Quantum Computation for Machine Learning, AI, and Optimization

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PROCESS SYSTEMS ENGINEERING

Time scale

- Year
- Week
- Day
- Hour
- Min
- S
- Ms
- Ns
- Ps

Length scale

- Pm
- Nm
- Mm
- Mm
- Km

Supply chain/logistics optimization
(Gounaris, Grossmann)

Plant design, control and operations
(Biegler, Gounaris, Grossmann, Sahinidis, Ydstie)

Unit operations design
(Biegler)

Material design
(Gounaris)

Molecular design
(Sahinidis)

Unit operations design
(Biegler)

Supply chain/logistics optimization
(Gounaris, Grossmann)
GLOBAL MINLP OPTIMIZATION

\[
\begin{align*}
\text{min} & \quad f(x, y) \\
\text{s.t.} & \quad g(x, y) \leq 0 \\
& \quad x \in \mathbb{R}^n, \ y \in \mathbb{Z}^p
\end{align*}
\]

- Multimodal objective
- Nonconvex constraints
- Integrality conditions

NP-HARD PROBLEM
Comparisons based on solver ability to prove global optimality
\( \min f(y) \)

- Here, \( y \in \{0,1\}^n \) and \( f \) is a polynomial
  - Each binary variable is mapped into a quantum spin (qubit)
  - The objective defines many-body interaction between spins
  - Exponentially faster than classic algorithms
- When \( f \) is quadratic, we have a Quadratic Unconstrained Binary Optimization (QUBO) problem
  - Ising model
- Integer nonlinear optimization problems and decision-making problems can be cast into QUBOs
  - All of Karp’s 21 NP-complete problems
  - Quadratic assignment, set partitioning, ...
  - Unsupervised machine learning
  - Supervised machine learning
CHALLENGES IN HYBRID ALGORITHMS

• Cast integer nonlinear optimization problems into QUBO problems
  – Lucas (2014); Glover et al. (2019)
• Embed QUBO into quantum hardware
  – Nonconvex integer nonlinear optimization
• Solve QUBO
  – Is it possible to obtain exact solutions?
  – Approximate solutions still of value
  – Randomization
• Recover solutions
• Programming challenges
• Hardware issues such as error correction