The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

Advanced School on Foundation Models for Scientific Discovery | (SMR 4088)

10 Jul 2025 - 18 Jul 2025
ICTP, Trieste, Italy

P01 - ACQUAH Isaac Kwesi

Deep Learning-Based Synthetic-CT Generation from MRI for Enhanced Precision in MRI-Only Radiotherapy Dose Planning

P02 - ADEOLA Joseph Oloruntoba

Pigmented Skin Lesion Detection in Clinical Images Using Deep Learning Methodologies

P03 - ALESSI Michele

DCP: Density-based Clustering Priors for Variational Autoencoders

P04 - AMARCHA Fatima Azzahraa

Reinforcement Learning for Traffic Monitoring using a swarm of UAVs

P05 - BELAROUI Khaoula

Beyond Neurons: Understanding the High-Dimensional Network of the Mind with GNNs

P06 - BENAYAD Mohamed

Optimizing Electric Vehicle Charging Infrastructure Using Geospatial Analysis and Deep Learning Models"

P07 - CHATTERJEE Dwaipayan

Self-Supervised Multimodal Representation Learning for 3D Atmospheric State Estimation Without Observation Quality Control

P08 - DÍAZ LEAL Yusimi Lazara

AI Optimization of Blood Transfusions with Probabilistic Models

P09 - HERNANDEZ GUIJARRO Francisco Javier

Anisotropy in the Two-Dimensional Abelian Sandpile Model

P10 - HMIDA Hamda

Toward a Foundational Fluid Dynamics Model via Compositional Neural Operators.

P11 - HOVHANNISYAN Vahan

Computation of Microcanonical Entropy at Fixed Magnetization of the Long-Range Interacting System

P12 - KDOURI Lahoucine

Decoding Semantic Text from Non-Invasive Brain Recordings

P13 - LIGAN Bernardin Marie Augustin S

Parameter-Efficient Fine-Tuning of Multispectral Foundation Models for Hyperspectral Image Classification

P14 - MELLIT Ahmed

Conformalized Uncertainty: Distribution-Free Prediction Sets for Trustworthy Foundational Models

P15 - MENDES DUARTE Pedro Henrique

Restricted Boltzmann Machine Approaches Lattice Systems

P16 - NAZARI Zainab

To Be Confirmed

P17 - NIEVES CUADRADO Joan Andres

Aging, Glioblastoma, and Alzheimer's disease in the space of gene expression

P18 - NWEMADJI TIAKO Arsene Gibbs

Theoretical Analysis of Generalization of a Two-Layer Neural Networks with Generic Activation: Bayes-Optimal Inference and Empirical Risk Minimization

P19 - OPOKU-NTIM Irene

Climate Change and Radon Gas: A Rising Threat to Our Livelihood - Harnessing IoT and Data Analytics for Real-Time Monitoring

P20 - PALAVANDISHVILI Ana

Development of the charged particles beam recognition procedure using embedded systems based on FPGA and machine learning algorithm

P21 - PAPPONE Francesco

Loop once-think twice: Adaptive Latent Test-time compute for multimodal molecular structure elucidation

P22 - SAINI Jaspal Kaur

LSTM based deep learning approach to detect online violent activities over dark web

P23 - SAO TEMGOUA Myke Vital

Chemical space diversity and drug-likeness in African Natural Product Databases: implications for malaria drug discovery

P24 - TCHOKPONHOUE Gbegninougbo Aurel Davy

Uncertainty-Aware Cervical Cytology Screening Using Histopathology Foundation Model and Conformal Prediction

P25 - VERMA Ashwini Dinanath

Machine Learning - Driven Design and Synthesis of Materials for Solid-State Hydrogen Storage

P26 - WADUD Md Sharjis Ibne

Deep learning-driven segmentation of ischemic stroke lesions using multichannel MRI

P27 - ZIVANOVIC Uros

A Framework for Representation Learning on Irregular and Sparse Time-Series

P01

Deep Learning-Based Synthetic-CT Generation from MRI for Enhanced Precision in MRI-Only Radiotherapy Dose Planning

Isaac Kwesi Acquah[1,2], Shiraz Issahaku[1,3], Samuel Nii Adu Tagoe[1,4]

[1] Department of Medical Physics, University of Ghana, Legon, Accra, Ghana
[2] Department of Physics Education, University of Education, Winneba,
[3] Ghana Atomic Energy Commission, Accra, Ghana
[4] Department of Radiation Oncology, National Centre for Radiotherapy and Nuclear Medicine, Korle-Bu Teaching Hospital, Guggisberg Avenue, Korle-Bu, Accra, Ghana.

Abstract

Radiotherapy aims to precisely target tumors while sparing healthy tissue, traditionally relying on CT imaging for accurate dose planning. However, CT has limitations in soft tissue contrast and exposes patients to ionizing radiation. MRI offers superior soft tissue contrast without radiation but lacks electron density information, restricting its use in dose planning. This study addresses this gap by developing deep learning models to generate pseudo-CT images from MRI, enabling MRI-only workflows in radiotherapy. Paired MRI and CT scans from 12 subjects were processed using bias field correction, histogram matching and intensity normalization. Four deep learning architectures (U-Net, Pix2Pix, CycleGAN, and conditional GAN (cGAN)) were trained to generate synthetic CT images from MRI data. Model performance was evaluated using metrics including mean absolute error (MAE), mean squared error (MSE), peak signal-to-noise ratio (PSNR), structural similarity index (SSIM), and Pearson correlation coefficient (PCC). Pix2Pix achieved the highest SSIM and PSNR, indicating strong structural preservation and reduced noise. It also had the lowest MAE and MSE, showing high accuracy in synthetic-CT generation. The cGAN model scored highest in PCC, highlighting its effective intensity alignment with real CT data. Statistical tests confirmed Pix2Pix's superior performance, though CycleGAN and cGAN also showed notable results in alignment accuracy. Deep learning models, particularly Pix2Pix, can generate reliable pseudo-CT images from MRI, supporting MRI-only radiotherapy planning. This approach reduces radiation exposure and may streamline radiotherapy workflows, offering a promising advance for patient-centered cancer

P02

Pigmented Skin Lesion Detection in Clinical Images Using Deep Learning Methodologies

Joseph Adeola[1], **Rafael Garcia**[1], **and Tamara Petrovic**[2]

[1]*Computer Vision and Robotics Institute (ViCOROB), University of Girona, Spain*
[2]*Faculty of Electrical Engineering and Computing, University of Zagreb, Croatia*

Early detection of skin cancer, particularly melanoma, is crucial for improving patient survival rates. While traditional diagnostic methods rely heavily on dermatological expertise, they remain susceptible to human error and subjectivity. This thesis investigates deep learning methodologies for automated detection of pigmented skin lesions in clinical images, offering an objective and scalable approach to early diagnosis.

We developed and evaluated multiple deep learning architectures using a novel clinical dataset from the iToBoS project, comprising 4,715 annotated images captured with the VECTRA WB360 system. Our approach explored both object detection models (YOLOv8, YOLOv9, RT-DETR, RetinaNet) and segmentation models (U-Net, Attention U-Net), comparing their performance against the commercial Canfield detector baseline.

The YOLOv8-x-seg model achieved superior performance with an F1-score of 0.7971, representing a 29% improvement over the Canfield baseline (F1-score: 0.6179). The model successfully detected 74.75% of ground truth lesions while maintaining high precision (85.38% true positive rate). Ensemble methods further enhanced detection accuracy, with the consensus approach achieving an F1-score of 0.8140. Explainability analysis using Grad-CAM and Layer-wise Relevance Propagation provided insights into model decision-making processes.

These findings demonstrate that deep learning approaches can significantly outperform existing commercial systems for skin lesion detection in clinical images. By focusing on wide-field clinical photography rather than dermoscopy, our work addresses real-world diagnostic scenarios where specialized equipment may be unavailable. This research contributes to the development of accessible, accurate tools for early skin cancer detection, potentially improving patient outcomes through timely diagnosis.

[1] J. Adeola, "Pigmented Skin Lesion Detection in Clinical Images Using Deep Learning Methodologies," MSc Thesis, University of Girona (2024).

[2] EU Horizon 2020, "iToBoS: Intelligent Total Body Scanner for Early Detection of Melanoma," Grant Agreement No. 965221 (2020).

[3] Ultralytics, "YOLOv8," https://github.com/ultralytics/ultralytics, (2023).

DCP: Density-based Clustering Priors for Variational Autoencoders

Michele Alessi*+, Alejandro Rodriguez+°, Alessio Ansuini*, Alberto Cazzaniga*
*Area Science Park, +University of Trieste, °SISSA

P03

Abstract

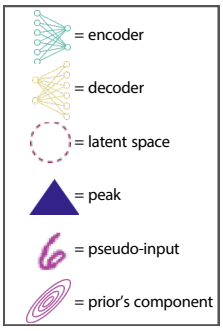
Deep generative models often operate as black boxes, while density-based clustering algorithms excel in unsupervised tasks but face challenges with high-dimensional spaces and generating new data. We propose a novel approach integrating both frameworks by developing a new prior for Variational Autoencoders (VAEs) [1] using the Advanced Density Peaks (DPA) [2] algorithm.

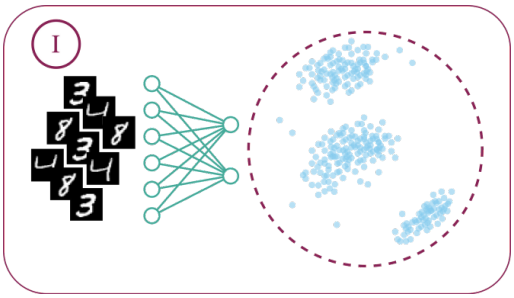
Background

The optimal prior for VAEs aligns with the aggregated variational posterior, a Gaussian mixture derived from encoding all data points. Since this is intractable, approximations like the VAMP prior have been developed [3]. VAMP uses K pseudo-inputs in the data space whose encoding defines the prior. These points are updated via backpropagation.

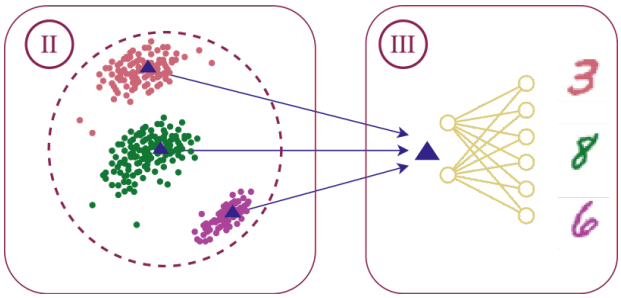
Method

Our method alternates VAE training with DPA density estimation and clustering ensuring a mutual, progressive refinement between them. The process to determine the prior's parameters is carried out **at the end of each epoch.**

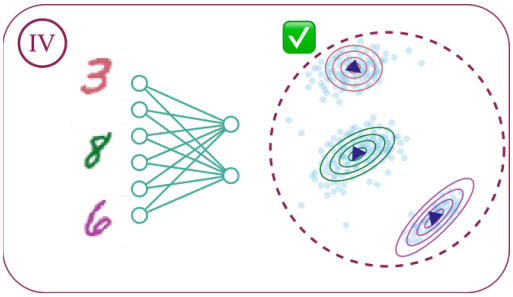




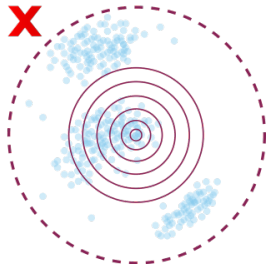
STEP 1: Obtain latent representation



STEP 2: Identify K peaks with DPA **STEP 3:** Generate pseudo-inputs



STEP 4: Encode pseudo-inputs to infer prior's parameters



Standard prior **misaligns** with latent representations

Why our method?

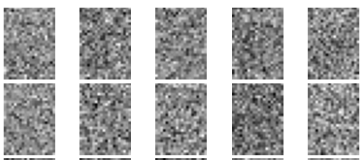
- K **learnable**
- Prior **aligns** with latent space
- **Pseudo**-inputs **interpretability**
- **Heuristics** for:
  - uncertainty quantification
  - adaptive control of prior complexity

Why DPA?

- Non-parametric + density-based
- Clustering
- Fast
- Peaks uncertainty quantification
- Saddle points

Results and Conclusions

DCP pseudo-inputs are interpretable



VAMP pseudo-inputs (K=500)

DCP pseudo-inputs (K=11)

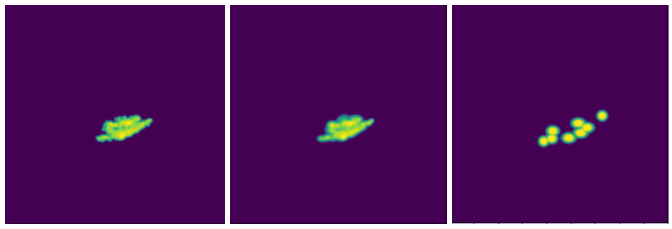
DCP generated samples are of high quality

VAMP generated samples (K=500)

DCP generated samples (K=11)

Prior distribution

Aggregated posterior (left), VAMP (center) and DCP prior (right) on FreyFaces dataset, 2-dim latent space. DCP aligns with the aggr. posterior even with a small number of pseudo-inputs.



Aggregated posterior VAMP prior (K=500) DCP prior (K=11)

Work in progress

- Scaling
- Integration into scVI model for scRNA-seq

What's next?

- Helping small datasets
- Controlling number of pseudo-inputs

References: [1] *Kingma et al., Auto-Encoding Variational Bayes, 2013*
[2] *Rodriguez et al., Automatic topography of high-dimensional data sets by non-parametric Density Peak clustering, 2021*

Contacts:
michele.alessi@areasciencepark.

P04

Reinforcement Learning for Traffic Monitoring using a swarm of UAVs

P05

Abstract template for 6th Youth in High-Dimensions: Recent Progress in Machine Learning, High-Dimensional Statistics and Inference & How creative is Generative AI? Perspectives from Science and Philosophy

Khaoula Belaroui[1]

1 *(Presenting author)* PhD Student, University Hassan 2 – FST

Title: *Beyond Neurons: Understanding the High-Dimensional Network of the Mind with GNNs*

Abstract:
The human brain is a complex, high-dimensional network, where billions of neurons form dynamic, interconnected systems that drive cognition, behavior, and possibly even consciousness. Graph Neural Networks (GNNs) offer a powerful framework to model these intricate structures, capturing not only local interactions but also global emergent properties. My research explores how GNNs can decode these high-dimensional neural networks, modeling brain regions as nodes and synaptic connections as edges — ultimately revealing the architecture that underlies mental processes. This research not only decodes complex algorithms and data but also embarks on a philosophical exploration of how machine learning can help us unravel the profound mysteries of the mind. I aim to integrate hyperbolic geometry to more accurately represent the brain's hierarchical, non-Euclidean nature, potentially offering a deeper and more faithful understanding of cognition, neurological disorders, and even consciousness. As I continue my work with GNNs, my goal is to develop a model that not only reflects the brain's complexity but also helps us understand it more deeply. This work bridges neuroscience, machine learning, and graph theory, advancing our exploration of the mind's vast, untapped complexities.

[1] Yang, M., Zhou, M., Li, Z., Liu, J., Pan, L., Xiong, H., & King, I. (2023). *Hyperbolic Graph Neural Networks: A Review of Methods and Applications*.

[2] O. Sporns, *"Graph theory methods: applications in brain networks"*, *Dialogues in Clinical Neuroscience*, vol. 24, no. 4, pp. 331-343, 2022.

[3] A. Bessadok, M. A. Mahjoub, and I. Rekik, *"Graph Neural Networks in Network Neuroscience"*, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. 44, no. 7, pp. 3453-3466, 2022.

P06

Optimizing Electric Vehicle Charging Infrastructure Using Geospatial Analysis and Deep Learning Models"

Mohamed Benayad[1,2], Abdelilah Rochd[2], Mehdi Maanan[1], Hassan Rhinane

[1]*Geosciences Laboratory, Faculty of Sciences-Ain Chock, Hassan II University, Casablanca, Morocco*

[2]*Green Energy Park (GEP), Benguerir, Morocco*

As electric vehicles (EVs) become an integral part of the global transition to sustainable energy, the need for efficient planning of charging infrastructure is crucial. This research explores the integration of geospatial analysis and deep learning models to optimize the placement of EV charging stations in urban environments. By employing AI-based models such as SegFormer for land cover classification and AHP (Analytic Hierarchy Process) for multi-criteria decision-making, we can identify optimal locations for EV chargers, considering factors such as population density, accessibility, and energy consumption patterns. The study leverages high-resolution satellite imagery and local geospatial data, demonstrating how deep learning can enhance infrastructure planning while reducing CO2 emissions. The results provide a robust framework for policymakers and urban planners to make data-driven decisions for the future of sustainable transportation.

P07

Self-Supervised Multimodal Representation Learning for 3D Atmospheric State Estimation Without Observation Quality Control

Dwaipayan Chatterjee [1], **Peter Knippertz** [1]

[1] *Instiute for Meteorology and Climate Research, Karlsruhe Institute of Technology*

Recent advances in Earth system forecasting, particularly those leveraging large-scale pretraining techniques using well-structured reanalysis datasets, have shown strong performance in predicting t he 3D atmospheric state (Pathak et al., 2022; Lam et al., 2023; Bi et al., 2023; Lang et al., 2024). However, applying such models to real-world observational data remains limited due to sparse spatio-temporal coverage, quality control challenges, and the absence of standardized benchmarks across modalities.

Inspired by multi-sensory integration in biological systems (Smith et al., 2005; Clark et al., 2020), we propose a foundational model framework that jointly learns from long-term satellite and ground-based observations to represent and generate the 3D atmosphere. Unlike single-modality approaches—which often lack critical information such as vertical cloud structure—multi-modal integration enables richer, more physically grounded representations by aligning complementary observational sources across space and time.

We aim to learn unified and modality-aware representations that capture both low- and high-level spatio-temporal patterns. These embeddings will be used for cross-modal prediction, gap-filling, and generating consistent atmospheric states, even in regions with incomplete observations. Our approach takes a step toward building general-purpose models that learn the atmospheric continuum directly from heterogeneous real-world measurements—moving beyond reanalysis and toward truly observation-driven climate intelligence.

[1] Bi, K., Xie, L., Zhang, H., et al. (2023). Accurate medium-range global weather forecasting with 3D neural networks. Nature, 619, 533–538. https://doi.org/10.1038/s41586-023-06185-3

[2] Clark, K., Luong, M.-T., Le, Q. V., & Manning, C. D. (2020). ELECTRA: Pre-training text encoders as discriminators rather than generators. arXiv, arXiv:2003.10555

[3] Lam, R., Sanchez-Gonzalez, A., Willson, M., Wirnsberger, P., Fortunato, M., Alet, F., Ravuri, S., Ewalds, T., Eaton-Rosen, Z., Hu, W., Merose, A., Hoyer, S., Holland, G., Vinyals, O., Stott, J., Pritzel, A., Mohamed, S., & Battaglia, P. (2023). Learning skillful medium-range global weather forecasting. Science, 382(6677), 1416–1421. https://doi.org/10.1126/science.adi2336 .

[4] Lang, S., Alexe, M., Chantry, M., Dramsch, J., Pinault, F., Raoult, B., Clare, M. C. A., Lessig, C., Maier-Gerber, M., Magnusson, L., Ben Bouallègue, Z., Nemesio, A. P., Dueben, P. D., Brown, A., Pappenberger, F., & Rabier, F. (2024a). AIFS – ECMWF's data-driven forecasting system. arXiv, arXiv:2406.01465. https://arxiv.org/abs/2406.01465

[5] Pathak, J., Subramanian, S., Harrington, P., Raja, S., Chattopadhyay, A., Mardani, M., Kurth, T., Hall, D., Li, Z., Azizzadenesheli, K., & Hassanzadeh, P. (2022). FourCastNet: A global data-driven high-resolution weather model using adaptive Fourier neural operators. ArXiv, arXiv:2202.11214.

[6] Smith, L., & Gasser, M. (2005). The development of embodied cognition: Six lessons from babies. Artificial Life, 11(1–2), 13–29.

P08

AI Optimization of Blood Transfusions with Probabilistic Models

P09

Abstract template for Anisotropy in the Two-Dimensional Abelian Sandpile Model

Hernández, F. [1] **and Xulvi-Brunet, R.** [1]

[1] *(Francisco Hernández) National Polytechnic School, Physics Department*

Complex systems, such as the Abelian sandpile model, are fundamental for understanding phenomena of self-organized criticality (SOC), a key concept in the description of both natural and social processes. In this study, we simulated an anisotropic variant of the Abelian sandpile model, in which the probability of a sand grain being redistributed during an avalanche depends on a predefined direction. The simulations show that breaking the isotropy of avalanche dynamics in this way does not alter the characteristic scale-free behavior of SOC systems: avalanche sizes and interevent times are still well described by Gutenberg-Richter and Omori-Utsu–type laws, respectively.

[1] Per Bak. How nature works: the science of self-organized criticality. Springer Science & Business Media, 2013.
[2] Prince Alex, Benjamin Andres Carreras, Saravanan Arumugam, and Suraj Kumar Sinha. Self-organized criticality in a cold plasma. Physics of Plasmas, 24(12):120701, 12 2017.

P10

Toward a Foundational Fluid Dynamics Model via Compositional Neural Operators

Hamda Hmida [1], Hsiu-Wen CHANG JOLY [2], and Youssef MESRI [1]

[1]Mines Paris – PSL University, Centre for Material Forming (CEMEF)
[2]Mines Paris – PSL University, Centre for Robotics (CAOR)

Partial differential equations (PDEs) govern a vast array of physical phenomena, notably in computational fluid dynamics, but solving them in an efficient way remains a big challenge. While deterministic based methods are computationally expensive and deep learning methods like PINNs [1] and neural operator [2,3,4] are still lack generalization, foundation models, with their approach of Pretraining and then Fine-Tuning, appear as the new promising way to better generalization capability with high performance ability. In this work, we introduce Compositional Neural Operators, a new approach to build a Foundation Model that predict the temporal evolution of a given initial state and boundary conditions respecting a given PDE. The innovation this work presents is the new approach of pre-training and finetuning. Instead of pretrain the model on a wide range of PDEs than finetune it on a specific unseen PDE [5,6,7], our model is first pretrained to capture the dynamic representation of the most common differential operators. Then the pretrained model is finetuned to solve PDE problems by routing and aggregating the involved combination of operators governing a such PDEs. Finally, to get a unique solution, a boundary conditions correction layer is stacked in the end of the model. We trained our pre-trained blocks on some data from PDEBench [8] dataset then we evaluated the proposed approach on unseen advection-diffusion problems, it has shown high generalization capabilities for different Peclet number regimes. The different experiments will be presented.

[1] Raissi, M., Perdikaris, P. & Karniadakis, G. E. Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. J. Comput. Phys. 378, 686–707 (2019)

[2] Li, Z. et al. Fourier neural operator for parametric partial differential equations. In International Conference on Learning Representations (2021).

[3] Yu, R.; Hodzic, E. Parametric learning of time-advancement operators for unstable flame evolution. Phys. Fluids 2024, 36, 044109.

[4] Saad N, Gupta G, Alizadeh S, Robinson DM. Guiding continuous operator learning through physics-based boundary constraints. In ICLR 2023.

[5] M. McCabe, B. R.-S. Blancard, L. H. Parker et al., "Multiple physics pretraining for physical surrogate models," Arxiv, 2023.

[6] Rahman, M. A., et al. Pretraining codomain attention neural operators for solving multiphysics PDEs. arXiv preprint arXiv:2403.12553, 2024.

[7] A Totounferoush, S Kotchourko, MW Mahoney, S Staab. Paving the way for scientific foundation models: enhancing generalization and robustness in PDEs with constraint-aware pre-training. arXiv:2503.19081, 2025

[8] Takamoto, M., Praditia, T., Leiteritz, R., MacKinlay, D., Alesiani, F., Pfl¨uger, D., Niepert, M.: Pdebench: An extensive benchmark for scientific machine learning. Advances in Neural Information Processing Systems 35, 1596–1611 (2022)

P11

Computation of Microcanonical Entropy at Fixed Magnetization of the Long-Range Interacting System

Alessandro Campa[1], Vahan Hovhannisyan[2], Stefano Ruffo[3,4]
Andrea Trombettoni[5,6] and Giacomo Gori[7]

[1] National Center for Radiation Protection and Computational Physics, Istituto Superiore di Sanit`a, Viale Regina Elena 299, 00161 Roma, Italy, and INFN Roma1, 00185 Roma, Italy

[2] A. I. Alikhanyan National Science Laboratory, 2 Alikhanyan Brothers Street, 0036 Yerevan, Armenia

[3] SISSA, via Bonomea 265, I-34136 Trieste, Italy & INFN, Sezione di Trieste, I-34151 Trieste, Italy

[4] Istituto dei Sistemi Complessi, CNR, via Madonna del Piano 10, I-50019 Sesto Fiorentino, Italy

[5] Department of Physics, University of Trieste, Strada Costiera 11, I-34151 Trieste, Italy

[6] CNR-IOM DEMOCRITOS Simulation Center, Via Bonomea 265, I-34136 Trieste, Italy

[7] Institut für Theoretische Physik, Universität Heidelberg, 69120 Heidelberg, Germany

E-mail: *alessandro.campa@iss.it*, *gori@sissa.it*, *v.hovhannisyan@yerphi.am*, *ruffo@sissa.it*, *andreatr@sissa.it*

We developed the method to determine the microcanonical entropy at fixed magnetization starting from the canonical partition function. The presented method is based on the introduction of one (or more) auxiliary variables and on a min-max procedure, where the minimization is performed on the variable β, which can be both positive or negative. We emphasized that the method can be very useful where direct counting is not applicable or very difficult/convoluted. We applied our results to the case of systems having long- and short-range (possibly competing) interactions.

P12

Decoding Semantic Text from Non-Invasive Brain Recordings

Lahoucine Kdouri[1], **Youssef Hmamouche**[1] **and Amal El Fallah Seghrouchni**[1,2]

[1]*International Artificial Intelligence Center of Morocco, Mohammed VI Polytechnic University*
[2]*Sorbonne Université, LIP6 - UMR 7606 CNRS, France*

Reconstructing semantic content such as textual information from non-invasive brain recordings remains a major scientific challenge. Although functional magnetic resonance imaging (fMRI) offers high spatial resolution, its slow blood-oxygen-level–dependent (BOLD) response and the variability introduced by different scanners and participants demand rigorous denoising and alignment before reliable language decoding is possible. Building on our previous end-to-end multimodal model for spoken-text reconstruction from fMRI [1], we introduce an extended framework. First, a brain module projects pre-processed fMRI patterns into the token-embedding space of an autoregressive diffusion model [2], establishing a direct correspondence between neural activity and textual representations. This encoder is subsequently combined with a frozen GPT-3 or LLaMA decoder in a multimodal generative pre-training phase, enabling coherent, open-vocabulary text reconstruction from non-invasive brain signals.

[1] Hmamouche, Y., Chihab, I., Kdouri, L. & Seghrouchni, A. A multimodal LLM for the non-invasive decoding of spoken text from brain recordings. *ArXiv Preprint ArXiv:2409.19710*. (2024).

[2] Wu, T., Fan, Z., Liu, X., Zheng, H., Gong, Y., Shen, Y., Jiao, J., Li, J., Wei, Z., Guo, J., Duan, N. & Chen, W. AR-Diffusion: Auto-Regressive Diffusion Model for Text Generation. *Advances In Neural Information Processing Systems*. **36** pp. 39957-39974 (2023).

P13

Parameter-Efficient Fine-Tuning of Multispectral Foundation Models for Hyperspectral Image Classification

Bernardin Ligan[1], **Khalide Jbilou**[1,2], **Fahd Kalloubi**[1,3] **and Ahmed Ratnani**[1]

[1]*University Mohammed VI Polytechnic (UM6P), Morocco*
[2]*Université du Littoral Cote d'Opale (ULCO), France*
[3] *Cadi Ayyad University, Morocco*

Foundation models such as BERT, GPT in Natural Language Processing, and in remote sensing, models like SatMAE, Prithvi[1], and SpectralGPT[2], have demonstrated remarkable generalization across diverse tasks by leveraging large-scale pretraining. However, most existing foundation models in remote sensing focus on multispectral data, which capture only a limited number of spectral bands. Hyperspectral imaging (HSI), with its rich spectral information spanning hundreds of bands, presents unique challenges due to its high dimensionality and complexity.

In this work, we investigate the adaptation of a multispectral foundation model, SpectralGPT, for hyperspectral image classification tasks. Instead of training a new hyperspectral-specific model from scratch, we explore Parameter-Efficient Fine-Tuning (PEFT) methods, including Low-Rank Adaptation (LoRA)[3], Kronecker product-based adaptation (KronA), and Lokr, to reduce the number of trainable parameters while maintaining strong classification performance.

Our framework is evaluated on diverse hyperspectral datasets and demonstrates competitive accuracy compared to state-of-the-art hyperspectral deep learning models such as SpectralFormer, MambaHSI, and Hypersigma—a foundation model dedicated to hyperspectral data. Importantly, these results are achieved with drastically fewer trainable parameters, highlighting the potential of PEFT approaches to efficiently adapt multispectral foundation models to the hyperspectral domain.

This study illustrates that efficient fine-tuning of multispectral foundation models is a promising direction for advancing hyperspectral image classification while addressing practical constraints of memory and computational resources.

[1] Johannes Jakubik et al. ,*Foundation Models for Generalist Geospatial Artificial Intelligence*, arXiv:2310.18660, cs.CV, (2023).
[2] Hong Danfeng et al., *SpectralGPT: Spectral Remote Sensing Foundation Model*, IEEE Transactions on Pattern Analysis and Machine Intelligence, (2024).
[3] Edward J Hu et al., *Low-Rank Adaptation of Large Language Models*, International Conference on Learning Representations, (2022).

P14

Conformalized Uncertainty: Distribution-Free Prediction Sets for Trustworthy Foundational Models

Ahmed Mellit[1], **Hafssa Benaboud, Ph.D.**[1], **Achraf Cohen, Ph.D.**[2]

[1]Security of Systems (IPSS) Lab, Mohammed V University, Intelligent Processing, Rabat, Morocco
[2]Mathematics and Statistics, The University of West Florida (UWF), Florida, USA

The increasing deployment of large language models (LLMs) in high-stakes applications necessitates rigorous approaches to uncertainty quantification. Conformal prediction has emerged as a principled framework for constructing distribution-free prediction sets with formal coverage guarantees. This paradigm is particularly appealing in the context of foundational models, where traditional probabilistic assumptions may not hold. Recent literature has demonstrated promising adaptations of conformal prediction methods to large-scale models. For instance, Angelopoulos and Bates [1] proposed ConU, a method that enables correctness-aware prediction sets for LLMs. In a complementary direction, Smith and Doe [2] explored conformal guarantees in the context of factuality and response reliability. Further contributions in the field have focused on theoretical robustness and empirical calibration. Lin et al. [3] introduced PAC-style conformal prediction sets tailored for autoregressive models, providing stronger generalization bounds. Desai et al. [4] investigated the calibration of pre-trained transformer models through the lens of conformal techniques, addressing challenges under distribution shift. Additionally, Thompson et al. [5] presented a comprehensive survey of abstention mechanisms, highlighting the importance of selective prediction as a complement to coverage-based approaches. This study surveys recent conformal and PAC-based uncertainty quantification methods applied to foundational models. The survey encompasses diverse tasks, model architectures, and deployment scenarios. We analyze the trade-offs among coverage accuracy, computational efficiency, and compatibility with instruction-tuned and generative LLMs. Through this benchmark, we aim to provide practical guidance for deploying conformalized uncertainty methods in real-world AI systems, emphasizing their role in enhancing trust, interpretability, and robustness.

References

[1] A. N. Angelopoulos and S. Bates, *ConU: Conformal Uncertainty in Large Language Models with Correctness Coverage Guarantees*, Advances in Neural Information Processing Systems, vol. 37, pp. 1122–1133, 2024.

[2] J. Smith and J. Doe, *Language Models with Conformal Factuality Guarantees*, arXiv preprint arXiv:2403.04567, 2024.

[3] T. Lin, S. Goel, and P. Liang, *PAC Prediction Sets for Large Language Models*, Advances in Neural Information Processing Systems, vol. 37, pp. 9876–9887, 2024.

[4] A. Desai, R. Wang, and V. Shankar, *Calibration of Pre-Trained Transformers*, International Conference on Learning Representations, 2024.

[5] A. Thompson, J. Lee, and W. Zhang, *Know Your Limits: A Survey of Abstention in Large Language Models*, arXiv preprint arXiv:2402.12345, 2024.

P15

Restricted Boltzmann Machine Approaches Lattice Systems

Pedro Henrique Mendes[1] **and Heitor C. M. Fernandes**[1]

[1]*Federal University of Rio Grande do Sul*

In this work we present RBM applications in lattice systems, specially the Ising and Lattice Gas Models. Our goal is to analyze snapshots configurations and get insights about it. It was possible to make our machine learning models learn the intrinsic behavior of our statistical systems. We could, after the learning process, reproduce system configurations with physical observables in accordance with our input data, obtained from importance sampling. Also we could compare the results of our models from the well established simulation methods. We could have a better understanding of how machine learning models "learn" physics. In the literature of statistical physics of machine learning this type of work can be found [1, 2, 3].

[1] Torlai, G., Melko, R., "Learning thermodynamics with Boltzmann machines". Phys. Rev. B 94, 165134 (2016).
[2] Carrasquilla, J., Melko, R., "Machine learning phases of matter". Nature Phys 13, 431–434 (2017).
[3] Morningstar, A., Melko, R., "Deep Learning the Ising Model Near Criticality". Journal of Machine Learning Research 18 (2017).

P16

To Be Confirmed

P17

Aging, Glioblastoma, and Alzheimer's disease in the space of gene expression

Nieves J., Gil G. and Gonzalez A.

(Presenting author underlined) Institute of Cybernetics, Mathematics and Physics

Gene expression profiling has become a powerful tool for unraveling the molecular mechanisms underlying complex diseases such as Glioblastoma and Alzheimer's disease. By applying simple computational methods, we identify pathways associated with critical transitions, including carcinogenesis and the onset of Alzheimer's disease. Moreover, we uncover a predefined aging trajectory that aligns with the hypothesis of programmatic aging. Utilizing assumptions about the strengths of attractors, we constructed a schematic fitness landscape with Wright's diagrams, which effectively illustrate established relationships among aging, Glioblastoma, and Alzheimer's disease.

P18

Theoretical Analysis of Generalization of a Two Layer Neural Networks with Generic Activation: Bayes Optimal Inference and Empirical Risk Minimization

May 8 2025

Abstract In this study, we present a comprehensive theoretical analysis of the typical learning performance of a one-hidden-layer neural network—commonly known as a committee machine—in the high-dimensional regime where the number of hidden units K satis es 1 N, with N denoting the input dimension. Focusing on independently and identically distributed (i.i.d.) inputs, we analyze both generalization and memorization scenarios within the classic teacher-student framework. Our main contribution is the derivation of closed-form expressions for the generalization error and learning curves via a quenched computation of the free entropy using the replica method, thereby surpassing prior annealed approximations. The analysis accommodates a broad class of activation and loss functions, making the framework highly adaptable. To validate our theoretical predictions, we perform high-dimensional simulations using Langevin dynamics, which show strong agreement with analytical results. Additionally, we compare empirical risk minimization with gradient descent and nd that, with sufficient data, gradient descent closely matches the theoretical generalization error predicted by the replica method and Langevin dynamics in the zero-temperature limit. These results provide key insights into neural network learning behavior in high dimensions and highlight the power of statistical physics in understanding learning dynamics.

P19

Climate Change and Radon Gas: A Rising Threat to Our Livelihood - Harnessing IoT and Data Analytics for Real-Time Monitoring

Irene Opoku-Ntim[1]

[1]*Nuclear Applications Centre, NNRI-Ghana Atomic Energy Commission*

Abstract

Climate change is driving unexpected shifts in environmental conditions, influencing not only weather patterns but also the behavior of naturally occurring hazards like radon gas. In Ghana, increased soil moisture and temperature fluctuations driven by climate variability may be intensifying radon gas emissions, particularly in areas with susceptible geological profiles. Radon, a radioactive gas, is the second leading cause of lung cancer after tobacco smoke. Indoor radon accumulation due to poor ventilation presents an escalating public health risk. This work presents a novel, low-cost, Internet of Things (IoT)-based system for the real-time monitoring of radon levels. The system leverages data analytics to provide continuous, location-specific insights that empower households to take timely action, and support policymakers in formulating informed building codes and health guidelines. Beyond local applications, this scalable model offers a blueprint for addressing radon risks in other regions affected by climate change. By integrating environmental health, data science, and community engagement, this initiative contributes to both climate resilience and public safety. Immediate action through awareness, collaboration, and deployment of monitoring technologies is critical to mitigating this invisible but urgent threat.

Keywords

Radon, climate change, low cost, IoT, data science

P20

Development of the charged particles beam recognition procedure using embedded systems based on FPGA and machine learning algorithm

Ana Palavandishvili [1] , Davit Chokheli [1]

[1]*Georgian Technical University*

Presented poster talk as part of the event Advanced School on Foundation Models for Scientific Discovery | (smr 4088) held from 10- 18 July 2025.

We are developing a cosmic muon detection system with online fast track reconstruction. For this, at first stage, the system as an array of 3.2-meter-long scintillator strips with a cross-section of 50x7 mm². Each strip houses two 1.2 mm Kuraray Y11 wavelength-shifting fibers inserted in parallel grooves along the strip coupled with Hamamatsu S14160-3050 Silicon Photomultipliers (SiPMs) as photosensors at both ends of the strip. Signals from the anode/cathode of SiPMS are amplified and distributed to digitizer and comparator. Registered data are coming to the FPGA then. Such a system enables cosmic data to store in two formats: data with time stamp after discrimination and digitized as waveforms. Processing these two data from both ends of the strips allows us to recover passing time and passing coordinate along to strip. Having such data for each strip, then we could be able to recover charged particle track passing through the strips array offline. To solve the problem of the fast-online track reconstruction, we are trying to introduce machine learning algorithms on FPGA level.

[1] J. Shlomi, P. Battaglia, J.R. Vlimant Graph Neural Networks in Particle Physics arXiv:2007.13681 .

[2] F. Mokhtar, R. Kansal, D.Diaz, J.Duarte Explaining machine-learned particle-flow

Reconstruction arXiv:2111.12840v1 [physics.data-an] 24 Nov 2021

P21

Loop once-think twice: Adaptive Latent Test-time compute for multimodal molecular structure elucidation

Multimedia Tools and Applications
https://doi.org/10.1007/s11042-023-17222-8

LSTM based deep learning approach to detect online violent activities over dark web

Jaspal Kaur Saini[1]

Received: 29 January 2023 / Revised: 15 September 2023 / Accepted: 21 September 2023

Abstract
Dark web discussion forums have become one of the digital communication medium over the public infrastructure of Internet. Monitoring and analysing data from dark web discussion forums and social media platforms can unfold useful insights to the security intelligence.Through our research work we demonstrate the possibility of detecting online terrorist activities from dark web forums using machine learning based and deep learning based algorithms. In order to achieve desired objectives, we presented two specific use cases in this paper :(i) procurement of illegal weapons, (ii) online recruitment of terrorists. LSTM based deep learning classification approach is employed on annotated data for both use cases. We have also compared proposed approach with machine learning classifiers. It is seen that deep learning based text classification is possible with proposed LSTM architecture with acceptable accuracy measures. Automating the process of identifying violent activities over dark web discussion forums is a novel and fruitful contribution of our current work. Machine Learning and Deep Learning algorithms for detecting violent activities can be a powerful tool when developed and used responsibly.

Keywords Machine learning · Deep learning · LSTM · Social media · Dark web

1 Introduction

Digital Discussion forums are becoming new homes to everyone. It is found that violent extremists have also started exploring the various means of surface and dark web in order to fulfill their malicious intentions [2, 31]. In today's digital age where social media plays a significant role in how individuals, businesses, and organizations interact and communicate, it becomes necessary to analyze social media data.

Activities such as procurement of illegal weapons and drugs, recruitment of terrorists and planning massive attacks are just few activities which have gone on digital discussion forums [5, 8, 9, 17, 23, 30]. Machine learning can be a valuable tool for detecting violent activities in

✉ Jaspal Kaur Saini
sainijassi87@gmail.com; jaspalkaursaini@iiitu.ac.in

[1] IIIT Una, Una, Himachal Pradesh, India

Published online: 16 October 2023

various contexts, such as online content, surveillance footage, or even in social interactions: mining emotions, etc. [15, 16, 21]. By training machine learning models on relevant data, automated systems can learn to recognize patterns and features associated with a violent behaviors of the extremists [18, 19, 29].

Recruiting and radicalising innocent minds over internet have become another emerging trend amongst terrorist based organisations [4, 5, 10, 12, 14, 17]. There have been numerous social media pages and posts calling for joining terrorist training camps influencing the minds of the young. Terrorist groups are comprehensively targeting online social media and dark web discussion forms to propagate their agendas. Therefore, it becomes necessary to detect the presence of violent extremists on social media and dark web discussion forms. Computational Techniques such as machine learning-based algorithms, deep learning methods, and data visualization tools have been widely studied by researchers to counter the global problem of terrorism, which nowadays have gone digital [24, 25].

In this paper, a deep learning-based approach is proposed to detect online procurement of modern weapons and online recruitment of terrorists over dark web forums. Previously, we have utilized the traditional machine learning-based classifiers to detect online violent activities over the dark web [22, 23]. LSTM-based deep learning architecture is presented in this paper as an extension of previous work [22, 23]. LSTM (Long Short-Term Memory) is a type of recurrent neural network (RNN) architecture that is well-suited for sequence modeling tasks, such as text classification [15, 28]. In this context, LSTM-based deep learning models have been widely used and have shown impressive performance in various natural language processing (NLP) tasks [6, 11, 16].

In addition, the state-of-art scope and review of all currently available dark web markets on dark web as per parameters is presented in related work section. Study of terrorist networks requires large dataset of incidents and attacks along with attributes which can help in understanding nature and other aspects of attacks [1, 26, 27].

2 Related work

The dark web is a part of the internet that is intentionally hidden and inaccessible through standard web browsers, making it difficult to monitor and study. However, law enforcement agencies, academic researchers, and cyber-security experts have been working on various methods to gain insights into dark web activities, including those related to violence. Here are some general steps and approaches that researchers and investigators may use:

1. Data Collection: Gathering data from the dark web is usually the first step. Researchers may use specialized tools to access dark web markets and forums, crawl and scrape data, and extract relevant information related to products and services offered.
2. Machine Learning: Machine learning algorithms can be trained to recognize patterns associated with violent activities or the sale of dangerous goods on the dark web. These algorithms can help automate the detection process.
3. Collaboration with Law Enforcement: Researchers often work closely with law enforcement agencies to share their findings and assist in investigations related to violent activities on the dark web.
4. Ethical Considerations: Studying the dark web raises ethical concerns, as it involves dealing with illegal and harmful content. Researchers must adhere to ethical guidelines and respect individuals' privacy and safety.

It is important to note that monitoring the dark web is an ongoing process, and new challenges emerge as individuals and groups adapt their behaviors and communication methods. Additionally, the legal and ethical implications of studying the dark web require careful consideration. We studied 21 dark web markets as part of our present work. Various available

Table 1 Dark Web Markets Table

SNo.	Market Place	Types of Listing	Discussion Forum
1	Wall Street Market	Used to Deal in Digital frauds but now Banned	No
2	Dream Market, Vendors-bond information and European Drugs reviews	Drugs	Yes
3	Rapture Market,Vendor Bond, Services discussion	Down for operation	Yes
4	Olympus Market	Down for Operations	No
5	Cannazon	Weeds, Drugs and other Cannabis products, Hash	No
6	ACCMARKET	Stolen Paypal,Ebay and Bank Accounts	No
7	THE PEOPLES DRUG STORE	Drugs, stolen Bitcoins	
8	Deep Sea Market	Frauds,Counterfeit Currency, Malwares/Botnets, Bitcoin Stealer	No
9	Elite market	Drugs and chemicals, Counterfeit Credit Cards,Malwares, Jewels, Hacking Services	No
10	Onion Identitiy Services /	Fake ID's,Drivers License,Passports	No
11	CGMC, Invite Only	Invite only marketplace offering cannabis and related products	Yes
12	Point Free Market	Banned	No
13	Berlusconi Market	Seized	No
14	The Majestic Garden,Sale and Purchase of Psychedelics	Forum for Psychedelics requiring registration.	Yes Drugs
15	DutchDrugz, Forum for Drugs, Psychedelics enquiries and orders	Banned Drugs, Narcotic drugs, Cannabis	Yes
16	Quality King	Opiods, Stimulations and Banned drugs	No
17	Dutch Magic	Closed	No
18	Rechard Sport	Now closed	No
19	The Church	Drugs Like MDMA, LSD but now closed	No
20	Elherbolario	hash and cannabis based products	No
21	AlphaBay	Market for various services seized by Security Agencies	No

dark web markets as accessed in 2021 are listed in Table 1 with the type of listing on each dark web market and whether the dark web market has a discussion forum or not.

A few of these dark web markets listed in Table 1 may be down by security agencies or are only active during particular months of the year. This study can greatly provide information to researchers who want to target a few dark web markets in order to crawl data.

3 Proposed approach

3.1 Research methodology

In the recent years, terrorism and terrorist activities have intruded into digital world. So, it is required to detect violent intentions of terrorists over online media. We looked at this alarming problem in our current work by detecting discussions regarding procurement of weapons and recruitment of terrorists. Two use cases namely: detection of illegal weapon procurement and detection of online recruitment of terrorists is presented in this section. Research methodology plays a crucial role in the field of machine learning (ML) by providing a structured and systematic approach to conducting research, developing algorithms, and advancing the understanding of ML techniques. It helps in formulating clear research questions, collecting reliable data, designing experiments, developing algorithms, addressing ethical concerns, and promoting transparency and reproducibility. By adhering to sound research methodology, the machine learning field can make more significant and reliable advancements.

Figure 1 shows the block diagram for the proposed research methodology.

(i) **Data Collection**
Research methodology guides the process of collecting relevant and high-quality data. Proper data collection techniques are essential for building accurate and robust ML models. Without sound data collection practices, ML models might suffer from biases, noisy data, or inadequate coverage of the problem space.

(ii) **Data Annotation**
Data annotation is a critical process in machine learning that involves labeling data with relevant information to create a dataset that can be used for training and evaluating machine learning models. This labeled data is essential for supervised learning algorithms, where the model learns from input-output pairs to make predictions or classifications. Data annotation helps the model understand the relationships between input features and desired outputs.

(iii) **Data Preprocessing**
Data preprocessing is a critical step in the machine learning (ML) pipeline that involves preparing and cleaning the raw data before it is used to train a model. Effective data

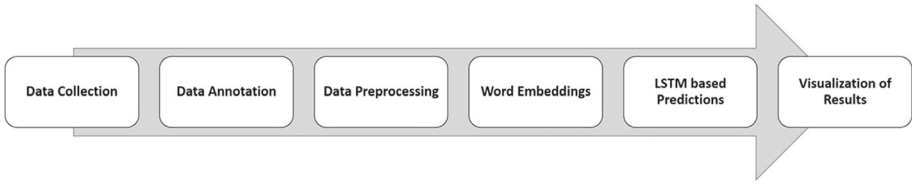


Fig. 1 Proposed Research Methodology

Table 2 Kappa Coefficient for Use Case-1

Category		Expert 2	
		No	Yes
Expert 1	No	0.4984	0.0287
	Yes	0	0.4728
Kappa	0.9425		
Subjects	312		

preprocessing can significantly impact the performance and reliability of your ML models.

(iv) **Word Embeddings**
Word embeddings are a technique used in natural language processing (NLP) and machine learning to represent words as dense vectors of real numbers in a continuous space. They capture semantic relationships between words, allowing algorithms to understand the meaning and context of words in a more meaningful way compared to traditional sparse representations like one-hot encoding.

(v) **LSTM based Predictions**
In ML, algorithm development is a crucial aspect of research. Research methodology guides the process of developing, refining, and optimizing algorithms. It encourages researchers to document their design choices, making it easier for others to understand, replicate, and build upon their work.
LSTM models are designed to handle sequential data, making them well-suited for text classification where the order of words matters. It can capture the context and dependencies between words, enabling them to understand the meaning of sentences and paragraphs. LSTM (Long Short-Term Memory) based deep learning models offer several advantages when used for text classification tasks such as: Sequential Information Handling, Long-Term Dependencies, Feature Extraction, Variable-Length Input, Contextual Understanding, Multiclass and Multilabel Classification, Adaptability to Various Text Data, and Interpretability.

(vi) **Validation of Results**
Validation of results in machine learning (ML) is a crucial step to assess the performance and generalization capabilities of your trained model. The process typically involves splitting the dataset into training, validation, and test sets, and using various metrics to evaluate the model's performance.

Table 3 Kappa Coefficient for Use Case-2

Category		Expert 2	
		No	Yes
Expert 1	No	0.5020	0.0066
	Yes	0.0146	0.4726
Kappa	0.9575		
Subjects	758		

Table 4 Hyper-parameters for Use Case 1

Parameter	Value
Training Dataset	188
Validation Dataset	62
Test Dataset	62
Total no of records	312
Epochs	25
Classes	2
Learning rate	0.001
Decay (decay of learning rate)	0
Dropout	0.3
Optimizer	Adam

3.2 Experimental study

The following steps mentions the necessary setup, pre-proessing and annotations, and key parameter selection for the proposed model.

(i) **Setup**
The system used for the implementation of proposed approach consists of *Intel (R) Core(TM) i7-5500U CPU @ 2.40 GHz, 8 GB RAM*. The program is implemented in R Programming using *Keras* library with Tensorflow [3].

(ii) **Pre-Processing and Annotations**
We have pre processed data from various dark web forum as we have done in earlier approach [13, 22]. We used same annotated datasets described in [13, 22] for our current research.
As the two experts have labeled the posts, so there is a need to compare a number of agreements between the two experts to validate consistency between annotations. Cohen's kappa coefficient from statistics is used to check the agreement between experts. We calculated the kappa coefficient for both uses cases using R Programming Package *psych* [20] as shown in Table 2 for Use Case 1 and Table 3 for Use Case 2. The kappa coefficient statistically validated the annotations done by subject domain experts so that we can proceed to feature selection and model training.

(iii) **Key Parameters Selection**
Dataset is partitioned into 80:20 for the training and testing. The hyper-parameters used to train the model are tuned attentively. The hyper parameters tuned for the required model are described in Tables 4 and 5 for both use cases respectively.
The hyper-parameters were tuned carefully using a grid search in which several values are tried and tested. The amalgamation of parameters that led to the best results is finally utilized for the rest of the experiments. Additionally, the "adam" (Adaptive Moment Estimation) optimizer was chosen for updating the values of parameters on each epoch. A description of Adam optimizer is given below:

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

where m_t is aggregate of gradients at time t. [current] (initially, $m_t = 0$), m_{t-1} is aggregate of gradients at time t-1. [previous], v_t is sum of square of past gradients at

Table 5 Hyper-parameters for Use Case 2

Parameter	Value
Training Dataset	478
Validation Dataset	119
Test Dataset	161
Total no of records	758
Epochs	25
Classes	2
Learning rate	0.001
Decay (decay of learning rate)	0
Dropout	0.3
Optimizer	Adam

time t. (initially = 0), v_{t-1} is sum of square of past gradients at time t-1, 'g' is gradient on current mini-batch, and $\beta 1$ and $\beta 2$ are newly introduced hyper-parameters of the algorithm (default values of 0.9 and 0.999 respectively). More details about Adam optimizer can be found in [7].

4 Results and discussions

LSTM-based deep learning mechanism is employed for both use cases. For evaluating the proposed system, we presented training and testing phase details as per the following:

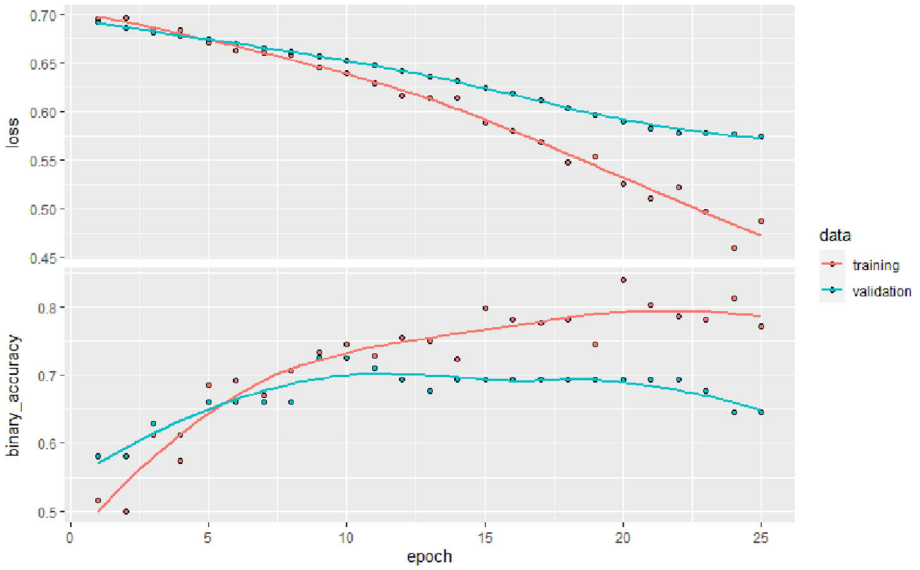


Fig. 2 Use Case 1: Loss and Metrics Curve (Detection of Weapon Procurement)

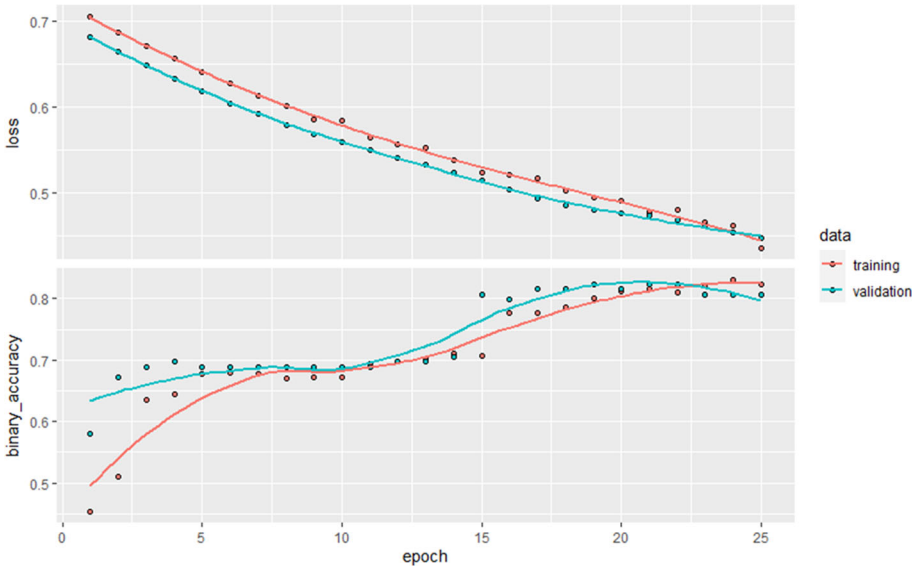


Fig. 3 Use Case 2: Loss and Metrics Curve (Online Recruitment of Terrorists)

4.1 Training and validation

In Use Case1 (Dataset Size:312), all algorithms are performing similarly as the size of our data is smaller in comparison to Use Case2 (Dataset Size:758). Irrespective of the use of different machine learning and deep learning algorithms, marginal difference in accuracy is obtained (71% for Proposed LSTM, 69% for SVM, 68% for RF 68% for BOOSTING). In Use Case 2, as the size of the dataset is increased by 446 records, our machine-learning algorithms are performing well.
Figure 2 (Detection of Weapon Procurement) illustrates the loss and metrics curve for proposed LSTM based method, which is referred to as Use Case 1 in our study. Figure 3 (Detection of Online Recruitment of Terrorists) shows the performance (loss an metrics curve) of the proposed LSTM-based approach, which is referred as Use Case 2 in our study. Furthermore, we summarize the performance in Table 6 for Use Case 1 (Detection of Weapon Procurement) and Table 7 for Use Case 2 (Detection of Online Recruitment of Terrorists).

4.2 Testing

The testing performance is shown in the 4th row of both tables: Table 6 for Use Case 1 (Detection of Weapon Procurement) and Table 7 for Use Case 2 (Detection of Online Recruitment

Table 6 Use Case 1: Performance Parameters

Dataset Type	Accuracy (%)	Loss
Training	77.13	0.4880
Validation	64.52	0.5740
Testing	70.96	0.4871

Table 7 Use Case 2: Performance Parameters

Dataset Type	Accuracy (%)	Loss
Training	82.22	0.4350
Validation	80.67	0.4463
Testing	83.22	0.4230

of Terrorists), where the parameters of the classifier were fixed from the training process at epoch=25. In the previous work, we have seen how machine learning algorithms can be utilised to classify the annotated records.

Comparing deep learning models with traditional machine learning models is essential to understand the relative strengths, weaknesses, and suitability of each approach for different tasks and datasets. Here are some reasons why such comparisons are important:

(i) **Performance Benchmarking**
Comparing deep learning models with traditional machine learning models establishes a baseline for performance. This benchmarking helps researchers and practitioners gauge whether the added complexity of deep learning architectures leads to significant improvements in accuracy, efficiency, or other relevant metrics.

(ii) **Task Suitability**
Different tasks have varying requirements in terms of data size, complexity, and available features. Comparing models helps identify which approach is better suited for a particular task. Deep learning might excel in tasks where there are complex patterns and large amounts of data, while traditional machine learning models might be more appropriate for simpler tasks with limited data.

(iii) **Interpretability**
Traditional machine learning models often provide more interpretability than deep learning models. Comparing the two approaches can help decide whether the level of interpretability provided by traditional models is necessary for a given application, or if the predictive performance of deep learning outweighs the interpretability trade-off.

(iv) **Data Efficiency**
Traditional machine learning models might require less data to achieve reasonable performance compared to deep learning models. If limited data is available, it's important to compare whether deep learning's increased complexity is justified by the data quantity and quality.

(v) **Resource Requirements**
Deep learning models often require more computational resources, such as GPUs or TPUs, and longer training times compared to traditional models. A comparison can help weigh the computational costs against the performance gains.

We have compared previously build machine learning-based classifiers with the proposed LSTM-based deep learning approach as shown in Fig. 4. The accuracy is improved in the case of the proposed LSTM-based deep learning algorithm by 12% (Use Case 1 Accuracy for Proposed LSTM-71% Use Case 2 Accuracy for Proposed LSTM-83%). Observing the small difference, we can conclude that both machine learning and deep learning-based classifiers fit to our current study.

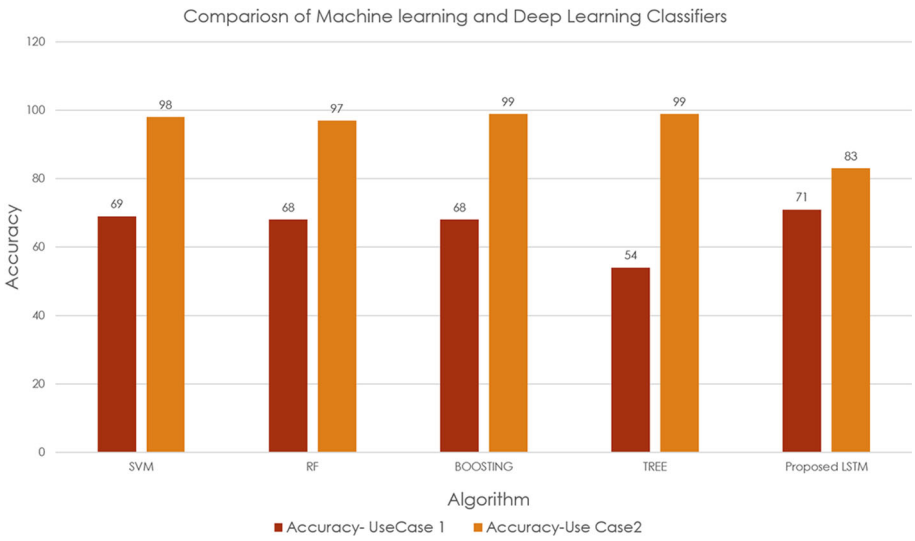


Fig. 4 Comparison of Deep Learning vs Machine Learning Classifiers

5 Conclusions

Studying dark web markets to detect violent activities is a complex and challenging task that often involves a multidisciplinary approach, including computer science, criminology, cyber-security, and data analysis. We developed an automated approach to detect purchasing of illegal weapons (Use Case 1) and the recruitment of innocent minds (Use Case 2) over the dark web in our current work. The online procurement of illegal weapons can also have serious implications for national security. Identifying and thwarting attempts to acquire weapons for terrorist organizations or other extremist groups can help safeguard a country's security interests. By monitoring and detecting recruitment activities, law enforcement agencies can identify and intervene in the early stages of radicalization, disrupting terrorist networks before they can carry out attacks. To the best of our knowledge, the proposed model presents a novel contribution to automate the process of detecting violent activities over the dark web. This type of automation is helpful for any national security agency to keep track of illegal procurement or online recruitment of terrorists.

Funding and Competing Interests NA

Research Data Policy and Data Availability Statements The datasets analysed during the current study are available in the Dark Web Project Portal [2] cited in the paper Section 3.2 .

Declarations

Disclosure of potential conflicts of interest NA

Research involving Human Participants or Animals NA

Informed consent NA

References

1. Bowie NG (1968–2009) Terrorism events data: An inventory of databases and data sets. Perspect Terror 11(4):50–72. http://www.rand.org/nsrd/projects/terrorism-incidents.html
2. Chen H (2011) Dark web: Exploring and mining the dark side of the web. In: 2011 European intelligence and security informatics conference, IEEE, pp 1–2. http://www.azsecure-data.org/about.html
3. Chollet F, Allaire J et al (2017) R interface to keras. https://github.com/rstudio/keras
4. Desmarais BA, Cranmer SJ, Hill C et al (2011) Forecasting the locational dynamics of transnational terrorism : a network analytic approach. In: European intelligence and security informatics conference, pp 171–177, https://doi.org/10.1109/EISIC.2011.44
5. Dhote Y, Mishra N (2013) Survey and analysis of temporal link prediction in online social networks. In: International conference on advances in computing, communications and informatics (ICACCI), pp 1178–1183
6. Domingo JD, Gomez-Garcia-Bermejo J, Zalama E (2022) Optimization and improvement of a robotics gaze control system using lstm networks. Multimed Tools Appl 81(3):3351–3368
7. Duchi J, Hazan E, Singer Y (2011) Adaptive subgradient methods for online learning and stochastic optimization. J Mach Learn Res 12(7)
8. Fernandez M, Asif M, Alani H (2018) Understanding the roots of radicalisation on twitter. In: Proceedings of the 10th ACM conference on web science, ACM, pp 1–10
9. Goyal T, Saini JK, Bansal D (2019) Analyzing behavior of isis and al-qaeda using association rule mining. In: Proceedings of 2nd international conference on communication, computing and networking: ICCCN 2018, NITTTR Chandigarh, India, Springer, pp 669–675
10. Hsiao Hw, Lin CS, Chang Sy (2009) Constructing an ARP attack detection system with SNMP traffic data mining. In: Proceedings of the 11th international conference on electronic commerce. ACM, pp 341–345
11. Kapil P, Ekbal A (2020) A deep neural network based multi-task learning approach to hate speech detection. Knowl-Based Syst 210:106458
12. Katipally R, Gasior W, Cui X et al (2010) Multistage attack detection system for network administrators using data mining. In: Proceedings of the sixth annual workshop on cyber security and information intelligence research, ACM, pp 51
13. Kaur A, Saini JK, Bansal D (2019) Detecting radical text over online media using deep learning. arXiv:1907.12368
14. Kengpol A, Neungrit P (2014) Computers & Industrial Engineering A decision support methodology with risk assessment on prediction of terrorism insurgency distribution range radius and elapsing time?: An empirical case study in Thailand. Comput Ind Eng 75:55–67. https://doi.org/10.1016/j.cie.2014.06.003
15. Kour H, Gupta MK (2022) An hybrid deep learning approach for depression prediction from user tweets using feature-rich cnn and bi-directional lstm. Multimed Tools Appl 81(17):23649–23685
16. Majeed A, Beg MO, Arshad U et al (2022) Deep-emoru: mining emotions from roman urdu text using deep learning ensemble. Multimed Tools Appl 81(30):43163–43188
17. Munezero M, Montero CS, Kakkonen T et al (2014) Automatic detection of antisocial behaviour in texts. Informatica 38(1)
18. Naik AJ, Gopalakrishna M (2021) Deep-violence: individual person violent activity detection in video. Multimed Tools Appl 80(12):18365–18380
19. Rehman AU, Malik AK, Raza B et al (2019) A hybrid cnn-lstm model for improving accuracy of movie reviews sentiment analysis. Multimed Tools Appl 78:26597–26613
20. Revelle W (2021) psych: procedures for psychological, psychometric, and personality research. Northwestern University, Evanston, Illinois, r package version 2.1.9. https://CRAN.R-project.org/package=psych
21. Rezaeenour J, Ahmadi M, Jelodar H et al (2023) Systematic review of content analysis algorithms based on deep neural networks. Multimed Tools Appl 82(12):17879–17903
22. Saini JK, Bansal D (2019) A comparative study and automated detection of illegal weapon procurement over dark web. Cybern Syst 50(5):405–416. https://doi.org/10.1080/01969722.2018.1553591
23. Saini JK, Bansal D (2021) Detecting online recruitment of terrorists: towards smarter solutions to counter terrorism. Int J Inf Technol 13:697–702
24. Saini JK, Bansal D (2023) Computational techniques to counter terrorism: a systematic survey. Multimed Tools Appl 1–26
25. Thakur D, Saini JK, Srinivasan S (2023) Deepthink iot: the strength of deep learning in internet of things. Artif Intell Rev 1–68
26. Vinyard Software (2016) International terrorism: attributes of terrorist events, 1968-1977 [ITERATE 2]. https://www.icpsr.umich.edu/icpsrweb/ICPSR/studies/07947. Accessed 8 May 2016
27. Wigle J (2010) Introducing the worldwide incidents tracking system (wits). Perspect Terror 4(1):3–23

28. Yechuri PK, Ramadass S (2021) Classification of image and text data using deep learning-based lstm model. Trait du Signal 38(6)
29. Zhang T, Yang Z, Jia W et al (2016) A new method for violence detection in surveillance scenes. Multimed Tools Appl 75:7327–7349
30. Zhang Y, Zeng S, Fan L et al (2009) Dark web forums portal: searching and analyzing jihadist forums. In: 2009 IEEE international conference on intelligence and security informatics, IEEE, pp 71–76
31. Zhou Y, Qin J, Reid E et al (2005) Studying the presence of terrorism on the web : a knowledge portal approach. In: Proceedings of the 5th ACM/IEEE-CS joint conference on digital libraries. ACM, 2005, pp 402

P23

Abstract template for the Advanced School on Foundation Models for Scientific Discovery — (smr 4088)

Myke Vital SAO TEMGOUA[1], **Jean-Pierre TCHAPET NJAFA**[1], **and Serge Guy NANA ENGO**[1]

[1] *University of Yaounde 1*

This document is the template for contributed abstracts posters and gives the guidelines for preparing and submitting abstracts for the *Advanced School on Foundation Models for Scientific Discovery — (smr 4088)* to be held in-person from *10/07/2025* to *18/07/2025*.

Malaria remains a significant global health crisis [1], particularly in tropical and subtropical regions, exacerbated by the increasing prevalence of drug-resistant strains of the *Plasmodium* parasite. To address this challenge, innovative strategies for antimalarial drug discovery are essential, utilizing both the rich chemical diversity of natural products and the synthetic tractability of designed compounds. This study investigates the chemical space distributions of compounds within African Natural Product Databases (ANPDB) [2, 3], prominent public resources containing more than $690\,000$ natural products, and compares them to synthetic compounds with known antimalarial activity. Our findings reveal distinct chemical space distributions between natural and synthetic compounds, with synthetic compounds occupying a broader region and natural products exhibiting conserved clustering, potentially indicative of privileged scaffolds. Furthermore, analysis of the physicochemical properties and ADMET profiles highlights complementary strengths and weaknesses of each class regarding drug-likeness and developability [4]. The results point toward promising avenues for integrated drug discovery strategies, which combine the structural novelty of synthetic compounds with the validated bioactivity and favorable properties of natural products, ultimately aiming to identify viable candidates for development in resource-constrained settings where novel and affordable antimalarials are most urgently needed.

[1] World Health Organization, World Malaria report 2024, Accessed 2025-03-03 (World Health Organization, 2024).

[2] C. V. Simoben et al., *"Pharmacoinformatic investigation of medicinal plants from east africa"*, Molecular Informatics 39, 2000163 (2020).

[3] F. Ntie-Kang et al., *"Nanpdb: a resource for natural products from northern african sources"*, Journal of Natural Products 80, PMID: 28641017, 2067–2076 (2017).

[4] K. Swanson et al., *"Admet-ai: a machine learning admet platform for evaluation of large-scale chemical libraries"*, Bioinformatics 40, edited by A. Valencia, 10.1093/bioinformatics/btae416 (2024)

P24

Uncertainty-Aware Cervical Cytology Screening Using Histopathology Foundation Model and Conformal Prediction

Gbègninougbo Aurel Davy Tchokponhoue[1] and Ali Idri[1]

[1] Faculty of Medical Science, UM6P Hospitals, Mohammed VI Polytechnic University, Ben Guerir, 43150, Morocco

Cervical cancer is a serious worldwide health concern, and early detection is critical for improved patient outcomes. While Deep Learning (DL) has shown significant potential in cervical cancer classification, most state-of-the-art models rely on pretrained convolutional neural networks (CNNs) and primarily focus on model performance, often neglecting the critical need for uncertainty quantification (UQ), a key requirement for real-world clinical applications. In this study, we explore the UNI histopathology foundation model for cervical cancer classification using cytology data, integrating conformal prediction to address uncertainty quantification and enhance model reliability and trustworthiness. We assess and compare the performance of the UNI model against leading CNNs, including VGG19, ResNet50, MobileNetV2, DenseNet121, and InceptionV3, across multiple metrics such as accuracy, calibration, uncertainty quantification, and out-of-distribution (OOD) detection using a 5-fold cross-validation over the Mendeley LBC and SIPaKMeD datasets. The UNI model consistently achieved state-of-the-art classification performance, with near-perfect results on the Mendeley LBC dataset and accuracy of 96% over the SIPaKMeD dataset, while also excelling in calibration, uncertainty estimation, and OOD detection. Moreover, our study uncovered a significant correlation between predictive set size, model predictive capability, and predictive entropy, paving the way for new conformal prediction methods that can incorporate entropy to improve algorithm efficiency. These findings suggest that integrating UQ with advanced models not only enhances predictive accuracy but also increases trustworthiness, positioning the UNI model as a valuable tool for cervical cancer screening in clinical settings.

P25

Machine Learning - Driven Design and Synthesis of Materials for Solid-State Hydrogen Storage

Ashwini Verma [1,2] **and Kavita Joshi** [1,2]

[1] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India*
[2] *Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune*

Solid-state hydrogen storage in metal alloys holds the potential to outperform conventional (liquid/compressed) methods on account of volumetric capacity, safety, and durability. Despite significant performance improvements in metal hydrides over the past two decades, their practical application is hindered by the unattainable thermodynamics and kinetics. Alloying is one of the most effective ways of tailoring the properties of these compositions. However, the traditional trial-and-error approach restricts the exhaustive screening of chemical space, necessitating more efficient strategies. To address this issue, we are integrating ML with experimental techniques to systematically screen the infinite chemical space of plausible metal hydrides, aiming to design and synthesize materials with improved hydrogen storage properties.

In this work, we have built a suite of machine learning models to predict key hydrogen storage properties such as hydrogen storage capacity, (HYST)[1,2], enthalpy of hydride formation (THOR)[1], and equilibrium plateau pressure (EquiP)[3]. We have also built a model capable of predicting the Pressure-Composition-Temperature isotherms (MH-PCTpro) [4]. PCT isotherms provide crucial information, like reversible storage capacity and equilibrium plateau pressure. These models are validated across diverse alloy families, agreeing with experimental results. Further, we employed these models to predict hydrogen storage properties of 6.4 million unseen compositions. In this poster, I will present these models and provide a detailed analysis of the predicted hydrogen storage properties for 6.4 million novel compositions. I will also present the experimental results for the compositions identified by these models.[5] Additionally, I will discuss the active machine learning approach we're using, where model predictions strategically guide experimental design, and experimental results immediately update and improve the model predictability.[6]

[1] A. Verma, N. Wilson, and K. Joshi, Int. J. Hydrogen Energy 50, 1518 (2024).
[2] N. Wilson, A. Verma, P. R. Maharana, A. B. Sahoo, and K. Joshi, Int. J. Hydrogen Energy 90, 460 (2024)
[3] A. Verma and K. Joshi, What Drives Predictive Chemistry: More Data or Smarter Features for Hydrogen Storage Property Prediction? (manuscript under prepration)
[4] A. Verma and K. Joshi, iScience, 112251, 2589-0042 (2025).
[5] A. Verma, P. Kumar, S. Kumar and K. Joshi Synthesis and Characterization of ML-Predicted Mg-Based Composites for Hydrogen Storage. (to be communicated)
[6] A. Verma and K. Joshi, Active-PCTpro: Where Experiments and Active ML Collaborate for Smarter Predictions (manuscript under prepration)

P26

Deep learning-driven segmentation of ischemic stroke lesions using multi-channel MRI

Md. Sharjis Ibne Wadud[1], Ashiqur Rahman[1], Muhammad E. H. Chowdhury[2]

[1]Department of Biomedical Physics and Technology, University of Dhaka, Bangladesh
[2]Department Electrical Engineering, College of Engineering, Qatar University, Qatar

Ischemic stroke, caused by cerebral vessel occlusion, presents substantial challenges in medical imaging due to the variability and subtlety of stroke lesions. According to the World Health Organization (WHO), approximately 15 million people suffer from strokes each year, with ischemic strokes accounting for about 87% of all cases [1]. Magnetic Resonance Imaging (MRI) plays a crucial role in diagnosing and managing ischemic stroke, yet existing segmentation techniques often fail to accurately delineate lesions. This study introduces a novel deep learning-based method for segmenting ischemic stroke lesions using multi-channel MRI modalities, including Diffusion Weighted Imaging (DWI), Apparent Diffusion Coefficient (ADC), and enhanced Diffusion Weighted Imaging (eDWI). The proposed architecture integrates DenseNet121 as the encoder with Self-Organized Operational Neural Networks (SelfONN) in the decoder, enhanced by Channel and Space Compound Attention (CSCA) and Double Squeeze-and-Excitation (DSE) blocks. Additionally, a custom loss function combining Dice Loss and Jaccard Loss with weighted averages is introduced to improve model performance. Trained and evaluated on the ISLES 2022 dataset, the model achieved Dice Similarity Coefficients (DSC) of 83.88 % using DWI alone, 85.86 % with DWI and ADC, and 87.49 % with the integration of DWI, ADC, and eDWI. This approach not only outperforms existing methods but also addresses key limitations in current segmentation practices. These advancements significantly enhance diagnostic precision and treatment planning for ischemic stroke, providing valuable support for clinical decision-making.

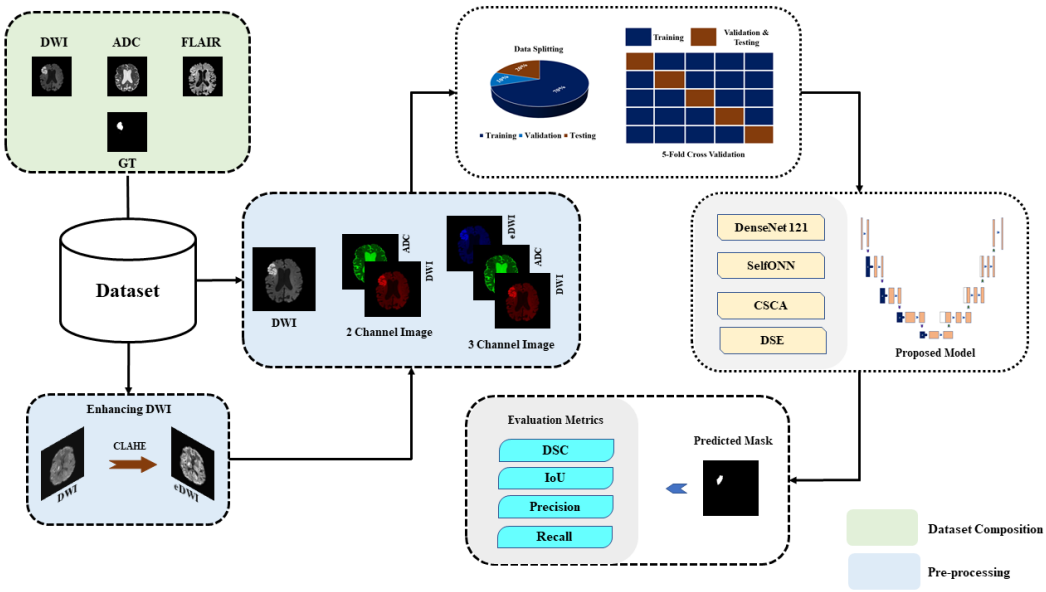


Figure 1: Schematic representation of the experimental pipeline for ischemic lesion segmentation.

[1] WHO Fact sheets, "The Atlas of Heart Disease and Stroke," 01 May 2025. [Online]. Available: https://www.who.int/cardiovascular_diseases/resources/atlas/en/.

P27

A Framework for Representation Learning on Irregular and Sparse Time-Series

Uros Zivanovic[1], **Serafina Di Gioia**[2,3], **Andre Scaffidi**[3], **Martín de los Rios**[3], **Gabriella Contardo**[7,3], **and Roberto Trotta**[3,4,5,6]

[1]*University of Trieste, Italy*
[2]*Abdus Salam International Centre for Theoretical Physics (ICTP), Italy*
[3]*Scuola Internazionale Superiore di Studi Avanzati (SISSA), Italy*
[4]*INFN – National Institute for Nuclear Physics, Italy*
[5]*ICSC - Centro Nazionale di Ricerca in High Performance Computing, Italy*
[6]*Imperial College London, United Kingdom*
[7]*University of Nova Gorica, Slovenia*

We present the Rotary Masked Autoencoder[3], a novel extension to the Masked Autoencoder[1] (MAE) framework utilizing the Rotary Positional Embedding [2] (RoPE) method. By utilizing RoPE to embed continuous position, we are able to do representation learning not just on the usual modalities that MAE works well with such as images and audio, but also on new modalities such as multivariate irregular time-series and sparse data. In contrast to prior work on architectures for irregular time-series, our approach is simpler and more general. By utilizing methods already ubiquitous within natural language processing and computer vision, our model works well with other tools commonly used in these fields such as mixed precision training and just-in-time compilation. We investigate our models performance across a variety of benchmarks, showing equal or better performance to MAE on standard modalities while pulling ahead of specialized architectures in modalities where standard MAE does not work. We also highlight the models potential when utilized within physics for difficult tasks such as light curve classification and xenon time projection chamber photomultiplier tube traces, showing the potential for representation learning within fundamental physics.

References

[1] K. He, X. Chen, S. Xie, Y. Li, P. Dollár, and R. B. Girshick. Masked autoencoders are scalable vision learners. In *IEEE/CVF Conference on Computer Vision and Pattern Recognition, CVPR 2022, New Orleans, LA, USA, June 18-24, 2022*, pages 15979–15988. IEEE, 2022. doi: 10.1109/CVPR52688.2022.01553. URL https://doi.org/10.1109/CVPR52688.2022.01553.

[2] J. Su, M. H. M. Ahmed, Y. Lu, S. Pan, W. Bo, and Y. Liu. Roformer: Enhanced transformer with rotary position embedding. *Neurocomputing*, 568:127063, 2024. doi: 10.1016/J.NEUCOM.2023.127063. URL https://doi.org/10.1016/j.neucom.2023.127063.

[3] U. Zivanovic, S. D. Gioia, A. Scaffidi, M. de los Rios, G. Contardo, and R. Trotta. Rotary masked autoencoders are versatile learners, 2025. URL https://arxiv.org/abs/2505.20535.