MAHMOUD EBRAHIMKHANI

Artificial Intelligence Scientist I

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SUMMARY

I am an AI Scientist experienced in developing generative AI models, including DDPMs, LLMs, and GANs, designed using transformers, GNNs, RNNs, and CNNs, for various chem- and bio-informatics applications. I am proficient in Python programming, deep learning tools like PyTorch and TensorFlow, and cloud platforms such as Azure and HPC. My work is to design, train, benchmark, and productionize ML models to tackle research challenges across image, time-series, text, and graph data.

EDUCATION

Ph.D. and M.Sc. in Biomedical Engineering, Stony Brook University, NY **2017 – 2022**

Thesis: "Machine Learning in Terahertz Spectroscopy: Burn Diagnosis and Material Characterization Applications"

B.Sc. in Electrical Engineering, Amirkabir University of Technology, Iran **2011 – 2016**

Thesis: "Denoising MRI Images Using the Fast 2D Stockwell Transform"

TECHNICAL SKILLS

Programming

Proficient: Python, R, MATLAB

Generative AI

Frameworks: PyTorch, TensorFlow

Models: VAE, CVAE, CGAN, CycleGAN, Denoising Diffusion, Masking Diffusion, Conditional Diffusion

Applications: Conditional Image Generation, Small Molecule Generation, Protein Generation, Motif Scaffolding

Deep learning

Frameworks: PyTorch, TensorFlow

Models: CNN, GNN, LSTM, EGNN, Transformer

Applications: Regression, Classification, Segmentation, Image-to-Image Translation, NLP, Molecule Generation

Machine learning

Techniques: Feature Extraction, Feature Selection, Dimensionality Reduction, Hyperparameter Optimization

Models: XGBoost, Random Forests, SVM, Linear/Polynomial Discriminant Analysis, Bayes Classifier

Tools: Scikit-learn, Optuna

Cloud & HPC

Expert: Microsoft Azure, Azure ML Studio

Proficient: AWS, HPC Clusters, Bash, SLURM (Linux)

Drug Discovery

Generative AI Models: RFDiffusion, DiffAb, ProtGPT, MolGPT, Pocket2Mol, TargetDiff, SBDD, DiffDock, AlphFold, ESMFold, RoseTTAFold

Datasets: PDB, ChemBL, Zinc, GuacaMol, PubChem, Moses, CrossDocked

Chem- and Bioinformatics:

Tools: RDKit, DeepChem, Py3DMol, NGLView, Open Babel, Autodock Vina, Gnina (Python)

Biomedical Data Analysis: ECG, PC-MRI, CTA, MRS, THz-TDS (Time-series, Medical Images, High-dimensional Datasets)

PROFESSIONAL EXPERIENCE

Artificial Intelligence (AI) Scientist I, 1910 Genetics, MA **2023 – Current**

Responsibilities

- Design, train, evaluate, and productionize generative AI models for structure-based small molecule/protein design.
- Lead data engineers in curating large-scale datasets for various molecular ML modeling and analysis tasks.
- Adapt, optimize, benchmark, and fine-tune existing ML models for molecular property prediction and reinforcement learning.
- Collaborate with medicinal chemists and biologists to optimize AI-generated compounds in drug campaigns.
- Stay updated with the latest advancements in generative AI, especially in bio- and chem-informatics applications.

Projects

- Developed a 3D E(3)-equivariant self-supervised, auto-regressive GNN model for structure-based small molecule design to inhibit an enzyme pertaining to a neurodegenerative disorder.
- Implemented training, finetuning, and reinforcement learning of RNN and Transformer-based LLMs to generate novel and diverse chemical SMILES strings in drug discovery campaigns.
- Adapted the TargetDiff and Pocket2Mol, DDPM and GNN-based models, for target-aware small molecule generation and optimization.
- Finetuned and productionized the ImageMol, a pretrained on 10 million molecular images, to predict the blood-brain barrier penetration on internal and public datasets.
- Curated the CrossDocked2020 dataset, containing over 20 million cognate and non-cognate docked receptor-ligand complexes from PDB.

Postdoctoral Research Associate, Northwestern University, IL **2022 – 2023**

Responsibilities

- Design, train, and productionize deep learning models for medical imaging and prediction of 3D cardiovascular hemodynamics using AI.
- Incorporate and standardize data from diverse imaging modalities, including PC-MRI, CTA, and wearable diagnostic devices.
- Design advanced signal and image processing methodologies, such as CWT, image segmentation and registration, for the analysis/curation of medical imaging datasets.
- Participate in scientific conferences and workshops; author and submit articles to peer-reviewed journals and conferences; and contribute to patent filings.
- Collaborate with radiologists, cardiologists, clinical teams, and engineering professionals to advance project objectives.

Projects

- Trained, finetuned, and optimized a Cycle-GAN model for 3D aortic hemodynamics prediction using anatomical data from CT Angiography. Validated using 4D Flow MRI ground truth [GitHub].
- Developed a hybrid deep learning framework combining CNN and MLP architectures for the diagnosis of aortic stenosis and regurgitation using wearable seismocardiography (SCG) data [GitHub].
- Authored a journal article, delivered presentations at two conferences, and filed a patent on the application of AI in diagnosing cardiac pathologies using SCG.

Graduate Research Assistant and Postdoctoral Researcher, Stony Brook University, NY **2017 - 2022**

Responsibilities

- Design, train, and evaluate NN and ML models to regress biological markers of in-vivo burn injuries, predicting indicators like apoptosis and reepithelialization rate using THz-TDS data.
- Design and implement techniques for feature extraction, feature selection, and dimensionality reduction to train ML models, including SVM, XGBoost, and LDA, for non-invasive depth assessment of burn injuries.
- Implement advanced signal and image processing methods such as wavelet denoising, Wiener deconvolution, and sparse deconvolution for enhanced SNR and image resolution.
- Collaborate with interdisciplinary teams to design and create a portable THz scanner.
- Design and implement computational techniques to mitigate Mie and Kirchhoff scattering at THz regime.
- Participate in scientific conferences, author peer-reviewed publications, contribute to patent applications, and assist in drafting grants.

Projects

- Developed ML models (DNN, SVM, XGBoost) for in vivo burn injury severity prognosis (predicting histological markers including apoptosis and re-epithelialization rates) using THz-TDS imaging and the double Debye (DD) dielectric theory.
- Designed and implemented a pipeline for enhancing THz imaging signals using wavelet denoising, Wiener deconvolution, and sparse deconvolution.
- Simulated scattered THz wave reflections in biological tissues using Monte Carlo methods and characterized chemical substances in the THz frequency range amid Kirchhoff surface scatterings.
- Innovated a THz imaging approach to visualize through diffusive cloaks, introducing the bimodality coefficient spectrum.
- Optimized optical alignment in THz-TDS with PCA and ASOPS technology.
- Contributed to over 35 peer-reviewed journal and conference articles, serving as the first author in 8 of them, and presented at 6 international conferences.

Graduate Teaching Assistant, Stony Brook University, NY **2020 – 2021**

- Assisted in teaching BME271: Introduction to Electric Circuits and Bioelectricity, and BME301: Bioelectricity.
- Duties included preparing lesson materials, conducting tutorial sessions, grading assignments and exams, and providing academic support to students.

Undergraduate Research Assistant, Amirkabir University of Technology (AUT), Iran **2015 – 2016**

Projects

- Programmed a binary classification model for brain tumor identification, using Stockwell transform and magnetic resonance spectroscopy (MRS).
- Programmed a denoising approach for MRI images using soft-thresholding based on 2D Stockwell transform.

Summer internship, Pardis Communications Co., Iran **2015 – 2015**

Projects

- Developed and simulated analog modulation and demodulation methodologies, including amplitude, frequency, single-sideband, and double-sideband modulations in MATLAB.

PUBLICATIONS LIST

- Collins et al., “Attentive graph neural network models for the prediction of blood brain barrier permeability,” **Nat. Communications** submitted.

- **Khani** et al., "A deep learning approach to using wearable seismocardiography (SCG) for diagnosing aortic valve stenosis and predicting aortic hemodynamics obtained by 4D Flow MRI," **Ann. Biomed. Eng.** 2023.
- **Khani** et al., "Triage of in vivo burn and prediction of wound healing outcome using neural networks and modeling of the terahertz permittivity based on the double Debye dielectric parameters," **Biomed. Opt. Express** 2023.
- **Khani** et al., "Deep learning-based prediction of aortic hemodynamics obtained by 4D flow MRI using seismocardiography of chest vibrations," **ISMRM** 2023.
- Berhane et al., "Highly resilient AI-derived 3D aortic hemodynamics from aortic geometry," **ISMRM** 2023.
- **Khani** et al., "Prediction of aortic hemodynamics using convolutional neural networks (CNN) and time-frequency transformation of chest vibrations measured by seismocardiography (SCG)," **SCMR** 2022.
- **Khani** et al., "Physical modeling of the permittivity of in vivo burn injuries using Debye dielectric parameters measured by the THz PHASR scanner," **Proc. Conf. Lasers Electro-Opt.** 2022.
- **Khani** et al., "Supervised machine learning for automatic classification of in vivo scald and contact burn injuries using the terahertz Portable Handheld Spectral Reflection (PHASR) Scanner," **Sci. Rep.** 2022.
- **Khani** et al., "Accurate and early prediction of the wound healing outcome of burn injuries using the wavelet Shannon entropy of THz time-domain waveforms," **J. Biomed. Opt.** 2022.
- **Khani** et al., "Multiresolution spectrally-encoded terahertz reflection imaging through a highly diffusive cloak," **Opt. Express** 2022.
- **Khani** et al., "Translation-invariant zero-phase wavelet methods for feature extraction in terahertz time-domain spectroscopy," **Sensors** 2022.
- Osman et al., "Deep neural network classification of in vivo burn injuries with different etiologies using terahertz time-domain spectral imaging," **Biomed. Opt. Express** 2022.
- **Khani** et al., "Diffuse terahertz spectroscopy in turbid media through a wavelet-based bimodality spectral analysis," **Sci. Rep.** 2021.
- **Khani** et al., "Chemical identification in the specular and off-specular rough-surface scattered terahertz spectra using wavelet shrinkage," **IEEE Access** 2021.
- **Khani** et al., "Acute burn assessment using terahertz spectroscopic feature extraction and support vector machines," **Proc. Conf. Lasers Electro-Opt.** 2021.
- **Khani** et al., "Accurate classification of burn injuries using support vector machines and the wavelet Shannon entropy of the THz-TDS waveforms," **Proc. of IEEE IRMMW-THz** 2021.
- **Khani** et al., "Phase function effects on identification of Terahertz spectral signatures using the discrete wavelet transform," **IEEE Trans. Terahertz Sci. and Technol.** 2020.
- Harris et al., "Terahertz time-domain spectral imaging using telecentric beam steering and an f-θ scanning lens: distortion compensation and determination of resolution limits," **Opt. Express** 2020.
- Harris et al., "Terahertz portable handheld spectral reflection (PHASR) scanner," **IEEE Access** 2020.

CONFERENCE PERESENTATIONS

- "Deep learning-based prediction of aortic hemodynamics obtained by 4D flow MRI using seismocardiography of chest vibrations," **ISMRM 2023 – Poster**.
- "Prediction of aortic hemodynamics using convolutional neural networks (CNN) and time-frequency transformation of chest vibrations measured by seismocardiography," **SCMR 2022 – Poster**.
- "Physical modeling of the permittivity of in vivo burn injuries using Debye dielectric parameters measured by the THz PHASR scanner," **CLEO 2022 – Oral**.
- "Highly accurate and early prediction of the wound healing outcome of in vivo burn injuries using the Terahertz PHASR Scanner and supervised machine learning," **NEBEC 2022 – Poster**.
- "Accurate classification of burn injuries using support vector machines and the wavelet Shannon entropy of the THz-TDS waveforms," **IRMMW-THz 2022– Oral**.
- "Acute burn assessment using terahertz spectroscopic feature extraction and support vector machines," **CLEO 2021 – Oral**.

- "Two wavelet-based algorithms for chemical recognition using transmission terahertz spectral imaging through turbid media," **IRMMW-THz 2021– Oral**.
- "Wavelet Shrinkage for Enhanced Chemical Recognition in the Rough Surface Diffused Terahertz Spectra," **IRMMW-THz 2021– Poster**.
- "Terahertz spectral imaging through turbid media: A wavelet approach to scattering mitigation," **CLEO 2020 – Oral**.
- "Wavelet multiresolution analysis for spectral imaging in scattering media," **OTST 2019 – Oral**.
- "Extraction of THz absorption signatures obscured by rough surface scattering using discrete wavelet transform," **IRMMW-THz 2018 – Oral**.

PATENTS

"Personalized chest acceleration derived prediction of cardiovascular abnormalities using deep learning," M. Ebrahimkhani, E. Johnson, and M. Markl, submitted.

PROFESSIONAL MEMBERSHIPS

- Institute of Electrical and Electronics Engineers (IEEE)
- Optical Society of America (OSA)
- American Physical Society (APS)
- Society for Cardiovascular Magnetic Resonance (SCMR)
- Radiological Society of North America (RSNA)

PROFESSIONAL SERVICE

Completed peer review assignments for the following journals:

- IEEE Transactions on Terahertz Science and Technology
- Optics Express
- Biomedical Optics Express
- Sensors
- Measurements
- Applied Optics
- Infrared Physics and Technology