Rustworkx

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https://github.com/mtreinish/rustworkx-presentation

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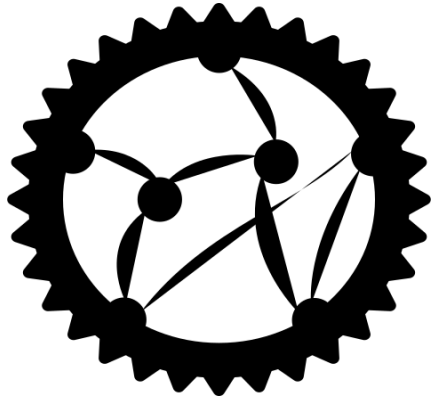
What is Rustworkx?

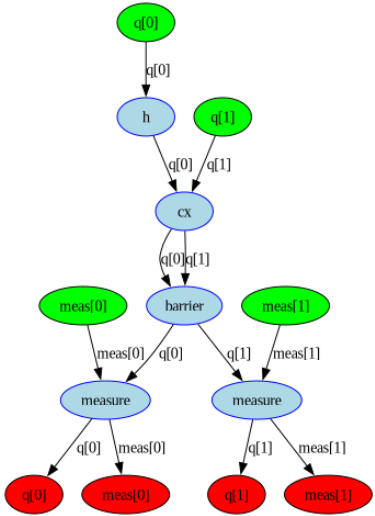
- Open source graph library written in Rust
- Primarily a library for Python
- Designed for high performance and flexibility
- Apache 2.0 Licensed



Unofficial logo proposal, see:
https://github.com/Qiskit/rustworkx/issues/824

Origin of the project

- Started as a library to replace NetworkX usage for the Qiskit[1] compiler's DAG IR.
- Use case where a graph is built, analyzed, mutated, and analyzed again as part of compiler transforms.
- Designed to be flexible so that any Python object can be attached to a graph
- Expanded to cover other graph functionality



[1] Javadi-Abhari, A., Treinish, M., Krsulich, K., Wood, C. J., Lishman, J., Gacon, J., ... & Gambetta, J. M. (2024). Quantum computing with Qiskit. arXiv preprint arXiv:2405.08810. https://doi.org/10.48550/arXiv.2405.08810

Why Rust?

- Rust is designed for safety with no runtime
- Compiler checks to make sure it's memory safe and has safe concurrency
- Performance of Rust code is equivalent to C or C++ but has the safety guarantees
- Rust packaging and build tooling make integration with Python simple

[1]Matsakis, N. D., & Klock, F. S. (2014). The rust language. ACM SIGAda Ada Letters, 34(3), 103-104. https://doi.org/10.1145/2692956.2663188

Two Language Bindings

Python Library

- Primary Interface
- Python library for creating graphs
- Enables using any Python object for node and edge payloads
- Visualization functions for using Matplotlib and Graphviz
- Fully type annotated
- Package available on PyPI for Linux (x86_64, i686, ppc64le, s390x, aarch64), Windows (32bit and 64bit), MacOS (x86_64, arm64).

Rust Library

- Rust language library that provides rust implementation of graph algorithms
- Currently built as an extension to petgraph library
- Pure Rust library (no Python needed)
- Designed to be generic to work with with arbitrary data types
- Used to build the Python library

Rust interface

```rust
use rustworkx_core::petgraph;
use rustworkx_core::max_weight_matching::max_weight_matching;
use rustworkx_core::Result;

// Create a path graph
let g = petgraph::graph::UnGraph::<i32, i128>::from_edges(&[
    (1, 2, 5), (2, 3, 11), (3, 4, 5)
]);
// Run max weight matching with max cardinality set to true
let matching = max_weight_matching(&g, true, |e| Ok(*e.weight()), true);
```

Python Interface

```
import rustworkx as rx

# Create a path graph
g = rx.PyGraph()
g.extend_from_weighted_edge_list([(0, 1, 5), (1, 2, 11), (2, 3, 5)])
# Run max weight matching with max caridnality set to True
matching = rx.max_weight_matching(g, max_cardinality=True, weight_fn=int)
```

Using Rustworkx

- Two classes PyGraph and PyDiGraph for undirected and directed graphs respectively

```
import rustworkx as rx

graph = rx.PyGraph()
graph.extend_from_edge_list([(0, 1), (1, 2)])
assert graph.has_edge(1, 0)
digraph = rx.PyDiGraph()
digraph.extend_from_edge_list([(0, 1), (1, 2)])
assert not digraph.has_edge(1, 0)
```

Using Rustworkx

- Two classes PyGraph and PyDiGraph for undirected and directed graphs respectively
- All nodes and edges are addressed with integer indices and data payloads can be any Python object

```
import rustworkx as rx

graph = rx.PyDiGraph()
node_a = graph.add_node("my_node_a")
node_b = graph.add_node("my_node_b")
assert node_a == 0
assert node_b == 1
graph.add_edge(node_a, node_b, None)
assert "my_node_a" == graph[node_a]
assert "my_node_b" == graph[node_b]
```

Using Rustworkx

- Two classes PyGraph and PyDiGraph for undirected and directed graphs respectively
- All nodes and edges are addressed with integer indices and data payloads can be any Python object
- Graphs can be multigraphs (the default)

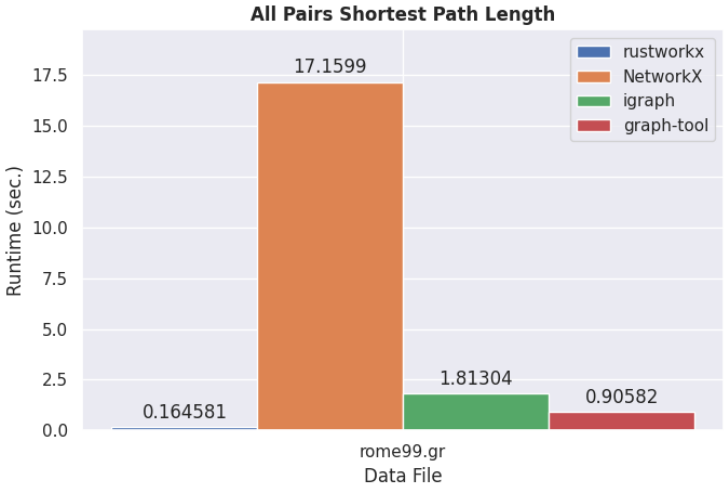
```
import rustworkx as rx

simple_graph = rx.PyGraph(multigraph=False)
multi_graph = rx.PyGraph()

simple_graph.extend_from_edge_list(
    [(0, 1), (1, 0)]
)
multi_graph.extend_from_edge_list(
    [(0, 1), (1, 0)]
)
assert simple_graph.num_edges() == 1
assert multi_graph.num_edges() == 2
```

Using Rustworkx

- Two classes PyGraph and PyDiGraph for undirected and directed graphs respectively
- All nodes and edges are addressed with integer indices and data payloads can be any Python object
- Graphs can be multigraphs (the default)
- Callbacks are typically used to convert data payloads to static types for algorithms

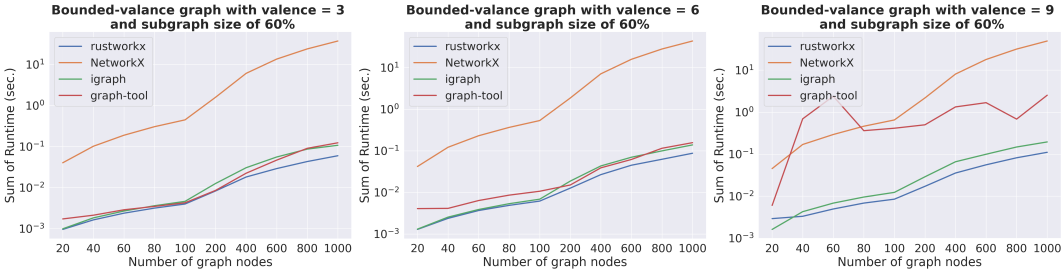
```
import rustworkx as rx

graph = rx.PyDiGraph()
graph.extend_from_weighted_edge_list(
    [
        (0, 1, {"weight": 1}),
        (0, 2, {"weight": 2}),
        (1, 3, {"weight": 2}),
        (3, 0, {"weight": 3}),
    ]
)
# Callback weight_fn to return float weight
dist_matrix = rx.floyd_warshall_numpy(
    graph, weight_fn=lambda edge: edge[weight]
)
```

All Pairs shortest path for Road Network of Rome, Italy in 1999[2]



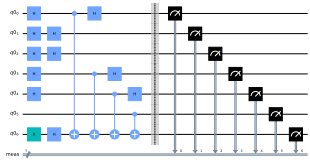
[3]Demetrescu, C., Goldberg, A., & Johnson, D. The Shortest Path Problem: Ninth DIMACS Implementation Challenge. https://doi.org/10.1090/dimacs/074

Subgraph isomorphism benchmarks using ARG database[3]

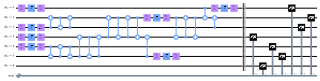


[4]Santo, M. D., Foggia, P., Sansone, C., & Vento, M. (2003). A large database of graphs and its use for benchmarking graph isomorphism algorithms. Pattern Recognition Letters, 24(8), 1067–1079. https://doi.org/10.1016/S0167-8655(02)00253-2

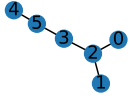
Subgraph Isomorphism based Quantum Circuit Layout[4]



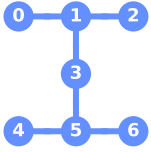
(a)



(b)



(c)



(d)

[5]Nation, P. D., & Treinish, M. (2023). Suppressing quantum circuit errors due to system variability. PRX Quantum, 4(1), 010327. https://doi.org/10.1103/PRXQuantum.4.010327

Subgraph Isomorphism based Quantum Circuit Layout[4]

```
import rustworkx as rx
# Build connectivity graph that models constraints of QPU
connectivity_graph = rx.generators.directed_heavy_hex_graph(9)
for index in connectivity_graph.node_indices():
    connectivity_graph[index] = {"rz", "sx", "x"}
for index in connectivity_graph.edge_indices():
    connectivity_graph.update_edge_by_index(index, {"cx"})
# Build interaction graph of circuit
interaction_graph = rx.PyDiGraph()
interaction_graph.add_nodes_from([set() for _ in range(dag.num_qubits)])
for node in dag.topological_sort():
    if len(node) == 2:
        if interaction_graph.has_edge(*node.qubits):
            interaction_graph.get_edge_data(*node.qubits).add(node.name)
        else:
            interaction_graph.add_edge(*node.qubits, {node.name,})
    else:
        interaction_graph[*node.qubits].add(node.name)
```

[5]Nation, P. D., & Treinish, M. (2023). Suppressing quantum circuit errors due to system variability. PRX Quantum, 4(1), 010327. https://doi.org/10.1103/PRXQuantum.4.010327

Subgraph Isomorphism based Quantum Circuit Layout[5]

```
def _target_match(a, b):
    return a.issuperset(b)
# Return an iterator of subgraphs mappings:
subgraphs = vf2_mapping(
    connectivity_graph,
    interaction_graph,
    node_matcher=_target_match,
    edge_matcher=_target_match,
    subgraph=True,
    id_order=False,
    induced=False,
)
best_layout = min(subgraphs, key=scoring_function)
```

Find best subgraph using VF2 with ordering heuristic from VF2++[4]

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[5] Nation, P. D., & Treinish, M. (2023). Suppressing quantum circuit errors due to system variability. PRX Quantum, 4(1), 010327. https://doi.org/10.1103/PRXQuantum.4.010327

[6] Jüttner, A., & Madarasi, P. (2018). VF2++—An improved subgraph isomorphism algorithm. Discrete Applied Mathematics, 242, 69-81. https://doi.org/10.1016/j.dam.2018.02.018

Uses Outside of Quantum Computing

- Rautila, O. S., Kaivola, K., Rautila, H., Hokkanen, L., Launes, J., Strandberg, T. E., . . . & Tienari, P. J. (2024). The shared ancestry between the C9orf72 hexanucleotide repeat expansion and intermediate-length alleles using haplotype sharing trees and HAPTK. The American Journal of Human Genetics, 111(2), 383-392. https://doi.org/10.1016/j.ajhg.2023.12.019
- Chen, R., Ding, Z., Zheng, S., Zhang, C., Leng, J., Liu, X., & Liang, Y. (2024, April). Magis: Memory optimization via coordinated graph transformation and scheduling for dnn. In Proceedings of the 29th ACM International Conference on Architectural Support for Programming Languages and Operating Systems, Volume 3 (pp. 607-621). https://doi.org/10.1145/3620666.3651330
- Tantos A, Kosmidis K. From Discourse Relations to Network Edges: A Network Theory Approach to Discourse Analysis. Applied Sciences. 2023; 13(12):6902. https://doi.org/10.3390/app13126902
- Caetano, J., Carriço, N., Figueira, J. R., & Covas, D. (2023). A novel methodology for pipe grouping and rehabilitation interventions scheduling in water distribution networks. Urban Water Journal, 20(7), 769–781. https://doi.org/10.1080/1573062X.2023.2209560
- Setiawan, T. H., Beltsazar, F., Aden, A., Gunawan, G., & Zarista, R. H. (2023). Graph coloring for determining courier frequency. Desimal: Jurnal Matematika, 6(3), 273 - 284.

Where to get more information

- These Slides: https://github.com/mtreinish/rustworkx-presentation
- Rustworkx Documentation: https://www.rustworkx.org
- Tutorial for NetworkX users: https://www.rustworkx.org/networkx.html
- Rustworkx on Github: https://github.com/Qiskit/rustworkx
- JOSS Paper: https://joss.theoj.org/papers/10.21105/joss.03968