Reports on Scientific Computing and Optimization 1/2019

Eds. Tero Tuovinen, Jacques Periaux & Pekka Neittaanmäki

Book of Abstracts:

Computational Sciences and AI in Industry - New digital technologies for solving future societal and economical challenges (CSAI) 2019

ECCOMAS Thematic Conference

UNIVERSITY OF JYVÄSKYLÄ
FACULTY OF INFORMATION TECHNOLOGY

Industry Interest Group ECCOMAS

Book of abstract

CSAI

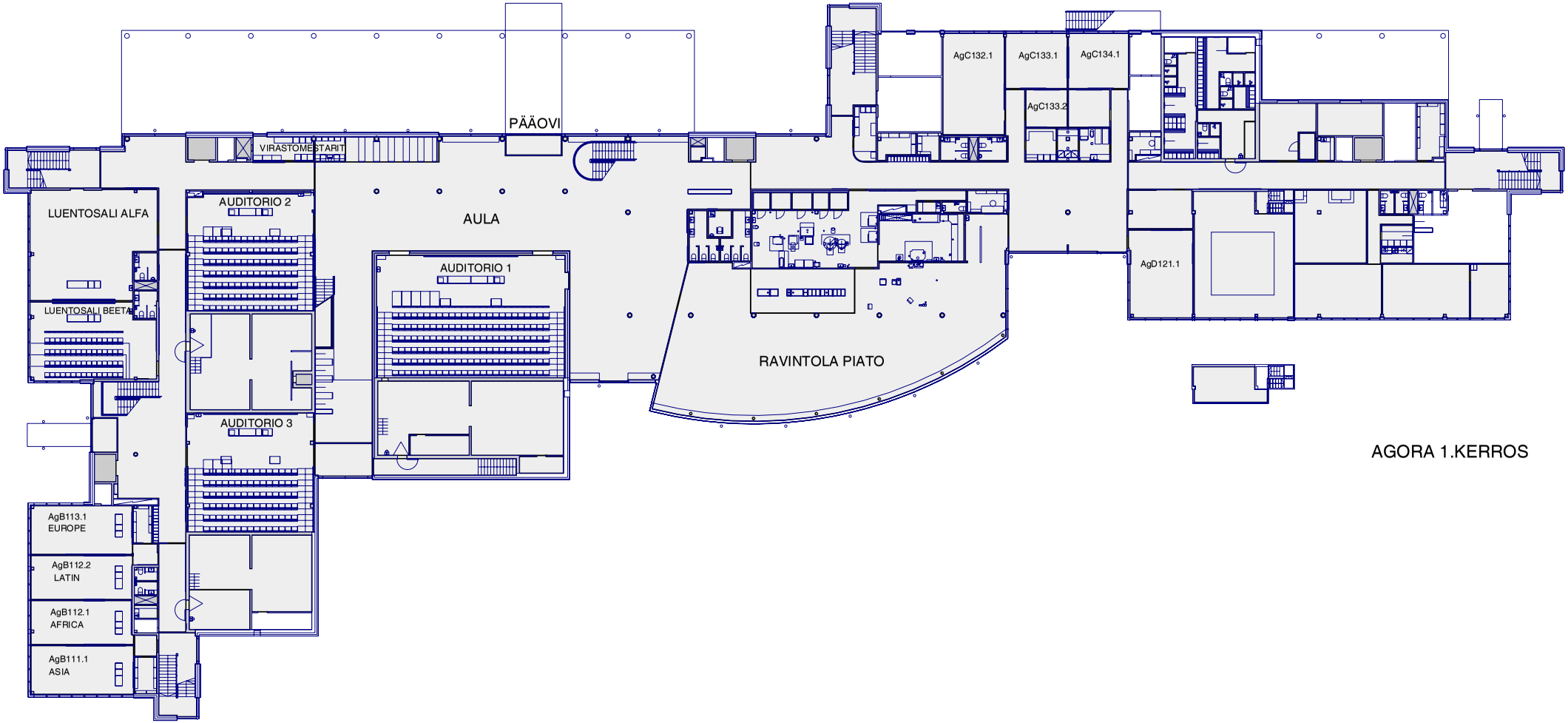
Computational Sciences and AI in Industry: new digital technologies for solving future societal and economical challenges

2019

12-14 June, 2019, Jyväskylä, Finland

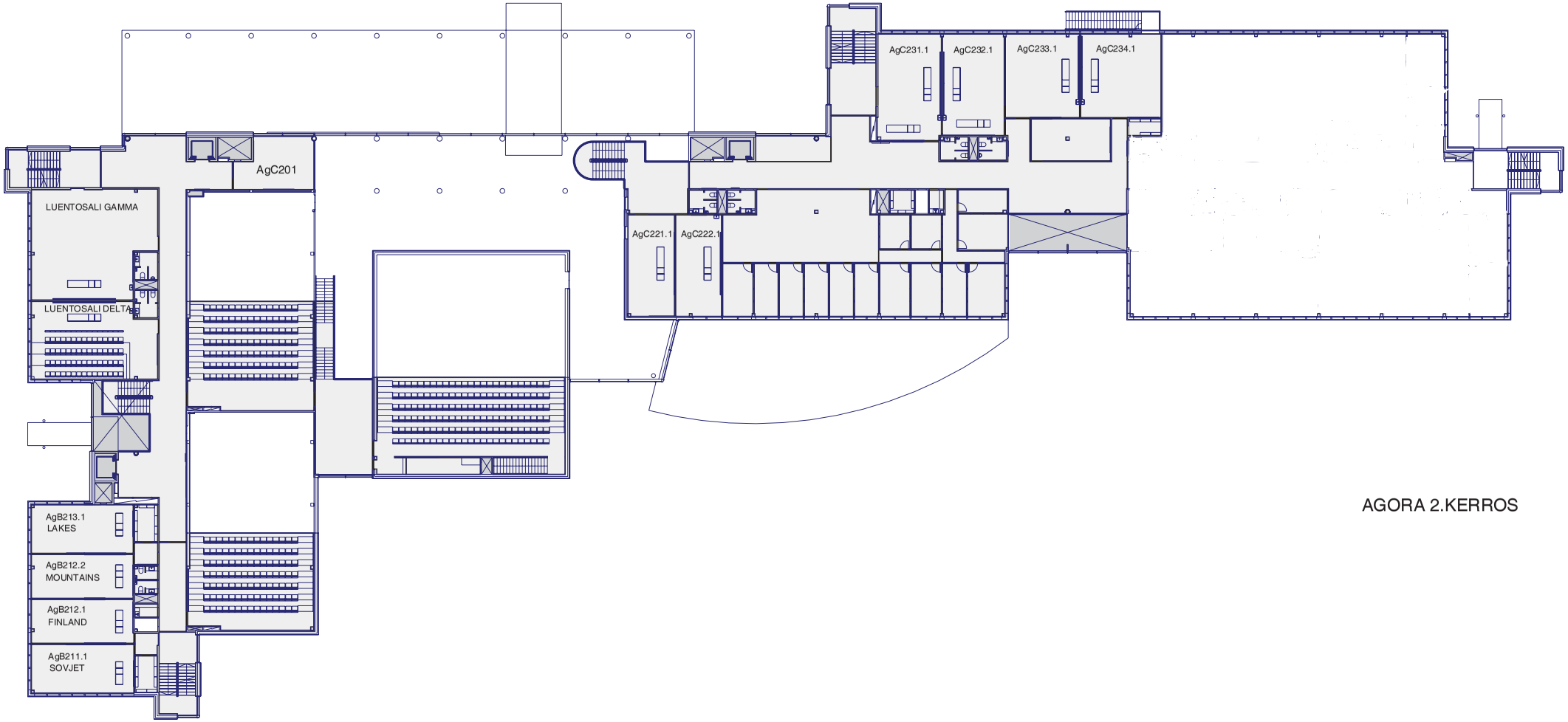
Reports on Scientific Computing and Optimization 1/2019
Editors Tero Tuovinen, Jacques Periaux & Pekka Neittaanmäki
University of Jyväskylä

ISBN 978-951-39-7788-7 (Print)
ISBN 978-951-39-7789-4 (e-publication)
ISSN 2489-351X



AGORA 1.KERROS

0 5 10m



AGORA 2.KERROS

0 5 10m

Preface

First of all and on behalf of the University of Jyväskylä organizers, we would like to extend our warm congratulations on the successful participation of the delegates of this conference, the first in Europe in 2019 of a series and to express our heartfelt thanks to people from all computational Sciences and Artificial Intelligence styles who are meeting this week in Jyväskylä in a friendly perspective of international cooperation in science and technology.

The rapid digitalization of industry and society is bringing opportunities and challenges to large and small industries, with target in significantly improving well being of citizens, in reducing their environmental impact (greener transport called essential and big data seen as a help in cutting emissions), in increasing safe autonomous urban, air and surface transport, mobility, in accessing efficient (big) data tools for medical applications and public health-care systems.

In fact, applications are multiplying and directly affecting our daily lives with image recognition, self-driving cars, disease detection, among others... Many artificial intelligence (AI) strategies dealing with the collection of large bodies of data will help mastering new challenges, in particular in modeling and simulation. Data is a key competitive advantage in the global AI race. A data policy taking into account AI requirements is therefore essential if the European Union and other countries wish to attain the goals of sovereignty and strategic autonomy.

These goals are ambitious, but they are necessary steps in the creation of an AI industry. CSAI 2019 is opening the door to these goals by the dual networking of two majors computational disciplines: Computational Science and Artificial Intelligence. The aim of CSAI is to provide an overview on the state of the Art and the technology trends in advanced computational methods and digitalization of industrial and societal applications.

In 1997 a International Conference took place in Tours, France with the title " Computational Science for the 21st Century" with a collection of papers reflecting the "State of the Art" in computational science. Two decades after this event, in 2019 a second wave or " marriage à la mode" with the digitalization of industry and society is launched with "Computational Science and Artificial Intelligence" in Jyväskylä, Finland: CSAI 2019 .

Perspective of the conference

AI of the future will mean creating the greatest values for all stakeholders: industry, services and users. To achieve this, the industry will have to be connected, and this is already a reality today. Progress is central to such change, made possible by the digital revolution. The Internet of Things, the Cloud and Big Data are an integral part of the industry's transformation as they gain momentum, affecting every aspect of society.

The world of data algorithmics with Computational Sciences is improving performance and productivity in several industrial sectors. The proliferation of sensors installed on complex systems found at every level of industry help both to fine-tune service in real time and to regulate all production sequences at the highest possible level. All stakeholders in the industry and society sectors are now up to speed with the digital age. Connected industry is hastening the pace of transformations that are already underway.

But this comes at a price. All connected objects, soon to be linked to developments in Artificial Intelligence, are potential points of entry for digital attacks. Improved performance has the paradoxical effect of increasing exposure to cyber threats. Cyber attack can exploit the logics of networks, spreading to contaminate the most established industrial systems, such as social networks and governmental systems.

This is a topic of utmost importance, since the progress achieved in connected industry and society is so great that no one can imagine any going back.

The pace and continuity of innovation relies largely on the confidence placed in the data generated and systems that suspend them. Security is now a major issue for the sustainability of states, smart territories and businesses. The rapid increase in surface and air transport, medicine and finance sectors, among others, is the most tangible demonstration of the above issue.

Organizers & Committees

Chairmen

Professor Pekka Neittaanmäki

Professor Jacques Periaux

Adj. Professor Tero Tuovinen

Local Organizing Committee: Jaana Räisänen, Marianne Lampi, Kati Valpe, Marja-Leena Rantalainen, Jasmin Suikki, Billy Braithwaite, Leevi Annala, Matti Eskelinen

Scientific and Technical Committee: Pekka Abrahamsson, University of Jyväskylä; Robert Azencott, Univerity of Houston; Ferdinando Auricchio, University of Pavia; Thomas Bäck, LIACS Marc Schoenauer, INRIA; Josef Eberhardsteiner, Vienna University of Technology; William Fitzgibbon, University of Houston; Carlos M. Fonseca,

Supporting organizations

ECCOMAS

ECCOMAS (European Community on Computational Methods in Applied Sciences) is a scientific organization grouping together European associations with interests in the development and applications of computational methods in science and technology. The mission of ECCOMAS is to promote joint efforts of European universities, research institutes and industries which are active in the broader field of numerical methods and computer simulation in Engineering and Applied Sciences and to address critical societal and technological problems with particular emphasis on multidisciplinary applications.

University of Jyväskylä (JYU)

The University of Jyväskylä is the fourth largest university in Finland and offers education and research in various fields. The special expertise areas of the university include Natural Sciences, Human Sciences, Sports and Health Sciences, as well as Teacher education. In the field of Information Technology, the university focuses on the areas of Computational Sciences, Software and Telecommunication Technology, Information Systems, Cognitive Science and Educational Technology, and Cyber Security.

Interest Group (IIG)

The Industry Interest Group is a special interest group operating under ECCOMAS. Its main objectives include strengthening the industrial liaison and

developing contacts between ECCOMAS and the different DGs of the European Commission. Most importantly, IIG wishes to promote the interaction between universities and businesses. The main means of the IIG to promote this interaction is by organizing various kinds of events, such as conferences, special technology sessions and workshops. These events can provide a great space for exchange, networking and discussion.

ICIAM2019

CSAI is a satellite conference of ICIAM2019.

The Federation of Finnish Learned Societies

The Federation of Finnish Learned Societies, established in 1899, is a national co-operative body for learned societies in Finland. It contributes to the co-operation between learned societies, supports and develops scholarly communication and publishing, and promotes awareness and usage of research results. It also supports and develops the role of its members in science policy discussion. The Federation has a membership of 275 societies and four academies from all branches of arts and sciences, in total 250,000 individual members. Every year these learned societies arrange hundreds of meetings and conferences, attended by the academic community and the general public. The societies and academies are among the foremost academic publishers in Finland: they issue more than 100 periodicals and some 250 new book titles each year. The Federation receives state subsidy for its activities from the Ministry of Education and Sciences.

Thanks to the Supporters

We would like first of all to thank the university of Jyväskylä team – and the helpers, in particular Jaana Räisänen, Marianne Lampi, Marja-Leena Rantalainen and Kati Valpe - and the Faculty of Information Technonoly (Prof. Pasi Tyrväinen, Dean) for welcoming this event in AGORA and setting and fixing up the many technical and logistics aspects of the CSAI 2019 Conference.

Format of the conference

The conference will include plenary and semi-plenary presentations on contemporary topics about Computational Science and AI, as well as parallel mini-symposiums and Special Technology sessions, in which there may be a keynote speaker. The plenary, semi-plenary and keynote speakers are all top experts in their field and will be completely or partially supported by the conference. Mini-symposiums and Special Technology Sessions are parallel sessions consisting of approximately 4-6 contributed presentations of 20 minutes (including discussion) and a possible keynote presentation of 40 minutes. The mini-symposiums are more scientific in nature, while the Special Technology Sessions are more industry oriented. In the end of the conference, we have Mini-Forum, discussion event about the topics of the conference.

Objectives

The objective of this conference is to be a forum of presenting and discussing the recent research, innovation and ideas in the bridged areas of Computational Sciences and AI. A special area of interest is the application of these scientific fields to the industrial sector and real-life problem solving.

In accordance with the Industry Interest Group (IIG) of ECCOMAS, the conference aims to promote the interaction between universities and business life. Therefore a central goal is to bring together representatives of the scientific community as well as the industrial sector to share their knowledge and learn expertize from each other. As networks are becoming more and more important, the conference aims to be a place of creating links and connections between participants with mutual interests.

Conference topics

The conference topics and areas of interest include, but are not limited to, the following.

Topics: Innovations in AI and Computational Sciences; Industrial application cases (e.g. transport, medicine, finance, police investigation etc.); Applications for societal issues; Computational applied mathematics; Big data predictive analysis; Computational intelligence; Intelligent information processing;

Figure 1: Central Finland has beautiful nature

Problem-solving algorithms; Use of algorithms with big data and AI; Optimization issues AI tools; Machine learning and deep learning; Human-machine interaction; Emerging technologies

Areas of interest: 1) Computational fluid dynamics 2) Computational solids and structural mechanics 3) Scientific computing 4) Multi-disciplinary design and optimization for manufacturing

Welcome to Jyväskylä!

Welcome to Jyväskylä, a Central Finnish town surrounded by beautiful lakes and forests! This lively town will be the setting of the CSAI 2019 conference. Due to its compact size and warm atmosphere, Jyväskylä is easily reachable and ideal for networking.

The town is home to 140,000 people and very friendly to international visitors. The people in Jyväskylä have excellent language skills and customer service attitudes. Jyväskylä is also active in organizing events: over 5,000 events are held here annually. Jyväskylä is especially known for education and sports, and offers a unique combination of urban life and proximity of nature.

Figure 2: Bridge of Ylistö (Picture: Jussi Jäppinen 2012)

Venue

The conference is held at the Agora building (Mattilanniemi 2) of the University of Jyväskylä, right beside the beautiful lake Jyväsjärvi and within reasonable distance from the city center. You can easily reach the venue by foot along the lake, or by bus no. 5. The bus stop in the city center is called Keskusta 6 and it is located in front of Forum shopping center along with other local bus stops, just a short distance from the Travel Center. The bus stop at the venue is called Mattilanniemi. Local bus schedules can be found here. If you wish to use a taxi, there is a taxi stand just behind the Travel Center building.

At Agora, the auditorium can be found on the right side of the lobby of the building, while the other conference halls are compactly located close to it in the first (rooms Alfa and Beeta) and second (rooms Delta and Gamma) floor. The hall called Lea Pulkkisen sali can be found in the 4th floor: just pass the janitor's desk on the right side of the lobby and take a lift up, and when you step out, go through the glass door right in front of you and all the way to the end of the hallway. The hall will be on the left side. You can also check the locations of the conference halls from the floor maps below.

All conference rooms are equipped with a computer and a projector. The conference participants can also utilize a computer room on the first floor (room code Ag B112.1 Africa): follow the hallway past the Alfa and Beeta rooms and through the glass door, and the computer room is situated at the very end of the hallway on the right side. To use the university's computers in this room, you need a guest username and password, which you can get at the conference info desk in the lobby. The building has a free WLAN network called agora-open.

The University restaurant Piato is conveniently located under the same roof, on the left side of the lobby, and another university restaurant Maija can be found nearby in the MaA building (5min walk).

Free-time activities in Jyväskylä city center

Despite its small size, Jyväskylä is far from boring. The main street Kauppakatu offers a great variety of restaurants, cafés and bars, and is also home to several street festivals and events throughout the year. Along the street you can also find the Handicraft Museum of Finland as well as Jyväskylä Art Museum. Kirkkopuisto, the park with the town church and a popular place for gathering among locals, is also located along the Kauppakatu street. If you stray a little further away from the street, you can find the Toivola Old Courtyard and its historic milieu, local handicraft shops, and a cozy little café.

Many of the town's buildings were designed by famous architect Alvar Aalto, and one great example is the main campus of the university at Seminaarinmäki. The Seminarium building houses a tiny Cultural History Museum exhibiting life at the University of Jyväskylä. If you stroll to the area of the university's Ruusupuisto campus, you can find the Alvar Aalto museum. Right next to it you can find the Museum of Central Finland and learn more about the history and culture of the area.

The town center is squeezed between the beautiful lakeside and harbor as well as the Harju ridge. If you climb up the stone stairs, you can find an observation tower which offers a magnificent view over the town and the surrounding hills and forests, as well as a small Nature Museum. For those looking for the proximity of nature, there is a walking trail of around 700m through the Tourujoki Natural Park. You can also take a walk along the lakeside on the Rantaraitti trail, which passes by the harbor and two university campuses. The harbor is the departing point of various cruises to lake Päijänne.

For the most up-to-date information about other attractions and activities as well as events, please visit the Tourist information center website.

Titles and abstracts of the computational sciences and AI in industry (CSAI) - conference 2019

Contents

1 Novel strategies for data-driven evolutionary optimization 13

2 Machine learning using distance-based methods 16

3 Counting cells and predicting immunoscore using gradient boosted convolutional neural networks 17

4 Kubelka-Munk model and stochastic model comparison in skin physical parameter retrieval using neural networks 18

5 A combined approach of neural networks and graphical models in skin cancer inference using spectral imaging 20

6 Using wave propagation simulations and convolutional neural networks to retrieve thin coating's thickness from hyperspectral images 22

7 Predicting future overweight and obesity from childhood growth data: A case study 25

8 Variable selection under a value acquisition budget 26

9 Stochastic approximation by successive piecewise linearization 27

10 Non-convex robust low-rank matrix recovery 28

11 Neural network learning via successive piecewise linearization 29

12 Learning for scientific computing purposes 30

13 Computational intelligence in design of new nanomaterials 31

14 Modeling flow, reactive transport and geomechanics in porous media 32

15 Physics constrained machine learning for industrial applications 34

16 Parameter and type identification in partial differential equations using deep neural networks 35

17 Stability maximization for layered moving web with total mass constraint 36

18 Similarity solutions for condensation on a non-isothermal vertical plate 37

19 Enhanced topology optimization approach using moving morphable components coupled with NURBS curves 38

20 Combined model order reduction and artificial neural network for data assimilation and damage detection in structures 40

21 Towards the optimization of fuzzy pattern trees by abs - linearization 42

22 Support vector machines in clusterwise linear regression 43

23 A Second-order method with enriched hessian information for composite sparse optimization problems 44

24 Missing value imputation via nonsmooth optimization and clusterwise linear regression 45

25 Parsimonious neural networks 46

26 Nobody can stop advancing artificial intelligence (AI) where developing 47

27 Computational sciences, physics field theories and geometry 48

28 Mini-symposium on ethics in AI 50

29 Essentializing software engineering practices for ethically designing and developing artificial intelligence systems 52

30 Ethics is important, but how can we implement it? Survey on software developers' views on AI ethics 54

31 Industrial IoT capabilities in reducing the LCOE of offshore wind energy: A review 56

32 High-Performance data analysis with the Helmholtz Analytics Toolkit (HeAT) 58

33 Dynamic data-driven application systems based on tensor factorization: learning the physics of model evolution 61

34 Predicting customer experience 63

35 Puhti-AI: Finland's new AI supercomputer 64

36 Using Artificial Intelligence to Classify Textual Applications for Reporting Purposes 65

37 Application of machine learning methods to error control of approximate solutions 68

38 Iterative data selection strategy in offline data-driven evolutionary multiobjective optimization 69

39 On surrogate management in interactive multiobjective building energy system design 71

40 A modified deep neural network for the rapid inversion of geophysical resistivity measurements 73

41 Using agents for automatic meta-modelling algorithm selection in data-driven multiobjective optimization problems 77

42 Mini-Forum: Future cooperation between Computational Science and AI in Industrial and Societal Applications - challenges, impact and expectations? 79

42.1 Artificial Intelligence, Deep Learning and Science Policy in France 81

42.2 AI and Digital Twin challenges in current EU arenas – in overall and from Finnish perspective 82

42.3 AI and Data Analytics at a Centre for Scientific Computing . . . 84

42.4 AI in the field of medical applications 86

1 Novel strategies for data-driven evolutionary optimization

Nirupam Chakraborti
Department of Metallurgical & Materials Engineering, Indian Institute of Technology, India.

In this presentation I will talk about some recent learning algorithms EvoNN (Evolutionary Neural Net), BioGP (Bi-objective Genetic Programming) and EvoDN2 (Evolutionary Deep Neural Net) developed by me and my global collaborators which are now being widely used in diverse areas of engineering metamodeling and multi-objective optimization of practical interest. Among them BioGP is now integrated in the commercial Kimeme software, the flagship product of Cyber Dyn Srl, an Italian software company. Open source codes of these algorithms are also available from me for academic research. These algorithms are based upon a nature inspired approach, trying to mimic some basic aspects of evolutionary biology in a non-biological context, and follow the principles of multi-objective optimization. The starting point is the noisy data from diverse sources that could be either from industry, experiments or simulation and the next step is to create a set of optimum models following an intelligent strategy for avoiding the random noise in the original information. For a given system, several such models can be created for various conflicting objectives pertinent to the system in hand, and all these algorithms allow the users to optimize them simultaneously following the notions of Pareto Optimality, which tends to find out the best possible tradeoffs between these conflicting requirements. Once a model is created, it also allows the users to evaluate the interaction between the decision variables, using a simple, intuitive approach tailor made for this purpose.

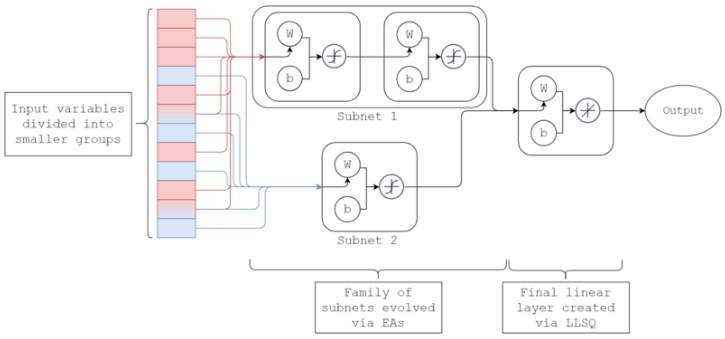


Figure 3: The schematics of EvoDN2 algorithm.

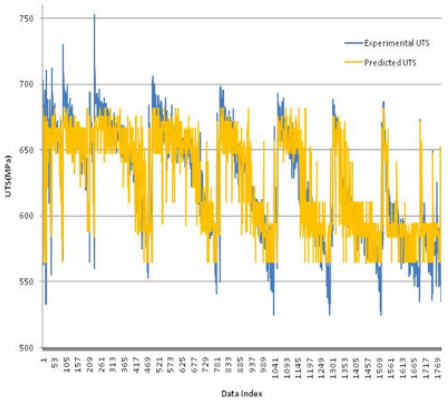


Figure 4: Noisy data for UTS of micro alloyed steel and model by obtained by the EvoNN algorithm.

In this presentation the basic working principles of these algorithms will be explained in a nutshell and their efficacy will be demonstrated based upon some recently conducted real-life engineering applications in my group. The results obtained using these three in house softwares will be shown and analyzed along with the information obtained through the commercial software Kimeme that provides the users with several alternate strategies.

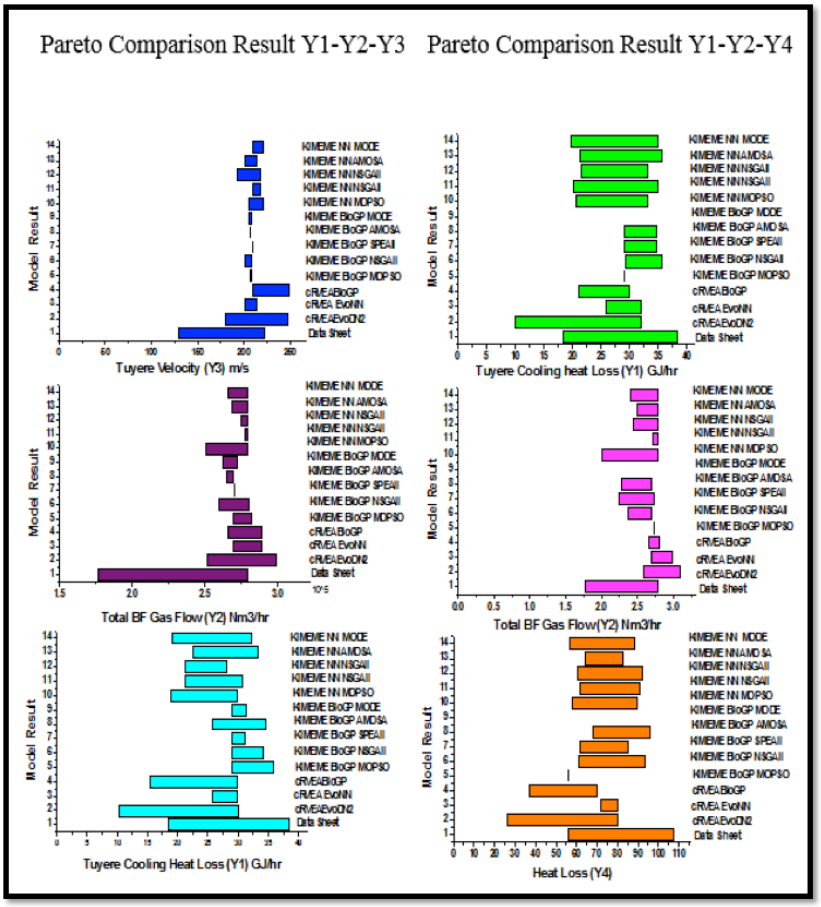


Figure 5: Parameter optimization for a working blast furnace.

2 Machine learning using distance-based methods

Tommi Kärkkäinen
University of Jyväskylä, Finland

Classically machine learning methods and algorithms have been given separately for unsupervised and supervised problems, with or without target variables. However, distance-based methods bridging the two domains appeared readily in 1980s in the form of the linear Radial Basis Function Networks. Supervised distance-based learning was rebirthed in 2013 when the Minimal Learning Machine (MLM) utilizing distance-regression was proposed [1]. In [2], the distance-based kernel from MLM was integrated with the extreme learning machine and the novel machine learning variant was referred as Extreme Minimal Learning Machine (EMLM). In this talk, I introduce both of these distance-based methods and describe some preliminary results from attempts to enforce sparsity in the EMLM models, by using the Douglas-Rachford operator-splitting method [3].

References

[1] de Souza Junior, A. H., Corona, F., Miche, Y., Lendasse, A., Barreto, G. A., & Simula, O. "Minimal learning machine: A new distance-based method for supervised learning". In International Work-Conference on Artificial Neural Networks, pp. 408-416, 2013.
[2] Kärkkäinen, T. "Extreme minimal learning machine: Ridge regression with distance-based basis". Neurocomputing, Volume 342, 21 May 2019, Pages 33-48.
[3] Kärkkäinen, T. and Glowinski, R. "A Douglas-Rachford method for sparse Extreme Learning Machine". Methods and Applications of Analysis, 17 pages, 2019 (to appear).

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 1: Contributed papers on AI in medical applications,

Chair: Tommi Kärkkäinen

Wednesday, 12 June, 11:00 - 11:20, Beeta

3 Counting cells and predicting immunoscore using gradient boosted convolutional neural networks

Timo Ojala[1], Rahkonen Samuli[1], Erkki-Ville Wirta[2], Teijo Kuopio[3], Sami Äyrämö, Ilkka Pölönen[1]
[1]University of Jyväskylä, Finland
[2]Tampere University Hospital, Finland
[3]Central Finland Central Hospital, Finland

In this paper we present a deep learning based model for counting CD3 and CD8 cells from histopathological images, which we then use to predict Immunoscore. The first stage of our model consists of ten instances of a Convolutional Neural Network (CNN) trained using gradient boosting. This model is used to estimate CD3 and CD8 populations, which we can use to form an estimate for the Immunoscore of our patient. The predictions of our model can also be explained using Integrated Gradients.

Keywords: *Colorectal Cancer, Immunoscore, Deep Learning*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 1: Contributed papers on AI in medical applications,

Chair: Tommi Kärkkäinen

Wednesday, 12 June, 11:20 - 11:40, Beeta

4 Kubelka-Munk model and stochastic model comparison in skin physical parameter retrieval using neural networks

Leevi Annala, Ilkka Pölönen
University of Jyväskylä, Finland

In this study we are retrieving physical parameters from a hyperspectral images of skin. Our objective is to use hyperspectral cameras and spectrometers to acquire the value of some physical parameter, such as melanin concentration in the skin. This is done by inversing models for light propagation in the skin. These models take the physical parameters as an input, and produce reflectance, absorbance or transmittance data for each wavelength. In this study we are using Kubelka-Munk model, which is based on differential equations, and stochastic model, that utilizes Markov chains. For inversion we use one dimensional convolutional neural network.

Skin related illnesses such as skin cancer are common, and non-invasive methods for diagnosing them are beneficial. As skin cancer occurance is increasing, their costs for the society is have same trend. Early detection and accurate treatment lowers these costs and improves life expectancy of patients. Hyperspectral imaging is one way for early detection and guidance for the treatment. Skin physical parameter retrieval with hyperspectral camera or spectrometer is a non-invasive method of measuring the pigment concentrations and other parameters in the skin. This method could be applied to for example recognizing healthy skin from unhealthy, provided that we know the parametrization of healthy or unhealthy skin. Interesting parameters include skin pigments,

thicknesses of different skin layers, blood hemoglobin concentration and blood oxygenation.

Hyperspectral camera is a device that captures multiple monochrome pictures in a rapid succession, while controlling the wavelength of the light that gets through to the imaging sensors. Each monochrome picture represents narrow wavelength range, such as 400nm – 405nm. There are usually about 100 of these monochrome images in one hyperspectral image. This hyperspectral image contains the same spatial data as the normal RPG-picture, but far more data in the spectral domain, that is, the interaction of the light and the subject in the image can be seen with more precision.

As said before, Kubelka-Munk model is based on differential equations by Kubelka and Munk. Our implementation of the model takes into account the thicknesses of two layers of the skin, epidermis and dermin, concentration of oxygen in the blood, amounts of hemoglobin, melanosome and blood, and three scattering and absorbtion related variables. When it's inversed, we get useful information on the blood and the skin melanosome concentration. Usually the Kubelka-Munk model is considered useful when transmittance is less than 20% and reflectance is more than 50%. This is the case with skin, when we use visible light and infrared.

Stochastic model on the other hand uses Markov chain. It takes into account the different pigments and absorbtion and scattering coefficients in different layers, as well as water content in the layers. When inversed, it gives information on the different pigments.

We are using one dimensional convolutional neural network to solve the inversion. Convolutional networks are proven to be capable in problems concerning images and other signals, and the data produced by both of the models is one dimensional signal.

Keywords: *convolutional neural network, deep learning, hyperspectral imaging, skin, physical parameter retrieval*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 1: Contributed papers on AI in medical applications,

Chair: Tommi Kärkkäinen

Wednesday, 12 June, 11:40 - 12:00, Beeta

5 A combined approach of neural networks and graphical models in skin cancer inference using spectral imaging

Billy Braithwaite, Ilkka Pölönen
University of Jyväskylä, Finland

Skin cancers, cause by melanoma and non-melanoma type cancers, is an incresing problem world wide. Continuous sun exposure due to travelling, also due to the aging population, melanoma type skin cancers is an increasing problem especially in the Nordic countries. For example, it is estimated that half of all annual skin cancer related costs are caused by melanomas. Therefore the need for tools for early stage skin cancer detection and separate them properly from healthy skin tissue. By doing early detection, it is possible to reduce the amount of re-surgeries, if and when part of a malignant skin tissue has been left after the original surgery. Early detection will also lower treatment costs and also ensure higher survival rates for patients.

Spectral imaging is an imaging modality which acquires an image using hundreds of narrow wavebands of light, which are imagined simultaneously. Each pixel in the spectal image represents an (almost) continuous spectrum of values. Spectral imaging offers a non-invasive way to imagine targets due to its use of only visible and near infra-red illumination to capture images. Furthermore, spectral imaging have been used in separating of tumor borders and distinguishin in-situ melanoma from malignant melanoma.

This work aims at doing early stage skin cancer detection using a combined approach of using neural networks (NN) and graphical models (GM), where spectal imaging has been applied as data acquisition. NNs gained a resurgence

of popularity in the past few years, as data collection and computing powers have increased, as well as improved software packages for constructing and implementing NNs. Today these modern NN implementations are coined as Deep learning. Typical examples of using NNs are learning huge data collections, for example an image database or a time-series of observations, and then doing either supervised or unsupervised learning for doing predictions. GMs on the other hand are a probabilistic network model for doing both learning and inference. The observations are treated as random variables, realizing a given probability distribution, and aims to solve most probable true values for the observed random variables. This assingment problem is known as maximum a posteriori problem, where a given set of random variables the true posterior distribution is solved. The benefit of using GMs, is that you can trace back on the inference task. That is, trace back which random variables encoded in the GM lead to the given inference output.

Our proposed framework is as follows: using acquired image data using spectral imaging, we use NNs to learn the data and extract physical quantities of the skin lesion. After we have determined the physical quantities, we then apply a GM model to do inference on the physical quantities. The aim with this inference task is to get information on which physical quantities could help us detect and classify different melanoma type skin cancers.

Keywords: *neural networks, Artificial intelligence, spectral imaging, graphical models, melanoma*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 1: Contributed papers on AI in medical applications,

Chair: Tommi Kärkkäinen

Wednesday, 12 June, 12:00 - 12:20, Beeta

6 Using wave propagation simulations and convolutional neural networks to retrieve thin coating's thickness from hyperspectral images

Ilkka Pölönen[1], Anna-Leena Erkkilä[1], Jukka Räbinä[1], Timo Sajavaara[2], Esa Alakoski[3], Tero Tuovinen[1]
[1]Faculty of Information Technology, University of Jyväskylä , Finland
[2]Department of Physics, University of Jyväskylä, Finland
[3]JAMK University of Applied Science, Finland

Ill-posed inversion problems are one of the main challenges when there is a need to combine measurements with the theory and numerical model. In this work we demonstrate how we can use wave propagation simulations to train inverse model which is able to retrieve thin sub-wavelength depth profiles of coatings from hyperspectral images. Hyperspectral images are captured in visible and near infrared wavebands [Saari et al., 2013]. Single image contains 120 intensity images, which are partly overlapping in spectral domain. Hyperspectral imaging is widely used in different monitoring applications. It can be used from the remote sensing to the clinical applications [Tuominen et al., 2017, Näsi et al., 2016, Neittaanmäki-Perttu et al., 2015]. Because of used wavelength region and coating thickness the main interfering phenomena in the imaged samples in this study is interference.

Wave propagation is done with discrete exterior calculus [Räbinä et al., 2018], which provides us accurate and reliable numerical model. Recent advance in practice of deep learning offers us tools to create inverse model [LeCun et al., 2015], which are able to map simulated spectra back to thickness variable

in the wave propagation model. Our model is based on convolutional neural networks, which have proven to be very efficient for example in pattern recognition [Krizhevsky et al., 2012].

We have produced, measured and simulated three different kind of coatings. The thin metal oxide films studied are prepared onto a silicon substrate using the deposition techniques PVD and ALD. In this study we are studying steady state in one dimension even thought discrete exterior calculus would allow simulations in the space-time. Our results show that we are able to deliver reliable inverse model, when refraction index of the coating is known.

References

[Krizhevsky et al., 2012] Krizhevsky, A., Sutskever, I., and Hinton, G. E. (2012). Imagenet classification with deep convolutional neural networks. In Advances in neural information processing systems, pages 1097–1105.

[LeCun et al., 2015] LeCun, Y., Bengio, Y., and Hinton, G. (2015). Deep learning. nature, 521(7553):436.

[Näsi et al., 2016] Näsi, R., Honkavaara, E., Tuominen, S., Saari, H., Pölönen, I., Hakala, T., Viljanen, N., Soukkamäki, J., Näkki, I., Ojanen, H., et al. (2016). Uas based tree species identification using the novel fpi based hyperspectral cameras in visible, nir and swir spectral ranges. International archives of the photogrammetry, remote sensing and spatial information sciences; Volume XLI-B1.

[Neittaanmäki-Perttu et al., 2015] Neittaanmäki-Perttu, N., Grönroos, M., Jeskanen, L., Pölönen, I., Ranki, A., Saksela, O., and Snellman, E. (2015). Delineating margins of lentigo maligna using a hyperspectral imaging system. Acta dermato-venereologica, 95(5):549–552.

[Räbinä et al., 2018] Räbinä, J., Kettunen, L., Mönkölä, S., and Rossi, T. (2018). Generalized wave propa- gation problems and discrete exterior calculus. ESAIM: Mathematical Modelling and Numerical Analysis.

[Saari et al., 2013] Saari, H., Pölönen, I., Salo, H., Honkavaara, E., Hakala, T., Holmlund, C., Mäkynen, J., Mannila, R., Antila, T., and Akujärvi, A. (2013). Miniaturized hyperspectral imager calibration and uav flight campaigns. In Sensors, Systems, and Next-Generation Satellites XVII, volume 8889, page 88891O. International Society for Optics and Photonics.

[Tuominen et al., 2017] Tuominen, S., Balazs, A., Honkavaara, E., Pölönen, I., Saari, H., Hakala, T., and Viljanen, N. (2017). Hyperspectral uav-imagery and photogrammetric canopy height model in estimating forest stand variables. Silva Fennica, 51.

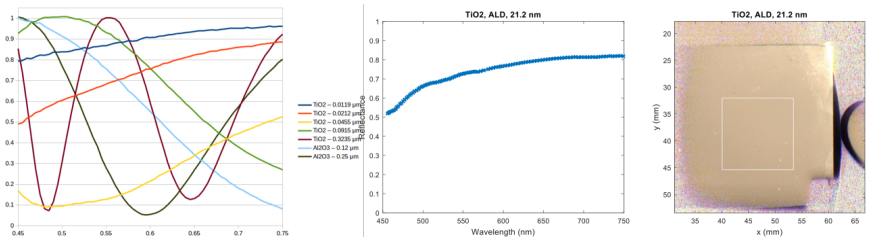


Figure 6: Left: Simulated spectra for different coatings and thickness. Center: Measured spectra for TiO2. Right: False color image of the coating sample composed from hyperspectral image.

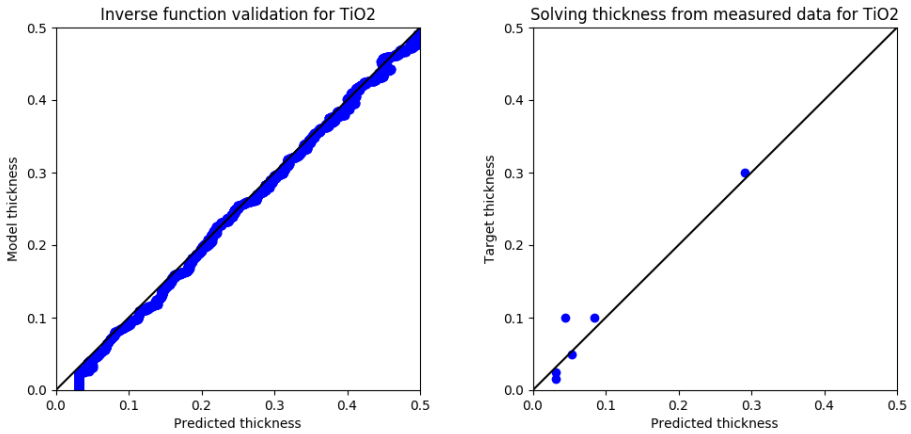


Figure 7: Results for the inverse function. Left: Simulated test set. Right: Average values of measured SiO2 hyperspectral images

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -
June 12-14, 2019, University of Jyväskylä, Finland
Parallel session 1: Contributed papers on AI in medical applications,
Chair: Tommi Kärkkäinen
Wednesday, 12 June, 12:20 - 12:40, Beeta

7 Predicting future overweight and obesity from childhood growth data: A case study

Ilkka Rautiainen[1], Toni Ruohonen[1], Eero Karhu[2], Keijo Lukkarinen[2], Sami Äyrämö[1]
[1]University of Jyväskylä, Finland
[2]Town of Äänekoski, Finland

Overweight, obesity and diseases associated to them have been increasing rapidly during the last few decades. A need has been identified for a model that reliably predicts future overweight/obesity status based on early childhood data. This study is based on a literature review that was conducted to find existing research on the topic. The focus of the review was in predictive modeling methods, i.e. research that validate their results by using independent data not used in training the model.

The case study presented here aimed to employ predictive modeling in a height/weight data collected in the health care system of Äänekoski. The study utilized nine existing study designs (e.g. to predict overweight status at age of five years based on data collected up to one year of age) presented in five research articles found during the literature review.

For each individual in the data, BMI development was tracked by 30 day intervals created using linear interpolation. This time series data was then utilized to form several predictive models using logistic regression, k-nearest neighbors with principal component analysis (PCA), support vector machine with and without PCA, decision tree and multilayer perceptron. In addition to these methods, k-means clustering was used to form body mass index trajectories for the data. The results were then compared to existing studies.

Keywords: *predictive modeling, obesity*

8 Variable selection under a value acquisition budget

Tapio Pahikkala
University of Turku, Finland

We consider the problem of learning sparse models under a budget on the variable value acquisition costs. As a representative example, we have survival prediction of prostate cancer patients based on an array of clinical measurements. A real-world price catalogue of hospital laboratory expenses is be utilized for computing the costs of the measurements. Accordingly, the budget can be interpreted as the maximum aggregate price of the measurements required by the model. One then has to select of such a subset of variables that provides maximal prediction performance meanwhile adhering to the budget. A comparison of embedded and greedy variable selection techniques for linear models on the survival prediction problem is presented. L1-type of regularization is shown shown to work well when the budget is non-existent or loose, while greedy selection is a better choice with tight budgets. These preliminary results pave the way for more sophisticated ideas on improving the budget constrained variable selection.

Keywords: *Budget, Variable selection, Machine learning*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 2: Minisymposium on Machine learning 1, Chair: Napsu Karmitsa

Wednesday, 12 June, 11:40 - 12:00, Alfa

9 Stochastic approximation by successive piecewise linearization

Jonathan Hüser, Uwe Naumann
RWTH Aachen University, Germany

Many machine learning tasks are solved by stochastic approximation of empirical risk minimizers with nonsmooth loss for large data sets (e.g. SVM, ReLU neural networks, l1 regression). Successive piecewise linearization (various papers by Griewank at al.) is an optimization method that obtains non-asymptotic linear convergence rates for certain deterministic nonsmooth convex optimization problems. We explain how to use successive piecewise linearization for large-step stochastic approximation and show how it improves upon the commonly used stochastic subgradient descent method. We analyze convergence in comparison with optimal asymptotic rates and show how convergence rates depend on condition number and noise scale.

Keywords: *convex optimization, piecewise linearization, nonsmooth optimization, stochastic approximation*

10 Non-convex robust low-rank matrix recovery

Xiao Li[1], Zhihui Zhu[2], Anthony Man-Cho So[1], Rene Vidal[2]
[1]CUHK, China
[2]Johns Hopkins University, USA

In this talk we present a non-smooth non-convex formulation of the problem of recovering a low-rank matrix from a number of random linear measurements that are corrupted by outliers taking arbitrary values. Our formulation explicitly enforces the low-rank property of the solution by using a factored representation of the matrix variable and employ an ℓ_1-loss function to robustify the solution against outliers. Under the Gaussian measurement model, we show that even when a constant fraction (which can be up to almost half) of the information-theoretically optimal number of measurements are arbitrarily corrupted, the resulting optimization problem is weakly sharp and weakly convex. Consequently, we show that when initialized close to the set of global minima of the problem, a subgradient method with geometrically diminishing step sizes will converge linearly to the ground-truth matrix.

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 2: Minisymposium on Machine learning 1, Chair: Napsu Karmitsa

Wednesday, 12 June, 12:20 - 12:40, Alfa

11 Neural network learning via successive piecewise linearization

Angel Rojas[1], **Andreas Griewank**[1]
[1]Yachay Tech, Ecuador

Neural networks using the hinge activation function (aka the Rectified Linear Unit) can only have minimizers that are nonsmooth. That means the experimental risk objective fails to be differentiable in some neighborhood of its global minimizers and most of its local ones as well. Yet continuous differentiability is assumed in practically all convergence statements presented in the context of machine learning, mostly for variations of steepest descent. Since the empirical risk is in fact piecewise smooth, we examine local and global optimization strategies that can be successively applied to their piecewise linear approximations. One of them is the application of Mixed Bilinear Programming by Branch and Cut methods. We present comparative numerical results on a variety of test problems.

Keywords: *Alternating Coordinate Search, Abs-Linear Form, Multi Piecewise Linearity, Abs-Normal Form, Averaged Descent*

12 Learning for scientific computing purposes

Bruno Despres
Lab JL Lions, Paris-Sorbonne, France

I will report on numerical experiments about the use of Tensorflow (Google) and Kers (Oneiros) for scientific computing purposes. The problems come from the identification of the order of a numerical scheme (with S.Bineta and O. Pironneau) and the identification of interface parameters (with H. Jourdren). Simple formulas will be proposed to interpret the results.

13 Computational intelligence in design of new nanomaterials

Tadeusz Burczynski
Institute of Fundamental Technological Research Polish Academy of Sciences, Poland

New potentially 2D nano-materials based on carbon and molybdenum are generated by the intelligent memetic strategy combining the evolutionary algorithm and the conjugate-gradient optimization technique and molecular model. The main goal of the optimization is to find stable arrangements of carbon atoms under certain imposed conditions. The fitness function is formulated as the total potential energy of an atomic system. The optimized structure is considered as a discrete atomic model and interactions between atoms are modeled using the AIREBO potential. The parallel approach used in computations allows significant reduction of computation time. Validation of the obtained results of new 2D graphene-like materials obtained using the described algorithm are presented, along with their mechanical properties. Apart from graphene one of the most prominent 2D material is the Single-Layered Molybdenum Disulfide (SLMoS2), which reveals polymorphism at the nano-level. The paper presents optimization technique which allows to obtain SLMoS2 heterostructures with desired mechanical properties. Proposed method combines the memetic global optimization of the potential energy of the nanostructure. The behavior and energy of the atoms is determined by the REAX-FF potential. Examples of such periodic SLMoS2 2H/1T heterostructures are presented with corresponding mechanical properties.

ACKNOWLEDGMENTS
This work was supported by the National ScienceCentre (NCN–Poland) Research Project:UMO-2016/21/B/ST8/02450.

14 Modeling flow, reactive transport and geomechanics in porous media

Mary F. Wheeler
The University of Texas at Austin, USA

In this presentation, we discuss enriched Galerkin (EG) algorithms for modeling Darcy flow, reactive transport, and geomechanics in porous media. This approach involves enriching the continuous Galerkin finite element method with discontinuous elements. For transport EG is coupled with entropy residual stabilization for transport. The method provides locally and globally conservative fluxes, which are crucial for coupled flow and transport problems. In particular, numerical simulations of viscous fingering instabilities in heterogeneous porous media and Hele-Shaw cells are illustrated as well as results for two phase flow. Here dynamic adaptive mesh refinement is applied in order to save computational cost for large-scale three dimensional applications. In addition, entropy residual based stabilization for high order EG transport systems prevents any spurious oscillations. Application of EG to acidizing in carbonate reservoirs and coupling with mechanics using fixed stress is also discussed. Computational results demonstrating the effectiveness of EG for flow, reactive transport and mechanics are provided. This work was done in collaboration with Sanghyun Lee at Florida State and Rencheng Dong at UT-Austin.

Presenter: Mary Fanett Wheeler is a world-renowned expert in computational science. She has been a member of the faculty at The University of Texas at Austin since 1995 and holds the Ernest and Virginia Cockrell Chair

in the departments of Aerospace Engineering and Engineering Mechanics, and Petroleum and Geosystems Engineering. She is also director of the Center for Subsurface Modeling (CSM) at the Institute for Computational Engineering and Sciences (ICES). Before joining the faculty at UT Austin, Dr. Wheeler was the Noah Harding Professor in engineering at Rice University in Houston.

Dr. Wheeler's research group employs computer simulations to model the behavior of fluids in geological formations. Her particular research interests include numerical solution of partial differential systems with application to the modeling of subsurface flows and parallel computation. Applications of her research include multiphase flow and geomechanics in fractured porous media, contaminant transport in groundwater, and sequestration of carbon in geological formations. Dr. Wheeler has published more than 300 technical papers and edited seven books; she is currently an editor of five technical journals.

15 Physics constrained machine learning for industrial applications

Karthik Duraisamy
University of Michigan, USA

With the recent growth in computational power and measurement resolution, there is an unprecedented opportunity to use data from fine-scale simulations, as well as critical experiments, to inform, and in some cases even define predictive models. While the general idea intuitive, the process of obtaining useful predictive models from data in complex problems is less straightforward than merely applying machine learning models on the data. This talk will discuss a coordinated approach of experimental design, statistical inference and machine learning with the goal of improving predictive capabilities, with an emphasis on enforcing the consistency between the model and data outputs and between inference and learning. Examples involving the use of data-augmented models for prediction and robust design will be provided. The final part of the talk will provide a vision towards developing digital twins for industrial applications.

Presenter: Karthik Duraisamy is an Associate Professor of Aerospace Engineering at the University of Michigan (UM), Ann Arbor. He obtained a doctorate in aerospace engineering and master's degree in applied mathematics from the University of Maryland, College Park. At UM, he is the Director of the Center for Data-driven Computational Physics, and the Air force center of excellence in Rocket combustor Dynamics. He is also the chief scientist and co-founder of the Silicon Valley-based startup Geminus.AI, which is focused on developing process centric digital twins for industrial applications.

16 Parameter and type identification in partial differential equations using deep neural networks

Olivier Pironneau
Paris-Sorbonne University, LJLL, France

Using either google's Tensorflow or a C++ toolbox called MiniDNN by Yi Xuan Qiu, we shall present the performance of DNN for the identification of parameters in a fluid-structure problem or in the Heston problem from the observation of part of the solution at final time. We shall show also that we can detect the type of a PDE (parabolic, hyperbolic etc) by observing a portion of the solution. Finally we shall compare with the stochastic evolutionary optimiser CMAES and discuss the results.

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 3: Contributed papers on Computational Solids, structural mechanics and fluid dynamics,

Chair: Tero Tuovinen

Thursday, 13 June, 11:00 - 11:20, Beeta

17 Stability maximization for layered moving web with total mass constraint

Nikolay Banichuk[1], Svetlana Ivanova[1], Evgeny Makeev[1], Pekka Neittaanmäki[2], Tero Tuovinen[2]
[1]Ishlinsky Institute for Problems in Mechanics RAS, Russia
[2]University of Jyväskylä, Faculty of Information Technology, Finland

In this paper we study the application of numerical evolutionary method (genetic algorithm) for the problems of instability velocity maximization and finding the best material properties distribution in axially moving layered webs (panels and plates) is presented. The thermomechanical model has been worked out for description of axially movement and transverse elastic deformations and vibrations of composite materials including instability phenomena and corresponding eigenvalue problem formulation. The aim of our studies has been to investigate an effective layers composition and perform sensitivity analysis of global optimal solutions and their dependence on geometric and physical-mechanical problem parameters. A key point of proposed evolutionary optimization algorithm is that the efficiency of the procedure is dependent on the used averaging techniques and obtained analytical expressions for effective modulas.

Keywords: *critical stability, Evolutionary optimization, Axial movement*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 3: Contributed papers on Computational Solids, structural mechanics and fluid dynamics,

Chair: Tero Tuovinen

Thursday, 13 June, 11:20 - 11:40, Beeta

18 Similarity solutions for condensation on a non-isothermal vertical plate

Jian-Jun Shu
Nanyang Technological University, Singapore

This paper gives similarity transformations for laminar filmwise condensation on a vertical flat plate with variable temperatures and finds analytical solutions for the arbitrary Prandtl numbers and condensation rates. The work contrasts with Sparrow and Gregg's assertion that wall temperature variation does not permit similarity solutions. Based on the similarity solutions, some useful formulas are obtained, including significant correlations for varying Prandtl numbers. Results are compared with the available experimental data.

Keywords: *Similarity solutions, non-isothermal plate, laminar filmwise condensation*

19 Enhanced topology optimization approach using moving morphable components coupled with NURBS curves

Rongzhen Zheng, Cheol Kim
Kyungpook National University, South Korea

An improved structural topology optimization method is developed newly in order to enhance the contour of optimum topology in this study based on the NURBS (non-uniform rational B-spline) curves and the moving morphable components (MMCs) algorithm. The basic MMC optimization is an explicit and geometrical method that uses a set of morphable structural components to create blocks of topology optimization. Optimal structural topologies may be obtained by optimizing the shapes, lengths, thicknesses, orientations and layout of these components. The proposed method adopts a different way of morphable components creation that combines with NURBS curves. The NURBS curve is widely used in the computer-aided-design (CAD) and advantageous on a B-spline curve. All kinds of complicated curved component can be built with NURBS curves or surfaces. NURBS curves are applied for shaping the geometries of structural components and the coordinates of control points system become the design variables. A MATLAB optimization code has been developed and two numerical examples of short cantilever and MBB beams are provided to prove that the geometric way of structural topology optimization coupled with NURBS curves using morphable components can get optimum shape and topology simultaneously. As results of comparison with others, we can obtain the same topologies for the two structures. The proposed approach can improve the smoothness of the structural boundaries which are similar to shape optimization results during the topology optimization process.

Keywords: *FEM-based, NURBS curve, Topology optimization, Enhanced contour, Shape optimization*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 3: Contributed papers on Computational Solids, structural mechanics and fluid dynamics,

Chair: Tero Tuovinen

Thursday, 13 June, 12:00 - 12:20, Beeta

20 Combined model order reduction and artificial neural network for data assimilation and damage detection in structures

Luca Rosafalco, Alberto Corigliano, Andrea Manzoni, Stefano Mariani
Politecnico di Milano, Italy

Structural Health Monitoring (SHM) of building and infrastructures aims to exploit sufficiently large measurement datasets to identify and quantify damage, which is defined as an irreversible reduction of the stiffness and strength characteristics of the structures themselves. This is especially crucial in Western countries, where a large amount of structures is about to reach the end of their life cycle. To assess their health state, damage identification must be performed in a reliable and robust way, and real-time data assimilation looks compulsory. Setting critical thresholds and sending out tweets whenever they look attained or even exceeded, well represent this demand of accuracy and real-time processing. A suitable methodological approach to SHM should be therefore able to detect novelties on the fly and, at the same time, should be already embedded into the monitored structure with an appropriate model of its mechanical response. A combined data- and model-driven approach is proposed here with this end: a physically-based structural model, obtained through any Reduced-Order Model (ROM) strategy, is coupled to an Artificial Neural Network (ANN) for novelty detection. While the ROM, which requires engineering judgement and numerical modelling expertise, is constructed offline, the ANN is trained as soon as a discrepancy between the recorded time series and the expected behavior

exceeds a pre-assigned threshold quantified via purely unsupervised, data-based algebraic tools. In case of drifts or biases away from the structural response foreseen in the training stage, the ANN provides the missing nonlinear contribution, assumed to be associated with damage only, to the ROM response, so as measurements can be consistently tracked. An ANN-based closure model is therefore proposed to fit the acquired data. Through the proposed approach, it is shown that damage events can be recognized, and an on-line ROM update strategy becomes possible. Results are reported for some numerical benchmarks, dealing with the time response of frames with an evolving damage in different critical locations.

Keywords: *Damage Detection, Structural Health Monitoring, Artificial Intelligence, Reduced Order Modelling*

21 Towards the optimization of fuzzy pattern trees by abs - linearization

Andrea Walther, Eyke Hüllermeier
Paderborn University, Germany

The notion of fuzzy pattern trees (FPTs) refers to a model class for classification and regression in machine learning. Formally, an FPT realizes a mapping from an input space X to an output space Y. An FPT can be thought of as a binary tree where each inner node corresponds to the evaluation of a possibly nonsmooth but continuous aggregation function. Learning an FPT is done by searching the space of tree topologies (including the type of aggregation functions in the inner nodes) in a systematic way. As part of this process, the parameters of the aggregation functions in each node need to be fit to the data. For this purpose, we employ the LiPsMin algorithm based on abs-linearization. In this talk, we introduce the problem formally, discuss the optimization strategy of LiPsMin and present preliminary results for the training of an FPT.

Keywords: *Abs-Linearization, Fuzzy Pattern Trees, Successive Piecewise Linearization*

22 Support vector machines in clusterwise linear regression

Kaisa Joki
University of Turku, Finland

In clusterwise linear regression (CLR), the aim is to simultaneously partition a data into a given number of clusters and find regression coefficients for each cluster. We will propose a novel approach to solve the CLR problem. The main idea is to utilize the support vector machines (SVM) approach to model the CLR problem by using the SVM for regression to approximate each cluster. This new formulation of the CLR problem is represented as an unconstrained nonsmooth optimization problem, where we minimize a difference of two convex (DC) functions. To solve this problem, a method based on the combination of the incremental algorithm and the double bundle method for DC optimization is introduced. Numerical results will be presented to validate the reliability of the new formulation for CLR and the efficiency of the proposed method. The results show that the SVM approach is beneficial in solving CLR problems, especially, when there are outliers in data.

Keywords: *Nonsmooth optimization, Data mining, Clusterwise regression*

23 A Second-order method with enriched hessian information for composite sparse optimization problems

Pedro Merino
Escuela Politecnica Nacional, Ecuador

In this talk we present a second order method for solving composite sparse optimization problems, which consist in minimizing the sum of a differentiable, possibly nonconvex function and a nondifferentiable convex term. The composite nondifferentiable convex penalization is given by 1–norm of a matrix times the coefficient vector. Our proposed method generalizes the previous second order algorithms designed for sparse problems in the optimizing variable. Here, we extend its three main ingredients to the case of the generalized composite optimization: orthant directions, projection step and, in particular, the full second–order information associated to the nondifferentiable terms.

Keywords: *Nonsmooth optimization, sparsity, second order*

24 Missing value imputation via nonsmooth optimization and clusterwise linear regression

Napsu Karmitsa
University of Turku, Finland

A new method of preprocessing incomplete data is introduced. The method is based on clusterwise linear regression and it combines two well-known approaches for missing value imputation: linear regression and clustering. The idea is to approximate missing values using only those data points that are somewhat similar to the incomplete data point. A similar idea is used also in clustering based imputation methods. Nevertheless, here the linear regression approach is used within each cluster to accurately predict the missing values, and this is done simultaneously to clustering. The underlying clusterwise linear regression problem is modelled as a nonsmooth optimization problem and solved using nonsmooth optimization techniques combined with an incremental approach. The proposed method is tested using some synthetic and real-world data sets and compared with other algorithms for missing value imputations. Numerical results demonstrate that the proposed method produces the most accurate imputations in data sets with a clear structure and the percentages of missing data no more than 25%.

Keywords: *nonsmooth optimization, imputation, incomplete data, clusterwise linear regression*

25 Parsimonious neural networks

Mohamed Masmoudi
Universite Paul Sabatier, France

ADAGOS has developed a new parsimonious approach that reduces the resources (including energy) required for implementing artificial intelligence algorithms by orders of magnitude. The state of the art of artificial intelligence is largely inspired by the biological brain, including its redundant nature. While this redundancy may ensure the continued functionality of the living brain despite regular, and sometimes accidental, loss of the neural cells, the same argument does not hold for artificial neural networks, which are made from inert matter. Occam's razor, also known as the principle of parsimony, proposes that from a set of competing hypotheses, the simplest solution is the most credible, or as Einstein phrased it: "Everything should be made as simple as possible, but no simpler." However, making things simple is not always itself a simple task and so the use of redundant neural networks persists in the state of the art. In accordance with Occam's razor, ADAGOS configures small, parsimonious neural networks in a fully automatic manner. Meanwhile, the state of the art is still limited by a tedious, manual trial and error process; this manual approach is itself a source of redundancy and cannot produce neural networks of a small size. In particular, our neural networks allow creation of highly reliable complex dynamical models, including for quasi-chaotic phenomena; a case in which even the slightest flaw of parsimony would have irremediable consequences on the quality of the model. We will present many results using data generated by static and dynamic scientific computing models.

26 Nobody can stop advancing artificial intelligence (AI) where developing

Yoshiyasu Takefuji
Keio University, Japan

AI applications are beyond our control. The hyper skills can be obtained by AI itself with or without human experts. A variety of AI-based applications are addressed. In order to build AI-based systems, skills of modularity and abstraction will play a key role in software engineering. What should we teach for children in the AI society?

27 Computational sciences, physics field theories and geometry

Lauri Kettunen, **Sanna Mönkölä, Tuomo Rossi**
University of Jyväskylä, Finland

Physics field theories and numerical solutions of boundary value problems is a significant part of computational sciences and essential in developing modern technology. As physics field theories are compartmentalized into strong branches –such as into elasticity, electromagnetism, thermodynamics, acoustics, and so on– this easily creates an impression the division of field theories into subclasses is dictated by the nature itself.

Ultimately, physics is, however, a model. It exploits abstract mathematical structures to explain and to predict the behavior of reality, and as condensed into an old saying, "the finger pointing to the moon is not the moon". Consequently, in building software systems for physics boundary value problems it justified to seek for a view that supported best the needs of modern technology and software development.

The physics field theories share common geometrical principles in terms of how observations are made in space-time and how they are formalized into algebra. This creates foundations for multi-physical software systems designed to tackle not only certain problems, but instead a large class of boundary value.

The key geometric principles are i) the Stokes theorem attaching differentiation and the boundary operator to each other, ii) the inner product needed to specify lengths, areas, volumes, and angles, and iii) a decomposition of volumes into products of "area" and "height". Formally, such a decomposition is about the so-called Hodge operator. The remaining key ingredient is the iv) action principle. The partial differential equations behind physics field theories involve the idea that small changes in their solutions do not change the underlying action up to the first order, and in this sense the differential equations are of

about conservation laws. The action itself is typically about energy, probability or some other significant notion of physics.

The presentation will introduce such a geometric view on physics field theories and explain how it is efficiently exploited in modern computational sciences.

Keywords: *Riemannian geometry, Field theories, Minkowski space, differential geometry*

28 Mini-symposium on ethics in AI

Pekka Abrahamsson
University of Jyväskylä, Finland

Artificial Intelligence (AI) systems are becoming increasingly ubiquitous, which has resulted in various ethical concerns being raised about different types of AI systems. Aside from the most visible ones such as autonomous vehicles, more invisible systems such as AI-based surveillance systems and systems dealing with personal data such as job application filter AIs have already resulted in real ethical issues out on the field. Concerns have been raised especially over safety (e.g. autonomous vehicles and robots), as well as data handling and bias (e.g. job application filtering systems). Larger issues on a societal scale have been discussed in relation to AI systems potentially resulting in large-scale changes in the work force distribution with AI systems replacing workers across industries at an accelerating rate.

These concerns are well-founded as AI systems differ from traditional information systems in that one largely cannot opt out of using them. Even those individuals that do not want to own an autonomous vehicle likely nonetheless have to drive alongside them on public highways in the future. Similarly, one cannot opt out of being surveilled using AI-based systems. Thus, ethical development of AI systems is important from a societal point of view as these systems have the potential to affect everyone regardless of their consent.

To address the ethical issues by means of scientific research, the CSAI Mini Symposium of Ethics in AI calls for papers to address ethical issues in AI systems. As ethics in AI is a multi-disciplinary area of research, we are interested in contributions across disciplines. More specifically, we welcome contributions of a wide range of topics including, but not limited to:

- Transparency in Systems and Systems Development
- Ethically Aligned System development
- Tools and theories for Ethically Aligned Design
- State of industry practice in Ethically Aligned Design
- Novel perspectives to Ethics & AI from UX, human-aspects and HCI fields of study
- Bias in AI systems
- Data Handling in AI systems
- Societal Effects of AI systems
- Regulations and Legal Issues in AI Systems
- Emerging Ideas

In this mini symposium, we are interested in new research ideas, lessons learned, experience reports, and emerging results. Work-in-progress type papers are welcome to spark discussion in the symposium.

29 Essentializing software engineering practices for ethically designing and developing artificial intelligence systems

Kai-Kristian Kemell
University of Jyväskylä, Finland

Ethics in Artificial Intelligence (AI) has recently become a more prominent area of research. Following technological advances in the field of AI, AI-based systems are becoming increasingly ubiquitous at an accelerating rate. Whereas some twenty years ago robots were largely confined to factories, handling repetitive conveyor belt tasks, AI-based Cyber-Physical Systems (CPS), including robots, are now entering the public sphere across industries. Autonomous vehicles have garnered mainstream media attention, and already operational AI-based surveillance systems have received negative public backlash over privacy concerns. Aside from CPSs, purely digital AI systems are also being used for various tasks ranging from automatic website content moderation to job application filtering.

These systems differ from conventional software systems in that one cannot fully opt out of using them. More importantly, one rarely uses AI systems as an active user. More often, it could be said that one is targeted by them, for e.g. data collection reasons, as these systems are independent actors (except to the organization in charge of the systems). From this follows that these systems should be designed ethically, as their potential impact is enormous on a societal level. The importance of ethically designing AI systems has been highlighted in practice by e.g. IEEE Global Initiative on Ethics of Autonomous and Intelligent Systems that seeks to raise awareness of the importance of ethics

as well as provide tools for doing so, as well as constructs for the discourse of AI ethics.

However, while the importance of ethics in AI systems has been highlighted in extant literature, few tools and methods for applying it in practice have been proposed. More general-purpose ethical tools such as the RESOLVEDD strategy from the field business ethics exist, but tools and methods specifically aimed at the field of IT, and more specifically AI design and development, are lacking. In order to help tackle this issue and to raise awareness of it, we discuss the act of essentializing software engineering practices as one potential approach for developing methods and practices that address ethical issues in AI development and design. We discuss the Essence Theory of Software Engineering, the background theory for doing so, and offer practical examples on how to carry out the process of essentializing software engineering practices.

Keywords: *essence, practice, artificial intelligence, method engineering, ethics*

30 Ethics is important, but how can we implement it? Survey on software developers' views on AI ethics

Ville Vakkuri
University of Jyväskylä, Faculty of Information Technology, Finland

The growing influence of Artificial Intelligence (AI) and autonomous systems (AS) to our lives force us to consider ethics and the values embedded into these systems. For example, looking biased algorithms in social media, decision making systems of autonomous cars, or even societal effects of new wave smart factories powered by AI it is clear that system development is not anymore only about technology or engineering question, it is also an ethical question. Concerning ethics as a part of system design has also gained attention from governmental, global and standardization level. However, on practical level the question of considering ethics as a part of system design is still widely open. How ethics should be implemented in practice into these systems? To answer this question, software developers hold a key role. Their development methods, tools, and personal commitments determine how ethical considerations are implemented in design and development of these systems.

In this study, we report the findings of two different surveys conducted on software developers which have experience working with AI solutions. On these survey developers' attitudes towards involving ethical considerations and practical means for implementing ethics in design were examined. Questions on surveys were related on individuals' both personal opinions and on experiences from working context. In both surveys implementing of ethics was seen mostly positive and important. There was no clear stand, how the implementing of

ethical consideration should be covered. A key finding from the study indicates that developers see ethical considerations important, but they are lacking means to implement ethics on practical level on design and development of AI systems. Findings of this study support the view that useful and tangible tools for implementing ethical considerations in design does not exist in practice for the software developers and designers. For future development of implementation ethics to AI new kind of tools are need, tools that are capable to transform developers' ethical considerations to the design.

Keywords: *software developer, Ethics, Practical implementation of ethics, Artificial Intelligence, AI ethics*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 5: STS - Special technology session, Chair: Olli Ventä

Friday, 14 June, 11:00 - 11:20, Alfa

31 Industrial IoT capabilities in reducing the LCOE of offshore wind energy: A review

Sean Loughney, Ariel Edesess
Liverpool John Moores University, United Kingdom

Wind power is recognised as one of the most promising sources of renewable energy. Increased generating capacity and recent technology advancements have led to a decrease in the Levelized Cost of Electricity (LCOE) in recent years for both onshore and offshore wind power generation. Although onshore wind still has greater capacity, offshore wind energy is forecast to be one of the most effective renewable energy sources due to the steady high winds found further out at sea and the potential for much larger wind turbines than are possible onshore.

Despite the potential for offshore wind power and recent reductions in the LCOE, several major challenges continue to imperil rapid deployment, including the expense and unpredictability of Operations & Maintenance (O&M) strategies and the grid power quality of the energy produced. At present, O&M for offshore wind farms is estimated to comprise 25-50% of the LCOE (Dalgic, 2015), 7% of which is estimated to be due to the need for unplanned maintenance (BVG Associates, 2012).

O&M challenges, especially for unscheduled maintenance, are expanded further for wind turbines in the extreme environments found at locations of more vast wind resources, namely further from the coast and in deeper water. In locations unsuitable for fixed wind turbines, floating wind platforms are being developed to harness the stronger, steadier wind found further at sea. The increased distance from shore and more extreme ocean conditions found in deeper water exacerbate challenges in accessing the wind turbines, and it is therefore more

vital than ever to develop non-intrusive systems for monitoring the integrity of the wind turbine structures and its individual systems and components.

Advances in computational capabilities and the increasing connection of sensor networks through the Internet of Things (IoT) have allowed for an expansion in the use Wireless Sensor Networks (WSNs), capable of monitoring the condition of individual components of a wind turbine, such as temperature and vibrations. Condition-based asset monitoring using WSNs can reduce turbine downtime through early detection and location of failures, thereby reducing the need for unplanned access for maintenance, which could greatly reduce O&M costs and the risk to workers.

Furthermore, WSNs can monitor and regulate the typically irregular current and voltage, which can lead to poor power-quality for grid-connected turbines. WSNs function by sensing properties within the environment, processing the data collected and communicating about the data within the network. WSNs are a subset of IoT, which encompasses a much broader description of objects communicating through an internet-like network. This paper aims to highlight the key areas where industry-led WSNs and IoT can be employed for condition monitoring of offshore wind turbines and regulating the grid power quality to further reduce the LCOE and increase turbine reliability.

Keywords: *Offshore wind energy, Sensor networks, O&M, IoT, condition monitoring*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 5: STS - Special technology session, Chair: Olli Ventä

Friday, 14 June, 11:20 - 11:40, Alfa

32 High-Performance data analysis with the Helmholtz Analytics Toolkit (HeAT)

Martin Siggel, Charlotte Debus, Philipp Knechtges, Alexander Rüttgers
German Aerospace Center (DLR), Germany

This work introduces the Helmholtz Analytics Toolkit (HeAT), an open source scientific big data analytics library for High-Performance Computing (HPC) and High-Performance Data Analytics (HPDA) systems. The large progress in big data analytics in general and machine learning/deep learning (ML/DL) in particular, has been considerably enforced by well-designed open source libraries like Hadoop, Spark, Storm, Disco, scikit-learn, H2O.ai, Mahout, TensorFlow, PaddlePaddle, PyTorch, Caffe, Keras, MXNet, CNTK, BigDL, Theano, Neon, Chainer, DyNet, Dask and Intel DAAL to mention only a few of them. Despite the large number of existing data analytics frameworks, a library taking the specific needs in scientific big data analytics under consideration is still missing. For instance, no pre-existing library operates on heterogeneous hardware like GPU/CPU systems while allowing transparent computation on distributed systems. Typical big data analytics frameworks like Spark are designed for distributed memory systems and consequently do not fully explore the shared memory architecture as well as the network technology of HPC systems. ML/DL frameworks like Theano or Chainer focus on single node computations or when providing mechanisms for distributed computation, as done by TensorFlow or PyTorch, they impose the details of the distributed computation to the programmer. Libraries designed for HPC like Dask and Intel DAAL do not provide any GPU support.

The presented library – HeAT – is designed for the specific needs of big data analytics in the scientific context. It is based on a distributed tensor data object on which operations can be performed like basic scalar functions, linear algebra algorithms, slicing or broadcasting operations necessary for most data analytics algorithms. The tensor data objects reside either on the CPU or on the GPU and, if needed, are distributed over various nodes. Operations on tensor objects are transparent to the user, i.e. they remain the same irrespective of whether the tensor object resides on a single node or if it is distributed over several nodes allowing to conveniently port algorithms from single nodes to multiple nodes or from CPUs to GPUs. HeAT's tensor module offers a Python-based API almost identical to NumPy, which allow a fast transition from vectorized NumPy code to a parallel and distributed HeAT code. HeAT builds on top of PyTorch, which already provides many required features like automatic differentiation, CPU and GPU support, linear algebra operations, and basic MPI functionality as well as an imperative programming paradigm allowing for fast prototyping essentially in scientific research. In addition to basic tensor operations, HeAT implements several common data analytics algorithms, e.g. k-means, logistic regression and neural networks, optimized for large scale distributed systems.

We demonstrate the runtime performance of HeAT by clustering image data of a rocket engine combustion captured by high-speed cameras. Compared to the performance of the k-means clustering algorithm on MATLAB or the serial HeAT implementation, the distributed computation with 16 MPI ranks leads to a runtime acceleration of about a factor of 20. Since the serial k-means clustering also has a very high memory requirement for these large data sets, the distributed computation even enables the computation of even larger data sets, which would not be possible with single node shared-memory only computation.

Keywords: *GPU, HeAT, MPI, Distributed, Python*

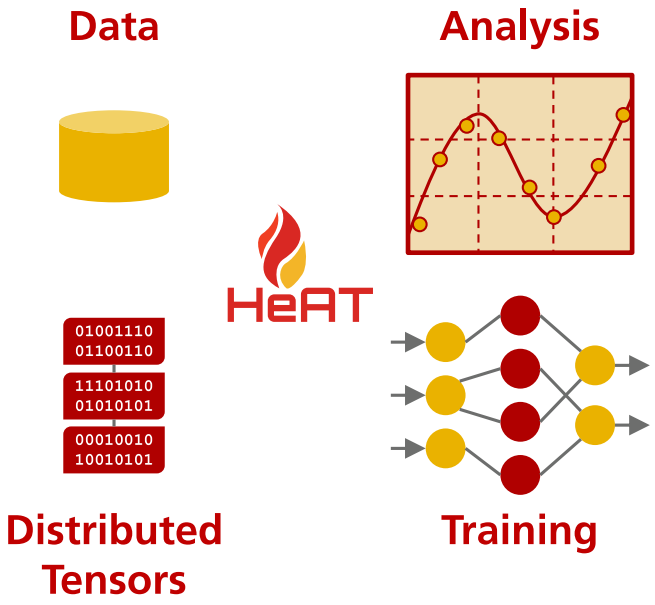


Figure 8: Distributed data analysis with HeAT.

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 5: STS - Special technology session, Chair: Olli Ventä

Friday, 14 June, 11:40 - 12:00, Alfa

33 Dynamic data-driven application systems based on tensor factorization: learning the physics of model evolution

Valentina Zambrano, Rafael Rodriguez-Barrachina, Javier Orus, Salvador Izquierdo
Instituto Tecnologico de Aragon, Spain

Dynamic Data-Driven Application Systems (DDDAS) is a paradigm that allows the evolution, and hence the improvement in time, of dynamic models for model-based control strategies and for digital twins. DDDAS aim to correct and update mathematical models in real-time, by constantly processing data obtained from the real system or related simulations.

In this paper we propose a DDDAS approach based on tensor factorization applied to electric vehicles' active suspension systems. A suspension system's behaviour can vary in time due to material degradation, deformations, etc.; all these variations can considerably affect the suspension system's performance in time and therefore it is of extreme importance to update the parameters of the mathematical model taking these changes into account. The DDDAS strategy we introduce in this paper aims to handle and include time dependant corrections into the suspension system's model; for this purpose we make use of tensor factorization, which is an excellent tool for learning the underlying physics of collected data, becoming an extremely relevant requisite when attempting to foresee the origin of faults in industrial systems.

In order to compute a mathematical model of a suspension system, data coming from it are fed to an algorithm for Reduced Order Model (ROM). ROM strategies are based on numerical methods for multivariable problems simplification through mathematical approximation techniques. ROMs computation can

be handful in such situations where a reduction in terms of system's variables should be taken into consideration, e.g. big data, uncertainties in the physics behind the system, system's equations' solution not trivial and/or computationally cumbersome.

In this article we compute ROMs using TWINKLE, an in-house built software. TWINKLE is a high performance library written in C++ for carrying out Canonical Polyadic Decomposition (CPD) on tensors. It allows processing and recovering highly sparse and unstructured data, which is not usually foreseen in CPD, e.g. Singular Value Decomposition (SVD), Principal Components Analysis (PCA), PARAllel FACtor analysis (PARAFAC) or CANonical DECOMPosition (CANDECOMP). The library uses Armadillo, an open source library for linear algebra and scientific computing, which is based on LAPACK (Linear Algebra PACKage) and BLAS (Basic Linear Algebra Subprograms) routines in turn.

In this paper we select the DDDAS paradigm to apply TWINKLE on incremental data coming from electric vehicles' active suspension systems, in order to analyse the efficiency and accuracy of the algorithm, as well as to explore a new strategy to prove the possibility of updating systems' mathematical models using tensor factorization.

Keywords: *system-modelling, data-analysis, DDDAS, tensor-factorization, model-order-reduction*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 5: STS - Special technology session, Chair: Olli Ventä

Friday, 14 June, 12:00 - 12:20, Alfa

34 Predicting customer experience

Marjaana Nokka
Telia Finland, Finland

Net Promoter Score (NPS) is used to measure customer experience and loyalty of the company's customer relationships. It is based on responses to a single question: *"How likely it is that you would recommend our company / product / service to a friend or colleague?"*, using a 0 – 10 scale. Respondents are grouped as Promoters (score 9 – 10), Neutrals (score 7 – 8), and Detractors (score 0 – 6). Net Promoter Score is calculated by subtracting the percentage of Detractors from the percentage of Promoters.

However, Net Promoter Score has some major weaknesses. For example, the number or respondents has been declining every year, which gives both inaccurate and biased results. In addition, it is a discrete method, so we only get results after asking the question.

To overcome these difficulties, we have developed a method to predict what the customer would answer if we asked the question, without actually asking the question. We don't have to bother our customer with questions, we have answers from all the customers (not only the customers who like to answer), and a continuous score. With our customer data, we can get the full view on our customer satisfaction. Furthermore, we can analyze the most crucial things to improve for different types of customers.

Keywords: *prediction, analytics, nps, customer relationship*

35 Puhti-AI: Finland's new AI supercomputer

Mats Sjöberg, Markus Koskela
CSC - IT Center for Science Ltd, Finland

CSC is a Finnish center of expertise in ICT that provides services for research, education, culture, public administration and enterprises. In this talk, we will introduce CSC's upcoming computing and data environment, currently in pilot test phase and scheduled for general availability in July. The environment includes an AI partition containing a total of 80 GPU nodes with a total peak performance of 2.7 Petaflops. In particular, the partition is engineered to allow GPU intensive workloads to scale well to multiple nodes. We will also illustrate large-scale distributed training of deep neural networks using the new environment.

Keywords: *distributed deep learning, supercomputer, high-performance computing, gpu computing*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 5: STS - Special technology session, Chair: Olli Ventä

Friday, 14 June, 12:40 - 13:00, Alfa

36 Using Artificial Intelligence to Classify Textual Applications for Reporting Purposes

Timo Lehtonen, Mikael Ahonen
Solita, Finland

Real-world implementations of artificial intelligence solutions in business context are advancing rapidly. In this case project, artifical intelligence was applied to the context of information systems of Business Finland which is the Finnish government organization for innovation funding and accelerator of global growth. The goal was to automate routine work performed by the officer users who manually classify incoming textual applications to predefined categories.

Classifications are assigned to define the topics which the application is related to, for instance, bioenergy or digitalization. The classification information is then used for reporting purposes. One of the reporting needs is to provide the ministry of economic affairs and employment a calculation of total amount of funding related to resource-efficient and carbon-neutral solutions. The classifications can be utilized to collect such information. It is noteworthy that the classification results are not criteria for Business Finland for approving applications.

To solve the classification problem of textual applications, we applied a natural language processing tool, namely FastText implemented by Facebook. FastText is an efficient, open-source and lightweight text analysis tool that is suitable for any language. The tool is based on a neural network approach that utilizes word vectors. The machine learning models created by the tool enable classification of any textual data. The model can be used to assign textual documents to one or multiple categories.

We applied the supervised learning method of the FastText tool to the combination of textual data in Finnish language and classifications assigned by officer users during last 20 years. We built a single machine learning model per classification category. The data set was splitted into training and test data set with proportions of 80% of training data and 20% of test data. A single model predicts several classifications for a single category based on textual data of an application. For instance, one of the models predicts classifications related to category of environment. These classifications define if the application is related to environmental classification such as bioenergy or wind energy, for instance. If the application is not related to any classification, value "None" is used. This category is the most common classification in the data set. For instance, in the category of environment classifications, 75% of applications have classification "None". A simple and naive model with precision of 75% would predict that the classification is always "None". We used this as a baseline.

The accuracy of the constructed machine learning model is better than the baseline. For instance, for one of the categories, the precision of the model was 80% while the precision of the baseline was 75%. Moreover, we are able to improve the accuracy of the model by taking use of FastTexts probability approximation functionality. With it, the model gives a P-value of the certainty of the predicted classification. For instance, the P-value of certainty could be 97% or 42% for a single classification. Now, we are able to set a limit to the P-value to filter out uncertain predictions. For instance, we can set P-value limit to 70% and filter out predictions with lower P-value. With this method, we are able to increase the accuracy to even 86% by using such a P-value limit that 70% of the classifications are still predicted.

The models have been deployed to production use. The software collects telemetry data regarding the usage of the automatic classifications in the production environment. Both the value set by the machine and the value possibly changed by the user are stored. In the future, we are able to analyze how the automatic classifications set by artificial intelligence are actually used in a business context.

Keywords: *usage data, artificial intelligence, text analysis*

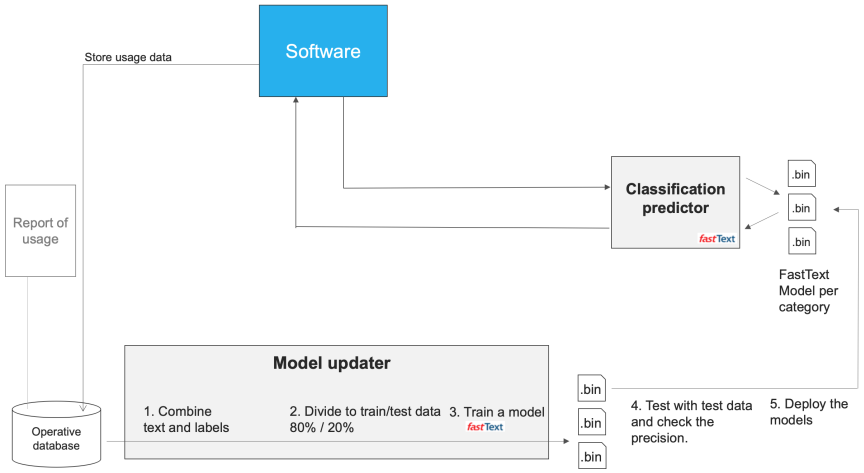


Figure 9: Flow of combining data to train/test set, training and testing the model, deploying the model, and finally, collecting usage data.

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 6: Contributed papers on machine learning and optimization,

Chair: Johannes Kraus

Friday, 14 June, 11:00 - 11:20, Beeta

37 Application of machine learning methods to error control of approximate solutions

Sergey Repin[1], **Pekka Neittaamäki**[1], **Aleksei Muzalevski**[2]
[1]University of Jyväskylä, Finland
[2]St. Petersburg Polytechnic University, Institute of Appled Mathematics and Mechanics, Russia

Modern computer simulation methods based on mathematical models described by partial differential equations typically use the conception of adaptivity in which a new discretisation (mesh) is generated by means of a posteriori error analysis of a numerical solution computed on the previous (coarser) mesh. A posteriori error indicators play the crucial role in it. In contrast to known approaches, in this paper we suggest a new modus operandi for the generation of error indicators by using deep learning methods. They generate neural nets and special representations which solve the error control problem very efficiently. Several series of numerical tests compare them with known error indicators and confirm the applicability and perceptiveness of the approach.

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 6: Contributed papers on machine learning and optimization,

Chair: Johannes Kraus

Friday, 14 June, 11:20 - 11:40, Beeta

38 Iterative data selection strategy in offline data-driven evolutionary multiobjective optimization

Atanu Mazumdar[1], Tinkle Chugh[2], Manuel Lopez-Ibanez[3], and Kaisa Miettinen[1]
[1]University of Jyväskylä, Finland
[2]University of Exeter, United Kingdom
[3]University of Manchester, United Kingdom

Surrogate-assisted optimization techniques are devoted towards solving computationally expensive optimization problems (e.g., simulations, lab experiments etc) in a comparably efficient way. In such techniques, inexpensive surrogate models are built to emulate the actual objective functions and these surrogates are used as objective functions instead of the original ones, which speeds up the optimization process.

In data-driven optimization, we make decisions based on data. If we have an offline data-driven optimization problem, further evaluation of the objective functions using a simulator or further experimentation is not possible, and we have to rely on pre-collected or sampled data. Thus, the quality of the solutions obtained is entirely dependent upon the accuracy of the surrogate model built. For solving a multiobjective optimization problem (with several conflicting objectives), an evolutionary multiobjective optimization algorithm can be used to find a set of Pareto optimal solutions (also called Pareto optimal set in decision space and Pareto front in objective space) that represent the tradeoffs between the objectives.

Kriging or Gaussian process regression is a popular choice as a surrogate model for solving data-driven optimization problems due to its ability to provide the uncertainty information of approximated values. However, the computational cost for building the Kriging surrogates is $O(n^3)$ and thus increases with the number of samples n. Data available from real-world problems might have a large sample size and thus building a global surrogate model such as Kriging becomes computationally challenging. Thus, reducing the computational complexity of Kriging models e.g. by reducing the size of the dataset and selecting representative data for building surrogates is a desirable way.

Existing approaches, such as active set selection, focus on selecting samples from the available dataset and simultaneously achieve accuracy comparable to a global model that uses all the available data. However, these approaches do not try to preserve the accuracy of the surrogates near the Pareto optimal solutions. Here, we propose an approach to tackle this problem by building surrogates only using those samples that enable us to achieve better accuracy near the Pareto front. Our approach consumes a fraction of the computation cost required for building a global surrogate model that uses all the data provided. Tests conducted using the standard benchmark problems demonstrate that the proposed approach builds surrogates faster for larger datasets without compromising the quality of solutions compared to optimizing a global model. It also provides solutions with higher accuracy than the existing active set selection approaches.

Keywords: *Computational Complexity, Active set selection, Evolutionary Computation, Metamodeling, Gaussian processes*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 6: Contributed papers on machine learning and optimization,

Chair: Johannes Kraus

Friday, 14 June, 11:40 - 12:00, Beeta

39 On surrogate management in interactive multiobjective building energy system design

Pouya Aghaei Pour[1], Tobias Rodemann[2], Markus Olhofer[2], Jussi Hakanen[1], and Kaisa Miettinen[1]
[1]University of Jyväskylä, Finland
[2]Honda Research Institute Europe, Germany

When thinking of possible extensions of energy systems for larger buildings, decision making consists of a series of complex investment decisions.

The consideration involves multiple objectives like investment and annual operation costs, CO_2 emissions and module lifetime to be considered simultaneously. Thus, in building energy system management, methods of multiobjective optimization are needed to support decision making.

We study a system upgrade problem with five objective functions: initial investment cost, running cost, CO_2 emissions, resilience to power outages and battery lifetime. We consider hardware additions and modifications of system controllers and use a building simulation software to simulate energy flows to analyze different investment options.

We use evolutionary algorithms for optimization because of their versatility. Unfortunately, they are very time-consuming in simulation-based problems since they deal with populations of solution candidates and simulations may take days or even weeks. In our case study of a building energy system design, we can vary the simulation period leading to a trade-off between the simulation time (seconds to minutes) and how realistic the solution is. For instance, if we set the simulation time for one week, the simulator cannot predict a good outcome

for the next year since there are many changes that do not happen in this short period of time, such as different weather, changes in the number of tenants etc. In order to solve optimization problems to get acceptable solutions, longer simulation periods have to be used but this results with long evaluation times for the objective functions. Therefore, using surrogate models help to expand the simulation period, so we can get solutions as close to reality as possible.

More specifically, we apply Kriging (or Gaussian processes) as surrogate models because they can provide uncertainty information about the surrogates. As an evolutionary algorithm, we apply the reference vector guided evolutionary algorithm (RVEA) and, as said, incorporate surrogate models in it.

Instead of settling for surrogate-assisted RVEA that tries to widely represent all solutions with different trade-offs among the objectives, we introduce an interactive method. Such a method has not been used before to solve this particular problem. Among the advantages of interactive methods are that the decision maker can learn about the trade-offs involved conveniently and can concentrate on those solutions that are interesting. The challenge here is that the decision maker usually has a limited time to spend on the solution process but updating the surrogate model may take a lot of time.

In this research, we focus on an adaptive method to update the Kriging model based on the decision maker's preferences. For example, we can spend more time on training the surrogate before the DM is involved or change when to update the model according to the DM's preferences.Moreover, we test Kriging models with different kernels for this problem and compare their performances with each other.

Keywords: *Interactive methods, Kriging, Multiobjective optimization, Smart buildings*

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 6: Contributed papers on machine learning and optimization,

Chair: Johannes Kraus

Friday, 14 June, 12:00 - 12:20, Beeta

40 A modified deep neural network for the rapid inversion of geophysical resistivity measurements

Mostafa Shahriari[1], David Pardo[2], Artzai Picon[3], Javier Del Ser[4], Sebastian Ossandon[5], Carlos Torres-Verdin[6]

[1]Euskampus Fundazioa, Bilbao, Spain. Basque Center for Applied Mathematics (BCAM), Bilbao, Spain.

[2]University of the Basque Country (UPV/EHU), Leioa, Spain. Basque Center for Applied Mathematics, (BCAM), Bilbao, Spain. Ikerbasque (Basque Foundation for Sciences), Bilbao, Spain.

[3]Tecnalia, Bilbao, Spain. University of the Basque Country (UPV/EHU), Leioa, Spain.

[4]Tecnalia, Bilbao, Spain. Basque Center for Applied Mathematics, (BCAM), Bilbao, Spain. University of the Basque Country (UPV/EHU), Leioa, Spain.

[5]Pontificia Universidad Catolica de Valparaiso, Valparaiso, Chile.

[6]The University of Texas at Austin, USA.

The oil industry is using different geophysical measurement methods to explore oil reservoirs and to increase their productivity. In this work, we focus on resistivity measurement which we categorize as: (a) on surface, including those obtained using controlled-source-electromagnetics (CSEM); (b) in the borehole, including those obtained using logging-while-drilling (LWD) devices. LWD instruments record measurements while drilling and transmit them to the surface for real-time interpretation. We use this real-time data to perform geosteering, which is the act of changing the direction of the instrument to reach a specific

geological target. The use of geosteering considerably increases the productivity of a reservoir.

Mathematically, we divide the problem of interpreting resistivity measurements into two: (a) the forward problem, denoted by function $\mathcal{F}$, which is governed by Maxwell's equations and for given subsurface properties $\mathbf{P}$, it produces the measurements $\mathbf{M}$ (i.e., $\mathcal{F}(\mathbf{P}) = \mathbf{M}$) [1]; (b) the inverse problem in which for given measurements $\mathbf{M}$, we evaluate the subsurface properties $\mathbf{P}$ (i.e., $\mathcal{I}(\mathbf{M}) = \mathbf{P}$) [2]. In this work, we focus on solving the inverse problem using deep learning.

Inverse problems are mathematically posed as the minimization of a cost function [3]. There exist two traditional families of methods to solve this minimization problem: (a) gradient-based algorithms, which only guarantee a local minimum, and (b) statistic-based methods, which require a large number of forward simulations. In both of the above families of methods, we need to repeat the entire inversion process for each set of new measurements, which escalates the computational time and often prevents real-time inversion. This occurs because these methods do not provide an approximation of the inverse operator $\mathcal{I}$, and they only evaluate it on a specific set of measurements.

In this work, we overcome the above limitations by using a deep neural network (DNN) $\mathcal{I}_h$ to approximate the inversion operator $\mathcal{I}$. Using this approach, we can train the DNN a priori, and perform the inversion by evaluating a trained DNN in the field in real time [4].

In this presentation, we shall emphasize the main computational advantages and limitations of using a DNN for inverting resistivity measurements for the oil industry. One crucial advantage of this method is that it enables a faster real-time inversion than other existing traditional methods. On the other side, a DNN approach requires computation of enormous data sets over parallel GPUs. We also discuss the effect of using different cost functions leading to different DNN architectures. Finally, we shall propose a specific DNN architecture and cost function which seem to provide adequate results for some of the inverse problems we analyzed. We also discuss the use of this technology for uncertainty quantification.

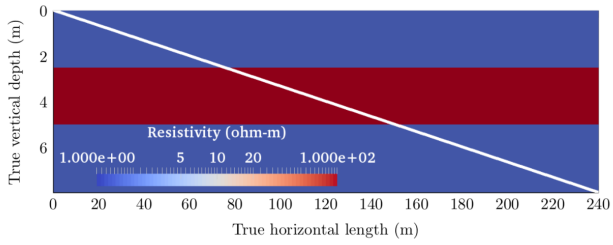
References

[1] M. Shahriari, S. Rojas, D. Pardo, A. Rodríguez-Rozas, S. A. Bakr, V. M. Calo, and I. Muga. A numerical 1.5D method for the rapid simulation of geophysical resistivity measurements. Geosciences, 8(6), 1–28, 2018.

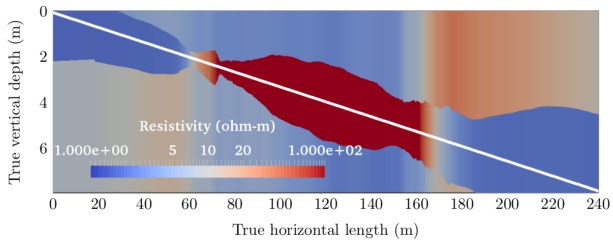
[2] D. Pardo and C. Torres-Verdín. Fast 1D inversion of logging-while-drilling resistivity measurements for the improved estimation of formation resistivity in high-angle and horizontal wells. Geophysics, 80(2), E111–E124, 2014.

[3] A. Tarantola, Inverse Problem Theory and Methods for Model Parameter Estimation, Society for Industrial and Applied Mathematics, 2005.

[4] M. Shahriari, D. Pardo, A. Picón, A. Galdran, J. Del Ser, C. Torres-Verdín. A Deep Learning approach to the inversion of borehole resistivity measurements. arXiv:1810.04522.

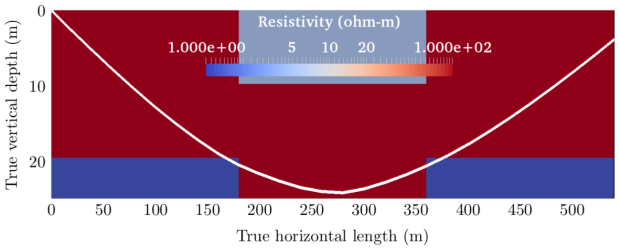


(a) Actual formation

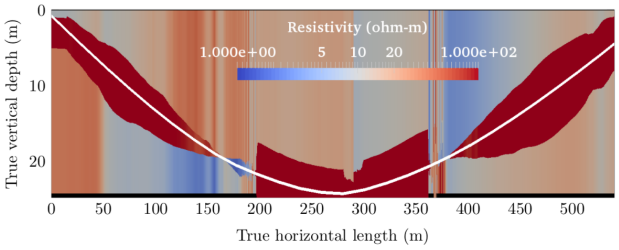


(b) Predicted (inverted) formation using new cost function

Figure 10: Model problem 1. Comparison between actual and predicted (inverted) formation.

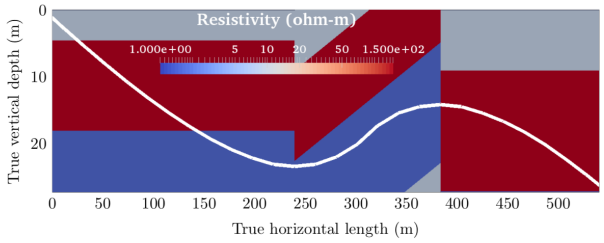


(a) Actual formation

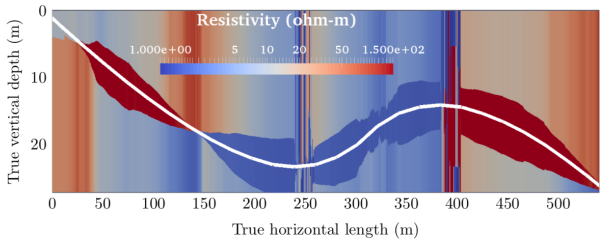


(b) Predicted (inverted) formation using new cost function

Figure 11: Model problem 2. Comparison between actual and predicted (inverted) formation.



(a) Actual formation



(b) Predicted (inverted) formation using the new cost function

Figure 12: Model problem 3. Comparison between actual and predicted (inverted) formation.

- COMPUTATIONAL SCIENCES AND AI IN INDUSTRY (CSAI) -

June 12-14, 2019, University of Jyväskylä, Finland

Parallel session 6: Contributed papers on machine learning and optimization,

Chair: Johannes Kraus

Friday, 14 June, 12:20 - 12:40, Beeta

41 Using agents for automatic meta-modelling algorithm selection in data-driven multiobjective optimization problems

Bhupinder Singh Saini[1], **Kaisa Miettinen**[1], **Manuel Lopez-Ibanez**[2]
[1]University of Jyväskylä, Finland
[2]University of Manchester, United Kingdom

Solving industrial multiobjective optimization problems (MOPs) in often requires expensive objective function evaluations. This expense can be financial (physical experiments may be required to calculate objective values) or computational (objective values may be the output of a time-consuming simulation models). The cost may be reduced by using meta-models or surrogate models created from datasets, which approximate the behaviour of objective functions, during the optimization process. Some of the surrogate modelling algorithms widely used in literature are Artificial Neural Networks and kriging models.

While many surrogate modelling techniques have been discussed in literature, there is no standard procedure or guide that can help researchers select the best technique for any given problem. More often than not, there is no reasoning behind the selection of a surrogate modelling technique apart from popularity of the technique in the research community and the researcher's familiarity with it. While this is not ideal, the alternative, due to a lack of an algorithm selection guideline, is a trial-and-error of the various surrogates modelling algorithms. This is a waste of time and resources.

In this study, we propose an agent that can automate the process of selection of a surrogate modelling algorithm. The agent, based on the features of a

dataset, tries to predict which surrogate modelling algorithm will perform the best on the dataset. The algorithms are selected from a subset of the regression algorithms available in the open-source Python library scikit-learn. The performance of the agent on benchmark and engineering problems is discussed. This research as a part of developing open source project DESDEO (desdeo.it.jyu.fi), will remove the unnecessary cognitive load of choosing surrogate modelling algorithms from the researchers, while improving the performance of the metamodels and thus leading to better results.

Keywords: *Automatic algorithm selection, Multiobjective optimization*

42 Mini-Forum: Future cooperation between Computational Science and AI in Industrial and Societal Applications - challenges, impact and expectations?

William Fitzgibbon[1], **Jacques Periaux**[2], **Tero Tuovinen**[3]
[1] Univ. of Houston, USA
[2] CIMNE, Spain and Univ. of Jyväskylä, Finland
[3] Univ. of Jyväskylä, Finland

Objectives:

AI is at the crossroads of several disciplines: computer science, mathematics (logic, optimization, analysis, probabilities, linear algebra), and cognitive science. The algorithms that underpin it are based on equally varied approaches: semantic analysis, symbolic representation, statistical and exploratory learning, neural networks. A recent boom in AI is due to significant advances in machine learning. AI is also developing quickly due to the international "data-ization" of all sectors (i.e. big data) and the exponential increase in computing power and data storage capacities. Many artificial intelligence (AI) strategies start with the collection of large bodies of data. Data isappearing as a key competitive advantage in the global CS-AI race. Four applications with sufficient maturity to launch major transformation operations in Medicine, Transport, Energy/Environment and Defense/Security

- are areas of world excellence;
- represent important challenges in terms of the public interest;
- attract the interest and involvement of public and private actors;
- require strong public leadership to trigger the transformations.

Due to the AI-automation of tasks, it is likely that most occupations and organizations will change. These four applications with lectures followed by questions / answers will be presented during this debate by experts in CS and AI to discuss the impacts related to the development of digital practices and services boosted by AI. Among the many challenging questions to be identified discussed by experts and the audience, does Artificial Intelligence technologies and Algorithms will really improve our well-being in the Era of Big Data and what are the actions to be taken by scientists, government, industry and civil society ?

42.1 Artificial Intelligence, Deep Learning and Science Policy in France

Olivier Pironneau
French Academy of Sciences, France

As most countries, France is deeply concerned with the development of AI, the problems related to ethics, reliability and the transformation of our society. Two important reports have been written for the government two years ago. It is also one of the 3 topics for the G7 meeting in Biarritz in August. Consequently the French Government has budgeted 500Million € to build 4 AI centers.

Presenter: Olivier Pironneau

42.2 AI and Digital Twin challenges in current EU arenas – in overall and from Finnish perspective

Olli Ventä
VTT, Finland

Artificial intelligence and digital twins are currently major topics, as enabling technologies as such, or as significant drivers in practically all application sectors of Europe and Finland. In my presentation or discussion in the intended panel, I want to summarize how these signifigant technologies appear in the SRA:s of Big Data Values Association (BDVA, a PPP for big data), ECSEL (Electronic Components and Systems for European Leadership), Factories of the Future, and SPIRE (Sustainable Process Industry through Resource and Energy Efficiency), in some CSA or roadmap deliverables, and in the end in some significant H2020 projects. All these key documents are contributing to European Commission activities producing the profiling and backgroung texts for respective calls for proposals in the coming few years.

VTT is participating in this future directing work and also in respective ongoing EU projects. In the presentation or panel I want to highlight some important Finnish subconsortia of larger projects, about how artificial intelligence and digital twins are being utilized.

Keywords: *public-private-partnerships, artificial intelligence, digital twin, reasearch agendas*

Presenter: Olli VENTÄ (male), D. Sc. Technology, Senior Principal Scientist of Intelligent Systems, Research Manager of Industrial Internet. Formerly Research Manager and Deputy Head of Research Area of VTT Life-Cycle Management research area (ca. 120). A board member of VTT Strategic Research, a Board Member and Deputy Chairman of Industrial Systems Management

Strategic Research Steering Group (2006–2013), Programme Manager of the former (2009–2012) VTT spearhead programme called e-Engineering. In 2001–2004, Dr. Ventä was the leader of the national technology programme Intelligent Automation Systems (Tekes). Also in the recent past, he has been the Programme Leader of VTT's internal research programmes Intelligent Products and Systems (2003–2006) and Complex Systems Design (2006–2008). Dr. Ventä is an active member of the Finnish Automation Society, currently a Board Member of Finnish Automation Foundation. On EU arenas, Olli Ventä active in ECSEL (e.g., an SRA chapter leader of Digital Industry and LIASE member of Industry4.e - an ECSEL lighthouse), in EFFRA, in BDVA (esp. Smart Industry) and in SPIRE. Dr. Ventä is a Knight, First Class, of the Order of the Lion of Finland, issued by the President of Finland on December 6, 2015.

42.3 AI and Data Analytics at a Centre for Scientific Computing

Markus Koskela
CSC - IT Center for Science Ltd, Finland

Dynamic Data-Driven Application Systems (DDDAS) is a paradigm that allows the evolution, and hence the improvement in time, of dynamic models for model-based control strategies and for digital twins. DDDAS aim to correct and update mathematical models in real-time, by constantly processing data obtained from the real system or related simulations.

In this paper we propose a DDDAS approach based on tensor factorization applied to electric vehicles' active suspension systems. A suspension system's behaviour can vary in time due to material degradation, deformations, etc.; all these variations can considerably affect the suspension system's performance in time and therefore it is of extreme importance to update the parameters of the mathematical model taking these changes into account. The DDDAS strategy we introduce in this paper aims to handle and include time dependant corrections into the suspension system's model; for this purpose we make use of tensor factorization, which is an excellent tool for learning the underlying physics of collected data, becoming an extremely relevant requisite when attempting to foresee the origin of faults in industrial systems.

In order to compute a mathematical model of a suspension system, data coming from it are fed to an algorithm for Reduced Order Model (ROM). ROM strategies are based on numerical methods for multivariable problems simplification through mathematical approximation techniques. ROMs computation can be handful in such situations where a reduction in terms of system's variables should be taken into consideration, e.g. big data, uncertainties in the physics behind the system, system's equations' solution not trivial and/or computationally cumbersome.

In this article we compute ROMs using TWINKLE, an in-house built software. TWINKLE is a high performance library written in C++ for carrying out Canonical Polyadic Decomposition (CPD) on tensors. It allows processing and recovering highly sparse and unstructured data, which is not usually foreseen in CPD, e.g. Singular Value Decomposition (SVD), Principal Components Analysis (PCA), PARAllel FACtor analysis (PARAFAC) or CANonical DECOMPosition (CANDECOMP). The library uses Armadillo, an open source library for linear algebra and scientific computing, which is based on LAPACK (Linear Algebra PACKage) and BLAS (Basic Linear Algebra Subprograms) routines in turn.

In this paper we select the DDDAS paradigm to apply TWINKLE on incremental data coming from electric vehicles' active suspension systems, in order to analyse the efficiency and accuracy of the algorithm, as well as to explore a new strategy to prove the possibility of updating systems' mathematical models using tensor factorization.

Presenter: Markus Koskela holds a PhD in computer science from Helsinki University of Technology. He works currently as senior applications specialist at CSC and has previously worked as a senior researcher at University of Helsinki, Aalto University, and Dublin City University. His professional interests are focused on machine learning, deep learning, GPU computing, intelligent information access, and computer vision. He has published over 60 scientific articles in these areas.

42.4 AI in the field of medical applications

Pirjo Mustonen
University of Jyväskylä

In this presentation I will outline the current status and the near future perspective of the use of artificial intelligence, and especially deep learning subtype in the field of medicine. The talk will focus mainly on three viewpoints: firstly of a real-life hospital-based practicing medical specialist, secondly of patient (self-care and status), and thirdly of the emerging field of strategic leadership of health systems. An overview of contemporary evidence of the performance of AI in comparison to traditional human approach will be presented. I will also discuss the present attitudes towards AI among health care professionals, as well as the current main limitations and barriers of AI technology introduction in hospitals.

Presenter: Pirjo Mustonen is MD, PhD, Specialist of Internal Medicine and Cardiology (University of Helsinki), Adjunct Professor in Internal Medicine (University of Eastern Finland) and eMBA (University of Tampere). She is a consultant in the field of Thrombosis and Haemostasis, the past president of the Working Group of Thrombosis of Finnish Cardiac Society, and the working group member of several National Current Care Guidelines. Her clinical expertise and educational skills in the field of cardiology have been acknowledged with the Pentti Halonen award. Currently she works as a Developer Chief Physician in Central Finland Health Care District, and in the Finnish National Institute for Health and Wellfare. In University of Jyväskylä, she is a Professor of Practice in the Faculty of Information Technology.

	Wednesday, 12 June 2019		Napsu Karmitsa: Missing value imputation via nonsmooth optimization and clusterwise linear regression
8:00-8:30	Registration (Room: Agora Lobby)	**13:00-14:00**	Lunch
8:30-9:00	Opening (Room: Alfa)	**14:00-14:40**	Semi-plenary 3: Mohamed Masmoudi: Parsimonious Neural Networks (Chair O. Pironneau) (Room: Alfa)
9:00-9:45	Plenary 1: N. Chakraborti: Novel Strategies for Data-driven evolutionary Optimization (Chair K. Miettinen) (Room: Alfa)	**14:40-15:20**	Semi-plenary 4: Yoshiyasu Takefuji: Nobody can stop advancing artificial intelligence (AI) where developing (Chair P. Neittaanmaki) (Room: Alfa)
9:45-10:30	Plenary 2: Tommi Kärkkäinen: Machine learning using distance-based methods (Chair P. Neittaanmäki)	**15:20-16:00**	Coffee break
10:30-11:00	Coffee break	**16:00-16:40**	Semi-plenary 5: Lauri Kettunen: Computational Sciences, Physics Field Theories and Geometry (Chair T. Tuovinen) (Room: Alfa)
11:00-13:00	Parallel session 1: Contributed papers on AI in medical applications (Chair T. Kärkkäinen) (Rom: Beeta)	**18:30-21:00**	Conference dinner. Conference dinner is held in cruise where we can enjoy Finnish summer and see beautiful lake Päijänne. (Agora harbor)
	Timo Ojala: Counting cells and predicting Immunoscore using Gradient Boosted Convolutional Neural Networks		**Friday, 14 June 2019**
	Leevi Annala: Kubelka-Munk model and Stochastic model comparison in skin physical parameter retrieval using neural networks	**8:30-9:00**	Registration (Room: Agora Lobby)
	Billy Braithwaite: A combined approach of neural networks and graphical models in skin cancer inference using spectral imaging	**9:00-10:30**	Minisymposium on ethics in AI (Chair P. Abrahamsson) (Room: Alfa)
	Ilkka Pölönen: Using wave propagation simulations and convolutional neural networks to retrieve thin coating's thickness from hyperspectral images		Pekka Abrahamsson: Ethics in AI
	Ilkka Rautiainen: Predicting future overweight and obesity from childhood growth data: A case study		Kai-Kristian Kemell: Essentializing Software Engineering Practices for Ethically Designing and Developing Artificial Intelligence Systems
11:00-13:00	Parallel session 2: Minisymposium on Machine learning 1 (Chair N. Karmitsa) (Room: Alfa)		Ville Vakkuri: Ethics is important, but how can we implement it? Survey on software developers' views on AI ethics
	Keynote: Tapio Pahikkala: Variable selection under a value acquisition budget	**10:30-11:00**	Coffee break
	Jonathan Hüser: Stochastic approximation by successive piecewise linearization	**11:00-13:00**	Parallel session 5: Special technology session (Chair O. Ventä) (Room: Alfa)
	Anthony Man-Cho So: Non-Convex Robust Low-Rank Matrix Recovery		Ariel Edesess: Industrial IoT capabilities in reducing the LCOE of offshore wind energy: A review
	Andreas Griewank: Neural Network Learning via Successive Piecewise Linearization		Martin Siggel: High-Performance Data Analysis with the Helmholtz Analytics Toolkit (HeAT)
13:00-14:00	Lunch		Salvador Izquierdo: Dynamic data-driven application systems based on tensor factorization: learning the physics of model evolution
14:00-14:40	Semi-plenary 1: Bruno Despres: Learning for scientific computing purposes (Chair S. Repin) (Room: Alfa)		Marjaana Nokka: Predicting customer experience
14:40-15:20	Semi-plenary 2: Tadeusz Burczyński: Computational intelligence in design of new nanomaterials (Chair T. Tuovinen)(Room: Alfa)		Markus Koskela & Mat Sjöberg: Puhti-AI: Finland's new AI supercomputer
15:20-16:00	Coffee break		Timo Lehtonen: Using Artificial Intelligence to Classify Textual Applications for Reporting Purposes
16:00-16:45	Plenary 3: Mary F. Wheeler: Modeling Flow, Reactive Transport and Geomechanics in Porous Media (Chair B. Despres) (Room: Alfa)	**11:00-13:00**	Parallel session 6: Contributed papers on machine learning and optimization (Chair J. Kraus) (Rom: Beeta)
16:45-19:00	Welcome coctails (Lea Pulkkinen hall, 4 th floor)		Sergey Repin: Application of machine learning methods to error control of approximate solutions
	Thursday, 13 June 2019		Atanu Mazumdar: Iterative Data Selection Strategy in Offline Data-Driven Evolutionary Multiobjective Optimization
8:30-9:00	Registration (Room: Agora Lobby)		Pouya Aghaei Pour: On Surrogate Management in Interactive Multiobjective Building Energy System Design
9:00-9:45	Plenary 4: K. Duraisamy: Physics constrained machine learning for industrial applications (Chair J. Periaux) (Room: Alfa)		Mostafa Shahriari: A Modified Deep Neural Network for the Rapid Inversion of Geophysical Resistivity Measurements
9:45-10:30	Plenary 5: Olivier Pironneau: Parameter and Type Identification in Partial Differential Equations using Deep Neural Networks (Chair M. Wheeler) (Room: Alfa)		Bhupinder Singh Saini: Using agents for automatic meta-modelling algorithm selection in data-driven multiobjective optimization problems
10:30-11:00	Coffee break	**13:00-14:00**	Lunch
11:00-13:00	Parallel session 3: Contributed papers on Computational Solids, structural mechanics and fluid dynamics (Chair T. Tuovinen) (Rom: Beeta)	**14:00-16:00**	Mini-forum: Future cooperation between Computational Science and AI in Industrial and Societal Applications: challenges, impact and expectations? (Room: Alfa)
	Nikolay Banichuk: Stability maximization for layered moving web with total mass constraint		Organisers: W. Fitzgibbon (U. of Houston, USA), J. Periaux (CIMNE, Spain), T. Tuovinen (JYU, Finland)
	Jian-Jun SHU: Similarity solutions for condensation on a non-isothermal vertical plate		Michael Kyriakopoulos, EC DirectorateTransport, Belgium, Transport
	Cheol Kim: Enhanced Topology Optimization Approach Using Moving Morphable Components Coupled with NURBS Curves		Pirjo Mustonen, JYU, Finland, Medical Applications
	Luca Rosafalco: Combined Model Order Reduction and Artificial Neural Network for data assimilation and damage detection in structures		Olivier Pironneau, French Academy of Sciences, A strategy for France in AI
11:00-13:00	Parallel session 4: Minisymposium on Machine learning 2 (Chair A. Griewank) (Room: Alfa)		Olli Ventä, VTT Espoo, Finland, Energy/Environment
	Keynote: Andrea Walther: Towards the optimization of fuzzy pattern trees by abs-linearization		Markus Koskela: AI and Data Analytics at a Centre for Scientific Computing
	Kaisa Joki: Support vector machines in clusterwise linear regression	**16:00**	Closing
	Pedro Merino: A Second-order method with enriched hessian information for composite sparse optimization problems		

ISBN 978-951-39-7788-7 (Print)

ISBN 978-951-39-7789-4 (e-publication)

ISSN 2489-351X