# Introduction to Quantum Machine Learning by Example

Ahmed El-Mahdy

11/8/2025

# Outline

- Quantum AI
  - Quantum Variational Circuits
  - Quantum Binary Classification for Micro-Organisms using Raman Spectroscopy

# Major Emerging Technologies to the Field

## The Generative AI

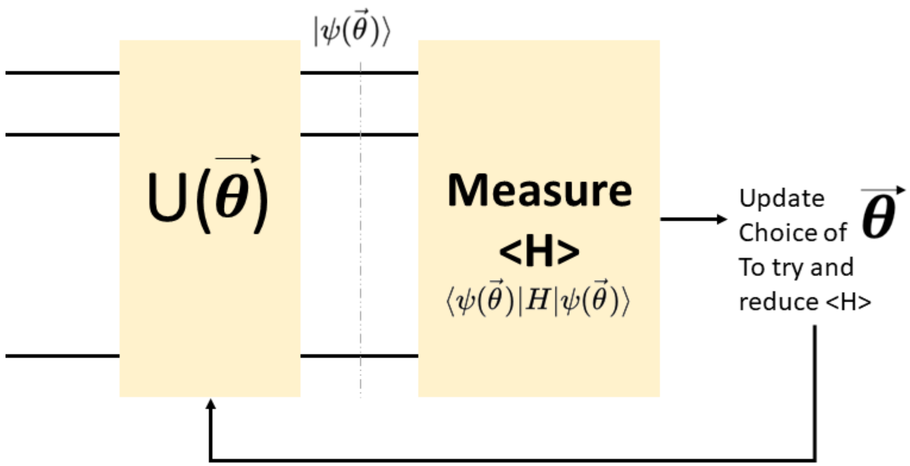
- **~$400 Billons** investment from Alphabet, Amazon, Apple, Meta, and Microsoft (Economist)
- Expected to increase the **global GDP by 7%** (Goldman Sachs)
- AI has **hacked the operating system of humans** (Yuval Harari)

## Quantum Computing

- It can make computers **exponentially faster**
- And has **exponentially less memory**
- Quadratic **better sensing** accuracy
- Provides 'true' **secure communication**
- They do exist!

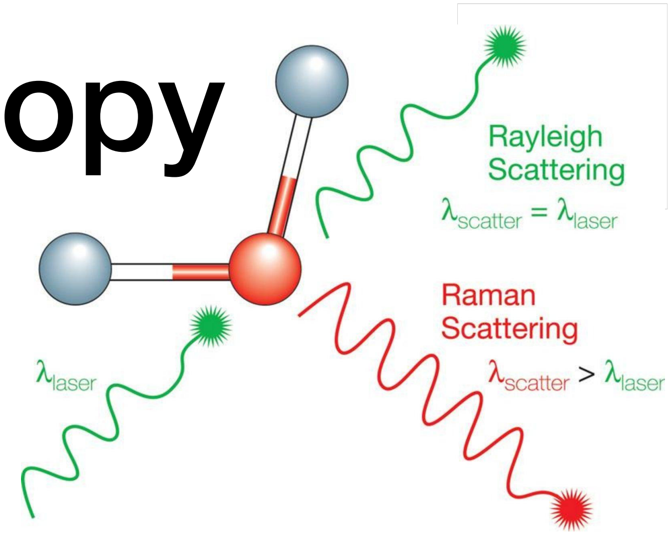
# Variational Quantum Circuits

- Hybrid classical-quantum computing
- Is showing promise in decreasing the number of trainable weights
- Still not well-explored

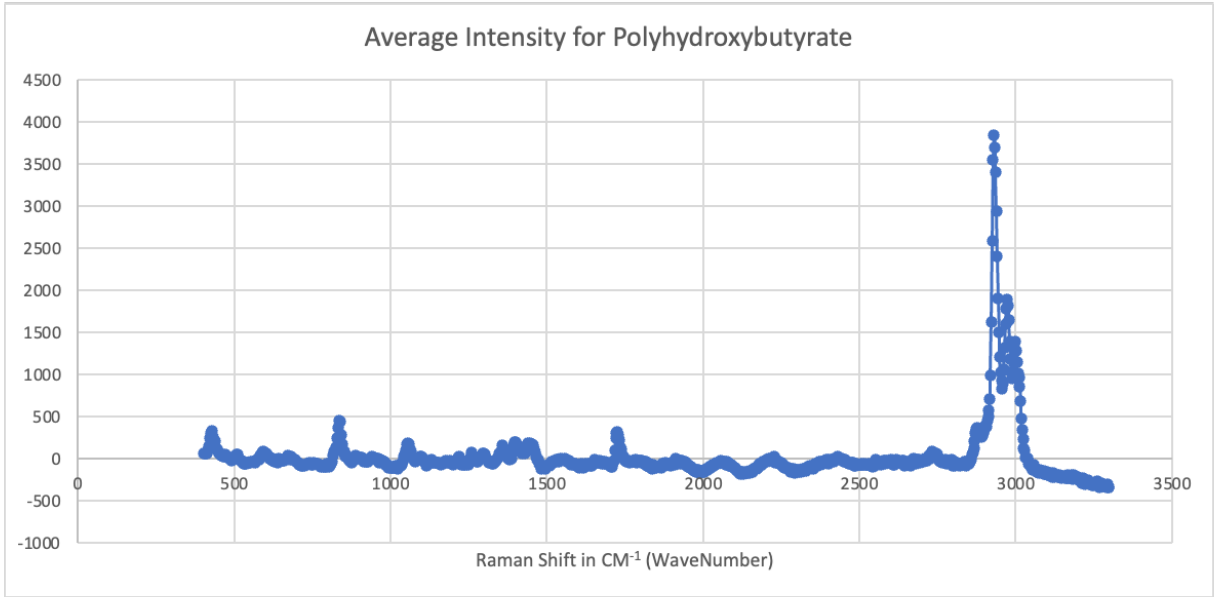



cc: Ketulmehta22

# Raman Spectroscopy




- Invented by R. C. Raman in 1928
- The vibration of molecules affects the scattered light (Vibration spectroscopy)
- Can identify molecules



# MicrobioRaman

- An open-access repository
- It includes ~7 different datasets for microbiological samples

**Correspondence**

https://doi.org/10.1038/s41564-024-01656-3

## MicrobioRaman: an open-access web repository for microbiological Raman spectroscopy data

Check for updates

Here we present the establishment of an open-access web-based repository for microbiological Raman spectroscopy data. The data collection, called 'MicrobioRaman' (https://www.ebi.ac.uk/biostudies/MicrobioRaman/studies), was inspired by the great success and usefulness of research databases like GenBank and UniProt. This centralized repository, residing within the BioStudies database[1] – which is maintained by a public institution, the European Bioinformatics advances in technology and data analysis now enable the investigation of molecular composition at the resolution of a single microorganism with high measurement sensitivity (Fig. 1a). By measuring the presence of peaks corresponding to specific macromolecules or differences in spectral shape, peak position and relative intensity of peaks, and often in conjunction with complementary techniques such as stable isotope probing (SIP)[3], fluorescence in situ hybridization (FISH)[4] or omics[5], Raman spectroscopy enables investigation of types, ranging from large nematodes (and beyond) to minuscule viruses measuring a few tens of nanometres, collected from various environments spanning oceans, soils and mammalian guts, and potentially even efforts to detect signals of life on other planets like Mars (see refs. 3,6–10 for comprehensive reviews about Raman technologies and applications in microbiology).

Despite the potential of Raman spectroscopy in microbiology, the reporting of analytical methods and data for microbiological

Lee, Kang Soo, Zachary Landry, Awais Athar, Uria Alcolombri, Pratchaya Pramoj Na Ayutthaya, David Berry, Philippe de Bettignies et al. "MicrobioRaman: an open-access web repository for microbiological Raman spectroscopy data." Nature Microbiology (2024): 1-5.

# Dataset Generation

Nile University
جامعة النيل الأهلية

- We have used 5 datasets:
  - Chaetoceros-affinis
  - Methanosuratincola-verstraetei
  - Polyhydroxybutyrate
  - Vibrio-alginolyticus
  - Escherichia-coli ( our target )

Richard A. Ingebrigtsen, Department of Aquatic Biosciences - University of Tromsø


Licensed by Google

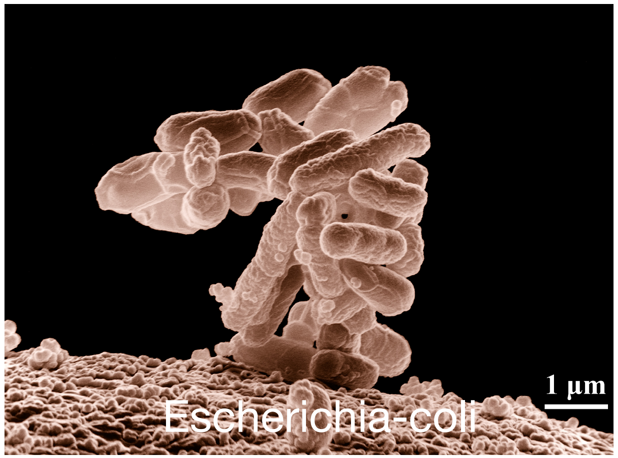
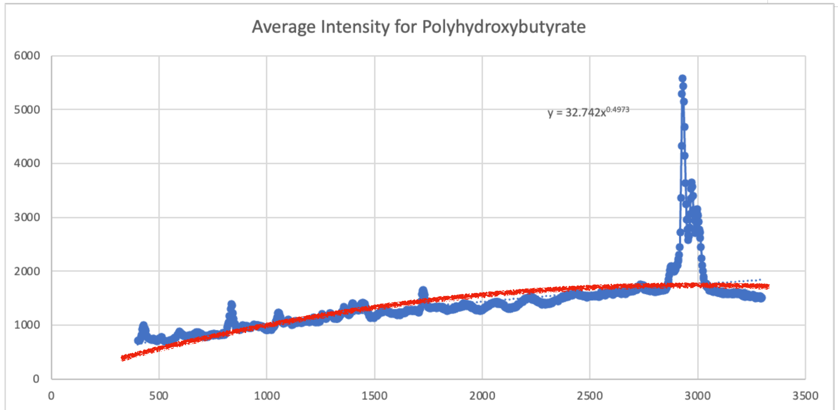
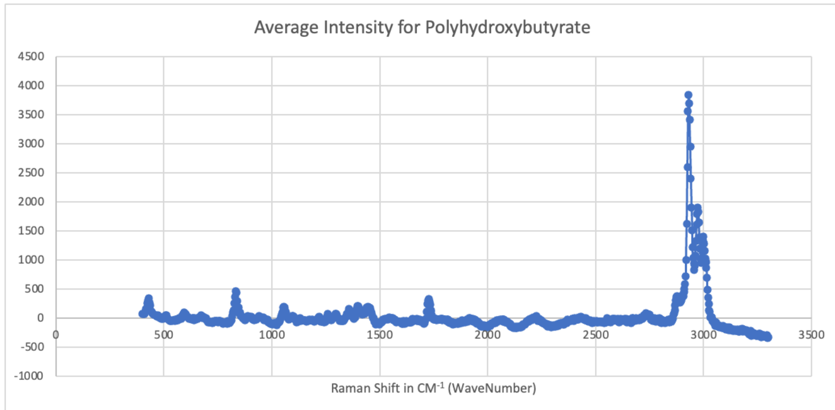




Photo byfkfkrErbe, digital colorization
by Christopher Pooley, both of USDA, ARS, EMU

# Dataset Generation: Preprocessing



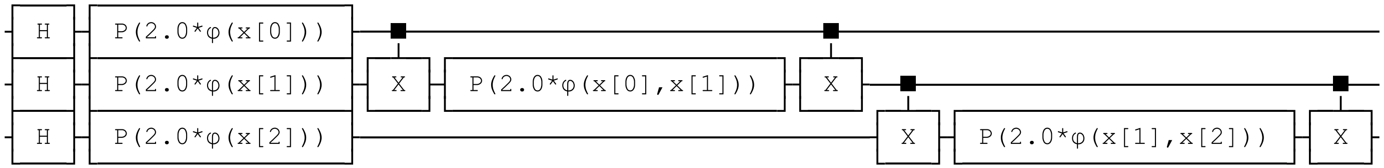




- Baseline subtraction
- Range reduction as not all data have the same domain
  - 410 - 3200 -> 410 - 1799
- Normalize so that the intensity vector has a unit length

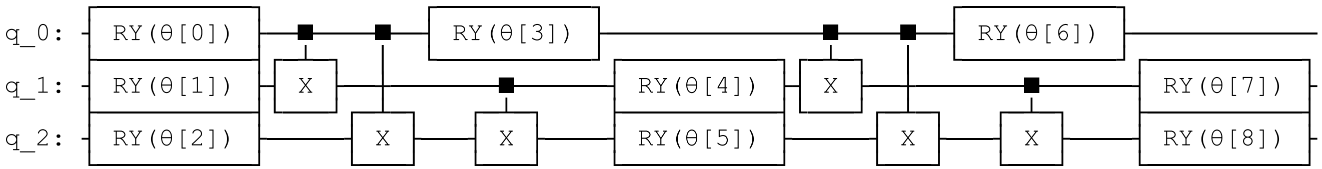
# Dataset Generation

- We have 5 spectra
- We randomly mix that data such that:
  - Each bacteria is present 50% of the time
  - When present, the weight is uniformly distributed from 0+ to 100%
- We then label each record as 1 if E.Coli is present, otherwise 0
- We generate 10,000 samples

# Variational Quantum Circuit Design

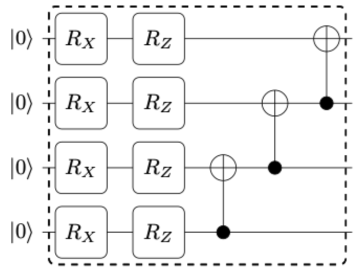



- ZZFeatureMap
- RealAmplitude (no complex part) Ansatz
- Depth 12
- Full entanglement
- Used 5 qubits
- Binned the data into 5 bins

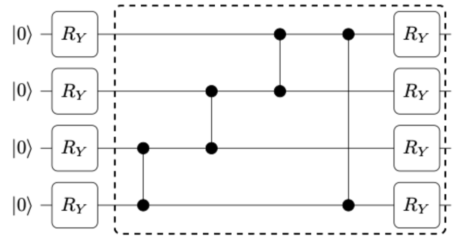


# Entanglement Type

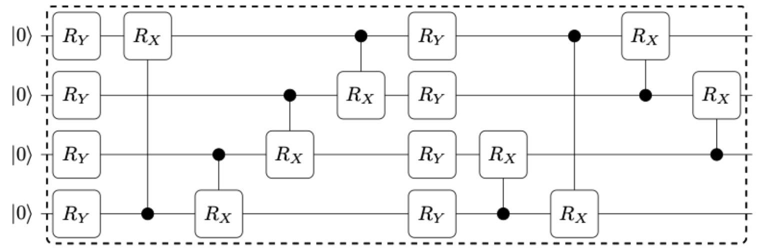
- Full: all pairs
- Linear: *i* with *i+1*
- Reverse-Linear: linear but in reverse order
- Pairwise: all even *i* with *i+1, and then all odd i* with *I+1*
- Circular: Linear by with ends connected
- Shifted Circular Alternating: first-last connected, shifted, and control/target alternates at each layer




Reverse-Linear




Circular



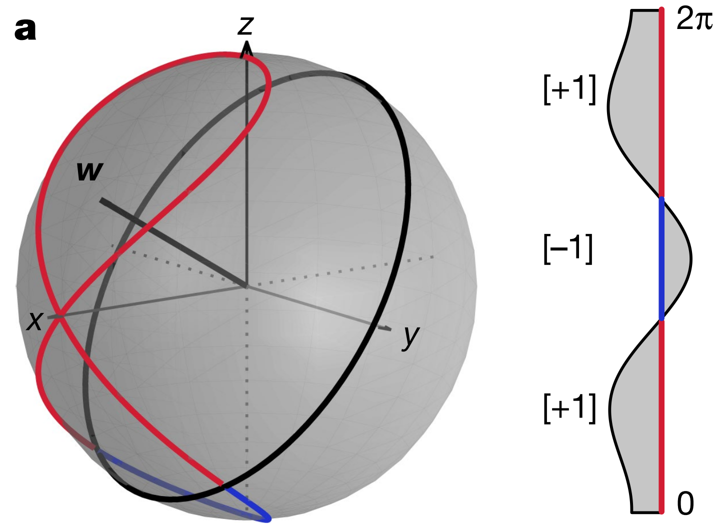

SCA

# Optimisers

- Constrained Optimization By Linear Approximation optimizer (COBYLA)
- Limited-memory Broyden-Fletcher-Goldfarb-Shanno Bound (L-BFGS-B)
    - Iterative
    - Solves unconstrained, non-linear optimisation problems
    - Identifies the steepest decent direction

# Feature Mapping

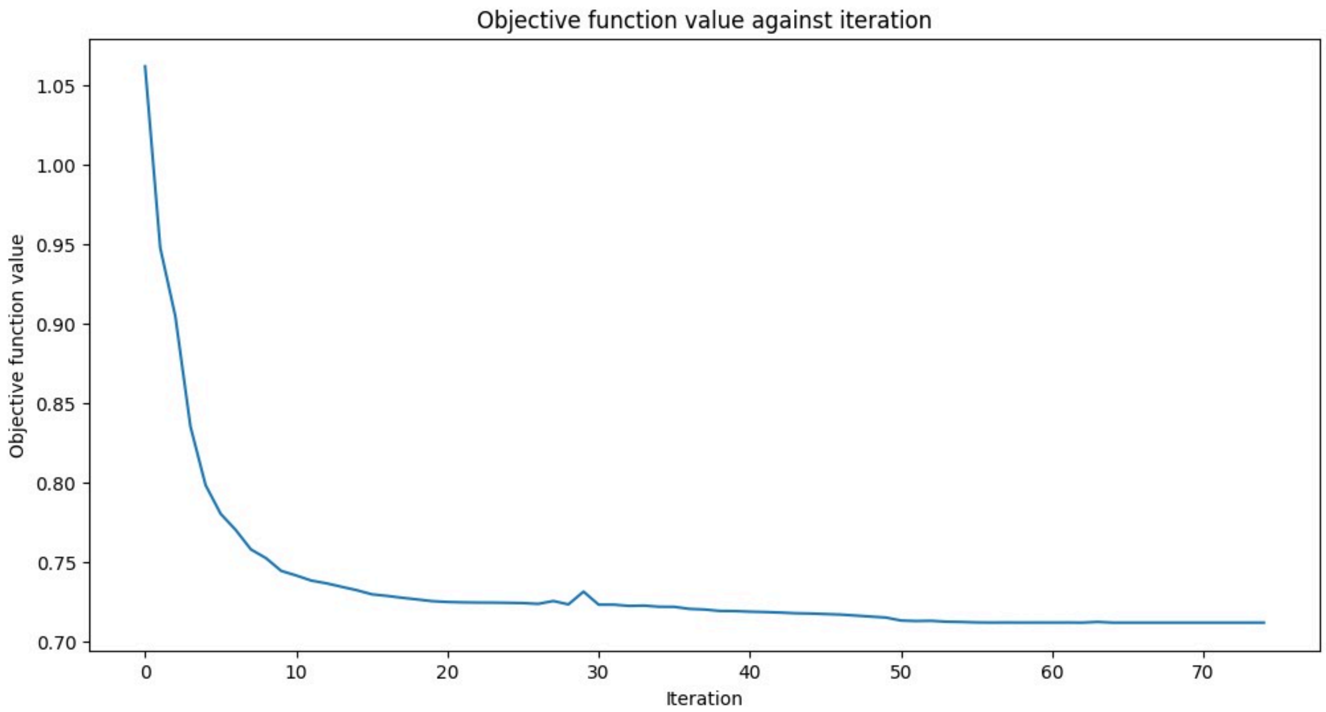
- For the feature vector $\vec{x} \in \mathbb{R}^n$
- $$U_{\Phi(\vec{x})} = \exp\left(i \sum_{S \in \mathcal{I}} \phi_S(\vec{x}) \prod_{i \in S} P_i\right)$$
- $$\phi_S(\vec{x}) = \begin{cases} x_i \text{ if } S = \{i\} \\ \prod_{j \in S}(\pi - x_j) \text{ if } |S| > 1 \end{cases}$$
- Havlíček, V. et al. Supervised learning with quantum-enhanced feature spaces. Nature 567, 209–212 (2019).



# Results

| | Default |
|---|---|
| **Default** | <50% |
| **Full Entanglement** | 65% |
| **Optimizer L_BFGS_B** | 71% |
| **Normalizing Features to be from 0 to 2pi** | 82% |

# Training Loss



# Conclusions

- The number of parameters is in the order of 10s, whereas the classical is in the order of 100,000s

- There is a strong potential, especially for quantum data, in material science, biochemistry, and high-energy physics

- Can potentially make a sea-change in data science

# Reading List


- Nielsen, Michael A., and Isaac L. Chuang. Quantum computation and quantum information. Cambridge University Press, 2010.

- Griffiths, David J., and Darrell F. Schroeter. Introduction to quantum mechanics. Cambridge University Press, 2018.

- Majidy, Shayan, Christopher Wilson, and Raymond Laflamme. Building Quantum Computers: A Practical Introduction. Cambridge University Press, 2024.

- Schuld, Maria, and Francesco Petruccione. Machine learning with quantum computers. Vol. 676. Berlin: Springer, 2021.

- Cerezo, Marco, Guillaume Verdon, Hsin-Yuan Huang, Lukasz Cincio, and Patrick J. Coles. "Challenges and opportunities in quantum machine learning." Nature computational science 2, no. 9 (2022): 567-576.

# Thank You

# شكرا جزيلا