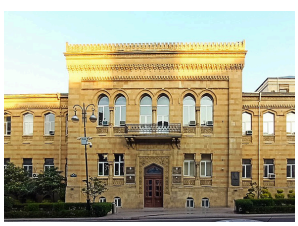
FOURTH INTERNATIONAL BILATERAL WORKSHOP ON NATURAL SCIENCE BETWEEN DOKUZ EYLUL UNIVERSITY AND AZERBAIJAN NATIONAL ACADEMY OF SCIENCES

ABSTRACT BOOK

DECEMBER 23, 2025 | ONLINE (ZOOM)

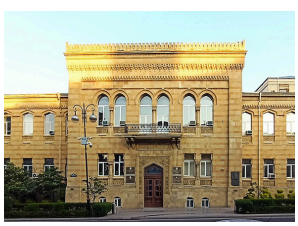
Contents



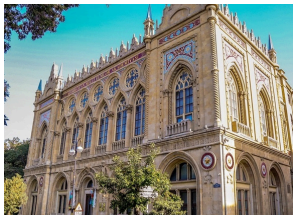



Contents






Contents

WORKSHOP PROGRAMME

OPENING SPEECHES

09:45-10:00 Aylin ALIN, Dean (DEU)
İsa HABIBBEYLI, President (AMEA)
İrada HUSEYNOVA, Vice President (AMEA)
Hamdi Şükür Kılıç, Vice-Rector (DEÜ)

10:00-10:05 **Workshop Group Photo (Online)**

10:05-10:35
"Lasers and Their Applications"
Hamdi Şükür Kılıç

10:35-11:05
"Electron Transfer in Photosystem II and Chlorophyll Fluorescence"
Yashar Feyziyev

BIOLOGY SESSION

11:10-12:30

Moderator: Dr. Gulnar Abdullayeva, Prof. Dr. Tamer Albayrak

11:10-11:30
"Studying Biochemical Responses of Tomato Varieties to Drought Stress and Subsequent Rehydration"
Naima Niyazova, Durna Aliyeva, Irada Huseynova

11:30-11:50
"Future Therapeutic Strategies in Cancer Treatment"
Muhammet Karaman

11:50-12:10
"Oxidative Stress-Linked Expression Dynamics of Key SOD Genes Throughout Drought-Driven Senescence"
Turana Isgandarova, Irada Huseynova

12:10-12:30
"Integrated Computational Analysis of the Impacts of Estrogen Metabolism on the BMP Pathway in the Context of Breast Cancer"
Mustafa İlhan

CHEMISTRY SESSION

11:10-12:30

Moderator: Prof. Dr. Ibadulla Mahmudov, Assoc. Prof. Elif Ant Bursalı

11:10-11:30
"Synthesis and Study of New Cu Complexes Based on Pyrazole and Dicyandiamide"
Ibadulla Mahmudov, Gunay Alizade, Vagif Farzaliyev, Afsun Sujayev

11:30-11:50
"Synthesis, Spectroscopic Characterization, and X-Ray Crystal Structures of Novel Halogenated Thiophene-Based Metal(II) Chelates"
Ozan Ali Dündar, Elif Subaşı , Serkan Öncüoğlu, Cevher Gündoğdu Hızlıateş, Aslı Şahiner, Ceylan Mutlu Balcı

11:50-12:10
"Biphenyl-Based Phenanthroimidazole Derivative: Synthesis, Antimicrobial Activity, DFT and Docking"
Vagif Abbasov, Ayaz Mammadov, Ulviyya Yolchuyeva, Emil Aydinsoy

12:10-12:30
"A Tutorial on Mass Spectrometric Imaging"
Şükrü Gökhan Elçi

COMPUTER SCIENCES SESSION

11:10-12:30

Moderator: Prof. Dr. Anar Rahimov, Asst. Prof. Erdem Alkım

11:10-11:30
"A Rag-Supported Hybrid Assessment Model For Coding Instruction in Higher Education"
Aynur Aliyeva

11:30-11:50
"Integration of Large Language Models into Multi-Agent Systems: Collaboration, Software Verification Processes, and Application Examples"
Esi Aşkın,Minel Üstgel, Barış Tekin Tezel

11:50-12:10
"On a Viewpoint-Invariant Algorithm for Identifying Infrastructure Objects from Images"
Ulviyya Goyushova, Ali Abbasov, Adalat Pashayev, Elkhan Sabziev

12:10-12:30
"On the Development of Python Library for FN-DBSCAN Clustering Algorithm"
Onur Mert Celdir, Efendi Nasiboglu

MATHEMATICS SESSION

11:10-12:30

Moderator: Prof. Dr. Başak Karpuz, Dr. Afig Mammadov

11:10-11:30
"A Study of the Isoperimetric Problem for Quadratic Variational Functionals under Jacobi-Type Conditions"
Narmina Gubatova

11:30-11:50
"Persistent Sannia Motions"
Derya Bayrıl Aykut

11:50-12:10
"t-Basicity of System from Generalized Faber Polynomials and Applications to Bochner–Smirnov Classes"
Sabina Sadigova

12:10-12:30
"Extremal Properties of Fractional Torsional Rigidity on Metric Graphs"
Sedef Özcan

PHYSICS SESSION

11:10-12:30

Moderator: Prof. Dr. Elchin Huseynov, Prof. Dr. Yusuf Yüksel

11:10-11:30
"Polaritonic Enhancement of Nonlinear Optical Response in 2D Materials"
Fadıl İyikanat, F. Javier García de Abajo

11:30-11:50
"New Generation of Optical Sensors: Status and Prospects"
Azer Sadigov

11:50-12:10
"Critical Dimensional Crossover in Periodically Driven Multilayer Ising Systems"
Erol Vatansever, Mikel Quintana, Andreas Berger

12:10-12:30
"Elemental and Structural Characterization of Nanocrystalline Titanium Carbide by Neutron Activation Analysis and XRD"
Raisa Hakhiyeva

STATISTICS SESSION

11:10-12:30

Moderator: Kaveh Babai, Prof. Dr. Özlem Ege Oruç

11:10-11:30
"A Novel Feature Extraction Method Using Chemosensory EEG for Parkinson's Disease Classification"
Begum Kara Gulay, Neslihan Demirel, Alper Vahaplar, Cagdas Guducu

11:30-11:50
"Research on Soil Fertility through Agrochemical Methods and Mathematical Models (Methodology)"
Yasin Rustamov, Eldar Abbasov

11:50-12:10
"Memory Type Estimator under Systematic Sampling"
Eda Gizem Koçyiğit

12:10-12:30
"Enhancing Conformational Priors for Small Rings in Structural Biology through Computational Energy Analysis"
Lala Ibadullayeva, Fei Long, Garib Murshudov

CLOSING SESSION, 12:30-12:45

PLENARY TALK

Lasers and Their Applications

Hamdi Şükür Kılıç[1]*

[1] *Dokuz Eylul University, Faculty of Engineering, Department of Metallurgical and Materials Engineering, Central Campus, 35390, Buca, İzmir Türkiye.*
* *hamdisukur.kilic@deu.edu.tr*

The most popular windows of science and technology is based on the material science which is set on the interaction of energy with materials which is actually augmented by optical spectroscopy.Optical spectroscopy works with the interaction of energy with materials and cam be defined to be the measurement of the response of the material to the energy when they interacted. In this concepts energy is a key parameter for performing spectroscopy. Laseris one of the most important energy sources to apply in this area of science and technology. The laser has an important and prominent property having the most intense sources of electromagnetic radiation with exceptional spatial and temporalcoherence with fully controlled parameters. After the first laser demonstration with its invention in 1960s, the development progress continuous in laser physicsand engineering, this progress has led to the development of a wide varietyof laser systems,including solid-state, gas, dye, semiconductor, and fiber lasers due to the active medium used to produce laser beam at the categories of continues and pulsed modes.

Laser, are a versatile technology with an output of a bright, intense, parallel, steerable and all parameters are controllable, has enabled its widespread applications over all a numerous scientific, industrial, medical, military and social applications. In material science and manufacturing, lasers are extensively used for precision sensing, detection, cutting, welding, surface modification (micromachining), lithography and additive manufacturing due to their high energy density and non-contact processing capabilities. In medicineand healthcare, lasers play a critical role in diagnostics, imaging, and minimally invasive treatments, including ophthalmic surgery, dermatology, oncology, and photodynamic therapy. Additionally, advanced applications in environmental monitoring, remote sensing, metrology, and fundamental research further demonstrate the broad impact of laser-based techniques.

Recent advances in ultrafast and high-power lasersystems have openednew frontiers in science and technology, enabling the investigation of nonlinear optical phenomena, attosecond dynamics, and extreme states of matter. As laser technology continues to evolve, ongoing research focuses on improving efficiency, compactness, wavelength tunability, and system integration. These developments are expected to further expand the capabilities and applications of lasers, reinforcing their central role in future scientific and technological.

Keywords: Lasers, active medium, stimulated emission, population inversion

Electron transfer in Photosystem II and Chlorophyll Fluorescence

Konul Jumshudlu[1], Yashar Feyziyev[1]*

[1] *Institute of Molecular Biology and Biotechnologies, Ministry of Science and Education of the Republic of Azerbaijan, Izzat Nabiyev 11, AZ1073, Baku, Azerbaijan.*

* *yafeyziyev@imbb.science.az*

Photosystem II (PSII) of oxygenic organisms – plants, algae and cyanobacteria realizes the conversion of light energy into electrochemical energy in series of oxidation-reduction reactions initiated through the absorption of photons by chlorophyll (Chl) molecules. This complex converts light energy into electrochemical energy with ≥98% efficiency. Its photochemical reaction center includes photoactive chlorophyll a molecule P_{680} as primary electron donor, pheophytine (Pheo) as initial electron acceptor and plastoquinone electron acceptor Q_A. The light absorption in the PSII results in the electron transfer from excited photoactive chlorophyll P_{680}^* to plastoquinone Q_A, through the charge separated state $P_{680}^{\bullet+}Pheo^{\bullet-}$. Reduction of Q_A leads to increase in the Chl fluorescence. The changes of Chl fluorescence serves as an indicator of the state of PSII. The Chl fluorescence is also used in the studies of the response of oxygenic species to the various environmental factors. Using the fluorescence techniques, we estimated the energy difference between $P_{680}^*PheQ_A^{\bullet-}$ and $P_{680}^{\bullet+}Pheo^{\bullet-}Q_A^{\bullet-}$ states of the PSII reaction center to be ~0.06 eV. This value is significantly lover than those (~0.12 eV) obtained in earlier studies for the state of PSII with double-reduced Q_A.

It has been shown that the lifetime (recombination) of the $P_{680}^{\bullet+}Pheo^{\bullet-}$ pair, formed when plastoquinone is double reduced, is ≥10 times greater than when plastoquinone is single reduced (recombination of charges, accordingly, occurs at a ≥10 times lower rate). Applications of the Chl fluorescence parameters (F_0, F_V, "maximum quantum efficiency" of PSII) used to evaluate the photochemical activity of the photosynthetic apparatus, and the physiological state of plants are discussed.

Keywords: Photosystem II, electron transfer, fluorescence, quantum efficiency, charge recombination, energy barrier, lifetime.

Acknowledgement: This work was supported by the Ministry of Science and Education of the Republic of Azerbaijan.

BIOLOGY SESSION

Integrated computational analysis of the impacts of estrogen metabolism on the BMP pathway in the context of breast cancer

Mustafa İlhan[1]*

[1] *Dokuz Eylül University, Faculty of Science, Department of Biology, İzmir, Türkiye.*
*mustafa.ilhan@deu.edu.tr

Breast cancer is the most common malignancy and leading cause of cancer-related morbidities among women. Metastasis is responsible for almost 90% of deaths. During metastasis, cancer cells enter the blood/lymph circulation and travel to distant organs to form secondary tumors. The formation of new capillaries through angiogenesis contributes to metastasis by facilitating intravasation/extravasation of cancer cells. Bone morphogenetic proteins (BMPs) are important members of the transforming-growth-factor-beta (TGF-β) superfamily and are mainly known for their role in osteogenesis. Similarly, estrogen modulates the growth and maturation of bone. Interestingly, breast cancer patients with the estrogen receptor-positive subtype have a higher metastasis rate to the bone. However, the impact of estrogen metabolism on the BMP pathway is still poorly understood. Here, we aim to (i) investigate the effects of β-estradiol treatment on the expression of BMP- and TGF-β pathway-related genes in the estrogen receptor-positive human breast cancer cell line MCF7 and (ii) to reveal the respective mechanism of the potential interaction in breast cancer progression. To do this, we plan to follow a computational biology approach by assessing the impact of β-estradiol treatment on DNA accessibility and gene expression by analyzing ATAC-seq, ChIP-seq and RNA-seq datasets, respectively. This will be further supported by validation experiments and functional assays to understand the mechanism of BMP-estrogen interaction in breast cancer progression. Our preliminary results suggest that β-estradiol treatment modulates the regulation of the BMP pathway through the upregulation of an antagonist of the BMP pathway, which has a pro-angiogenic function and suppresses the expression of the majority of BMP-related core genes. Of note, some of them (e.g., BMPR2) have pivotal functions in vascular integrity by limiting endothelial cell proliferation. Therefore, it is also planned to investigate their role in angiogenesis using different functional assays such as in vitro tube formation and 3D bead assay for sprouting.

Keywords: Metastasis, breast cancer, estrogen metabolism, BMP pathway.

Oxidative Stress–Linked Expression Dynamics of Key SOD Genes Throughout Drought-Driven Senescence

Turana Isgandarova[1*], Irada Huseynova[1]

[1] *Institute of Molecular Biology and Biotechnologies, Ministry of Science and Education of the Republic of Azerbaijan, AZ1073, Baku, Azerbaijan.*

* turanaisgandarova@gmail.com

Drought stress accelerates leaf senescence by disrupting redox homeostasis and increasing the accumulation of reactive oxygen species (ROS). To better understand the antioxidant response associated with this process, the expression patterns of Cu/ZnSOD, FeSOD, and MnSOD were evaluated in contrasting wheat genotypes subjected to natural and drought-induced senescence. Contrasting durum and bread wheat genotypes were obtained from the GenBank of the Research Institute of Crop Husbandry. Plants were grown under controlled conditions, and the progression of senescence was monitored at defined developmental stages under both natural and drought treatments. Total RNA was extracted using the Monarch RNA kit, quantified with a NanoDrop spectrophotometer, and converted into cDNA using the LunaScript system. The expression levels of Cu/ZnSOD, FeSOD, and MnSOD were measured by qRT-PCR on a Mic real-time PCR platform and analyzed using the 2^−ΔΔCt method. Cu/ZnSOD and FeSOD showed strong early induction under drought, indicating rapid activation of detoxification pathways in the cytosol and chloroplasts. In contrast, MnSOD exhibited a delayed but pronounced increase during the late stages of senescence, consistent with its mitochondrial role in mitigating oxidative damage. In sensitive genotypes, early repression of all three genes was accompanied by increased lipid peroxidation and decreased membrane stability. These results demonstrate that coordinated expression of SOD genes plays a critical role in reducing oxidative stress and that these genes may serve as potential markers for drought tolerance. Furthermore, the findings confirm that these genes act as promising indicators for identifying wheat genotypes with enhanced resilience during drought-induced senescence.

Keywords: Superoxide dismutase, Cu/ZnSOD, FeSOD, MnSOD, drought stress, leaf senescence, oxidative damage, wheat.

Acknowledgement: This work was supported by the Institute of Molecular Biology and Biotechnologies, Ministry of Science and Education of the Republic of Azerbaijan.

Future Therapeutic Strategies in Cancer Treatment

Muhammet Karaman[1]*

[1] *Dokuz Eylül University, Faculty of Science, Department of Biology, İzmir, Türkiye.*
*muhammet.karaman@deu.edu.tr

Humanity has utilized plant-derived medicinal substances for healing, relief, and pain management since as early as 3300 BC. Today, bioactive compounds obtained from plants and their structural derivatives continue to play a significant role in pharmaceutical development. However, advances in technology have profoundly transformed both therapeutic strategies and drug development processes.

Modern pharmaceuticals now encompass a wide range of classes, including synthetic small molecules, biotechnological therapeutics, peptides and oligonucleotides, nucleic acid–based medicines, and targeted conjugated drugs. The rapid evolution of computer-aided design and artificial intelligence- driven approaches has enabled the development of highly specific, more effective, and pharmacokinetically favorable therapeutic agents. In addition, the success of contemporary treatment modalities depends not only on rational drug design but also on the advancement of drug delivery systems and AI-based diagnostic and therapeutic technologies. The functionalization of nanotechnology-based drug delivery materials has markedly improved therapeutic efficiency by enabling precise targeting and controlled release of active agents. These technological innovations in diagnostics and therapeutics have further accelerated the shift toward targeted and personalized treatment strategies in modern medicine.

Keywords: Drug Discovery, Personalized Treatment, Artificial Intelligence.

Studying Biochemical Responses of Tomato Varieties to Drought Stress and Subsequent Rehydration

Naima Niyazova[1]*, Durna Aliyeva[1], Irada Huseynova[1]

[1] *Institute of Molecular Biology and Biotechnologies, Ministry of Science and Education of the Republic of Azerbaijan, AZ1073, Baku, Azerbaijan.*
*naimeniyazova@gmail.com

Climate change is widely recognized as one of the most critical challenges to global agriculture, with increasing water scarcity and more frequent, severe droughts posing significant threats to crop production. Water scarcity triggers a series of physiological and biochemical changes in plants that play an essential role in their adaptive responses. Tomato (Solanum lycopersicum L.) is one of the most widely cultivated and economically significant vegetable crops due to its global dietary importance and high nutritional value. However, tomato plants are highly sensitive to drought stress, which leads to substantial reductions in yield and a decline in fruit quality. Therefore, investigating the biochemical alterations induced by drought stress and the subsequent recovery processes in tomato plants is of great importance.

In this study, the biochemical responses of ten local tomato varieties to drought stress and their recovery at 3 and 7 days after rehydration were examined. The concentrations of stress markers, including hydrogen peroxide (H_2O_2) and malondialdehyde (MDA), as well as the activities of the antioxidant enzymes ascorbate peroxidase (APX) and guaiacol peroxidase (POX), were determined using spectrophotometric methods. The isoenzyme profiles of these enzymes were analyzed through native polyacrylamide gel electrophoresis.

The contents of H_2O_2 and MDA increased in all drought-exposed tomato plants and subsequently decreased upon rewatering. The activities of APX and POX also exhibited a marked increase under drought stress, followed by a decline after rehydration. 8 constitutive APX isoforms and 2 constitutive POX isoforms were detected, and their activity patterns showed notable modulation in response to drought stress and rewatering in all studied varieties. Understanding the responses of tomato plants to drought and subsequent recovery is essential for screening and selecting drought-tolerant cultivars and for developing strategies to enhance crop productivity under adverse environmental conditions.

Keywords: Drought, tomato, rehydration, antioxidant enzyme

CHEMISTRY SESSION

A Tutorial on Mass Spectrometric Imaging

Şükrü Gökhan Elçi[1]*

[1] *Dokuz Eylul University, Faculty of Science, Department of Chemisty, 35390, İzmir, Türkiye.*

* *sukrugokhan.elci@deu.edu.tr*

The ability to observe structures smaller than the human eye has driven major scientific advances across fields such as materials science, structural biology, forensics, and medical diagnostics. While modern imaging techniques offer impressive spatial resolution, most lack chemical specificity; their signals often cannot be traced to individual molecular species, particularly on complex biological surfaces. Conventional optical and electron microscopy provide detailed visualization of cellular structures but reveal little about underlying biochemical composition such as proteins or metabolites. Labeled imaging approaches, including immunofluorescence, offer molecular insights but remain limited by spectral overlap, labor-intensive preparation, and the scarcity of suitable labels. Given that each cell contains millions of molecular species, these approaches cannot capture a meaningful fraction of its proteome, metabolome, or lipidome.

Yet biochemical changes underpin nearly all diseases, emphasizing the need for techniques that can detect, identify, quantify, and spatially localize large numbers of molecules in situ. Bulk analytical tools like HPLC–MS provide deep molecular information but lack spatial context, obscuring critical variations in tissue microenvironments where molecules can function differently depending on their location and concentration.

Mass Spectrometry Imaging (MSI) has emerged as a powerful method to bridge this gap between molecular depth and spatial resolution. MSI visualizes spatial distributions of atoms and molecules on surfaces and identifies them via mass spectrometry. It offers unmatched molecular information density, high sensitivity, and applicability to chemically complex samples without labels or extensive preparation. Although MSI currently lags behind traditional imaging in resolution and throughput, rapid technological advancements are steadily narrowing this gap, making MSI a promising tool for comprehensive molecular imaging.

Keywords: Mass Spectrometry, Imaging, tissue samples, spatial information.

Synthesis, Spectroscopic Characterization, and X-Ray Crystal Structures of Novel Halogenated Thiophene-Based Metal(II) Chelates

Ozan Ali Dündar[1]*, Elif Subaşı[1], Serkan Öncüoğlu[1], Cevher Gündoğdu Hızlıateş[1], Aslı Şahiner[2], Ceylan Mutlu Balcı[3]

[1] *Dokuz Eylul University, Faculty of Science, Department of Chemisty, 35390, İzmir, Türkiye.*
[2] *Ege University, Faculty of Science, Department of Biology, 35100, Izmir, Türkiye.*
[3] *Gebze Technical University, Faculty of Basic Sciences, Department of Biology, 41400, Kocaeli, Türkiye.*
** o.dundar@deu.edu.tr*

Thiosemicarbazones are a versatile class of Schiff bases valued in medicinal chemistry for their pharmacological activity and ability to overcome multi-drug resistance. Their biological properties can be tuned through transition-metal coordination. This study presents the rational design, synthesis, and full characterization of a new chloro-substituted thiophene thiosemicarbazone ligand (HL) and its Co(II), Zn(II), Ni(II), and Pd(II) complexes. The chloro-thiophene unit was introduced to improve lipophilicity and bioavailability.

Structural characterization was carried out using elemental analysis, FT-IR, UV-Vis, ^{1}H NMR, mass spectrometry, molar conductivity, and single-crystal XRD. Spectroscopic data showed shifts in the C=N and C=S bands, consistent with metal–ligand coordination, while XRD revealed distinct metal-dependent geometries: Co(II) and Zn(II) formed distorted tetrahedral structures with neutral, monodentate HL ligands, whereas Ni(II) and Pd(II) adopted square-planar geometries with the ligand binding in a deprotonated N,S-bidentate mode. Crystal packing was stabilized by hydrogen bonding and π–π interactions.

DFT calculations provided insight into electronic features, with Pd(II) and Ni(II) complexes showing narrower HOMO–LUMO gaps than HL, indicating increased chemical softness. In vitro antimicrobial tests against Gram-positive, Gram-negative, and fungal strains demonstrated that metal coordination markedly enhanced activity via a chelation-driven increase in lipophilicity. The Co(II) complex showed broad-spectrum activity—particularly against Pseudomonas aeruginosa and Candida albicans—while the Pd(II) complex exhibited strong, selective action against Escherichia coli (MIC = 78 µg/mL). Overall, the results support halogen-substituted thiosemicarbazone metal complexes as promising antimicrobial agents.

Keywords: Thiosemicarbazone derivatives, Metal(II) complexes, X-ray crystallography, DFT calculations, Antimicrobial activity.

Enhancing Conformational Priors for Small Rings in Structural Biology through Computational Energy Analysis

Lala Ibadullayeva[1]*, Fei Long[2], Garib Murshudov[1,2]

[1] *Institute of Molecular Biology and Biotechnologies, Ministry of Science and Education of the Republic of Azerbaijan, AZ1073, Baku, Azerbaijan.*
[2] *MRC Laboratory of Molecular Biology, Cambridge Biomedical Campus, CB2 0QH, UK.*
* *lala.ibadullayeva@gmail.com*

In macromolecular crystallography and cryo-EM, accurate three-dimensional(3D) structure determination relies on combining prior stereochemical knowledge with noisy and limited experimental data. Although the use of bond lengths and angles is well established, the use of conformational information-particularly for small, non-aromatic rings-still requires improvement. The main reason is that conformations depend on both bonding and non-bonding interactions. In the case of small rings, additional constraints arise from ring closure, which reduces the degrees of freedom.

The design and use of probability distributions describing conformational variety is the subject of this work. This study builds on earlier research by incorporating computational energy calculations to refine conformational priors for ring systems. Using a Python-based computational pipeline, we generated and assessed the conformational landscape of ensembles for representative ring systems taken from the Crystallography Open Database (COD). The pipeline combines RDKit for conformer generation and geometry optimization with force-field energy calculations, followed by visualization of low-energy conformers. In our work, we observed that one of the most significant limitations of the most widely used schemes for classifying ring systems is the failure to account properly for chirality. Without considering chirality, distinct stereoisomers appear in a single ring class, allowing multiple stereoisomers with the same energy in the conformational library.

This results in many conformations of the same ring class, resulting in inaccurate ring classes. Our findings also emphasize the importance of incorporating stereo chemical specificity when creating conformational priors. The approach adopted here merges high-quality, experimentally derived data from the COD with physics-based energy evaluations to produce an optimized, energy-weighted conformational library. Such energy-weighted conformational libraries may enhance the accuracy of macromolecular structure refinement, particularly for ligand modelling and density fitting when working with low-resolution data.

Keywords: Conformational analysis, ring puckering, computational chemistry, RDKit.

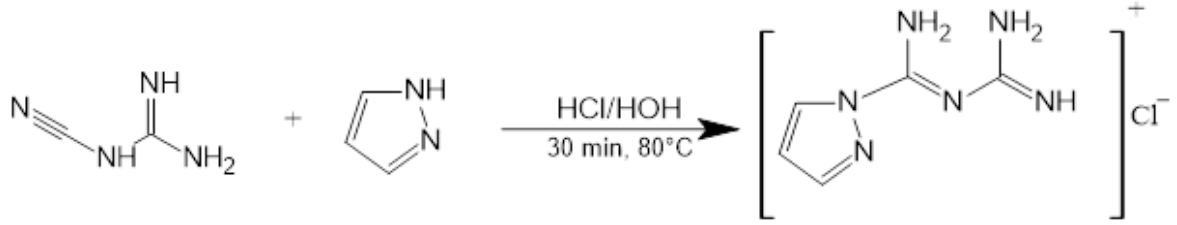
Acknowledgement: This work was supported by the MRC Laboratory of Molecular Biology. Computational resources were provided by the Institute of Molecular Biology and Biotechnologies, Baku, Azerbaijan.

Synthesis and study of new Cu complexes based on pyrazole and dicyandiamide

Ibadulla Mahmudov[1,2]*,Gunay Alizade[3], Vagif Farzaliyev[1], Afsun Sujayev[1]

[1] *Institute of Additive of Chemistry named after Academician A.Guliev, Ministry of Science and Education of the Republic of Azerbaijan, AZ1029, Baku, Azerbaijan.*
[2] *Baku Engineering University, Khirdalan city, 120 Hasan Aliyev Str., AZ0101, Absheron, Azerbaijan.*
[3] *Baku Higher Oil School, Khatai district, White City 1, 5 Khazar Str., AZ1025, Baku, Azerbaijan.*
* *ibadullamahmudov@gmail.com*

Copper (Cu) pyrazole metal-organic frameworks (MOFs) are important materials in reticular chemistry due to the pyrazole ligand's unique ability to form robust, stable, and tunable porous structures with copper ions. This combination leads to a variety of applications across different scientific and industrial fields. Pyrazole based ligand with dicyandiamide was synthesized in water usin hydrochloric acid. (Scheme 1):



Scheme 1. Sysntesis of (E)-N'-carbamimidoyl-1H-pyrazole-1-carboximidamide

Initially, (E)-N'-carbamimidoyl-1H-pyrazole-1-carboximidamide was synthesized. In this reaction Pyrazole, Dicyandiamide, water, and HCl were used in the synthesis of the product in Scheme 1. Following ligand used with Cu-copper metal salt in water to obtain metal complexes . For this processes used salt was $Cu(ClO_4)_2$ $^*6H_2O$ added into water heating and stirring 20 minutes and then addeed into the ligand water mixture. There were obtained some crystals in 2-3days.
Reaction carried out around 20-30 minutes temperature was less than boiling point of water. Reaction scheme salt with pyrazole based ligand
Obtained crystal analysed with FT-IR spectroscopy and result showed there is new compound which is differ from starting ligand.

Keywords: Pyrazole, FT-IR, Ligand.

Acknowledgement: This work was supported by the Azerbaijan Science Foundation - Grant № AEF-BQM-BRFTF-4-2024-5(53)-06/06/4-M-06

COMPUTER SCIENCES SESSION

On the development of Python library for FN-DBSCAN clustering algorithm

Onur Mert Celdir[1]*, Efendi Nasiboglu[1]

[1] *Dokuz Eylul University, Faculty of Science, Deptartment of Computer Science, 35190, İzmir, Türkiye.*

* onurmert.celdir@deu.edu.tr

The clustering problem is one of the most frequently used problems in data science. The aim of clustering is to group samples in a dataset based on similarity and to discover hidden patterns. In this context, there are many algorithms that offer various approaches that may be more suitable for the structure of the dataset. Among these algorithms, the Density-Based Spatial Clustering of Applications with Noise (DBSCAN) algorithm stands out, with its high capacity to distinguish all shapes of data structures and noise points. However, the results of the DBSCAN algorithm are very sensitive to parameters. Optimally adjusting its parameters to achieve accurate clustering results is a challenging process. In 2009, Nasibov and Ulutagay proposed the Fuzzy Neighborhood DBSCAN (FN-DBSCAN) algorithm, an improvement of the DBSCAN algorithm based on fuzzy neighborhood relationships. The FN-DBSCAN algorithm is a more robust algorithm compared to the classical DBSCAN algorithm and can produce accurate results over a wide range of parameters. Although numerous scientific studies have been conducted on the FN-DBSCAN algorithm, a standard Python library for this algorithm was not available. Considering the high interest of researchers in the FN-DBSCAN algorithm, in order to increase its practicality, in this study, a Scikit-learn compatible Python library for the algorithm was developed. The library can be downloaded with the pip install fn-dbscan command and integrated into any Python code with the from fn-dbscan import FN_DBSCAN command. The library is published at https://pypi.org/project/fn-dbscan/, and the user manual and code are available at https://github.com/onurceldir123/fn-dbscan. We believe the developed library will be useful to researchers working in the fields of data science and machine learning.

Keywords: Data science, Machine learning, Clustering, Fuzzy relation, FN-DBSCAN algorithm.

Integration of Large Language Models into Multi-Agent Systems: Collaboration, Software Verification Processes, and Application Examples

Esi Aşkın[1] ,Minel Üstgel[1], Barış Tekin Tezel[1]*

[1] *Dokuz Eylul University, The Graduate School of Natural and Applied Sciences, Department of Computer Science, 35160, İzmir, Türkiye.*

* *baris.tezel@deu.edu.tr*

Multi-Agent Systems (MAS) represent sophisticated computational architectures where multiple intelligent software agents collaborate to execute complex tasks that are often difficult for monolithic systems to handle. Each agent in these systems is characterized by its autonomy, enabling it to perceive its environment, make independent decisions based on its beliefs and goals, and communicate effectively with peers. While traditional agents are proficient in operational tasks, the recent integration of Large Language Models (LLMs) has significantly revolutionized their capabilities, particularly within the critical domain of software verification and validation. By leveraging the advanced natural language processing, context comprehension, and reasoning capabilities of LLMs, agents can now assume more strategic roles in quality assurance, moving beyond simple execution to intelligent analysis.

This study investigates the synergy between LLMs and Multi-Agent Systems, focusing specifically on their application in automating software testing activities. The primary objective is to demonstrate how agents, empowered by LLMs, can autonomously manage the lifecycle of software verification. In frameworks such as JaCaMo, agents interact with LLMs to interpret requirement documents, generate comprehensive test scenarios, and execute test scripts. Crucially, this collaboration extends to the evaluation phase, where agents analyze test outputs and error logs to provide actionable insights. Unlike static testing tools, these intelligent agents establish dynamic feedback loops, iteratively refining their testing strategies based on the LLM's interpretation of previous results.

Moreover, the research critically addresses the inherent challenges of this hybrid approach. Significant issues such as the computational cost of LLM inference, the stochastic nature of model outputs leading to potential inconsistencies, and the necessity for ensuring the reliability of generated test cases are examined in depth. Ultimately, this work provides a comprehensive overview of how LLM-enhanced agent-based approaches are redefining the boundaries of automated software testing in complex environments.

Keywords: Multi-Agent Systems, Large Language Models, Software Verification, Autonomous Testing Processes, LLM Integration.

On a Viewpoint-Invariant Algorithm for Identifying Infrastructure Objects from Images

Ulviyya Goyushova[1,3*], Ali Abbasov[1], Adalat Pashayev[1,2], Elkhan Sabziev[1,2]

[1] *Institute of Control Systems, Ministry of Science and Education of the Republic of Azerbaijan, AZ1141, Baku, Azerbaijan.*
[2] *National Defence University, AZ1065, Baku, Azerbaijan.*
[3] *Faculty of Digital Economics, Azerbaijan State University of Economics, Baku, Azerbaijan.*
* kadaseva.ulviyye@gmail.com

Navigation of a UAV based on images captured by the onboard camera, first of all, implies the identification of known objects in these images. Among such objects, one can mention buildings with characteristic shapes, large water bodies, the outlines of residential and forest areas, rivers, roads, and other objects that remain unchanged or change very little over a certain relevant period of time. For definiteness, in this paper, winding roads are chosen as such objects.

In traditional recognition problems, it is usually assumed that there is a training database containing samples of the object of identification captured from different viewpoints. However, depending on the specifics of the problem, in a number of cases, recognition methods that are invariant to the orientation of the object in the image can also be used. In this case, the volume of the training database is significantly reduced, and the execution time of the algorithm becomes shorter.

From this point of view, it is required that the recognition method used for the identification of winding roads in images be invariant with respect to the viewpoint. In this study, the research object is defined as winding roads that can be represented in the form of straight-line segments, and as object characteristics, the parameters included in the normal equations of the planar lines to which these segments belong, as well as their frequency of occurrence, are used. The calculation of these parameters is carried out in several stages: first, the colored images are converted to grayscale, then to binary (black-and-white) form, and afterward a finite set of three-dimensional elements is constructed by applying the Hough Transform algorithm to these images.

Keywords: UAV navigation, autonomous navigation, pattern recognition, invariant, object identification.

Acknowledgement: This work was supported by the Institute of Control Systems, Ministry of Science and Education of the Republic of Azerbaijan.

A Rag-Supported Hybrid Assessment Model for Coding Instruction in Higher Education

Aynur E. Aliyeva[1*]

[1] *Institute of Control Systems of Ministry of Science and Education of Republic of Azerbaijan*

* aynur.aliyeva@gmail.com

The article explores how retrieval-augmented generation (RAG) can be incorporated into formative assessment within computer science education. Conventional automatic short-answer grading (ASAG) systems rely mainly on text similarity and therefore struggle to analyze the deeper meaning, context, and conceptual accuracy of student responses. To address this limitation, a hybrid framework that integrates RAG with ASAG is introduced. Using enriched assessment criteria, the model evaluates student answers not only linguistically but also in relation to computer science concepts, curriculum resources, and expert-level solution examples. This enables a more objective and transparent evaluation of students' ability to apply knowledge, think critically, and demonstrate creativity.

The short written responses produced by students during coding instruction—such as explaining an algorithm, determining the output of a program, or analyzing a code structure—cannot be reliably evaluated using traditional text-similarity methods. Manual grading of such responses is time-consuming, resource-intensive, and vulnerable to subjectivity and inconsistency. Therefore, automatic short answer assessment (ASAG) systems have been introduced to automate this evaluation process, aiming to replicate human scoring as closely as possible. In traditional ASAG approaches, a student's response to a task x is mapped to a predefined set of scores $y_i \in \{y_1, y_2, \dots, y_n\}$. The goal is to achieve a high level of agreement with human judgment while ensuring efficiency, scalability, and transparency.

In the proposed system, the assessment model is not based solely on the student's response. Instead, the model makes decisions based on the interaction of the following three main components:

$$y_i = F(x_i, I, E),$$

where, is the answer given by the student, is the related information and teaching context related to the question and answer obtained as a result of searching the knowledge base of the subject, and is similar answers, their grades and explanations taken from the expert assessment sample database.

Keywords: Hybrid assessment model, code evaluation, automated grading, automatic short answer assessment (ASAG), RAG technology.

MATHEMATICS SESSION

Extremal Properties of Fractional Torsional Rigidity on Metric Graphs

Sedef Özcan[1]*

[1] *Dokuz Eylül University, Faculty of Science, Department of Mathematics, 35390, İzmir, Türkiye.*
* *sedef.taskin@deu.edu.tr*

Metric graphs equipped with differential operators, often referred to as quantum graphs, serve as versatile models in various fields of mathematical physics and spectral geometry. Within this framework, the torsional rigidity of a domain is a fundamental geometric quantity. In the classical setting involving the standard Laplacian, this quantity is associated with the solution of the Poisson equation with a constant source term and admits clear probabilistic interpretations related to the mean exit time of Brownian motion from the graph. While the spectral and geometric properties of the standard Laplacian on metric graphs are well-established, the extension of these concepts to nonlocal operators remains a developing area of research.

In this talk, recent work focusing on the fractional Laplacian on compact, connected metric graphs is presented. Motivated by the growing interest in nonlocal analysis and anomalous diffusion processes, the concept of fractional torsional rigidity is introduced. It is rigorously defined as the total integral of the fractional torsion function, which arises as the unique solution to a Dirichlet boundary value problem involving the fractional Laplacian.

A primary focus of the presentation is the derivation of upper and lower bounds for this new quantity. By employing surgery principles, such as cutting and gluing edges, explicit upper and lower bounds are obtained for the fractional torsional rigidity across the class of metric graphs with a fixed total length. It is demonstrated that, analogous to the classical case, the path graph (interval) maximizes the rigidity, whereas the flower graph acts as the minimizer.

Keywords: Fractional Laplacian, Metric Graphs, Torsional Rigidity, Nonlocal Operators.

Persistent Sannia Motions

Derya Bayrıl Aykut[1]*

[1] *Dokuz Eylül University, Faculty of Science, Department of Mathematics, 35390, İzmir, Türkiye.*
* derya.bayril@deu.edu.tr

Rigid body motions play a fundamental role in kinematics, motion planning and mechanism design. A deeper understanding of the kinematic and geometric behavior of special rigid-body motions can be useful for potential applications and for designing new systems. Although special motions are often more tractable than general motions, their restrictive nature may limit their applicability in certain contexts. Therefore, expanding the set of special motions can be beneficial, offering valuable insights for both theoretical developments and practical applications.

Sannia motions are a special type of rigid-body motions defined by using the Sannia frame at the striction point of a ruled surface. Since any regular space curve can be seen as a striction curve of its tangent developable or its binormal developable ruled surface, Sannia motions can be defined for any regular space curves. Persistent motions are defined as rigid-body motions whose velocity twist is characterized by a constant pitch, meaning that the ratio between the translational and rotational components of the twist remains invariant under the motion. When this constant pitch is equal to zero, the motion reduces to a Ribaucour motion, a classical subclass in which the instantaneous screw reduces to a pure rotation.

In this work, the kinematic and geometric properties of Persistent Sannia motions will be investigated. First, we derive the necessary and sufficient geometric conditions for a given Sannia motion to be persistent by using its velocity twist. We then investigate on which ruled surfaces, the associated Sannia motions reduce to Ribaucour motions. Furthermore, Sannia motions defined on ruled surfaces with constant invariants will be presented as special examples of Persistent Sannia motions. In particular, this study highlights the relations between Persistent Sannia motions and the classical differential geometry of curves and ruled surfaces.

Keywords: Rigid-body motions, Sannia motions, Persistent motions, Ruled surfaces.

t-Basicity of System from Generalized Faber Polynomials and Applications to Bochner–Smirnov Classes

Sabina Sadigova[1,2*]

[1] *Institute of Mathematics and Mechanics, Ministry of Science and Education of the Republic of Azerbaijan, Baku, Azerbaijan.*
[2] *Department of Mathematics and Digital Technologies, Odlar Yurdu University, Baku, Azerbaijan.*
* *s_sadigova@mail.ru*

In this work, we consider X-valued Lebesgue (Bochner) space $L_p(\Gamma;\mathrm{X}), 1 < p < +\infty$, on the closed, simple Lyapunov (or Radon) curve Γ in the complex plane. The concept of a t-basis is introduced for $L_p(\Gamma;\mathrm{X})$ and the systems from generalized Faber polynomials, associated with the domains intΓ and extΓ are considered. We define certain operators acting on the Hardy–Bochner classes $H_p^{\pm}(X)$ into $L_p(\Gamma;\mathrm{X})$, where X is a UMD (Unconditional Martingale Difference) space, and prove their invertibility by applying t-basicity results for subsystems of the exponential system in the Bochner-Hardy classes $H_p^{\pm}(X)$.
Furthermore, we introduce the X-valued Smirnov classes $E_p^{\pm}(X)$, corresponding to domains intΓ and extΓ respectively. It is proved that the system from Faber polynomials forms t-basis for Smirnov-Bochner classes, and this fact allows us to establish the t-basicity of the double system from Faber polynomials for Bochner spaces for $L_p(\Gamma;\mathrm{X}), 1 < p < +\infty$, where X is a UMD space, some properties of the Smirnov-Bochner classes are also studied.

Keywords: Smirnov-Bochner classes, t-basicity, Faber polynomials.

Acknowledgement: The author would like to express her deepest gratitude to Professor B.T. Bilalov for his valuable guidance throughout this research. This work is supported by the Azerbaijan Science Foundation- Grant No. AEF-MGC-2024-2(50)-16/02/1- M-02.

PHYSICS SESSION

Critical Dimensional Crossover in Periodically Driven Multilayer Ising Systems

Erol Vatansever[1]*, Mikel Quintana[2], Andreas Berger[2]

[1] *Dokuz Eylul University, Faculty of Science, Department of Physics, 35160, İzmir, Türkiye.*

[2] *CIC NanoGUNE BRTA,E-20018 Donastia-San Sebastian, Spain.*

* *erol.vatansever@deu.edu.tr*

We investigate the dimensional crossover of critical behavior in periodically driven multilayer Ising systems by performing large-scale Monte Carlo simulations of the kinetic Ising model. Under a time-dependent external magnetic field, these systems exhibit a dynamic phase transition (DPT), characterized by the scaling properties of a dynamic order parameter. By systematically varying the film thickness and analyzing the distance to the critical point, we determine how the effective critical exponents evolve as the system transitions from two-dimensional (2D) to three-dimensional (3D) regimes.

Our results reveal a clear and continuous crossover: thin films display 2D-like scaling, while sufficiently thick films recover the expected 3D critical behavior. We further compare these findings with those obtained for the thermodynamic phase transition (TPT) in the same multilayer geometry. Although both transitions exhibit dimensional crossover, the onset of 3D-like behavior occurs at noticeably larger thicknesses for the DPT than for the TPT. This demonstrates that the dynamic and thermodynamic transitions are governed by distinct characteristic length scales and that surface effects influence them differently. The slower crossover of the DPT implies a stronger sensitivity to nonequilibrium fluctuations and a more pronounced role of the external driving field. Our observations align with experimental studies on ultrathin Co films, where the dynamic and thermodynamic critical exponents were found to differ significantly.

Altogether, this work provides a comprehensive and unified interpretation of how thin-film geometry, surface contributions, and nonequilibrium driving collectively shape critical behavior. By elucidating the contrasting dimensional crossover properties of the DPT and TPT, we offer valuable numerical outputs relevant to magnetic thin films and other layered nonequilibrium systems.

Keywords: Dimensional crossoever, Monte Carlo simulations, critical exponents, universality.

Polaritonic Enhancement of Nonlinear Optical Response in 2D Materials

Fadil Iyikanat[1]*, F. Javier García de Abajo[2,3]

[1] *Dokuz Eylul University, Faculty of Science, Department of Physics, 35160, İzmir, Türkiye.*
[2] *ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Barcelona, Spain.*
[3] *ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain.*
* *fadil.iyikanat@deu.edu.tr*

Understanding the mechanisms that govern optical response in materials is essential for designing systems with strong nonlinearities at reduced light-intensity thresholds and identifying their potential applications. The emergence of pronounced photon-polariton interaction signatures in the linear optical spectrum of two-dimensional (2D) materials, attributed to the reduction in Coulomb screening and the amplification of quantum-confinement effects, has sparked active research into polaritonic effects in the nonlinear optical response of these materials. In this talk, we will highlight key studies that showcase the nonlinear optical response observed in 2D materials.

We introduce a specific collection of 2D materials, along with a range of excitation modes such as phonons, excitons, and plasmons, which provide a suitable arena for monitoring the interactions between light and matter. Using first-principles methods, including density functional theory (DFT) and post-DFT approaches (e.g., GW and Bethe-Salpeter equation), we reveal the detailed electronic and vibrational properties of 2D materials and predict their optical response in the presence of polaritons. Then, solving the equation of motion either in the time domain or with perturbative approaches, we obtain the nonlinear susceptibilities associated with second- and third-harmonic generation.

In brief, our work demonstrates that various types of polaritons exhibit a robust, optically and electrically controllable nonlinear response in 2D materials. The resulting polaritonic nonlinearities provide a versatile platform for optical manipulation across multiple spectral regimes.

Keywords: 2D materials, Polaritons, Nonlinear optical response, Harmonic generation.

New Generation of Optical Sensors: Status and Prospects

Azer Sadigov[1,2]*

[1] *Institute of Radiation Problems, Ministry of Science and Education of the Republic of Azerbaijan, 9 B.Vahabzade, AZ1143, Baku, Azerbaijan.*
[2] *Innovation and Digital Development Agency of MDDT.*
* *saazik626@gmail.com*

Optical sensors and detectors are key high-technology components in applications ranging from optical communications and high-speed data transmission to the detection of cosmic and elementary particles. Their continued development is driven by the demand for ultra-sensitive, compact, reliable, and energy-efficient photon detection systems capable of operating in harsh environments.

Our research group pioneered micro-pixel silicon detectors, first introduced in 1993 and now known as MAPD (Micro-pixel Avalanche Photodiodes) or SiPM (Silicon Photomultipliers). These solid-state sensors have largely replaced traditional photomultiplier tubes due to their compactness, robustness, low operating voltage, magnetic-field immunity, and compatibility with modern electronics.

Advances in SiPM technology focus on improving photon detection efficiency, timing resolution, scalability, and power consumption. Modern devices offer high gain, single-photon sensitivity, low noise, and seamless integration into pixelated and system-on-chip architectures. Within our recent research, we have developed and experimentally validated high-sensitivity SiPM/MAPD sensors with buried-pixel architectures, high pixel densities, and gains of 10^4–10^5, achieving enhanced photon detection efficiency, reduced optical crosstalk, and improved radiation hardness.

SiPM-based detectors are now widely used in medical imaging, nuclear and radiation physics, LIDAR, environmental monitoring, and advanced scientific and industrial systems. Our group actively contributes to international and regional projects in detector development, supporting both fundamental research and the transfer of innovative technologies into practical applications.

Keywords: Optical sensors and detectors, Micro-pixel Avalanche Photodiodes, Silicon Photomultipliers.

Elemental and Structural Characterization of Nanocrystalline Titanium Carbide by Neutron Activation Analysis and XRD

Raisa Hakhiyeva[1]*

[1] *Institute of Radiation Problems, Ministry of Science and Education of the Republic of Azerbaijan, 9 B.Vahabzade, AZ1143, Baku, Azerbaijan.*

** raisahakhiyeva@gmail.com*

Titanium carbide (TiC) is an advanced ceramic material distinguished by its high mechanical strength, thermal stability, and resistance to radiation damage, making it a promising candidate for nuclear and aerospace applications. At the nanoscale, however, its structural behavior becomes highly sensitive to ionizing radiation, necessitating a detailed investigation of its radiological and crystallographic stability.

Prior to structural analysis, the chemical purity of nanocrystalline TiC was verified using the k_0-based Instrumental Neutron Activation Analysis (k_0-INAA) method. The samples were irradiated in a TRIGA Mark II research reactor at a neutron flux of $2\times10^{13} n\cdot cm^{-2}\cdot s^{-1}$, and induced radionuclides were identified by high-resolution gamma-ray spectrometry. The results confirmed a high degree of chemical purity, with only trace amounts of impurities detected. The induced radioactivity was mainly attributed to minor impurities rather than the TiC matrix itself, ensuring the reliability of subsequent radiation-induced structural interpretations.

Following purity verification, gamma irradiation effects on the crystal structure of TiC nanoparticles were examined by X-ray diffraction (XRD). Structural parameters were evaluated using Rietveld refinement, the Scherrer equation, and the Williamson–Hall approach.

XRD patterns revealed that gamma irradiation does not induce phase transformation, and the face-centered cubic ($Fm\bar{3}m$) structure of TiC remains stable. Nevertheless, diffraction peak broadening and slight peak shifts were observed, indicating lattice expansion, increased microstrain, and radiation-induced defect formation. A decrease in crystallite size and an increase in dislocation density were also determined.

Overall, the combined use of k_0-INAA and XRD provides a comprehensive evaluation of both the radiological behavior and structural response of nanocrystalline TiC under ionizing radiation, confirming its structural stability and suitability for radiation-intensive environments.

Keywords: Nanocrystalline Titanium Carbide (TiC), Ionizing Radiation Effects, k_0-Instrumental Neutron Activation Analysis (k_0-INAA), Gamma Irradiation.

STATISTICS SESSION

Memory type estimator under systematic sampling

Eda Gizem Koçyiğit[1]*

[1] *Dokuz Eylül University, Faculty of Science, Department of Statistics, 35390, İzmir, Türkiye.*

* *eda.kocyigit@deu.edu.tr*

This study aims to enhance estimation accuracy in systematic sampling by introducing a novel Exponentially Weighted Moving Average (EWMA)-based memory-type ratio estimator specifically developed for this sampling framework. Systematic sampling is widely preferred in practical applications because it ensures uniform coverage of the entire population and often yields higher efficiency than simple random sampling. Its operational simplicity, coupled with strong performance when population units follow an ordered structure, has led to a growing body of research focused on developing new sampling schemes and improved estimators within this design. Despite the breadth of studies addressing systematic sampling, no prior work has incorporated memory-type estimation—particularly approaches based on EWMA control chart statistics—into ratio estimators for systematic sampling.

The proposed EWMA-based ratio estimator leverages information not only from the current sample but also from historical or previously observed values of the study and auxiliary variables. By allowing the estimator to "remember" past trends, the EWMA structure enhances stability and efficiency, especially when the variables under consideration exhibit autocorrelation or smooth transitions across ordered units. The weight parameter within the EWMA formulation controls the degree to which past information influences the estimator, offering flexibility in adapting to varying population patterns.

To evaluate the estimator's performance, extensive simulation studies using both artificial and real-world datasets were conducted. The results demonstrate that the EWMA-based ratio estimator significantly outperforms classical ratio estimators under systematic sampling, achieving notable reductions in bias and mean squared error. The estimator performs particularly well in symmetric populations when the weight parameter is set to moderate levels, indicating an optimal balance between past and present information.

Overall, this study fills a critical methodological gap by integrating a memory-type estimation mechanism into systematic sampling. The findings highlight the practical advantages of incorporating exponentially weighted historical information in improving finite population mean estimation. The proposed estimator is especially relevant in structured data environments, such as environmental monitoring, agricultural surveys, market research, and official statistics, where systematic sampling is routinely applied.

Keywords: Systematic sampling, mean estimator, EWMA, control chart, efficiency.

A novel feature extraction method using chemosensory EEG for Parkinson's disease classification

Begum Kara GÜlay[1]*, Neslihan Demirel[1], Alper Vahaplar[2], Çağdaş Güdücü[3]

[1] *Dokuz Eylul University, Faculty of Science, Department of Statistics, 35390, İzmir, Türkiye.*
[2] *NETAS Telecommunication, İstanbul, Türkiye.*
[3] *Dokuz Eylul University, Faculty of Medicine, Department of Biophysics, 35330, İzmir, Türkiye.*
* *begum.kara@deu.edu.tr*

Parkinson's disease (PD) is an incurable nervous system disease that affects millions of people all around the world. The loss of smell is one of the first symptoms that come into prominence in the early diagnosis of PD.

The main motivation of this study is to provide a more accurate diagnosis in the early period of the disease using chemosensory electroencephalography (EEG) signals, which are difficult to study and also less studied. For this purpose, we proposed a hybrid feature extraction method called EEMD_VAR that combines Ensemble Empirical Mode Decomposition (EEMD) and Vector Autoregressive Model (VAR). In contrast to conventional feature extraction methods, the proposed method is to prevent arbitrary selection of features and to determine the number of features. The pre-processed EEG signals were decomposed using EEMD and the obtained intrinsic mode functions (IMFs) used as independent variables in VAR. The coefficients of the VAR model were employed as features in frequently used supervised classification algorithms. The performance metrics of the EEMD_VAR were compared to the performance metrics of the autoregressive (AR) model and Hjorth parameters.

The maximum classification accuracy of the proposed method was 100% using artificial neural networks (ANN) in C2 electrode, while the AR method and Hjorth parameters only obtained a maximum of 72%. The other metrics also corroborate the proposed method's ability to perform well in the classification. In addition, the higher results from right side electrodes may lead to the conclusion that the right side of the brain is more sensitive to odor stimuli.

Keywords: Classification, Feature extraction, Electroencephalogram, Parkinson's disease, Chemosensory.

Research on Soil Fertility through Agrochemical Methods and Mathematical Models (Methodology)

Yasin Rustamov[1], Eldar Abbasov[2]*

[1] *Institute of Control Systems, Ministry of Science and Education of the Republic of Azerbaijan, AZ1141, Baku, Azerbaijan.*

[2] *Institute of Mathematics and Mechanics Ministry of Science and Education of the Republic of Azerbaijan, Baku, Azerbaijan.*

* *eldarab@gmail.com*

The variation order of the statistical parameters obtained as a result of any research conducted to determine the fertility of the soil (mechanical, chemical, agrochemical, etc.) is compiled. The max and min values of the obtained variation orders are found separately. Since the parameters characterizing the fertility of the soils are variable depending on time and space and these changes occur in a stochastic system as a hypothesis, the possibility of applying the reliability theory is accepted.

First, considering that the experimental area has not been studied in sufficient detail, that is, the absence of other information characterizing the fertility, it is accepted that the obtained parameters are subject to the law of normal distribution. The parameters characterizing the soil are divided into first and second orders according to their effect on fertility. A block diagram corresponding to these is compiled and a suitable model is given.

According to the reliability theory, the system or facilities are divided into two parts: renewable and non-renewable. The reliability limit is determined in accordance with these. Since the soil is a renewable system, the reliability - fertility limit should be accepted here.

Based on the statistical data obtained as a result of laboratory analysis of soil samples taken from lithological layers suitable for the plant root system, the probability integral of the parameters is calculated separately for each layer. Finally, the total fertility of the soil is determined through the model developed.

Keywords: Soil, fertility, probability, statistics, reliability, flowchart.

Enhancing Conformational Priors for Small Rings in Structural Biology through Computational Energy Analysis

Lala Ibadullayeva[1]*, Fei Long[2], Garib Murshudov[1,2]

[1] *Institute of Molecular Biology and Biotechnologies, Ministry of Science and Education of the Republic of Azerbaijan, AZ1073, Baku, Azerbaijan.*

[2] *MRC Laboratory of Molecular Biology, Cambridge Biomedical Campus, CB2 0QH, UK.*

* lala.ibadullayeva@gmail.com

In macromolecular crystallography and cryo-EM, accurate three-dimensional(3D) structure determination relies on combining prior stereochemical knowledge with noisy and limited experimental data. Although the use of bond lengths and angles is well established, the use of conformational information-particularly for small, non-aromatic rings-still requires improvement. The main reason is that conformations depend on both bonding and non-bonding interactions. In the case of small rings, additional constraints arise from ring closure, which reduces the degrees of freedom.

The design and use of probability distributions describing conformational variety is the subject of this work. This study builds on earlier research by incorporating computational energy calculations to refine conformational priors for ring systems. Using a Python-based computational pipeline, we generated and assessed the conformational landscape of ensembles for representative ring systems taken from the Crystallography Open Database (COD). The pipeline combines RDKit for conformer generation and geometry optimization with force-field energy calculations, followed by visualization of low-energy conformers. In our work, we observed that one of the most significant limitations of the most widely used schemes for classifying ring systems is the failure to account properly for chirality. Without considering chirality, distinct stereoisomers appear in a single ring class, allowing multiple stereoisomers with the same energy in the conformational library.

This results in many conformations of the same ring class, resulting in inaccurate ring classes. Our findings also emphasize the importance of incorporating stereo chemical specificity when creating conformational priors. The approach adopted here merges high-quality, experimentally derived data from the COD with physics-based energy evaluations to produce an optimized, energy-weighted conformational library. Such energy-weighted conformational libraries may enhance the accuracy of macromolecular structure refinement, particularly for ligand modelling and density fitting when working with low-resolution data.

Keywords: Conformational analysis, ring puckering, computational chemistry, RDKit.

Acknowledgement: This work was supported by the MRC Laboratory of Molecular Biology. Computational resources were provided by the Institute of Molecular Biology and Biotechnologies, Baku, Azerbaijan.

FOURTH INTERNATIONAL BILATERAL WORKSHOP ON NATURAL SCIENCE BETWEEN DOKUZ EYLUL UNIVERSITY AND AZERBAIJAN NATIONAL ACADEMY OF SCIENCES

DOKUZ EYLÜL ÜNİVERSİTESİ REKTÖRLÜĞÜ

Cumhuriyet Bulvarı, No: 144, 35210 Alsancak/ İZMİR.

+90(232) 412 12 12 deu.edu.tr

DEÜ FEN FAKÜLTESİ

DEÜ Merkez Yerleşke, 35390 Buca/ İZMİR

+90 232 301 85 02 fen.deu.edu.tr

AZƏRBAYCAN MİLLİ ELMLƏR AKADEMİYASI

AZ1001, Azərbaycan Respublikası, Bakı ş., İstiqlaliyyət küç., 30.

(+994 12) 539 24 72 science.gov.az