel investment. Price of oil tumbled, for the first-time making oil countries aware of the end of century of oil. Coal and oil investments collapsed, coal power plants started to shut down in masses, slowly creating snowball effect.

Can we do it? We need to reduce greenhouse gas emissions in European Union for 55-60% by 2030, and at least 45% on global level. That means we need to rapidly invest in renewables and phase out fossil fuel technologies for which we have alternative, such as coal power plants, gas boilers and internal combustion engine cars. Fossil fuel industries will put up heroic fight, but they lost an important ally, financial sector.

Can we save climate by reducing our impact on environment by voluntary measures? No! We need to reduce emissions by 100% and we cannot do that by change of lifestyle. We can only

do that by rapid investment in clean technologies. Should we change lifestyle? Probably yes, because human happiness is perhaps not proportional to the quantity of material things after some minimum has been satisfied, but this is NOT a way to save climate.

Key words: COVID-19, energy transition, climate change

Lecithin as a putative biodegradable inhibitor of SARS-CoV-2

Edgar Roldan
International Center for Theoretical Physics, Trieste, Italy

Understanding the physical and chemical properties of viral infection at molecular scales is a major challenge of the scientific community in the fight against the Coronavirus (COVID-19) pandemic.
We employ all-atoms molecular dynamics simulations to study the interaction between the receptor-binding domain of the SARS-CoV-2 spike protein and the surfactant lecithin in water solutions. Our microsecond simulations reveal a preferential binding of lecithin to the receptor-binding motif (RBM) of SARS-CoV-2. Furthermore, we find that the lecitin-RBM binding events are mainly dominated by the hydrophobic interactions, which are accompanied by dewetting of water molecules near the RBM. These proof-of-concept simulations provide a demonstration of the use of biodegradable phospholipids as blockers of binding of SARS-CoV-2 with the human Angiotensin-Converting Enzyme 2 (ACE2) receptor.

[1] Qaisrani et al., chemrxiv.12670952.v1 (2020)

Keywords: all-atoms molecular dynamics simulations, SARS-CoV-2 spike protein, lecitin-RBM binding events

BirdbrAIn Genius – the Reach and Limitations of Machine Intelligence

Ivan Štajduhar
University of Rijeka, Faculty of Engineering, Rijeka, Croatia

Creating machines that think and act like human beings has puzzled scholars from the dawn of time. While pondering on this concept, ancient Greek philosophers have established the rules that govern correct thought, consequently laying out the foundation for contemporary theorem provers and deduction systems. For quite some time, we believed that computation could be used to mimic reasoning, which in turn would lead to understanding the processes influencing behavioural patterns –it turned out, however, that it is difficult to encode rational thought. On the other hand, mimicking the thought processes going on in our brains, by reverse engineering of the brain, has proven to be infeasible, albeit it led to advances in some other fields of research. Regardless of the approach used for modelling the thought process behind decision making, working on machines that act like people was more or less abandoned because performing well in the imitation game (e.g. the Touring test) did not help in understanding human intelligence.

Noticeable advances in artificial intelligence (AI) were reported only when the core focus shifted towards rational acting, disregarding the gist of previous approaches.

Nowadays, AI deals with the concept of creating machines thinking and acting like human beings in a rational sense, i.e. agents behaving optimally. Optimal behaviour can be learned (taught) using state-space search algorithms and self-play. Whereas rational acting by an autonomous agent can be considered solved for smaller scale problems in a simulated environment (games and such), the same cannot be stated for large scale problems, those involving uncertainty in a dynamic, ever-changing, environment (i.e., the real world). Here, an agent's performance largely depends on its ability to learn quickly, and from fewer examples – which can be helped by embedding the agents percepts with machine learning (abstraction of the state space) and enhancing their search strategies using q-learning.

Recent advances in machine learning provided an end-to-end modelling framework for learning adequate feature embeddings, via stacked representations, directly from data (i.e. deep learning), which has proven to be rather useful for dealing with highly-nonlinear problems (e.g. those related to sound or vision). This, in turn, resulted in significant improvements in modelling numerous complex problems, previously considered infeasible for real-world applications (because of low fidelity), e.g. image to image translation, translation between written or spoken languages, and image inpainting, just to name a few. The same technology also triggered the development of techniques mimicking human abilities or appearance, e.g. artistic style transfer, speech synthesis, and so on. Although the aforementioned technologies can be utilised for building autonomous agents surpassing human experts in performing numerous highly specialised menial tasks, their intelligence (optimal rationality) is strictly limited to the task at hand, and they can often be easily fooled into suboptimal acting.

Key words: artificial intelligence; rational acting; game playing

Companion Healthcare - a new paradigm in treatment of chronic patients

Mislav Malenica
Mindsmiths d.o.o., Zagreb, Croatia

Health systems in the EU are built on common values: universality, access to good quality care, equity and solidarity. Because European population is ageing and getting more exposed to multiple chronic diseases this leads to higher demand for healthcare and increases fiscal pressure. Usually around 80% of the healthcare budget is dedicated for chronic conditions.

We believe that by introducing digital assistants based on AI to assist medical workers in treating chronic patients, we can significantly improve quality of care and at the same time reduce the cost. During the presentation the speaker will show results from two pilots:

1. digital assistant Andrija who is helping Croatian ministry of health to efficiently communicate with citizens during COVID-19 pandemics, and
2. digital assistant Megi who is for the last 11 months helping doctors at Magdalena clinic to manage the treatment of hypertension patients.

Key words: chronic conditions, artificial intelligence, digital assistant, Andrija, COVID-19

A multilayer network approach for fake news detection during the COVID-19 crisis

Ana Meštrović
University of Rijeka, Department of Informatics, Rijeka, Croatia

Digital communication technologies and social media accelerate information spreading. This trend is reflected in the infodemics – the rapid diffusion of information and misinformation. Infodemic is potentially dangerous, especially during the crisis because it makes it difficult for individuals and groups to find reliable sources of information. The COVID-19 outbreak infodemic resulted in misinformation and fake news spreading.

In this light, automatic detection and prediction of the spread of fake news plays an important role and may improve various aspects of crisis communication. In last ten years, a vast number of research papers addressing the problem of the automatic detection of fake news have been published, however, it remains a challenging task, especially in the context of COVID-19 crisis communication.

The aim of our research is to define an approach that captures various features of information spreading over social media and thus enables a classification into two categories: true information and false information. More precisely, we will propose a multilayer framework that defines a set of models and approaches that integrates three aspects of the analysis of the information spreading: (i) content, (ii) context and (iii) dynamic. Message content captures semantics and it can be numerically represented as a low dimensional vector called embedding using deep learning models (for example BERT). Message context refers to the features extracted from the structure of a social network related to the message and can be described through various layers. For example, the features of Twitter messages extend to the reply layer, the retweet layer, the mention layer and the quote layer. To represent all these features in one formalism, we propose a multilayer network. The third aspect of a message is its dynamics that can be described in terms of how for example depth, breadth, and size of diffusion change over the time. Thus, the main idea of the proposed approach is to extend the embedding of a message's content with other features and to construct a multilayer embedding which will be used in the task of fake news detection.

Within the proposed framework, we will study empirical data related to the communication of the COVID-19 crisis crawled from various social media sources, such as Twitter, Facebook and online portals. The focus of our datasets will be texts in the Croatian language, however, to be comparable with other studies, we will perform experiments with texts in the English language as well.

We expect that the results of this research will enable a better understanding of the spread of fake news and help in the future development of systems for the detection and prevention of misleading and harmful information on social media.

Key words: fake news detection, deep learning, natural language processing, social networks analysis, COVID-19

Blockchain solutions for postpandemic society

Kristijan Lenac

University of Rijeka, Faculty of Engineering, Rijeka, Croatia

Covid-19 pandemic accelerated the process of digital transformation of the society in some important areas like provisioning of health services, data sharing, remote work, and others. The pandemic rapidly brought to attention the needs for trusted real-time access to critical information, efficient supply chain management, frictionless health and financial services, contact tracing and others.
In this talk I will use several examples to show how blockchain solutions can help coping with Covid-19 by addressing these needs and in the process radically transform the way services are provided in the postpandemic society. I will argue that in some cases blockchain is currently the only viable solution capable of fully addressing these needs while still providing provenance and trust in the shared data without compromising on transparency and user privacy.

Key words: blockchain, health, security, society, data sharing, transparency

Application of soft computing in peptide design

Goran Mauša
University of Rijeka, Faculty of Engineering, Rijeka, Croatia

Peptides are of great interest in biomedical field as they can act as safe therapeutic agents as they show low toxicity and because they are the building blocks of life. They can be designed to mimic nature while incorporating new activities, such as antiviral, antibacterial or anticancer. However, the discovery of new peptides with desired properties based on their sequence is a challenging task, as they are part of a very large search space and the principles responsible for the target properties are not yet fully understood. To avoid expensive and time-consuming guesswork and experimental failure, a novel strategy is to apply soft computing techniques to address these issues. Search based algorithms allow for a faster exploration of peptide permutation space which grows exponentially with peptide length and whose amount and dimensionality is too overwhelming to rationally comprehend. Machine learning is able to find patterns or regularities in data, build mathematical models based on the theory of statistics and to make up for the lack of knowledge. To date, soft computing has been applied to a variety of chemical problems to maximize the chance of successful and rapid solving of complex issues.

Genetic algorithms have been reported successful for the optimisation of the antimicrobial activity of peptides found in nature, while evolutionary molecular design algorithm optimized

the selectivity of predicted peptides towards cancer cells. On the other hand, Support Vector Machine and Random Forest algorithms were applied to find highly effective antiviral peptides, while artificial neural network were used to measure the anticancer abilities of promising peptide candidates. In addition, a combination of these two soft computing approaches was formed for the discovery of *de novo* peptide substrates for enzymes and presents a motivation for our own research direction.

Our team has already reported on a multi-objective evolutionary approach for the exploration of mass and sequence diversity-oriented random peptide libraries and on a bottom-up design methodology for their design, which combines physico-chemical properties obtained experimentally and theoretically to cover larger parts of the peptide chemical space. Our current project activities involve the application of soft computing techniques to find peptides with catalytic activity, to predict their predisposition towards self-assembly and to estimate the antiviral activity of selected candidates for peptide binders. The aim behind these objectives is to rationally design supramolecular peptide-based viral mimetics for SARS-CoV-2 entrapment, thus aiding in the worldwide struggle against the COVID-19 infection.

Keywords: Peptide design, evolutionary algorithms, machine learning