Research Summary

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Outline of the Presentation

1. Background
2. Research Projects (2019-Present)
3. Part-time Projects
4. Major interests and Research themes
5. Why QML?

Beginnings

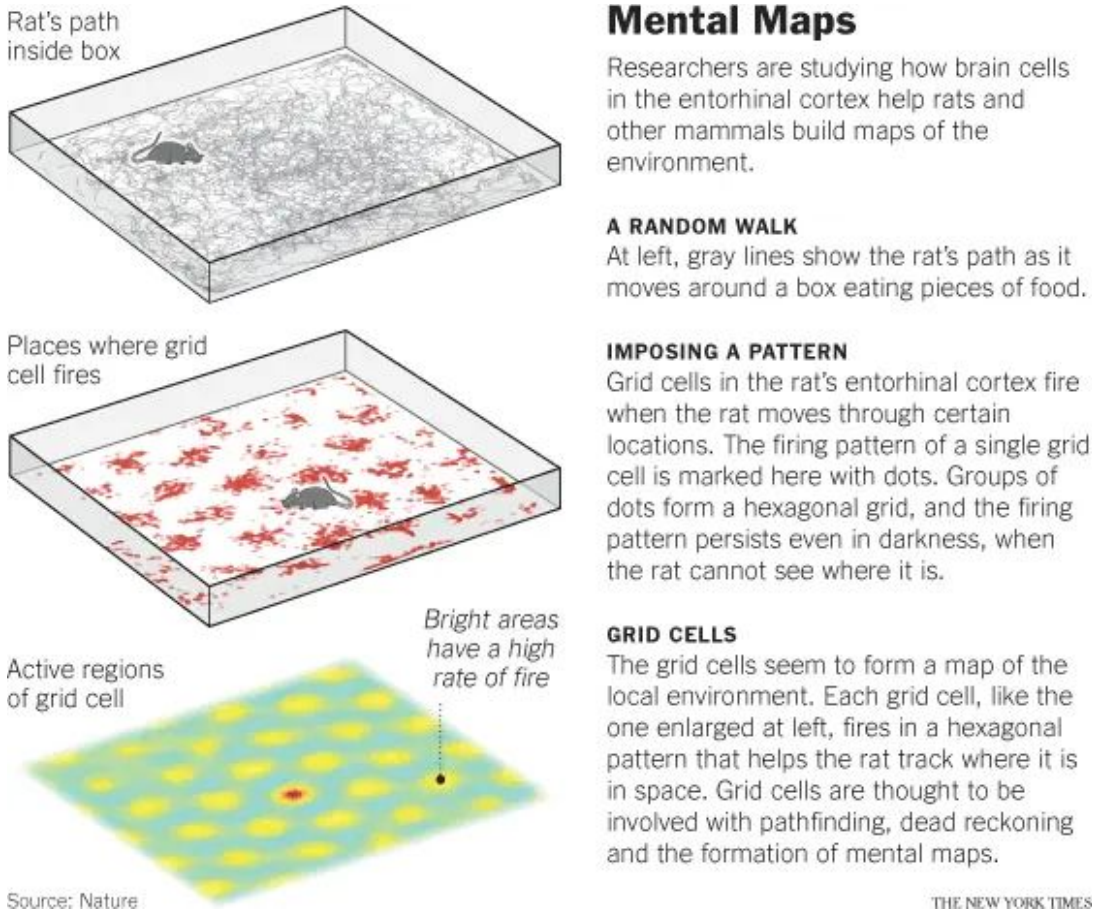
- Born and brought up in Bangalore, India
    - Languages: English, Kannada, Hindi, Marathi, Tamil
- Sri Kumaran Childrens' Home – State Board ('06 - '16)
    - 99% in 10th Board Exams
    - School Head Boy
    - Best Outgoing Quizzer | Best Science Project | Best Quizzer
- RV PU College ('18)
    - 97% in 12th Board Exams [Subjects: PCMB-ES]
    - JEE-Advanced AIR[1] 7000 | KVPY AIR 265 | KCET AIR 208
    - National Physics & Chemistry Olympiad
- IISER Pune (2018 – 2023 (*expected)*)
    - Major : Physics | Minor : Data Science
    - Part time Quiz-master at IISER Pune Quiz Club
    - CGPA 8.8/10 (8th / 228 students)

[1]All India Rank

Research Projects

Theoretical Neuroscience Lab, IISER Pune [2019]

- Worked with Dr.Collins Assisi [Nov 2019 – Feb 2020]
- **Problem**:
  - Grid cell neurons produce a tessalating firing pattern with consecutive modules exhibiting a spacing-ratio of ~ $\sqrt{2}$ [1,2]
- **Goal**:
  - Study the dynamics of Grid cell neurons in the entorhinal cortex of the Hippocampus by modelling its dynamics using a geometric attractor.
- **Contributions**:
  - Reviewed Literature on grid cell neuroscience and nonlinear dynamics on Networks.
  - Programmed and analysed different neural architectures using the Hodgkin-Huxley model for action potentials using Tensorflow 2.0 and Python 3.6



[1] Stensola, H., et al (2012). The entorhinal grid map is discretized. *Nature*, *492*(7427), 72-78.

[2] Kang, L., & Balasubramanian, V. (2019). A geometric attractor mechanism for self-organization of entorhinal grid modules. *Elife*, *8*, e46687.

[3] Mohanta, S. S., & Assisi, C. (2019). Parallel scalable simulations of biological neural networks using TensorFlow: A beginner's guide. *arXiv preprint arXiv:1906.03958*.

International Genetically Engineered Machine [2020]

- Led a team of 16 undergraduates that represented IISER Pune at iGEM ’20 under the supervision of Prof. Sanjeev Galande [Apr ‘20 – Nov ‘20]
- **Problem**:
  - Growing antibacterial resistance against malarial parasites.
  - Increasing costs, inaccessibility of blood-related diagnostic tests
- **Goal**:
  - Design novel class of orally administrable antimalarial peptides
  - Create a portable diagnostics kit that based on Artificial Intelligence
- **Contributions**:
  - Identified potential therapeutic peptide drugs against falciparum cerebral malaria with an insilico efficinecy of ~93%. (Publication) and developed **PACMal** (Peptides against Cerebral Malaria)
  - Supervised big-data analytics projects and equilibrium molecular dynamics simulations on the Parambrahma Supercomputer facility at IISER Pune.
  - Designed, programmed and deployed **DeleMa-Detect**, an open-source deep learning application for real-time Malaria diagnosis through blood-smear images with **Mobilenetv2 transfer learning** and an accuracy of 96%.
  - Cofounded Curem Biotech, the first student startup at IISER Pune, seeded at the Atal Innovation center, IISER Pune
- Won IISER Pune’s first Gold Medal and the best project award among >250 contesting teams from >40 countries at iGEM at Boston, MIT.
- Contributed to the final product that won first place at the iGEM 2021 Startup Showcase competition along with a $10,000 cash price

14 researchers from IISER-Pune win gold medal at iGEM

A project that entailed detecting malaria using a cost-effective tool helped 14 researchers from the Indian Institute of Science, Education and Research (IISER) - Pune win the top medal in the competition.

iGEM-IISER-Pune-India

Anopheles | The Half-Blood Princess

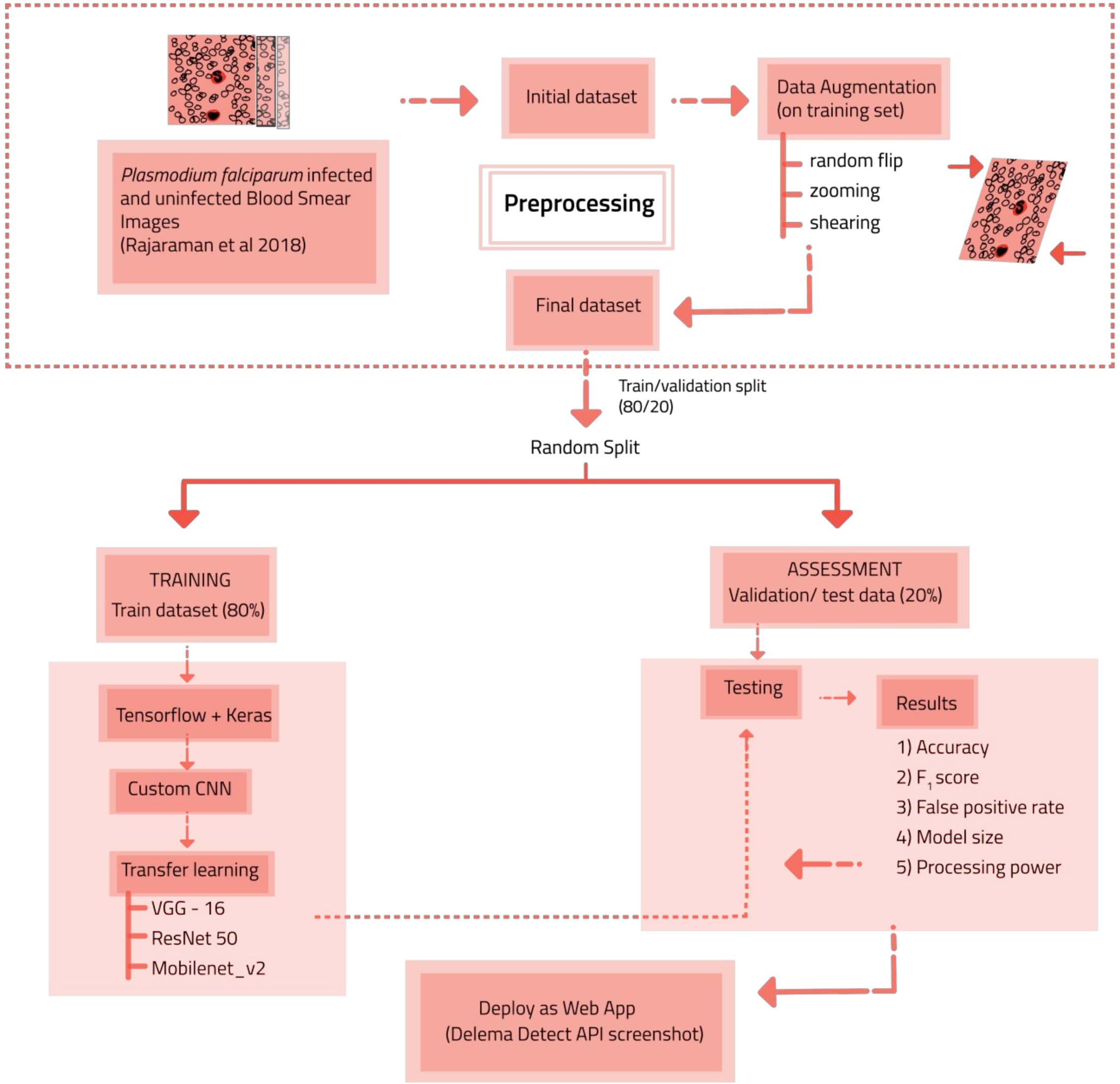
14 IISER students accomplish unique project on malaria

By Sukhada Khandge | Sat, 10 Oct 2020

14 IISER students accomplish unique project on malaria

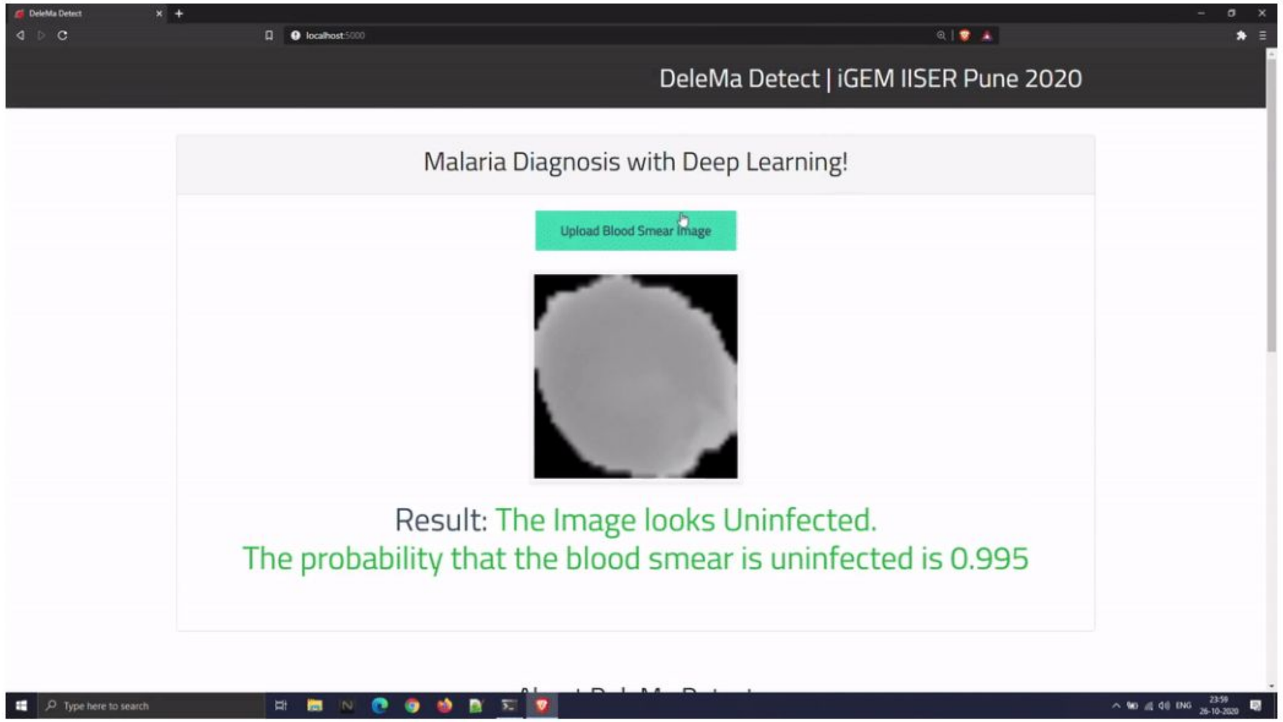
Research on drug development and diagnostics for the disease will soon be presented at the international iGEM competition

Sources: https://2020.igem.org/Team:IISER-Pune-India



DeleMa Detect

DEep LEarning for MAlaria Detection



[1] github.com/igemsoftware2020/IISER-Pune-India
[2] 2020.igem.org/Team:IISER-Pune-India/Software

Our Work

The Situation

Malaria

338,500 cases every year in India

Sickle Cell Disease

Upto 44.5% allele frequency

35-40% in Southern India

Leukemia

105,000 cases every year in India

Expensive therapies

Low Awareness

The Problem

Lack of Accessible and Accurate diagnostic tests for diseases in rural populations

Rapid Diagnostic Kit

- Fast Diagnosis
- High Error Rate
- High Cost

PBS Microscopy

- Expensive
- Delayed diagnosis
- Variable accuracy

Our Solution

A **Portable** diagnostic device which provides a **Rapid**, **Cost effective** and **Accurate** Diagnosis, requiring **Minimal Human Intervention**

Portable
AI-based
Accurate
Fast

curembiotech.com

Undergraduate Research Assistant, IISER Pune [2021]

- Worked with Prof MS Santhanam, IISER Pune [Dec 2020 - May 2022]
- **Problem**:
  - Understanding information scrambling in quantum chaotic systems.
- **Contributions**:
  - Reviewed and reproduced literature results by simulating the dynamics of a classical kicked rotator, quantum kicked rotor in 1D (QKR) and 3D, also called, quasi-periodic kicked rotor (QPKR) in different electronic phases.
  - Numerically evaluated the OTOC (Out-of-Time-ordered-Correlators), a proposed measure of quantum chaos for the QKR and QPKR.
  - Currently working on developing Restricted-Boltzmann-machine inspired models for OTOC computations.
  - Material :
    - Currently finishing up paper-draft.
    - Code: https://github.com/Anantha-Rao12/QuantChaos

3D Quantum Kicked rotor

- The quantum kicked rotor represents a particle on a ring periodically kicked by a smooth potential. Mathematically, these kicks are modelled as delta functions in time and between the kicks the particle undergoes free-particle time evolution.
- The quasi-periodic kicked rotor is obtained from the standard kicked rotor by an additional quasi-periodic temporal modulation of the kick strength. The Hamiltonian is written with two additional frequencies as follows:

$$H = \frac{1}{2M}(p_1^2 + p_2^2 + p_3^2) + \widetilde{K}\cos\theta\delta_T(t)$$
$$= \frac{1}{2M}(P^2) + \widetilde{K}\cos\theta\delta_T(t)$$

where:

- $\widetilde{K} = K\left[1 + \epsilon\cos(\omega_2 t + \phi_2)\cos(\omega_3 t + \phi_3)\right]$
- In the above expression, (ω_2, ω_3) are the two additional frequencies.
- $\delta_T(t)$ represents the delta function in time with a time-period 'T'

- Since the quasi-periodic kicked rotor requires only one spatial dimension, it is straightforward to be numerically evaluated while offering the richness of 3d systems.

Hashimoto, K., Murata, K., & Yoshii, R. (2017). Out-of-time-order correlators in quantum mechanics. Journal of High Energy Physics, 2017(10), 138–169. https://doi.org/10.1007/jhep10(2017)138

Google Summer of Code (2021)
Machine Learning for Science Organization

Google
Summer of Code

@

ML4SCI
Machine Learning
for Science

- Worked with an international collaboration of researchers (Dr. Stephen Carr, Prof Vesna Mitrovic, Prof Chandrasekhar Ramanathan, Prof Brad Marston) to identify novel quantum materials using magnetic resonance.
- **Goal**:
  - Develop novel quantum materials and achieve quantum control using NMR by leveraging Artificial Intelligence
- **Contributions**:
  - Developed, and programmed NMR_ML, a general-purpose python package to read, preprocess, extract, and interpret important features from the Nuclear Magnetic Resonance raw-data.
  - Evaluated and optimized the performance of multiple Machine learning models on time-series classification, multi-parameter regression and achieved a state-of-the-art performance of 0.9 F1-score on the classification of materials and R2 of 0.81 on predicting electronic properties of materials from NMR experiments.
  - Resulted in a first-author publication (currently under review)

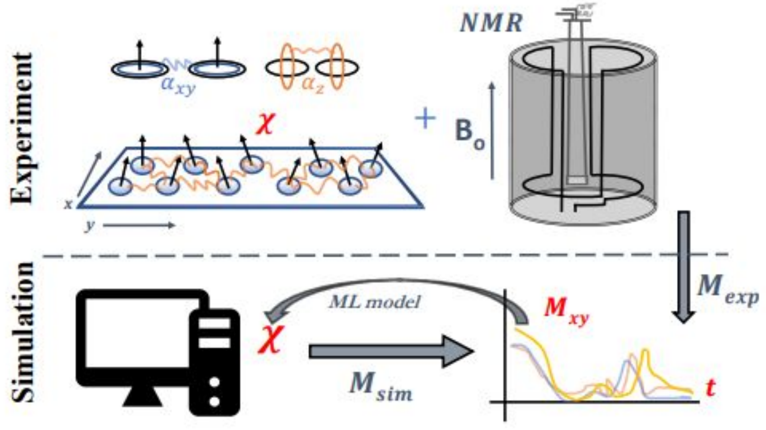


FIG. 1. **A schematic for material discovery via NMR** Top: A magnetic resonance experiment in a fixed field B_0 allows for the controlled evolution of many nuclei, with interactions between spins mediated by the electron susceptibility χ. This susceptibility is sometimes strongly polarized along either the out-of-plane (α_z) or in-plane (α_{xy}) spin axes. Bottom: Our machine learning (ML) model can predict the parameters of χ from raw magnetization data, which are generated by spin-echo simulations, represented by the map $M : \chi \to M_{xy}$.

[1] Carr, Stephen, et al. "Signatures of electronic correlations and spin-susceptibility anisotropy in nuclear magnetic resonance." *Physical Review B* 106.4 (2022): L041119.

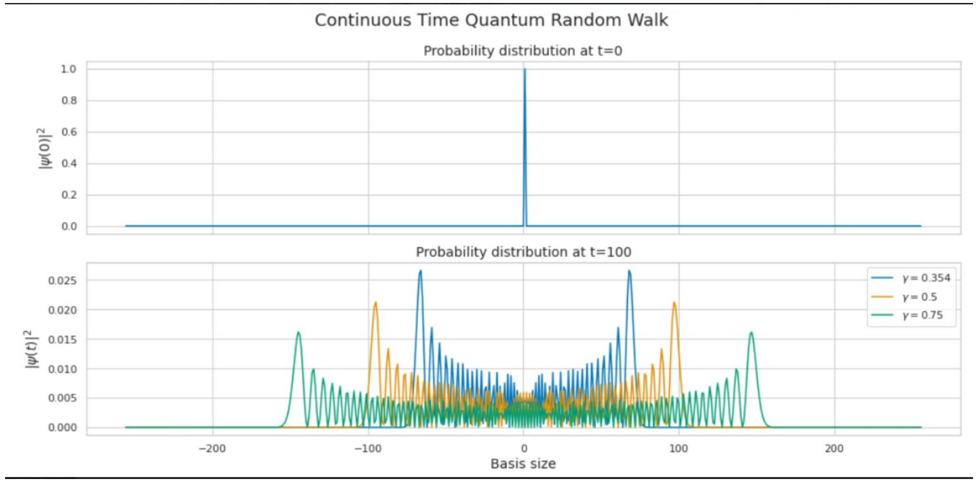
[2] Rao, Anantha, et al. "Machine learning assisted determination of electronic correlations from magnetic resonance." *arXiv preprint arXiv:2212.01946* (2022)..

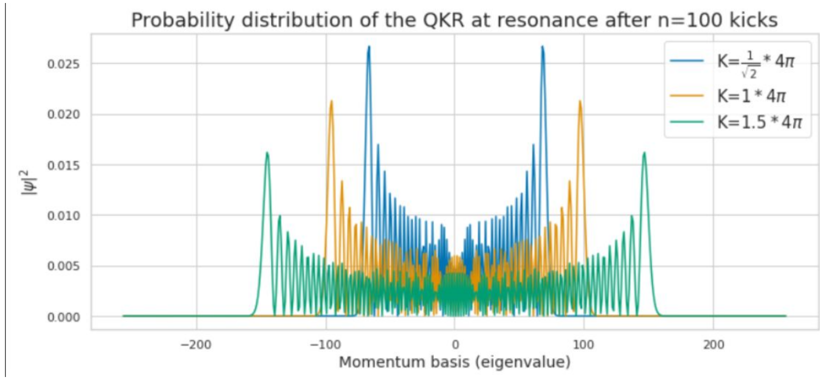
Undergraduate Research Assistant, IISER Pune [2022]

- Working with Prof MS Santhanam, IISER Pune [Dec 2021 - *May 2022*]

- **Problem**:
  - Developing physical realizable algorithms using the continuous-time quantum walk as a search algorithm.

- **Contributions**:
  - Studied the relationship between continuous time quantum random walks and the resonant quantum kicked rotor in higher dimensions to develop search protocols with quantum speedup.
  - Developed a formalism to test the first-hitting time distributions for the resonant quantum kicked rotor experimentally using ultracold atoms and probe coherence times in quantum systems.
  - Project report [link]





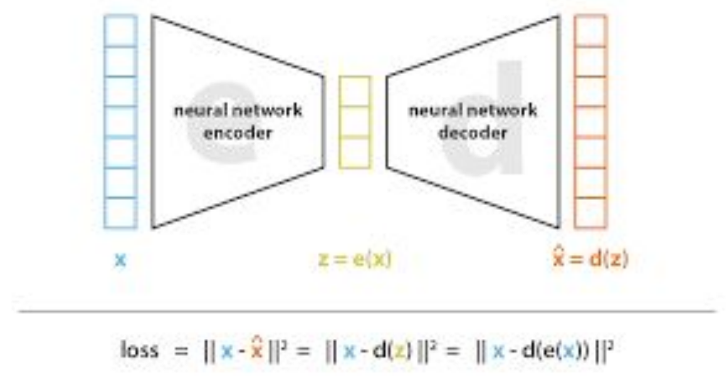
[1] Delvecchio, M., Petiziol, F., & Wimberger, S. (2020). Resonant quantum kicked rotor as a continuous-time quantum walk. *Condensed Matter*, *5*(1), 4.

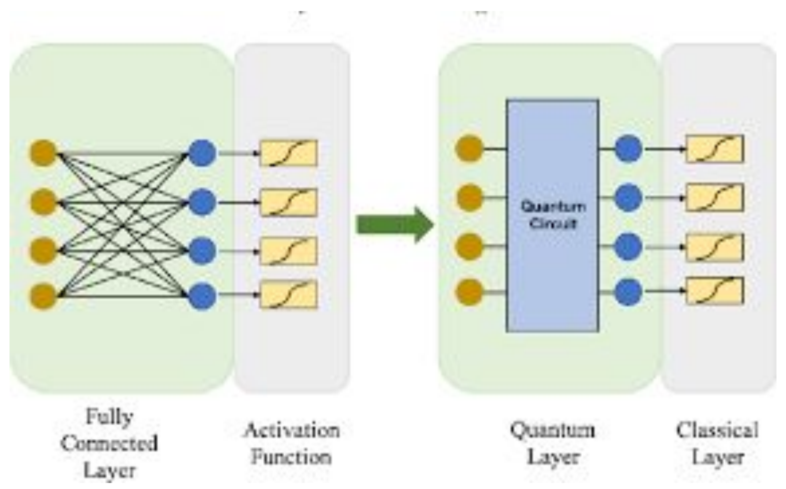
[2] Delvecchio, M., Groiseau, C., Petiziol, F., Summy, G. S., & Wimberger, S. (2020). Quantum search with a continuous-time quantum walk in momentum space. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *53*(6), 065301.

Master’s thesis student @ IBM Research

Supervisors: Dr L Venkata Subramaniam, Dr Dhinakaran Vinayagamurthy

1. Developing a hybrid quantum-classical neural network for generative learning under the variational autoencoder framework.
2. Benchmarking the model on various classical and quantum datasets and showed performance and training advantage over purely classical models.
3. Currently verifying results on IBM hardware.





Part-time Projects

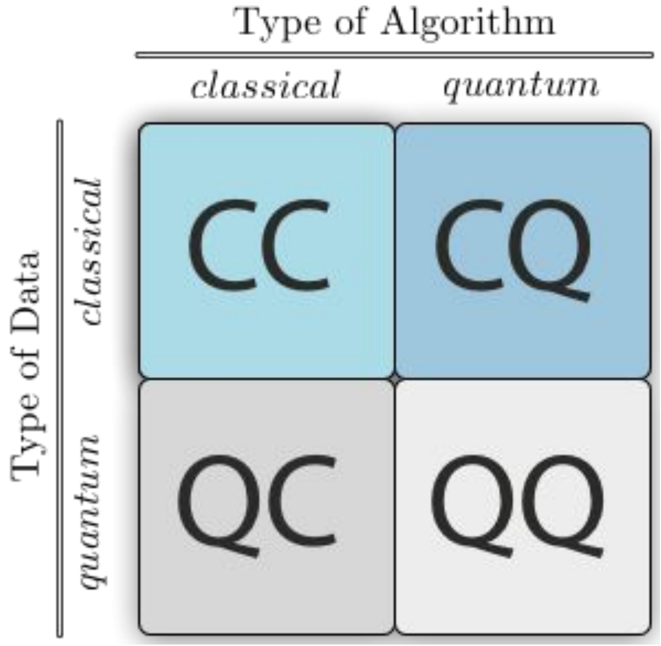
1. **QCompiler** (Anantha-Rao12/QCompiler)
    - Implemented a basic Quantum Circuit Simulator, as part of the Quantum Information course at IISER Pune, that performs:
        - The basic single-qubit gates (X,Y,Z,I,H,S,T) and the CNOT gate
        - Multi-shot measurement of all qubits using a weighted random technique
        - Addendum: Need to implement variational circuits
2. **Benchmarking Quantum computers** (TBA)
    - Performing volumetric Application-oriented benchmarking tests on the latest available quantum devices as part of the Chanakya UG fellowship program at iHUB Quantum Technology center, IISER Pune *(proposal submitted)*
3. **ComPhys** (Anantha-Rao12/ComPhys)
    - Fortran95 code for solving various Physics problems numerically.
    - Includes: Differential equations, MonteCarlo methods, Numerical integration, Molecular dynamics
4. **Machine-Learning** (Anantha-Rao12/Machine-Learning)
    - Implementation of Standard algorithms and methods of Machine Learning from scratch
    - Includes: Linear regression, Logistic regression, KNN, Decision Trees, *(working on adding new methods)*
5. **Bioinformatics** (Anantha-Rao12/Bioinformatics-BIO314)
    - Programmed and developed scripts for concepts useful for the BIO314 (Bioinformatics) course at IISER Pune.
    - Includes scripts for Sequence alignment of DNA, Protein sequences, Burrow-Wheeler Transforms for Next-Generation sequencing, Implementation of Hidden Markov models(evaluation, decoding, learning)
6. Implementation of Quantum Algorithms on Qiskit, and Cirq. Basic Knowledge of AWS Braket
7. Implementation Deep Learning Algorithms on Tensorflow, PyTorch

MOOCs and Certifications:

- Machine Learning,
- Computational Neuroscience,
- Deep Learning specialization,
- Qiskit Global Summer School 2020 (Introduction to Quantum computation),
- Qiskit Global Summer School 2021 (Quantum Machine Learning)

Project themes *(till now)*

- Quantum Machine learning
- Quantum Chaos
- Quantum Information and computation
- Machine Learning, Deep Learning
- Bioinformatics



Project themes I would like to explore:

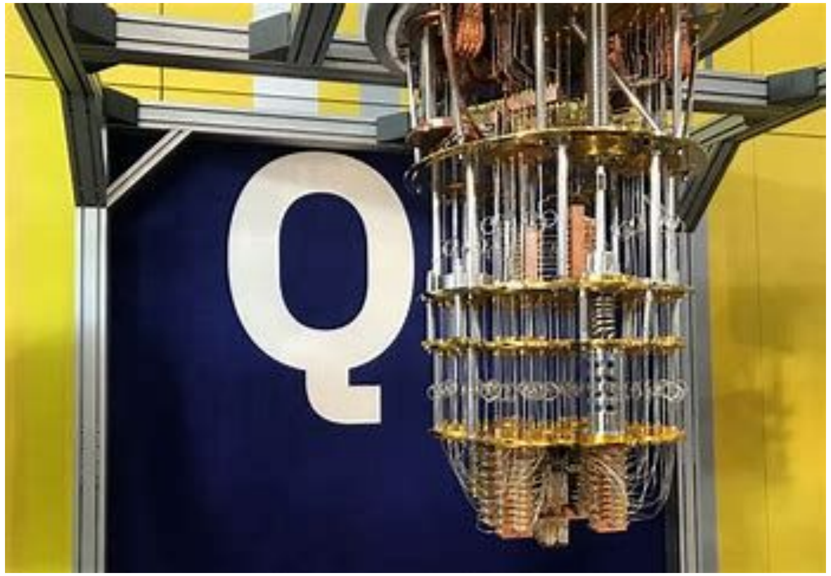
1. Quantum Control and optimization

2. Quantum simulation
   a. Hamiltonian problems (spectrum, simulation)

3. Application of ML methods in physics and chemistry:
   a. Solving many-body quantum physics problems
   b. Quantum error mitigation techniques using Machine Learning

4. Quantum Error-correcting codes

5. Developing novel algorithms for NISQ devices



Thank you!