STQM Term Project

Jyotirmaya Shivottam
1711069

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Noninteracting multiparticle quantum random walks applied to the graph isomorphism problem for strongly regular graphs

Kenneth Rudinger,[1,*] John King Gamble,[1] Mark Wellons,[2] Eric Bach,[2] Mark Friesen,[1] Robert Joynt,[1] and S. N. Coppersmith[1,†]
[1]*Physics Department, University of Wisconsin–Madison, 1150 University Avenue, Madison, Wisconsin 53706, USA*
[2]*Computer Sciences Department, University of Wisconsin–Madison, 1210 West Dayton Street, Madison, Wisconsin 53706, USA*
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Outline

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Graph Isomorphism

- Let us denote two graphs as $G(V, E)$ and $H(V', E')$.
- A graph isomorphism is an edge-preserving bijection between the vertices of two graphs.

$$f : V \to V'$$

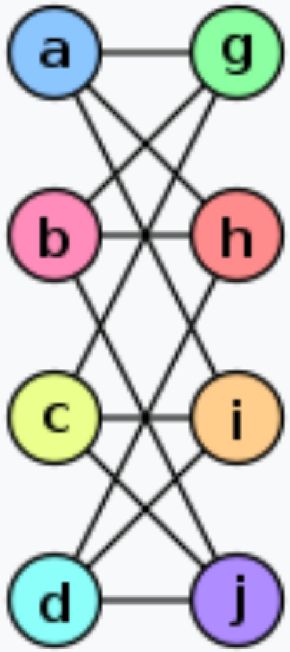
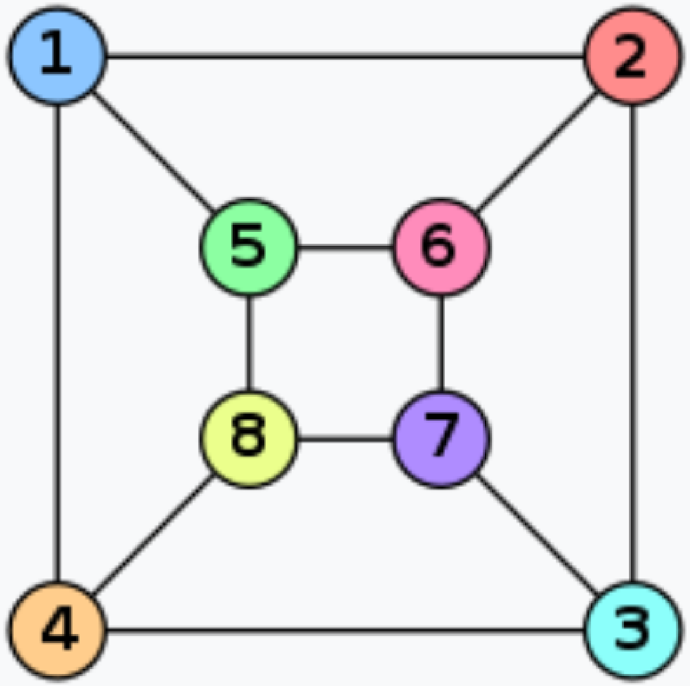
- If such a bijection exists, we call G and H isomorphic or $G \simeq H$.
- The GI problem is to determine whether two graphs are isomorphic or not, i.e. if one can be transformed into the other by a relabeling of vertices.

Graph Isomorphism

- Adjacency matrix:

$$A_{ij} = \begin{cases} 1, & \text{if } i \text{ and } j \text{ are connected} \\ 0, & \text{otherwise} \end{cases}$$

- A graph with N vertices has an $N \times N$ adjacency matrix.
- $G \simeq H$, iff there exists a permutation matrix, P, such that $A_G = P^{-1} A_H P$.
- Permutation matrix represents a relabeling of vertices.
- This problem is in the NP complexity class and is purported to be NP-Intermediate (if $P \neq NP$).

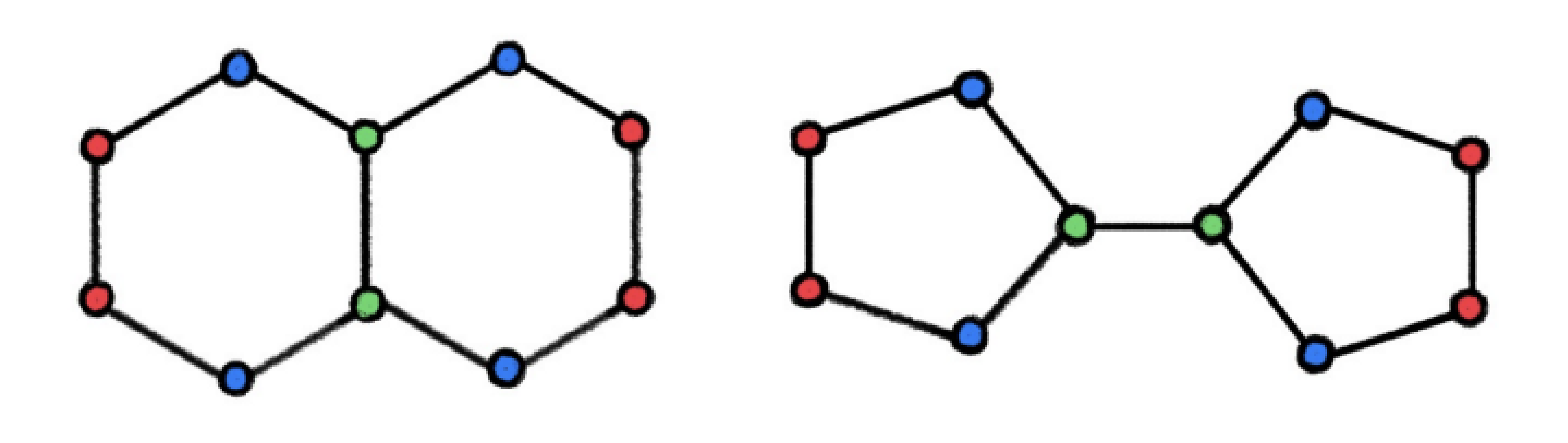
Graph G	Graph H	An isomorphism between G and H
		$f(a) = 1$ $f(b) = 6$ $f(c) = 8$ $f(d) = 3$ $f(g) = 5$ $f(h) = 2$ $f(i) = 4$ $f(j) = 7$

Classical tests

- Weisfeiler-Lehman (WL) test
  - Heuristic-based - *color-refinement*.
  - Produces canonical vertex-label sets.
  - Iterative
  - A necessary but insufficient condition.
- VF(1, 2, 2++) algorithm for Graph Matching
  - Uses *partial edge-matching*.
  - Recursive.
  - Memory requirements grow exponentially with the number of vertices.
  - State-of-the-art.
- Best classical algorithm has a worst-case time complexity of $O(c^{\sqrt{N}\log N})$.

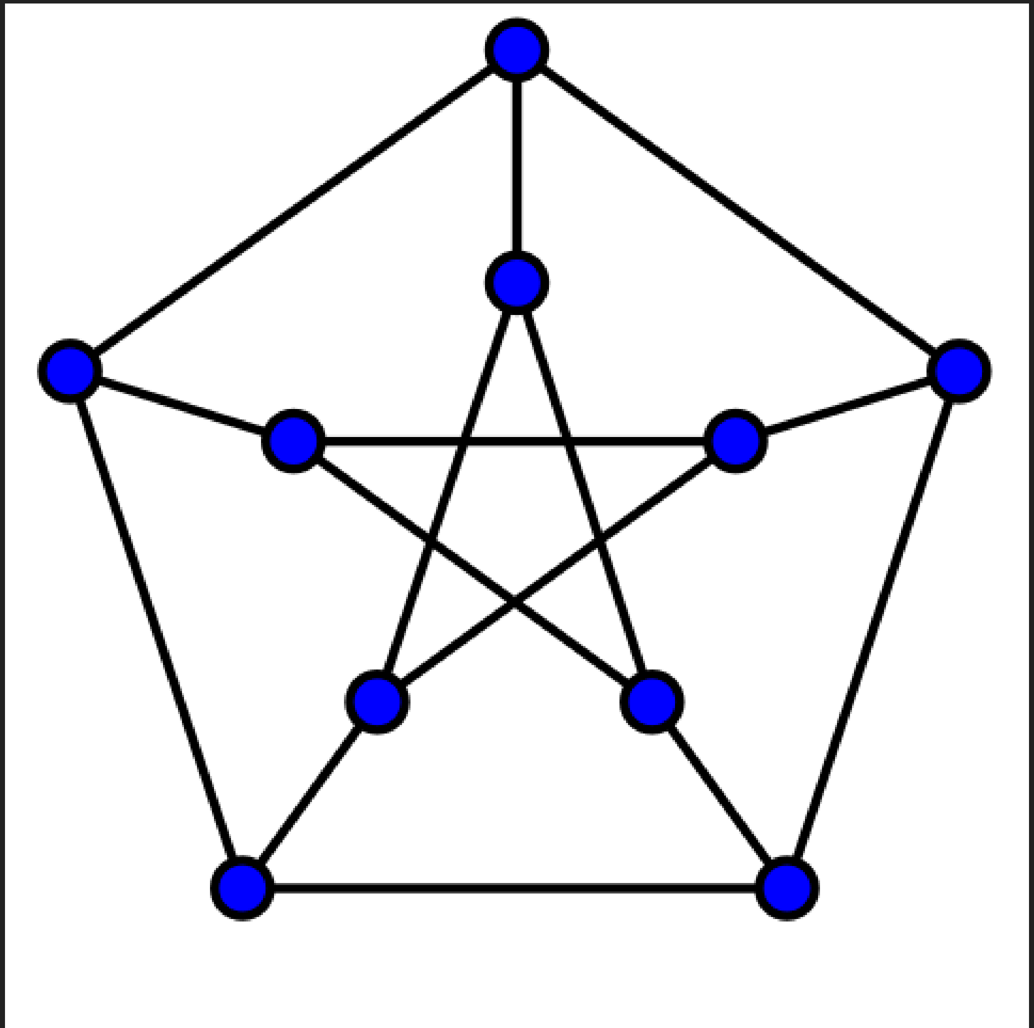
WL test - Failure

- These two non-isomorphic graphs are reported as isomorphic (false-positive).



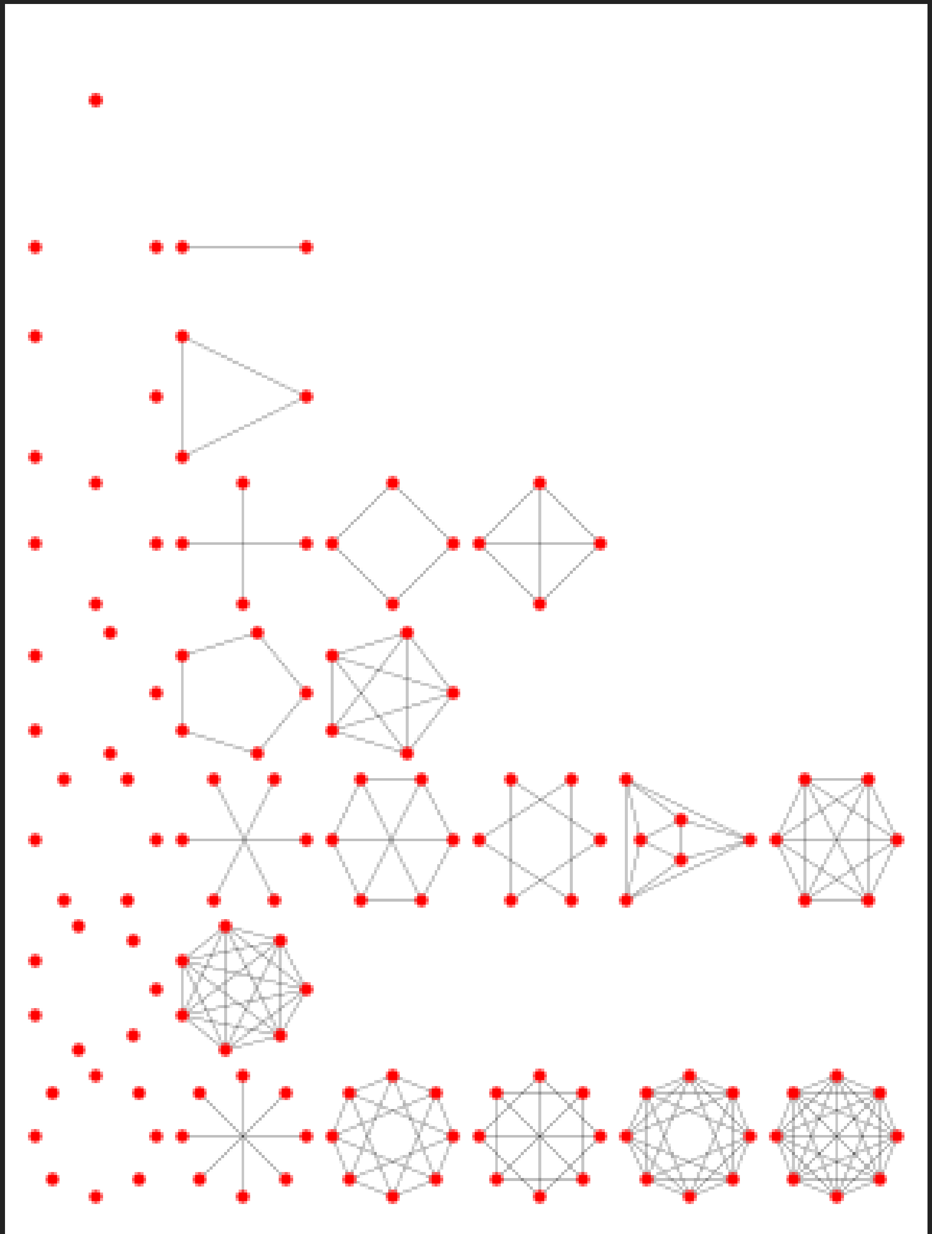
WL test - Failure

- Fails in presence of graph automorphisms.
- Regular graphs usually have a large number of automorphisms.



Strongly Regular Graphs (SRGs)

- Is a *distance-regular* graph with two properties:
  - Every two adjacent vertices have λ common neighbours.
  - Every two non-adjacent vertices have μ common neighbours.
- Collectively, $\mathrm{srg}(|V| = v, k, \lambda, \mu)$ denotes a SRG family (of graphs).
- Petersen graph is a SRG parameterized as $\mathrm{srg}(10, 3, 0, 1)$.



Some SRG properties

- Adjacency matrix for a SRG satisfies:

$$A^2 = (k-\mu)I + \mu J + (\lambda - \mu)A$$
$$JA = AJ = kA$$
$$J^2 = NJ$$

- Here, J is a matrix of all ones and I is identity.
- $\{I, J, A\}$ form a commutative 3-dimensional algebra, which leads us to;

$$A^n = \alpha_n I + \beta_n J + \gamma_n A$$

- $\alpha_n, \beta_n, \gamma_n$ are constants.

Difficulties in distinguishing SRGs

- In principal, the GI problem can be retooled as calculating the canonical labeling via the automorphism group, which is also what classical approaches exploit.
  - The automorphism group of a SRG family is a non-trivial group.
  - Calculating the automorphism group is a problem at least as hard as the GI problem.
  - There are no known polynomial time solutions to either problem.
  - There are no known perfect oracles for either problem.
- Graphs in the same SRG family are co-spectral.
- Each SRG signature defining a family can contain several graphs. For instance, $\mathrm{srg}(36, 15, 6, 6)$ has 32_548 graphs.

Paper's approach

- Defines Continuous Time Quantum Walks (CTQW) on graphs.
- Uses the Hubbard model, without the short-range interaction term, where each site corresponds to a vertex.

$$H = -\sum A_{ij} c_i^\dagger c_j$$

- For bosons: $[c_i, c_j^\dagger] = \delta_{ij}. [c_i, c_j] = [c_i^\dagger, c_j^\dagger] = 0 \implies$ symmetrized basis states, with multi-occupancy.
- For fermions: $\{c_i, c_j^\dagger\} = \delta_{ij}. \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \implies$ anti-symmetrized basis states, with single-occupancy.

Paper's approach

- p-boson or p-fermion Hamiltonian can be given as:

$$
\begin{aligned}
{}_B\langle i_1, \ldots, i_p | H_{p,B} | j_1, \ldots, j_p \rangle_B &= -{}_B\langle i_1, \ldots, i_p | A^{\oplus p} | j_1, \ldots, j_p \rangle_B \\
{}_F\langle i_1, \ldots, i_p | H_{p,B} | j_1, \ldots, j_p \rangle_F &= {}_F\langle i_1, \ldots, i_p | A^{\oplus p} | j_1, \ldots, j_p \rangle_F
\end{aligned}
$$

- Where, $A^{\oplus p} = A \otimes I \otimes \cdots + I \otimes A \otimes \cdots + \cdots + I \otimes \cdots \otimes A$.
- The evolution operator is defined as usual:

$$
U(t) = e^{-iHt}
$$

- The elements of the resulting matrix are also termed *Green's functions* (in the *correlator* sense).

Algorithm

1. Begin with the (complex) evolution matrix U.
2. Take the magnitude of each element.
3. Write all the (real) entries in a list, X_A.
4. Sort the list.
5. Compare the list using:

$$\Delta = \sum_v |X_A[v] - X_B[v]|$$

- If $\Delta \neq 0$, then A and B are non-isomorphic or distinguished.
- The converse is however not true, because non-isomorphic non-distinguished graphs (false negatives) can also have $\Delta = 0$.

Intuition

- As an example, for the 3-particle walk, U can be decomposed as: $U_{3B} = U_1^{\otimes 3}$ or $U_{3F} = \overline{U}_1^{\otimes 3}$, where $U_1 = e^{iAt}$ and $\overline{U}_1 = e^{-iAt}$.
- Recall the 3-algebra and decompose $U_1 = \alpha_n I + \beta_n J + \gamma_n A$.
- These constants depend only on SRG family parameters and t. Therefore:
    - All possible values of the Green's functions are determined by the family parameters.
    - Distinguishing power of the walks comes from the existence of at least one Green’s function with different multiplicities for nonisomorphic graphs in the same family.
    - Also see Gamble et al (2010).

Limitations

- The multiplicity of G (Green's functions) in a p-particle walk depends on how many shared neighbors a collection of up to p vertices has.
  - For 1 & 2-particle walks, G are a function of only the family parameters, because strong regularity uniquely determines the number of shared neighbors.
  - For $p \geq 3$, this may not always be true, because the number of shared neighbors is dependent on the number of shared neighbors among sets of p vertices.
  - This is the primary reason why the algorithm might return false negatives.
- Another reason is the choice of ordering of basis sets, which can flip the signs of the Green's functions, resulting in false-positives. The authors therefore take the absolute value to avoid this scenario and to avoid an exhaustive search for all p^N orderings. This however results in a loss of phase information.

Limitations

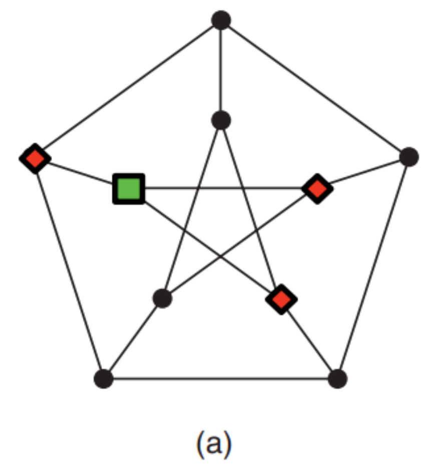


FIG. 4. (Color online) Two copies of the Petersen graph, an SRG with parameters (10,3,0,1). In each graph, three mutually nonadjacent vertices are highlighted as (red) diamonds. In (a), the three vertices share one common neighbor, shown as the (green) square. In (b), the three vertices share no common neighbors. This demonstrates that the number of neighbors common to a triple of vertices in a strongly regular graph is not strictly a function of the SRG family parameters, thus showing why widget multiplicity is not strictly governed by family parameters when $p \geqslant 3$.

Limitations

Forming the evolution operators $\mathbf{U} = e^{-it\mathbf{H}}$, we have

$$\mathbf{U}_A = \begin{pmatrix} \left(\frac{\cos(\sqrt{2}t)}{2} + \frac{1}{2}\right) & -\frac{i\sin(\sqrt{2}t)}{\sqrt{2}} & \left(\frac{\cos(\sqrt{2}t)}{2} - \frac{1}{2}\right) \\ -\frac{i\sin(\sqrt{2}t)}{\sqrt{2}} & \cos(\sqrt{2}t) & -\frac{i\sin(\sqrt{2}t)}{\sqrt{2}} \\ \left(\frac{\cos(\sqrt{2}t)}{2} - \frac{1}{2}\right) & -\frac{i\sin(\sqrt{2}t)}{\sqrt{2}} & \left(\frac{\cos(\sqrt{2}t)}{2} + \frac{1}{2}\right) \end{pmatrix} \quad (28)$$

and

$$\mathbf{U}_B = \begin{pmatrix} \cos(\sqrt{2}t) & -\frac{i\sin(\sqrt{2}t)}{\sqrt{2}} & \frac{i\sin(\sqrt{2}t)}{\sqrt{2}} \\ -\frac{i\sin(\sqrt{2}t)}{\sqrt{2}} & \left(\frac{\cos(\sqrt{2}t)}{2} + \frac{1}{2}\right) & \left(\frac{1}{2} - \frac{\cos(\sqrt{2}t)}{2}\right) \\ \frac{i\sin(\sqrt{2}t)}{\sqrt{2}} & \left(\frac{1}{2} - \frac{\cos(\sqrt{2}t)}{2}\right) & \left(\frac{\cos(\sqrt{2}t)}{2} + \frac{1}{2}\right) \end{pmatrix}. \quad (29)$$

Results

SRG family (N, k, λ, μ)	No. of graphs	Comparisons	Boson failures	Fermion failures
(16,6,2,2)	2	1	0	0
(16,9,4,6)	2	1	0	0
(25,12,5,6)	15	105	0	0
(26,10,3,4)	10	45	1	1
(28,12,6,4)	4	6	0	0
(29,14,6,7)	41	820	0	0
(35,18,9,9)	227	25 651	38	38
(36,14,4,6)	180	16 110	89	89
(40,12,2,4)	28	378	8	8
(45,12,3,3)	78	3 003	7	7
(49,18,7,6)	147	10 731	21	21
(64,18,2,6)	167	13 861	92	92

- 3-particle walks: 70_712 graph comparisons, with 256 failures (success > 99.6%).

Results

Family (N, k, λ, μ)	3-particle failures	4-fermion failures
(26,10,3,4)	1	0
(35,18,9,9)	38	0
(36,14,4,6)	89	1
(40,12,2,4)	8	0

- 4-particle walks, with near 100% accuracy.
- It should be noted that, in both cases, the authors have chosen subsets of families for large N, in order to reduce the number of comparisons.
- Also from these tables, it is clear that for $p = 3$, there is no difference between bosons and fermions.

Own calculations

- I could not calculate U_4, and even for U_3, the largest family handled for all cases was $\mathrm{srg}(16, 6, 2, 2)$, with 2 graphs (with correct results). (Updated post-talk)
- The code is available on GitHub.
- Issues faced:
  - A and H are large and non-sparse. So, diagonalization has to use slower methods.
  - Since we want accurate elements, iterative methods cannot be used.
  - The memory requirement blows up (exponential) in N.
  - The classical test also requires a long time to go through all the graphs and more importantly, is not guaranteed to be correct for large N.

Extensions to this work

- The authors had purported that including the phase-information might improve the algorithm's results, especially for larger-p or larger-N. Mahasinghe et al however showed that phase-modified CTQW is still unable to distinguish strongly regular graphs, since the Green's functions are still not unique.
- Alternative approaches to this problem have also been published:
  - It has been shown that DTQW evolves in a higher dimensional space, allowing it to possess extra distinguishing power on SRGs.
  - Wang et al present an optimizing heuristic that omits the sorting step.
  - Tamascelli et al present a QW-inspired adiabatic algorithm to reduce the search space and translate the problem to $2-$SAT.

References

- [Link to GitHub repo for the code]
- Using hyperlinks-only to preserve space.
- Main papers:
  1. Rudinger et al; Noninteracting multiparticle quantum random walks applied to the graph isomorphism problem for strongly regular graphs
  2. Gamble et al; Two-particle quantum walks applied to the graph isomorphism problem
- Classical approaches to GI:
  1. A (sub)graph isomorphism algorithm for matching large graphs
  2. VF2++—An improved subgraph isomorphism algorithm
  3. On the Complexity of Canonical Labeling of Strongly Regular Graphs

- SRG Data:
  1. Public paramter database - A.E. Brouwer
  2. Strongly Regular Graphs on at most 64 vertices
  3. Collection of graphs
  4. Strongly Regular Graph - Mathematica
- More recent works
  1. Rudinger et al; Comparing algorithms for graph isomorphism using discrete- and continuous-time quantum random walks
  2. Mahasinghe et al; Phase-modified CTQW unable to distinguish strongly regular graphs efficiently
  3. Wang et al; A graph isomorphism algorithm using signatures computed via quantum walk search model
  4. Tamascelli et al; A quantum-walk-inspired adiabatic algorithm for solving graph isomorphism problems

- Image sources:
  - Slide 5 - Wikipedia contributors. (2022). Graph isomorphism -- Wikipedia, The Free Encyclopedia.
  - Slide 7 - Sato, R. (2020). A Survey on The Expressive Power of Graph Neural Networks. arXiv e-prints, arXiv:2003.04078.
  - Slide 8 - Wikipedia contributors. (2022). Petersen graph -- Wikipedia, The Free Encyclopedia.
  - Slide 9 - Weisstein, Eric W. "Strongly Regular Graph." From MathWorld -- A Wolfram Web Resource.
  - Slides 17-20 - Rudinger et al

Post-talk Questions

- Non-interacting CTQW with particle number, $p = 1$ or $p = 2$:
  - The $p = 1$ & $p = 2$ walks are unable to distinguish between graphs from the same SRG family since the elements of U are only dependent on the family parameters ($\alpha,\ \beta,\ \gamma$), and are therefore all identical.
  - Analytical proof of non-distinguishability is available in [this paper]. This was also discussed by the authors in their previous work ([Gamble et al]).
  - I have also shown this in code with a specific example taken from [Gamble et al]. Check the latter portion of `./code/example.ipynb` on [GitHub]).
- In contrast, $p = 3$ (& $p = 4$) non-interacting CTQW has sufficient power to distinguish between non-isomorphic graphs from the same SRG family. I have replicated this result for $\mathrm{srg}(16, 6, 2, 2)$ with $p = 3$ & $p = 4$, and $\mathrm{srg}(26, 10, 3, 4)$ with only $p = 3$. CTQW with $p = 4$ led to an *OutOfMemory* error.

- For $\mathrm{srg}(16, 6, 2, 2)$ with 2 graphs and ${}^2C_2 = 1$ comparison:

p	Boson failures	Fermion failures	Peak Mem Usage (in GB)	Avg. CPU Time (in s)
1	1	1	0.009	4.8
2	1	1	0.009	5.1
3	0	0	0.5	9.1
4	0	0	156	525.1

- For $\mathrm{srg}((26, 10, 3, 4)$ with 10 graphs and ${}^{10}C_2 = 45$ comparisons:

p	Boson failures	Fermion failures	Peak Mem Usage (in GB)	Avg. CPU Time (in s)
1	45	45	1.39	21.4
2	45	45	1.92	35.4
3	1	1	112	2547.5