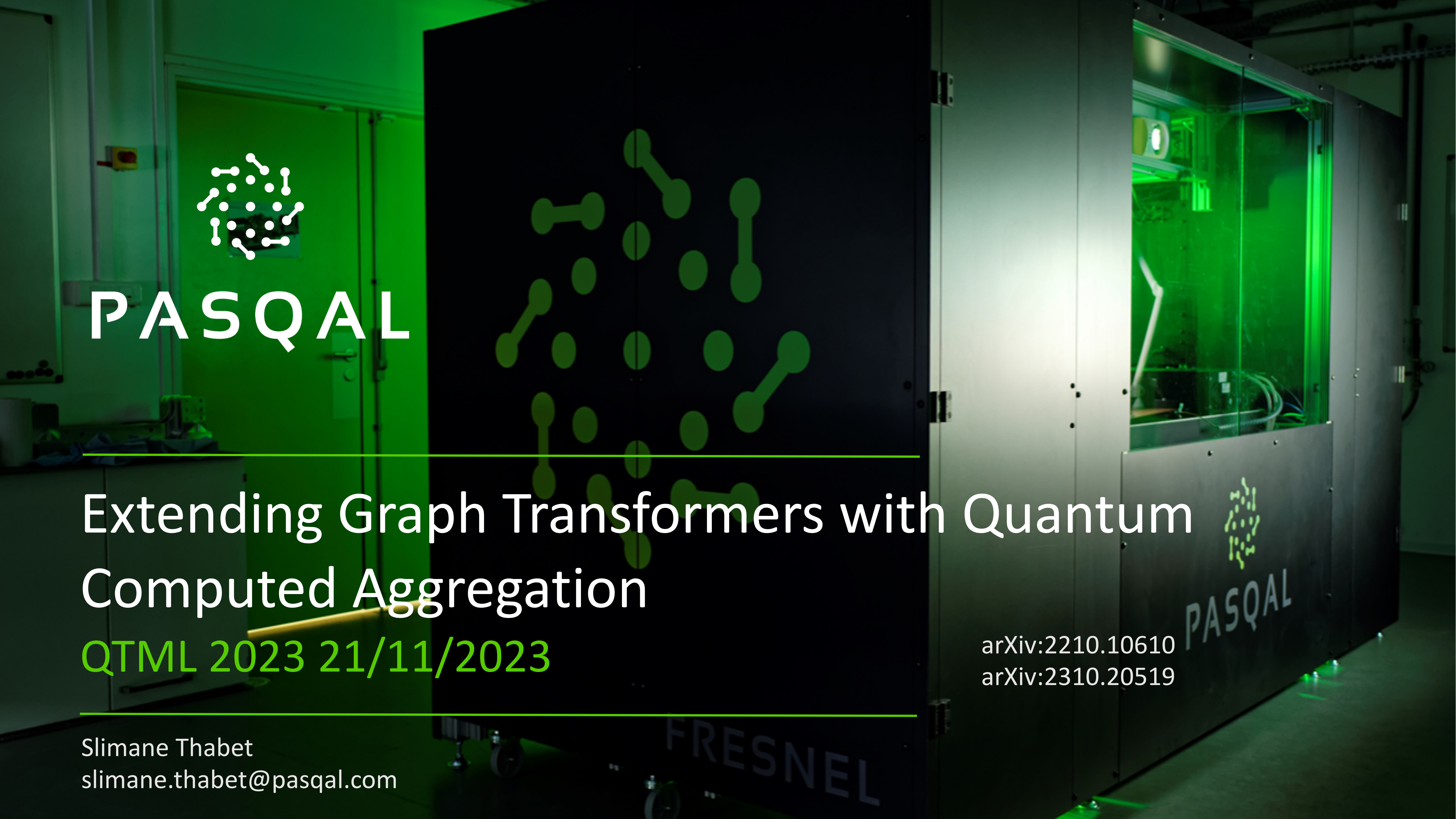

PASQAL

Extending Graph Transformers with Quantum Computed Aggregation

QTML 2023 21/11/2023

arXiv:2210.10610
arXiv:2310.20519

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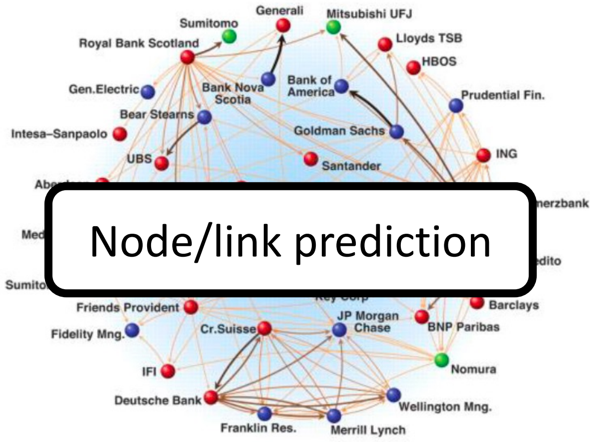
Graph-structured data

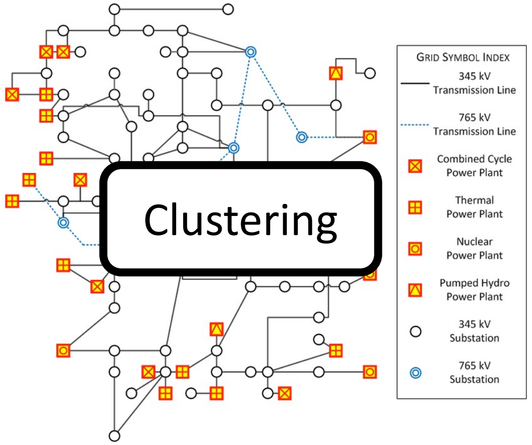
Machine learning tasks on graph-structured data



Node/link prediction

Economic networks

Anticipating new partnerships



Clustering

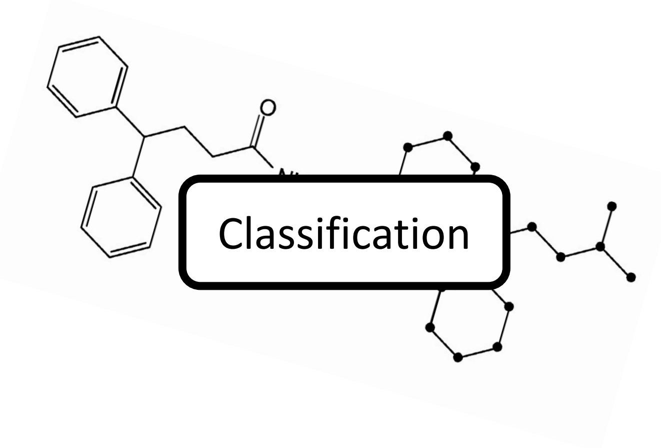
Power grid

Segmenting highly-connected zones

Community detection

Social networks

Marketing to like-minded users



Classification

Molecules

Predicting toxicity of compounds

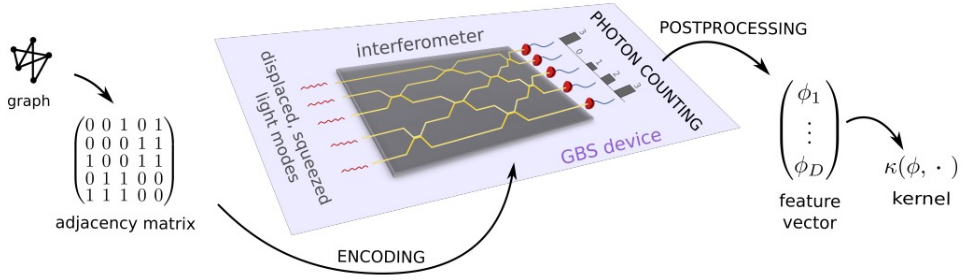
Graph Machine Learning with Quantum Computers

Theoretical protocols

- Verdon, G., McCourt, T., Luzhnica, E., Singh, V., Leichenauer, S., & Hidary, J. (2019). Quantum graph neural networks. *arXiv preprint arXiv:1909.12264*.

- Schuld, M., Brádler, K., Israel, R., Su, D., & Gupt, B. (2020). Measuring the similarity of graphs with a Gaussian boson sampler. *Physical Review A*, *101*(3), 032314.

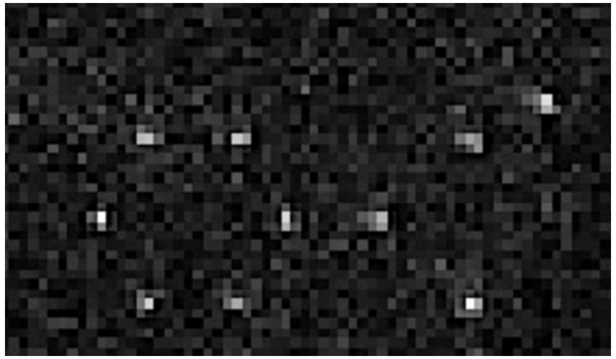
- Henry, L. P., Thabet, S., Dalyac, C., & Henriet, L. (2021). Quantum evolution kernel: Machine learning on graphs with programmable arrays of qubits. *Physical Review A*, *104*(3), 032416.



Schuld et al.

Experiemental implementation on neutral atoms platforms

- Albrecht, B., Dalyac, C., Leclerc, L., Ortiz-Gutiérrez, L., Thabet, S. et al. (2023). Quantum feature maps for graph machine learning on a neutral atom quantum processor. *Physical Review A*, *107*(4), 042615.

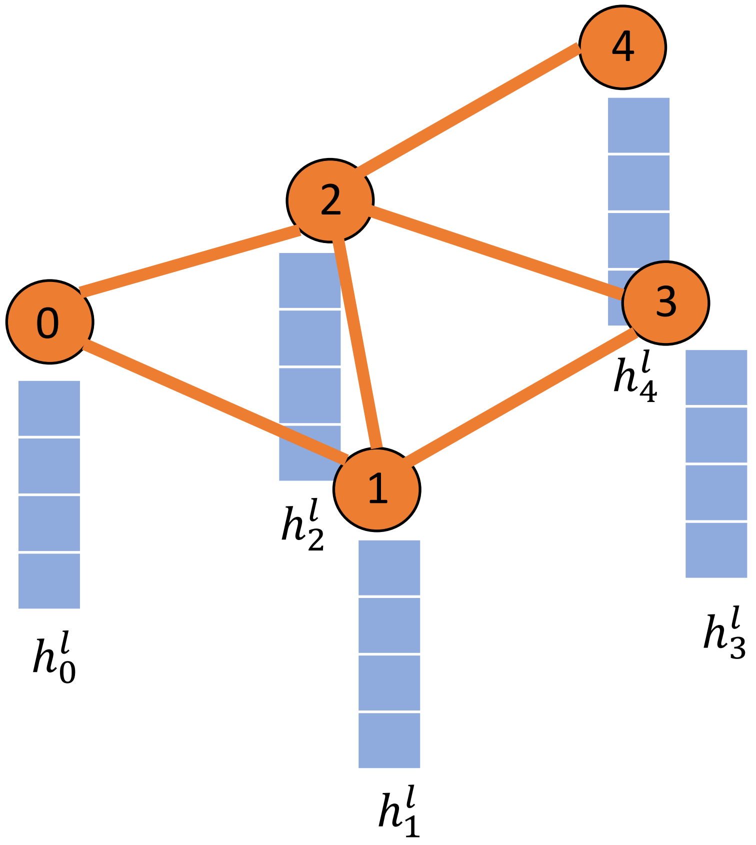


Albrecht et al.

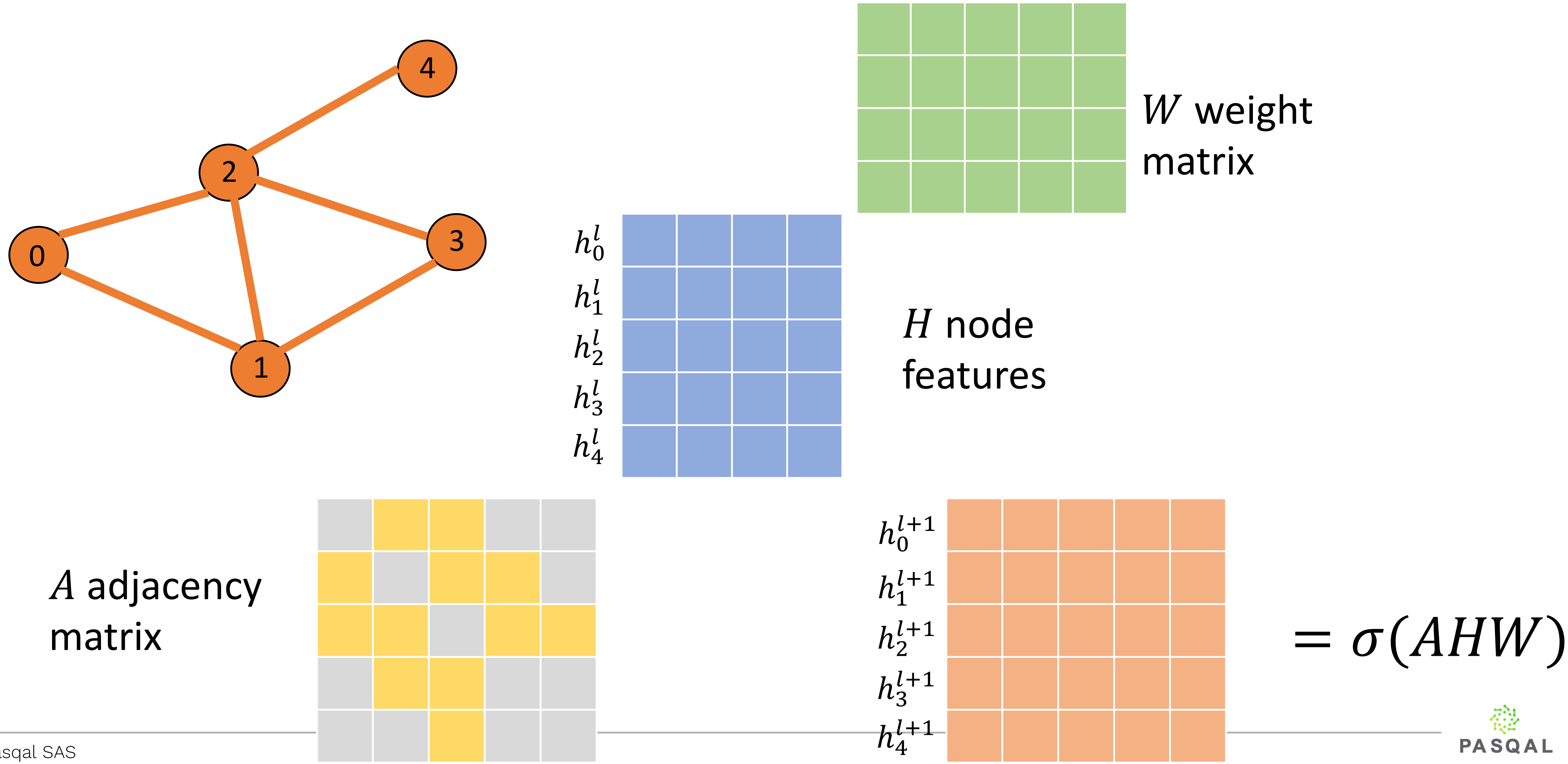
These protocols work for graph level tasks (classification or regression)

Graph Neural Networks (classical)

- Objective: learn representation of nodes (or edges) in a graph, with the use of neural networks.
- Each node is associated at the end with a vector of dimension d.
- These vectors can be the input of a machine learning algorithm. Can be used on many tasks.
- Can be done on one big graph, or several small graphs.

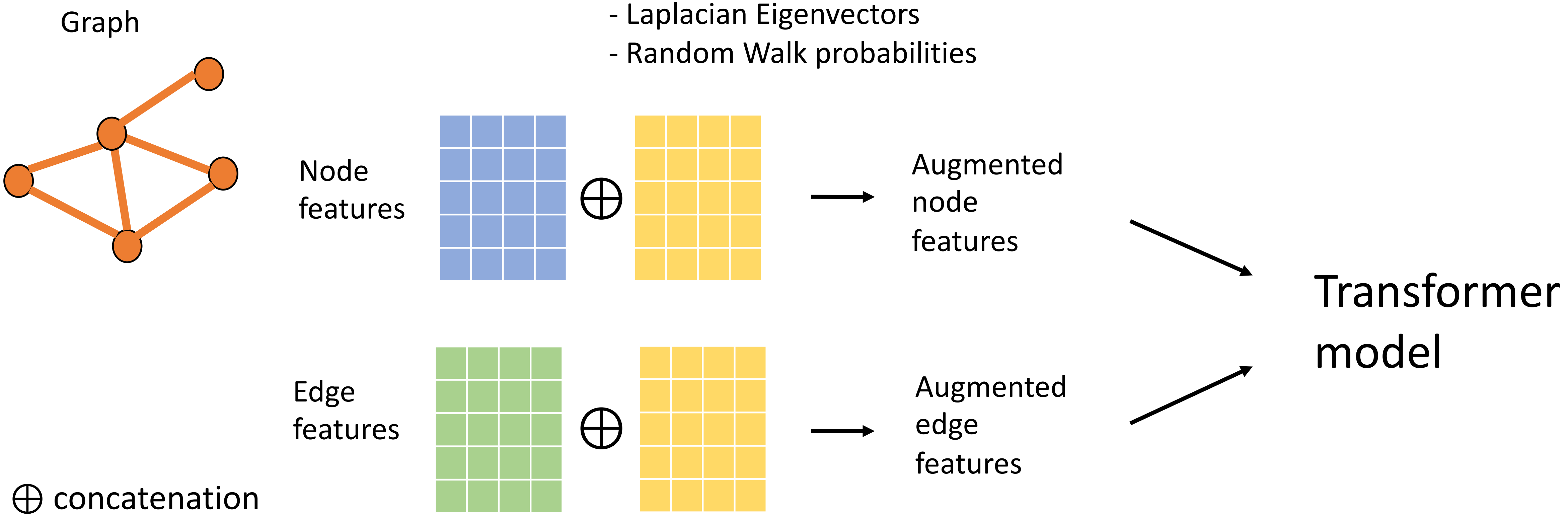


Graph Convolution Networks layer



Graph Transformers

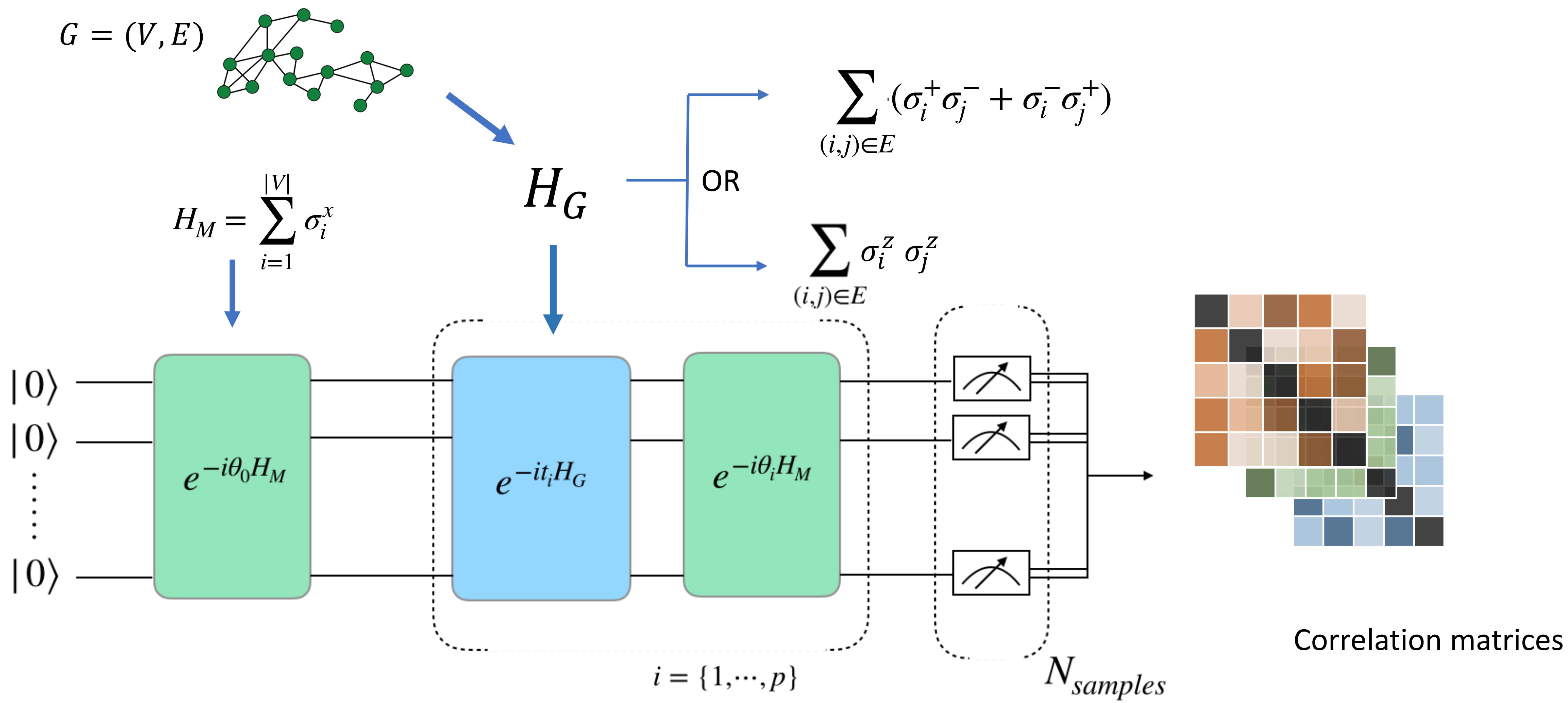
Positional Encodings:
- Laplacian Eigenvectors
- Random Walk probabilities



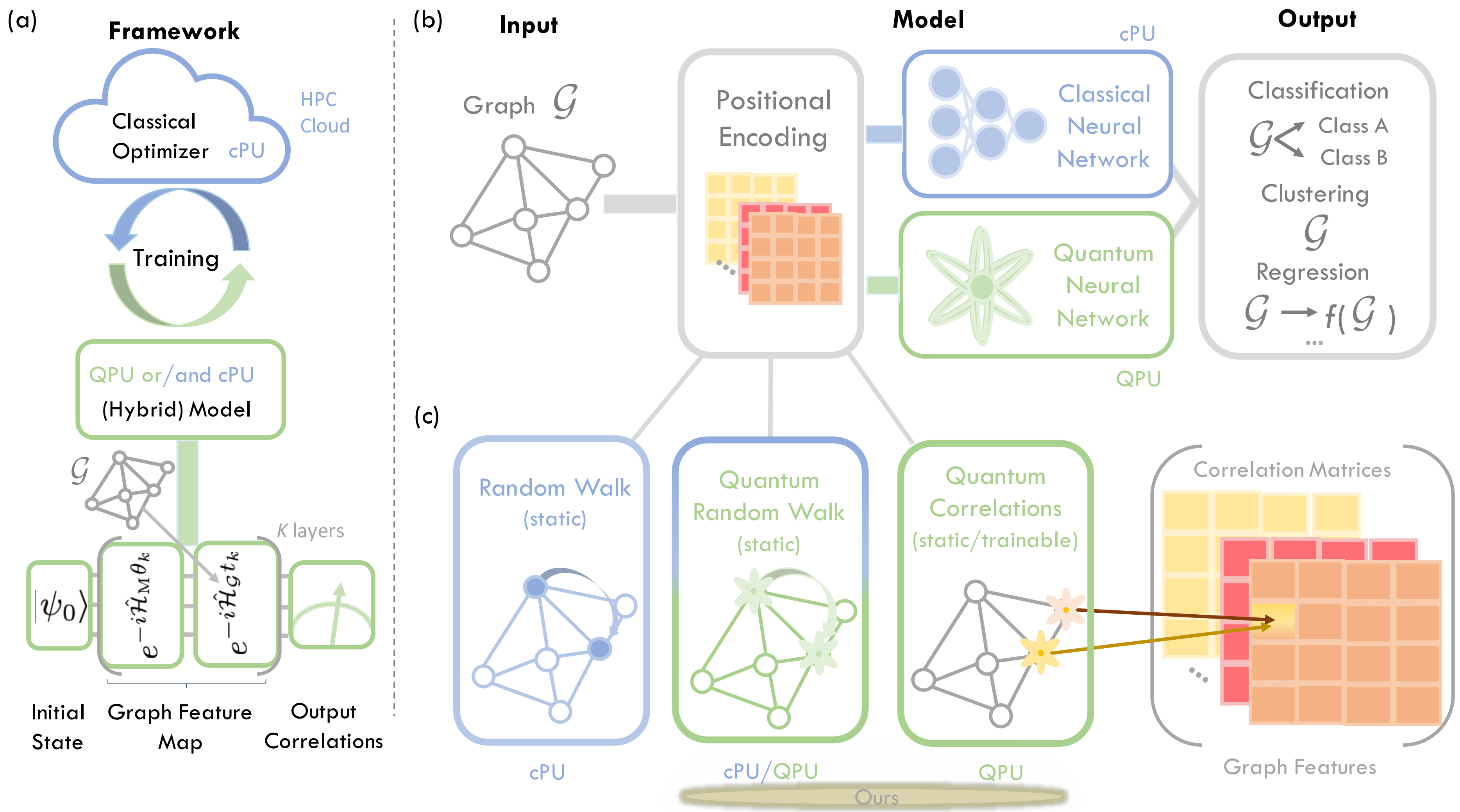
⊕ concatenation

- Kreuzer, D., Beaini, D., Hamilton, W., Létourneau, V., & Tossou, P. (2021). Rethinking graph transformers with spectral attention. *NeurIPS 2021*
- Ying, C., Cai, T., Luo, S., Zheng, S., Ke, G., He, D. et al. Do transformers really perform bad for graph representation? arXiv 2021. *arXiv:2106.05234*.
- Rampášek, L., Galkin, M., Dwivedi, et al. (2022). Recipe for a general, powerful, scalable graph transformer. *NeurIPS 2022*
- Ma, L., Lin, C., Lim, D., Romero-Soriano, A. et al. (2023). Graph Inductive Biases in Transformers without Message Passing. *arXiv:2305.17589*.

Quantum correlations as graph features



Quantum position encodings and aggregation



Properties of our method

- Learn a representation that can be reused on many tasks, graph level, node level etc
- Naturally equivariant by permuting the labeling of the nodes
- One can compute intractable features e.g correlation on ground state
- The quantum features can be adapted with new classical algorithms

Open questions:

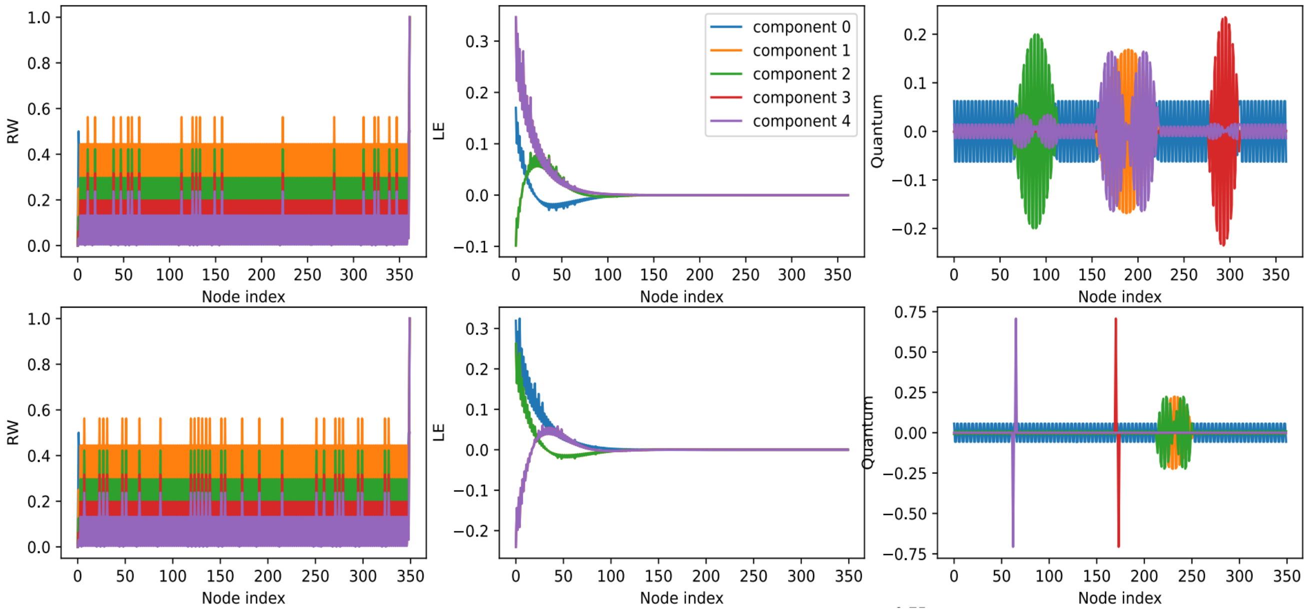
- Are there learning tasks that for which quantum features bring a significant advantage ?
- Is this advantage worth the cost of running a quantum computer ?

Experiments

Theorem 1 *GD-WL test with RRWP embedding fails to distinguish non isomorphic strongly regular graphs. 2 particle-QRW can distinguish some of them.*

Class 0

Class 1



Features on artificial datasets

Model	ZINC-full (MAE ↓)	PCQM4Mv2 (MAE ↓)
GIN	0.088 ± 0.002	0.1195
GraphSAGE	0.126 ± 0.003	—
GAT	0.111 ± 0.002	—
GCN	0.113 ± 0.002	0.1195
SignNet	0.024 ± 0.003	—
Graphormer	0.052 ± 0.005	0.0864
Graphormer-URPE	0.028 ± 0.002	—
Graphormer-GD	0.025 ± 0.004	—
GPS-medium	—	0.0858
GRIT (our run)	0.025 ± 0.002	0.0842
GRIT 1-CQRW (ours)	0.025 ± 0.003	0.0947*
GRIT 2-QiQRW (ours)	0.023 ± 0.002	0.0838

Benchmarks on real datasets

Thanks for your attention

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PASQAL

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