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STADIUS
Center for Dynamical Systems, Signal Processing and Data Analytics



October 2024

RESEARCH ▪ AWARDS ▪ NEWS ▪ EVENTS ▪ STAFF UPDATE ▪ DEFENDED PHD ▪ PUBLICATIONS

Welcome

Welcome to the October edition of the STADIUS Newsletter!
Scroll down to explore the latest news, meet our newest researchers, and discover upcoming events and other exciting highlights from STADIUS.
Enjoy the read!



New Professor @ STADIUS

In October 2024, **Pedro Gonçalves** began his joint appointment as a **VIB-KUL professor**, affiliated with both the Department of Computer Science and the **STADIUS division** within the ESAT Department.

Pedro is a **Group Leader at VIB-NERF** since May 2023, and an **affiliated PI at VIB Center for AI & Computational Biology**. He is also a member of KU Leuven ELLIS unit (European Laboratory for Learning and Intelligent Systems).
Before starting his lab, Pedro did a postdoc with Maneesh Sahani at the Gatsby Unit, UCL, London, followed by a postdoc in Jakob Macke's lab at the University of Tuebingen, Germany. His PhD was supervised by Christian Machens at Ecole Normale Supérieure, Paris.
Pedro's lab **develops and applies probabilistic machine learning tools to derive mechanistic insights from neural data**, to ultimately uncover the mechanisms underlying neural computations, across species and brain areas.

More details at https://goncalveslab.sites.vib.be/en



Newcomers Reception

Thank you for participating in the Newcomers Seminar and Reception that took place on 23rd October! It was a great afternoon and evening with an unforgettable trip between STADIUS offices, losts of tasty food and competitive games. Thank you Newcomers for organising it!!

On the **STADIUS Wiki** you can find the presentation about STADIUS given by Alexander Bertrand, the Presentation by the Newcomers and also a few pictures.

Revisit the presentations,
look at the pictures

Research of the month by Martijn Oldenhof

"Machine Learning for Advanced Chemical Analysis and Structure Recognition in Drug Discovery"

Work under the supervision of Yves Moreau

Introduction / Objective
The essence of successful Quantitative Structure-Activity Relationship (QSAR) modeling for drug discovery lies in the availability of diverse and high-quality data. However, acquiring such data in the pharmaceutical industry is not only challenging and expensive but also

constrained by its proprietary nature, limiting sharing opportunities. To overcome these challenges, this work introduces innovative methods aimed at accessing literature and cross-pharma data, thereby enabling the utilization of larger datasets for the training of machine learning models.

Research Methodology

In the first part of this research, we merge the concepts of **multi-task learning** and **federated learning** to facilitate cross-pharma federated learning on the confidential data of 10 pharmaceutical partners to improve predictive performance of drug discovery machine learning models [1] (as visualized in Figure 1).

Secondly, an integral component of this research involves the introduction of the **Optical Chemical Structure Recognition (OCSR)** technique, known as ChemGrapher [2]. While showcasing its potential, a notable limitation comes to light, emphasizing the indispensability of atom-level entity labels. These labels, providing precise details about the localization of individual elements within chemical compounds, prove essential for effective training and are crucial for atom-level OSCR methods. Atom-level OCSR methods not only predict the molecular graph given a depicted chemical structure but also the localization of the different components in the original image. Previous research has shown that atom-level entity prediction methods, compared to pure molecular graph prediction methods, typically enjoy better training sample efficiency, requiring less images for achieving the same level of performance. Therefore the methods developed in this work [3,4] (as visualized in Figure 2) aim to improve atom-level OCSR methods by treating atom-level entities as discrete objects highlighting the **convergence of OCSR with object detection methodologies**.

Figure 2: **Weakly supervised training**. ProbKT* will perform backpropagation to update the object detection backbone using probabilistic reasoning to be able to train atom-level OCSR using only SMILES supervision.

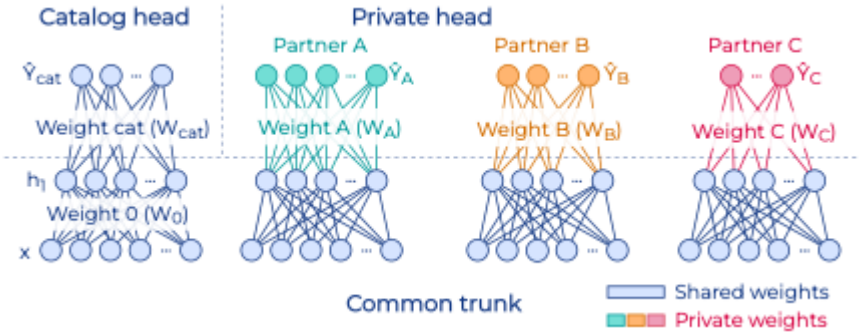
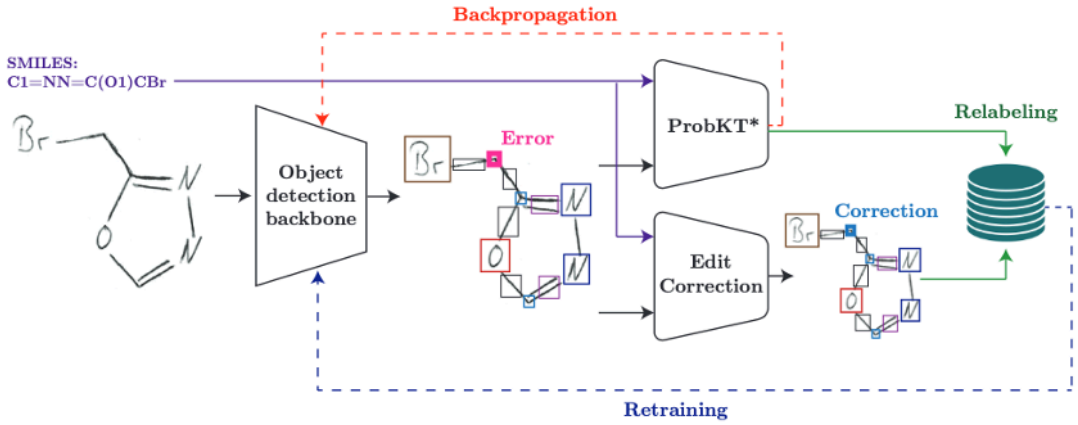


Figure 1: The contributing partners to the global federated model can all have different tasks which should be kept private to each partner; this is therefore split into a private head and a common trunk



Results & Conclusions

The jointly learned shared representation using cross-pharma federated learning resulted in the **improvement of predictive models**, supporting the drug discovery process. **ChemGrapher** [2] , **ProbKT** [3] and **AtomLenz** [4] represent a pioneering advancement in the realm of machine learning for Optical Chemical Structure Recognition by converging object detection methodologies and OCSR.

Major publications

[1] Oldenhof, Martijn, et al. "Industry-scale orchestrated federated learning for drug discovery." Proceedings of the AAAI Conference on Artificial Intelligence. Vol. 37. No. 13. 2023.
[2] Oldenhof, Martijn, et al. "ChemGrapher: optical graph recognition of chemical compounds by deep learning." Journal of chemical information and modeling 60.10 (2020): 4506-4517.
[3] Oldenhof, Martijn, et al. "Weakly Supervised Knowledge Transfer with Probabilistic Logical Reasoning for Object Detection." The Eleventh International Conference on Learning Representations. 2023
[4] Oldenhof, Martijn, et al. "Atom-Level Optical Chemical Structure Recognition with Limited Supervision." Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition. 2024.

News



Keynote by Toon van Waterschoot

On October 2, 2024, **Toon van Waterschoot** delivered a keynote lecture at the **IEEE International Symposium on the Internet of Sounds** at the **International Audio Laboratories Erlangen** in **Germany**. This was the 5th edition of a multidisciplinary symposium that brings together scientists, engineers, students, creative practitioners, entrepreneurs, and industry leaders around one central theme: the Internet of Sounds, an emerging research field at the intersection of the **Internet of Things (IoT) and Sound and Music Computing**. In his keynote, Toon gave an overview of the **results obtained in H2020 MSCA European Training Network** "Service-Oriented, Ubiquitous, Network-Driven Sound (SOUNDS)" that is coordinated at STADIUS, before diving into a more technical presentation about the use of consensus optimization in distributed audio signal processing.



John Hopfield and Geoffrey Hinton receive the 2024 Physics Nobel prize!

In the 90s, we were very much honored at **ESAT-Stadius** to **welcome John Hopfield** who opened at that time the ICNN Interdisciplinary Center for Neural Networks at KU Leuven. The ICNN was founded by **Joos Vandewalle (ESAT-Stadius)**, Desire Bolle (Physics dept) and Guy Orban (Neuroscience dept). It was providing a stimulating environment for researchers who could meet at interdisciplinary seminars that were regularly organized.

Since the early days up till now several research at ESAT-Stadius is connecting in a broad sense **to the works of Hopfield and Hinton**. It includes e.g. research on capacity in Hopfield associative memories, locally implementable matrix flows, cellular neural networks, equilibria and bifurcations in recurrent neural networks, stability theory of multilayer recurrent neural networks with applications in nonlinear modelling, neural control and robust control, learning genetic networks, continuous-time and fast global optimization algorithms,

deep kernel machines, generative restricted kernel machines and deep kernel principal component analysis.
The course on **Artificial Neural Networks and Deep Learning**, currently taught by J**ohan Suykens (ESAT-Stadius)** and previously by J**oos Vandewalle** and Desire Bolle, **covers the work by Hopfield and Hinton**. Associative memories and Hopfield networks are addressed within the lecture on recurrent neural networks and associative memories, and restricted Boltzmann machines and deep Boltzmann machines by Hinton et al. within generative models. The new course on Advanced data mining and neural networks also includes these topics.
Furthermore, the ESAT-Stadius research group appreciates the interdisciplinary nature of the Physics Nobel prize, which is highly stimulating for the future.
In line with this, we are pleased to share a related thought-provoking text by **Rodolphe Sepulchre (ESAT-Stadius)** on the intersections on physics and AI, titled "Reconciling Physics and Algorithmics". This recent editorial explores the future of AI, **influenced by the works of pioneers like John Hopfield.**

^

VAIA presented as best practice in SMERALD project (Erasmus+)

Flanders AI Academy (VAIA) is gaining recognition beyond Flanders. Recently, VAIA was invited by the Erasmus+ project SMERALD to present its approach as a best practice for awareness and learning on digital data, data analysis, and artificial intelligence in SMEs across Europe. Prof. Bart De Moor chairs VAIA, and the coordination of this inter-university project resides within STADIUS.
Check out the recording: https://youtu.be/oDCK39Elok0?si=qltwmNNIvFNoy3yz&t=2228

STADIUS Colloquium Series

- **6/11/2024 Prof. Andre Dekker "AI for Better Health Care"**
  - Wednesday 6/11/2024, 14:30 - 15:30
  - Location: MTM 00.13
- **4/12/2024 Dr. John Veitch "Analysing Black Hole and Neutron Star Merger Signals**
  - Wednesday: 4/12/2024, 15:00 - 16:00
  - Location: Aula C

For more detailed abstract and biographies, please consult the STADIUS Event website

Other events @ STADIUS

Meet the Jury Seminar
When: **7/11/2024, 14:30 - 16:00**
Where: **ELEC.01.0060**
By: **Dr. Huy Phan** and **Prof. Pieter Van Mierlo**

PhD defense - Jingwei Zhang
When: **7/11/2024, 17:00**
Where: **GA2 Auditiorium - 04.14 - O N1 Gasthuisberg**

For more information about STADIUS events please visit the STADIUS Event webpages.

Don't forget to check the website of VAIA for a wide choice of courses on (aspects of) AI: www.vaia.be

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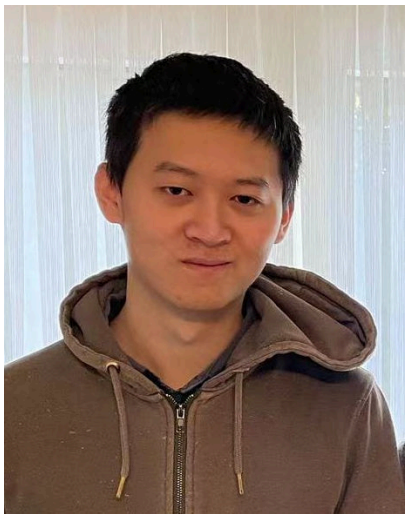
STADIUS seminar - *A Kernelizable Primal-Dual Formulation of the Multilinear Singular Value Decomposition*
When: **12/11/2024, 11:00 - 12:00**
Where: ESAT B00.35
By: **Kim Batselier**

New colleagues

A warm welcome to new personnel at STADIUS!



Hello everyone,

My name is **Jan Quan**. I have a MSc in Mathematical Engineering from KU Leuven and am now starting my PhD here at KU Leuven under the supervision of Prof. Panos Patrinos. The goal of my PhD project "Rethinking transformers through duality" is to develop a framework using generalized duality to understand and improve transformer architectures. I enjoy playing guitar, solving logic puzzles, and competing in programming and cybersecurity competitions. As for sports, I like swimming, badminton, indoor climbing, and archery.

Looking forward to working with you all



Dear all,
I am **Tom Colemont**. In 2022, I graduated with a bachelor's degree in Engineering Science from KU Leuven, majoring in Electrical Engineering and minoring in Mechanical Engineering. Last June, I completed my master's in Electrical Engineering at KU Leuven, specializing in information systems and signal processing. As of October, I have started my PhD at STADIUS under the supervision of Prof. Tjonnie Li and Prof. Marc Moonen. During my PhD, I will be exploring the fields of signal processing and data analysis, specifically addressing the data analysis challenges associated with the detection of gravitational waves with the next-generation Einstein Telescope gravitational interferometer.
In my free time, I enjoy going for runs and playing guitar. I also love to read a good book or watch an engaging series.
I'm looking forward to meeting all of you!

Hi everyone,
My name is **Hayden Johnson.** I have a BSc in computer science from the University of Minnesota. During my bachelor's, I spent a semester on exchange, studying artificial intelligence at the University of Amsterdam. After finishing my degree, I worked for a year as a full-time researcher in a computational neuroscience lab, again at



the University of Minnesota. I am currently beginning my predoctoral studies here at KU Leuven under the supervision of Dr. Pedro Gonçalves, where I will be working to develop methods of simulated-based inference for application in computational neuroscience. In my free time, I love reading, watching movies, and going to concerts.
Looking forward to meeting you all!



Hi,

I'm **Mustafa Enes Aydın** and I'm in the Biomed group under the supervisions of Prof. Alexander Bertrand and Prof. Maarten De Vos. I obtained my B.Sc. and M.Sc. degrees in Electrical and Electronics Engineering from Bilkent University in Ankara, Turkey. I'll be trying to develop techniques for quantifying and possibly improving the quality of time series data with regards to artifacts and noise. I like programming, chess and programming for procrastination.

Best Regards,
Mustafa Enes Aydın



Hi Everyone,
I'm **Anna Martens.** I obtained my master's degree in Biomedical Engineering from KU Leuven in June. Afterwards, I enjoyed a relaxing holiday and recharged my batteries. Now I'm ready for a new adventure as part of the STADIUS biomed group. I will be working under the supervision of Prof. De Vos and Dr. Lieven Lagae on childhood epilepsy. For my PhD project, the aim is to use analysis techniques to help in the daily clinical decision making. More specifically, we hope to identify specific EEG biomarkers that could detect abnormal brain activity, help in the diagnosis of specific epilepsy syndromes, predict co-morbidities and the effect of prescribed anti-seizure medication. If I'm not at work, you can find me on the dance floor, with my friends or at home reading a good book.
I look forward to getting to know everyone in the following weeks and months!
-Anna

Hello everybody!

I am **Maarten Vanmarcke**. I received my Master's degree in Engineering - Computer Science, with the



option Artificial Intelligence, at KU Leuven. Due to a strong interest in healthcare, I started a PhD at the BioMed group at Stadius under the supervision of Prof. Maarten De Vos. My research will focus on improving automatic epilepsy seizure detection using multimodal data from wearable sensors and investigating the potential use of foundation models.
I am really passionate about music and theatre. I have played the piano for a couple of years and I've just started with some courses on music composition and orchestration during my free time. Besides that, I like to read a comic book to look at all the wonderful art, play a (board or video) game or take a walk.

See you soon!



Hi

I am **Anastasia Krouglova** (or Nastya). I obtained an MSc in Computer Science (Artificial Intelligence) and joined in October 2023 the Gonçalves lab. The focus of my current research lies in the field of computational neuroscience, which is the investment of brain function using mathematical tools and machine learning techniques. If I am not in the lab, then you can typically find me at the ice rink training for the next competition or at the music school.

Nastya

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We wish the best of luck to the researchers who are leaving STADIUS

Best of luck!

Elisabeth Heremans defended her PhD in October and will now join the Belgian American Educational Foundation (BAEF) at Stanford, working with a group led by E. Mignot.

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Recently defended PhDs

21/10/2024: Elisabeth Heremans, *Automated sleep analysis: from the hospital to the home environment*, supervised by Prof. M. De Vos and W. Van Paesschen.

Congratulations to Elisabeth on defending **cum laude** (with the congratulations of the Examination Committee)

Newly approved FWO Scholarships

We wish to congratulate the researchers who recently got their FWO scholarship approved:

- FWO Strategic Basic Research
  - Helene Huts "*Data-driven approaches for personalized medicine*"
- FWO Fundamental Research:
  - Lore van Santvliet "*Data-driven approaches in computational cardiology"*
  - Guanchun Tong "*Physical computation: an energy-based approach*"

New Projects Starting

KUL C1 Project
Rethinking Transformers Through Duality Principles

- 01/10/2024 - 30/09/2028
- STADIUS PI - Johan Suykens & Panos Patrinos

KUL C3 Project
NEONAID: Neonatal Online Neuro-Analysis for Interpretation and Decision-support - Bringing automated neonatal monitoring to the bedside

- 01/10/2024 - 30/09/2026
- STADIUS PI - Maarten De Vos

KUL C3 Project
Flexibele activiteitsmeting ter ondersteuning van fysieke activiteit

- 01/10/2024 - 30/09/2026
- STADIUS PI - Bart Vanrumste

PhD scholarships for researchers from the South

- 01/10/2024 - 28/02/2028
- Grantee: Xuan Phu Nguyen

FWO-SBO Project
New Perspectives on Medieval and Renaissance Courtly Song

- 2024-10-01 - 2028-09-30
- STADIUS PI: Toon van Waterschoot

IDN - Interdisciplinary Networks
AI-guided computational design of anti-virulence proteins as sustainable alternative antibacterials

- 2024-10-01 - 2028-09-30
- STADIUS PI: Yves Moreau

Publication Digest

Here's the monthly STADIUS Publications Digest, including new reports that have been added to the publications database.
Please remember to have your own reports added in the publications database and make sure your entries are kept up to date (status submitted/accepted/published) at all times.

Contact Ida for new additions and updates, do not add/update database content yourself.

24-137

Attwood T.K., Blake J., Bourne P.E., Conesa A., Gaasterland T., Hunter L., Kingsford C., Kohlbacher O., Lengauer T., Markel S., Moreau Y., Noble W.S., Orengo C., Ouelette F., Parida L., Przulj N., Pop M., Przytycka T.M., Ranganathan S., Schwartz R., Schwede T., Valencia A., Warnow T., ``Biological databases in the age of generative artificial intelligence'', Technical Report 24-137, ESAT-STADIUS, KU Leuven (Leuven, Belgium), 2024. Accepted for publication in *Bioinformatics Advances*.
Lirias number: 4188827.

24-139

MacWilliam K., Dietzen T., Ali R., van Waterschoot T., ``State-space estimation of spatially dynamic room impulse responses using a room acoustic model-based prior'', *Frontiers in Signal processing*, Sec. Audio and Acoustic Signal Processing, vol. Volume 4, Sep. 2024, pp. 1-18.
Lirias number: 4191253.

24-140

Parul A., van Waterschoot T., ``Correlation among courses in mathematics trajectory of engineering technology'', Technical Report 24-140, ESAT-STADIUS, KU Leuven (Leuven, Belgium), 2024. Accepted for publication in *SEFI 2024*.
Lirias number: 4190382.

24-141

Seeuws N., De Vos M., Bertrand A., ``A Human-in-the-Loop Method for Annotation of Events in Biomedical Signals'', *IEEE Journal of Biomedical and Health Informatics*, vol. 71, no. 8, Aug. 2024, pp. 2442-2453.
Lirias number: 4186986.

24-142

Didier P., van Waterschoot T., Doclo S., Bitzer J., Moonen M., ``A Swiss-Knife Algorithm for Distributed Adaptive Node-Specific Signal Estimation in Ad-Hoc Wireless Acoustic Sensor Networks'', Technical Report 24-142, ESAT-STADIUS, KU Leuven (Leuven, Belgium), 2024.

24-143

Roebben A., van Waterschoot T., Moonen M., ``A Comparative Analysis of Generalised Echo and Interference Cancelling and Extended Multichannel Wiener Filtering for Combined Noise Reduction and Acoustic Echo Cancellation'', Technical Report 24-143, ESAT-STADIUS, KU Leuven (Leuven, Belgium), 2024.

24-144

Ingelaere S., Villa A., Varon C., Van Huffel S., Willems R., Vandenberk B., ``Detection of AI-enabled QRS fragmentation from 12-lead electocardiogram and its clinical relevance for predicting malignant arrhytmia onset'', Technical Report 24-144, ESAT-STADIUS, KU Leuven (Leuven, Belgium), 2024. Accepted for publication in *Frontiers in Cardiovascular Medicine, Section Cardiac Rhythmology*.
Lirias number: 4192198.

24-146

Nguyen N. D. T., Phan H., Geirnaert S., Mikkelsen K., Kidmose P., ``AADNet: An End-to-End Deep Learning Model for Auditory Attention Decoding'', Technical Report 24-146, ESAT-STADIUS, KU Leuven (Leuven, Belgium), 2024.

24-147

Musluoglu C. A., Bertrand A., ``Distributed Blind Source Separation based on FastICA", Technical Report 24-147, ESAT-STADIUS, KU Leuven (Leuven, Belgium), 2024.

24-148

Heremans E., *Automated sleep analysis : from the hospital to the home environment*, PhD thesis, Faculty of Engineering, KU Leuven (Leuven, Belgium), Oct. 2024, 274 p.
Lirias number: 4185409.



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ida.tassens@kuleuven.be .

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