



IWANN INTERNATIONAL
WORK CONFERENCE
ON ARTIFICIAL NEURAL NETWORKS

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JUNE 19-21, 2023

ABSTRACT PROCEEDINGS

19-21 June, 2023

**IWANN INTERNATIONAL WORK CONFERENCE ON ARTIFICIAL NEURAL
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Autores:

Ignacio Rojas

Gonzalo Joya

Andreu Catalá

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Julio Ortega Lopera

More than a friend of IWANN's friends

IN MEMORIAM

IWANN 2023.

Preface.

We are proud to present the set of abstract for the 17th International Work-Conference on Artificial Neural Networks (IWANN-2023), which will take place in June, 19th-21th, 2023 in Ponta Delgada (Sao Miguel, Azores Islands, Portugal).

This gathering will bring people physically together again after 4 years in the one of the most beautiful Atlantic's islands, conducive to creativity and inspiration.

We will continue with the structure of previous editions (Plenary Sessions, Special Sessions, Tutorials on relevant topics and Open Discussion forum), favouring the connection/interaction among attendees to facilitate the debate.

IWANN is a biennial conference that seeks to provide a discussion forum for scientists, engineers, educators, and students about the latest ideas and realizations in the foundations, theory, models, and applications of hybrid systems inspired by nature as well as in emerging areas related to these topics. As in previous editions of IWANN, this year's conference aimed to create a friendly environment that could lead to the establishment of scientific collaborations and exchanges among attendees. As in previous editions, we strongly emphasize the wide range of topics comprised under the umbrella of IWANN2023 and, in particular, we focus on trending topics such as Deep Learning and Ethics in AI. It's confirmed one tutorial about "From Deep Learning to Deep Understanding".

Since the first edition in Granada (LNCS 540, 1991), the conference has evolved and matured. The list of topics in the successive Call for Papers has also evolved, resulting in the following list for the present edition:

1. **Mathematical and theoretical methods in computational intelligence.** Mathematics for neural networks. RBF structures. Self-organizing networks and methods. Support vector machines and kernel methods. Fuzzy logic. Evolutionary and genetic algorithms.
2. **Deep Learning.** Deep Learning applied to Computer Vision. Deep Learning and Time Series Forecasting. Deep Learning and Biomedicine. New advances in Deep Learning.
3. **Neurocomputational formulations.** Single-neuron modelling. Perceptual modelling. System-level neural modelling. Spiking neurons. Models of biological learning.
4. **Learning and adaptation.** Adaptive systems. Imitation learning. Reconfigurable systems. Supervised, non-supervised, reinforcement, and statistical algorithms.
5. **Emulation of cognitive functions.** Decision-making. Multi-agent systems. Sensor mesh. Natural language. Pattern recognition. Perceptual and motor functions (visual, auditory, tactile, virtual reality, etc.). Robotics. Planning motor control.
6. **Bio-inspired systems and neuro-engineering.** Embedded intelligent systems. Evolvable computing. Evolving hardware. Microelectronics for neural, fuzzy, and bioinspired systems. Neural prostheses. Retinomorphic systems. Brain-computer interfaces (BCI), Nanosystems. Nanocognitive systems.
7. **Advanced topics in computational intelligence.** Intelligent networks. Knowledge-intensive problem-solving techniques. Multi-sensor data fusion using computational intelligence. Search and meta-heuristics. Soft computing. Neuro-fuzzy systems. Neuro-evolutionary systems. Neuro-swarm. Hybridization with novel computing paradigms.
8. **Applications.** Expert systems. Image and signal processing. Ambient intelligence. Biomimetic applications. System identification, process control, and manufacturing. Computational biology and bioinformatics. Parallel and distributed computing. Human computer interaction, Internet modeling, Communication and networking. Intelligent systems in education. Human-robot interaction. Multi-agent systems. Time series analysis and prediction. Data mining and knowledge discovery. Machine Learning for 4.0 industry solutions.

During IWANN 2021, several special sessions were held. Special sessions are a very useful tool for complementing the regular program with new and emerging topics of particular interest for the participating community. Special sessions that emphasize multi-disciplinary and transversal aspects, as well as cutting-edge topics are especially encouraged and welcome, and in this edition of IWANN 2019 comprised the following:

- SS01: Ordinal Classification.
Organized by Victor M. Vargas, David Guijo-Rubio and Pedro A. Gutiérrez
- SS02: Machine Learning in Mental Health.
Organized by: Pepijn van de Ven
- SS03: Interaction with neural systems in both health and disease.
Organized by Pablo Martínez Cañada and Jesus Minguillón Campos
- SS04: Deep Learning applied to Computer Vision and Robotics.
Organized by: Enrique Dominguez, José García-Rodríguez and Ramon Moreno Jiménez
- SS05: Applications of Machine Learning in Biomedicine and Healthcare.
Organized by Miri Weiss Cohen, Daniele Regazzoni and Catalin Stoean
- SS06: Neural Networks in Chemistry and Material Characterization.
Organized by Ruxandra Stoean, Patricio García Báez and Carmen Paz Suárez Araujo
- SS07: Real World Applications of BCI Systems.
Organized by Ivan Volosyak
- SS08: Spiking Neuron Networks: Applications and Algorithms.
Organized by Elisa Guerrero Vázquez and Fernando M. Quintana Velázquez
- SS09: Deep Learning and Time Series Forecasting: Methods and Applications.
Organized by Francisco Martínez Álvarez, Verónica Bolón-Canedo and David Camacho
- SS10: ANN HW-Accelerators.
Organized by Mario Porrman and Ulrich Rückert

The 17th edition of the IWANN conference was organized by the University of Granada, the University of Malaga, and the Technical University of Catalonia.

We would also like to express our gratitude to the members of the different committees for their support, collaboration and good work. We specially thank to our Steering Committee (Davide Anguita, Andreu Catalaj, Marie Cottrell, Gonzalo Joya, Kurosh Madani, Madalina Olteanu, Ignacio Rojas, and Ulrich Rueckert), the Technical Assistant Committee (Miguel Atencia, Francisco García-Lagos, Luis Javier Herrera, and Fernando Rojas), the Program Committee, the reviewers, invited speakers, and special session organizers. Finally, we want to thank Springer and especially Ronan Nugent, and Anna Kramer for their continuous support and cooperation.

June 2023

Ignacio Rojas
Gonzalo Joya
Andreu Catala

IWANN 2023.

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Forecasting passenger demand in competitive railway markets: an approach based on Temporal Fusion Transformer (TFT)^{*}

E.A. Villarrubia-Martin^{1[0009-0002-8006-5711]}, D.
Muñoz-Valero^{2[0000-0002-2509-9911]}, L. Jimenez-Linares^{1[0000-0002-2737-5887]},
and L. Rodriguez-Benitez^{1[0000-0002-7665-943X]}

¹ Escuela Superior de Informática, Universidad de Castilla-La Mancha, Paseo de la
Universidad, 4, Ciudad Real, Spain

² Escuela de Ingeniería Industrial y Aeroespacial, Universidad de Castilla-La
Mancha, Avenida Carlos III, s/n, Toledo, Spain

Abstract. The liberalization of the railway market in the European Union and especially in Spain has led to international competition in the markets that require new and adaptive planning methodologies to respond to demand changes as quickly as possible. In this paper, we present an interpretable competitive passenger rail services demand forecasting model using Temporal Fusion Transformer (TFT). It can predict with promising results the distribution of tickets sold, which can be used to adjust the rail services to maximize the economic benefits while being environmentally sustainable by modifying the ticket prices, the number of different seat classes (e.g. tourist and business class), schedule and frequency of services, among others variables. In addition, expert domain knowledge has been included in the TFT model, such as the location of the stations, meteorological warnings, and their severity, as well as, local, regional, and national holidays that can impact the demand for rail services.

Keywords: Demand forecasting · Railroad transportation · Time series · Deep learning · Explainable AI · Attention mechanisms

1 Introduction

Forecasting passenger demand for rail services is essential for efficient and effective service planning, infrastructure investment, and policymaking. Over the years, various demand forecasting techniques have been developed to capture complex patterns and trends in passenger demand data including time series

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methods, causal models, and machine learning algorithms [1]. However, accurate and interpretable demand forecasting remains a significant challenge due to the complexity of passenger behavior, changing market conditions, and external factors such as special events, holidays and meteorological conditions.

2 Proposed model

The proposed demand forecasting model is based on the Temporal Fusion Transformer architecture (TFT) [2] which incorporates known past inputs (distribution of tickets sold, the hour of the day, day of the week, etc), known future inputs (discounts, holidays, etc) and static covariates (station number, city, geographic location, etc), allowing to capture the complex temporal patterns in passenger demand data while also accounting for external factors that may influence demand. The processing of time-dependent information in the TFT architecture is accomplished through the use of LSTMs for local processing and multi-head attention for integrating information from any time step. Finally, the TFT architecture has been shown to outperform traditional time series models and other machine learning techniques in electricity, traffic, and retail real-world datasets, providing a suitable model for accurate and interpretable demand forecasts for passenger rail services (Figure 1).

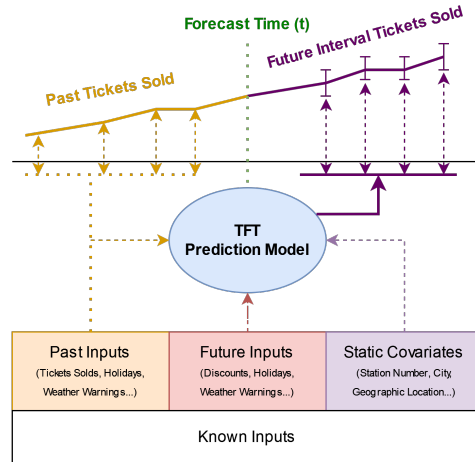


Fig. 1. Demand forecasting model architecture based on TFT [2]

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Frequency, space and time tensor decomposition of motor imagery EEG in BCI applied to post-stroke neurorehabilitation*

Roman Rosipal^{1,2}[0000–0002–0276–4579], Zuzana Roščáková¹[0000–0002–0192–9626],
Natália Porubcová¹, and Leonardo J Trejo²[0000–0003–1025–8585]

¹ Institute of Measurement Science, Slovak Academy of Sciences, Bratislava 84104, Slovakia

{roman.rosipal, zuzana.rostakova, umerporu}@savba.sk

² Pacific Development and Technology, LLC, Capitola CA 95010, USA
ltrejo@pacdel.com
<http://www.pacdel.com>

Abstract. We present a novel method of tensor decomposition of EEG for precise measurement and real-time tracking of narrowband brain oscillations (NBO) for brain-computer interfaces (BCI). To determine NBOs associated with specific limb movements, we used mirror-box therapy, in which users view mirror images of one limb moving to alter the NBO associated with the movement of the contralateral limb. Unlike purely imaginary motion, mirror-box imagery is specific and easy for users to control. Tensor decomposition is a machine-learning algorithm that separates the NBOs present in a multi-channel EEG and provides a spectral-spatial signature for precise measurement of each NBO. Using the signature of a NBO we can track its activity in real time by back-projecting the signature on a live multichannel EEG recording. This enables continuous monitoring of the synchronization and desynchronization of selected NBOs and the construction of an elegant BCI protocol. We applied this approach to rehabilitating post-stroke patients using the BCI control of a robotic splint and a virtual reality avatar hand.

Keywords: Tensor decomposition · Oscillations · Neurorehabilitation.

1 Introduction

A frequently used principle for creating motor imagery BCI protocols is the discrimination of event-related synchronization and desynchronization of sensorimotor rhythms, such as the well-known μ -rhythm. These rhythms have a narrow-band, oscillatory character, and their dominant frequency has high inter-subject variability [1]. Therefore, monitoring the activity of sensorimotor rhythms requires abandoning the generally defined wide-frequency EEG bands, such as 8-12 Hz for α rhythm, and focusing on extracting subject-specific NBOs. Tensor decomposition based on PARAFAC or Tucker models represents an elegant

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solution for extracting and monitoring NBOs in BCI protocols. By introducing frequency and spatial constraints to improve the physiological plausibility of the EEG tensor decomposition, we demonstrated excellent performance of tensor decomposition on simulated, and real EEG data [2]. We validate and discuss the practicality of a system that combines tensor decomposition of EEG and mirror-box therapy in a BCI system to rehabilitate post-stroke patients.

2 Methods

We obtain EEG data for a training set in single subject over several mirror-box therapy sessions. Preprocessing involves cleaning the EEG signal of artifacts and decomposing it into oscillatory and fractal components. Working only with the oscillatory component allows us to suppress the effect of broadband cortical activity, which is an unwanted signal. This is followed by tensor decomposition of the oscillatory component, which extracts latent EEG elements or atoms, each of which has a specific spectral-spatial signature. Incorporating certain constraints on the tensor decomposition ensures that each atom represents a unique NBO [2]. In the mirror-box system, these atoms represent the sensorimotor NBOs associated with the movement observation and reflect the sensorimotor rhythms activated during mental imagery. The atoms derived from the training set are used to start the BCI protocol, and their signatures can be continuously adapted as the neurorehabilitation training continues. We built the given procedure into the BCI process of motor neurorehabilitation using a robotic splint control and avatar hand control tasks in virtual reality (VR).

3 Results

We used the mirror-box, tensor-decomposition BCI system for motor neurorehabilitation training of four post-stroke patients. Two patients controlled a robotic splint and two an avatar hand in the VR. One patient participated in both tasks. The training generally ranged from 10 to 12 days, but we looked at longitudinal effects by training for several months in one patient. Consistent clinical evaluation was part of the training protocol. In our contribution, we will report the performance, user acceptability, clinical results, and overall experience with the concept of tensor decomposition for BCI.

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Reconfigurable Accelerators for Heterogenous Computing in AIoT^{*}

M. Tassemeier¹, M. Porrman¹, R. Griessl², J. Hagemeyer², and P. Trancoso³

¹ Osnabrück University, Germany

² Bielefeld University, Germany

³ Chalmers University of Technology, Sweden

1 Introduction

Efficient processing in the realm of Artificial Intelligence of Things (AIoT) necessitates highly scalable approaches that encompass the entire spectrum of cognitive computing, ranging from embedded devices through the edge to the cloud. This study presents findings related to deep learning accelerators utilizing reconfigurable computing within the H2020 VEDLIoT project [1]. The project emphasizes the significance of Machine Learning (ML), particularly Deep Learning (DL), in IoT, leading to demanding computational and memory needs while maintaining a low energy consumption. The cognitive IoT hardware platform employed in VEDLIoT, known as RECS, is based on a modular microserver architecture that allows for scalable and heterogeneous computing across the cognitive computing continuum.

2 Reconfigurable Accelerators

One of the main topics in VEDLIoT is the development and evaluation of resource-efficient accelerators for deep learning, based on FPGAs, which allow for fine-grained adaptation to a specific application. IP cores like the Deep Learning Processor Unit (DPU), provided by Xilinx, enable the acceleration of a wide variety of deep learning models utilizing a versatile, highly parallel architecture. Other approaches like FINN [3] create specific IP cores for given deep learning models. Within VEDLIoT, the Xilinx DPU is used as a baseline for comparison to own custom developments like FiBHA (Fixed Budget Hybrid CNN accelerator), which provide dedicated engines for the different CNN layers or combinations of layers [2].

A wide variety of FPGAs are already available in the different RECS platforms. In addition to classical reconfigurable SOCs comprising FPGA fabrics and embedded CPUs, the new Versal ACAPs (Adaptive Compute Acceleration Platform) are used. With their integrated AI Engines and a Network-on-Chip

^{*} This publication incorporates results from the VEDLIoT project, which received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957197.

for high-speed data transfer, they promise enhanced performance and energy efficiency. A base design has been developed, abstracting from the different architectures and providing an easy yet efficient integration of different accelerator designs into RECS.

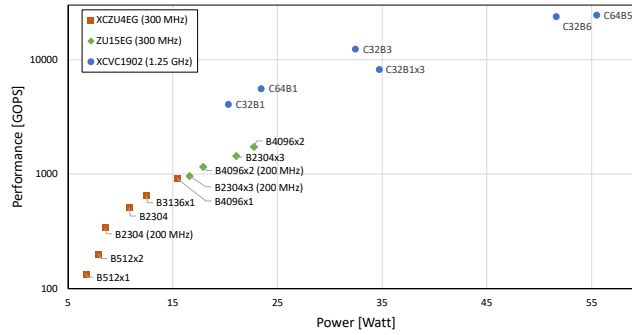


Fig. 1. Performance vs. power for YoloV4 utilizing various DPU variants on different reconfigurable SoCs

Figure 1 shows the performance and power of YoloV4 utilizing different DPUs on three Xilinx devices. The evaluation was performed on two Xilinx UltraScale+ SoCs (ZU4EG and ZU15EG) and on a Xilinx Versal VC1902. The DPU offers different parameters to match the application requirements. One of the most important is the internal parallelism, defining the peak number of operations per clock cycle. For UltraScale+, e.g., the B4096 DPU can perform 4096 INT8 operations per clock cycle. For the Versal architecture, the DPU naming refers to the number of used AI engines and the batch size. The C32B6 DPU, e.g., uses 32 AI engines for each of its six batch handlers. Results show an average efficiency of around $60 \frac{\text{GOPS}}{\text{Watt}}$ for UltraScale+ and up to $460 \frac{\text{GOPS}}{\text{Watt}}$ for specific Versal variants. A special feature of the base design used for integration of the DPUs is the capability for dynamic partial reconfiguration. Hence, the DPU implementation can be changed at runtime based on changing application or environmental conditions, enabling further improvements of energy efficiency.

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Texture Detection with Tactile Sensors based on the Goertzel Algorithm

Raúl Lora-Rivera¹[0000-0002-8746-3117], Óscar Oballe-Peinado¹[0000-0003-1185-4864] and Fernando Vidal-Verdú¹[0000-0002-54598306]

¹ Universidad de Málaga(UMA), Instituto Universitario de Investigación en Ingeniería Mecatrónica y Sistemas Ciberfísicos (IMECH.UMA), Málaga, Spain
fvidal@uma.es

Abstract. This paper focuses on the detection of the texture of an object with smart tactile sensors. To ease the implementation on the embedded electronics of these sensors, the Goertzel algorithm instead of the fast Fourier Transform is considered. Twelve different textures are explored through active touch. A *k-means* classifier is trained with the output of the Goertzel algorithm for eight frequencies and a classification accuracy of 85.4% is achieved.

Keywords: Smart tactile sensors, texture detection, Goertzel algorithm.

1 Introduction

Texture detection with tactile sensors can be done through active touch, that consists of moving the sensor in contact with the texture and processing the so obtained signal. The common procedure to detect textures with active touch is to perform the Fast Fourier Transform (FFT) and use classification algorithms that take the output of the transform as input [1]. However, the implementation of the FFT is complex and requires a lot of hardware resources, as well as high power consumption. For smart tactile sensors with embedded electronics, simpler alternatives that consume less resources are looked for. For instance, an algorithm is proposed in [2] that basically decomposes the signal into frequency bands and calculates the signal power in each band, using the result as the set of input descriptors (one per band) to the classifier. This work explores the use of the Goertzel algorithm as an alternative to the FFT [3]. The Goertzel algorithm is especially interesting for embedded applications if only a reduced set of K frequencies are processed.

2 Materials and Methods

A Cartesian robot with a smart tactile sensor mounted on an artificial finger [4] is used to explore a set of different textures that include fabrics, 3D printed textures, and textures made with laser engraving on methacrylate. The spatial wavelengths of these textures are in the range between 1.3mm and 39mm. 200 vectors with 2048 samples

each are obtained from active touch of the textures at a constant speed of 30mm/s. The Goertzel algorithm in [3] is then computed for K frequencies. It is observed in the frequency spectrum that most information of the signal is concentrated at low frequencies. Therefore, we proposed a non-linear distribution of the K selected frequencies in the spectrum instead of a linear one. 60% of the output vectors from the Goertzel algorithm were used to train a k -means classifier implemented on Matlab®.

3 Results and Conclusion

The remaining 40% of the output vectors from the Goertzel algorithm were used for testing. 85.4% classification accuracy was obtained for $K = 8$, and Fig. 1 shows the confusion matrix. 88.5% accuracy was obtained for $K = 16$. When compared to the FFT, for input vectors of N samples, the Goertzel algorithm has less computational complexity if $K < 2\log_2 N$ and it is less memory-demanding if $K < 4N/7$ [3]. $N = 2048$ in our case, and previous conditions reduce to $K < 22$, so our proposal is advantageous.

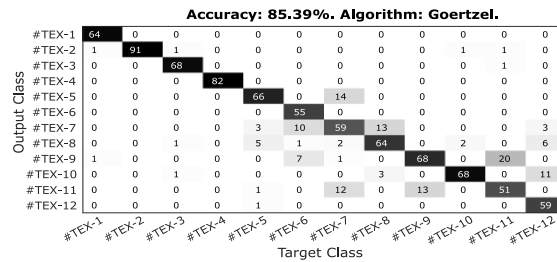


Fig. 1. Confusion matrix obtained from the output of the Goertzel algorithm for eight frequencies and twelve different textures.

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Coordination of Autonomous Mobile Robot Teams with Anticipatory Networks

Andrzej M.J. Skulimowski^{1,2} [0000-0003-0646-2858]

¹AGH University of Science and Technology, Decision Science Dept., 30-059 Kraków, Poland

²International Centre for Decision Sciences and Forecasting
Progress & Business Foundation, 30-048 Kraków, Poland
ams@agh.edu.pl

1 Introduction

This paper shows how recent advances in the theory of anticipatory robotic decisions can be applied to derive new principles of cooperation and compromise decision selection by autonomous harvesting robots. The preference model of autonomous anticipatory decision agents is based on two main assumptions, namely that the decision outcomes and decision scope of temporally ordered agents are linked by an acyclic causal relation. Furthermore, it has been assumed that the decisions of some agents take into account the anticipated solutions of certain future problems. The above assumptions allow the robot team modeler to construct a multigraph of decision problems termed anticipatory networks (ANs) [5]. ANs generalize earlier models of consequence anticipation in multicriteria decision problem solving (Skulimowski 1985) and extend the theory of anticipatory systems of Rosen [1] towards applications in autonomous robotics [2]. Specifically, cooperating robot formations are modelled as evolving (timed) anticipatory networks driven by a discrete event system with a virtual supervisor [6]. It is assumed that robots are endowed with autonomous decision making capacity and the knowledge of other robot decision algorithms.

We will present an application of the above model to establish efficient collaboration of teams consisting of autonomous harvesting robots and human supervisors [7]. This problem is formulated as a bi-level multicriteria optimization problem embedded in an anticipatory network. The optimization criteria at the higher level refer to the overall team performance, such as harvest efficiency and total harvest yield, while at the lower level each robot optimizes its individual criteria of minimal energy consumption and minimal damage. The proposed solution method of this real-life problem refers to the theory of cooperative systems, robot preferences, anticipatory robotics, and supervisory control. We will also present a nested simulation approach that has been implemented to model the anticipatory behavior of an autonomous fruit harvesting robot team. This application refers to an ongoing research project aimed at design, construction and deployment of teamed intelligent and fully autonomous anticipatory fruit picking robots. An illustrative example referring to finding an optimal formation evolution strategy will also be presented. Finally, we will recall how the theory of anticipatory robotic decisions emerged as a parsimonious effect of a foresight project devoted to modelling the AI futures.

2 Basic notions in the theory of anticipatory robot coordination

To build an *anticipatory network* (AN) modelling the coordination of a robot team, we assume that the decisions of some robotic agents determine the scope of future admissible decisions of other agents. This impact is modeled by the causal acyclic relation r . When making their decisions, agents may take into account the forecasted (based on extrapolation or judgments) or anticipated (forecasts based on the knowledge of decision algorithms) solutions of certain future problems. The influence of expectation regarding the future decisions is modelled by another acyclic relation termed anticipatory feedback (AF). Both relations are mutually weakly asymmetric, i.e. $AfB \Rightarrow BrA$ (but not vice-versa) and constitute the basic structure of ANs.

The above assumptions allow the robot team modeler to construct a multigraph of decision problems linked causally and by AF relations. Another key notion for our team coordination approach is *virtual formation* which explores arbitrary relations linking robots in a team. Robots are in a causal virtual formation if their decisions are temporarily ordered and the decision outcomes of some of them influence the scope of decisions of other agents. A causal virtual formation is anticipatory if, in addition, robots make their decisions taking into account their expected consequences on the decisions of other agents. The coordination problem for anticipatory formations consisting of N agents is formulated as a consensus optimization task $(F, F_1, \dots, F_N) \rightarrow \text{opt}$, where the function F is optimized over the set of coordinated actions, $U := U_1 \times \dots \times U_N$, while F_i are defined on U_i . *Anticipatory coordination* consists in making agents to optimize F rather than F_i by an appropriate definition of constraints r in AN. The decision mechanisms of autonomous robots in ANs may also lead to forming a physical formation to accomplish common tasks, with virtual links between the team members.

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What are the ethical paradoxes of using artificial intelligence in online communities?

Cristina Fernandes¹[0000-0001-8560-0758] and Pedro Mota Veiga²[0000-0003-2722-9510]

¹ University of Beira Interior, Department of Management and Economics & NECE Research Unit in Business Sciences, Portugal. Centre for Corporate Entrepreneurship and Innovation at Loughborough University, UK

² Polytechnic Institute of Viseu, Higher School of Education, Portugal
NECE Research Unit in Business Sciences, University of Beira Interior, Portuga

The accelerated and exponential growth of the Internet and consequently the online communities has led the most diverse researchers into making discoveries and advances in highly varied scientific fields, such as healthcare [1], psychology [2], management and marketing [3]. For each respective field, there have been systems and services proposed focused on the needs and interests of their users [4]. Irrespective of such growth, the advantages to this rapid access to the information that online communities provide, both to their users and to their researchers, have drawn concerns over issues around the ethics and safety [5] associated with these communities [1]. Such issues essentially derive from the growing piracy of software [6], which inevitably compromises the trust both of organisations and in organisations [7], given this calls into question the credibility of the information made available by online communities [8]. Furthermore, the growing dependence of society on information technologies combines with the increasing scale, frequency and sophistication of cyberattacks, committed by criminals operating on the Darknet [9]. Another problem faced by these communities interrelates with online aggression, such as cyberbullying, the “calls” for suicides, among other challenges that arise for their users and that they themselves end up following [10]. However, despite the rising concerns over the ethics and the dark side of online communities, we may confirm that there is hitherto no systematic overview of the literature that would enable the identification of just which questions relate to ethics and the dark side of online communities while also grasping their origins and future trends. This therefore verifies the need to undertake a review of the research and provide an integrated, systematic structure to the literature existing on ethics and the dark side of online communities, with this precisely constituting our objective here. Hence, in this study, we apply bibliometric analysis to explore the relational nature of the creation of knowledge in the field of ethics and the dark side of online communities and identifying the different subfields to this theme and characterise them in relation to their underlying assumptions, the research design, contributions to the field and future research trajectories. Our research makes two essential contributions. Firstly, this sets out a quantitative-based methodology on the current research trends into the ethics and the dark side of online communities. This is a step forward in identifying growth and changes in the research field on the ethics and the dark side of online communities and on which future research may focus to further deepen this field of knowledge. Secondly, we contribute to the research on this field, reporting its internal structure, exploring the trends, patterns and trajectories to culminate in a future research agenda. At the general field level, we put forward an organised framework that provides a balance of progress in this field of study. While

we encounter a series of very encouraging developments in the literature on the ethics and the dark sides of online communities, most notably the proliferation of various levels of analysis as well as the diversity of the research questions therein approached, there remains a series of areas that remain lacking in research. At the level of the sub-fields of ethics and the dark side of online communities, we convey how these define future research trajectories.

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A Quantum Computing Artificial Neuron ^{*}

Hernan I. de la Cruz^{1[0000-0001-6445-5256]}, Jesus A. Fernandez¹, Jose J. Paulet^{1[0000-0002-0777-4119]}, Fernando Cuartero^{1[0000-0001-6285-8860]}, and Fernando L. Pelayo^{1[0000-0001-7849-087X]}

Departamento de Sistemas Informaticos. Universidad de Castilla - La Mancha, Albacete-02071, Spain {HernanIndibil.Cruz, . . . , FernandoL.Pelayo}@uclm.es

Abstract. This piece of research presents the first quantum computing implementation of an artificial neuron over continuous domain.

Keywords: Quantum Computing · Artificial Neural Network · Quantum Information Theory

1 Enhancing Tachinno´s quantum neuron model

Four years ago Tachinno et al. proposed in [2] the former quantum computing model of an artificial neuron (McCulloch & Pitts model). This primary proposal ranged over neurons with binary domain which encodes qubits as if they were just bits. Instead, we take advantage of superposition issue when encoding m inputs and m weights by means of N qubits according to $N = \lceil \log_2(m) \rceil$, i.e. we use probability amplitudes of the computational base in order to encode data. Nevertheless, there are a couple of drawbacks coming from quantum mechanics:

1. The values must be normalised to held the sum of probabilities being 1
2. The rest of non used base elements $n - m$ where $n = 2^M$ must be set to 0

Let \vec{i} be the vector of inputs and \vec{w} be the vector of weights. Our state once considered previous two considerations is defined in the following equation:

$$\hat{i} = \begin{bmatrix} i'_1 \\ \vdots \\ i'_n \end{bmatrix} = \left[\frac{i_1}{\|\vec{i}\|} \dots \frac{i_m}{\|\vec{i}\|} (0 \dots 0) \right]^T \quad \hat{w} = \begin{bmatrix} w'_1 \\ \vdots \\ w'_n \end{bmatrix} = \left[\frac{w_1}{\|\vec{w}\|} \dots \frac{w_m}{\|\vec{w}\|} (0 \dots 0) \right]^T$$

$$\forall k \in \mathbf{N}_{\leq m}^* \quad i_k, w_k \in [0, 1] \wedge \|\vec{i}\|, \|\vec{w}\| \neq 0$$

We use an oracle that can set the state vector to a desired arbitrary value for which we follow [1] where the steps needed to create a quantum gate that has the desired amplitudes as its first column, and garbage unknown values in other columns are described. This would let us initialise the state vector as we want, yet we still require computing the effect of weights over inputs, i.e. $\sum_{k=1}^m i_k w_k$.

To do so, we need an oracle with the values of \vec{w} as its first row. Said oracle can follow the same strategy but over the complex conjugate of the numbers we need instead. Afterwards the conjugate transpose must be computed. Applying the inverses of the referred quantum gates in the opposite order will provide us with the appropriate weights oracle. These two processes results in $U_{\hat{i}}$ and $U_{\hat{w}}$:

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$$U_{\vec{i}} = \begin{bmatrix} i'_1 & g_{1,2} & \cdots & g_{1,n} \\ \vdots & \vdots & \ddots & \vdots \\ i'_n & g_{n,2} & \cdots & g_{n,n} \end{bmatrix} U_{\vec{w}} = \begin{bmatrix} w'_1 & \cdots & w'_n \\ g_{2,1} & \cdots & g_{2,n} \\ \vdots & \ddots & \vdots \\ g_{n,1} & \cdots & g_{n,n} \end{bmatrix} \text{ where } g \text{ denotes garbage values.}$$

In order to keep $\|\vec{i}\|, \|\vec{w}\| \neq 0$ we use three extra qubits in this way (the most significant qubits are those most to the "left"):

1. Initialising the Ψ quantum system of $N + 3$ qubits to 0: $|\Psi_1\rangle = |0\rangle$
2. Applying the $U_{\vec{i}}$ gate to the least significant N qubits, leaving the first three untouched: $|\Psi_2\rangle = (I_{2^3} \otimes U_{\vec{i}}) |\Psi_1\rangle = \sum_{k=1}^m i'_k |k-1\rangle$
3. Applying the $U_{\vec{w}}$ oracle over the same qubits: $|\Psi_3\rangle = (I_{2^3} \otimes U_{\vec{w}}) |\Psi_2\rangle = (I_{2^3} \otimes U_{\vec{w}}) \sum_{k=1}^m i'_k |k-1\rangle = \left(\sum_{k=1}^m i'_k w'_k \right) |0\rangle + \sum_{k=1}^{n-1} g''_k |k\rangle$
At this point the probability amplitude associated with the state 0 of the quantum system contains almost what we required to be computed.
4. Applying a *NOT* quantum gate (anti-controlled by the N least significant qubits) to the 3^{rd} qubit: $|\Psi_4\rangle = (I_{2^2} \otimes AC_{N-3} NOT) |\Psi_3\rangle = \sum_{k=1}^{n-1} g''_k |k\rangle + \frac{\sum_{k=1}^m i'_k w'_k}{\|\vec{i}\| \cdot \|\vec{w}\|} |n\rangle$
5. Applying an oracle $U_{\vec{\gamma}}$ similar to $U_{\vec{w}}$ over 2^{nd} and 3^{rd} qubits, where $\vec{\gamma} = \begin{bmatrix} \|\vec{i}\| \cdot \|\vec{w}\| \\ 0 & \gamma_4 \end{bmatrix}$ with γ_4 such that $\|\vec{\gamma}\| = 1$:
 $|\Psi_5\rangle = (I_2 \otimes U_{\vec{\gamma}} \otimes I_n) |\Psi_4\rangle = \frac{\sum_{k=1}^m i'_k w'_k}{m} |0\rangle + \sum_{k=n}^{2^{N+2}-1} g'''_k |k\rangle$
6. Applying a *NOT* q. gate to the first qubit, anti-controlled by the following two qubits: $|\Psi_6\rangle = (AC_2 NOT \otimes I_n) |\Psi_5\rangle = \frac{\sum_{k=1}^m i'_k w'_k}{m} |2^{N+2}\rangle + \sum_{k=n}^{2^{N+2}-1} g'''_k |k\rangle$

The only probability amplitude associated with the first qubit stated to 1 is $\frac{\sum_{k=1}^m i'_k w'_k}{m}$, from which we get:

$$\sum_{k=1}^m i'_k w'_k = \begin{cases} \sqrt{P(M(q_1) = 1)} \cdot m, & \text{if } \|\vec{i}\| \neq 0 \wedge \|\vec{w}\| \neq 0 \\ 0, & \text{otherwise} \end{cases}$$

This shows that we have been able to compute $\sum_{k=1}^m i'_k w'_k$ requiring just $\lceil \log_2(m) \rceil + 3$ qubits, which means an exponential saving on the space computational complexity and a huge improvement on accuracy with respect to Tacchino's binary domain neuron [2].

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Global Feature Importance in Dynamic Environments

Fabian Fumagalli¹, Maximilian Muschalik², Eyke Hüllermeier², and Barbara Hammer¹

¹ Bielefeld University, D-33615 Bielefeld, Germany

² LMU Munich, D-80539 Munich, Germany

Theoretical Background

Black-box machine learning models have shown impressive predictive accuracy in a variety of applications. The increasing use of these models in real-world settings with high-stake decisions yielded a growing interest in their interpretability alongside their predictive performance. Explainable Artificial Intelligence (XAI) emerged to evaluate and understand their reasoning to guarantee reliable deployment. Quantifying feature importance (FI), that is, the contribution of an individual feature to the model’s reasoning, is a well-established method in this field. [1] Recent work has unified FI methods in *removal-based explanations* [2], which consist of three components. First, *feature removal* refers to how a model function is restricted to a subset of features when a group of which is assumed to be unknown. Second, *model behavior* describes a property of the model for which the feature’s contributions are quantified. Third, *summary technique* refers to the aggregation of model behavior evaluated for different features sets to obtain FI scores, often related to cooperative game theory and the Shapley value [2].

Incremental Global Feature Importance

In this work, we are interested in model-agnostic global FI measures, where the model behavior is given as the expected improvement in loss over the mean prediction loss. While removal-based explanations consider a static *batch* learning scenario, recent work has shown the significance of adaptive global FI measures in dynamically changing environments [3,6]. In extreme cases, a model learns in real-time on a data stream, known as *online learning* [4,5]. In this setting, the model observes a new data point, updates the model efficiently and then discards the observation. It is common that the underlying data-generating distribution changes over time, known as *concept drift*, which necessitates substantial changes in the model and consequently the global FI scores. Thus, we seek to update global FI scores incrementally, jointly with the updates of the model itself as illustrated in Figure 1.

Formally, we define a novel mathematical framework that considers incremental global FI and extends on [2] for dynamic environments. Given a model f_t and data-generating random variables (X_t, Y_t) at time t , we aim to explain the

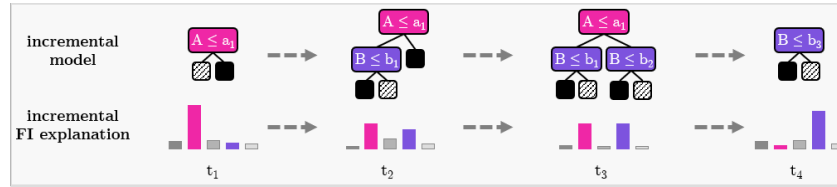


Fig. 1. An incremental model is updated over time resulting in different architectures. Incrementally computing FI scores enables any-time quantification of the model’s state.

improvement in loss over the mean prediction loss $\mu := \mathbb{E}_{Y_t} [\ell(\mathbb{E}_{X_t}[f_t(X_t)], Y_t)]$, i.e. $\nu_t(D) := \mu - \mathbb{E}_{(X_t, Y_t)} [\ell(f_t(X_t), Y_t)]$, where ℓ is a loss function and D the set of features, i.e. the dimensions of X_t . If only a subgroup of features $S \subset D$ is known, we define the restricted improvement in loss with $\nu_t(S) := \mu - \mathbb{E}_{(X_t, Y_t)} [\ell(f_t^S(X_t^{(S)}), Y_t)]$ and $f_t^S(x^{(S)}) := \mathbb{E}_{\tilde{X} \sim \mathbb{P}_t} [f(x^{(S)}, \tilde{X})]$, where $x^{(S)}$ denotes the features of x in S and $\tilde{X} \sim \mathbb{P}_t$ is the distribution of features in $D \setminus S$ at time t , which could also depend on $x^{(S)}$. Our goal is to incrementally update time-dependent FI scores $\phi_t(i)$ for $i \in D$ at time t with $\sum_{i \in D} \phi_t(i) = \nu_t(D)$ by summarizing $\nu_t(S)$ for different $S \subset D$. This already constitutes a difficult task in the static batch setting, as Shapley-based explanations encounter computational limitations [2]. In an incremental learning scenario, however, we describe and address the following additional challenges:

1. Concept drift changes the data-generating distribution (X_t, Y_t) , which affects f_t^S as well as $\nu_t(S)$. Hence the model f_t itself may change significantly over time. This requires a time-dependent weighting mechanism to estimate $\hat{\nu}_t(S)$ and $\hat{\phi}_t$, favoring recent updates over older, possibly out-dated, computations.
2. For feature removal, the time-dependent distribution \mathbb{P}_t must be maintained with minimum storage capacity of previous observations or efficient generative models. This can be achieved with time-sensitive marginal sampling or time-sensitive maintenance of conditional distributions.

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Deep Learning Algorithms For Diagnosis of Coffee Plants Disease

Nameer Baht¹[0009–0006–3684–4629] and Enrique Domínguez^{2,3}[0000–0002–2232–4562]

University of Malaga, Dept. of Computer Science, Malaga, Spain
nameer.m.b.88@gmail.com enriqued@lcc.uma.es

Abstract. Coffee production faces a variety of difficulties, including the prevalence of coffee diseases that cause significant losses in production in terms of quantity and quality. The article aim to identify that artificial neural networks, specifically CNN, are one of the most important algorithms that work effectively in disease detection and image classification compared to other algorithms. this study helps researchers to use deep learning techniques to solve the current problem and classify the most essential and common diseases that affect coffee plants. Based on the Arabica dataset (JMuBEN1) CNN achieved an overall 95% accuracy in diagnosing coffee leaf disease.

Keywords: CNN · Deep Learning · Coffee · JMuBEN Dataset.

1 Introduction

Coffee is grown in 50 countries around the world and consumed on all continents[1]. One of the challenges facing coffee-exporting countries is the spread of diseases and pests that reduce production and lead to a decline in coffee exports[2]. Therefore, deep learning techniques and deep neural networks are the latest revolutions in detecting plant diseases and object detection, taking advantage of their time and effectiveness without the need for people who are experts in detecting and helping poor families who manage cultivation in various countries whose economy depends on the coffee plant. the researchers instead conducted experiments with attribute vectors containing a relatively small number of input elements for the neural network to classify the images of coffee leaves[3].

2 Experimental Results

Convolutional neural networks are, one of the advanced algorithms and techniques for classifying and detecting objects and computer vision[4]. the data set is considered the important and main part of this work to achieve a system capable of detecting diseases that affect coffee plant plants The Arabica dataset (JMuBENnand JMuBEN1) contains(58,555) images that are useful in training and validation during the utilization of deep learning algorithms used in plant

disease recognition and classification. We trained and tested the JMuBEN1 data set that contains (35,964) An image and two classes of diseases healthy and Miner [5]. Figure 1 shows the types of diseases that affect plant coffee. our CNN proposed model shows results of the preliminary comparison showed that our approach is very effective and fast for detection, as the accuracy of the proposed model achieved 95% for detecting coffee diseases.

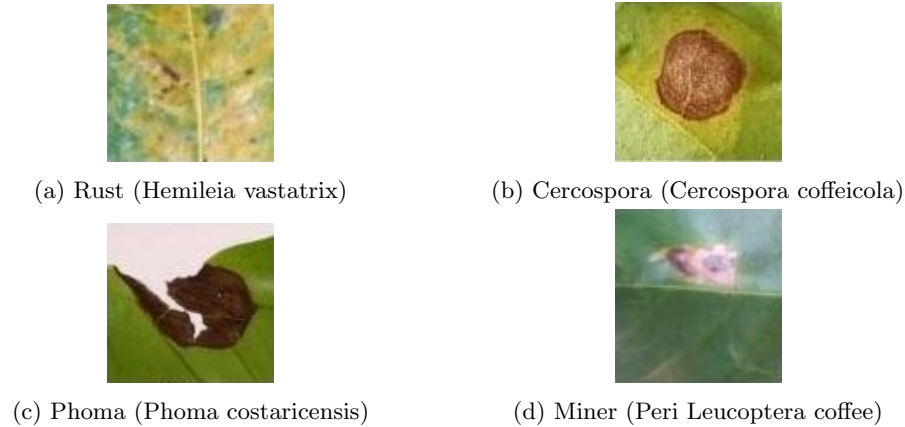


Fig. 1: Most common types of coffee diseases. (a) Color from yellow to brown, (b) bright halo around it, (c) a leaf that turns brown, (d) white caterpillars in the new mines.

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Interpretability of autoencoder latent space for passengers demand-sensitive planning on high-speed railways*

D. Muñoz-Valero¹[0000-0002-2509-9911], E.A. Villarrubia-Martin²[0009-0002-8006-5711], J.A. López-Gómez³[0000-0001-6291-6637], and J. Moreno-García¹[0000-0003-2430-145X]

¹ Escuela de Ingeniería Industrial y Aeroespacial, Universidad de Castilla-La Mancha, Avenida Carlos III, s/n, Toledo, Spain

² Escuela Superior de Informática, Universidad de Castilla-La Mancha, Paseo de la Universidad, 4, Ciudad Real, Spain

³ Escuela de Ingeniería Minera e Industrial de Almadén, Universidad de Castilla-La Mancha, Plaza Manuel Meca, s/n, Almadén, Spain

Abstract. The liberalization of the High-Speed Railway (HSR) passenger market in Spain presents challenges related to infrastructure management and competition among operators. This study proposes a demand-sensitive planning approach using autoencoders (AEs) in order to analyze and represent the underlying characteristics of demand in the latent space. The interpretability of the latent space allows to obtain valuable information from demand which can be used to generate railway services tailored to the needs of consumers.

Keywords: Autoencoder · Latent Space Interpretability · High-Speed Railways · Planning.

1 Introduction

The liberalization of the High Speed Railways (HSR) market in Spain poses a challenge for all parties involved. Different operators must compete for the use of the infrastructure in order to provide their services. In this context, a service can be described as the capacity of a Train Service Provider (TSP) to provide journeys between pairs of stations, catering to specific characteristics such as seat types, schedules, prices, etc. Focusing on the passengers transport on HSR's, an efficient use of the infrastructure is done when the services provided by TSP's (supply) match the potential passengers requirements (demand).

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Adjusting services based on the characteristics observed in demand can lead to a series of benefits, both from the standpoint of efficiency in the use of available infrastructure and economic benefit [1].

Within this context, the main goal of this work focuses on the analysis of the demand data. The information obtained in this analysis could be valuable in order to generate demand-sensitive services, improving the factors discussed above.

2 Methodology

We propose the use of a specific type of neural network known as autoencoders (AEs), applied to demand analysis. An autoencoder is composed by two elements. On the one hand, the encoder must be able to extract and represent the features that define the input, with this information compressed in the bottleneck (latent space). On the other hand, the decoder is then responsible for “decompressing” this information with the ultimate goal to obtain at the output a reproduction as faithful as possible to the input.

The objective is to obtain within the latent space distribution an aggregated representation of the underlying characteristics in demand. Subsequently, an analysis of the obtained latent distribution will be carried out, focusing on the interpretability of this latent distribution. From this analysis, valuable information may be obtained to be used in generating efficient railway services.

To carry out the tests and validations of this study, the use of the RoBin simulator [2] is proposed, which is capable of receiving railway services (supply) and potential passengers (demand) as input, and simulate the aggregation of both parts.

3 Conclusions

The liberalization of the passenger HSR market in Spain entails a series of challenges related to infrastructure management and competition among operators. In this context, a demand-sensitive planning approach is proposed with the goal of offering an efficient supply that aligns with consumers’ needs. To achieve this, the use of an autoencoder is proposed with the aim of obtaining a representation of demand characteristics in the latent space.

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Simulation of HREM crystalline nanoparticles images using Conditional Generative Adversarial Network

Rubén Muñoz García¹, Guillermo Bárcena-González^{1*}, Juan Carlos de la Torre Macías¹, Arturo Ponce² and Pedro L. Galindo¹

¹ Univ. of Cádiz, Department of Computer Science and Engineering, Puerto Real, Cádiz, Spain.
Guillermo.barcena@uca.es

²Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, Texas 78249, USA

Abstract. In the electron microscopy field, sample preparation and the acquisition of images is a complex and expensive task. This exploratory work affords the task of simulating High Resolution Electron Microscopy (HREM) images using a Conditional Generative Adversarial Neural Network (CGAN) for the simulation of nanoparticles. The results obtained are promising and open the way to the generation of large electron microscopy image datasets for deep learning applications.

Keywords: Nanoparticles, Generative Adversarial Network (GAN), Conditional Generative Adversarial Network (CGAN).

1 Introduction

In the field of electron microscopy, more and more effort are being put into the design of high-performance nanomaterials that allow the use of automated methods for the extraction of material features, size, shape and defects, relating them to the characteristics and properties of the materials [1]. This is where Deep Learning [2] comes into play, not without a major problem of requiring a huge set of images for training. Sometimes, collecting many images for this purpose is a simple task. However, in the field of electron microscopy, imaging can become a major constraint for research. To solve this problem, the need arises to create a nanoparticle imager, guaranteeing its speed and without using a high number of resources.

1.1 Conditional Generative Adversarial Network

The first is the generator, which is in charge of generating the synthetic images, while the discriminator tries to find out whether an image is authentic or generated. The generator tries to generate images as detailed and like the real ones as possible, so that the discriminator cannot differentiate them from the real ones. In parallel, the discriminator receives as many real images as the generator generates to distinguish when an image is not real. As both neural networks compete, they become significantly more efficient at solving the task for which they have been trained, even generating significantly realistic images of crystalline nanoparticles (see figure 1). Such networks have

the limitation of not being able to select the kind of image we want to generate. This drawback is solved by using CGAN networks (Conditional Generative Adversarial Networks) [3]. These are like GANs, with the difference that, with them, the generator can elaborate images of a specific class. During the training of the generator, it receives as additional input a condition, making it associate this condition to the generation of a specific type of image.

1.2 Training & Results

A database of 20000 Conventional transmission electron microscopy (CTEM) images has been generated using the ‘Computem’ simulation software [3]. Each image contains a nanoparticle between 1 and 1.5 nanometers on a variable substrate between 2 and 4 nanometers thick. The images have been created at a size of 256x256 pixels to reduce computational time. The training of the CGAN network consists of sending a certain number of nanoparticle images to the discriminator (50% of the images are generated by the generator and the rest belong to the image dataset). The discriminator attempts to determine which of these images are real and which are synthetic. This allows the generator weights to be properly adjusted and to generate images with a higher degree of analogy. On the other hand, the weights of the discriminator are adjusted to extract features from the images that allow them to obtain optimal results.

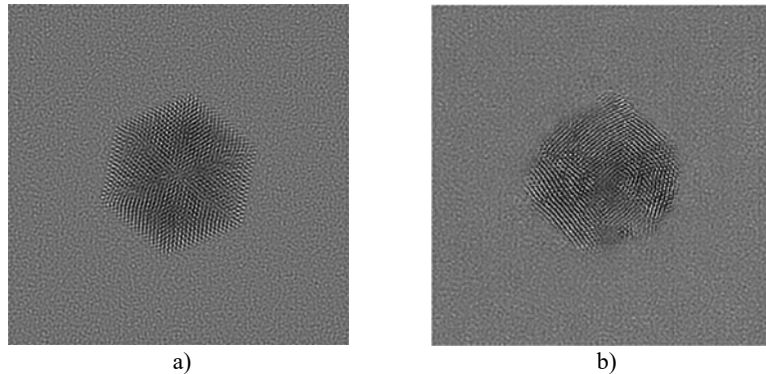


Fig. 1. a) Simulated image of 8-sided nanoparticle. b) Generated image of 8-sided nanoparticle

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Fall Detection in Smart Environments: A Comparative Study between Thermal Cameras and IMU-based Devices

Marcos Lupión¹[0000-0001-7697-8062], Luz López¹, Vicente González-Ruiz¹[0000-0001-6495-4856], Juan F. Sanjuan¹[0000-0002-2874-0903], and Pilar M. Ortigosa¹[0000-0001-6514-6543]

Department of Informatics, University of Almería, CEiA3, Sacramento Road, Almería, 04120, Spain

{marcoslupion,vruiz,jsanjuan,ortigosa}@ual.es
{luzlopez376}@gmail.com

Abstract. Falls are a major concern among older adults due to their declining psychomotor skills, leading to adverse health outcomes and frequent placement in long-term care centers. Smart environments utilizing IoT technology have been developed to detect falls accurately and quickly, enabling older adults to live independently. Wearable devices such as wristbands and cameras have been proposed for this purpose, but limitations such as battery autonomy and privacy concerns can hinder their deployment. In this work, two IMU-based devices and three thermal cameras were deployed in a Smart Home to assess the advantages and disadvantages of each type of device in a common setup. Preliminary results show that both types of devices achieve more than 90% accuracy, indicating a promising performance when used together.

Keywords: Fall detection · IMU · Thermal cameras · Smart Environments

1 Project Statement

As individuals age, their psychomotor skills and reflexes decline, resulting in an increased risk of falls and making falls the second leading cause of death among those over the age of 60 worldwide [5]. Immediate action is necessary to avoid adverse health outcomes in this population [4].

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Smart environments that utilize IoT technology and sensors placed within the environment have been developed to detect falls accurately and quickly, allowing older adults to live independently with the assurance of emergency alerts being sent when needed. Wearable devices such as wristbands are becoming popular and can be used to detect events such as falls using the IMU sensors incorporated in them. Their accuracy can achieve 100% of sensitivity and 97.9% of specificity [2]. However, there exist several limitations such as battery autonomy and invasiveness that can make these devices not to be fully incorporated into real environments. Visible cameras can also be used for this purpose, but concerns regarding privacy can hinder their deployment. Therefore, low-resolution thermal vision sensors have been proposed, providing privacy for the user while still enabling fall detection [3]. These cameras achieve nearly 93% accuracy [1].

The evaluation of these devices has been carried out by different authors and environments in different contexts. Therefore, in this work, we deploy two IMU-based devices (wristband and smartphone) and three thermal cameras in the Smart Home of the University of Almería in order to assess the advantages and disadvantages of each type of device in a common setup.

On the one hand, thermal images from three perspectives were recorded using three IoT devices composed of Raspberry Pi and FLIR Lepton 3.5 cameras. They were synchronized using the MQTT protocol. A Convolutional-LSTM neural network is proposed to identify falls in these images. Images from the three cameras are fused assembling a 3-channel image.

On the other hand, IMU data from a wristband and a smartphone was collected using a custom Wear OS app. From the given signals, two methods are compared: i) a machine learning algorithm using features such as mean, standard deviation, minimum, maximum, and range, and ii) a convolutional neural network processing the raw input signal, with a frequency of 50 Hz.

The experimentation consisted of 6 users simulating falls in the Smart Home of the University of Almería.

Preliminary results show that both types of devices achieve more than 90% of accuracy, showing a very promising performance when used together.

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Automatic recording and processing of saccadic electrooculograms

R. A. Becerra-García¹[0000-0002-6966-6690], G. Joya¹[0000-0001-9256-0870], R. García-Bermúdez²[0000-0002-0643-4745], and F. García-Lagos¹[0000-0002-9664-0832]

¹ University of Málaga, Málaga, Spain {idertator,gjoya,fgl}@uma.es

² Centro Docente de Formación Profesional CENEC, Málaga, Spain
rodgarberm@gmail.com

Keywords: Electrooculogram processing · Saccades identification · Saccadic biomarkers extraction · Machine learning

This work presents the development of a technology that processes human eye movement records in a fully automatic way. Since it is part of a collaboration with the Center for Rehabilitation and Research of Hereditary Ataxias (CIRAH) of Cuba, we focus on records of subjects suffering Spinocerebellar Ataxia type 2 (SCA2). The SCA2 is a neurodegenerative disease which has a very high prevalence in Cuba.

Our research has two complementary objectives: (i) design a fully automatic method to extract the relevant medical data from saccadic eye movement recordings; (ii) design and testing a low-cost device to record eye movements for clinical purposes.

To accomplish the first goal, we have defined a processing pipeline (Fig 1) which comprises the following blocks: filtering, differentiation, segmentation and biomarkers extraction.

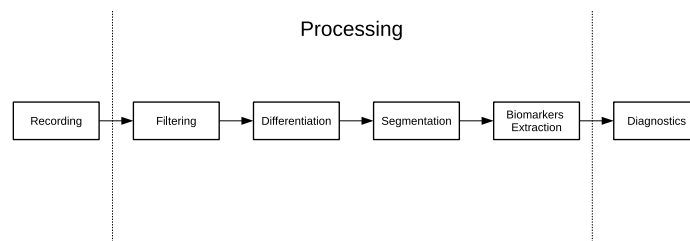


Fig. 1. Electrooculogram processing pipeline

For each one of these blocks, we have analyzed the current methodology employed and obtained a set of methods and algorithms that fit best for our kind of signals. For **Filtering** we have used median filters, which are mostly recommended in the literature on saccadic signals. Numerical **Differentiation**

is used to obtain the velocity profile of the saccadic signals; we have evaluated 16 methods, selecting the Lanczos with 11 points as the best fit for this task [1]. **Segmentation** is the operation where we identify induced saccades (those provoked by the stimulus). First, we separate all saccades (induced and spontaneous) from the rest of spurious events present in the signal by using both Multilayer Perceptron and Random Forest [2] with similar results. Second, we separate induced saccades from spontaneous ones. For this specific task we also evaluate four supervised machine learning techniques: Support Vector Machines (SVM), K-Nearest Neighbors (KNN), Classification and Regression Trees (CART) and Naive Bayes. Among these, we recommend to use CART because its high performance and explainability [3]. Induced saccades are clinically useful because they follow a visual stimulus that allows us to calculate biomarkers which are not computable from spontaneous saccades. Thus, **Biomarker Extraction** is finally carried out obtaining the following relevant clinical biomarkers: peak velocity, latency, duration, amplitude.

To fulfill the second goal, we present the development of a low-cost equipment that uses electrooculography to record eye movements. The hardware part of this equipment is based on the OpenBCI Cyton board, but with our own custom firmware that we named *OpenEOG*. To record and visualize the signals obtained by the *OpenEOG* we developed our own software. In order to use it in clinical environments, this software includes a visual stimulator that allows us to record saccadic eye movements in a controlled way. The system was tested by analyzing the data recorded to 10 healthy volunteers and comparing them against data from professional equipment and results in literature [4].

Our work shows how a fully automatic method can extract the saccadic information required by professional medical doctors to help them study neurological diseases such as SCA2. Also, we have shown that implementing a low-cost eye movement recording system is possible.

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Pilot Program to Attract Talented Students in STEM, with a Focus on Girls

Marta Musté¹ Marta Díaz¹, Xavier Parra¹ and Andreu Català¹

¹ TOC-UPC, Technical University of Catalonia, Vilanova i la Geltrú, Spain.

marta.muste@upc.eu

1 Introduction

STEM (Science, Technology, Engineering, and Mathematics) jobs, particularly in the field of Computer Science and ICT, are in high demand globally. The European Centre of Development for vocational training predicts a 12.8% increase in demand for ICT professionals by 2030. However, despite women comprising nearly half of the workforce, only 27% are working in STEM. The number of women employed in Engineering has remained constant at around 10%, while Computer Science shows a decreasing trend with only 20% women in this field in 2019. This is alarming considering the move towards a digital society where many jobs will be in STEM fields and gender balance is necessary [1].

Despite expressing an interest in STEM fields during their primary and early teenage years, the number of girls pursuing STEM declines rapidly after the age of 15-16. By the time they graduate from university, only 19% of women have STEM-related degrees [2]. Several factors may explain this gender imbalance in STEM. One factor is the lack of role models. With few women in STEM fields, young girls have fewer examples to follow. To address this issue, initiatives like STEAM UPC in Catalonia, aim to attract female talent to study technology and engineering by providing female role models through visits to schools and talks [3]. Another factor is unconscious bias. The stereotype that STEM fields are masculine and humanities and arts fields are feminine can be an obstacle to women's success in STEM. Additionally, media portrayals of STEM fields often feature male characters, making it harder for girls to see themselves in STEM roles [4]. A confidence gap may also contribute to the underrepresentation of women in STEM. Research has shown that girls often lose confidence in math by third grade, while boys are more likely to have strong math skills by second grade. This confidence gap may persist into adulthood and affect women's willingness to take risks and apply for jobs [2]. The lack of supportive social networks and unfriendly academic climate in STEM fields may also discourage women from pursuing careers in STEM. Women faculty in STEM may perceive their academic environment as unwelcoming and threatening, experiencing discrimination and sexual harassment [5].

In conclusion, STEM jobs, especially in ICT, are crucial for the digital society and will continue to be in high demand. However, despite comprising almost half of the workforce, women's representation in STEM fields is low. Achieving gender balance in STEM is necessary for the overall progress of humanity

2 Work line proposed

The Community Driven Technology (TOC) research group at UPC is proposing a cutting-edge pilot program in Catalonia to attract talented students, with a special focus on girls. Our objective is to analyse the outcomes and implement the program in other schools in Catalonia. The program will be specifically designed for children between the ages of 7 and 14 and will include five different modules: Mathematics, Mechanics, Electricity, Electronics-Robotics, and Computer Science. Throughout the academic year, students will complete three activities in each module, providing feedback for each activity. The strategy prepared for the development of a database includes qualitative and quantitative methods in order to get significant knowledge on the levels of: *difficulty*, *stress*, *enjoyment*, and *interest*. The first part of the work will be treated as a transversal study to acquire a general overview of the situation in a few different schools while the second part will be structured as a longitudinal study to analyse the evolution of the proposed activities over time. Such complex database will be processed with the most advanced Machine Learning tools that feeds the typology of data.

We are committed to paying special attention to girls in this program, supporting them to work autonomously and gain confidence in STEM activities, and breaking any gender stereotypes that may exist. *Using the data collected*, we will analyse the results for each student, tracking the evolution of their interest in technology over time to identify their strengths and possible career paths. We will provide support measures for each module to overcome any challenges and avoid letting talented students slip through the cracks due to stereotypes and social influences, particularly in the case of girls. We will empower them to learn from mistakes, and provide essential tools and support to enable them to achieve their goals in STEM fields.

Acknowledgements This work was partially supported by the UPC's Emerging Research Groups Action.

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Enhancing Efficiency at BAMline: Employing Data Science and Machine Learning for X-Ray Research

Martin Radtke, Cafer Tufan Cakir and Ana Guilherme Buzanich

BAM, Richard Willstätter Str- 11, 12489 Berlin, Germany
martin.radtke@bam.de

Abstract. This contributions investigates the use of Bayesian optimization and Gaussian processes at BAMline, a potent synchrotron research tool, to address challenges in data acquisition, processing, analysis, and interpretation. These methods substantially improve beamline component alignment and sample scanning efficiency, enabling researchers to achieve comparable results with fewer measurements and less time. As X-ray research progresses, these techniques will be vital for tackling complex synchrotron data challenges and opportunities.

Keywords: Bayesian Optimization, Active Learning, Synchrotron

1 Introduction

The BAMline[1], BAMs hard X-ray beamline at BESSY, enables the study of matter structure and properties at various scales. As measurement techniques advance, challenges arise in data acquisition, processing, analysis, and interpretation. Data science and machine learning offer solutions, and we have implemented these methods throughout the BAMline's experimental workflow. Successful applications include X-Ray Fluorescence (XRF) quantification via artificial neural networks[2] and coded aperture image reconstruction using mixed-scale dense convolutional neural networks[3]. Limited synchrotron beamline measurement time demands efficiency, with alignment and sample scanning often causing time loss. To address this, we developed routines utilizing Bayesian statistics and Gaussian Processes.

2 Optimisation of Optical Components

Proper component alignment during experiments, such as XANES, is critical yet challenging due to numerous parameters. To optimize parameters like angles and translations of multilayers and crystals, a user-friendly program based on Bayesian optimization with Gaussian processes was developed. This method can handle noise, complex functions, and high-dimensional inputs while providing confidence intervals for predictions. Compared to traditional scanning and manual adjustments, the Bayesian method significantly reduces optimization time (from 30 minutes to 10 minutes) and achieves a 5% higher flux.

3 Active Learning for XRF Scans

Bayesian optimization was applied to XRF scanning for efficient information acquisition in limited time. Compared to standard 2D step scans, continuous scanning schemes and elaborated tracks reduced measurement time, though predefined step sizes and point numbers remained limitations. The Bayesian approach maximized information gain by optimizing point selection. Figure 1 demonstrates the effectiveness of this method, comparing a 8991-point scan to a 2466-point optimized scan, both depicting an extinct cephalopod, an ammonite. Despite the fewer points, a comparable image was achieved with three times fewer measurements.

4 Summary and Outlook

In summary, the integration of Bayesian optimization, Gaussian processes, and the installation of a digital twin have significantly enhanced the efficiency of experiments at BAMline. The future outlook includes the development of further automation in data evaluation and experimental processes, ensuring continued progress in addressing complex synchrotron data challenges.

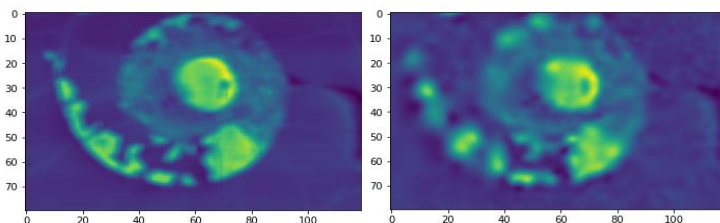


Figure 1: Comparison of an XRF step by step scan with 8991 points on the left and a Bayesian scan with 2466 points on the right.

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On macroscopic observations about COVID-19 mortality in Israel

Manuel Graña, Goizalde Badiola

Computational intelligence group, University of the Basque Country, Spain

The COVID-19 pandemic declared by the WHO in January 2020 has been a strong shock for the entire world at economic, political, and health care levels. Cost of the pandemic response is measured in the orders of trillions of dollars, and the pandemic emergency end has not been declared yet by the WHO. In this context, Israel has been selected by the Pfizer company as the showcase for the effects of its treatments against the disease, being the exclusive preventive treatment applied since early 2021. Recent studies on excess mortality in Israel during the first year of the pandemic show the existence of relevant mortality patterns related to COVID-19 [3] that partially explained the observed excess mortality. Other studies show a definitive impact of the pandemic response on the management and the outcomes of specific pathologies, namely heart failure [1]. Regarding studies about COVID-19 mortality, the predominant approaches in the literature are machine learning models trying to predict the time series on the basis of previous observations independently of other relevant time series (e.g. [2]). In this extended abstract and subsequent presentation at the conference, if accepted, we would like to address the issue of the relation among diverse measures of pandemic evolution on the basis of the data published at the well known ourworldindata.org site (OWD).

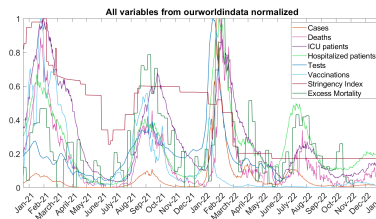


Fig. 1. Joint plot of OWD relevant variables along the pandemic duration, normalized independently in the $[0,1]$ interval.

Figure 1 shows the joint plot of relevant variables extracted from the OWD site as seen first of February 2023. Though the plot has much clutter it is apparent a wave like pattern, where relevant variables show some kind of synchronization. In our presentation we will dissect the correlations and partial synchronization effects that can be observed in the data. Intervention variables are the stringency index and the number of vaccination doses, while the outcomes of the pandemic

that are partially affected by the interventions are the COVID-19 mortality, cases, and Hospitalized and ICU patients. The excess mortality should be also affected by the interventions as long as they affect the COVID-19 mortality. It is well recognized by the scientific community that the immune response produced by the Pfizer-Biontech treatment decays in time, becoming very low three months after injection (e.g. [4]). Paradoxically, the OWD shows that minimal values of COVID-19 mortality, cases, and patients are achieved three months after the surge of vaccination doses, remaining low for some time, i.e. when the protection claimed by the vaccine is at its lowest levels.

Figure 2 shows the heat map of correlations among the pairs of OWD time series as a whole, restricted to the time period after the beginning of the massive vaccination intervention. Notice the positive strong correlation of COVID-19 mortality and ICU patients with the pharmacological intervention variable, among other surprising findings that will be discussed at length in the conference presentation, if this abstract proposal is accepted.

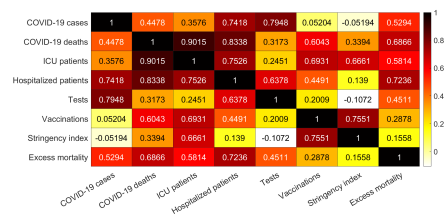


Fig. 2. Correlation between the time series of the OWD variables.

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On the use of artificial neural networks for automatic heliostat aiming^{*}

J.A. Carballo¹[0000-0003-0529-5672], N.C. Cruz²[0000-0002-5839-9451], J. Bonilla¹[0000-0002-2322-2867], J.D. Álvarez³[0000-0003-2791-8105], and M. Berenguel³[0000-0002-3349-7506]

- ¹ CIEMAT - Plataforma Solar de Almería (PSA). Ctra. de Senés km 4.5, E-04200 Tabernas, Almería, Spain
`{joseantonio.carballo,javier.bonilla}@psa.es`
- ² Dept. of Computer Architecture and Technology, University of Granada, Periodista Daniel Saucedo Street, 18071, Granada, Spain
`ncalvocruz@ugr.es`
- ³ Dept. of Informatics, University of Almeria, ceiA3 Excellence Agri-food Campus, 04120, Almería, Spain
`{jhervas,beren}@ual.es`

Abstract. One of the aspects to manage when operating solar power tower plants is the aiming of heliostats. Although the naive approach might be to aim all of them at the center of their receiver, it is inappropriate. Receivers have specific operation conditions, and radiation peaks can reduce their working life. Different strategies deal with this control problem, yet the most established methods still rely on fixed patterns, alarms, and human supervision. Nevertheless, an active research line seeks new control solutions using advanced methods, such as meta-heuristic optimizers and field models. This work tries to develop an advanced automatic control system for heliostat fields. It is based on an artificial neural network trained with an accurate model of the field to keep uniform flux distributions while maximizing the absorbed power. Preliminary results in a model of the Solar Platform of Almería are promising.

Keywords: Solar power tower · Artificial neural network · Automatic aiming.

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1 Project statement

Most countries aim to replace fossil-based energy sources with renewable ones to minimize pollution and reduce external dependencies [4]. Among the alternatives, solar energy is the most abundant resource, and concentrated solar technologies stand out from exploitation methods [2]. Solar power plants (SPT) belong to concentrated solar technologies and offer remarkable conversion efficiency and dispatchability due to the high temperatures reached and energy storage [2].

An SPT deploys mirrors called heliostats that track the sun and concentrate radiation onto a receiver generally placed on top of a tower [2]. A working fluid flows inside the receiver, and once it is hot enough, this fluid serves as the input of a power cycle, e.g., to produce steam and move a turbine. In this context, aiming the set of heliostats is a non-trivial task in which radiation peaks and temperature gradients can end the working life of receivers prematurely [2, 3].

As concisely reviewed in [3], multiple solutions have been designed. The simplest ones rely on plain temperature sensors and a reduced set of possible aiming points, including de-focusing or standby ones (as it is common to oversize the field for low-radiation situations). This kind of strategy is complemented by anomaly detection and human supervision. However, there are more advanced approaches that pay attention to optimizing flux distributions, e.g., by minimizing spillage. For this purpose, meta-heuristic algorithms, such as TABU search, ant colony optimization, and genetic algorithms, are powerful tools [2]. As this kind of method relies on system models, simulating the receiver and its field is also of great importance. For example, the work in [2] culminates the authors' research by combining i) a field-tailored model built through machine learning and accurate ray-tracing with ii) a general-purpose offline aiming tool based on a genetic algorithm, and iii) a closed-loop control logic. Unfortunately, it is necessary to combine multiple complex stages, and there is still room for improvement.

Artificial neural networks can be valuable for automatic heliostat aiming due to their ability to learn patterns implicitly [1]. This work will study the design of a deep neural network to be trained with accurate field-specific models to control a whole heliostat field autonomously. Preliminary results in a model of the Solar Platform of Almería, Spain, are promising.

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Adaptive Surrogate Modelling in Continuous Black-Box Optimization

Jiří Tumpach¹, Jan Koza², and Martin Holeňa³

¹ Faculty of Mathematics and Physics, Charles University Prague, Czech Republic

² Faculty of Information Technology, CTU Prague, Czech Republic

³ Institute of Computer Science, Czech Academy of Sciences, Prague, Czech Republic

A crucial kind of real-world optimization tasks is nowadays *black-box optimization*, i.e. optimization of objective functions for which no analytical description is provided. Black-box optimization methods are most often evolutionary and typically need many values of the objective function. This is a problem if evaluating the black-box objective function is time-consuming and/or expensive, e.g. if it is evaluated empirically in experiments. For example, for the tasks described in the book [1], the evaluation of a comparatively small generation of a genetic algorithm can sometimes take more than a week and cost more than 10000 €. To tackle such problems In continuous optimization, an approach called *surrogate modelling* has emerged more than 20 years ago. It evaluates the true, black-box objective function only in some points and evaluates a suitable regression model, surrogate of the true objective, in all remaining points. The model is trained on points with known value of the true objective. Apart from the model itself, surrogate modelling always needs a strategy when to evaluate the true objective function and when the model, which is in the context of evolutionary black-box optimization usually called evolution control. .

This extended abstract reports a recently started investigation into combinations of several evolution control strategies with a large number of surrogate models, including various kinds of composed models, which is a comprehensive continuation of the research reported in [6]. Like in [6], the employed optimization method is the state-of-the-art method for single-objective unconstrained continuous black-box optimization, the Covariance matrix adaptation evolution strategy (CMA-ES) [4]. However, the present research is performed within the framework of adaptive surrogate modelling, when the surrogate model and evolution control to be used are updated in every iteration of CMA-ES.

In the reported work-in-progress research, the following aspects of adaptive surrogate modelling for CMA-ES are investigated:

1. *Surrogate models* of the kinds polynomial, Gaussian process (GP) using as covariance function some of the kernels considered in [7], and random forest. In addition, models obtained using composition of functions: GPs with covariance functions composed according to the general approach proposed in [3], using GP as the last layer of a MLP [8], and deep GPs [5].
2. The four *evolution control* strategies considered in [6].
3. If the output of the surrogate model is produced by a GP, four different *acquisition functions* according to which the evolution control in 2. determines the points to evaluate the true objective function.
4. Two ways of measuring *predictive error* on validation data. Both of them take into account the invariance of CMA-ES to order-preserving transformations: (i) ranking difference error [2], (ii) several Euclidean-space distances between

the actual sequence of data and its reordering according to the values of the objective function.

5. *Classification* of the considered combinations of surrogate model, evolution control and acquisition function from 1.-3. with respect to their optimality as well as with respect to 99 %, 95 % and 90 % suboptimality. As classifiers serve a classification tree, an RF, a support vector machine (SVM) and an RF-SVM team, each of which is combined with every measure of predictive error considered in 4. In addition, for each of the four considered classifiers, their combinations with all considered measures are aggregated to teams according to those measures. Notice that for the RF-SVM team, this second aggregation leads to a hierarchical team.

In expensive black-box optimization, the evaluation of the true objective function needs many orders of magnitude more time than training any surrogate model. Therefore, the final objective of the reported research is to develop a surrogate-assisted version of CMA-ES that between each two iterations trains a large preselected set of combinations of values of the aspects 1.-3., among which a given classifier using a given measure of predictive error selects the one to determine the points in which the true objective function will be evaluated. With respect to the aspects 4. and 5., we investigate how suitable for this purpose each classifier-measure combination is.

The reported research started recently, that is why only some preliminary results could be obtained so far, though already including some unexpected ones, such as that the combination of GP and MLP proposed in [8] seems not to decrease the predictive error. Till the time of the conference, substantially more results should be available, which could shed further light at the relationship between surrogate models and evolution control, as well as at the suitability of particular classifiers and measures of predictive error for adaptive surrogate modelling in the context of CMA-ES.

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