Quantum-Inspired Graph Simulation of Contaminant Spread in Physical Networks

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**Abstract**

This project investigates the application of quantum-inspired optimization methods to simulate and mitigate the spread of contaminants across networked physical systems. Motivated by real-world challenges in environmental safety and public health, the study models contamination dynamics within graph-based representations of pipe networks, urban structures, or other physical infrastructures. Using toy graphs implemented via Python and networkx, the contaminant flow is simulated from source nodes, spreading through edges weighted by transmission probability or flow capacity. The intervention strategy is formulated as a Quadratic Unconstrained Binary Optimization (QUBO) problem, solved using D-Wave’s dimod library. The aim is to identify optimal configurations for containment or filtration node placement to reduce system-wide spread. Preliminary results compare baseline simulations against QUBO-optimized outcomes, offering visualizations of infection propagation and intervention effectiveness. This study explores the intersection of computational physics, graph theory, and quantum logic, contributing to interdisciplinary approaches in environmental modeling and optimization.

**Objective**

The core objective is to model and minimize the spread of a contaminant in a network using optimization techniques derived from quantum computing. The project aims to answer:

*How can QUBO models be applied to simulate and improve intervention strategies in physical networks prone to contamination?*

**Background**

The spread of harmful agents through physical infrastructure such as water pipelines or urban streets can be modeled as a diffusion process across graphs. Conventional simulations offer heuristic approaches, but recent developments in quantum computing—especially in combinatorial optimization—open pathways for more efficient and potentially more scalable intervention modeling.

**Methods**

1. Graph Construction

* Construct toy graphs (e.g., grids or small-world networks) using Python and network
* Nodes represent units of space (e.g., intersections, tanks)
* Edges represent flow paths with associated weights (distance, pressure, or transmission chance)

2. Contaminant Spread Simulation

* Simulate step-based contaminant diffusion from a source node
* At each timestep, affected nodes transmit to neighbors probabilistically
* Visualize the spread using matplotlib

3. QUBO Formulation

* Define binary decision variables per node (1 = intervention/filter placed)
* Formulate objective function to minimize total number of infected nodes after t steps, given a limited number of filters
* Solve the QUBO using dimod.ExactSolver() or simulated annealing

4. Evaluation

* Compare contamination spread with and without QUBO-optimized interventions
* Evaluate solution robustness across different graph structures and initial conditions

**Expected Results**

* A set of optimized intervention strategies (e.g., nodes where filters are placed)
* Visual side-by-side comparisons of spread maps before and after optimization
* Analysis of how graph structure influences QUBO solution effectiveness

**Significance**

This study applies accessible computational tools to simulate a physics-rooted process through the lens of quantum optimization. It provides insight into the applicability of QUBO models in environmental contexts and demonstrates how undergraduate-level research can intersect with frontier computation models. The framework is extensible to other network-based physical phenomena such as epidemic modeling, signal degradation, or heat transfer.