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# Artificial Neural Networks and Machine Learning – ICANN 2019


## Deep Learning


28th International Conference on Artificial Neural Networks  
Munich, Germany, September 17–19, 2019  
Proceedings, Part II

### *Editors*

Igor V. Tetko   
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Forschungszentrum für Gesundheit  
und Umwelt (GmbH)  
Neuherberg, Germany

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Forschungszentrum für Gesundheit  
und Umwelt (GmbH)  
Neuherberg, Germany

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Helmholtz Zentrum München - Deutsches  
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und Umwelt (GmbH)  
Neuherberg, Germany

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# Preface

The fast development of machine learning methods is influencing all aspects of our life and reaching new horizons of what we have previously considered being Artificial Intelligence (AI). Examples include autonomous car driving, virtual assistants, automated customer support, clinical decision support, healthcare data analytics, financial forecast, and smart devices in the home, to name a few, which contribute to the dramatic improvement in the quality of our lives. These developments, however, also bring risks for significant hazards, which were not imaginable previously, e.g., falsification of voice, videos, or even manipulation of people's opinions during elections. Many such developments become possible due to the appearance of large volumes of data ("Big Data"). These proceedings include the theory and applications of algorithms behind these developments, many of which were inspired by the functioning of the brain.

The International Conference on Artificial Neural Networks (ICANN) is the annual flagship conference of the European Neural Network Society (ENNS). The 28th International Conference on Artificial Neural Networks (ICANN 2019) was co-organized with the final conference of the Marie Skłodowska-Curie Innovative Training Network European Industrial Doctorate "Big Data in Chemistry" (<http://bigchem.eu>) project coordinated by Helmholtz Zentrum München (GmbH) to promote the use of machine learning in Chemistry. The conference featured the main tracks "Brain-Inspired Computing" and "Machine Learning Research." Within the conference the First International Workshop on Reservoir Computing as well as five special sessions were organized, namely:

Artificial Intelligence in Medicine

Informed and Explainable Methods for Machine Learning

Deep Learning in Image Reconstruction

Machine Learning with Graphs: Algorithms and Applications

BIGCHEM: Big Data and AI in chemistry

A Challenge for Automatic Dog Age Estimation (DogAge) also took place as part of the conference. The conference covered all main research fields dealing with neural networks. ICANN 2019 was held during September 17–19, 2019, at Klinikum rechts der Isar der Technische Universität München, Munich, Germany.

Following a long-standing tradition, the proceedings of the conference were published as Springer volumes belonging to the *Lecture Notes in Computer Science* series. The conference had a historical record of 494 article submissions. The papers went through a two-step peer-review process by at least two and in majority of cases by three or four independent referees. In total, 503 Program Committee (PC) members and reviewers participated in this process. The majority of PC members had Doctoral degrees (88%) and 52% of them were also Professors. These reviewers were assigned 46 articles. The others were PhD students in the last years of their studies, who

reviewed one to two articles each. In total, for the 323 accepted articles, 975 and 985 reports were submitted for the first and the second revision sessions. Thus, on average, each accepted article received 6.1 reports. A list of reviewers/PC Members, who agreed to publish their names, are included in these proceedings.

Based on the reviewers' comments, 202 articles were accepted and more than 100 articles were rejected after the first review. The remaining articles received an undecided status. The authors of the accepted articles as well as of those with undecided status were requested to address the reviewers' comments within two weeks. On the basis of second reviewers' feedback, another 121 articles were accepted and the authors were requested to include reviewers' remarks into the final upload. Based on these evaluations, diversity of topics, as well as recommendations of reviewers, special session organizers, and PC Chairs, 120 articles were selected for oral presentations. Out of the total number of 323 accepted articles (65% of initially submitted), 46 manuscripts were short articles with a length of five pages each, while the others were full articles with an average length of 13 pages.

The accepted papers of the 28th ICANN conference were published as five volumes:

Volume I Theoretical Neural Computation

Volume II Deep Learning

Volume III Image Processing

Volume IV Text and Time series analysis

Volume V Workshop and Special Sessions

The authors of accepted articles came from 50 different countries. While the majority of the articles were from academic researchers, the conference also attracted contributions from manifold industries including automobile (Volkswagen, BMW, Honda, Toyota), multinational conglomerates (Hitachi, Mitsubishi), electronics (Philips), electrical systems (Thales), mobile (Samsung, Huawei, Nokia, Orange), software (Microsoft), multinational (Amazon) and global travel technology (Expedia), information (IBM), large (AstraZeneca, Boehringer Ingelheim) and medium (Idorsia Pharmaceuticals Ltd.) pharma companies, fragrance and flavor (Firmenich), architectural (Shimizu), weather forecast (Beijing Giant Weather Co.), robotics (UBTECH Robotics Corp., SoftBank Robotics Group Corp.), contract research organization (Lead Discovery Center GmbH), private credit bureau (Schufa), as well as multiple startups. This wide involvement of companies reflects the increasing use of artificial neural networks by the industry. Five keynote speakers were invited to give lectures on the timely aspects of intelligent robot design (gentle robots), nonlinear dynamical analysis of brain activity, deep learning in biology and biomedicine, explainable AI, artificial curiosity, and meta-learning machines.

These proceedings provide a comprehensive and up-to-date coverage of the dynamically developing field of Artificial Neural Networks. They are of major interest both for theoreticians as well as for applied scientists who are looking for new

innovative approaches to solve their practical problems. We sincerely thank the Program and Steering Committee and the reviewers for their invaluable work.

September 2019

Igor V. Tetko  
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## **Keynote Talks**



# **Recurrent Patterns of Brain Activity Associated with Cognitive Tasks and Attractor Dynamics (John Taylor Memorial Lecture)**

Alessandro E. P. Villa

NeuroHeuristic Research Group, University of Lausanne,  
Quartier UNIL-Chamberonne, 1015 Lausanne, Switzerland  
[alessandro.villa@unil.ch](mailto:alessandro.villa@unil.ch)  
<http://www.neuroheuristic.org>

The simultaneous recording of the time series formed by the sequences of neuronal discharges reveals important features of the dynamics of information processing in the brain. Experimental evidence of firing sequences with a precision of a few milliseconds have been observed in the brain of behaving animals. We review some critical findings showing that this activity is likely to be associated with higher order neural (mental) processes, such as predictive guesses of a coming stimulus in a complex sensorimotor discrimination task, in primates as well as in rats. We discuss some models of evolvable neural networks and their nonlinear deterministic dynamics and how such complex spatiotemporal patterns of firing may emerge. The attractors of such networks correspond precisely to the cycles in the graphs of their corresponding automata, and can thus be computed explicitly and exhaustively. We investigate further the effects of network topology on the dynamical activity of hierarchically organized networks of simulated spiking neurons. We describe how the activation and the biologically-inspired processes of plasticity on the network shape its topology using invariants based on algebro-topological constructions. General features of a brain theory based on these results is presented for discussion.

# Unsupervised Learning: Passive and Active

Jürgen Schmidhuber

Co-founder and Chief Scientist, NNAISENSE, Scientific Director,  
Swiss AI Lab IDSIA and Professor of AI, USI & SUPSI, Lugano, Switzerland

I'll start with a concept of 1990 that has become popular: unsupervised learning without a teacher through two adversarial neural networks (NNs) that duel in a mini-max game, where one NN minimizes the objective function maximized by the other. The first NN generates data through its output actions while the second NN predicts the data. The second NN minimizes its error, thus becoming a better predictor. But it is a zero sum game: the first NN tries to find actions that maximize the error of the second NN. The system exhibits what I called "artificial curiosity" because the first NN is motivated to invent actions that yield data that the second NN still finds surprising, until the data becomes familiar and eventually boring. A similar adversarial zero sum game was used for another unsupervised method called "predictability minimization," where two NNs fight each other to discover a disentangled code of the incoming data (since 1991), remarkably similar to codes found in biological brains. I'll also discuss passive unsupervised learning through predictive coding of an agent's observation stream (since 1991) to overcome the fundamental deep learning problem through data compression. I'll offer thoughts as to why most current commercial applications don't use unsupervised learning, and whether that will change in the future.

# **Machine Learning and AI for the Sciences— Towards Understanding**

Klaus-Robert Müller

Machine Learning Group, Technical University of Berlin, Germany

In recent years machine learning (ML) and Artificial Intelligence (AI) methods have begun to play a more and more enabling role in the sciences and in industry. In particular, the advent of large and/or complex data corpora has given rise to new technological challenges and possibilities.

The talk will connect two topics (1) explainable AI (XAI) and (2) ML applications in sciences (e.g. Medicine and Quantum Chemistry) for gaining new insight. Specifically I will first introduce XAI methods (such as LRP) that are now readily available and allow for an understanding of the inner workings of nonlinear ML methods ranging from kernel methods to deep learning methods including LSTMs. In particular XAI allows unmasking clever Hans predictors. Then, ML for Quantum Chemistry is discussed, showing that ML methods can lead to highly useful predictors of quantum mechanical properties of molecules (and materials) reaching quantum chemical accuracies both across chemical compound space and in molecular dynamics simulations. Notably, these ML models do not only speed up computation by several orders of magnitude but can give rise to novel chemical insight. Finally, I will analyze morphological and molecular data for cancer diagnosis, also here highly interesting novel insights can be obtained.

Note that while XAI is used for gaining a better understanding in the sciences, the introduced XAI techniques are readily useful in other application domains and industry as well.

# **Large-Scale Lineage and Latent-Space Learning in Single-Cell Genomic**

Fabian Theis

Institute of Computational Biology, Helmholtz Zentrum München (GmbH),  
Germany

<http://comp.bio>

Accurately modeling single cell state changes e.g. during differentiation or in response to perturbations is a central goal of computational biology. Single-cell technologies now give us easy and large-scale access to state observations on the transcriptomic and more recently also epigenomic level, separately for each single cell. In particular they allow resolving potential heterogeneities due to asynchronicity of differentiating or responding cells, and profiles across multiple conditions such as time points and replicates are being generated.

Typical questions asked to such data are how cells develop over time and after perturbation such as disease. The statistical tools to address these questions are techniques from pseudo-temporal ordering and lineage estimation, or more broadly latent space learning. In this talk I will give a short review of such approaches, in particular focusing on recent extensions towards large-scale data integration using single-cell graph mapping or neural networks, and finish with a perspective towards learning perturbations using variational autoencoders.

# **The Gentle Robot**

Sami Haddadin

Technical University of Munich, Germany

Enabling robots for interaction with humans and unknown environments has been one of the primary goals of robotics research over decades. I will outline how human-centered robot design, nonlinear soft-robotics control inspired by human neuromechanics and physics grounded learning algorithms will let robots become a commodity in our near-future society. In particular, compliant and energy-controlled ultra-lightweight systems capable of complex collision handling enable high-performance human assistance over a wide variety of application domains. Together with novel methods for dynamics and skill learning, flexible and easy-to-use robotic power tools and systems can be designed. Recently, our work has led to the first next generation robot Franka Emika that has recently become commercially available. The system is able to safely interact with humans, execute and even learn sensitive manipulation skills, is affordable and designed as a distributed interconnected system.

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