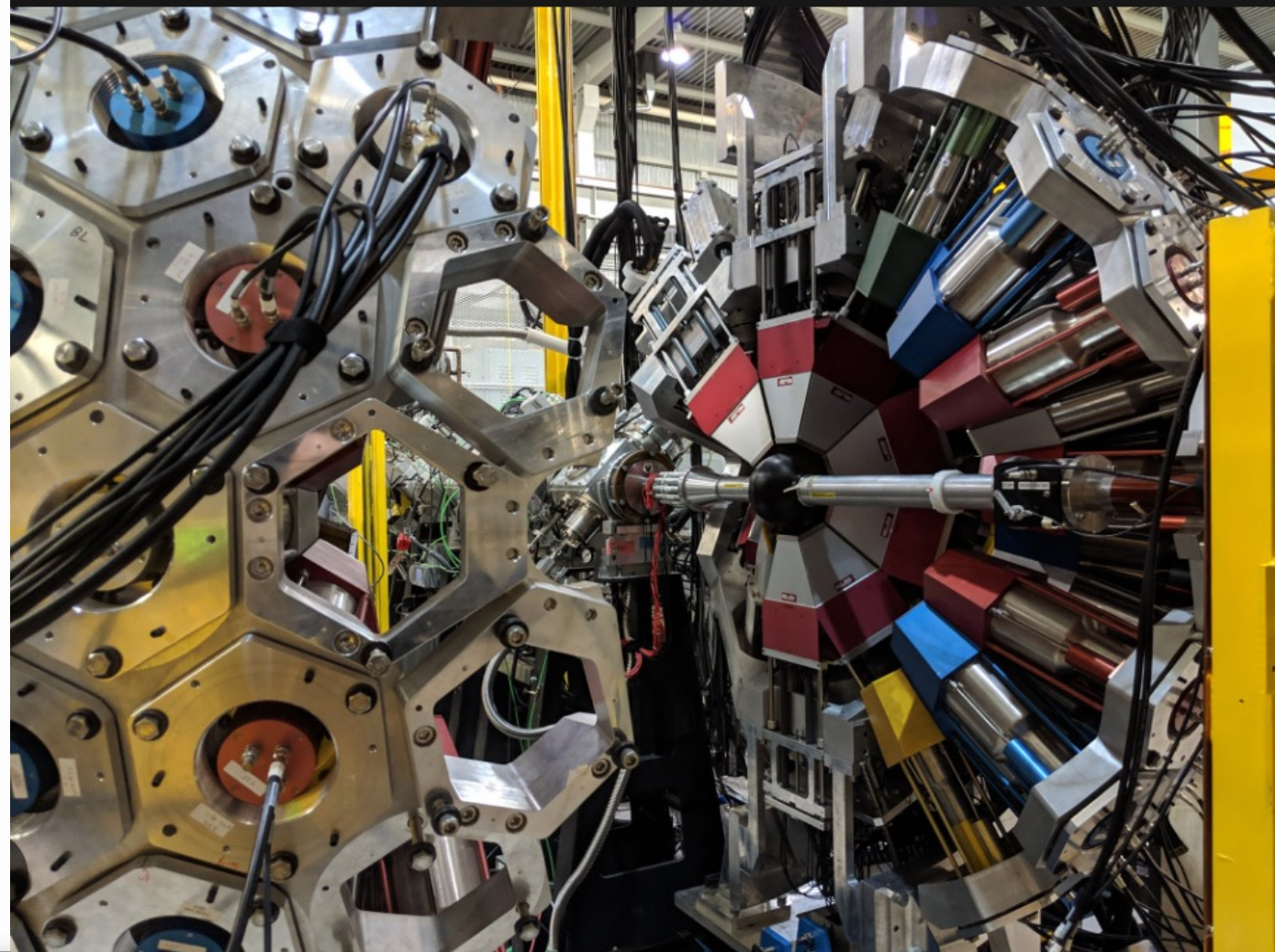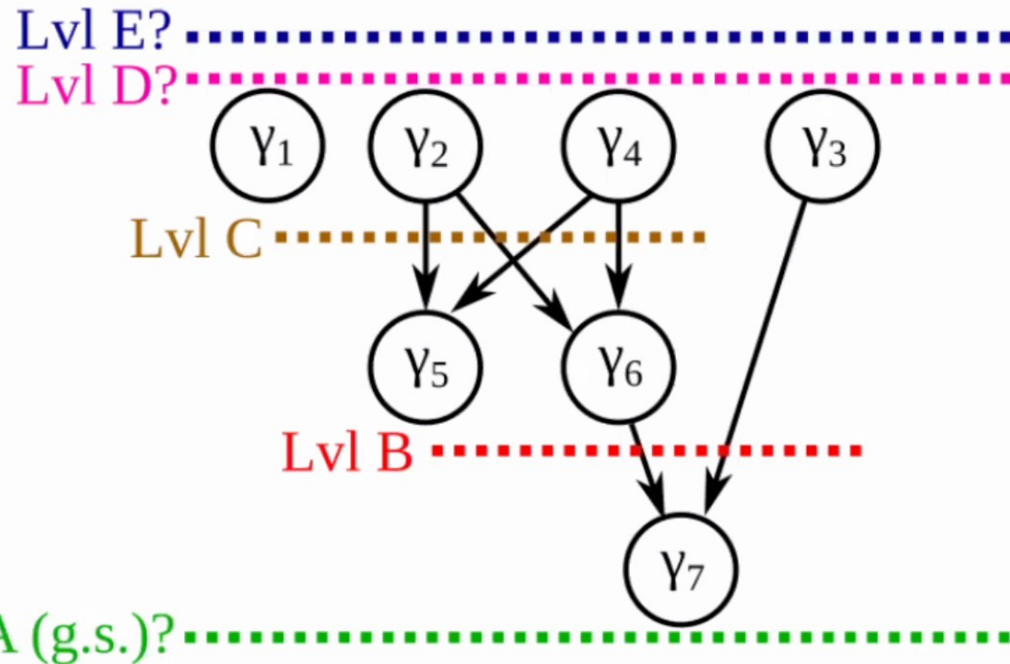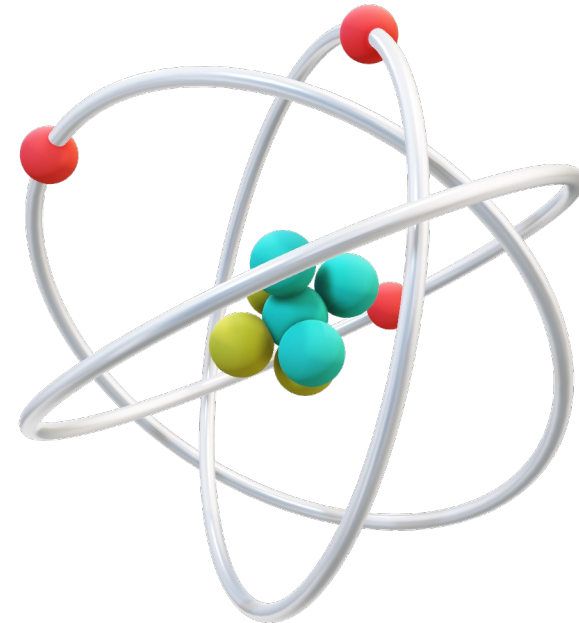# Quantum Machine Learning Towards the Development of Automated Analysis of Data from Large–Scale Gamma–Ray Spectrometers

University of Guelph, Samantha Buck
WNPPC 2024 : Feb 16, 2024
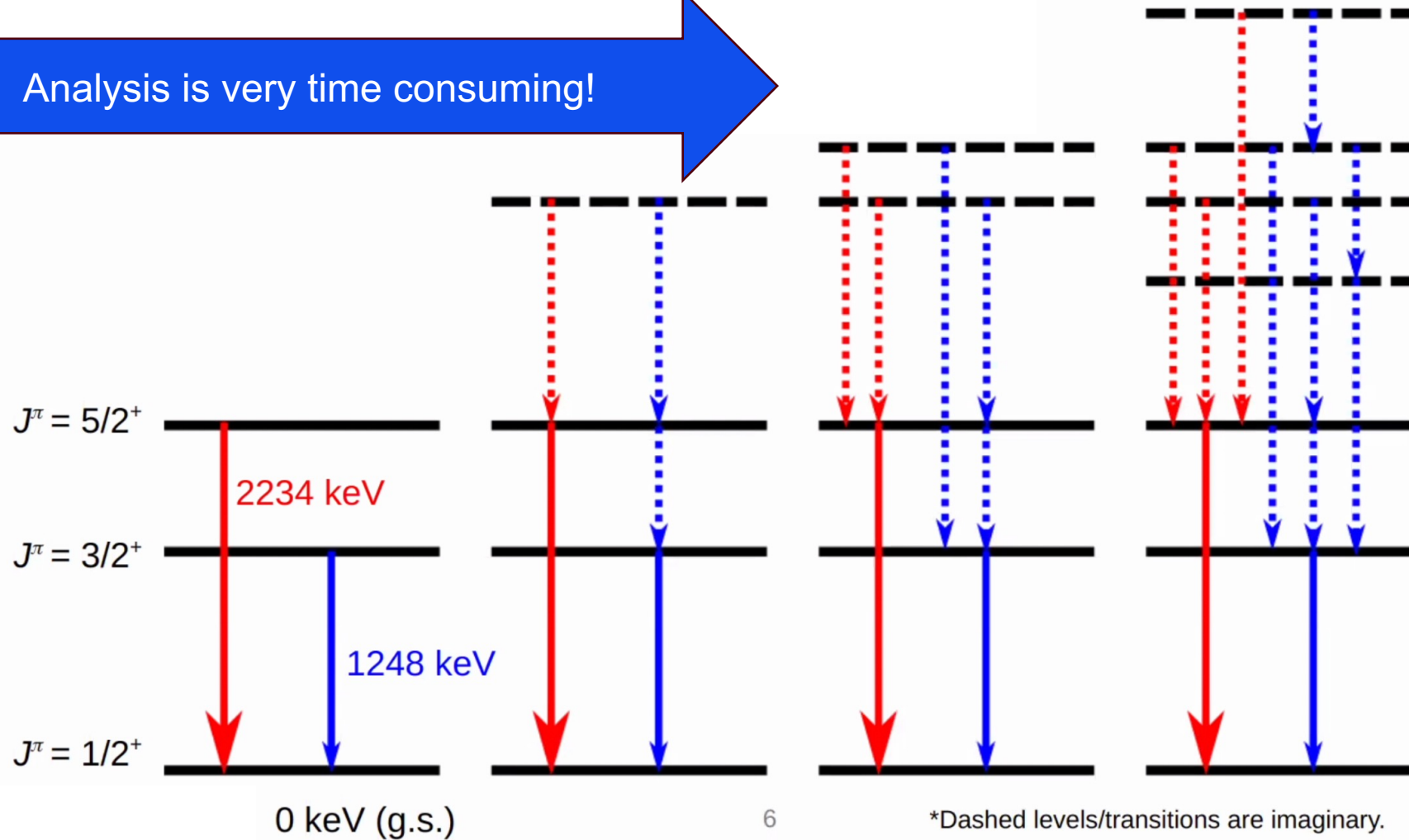
Outline

- Define Objective:
  - ➢ Traditional decay-scheme generation
  - ➢ A novel approach using graph theory representation (G.Demand & P. E. Garrett, University of Guelph)

- Reformulating the Problem:
  - ➢ Generating matrix representation
  - ➢ Numerical optimization

- Reformulating the Solution:
  - ➢ Machine learning investigation
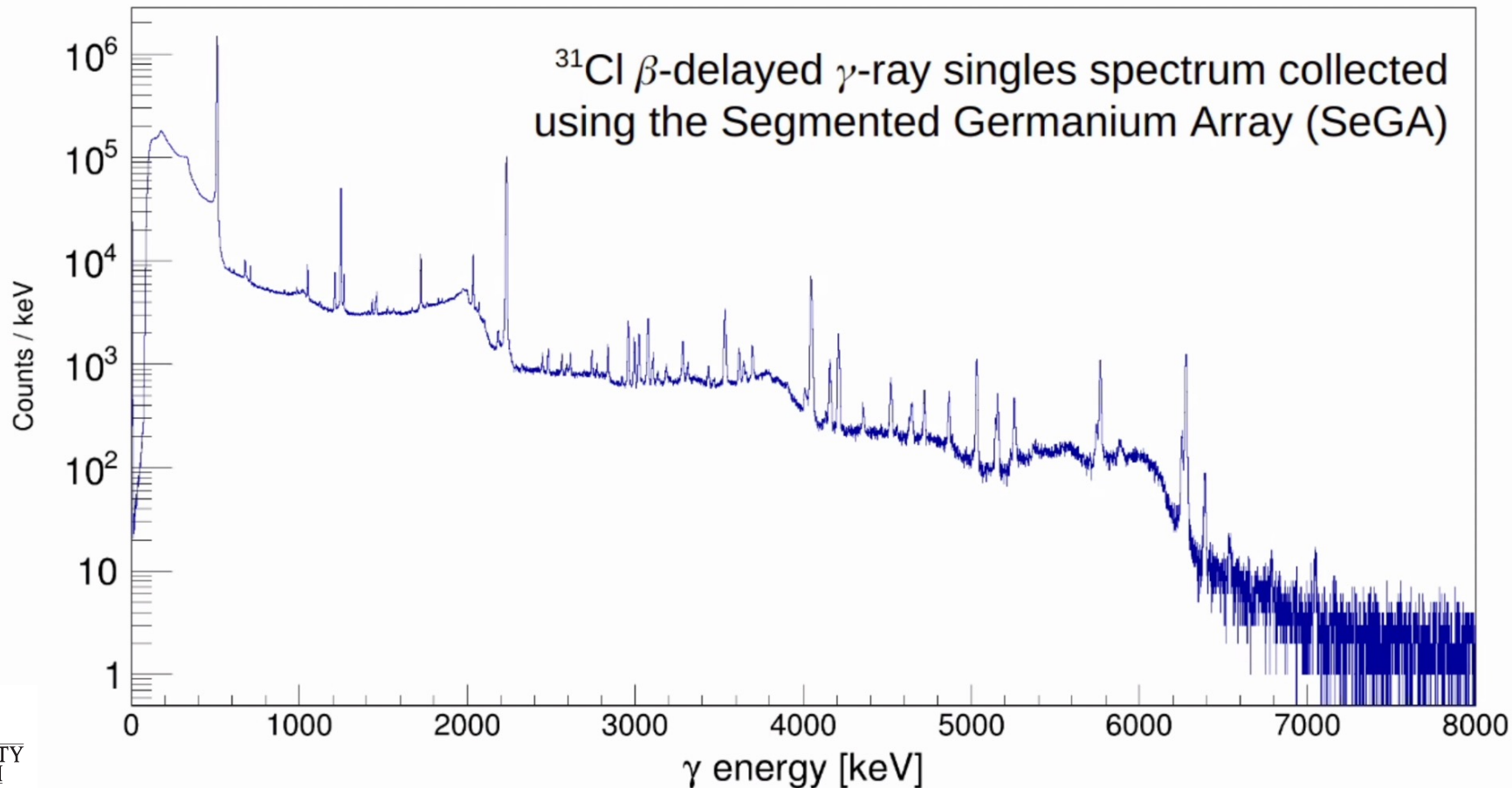 - ➢ Quantum Algorithms

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Building a Nuclear Decay Scheme

Analysis is very time consuming!

$J^\pi = 5/2^+$

2234 keV

$J^\pi = 3/2^+$

1248 keV

$J^\pi = 1/2^+$

0 keV (g.s.)

6

*Dashed levels/transitions are imaginary.

1D Gamma-Ray Singles Spectrum

- All statistics for n total γ transitions as measured by spectrometer

- The intensity of the ith γ-ray transition is stored as S_i in vector S

^{31}Cl β-delayed γ-ray singles spectrum collected using the Segmented Germanium Array (SeGA)

$$S = \begin{pmatrix} S_1 \\ S_2 \\ .. \\ S_n \end{pmatrix}$$

Tamas Budner, ^{31}Cl β-Delayed Proton Decay and Classical Nova Nucleosynthesis, PhD Thesis, MSU, 2022

2D Gamma-Gamma Coincidence Matrix

- All gamma events detected in coincidence with other γ-rays

- The number of $\gamma_i - \gamma_j$ coincidences is stored in each element $C_{i,j}$ within the reduced coincidence matrix C

- No temporal information; symmetry $C_{i,j} = C_{j,i}$
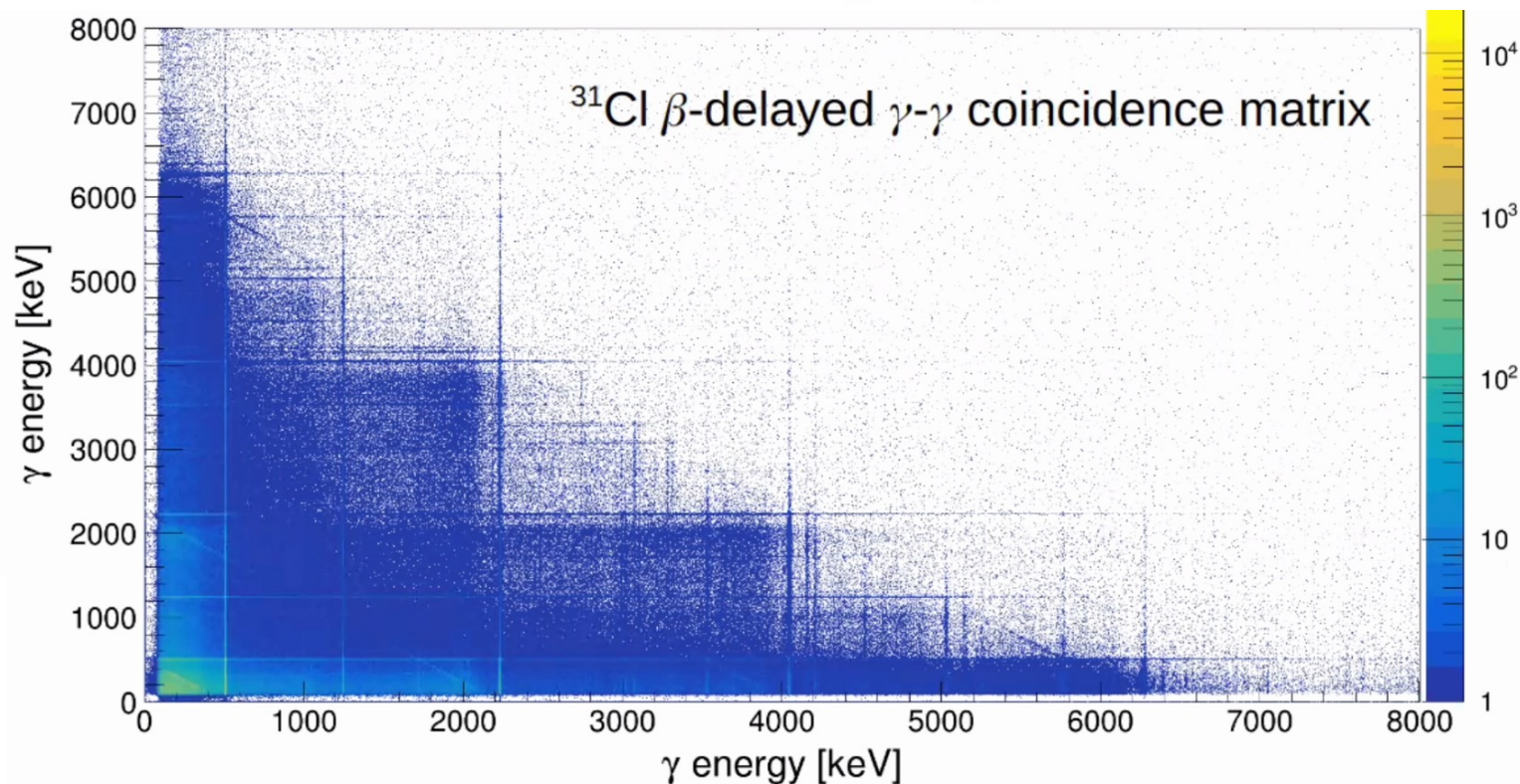
$$C = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1n} \\ C_{21} & C_{22} & \cdots & C_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ C_{n1} & C_{n2} & \cdots & C_{nn} \end{pmatrix}$$

Tamas Budner, ^{31}Cl β-Delayed Proton Decay and Classical Nova Nucleosynthesis, PhD Thesis, MSU, 2022

"Level-Centric" Decay Scheme

Decay schemes can be represented as graphs:

- Each level within the decay scheme corresponds to a vertex (or node), and the edges connecting these vertices correspond to γ-ray transitions between levels.

- Gamma-ray branching ratios correspond to edge weights.
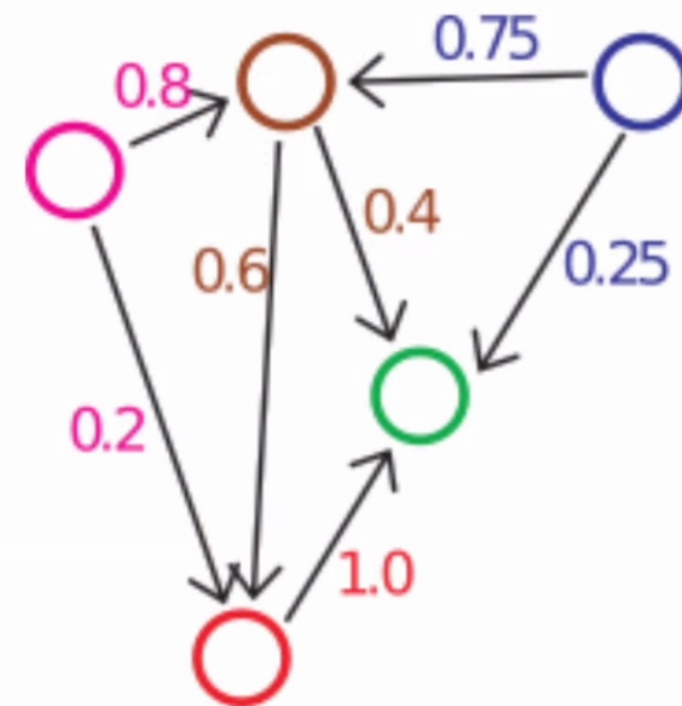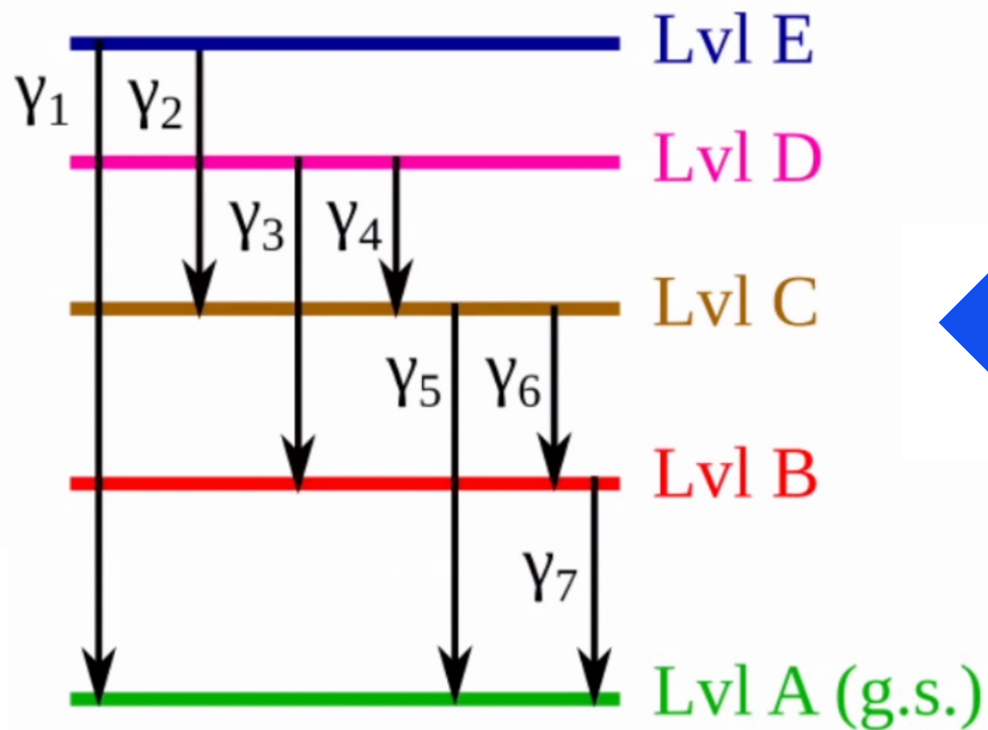
G. Demand, *Development of a Novel Algorithm for Nuclear Level Scheme Determination*. Master's thesis, University of Guelph, 2009.

Expressing Network in Terms of Statistical Observables:

- In this representation, vertices correspond to observable γ-rays, while edges connect γ-ray transitions detected in coincidence.

- A unique transition-centric graph exists for every level-centric decay scheme, but additional information required to reconstruct level-centric decay scheme from transition-centric graph.
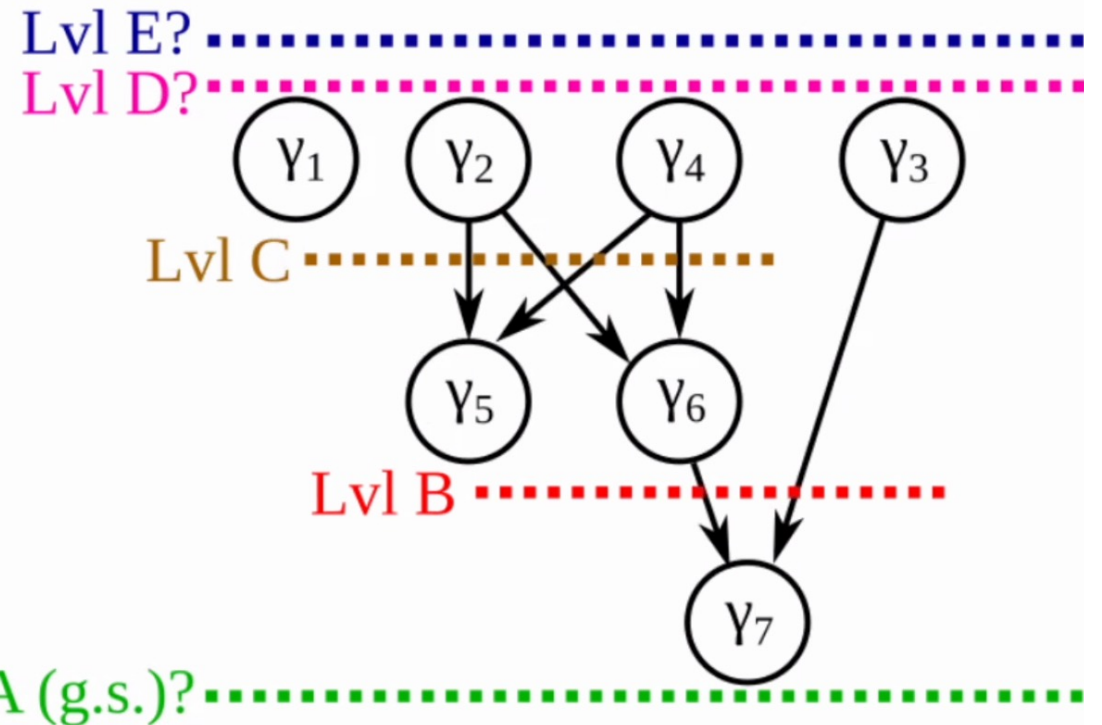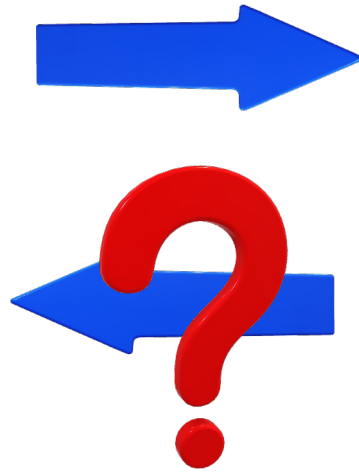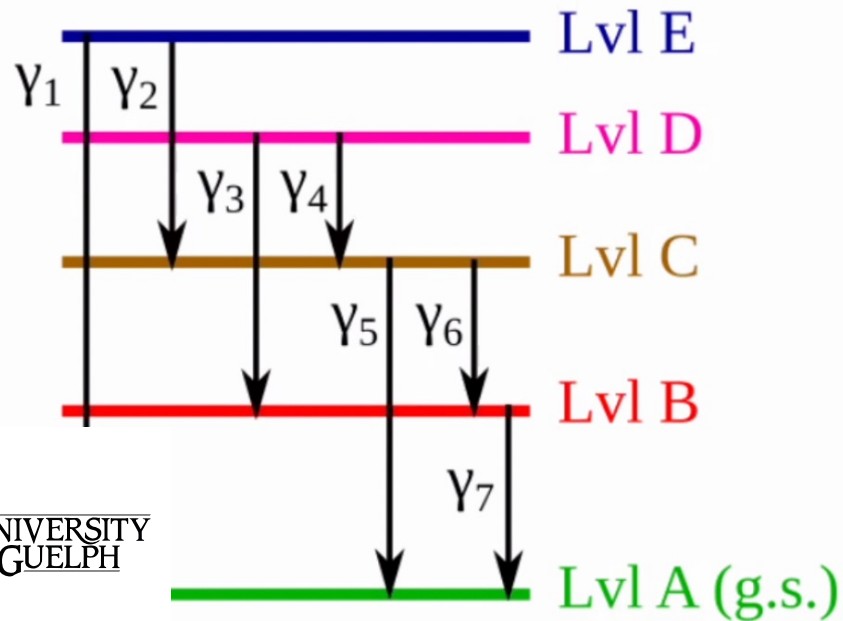
Every weighted, directed graph has a unique adjacency matrix A

Given a start position of vertex i, element $A_{i,j}$ is the probability of transitioning directly to vertex j (non-zero numbers=branching ratios)
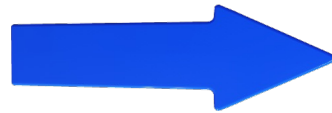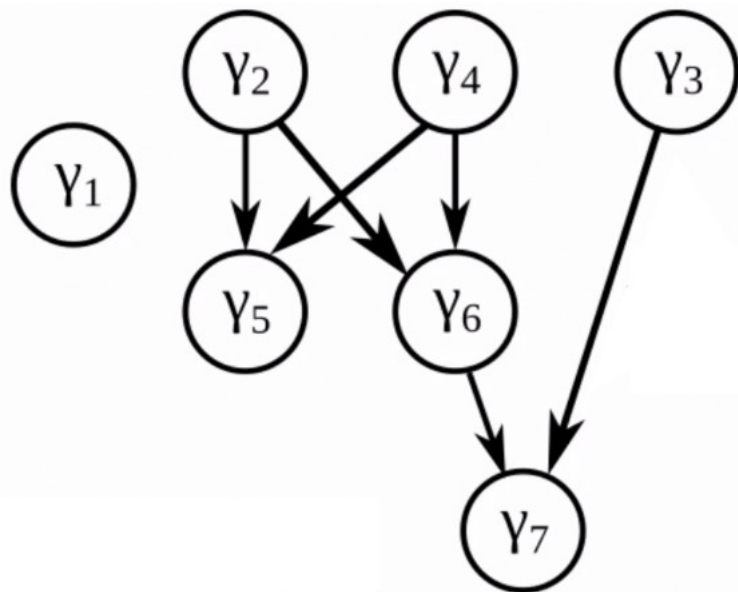
$$
A = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.4 & 0.6 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1.0 \\
0 & 0 & 0 & 0 & 0.4 & 0.6 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1.0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\begin{matrix}
Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \\ Y_6 \\ Y_7
\end{matrix}
$$

$$Y_1 \quad Y_2 \quad Y_3 \quad Y_4 \quad Y_5 \quad Y_6 \quad Y_7$$

Equations to Solve for Optimization

Every weighted, directed graph has a unique adjacency matrix A.

- Adjacency matrix elements $A_{i,j}$ give the probability of vertex i decaying directly to vertex j in a weighted, directed graph.

- Using matrix multiplication, $A^2{}_{i,j}$ gives the probability of vertex i decaying to vertex j in exactly two steps.

- It can be proven via induction that the probability of decaying from vertex i to vertex j in n steps is given by $A^n{}_{i,j}$

- Thus, the probability P of decaying from vertex i to vertex j in any number of steps is

$$P_{ij} = \left(A + A^2 + A^3 + \ldots \right)_{ij}$$

- Using the identity $I + A + A^2 + A^3 + \ldots = (I - A)^{-1}$, this implies

$$P = (I - A)^{-1} - I$$

G. Demand, *Development of a Novel Algorithm for Nuclear Level Scheme Determination*. Master's thesis, University of Guelph, 2009.

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Equations to Solve for Optimization

Defining the Directed Coincidence Matrix D:

- The product of the observed γ-ray singles vector S_i with the probability $P_{i,j}$ of γ_j decay occurring immediately after γ_i decay defines the (reduced) directed coincidence matrix:

$$D_{i,j} = SP_{i,j}$$

- Substituting our expression for probability in terms of the adjacency matrix:

$$D = S\left((I - A)^{-1} - I\right)$$

- The matrix sum of D and its transpose yields the observable, undirected coincidence matrix:

$$C = D + D^T$$

G. Demand, *Development of a Novel Algorithm for Nuclear Level Scheme Determination*. Master's thesis, University of Guelph, 2009.

Machine Learning Tools for Level-Scheme Design

Numerical Solution:

- Goal: Given S, C, find A, D such that

$$D = S\left((I - A)^{-1} - I\right) \text{ and } C = D + D^T$$

- Therefore we have two governing equations:

$$D = S\left((I - A)^{-1} - I\right)$$
$$C = D + D^T$$

- Satisfying both equations leads to the nonlinear optimization problem:

$$\min_{A,D} \left\| D - S\left((I - A)^{-1} - I\right) \right\|^2$$

subject to: $\boxed{A \geq 0, \sum_j A_{ij} \leq 1}$ $C = D + D^T$ PHYSICS!

Enforce constraints such as conservation of energy, non-negative decay intensities, etc.

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Finding A, D that produce the global minimum value is equivalent to finding A, D that satisfy the governing equations (and thus describe the true level scheme)

Level-Scheme Reconstruction

Mathematical Formulation for Writing Level Scheme Construction as Matrix Equations

- Start with data from Gamma-Ray Spectroscopy experiment:
  - $\rightarrow$ S : γ-ray transitions & intensities (as diagonal matrix)
  - $\rightarrow$ C : $\gamma\gamma$ coincidence data

- Following Demand (2013), try to satisfy two equations simultaneously:

$$D = S\left((I - A)^{-1} - I\right) \text{ and } C = D + D^T$$

- Inverse optimization problem results in two matrices:
  - $\rightarrow$ A: the matrix of branching ratios between subsequent y-rays
  - $\rightarrow$ D: the directed coincidence data

- Final Step: Create energy level scheme from matrix output

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 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0. ]
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 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0. ]
 [4229.02 4229.02 5708.98    0.      0.      0.      0.      0.      0.      0. ]
 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0. ]
 [1731.1  1731.1  2336.9  4068.      0.      0.      0.      0.      0.      0. ]
 [1486.44 1486.44 2006.62    0.   4097.94 3493.06    0.      0.      0.      0. ]
 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0. ]]
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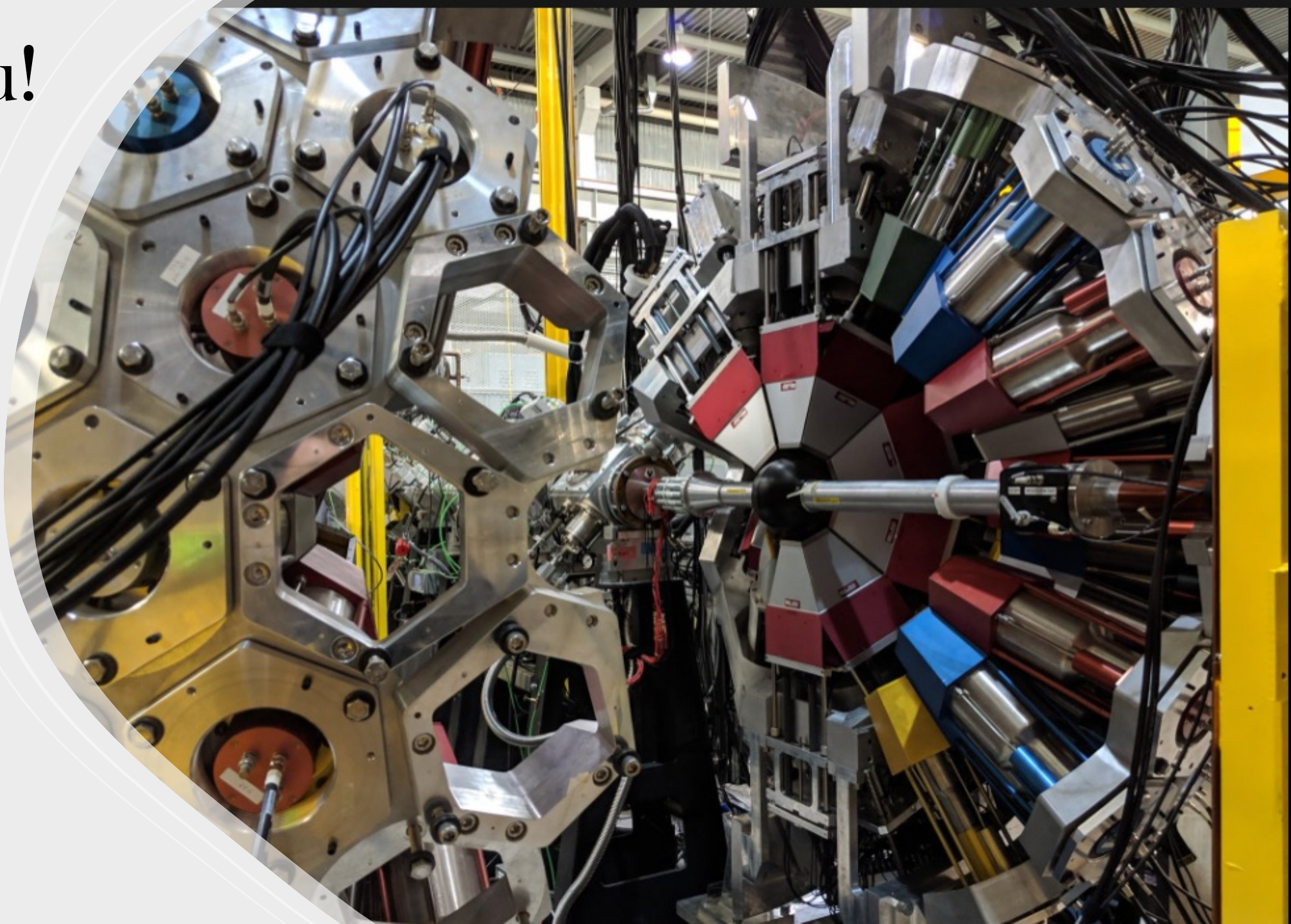
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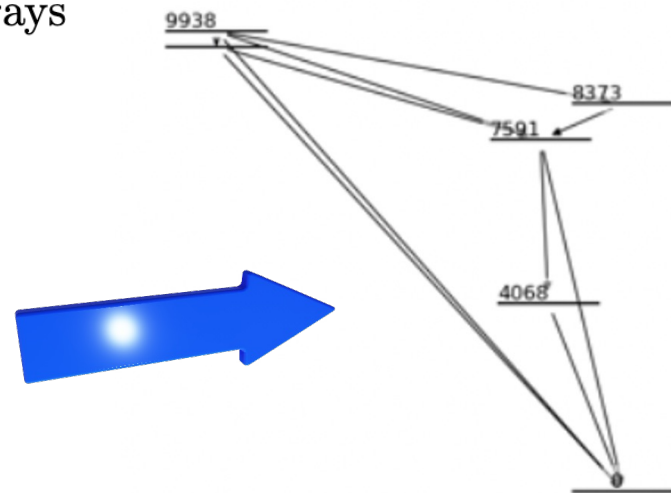
Quantum Algorithm Augmentation

Quantum Approximate Optimization Algorithm

Quantum Annealing

Quantum Gradient Descent

All three approaches are aimed at optimization, they differ in their underlying principles, the types of problems they are suited for, and the techniques they employ. QAOA is a parameterized quantum circuit algorithm for combinatorial optimization, Quantum Annealing is a method for finding the ground state of a quantum system to solve optimization problems, and Quantum Gradient Descent is a quantum optimization algorithm inspired by classical gradient descent methods.

Thank you!

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Quantum Annealing

Quantum annealing is a quantum optimization technique that is inspired by the physical process of annealing, which is the gradual cooling of a material to reach its lowest energy state. Quantum annealing works by encoding the optimization problem into a Hamiltonian, which is a mathematical operator that describes the energy of a quantum system. The Hamiltonian has two terms: one that represents the objective function to be minimized, and one that induces quantum fluctuations. The algorithm starts with a high value of the quantum fluctuation term, which puts the system in a superposition of all possible states. Then, the algorithm gradually decreases the quantum fluctuation term and increases the objective function term, which drives the system towards the lowest energy state, which corresponds to the optimal solution.

Quantum annealing has been implemented on specialized hardware devices called quantum annealers, such as those developed by D-Wave Systems. Quantum annealers have thousands of qubits, which are the basic units of quantum information, and can solve large-scale optimization problems in seconds. However, quantum annealing also has some drawbacks, such as noise, decoherence, and limited connectivity between qubits. Moreover, quantum annealing is not guaranteed to find the global optimum, and may get stuck in local minima.

Quantum Approximate Optimization Algorithm (QAOA)

QAOA is a quantum optimization algorithm that is based on the idea of variational quantum algorithms, which are hybrid algorithms that combine quantum and classical computation. QAOA works by encoding the optimization problem into a Hamiltonian, similar to quantum annealing. However, instead of gradually changing the Hamiltonian, QAOA applies a sequence of unitary operators to an initial state, which are parameterized by some angles. The unitary operators are chosen to alternate between the objective function term and the quantum fluctuation term. The algorithm then measures the final state and evaluates the objective function value. The algorithm repeats this process for different values of the angles, and uses a classical optimizer to find the optimal values that minimize the objective function.QAOA has some advantages over quantum annealing, such as being more robust to noise and decoherence, and being able to run on general-purpose quantum computers. However, QAOA also has some challenges, such as requiring many measurements and classical optimization steps, and having a trade-off between the quality of the solution and the depth of the circuit.

Quantum Gradient Descent

Quantum gradient descent is another variational quantum algorithm that is inspired by the classical gradient descent method, which is one of the most widely used optimization techniques in machine learning. Quantum gradient descent works by encoding the optimization problem into a parametrized quantum circuit, which acts as an ansatz or a guess for the optimal state. The algorithm then measures the output of the circuit and evaluates the objective function value. The algorithm then computes the gradient of the objective function with respect to the parameters of the circuit, either analytically or numerically, and updates the parameters accordingly. The algorithm repeats this process until convergence or until a stopping criterion is met.

Quantum gradient descent has some benefits over classical gradient descent, such as being able to explore a larger space of possible solutions and being able to leverage quantum speedups for certain subroutines. However, quantum gradient descent also faces some difficulties, such as having high circuit complexity and measurement cost, and being sensitive to noise and barren plateaus.

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