POLARISqb Demonstrates Menu Optimization via Constrained Quadratic Model on D-Wave Annealing Quantum Computer

POLARISqb has published a white paper that demonstrates quantum annealing-based optimization using a Constrained Quadratic Model, or CQM.

DURHAM, NC, USA, April 11, 2023 /EINPresswire.com/ -- The scientists at POLARISqb designed and engineered the first drug discovery engine built for an annealing quantum computer. This amplified search power allows the company to investigate a virtual chemical space of up to 10^23 molecules and to design a set of molecules that fit a particular binding pocket and have certain drug-like characteristicsThese drug-like characteristics include solubility, synthesizablity, binding pocket fit, etc., and these are the “multi-variables” of interest in the area of drug discovery. The company has published a white paper that demonstrates quantum annealing-based optimization using a Constrained Quadratic Model, or CQM. The CQM solves a multi-variable optimization problem that is designed for implementation on the D-Wave Advantage annealing quantum computer.

In order to make the topic more approachable to an audience that includes people outside of the field of chemistry, the team at POLARISqb used the example of a diner choosing a single meal from a complex menu at a Chicken and Waffles restaurant. With this scenario, the white paper demonstrates how to define a multi-variable menu by its mathematical options, formulate the optimization problem as a Constrained Quadratic Model, and submit it to the annealing quantum computer.

POLARISqb is one of the companies at the forefront of quantum combinatorial optimization,

which is accomplished using the Advantage quantum computing system from D-Wave Systems. The greatest strength of these annealing quantum computers is their ability to handle complex multi-variable optimization problems. In order to solve the menu problem, POLARISqb submitted their Constrained Quadratic Model to the annealing computer, which uses low-minima calculations to search for an objective that is subject to multiple equality and inequality constraints. This objective is handled on the D-Wave Advantage system through its Ocean™ SDK, which is where the team defines the CQM model and variables and sets the constraints and objectives for the process. The system is then able to return a solution defined by a diner's particular economic and dietary constraints in a fast and efficient method powered by the ability of annealing quantum computers to formulate optimization solutions. You can find the published whitepaper here, and if you are interested in trying the process yourself, download the source code at D-Wave's gitlab repository here and sign up for time on the Advantage system via the Leap™ quantum cloud service here.

This constraint optimization model running via the D-Wave annealing quantum computer holds great promise for addressing problems in fields like logistics and sustainability, as well as for the chemical optimization that POLARISqb does to accelerate drug research. The Tachyon drug design platform allows the chemists at POLARISqb to search enormous molecular libraries for targets that fit a particular protein and fulfill certain drug-defining properties that determine its effectiveness as a treatment. This platform is able to help drug developers target a better set of treatment molecules in a much shorter timeframe, enabling more efficient research into more conditions and potential treatments.

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