Quantum Algorithms for Multiobjective Optimization

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Núcleo de Investigación y Desarrollo Tecnológico (NIDTEC)

- **Computational Optimization**
- **Applied Mathematics and Scientific Computation**
- **Bioinformatics**
- **Biomaterials**
- **Software Engineering**
- **Theoretical Computer Science**

Theoretical Computer Science Group at NIDTEC

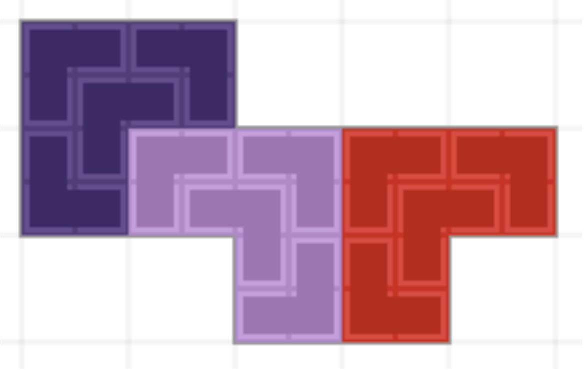
Professors
- **Eduardo Canale (UNA/Udelar)**
- **Marcos Villagra**

Doctor students
- **Cristhian Martínez (algebraic complexity)**
- **Pedro Villagra (algebraic complexity)**

Master students
- **Marcos Ibarra (quantum computing)**
- **Fabricio Mendoza (espectral algorithms)**
- **Sergio Mercado (espectral algorithms)**

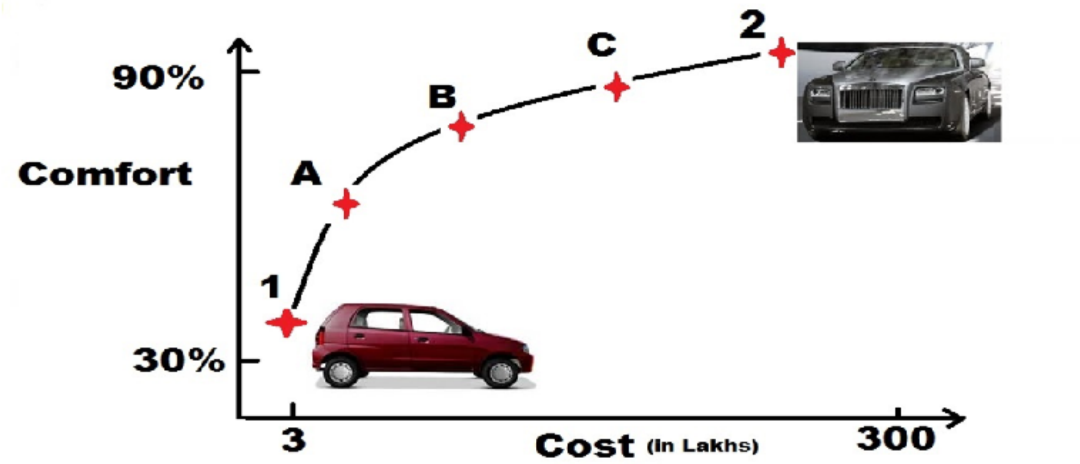
Undergrad students
- **Tadashi Akagi (tilings and graph theory)**

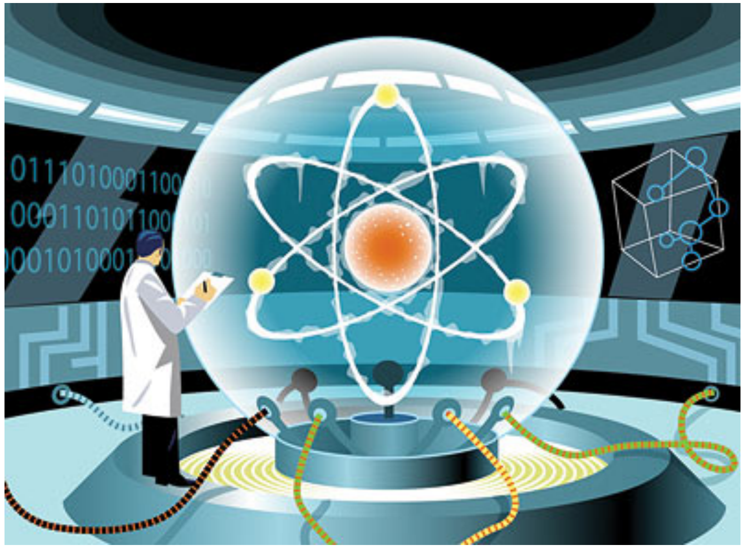
Research
- **Algorithms**
- **Graph theory**
- **Computational Complexity**
- **Quantum computing**



This talk is about…

How to solve Multiobjective Optimization Problems
using a Quantum Computer





Why?

In the early days it was very difficult to design quantum algorithms for optimization problems for most quantum computing models.

There were, however, papers with empirical results, like

- Crhistoph Dürr, Peter Høyer. **A quantum algorithm for finding the minimum**.
  arXiv:quant-ph/9607014 (1999)
- Baritompa et al. **Grover's quantum algorithm applied to global optimization.**
  SIAM Journal on Optimization 15(4), 2005.

Quantum adiabatic computing [Farhi et al. 2000], however, is made for optmization problems.

Why? (cont'd)

More recently,

1- A. Harrow, A. Hassidim, S. Lloyd. **Quantum algorithm for solving linear systems of equations.** arXiv:0811.3171.

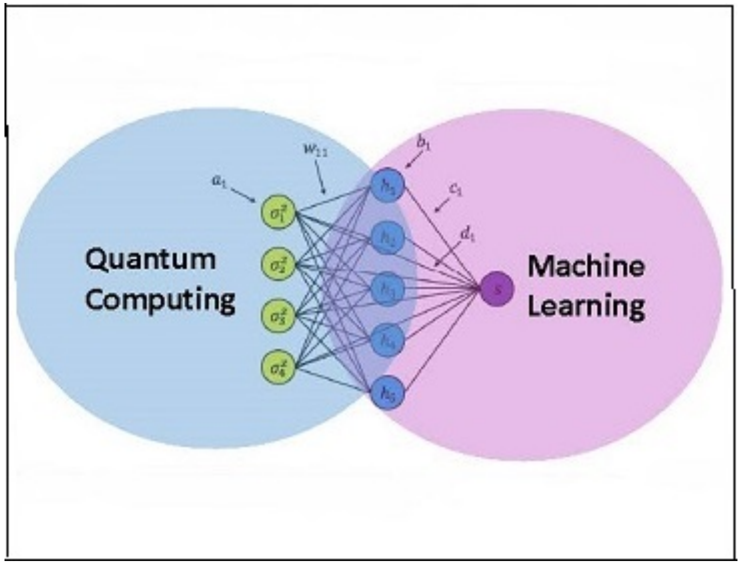
2- F. Brandao, K. Svore. **Quantum speed-ups for semidefinite programming.** arXiv:1609.05537.

3- I. Kerenidis, A. Prakash. **A quantum interior point method for LPs and DSPs.** arXiv:1808.09266

Quantum Optimization

Applications in:

1- Big data.
2- Artificial Intelligence
3- Machine Learning
4- Engineering



Anything that needs to be optimized!

But what about **Multiobjective Optimization Problems**?

Outline

- Multiobjective Combinatorial Optimization
- Empirical results using an adaptive strategy
- Theoretical results using quantum adiabatic computing
- Concluding remarks and open problems

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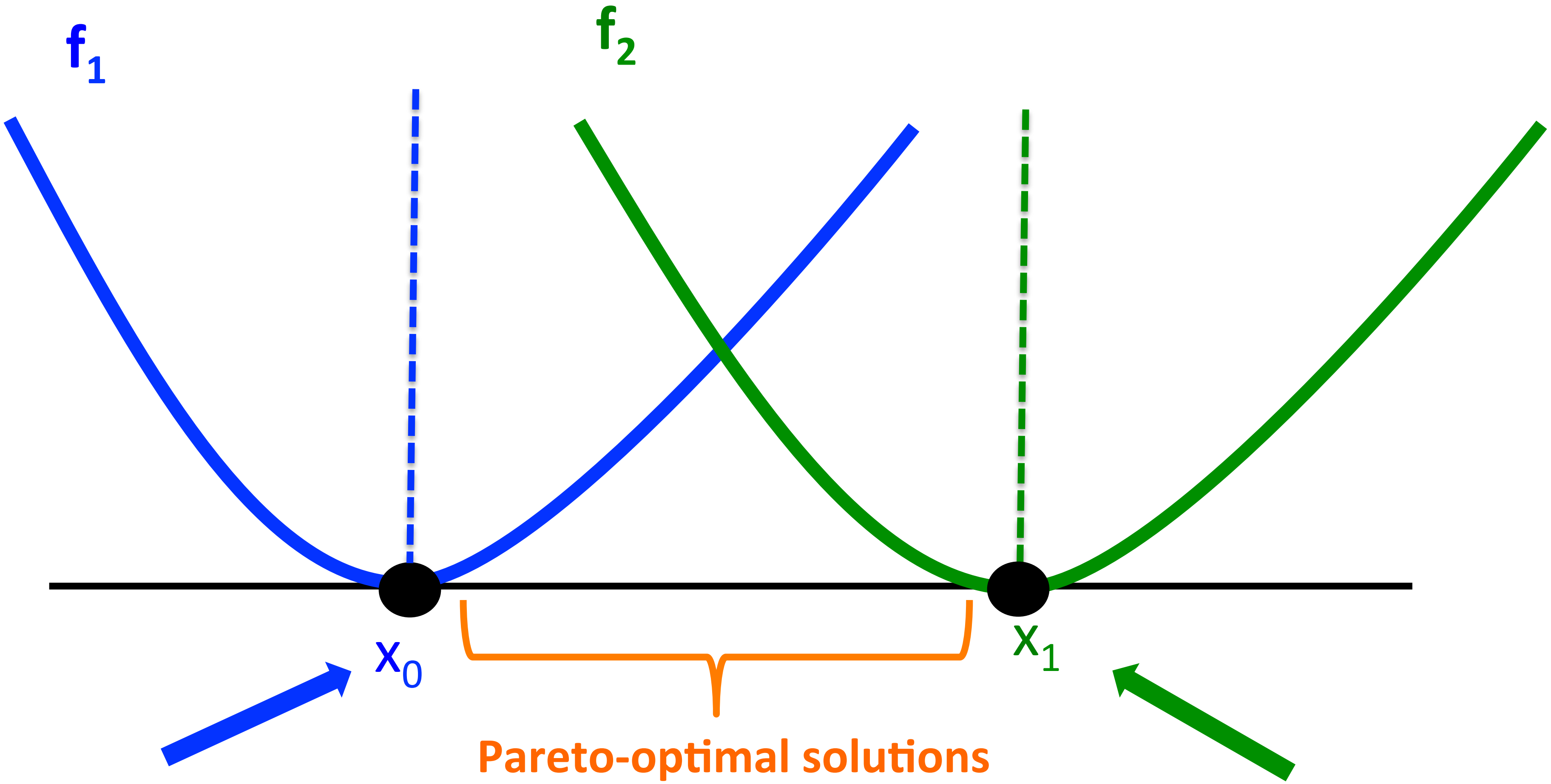
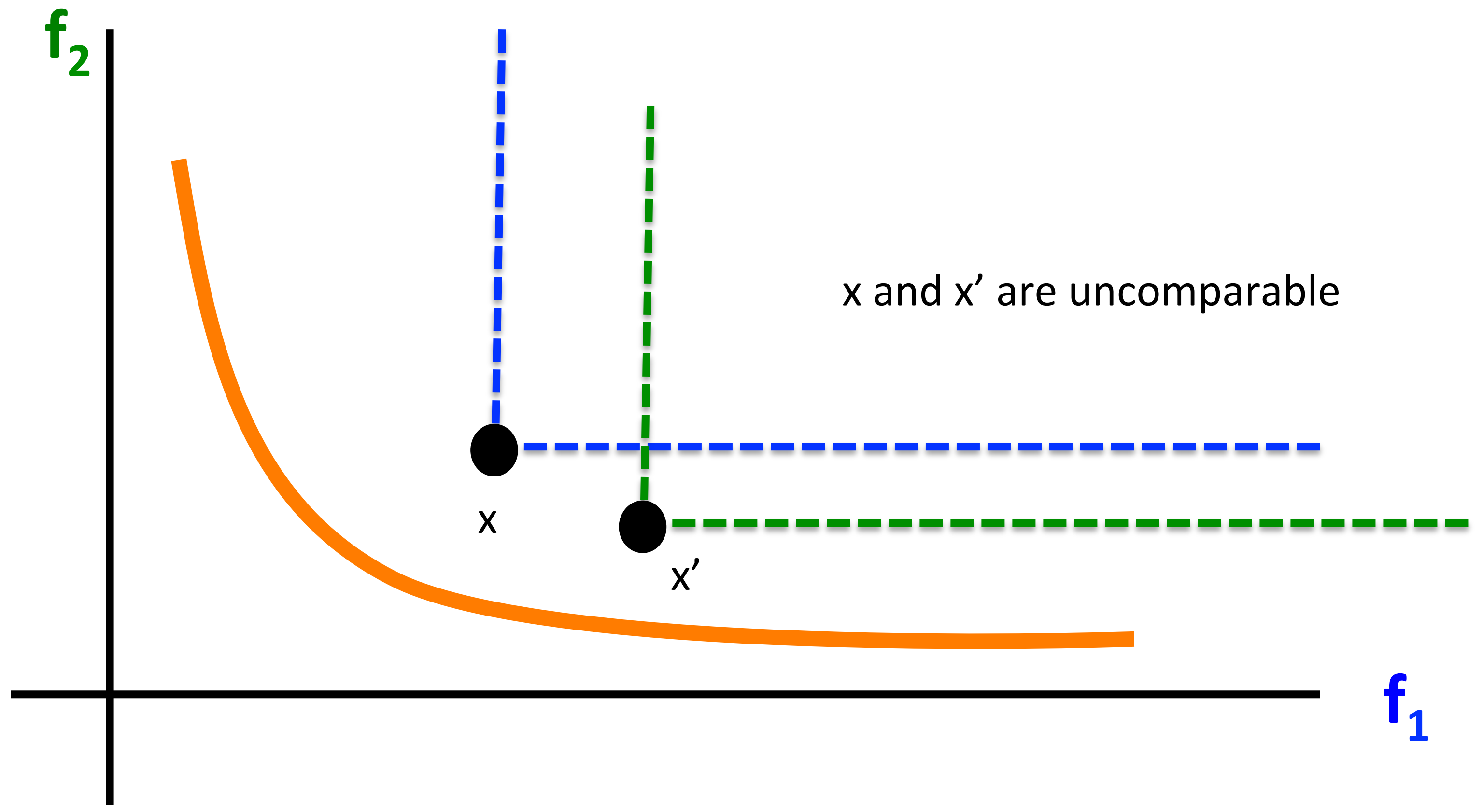
Multiobjective Optimization



Optimal solution of f_1

Optimal solution of f_2

Multiobjective Optimization (cont'd)



x and x' are uncomparable

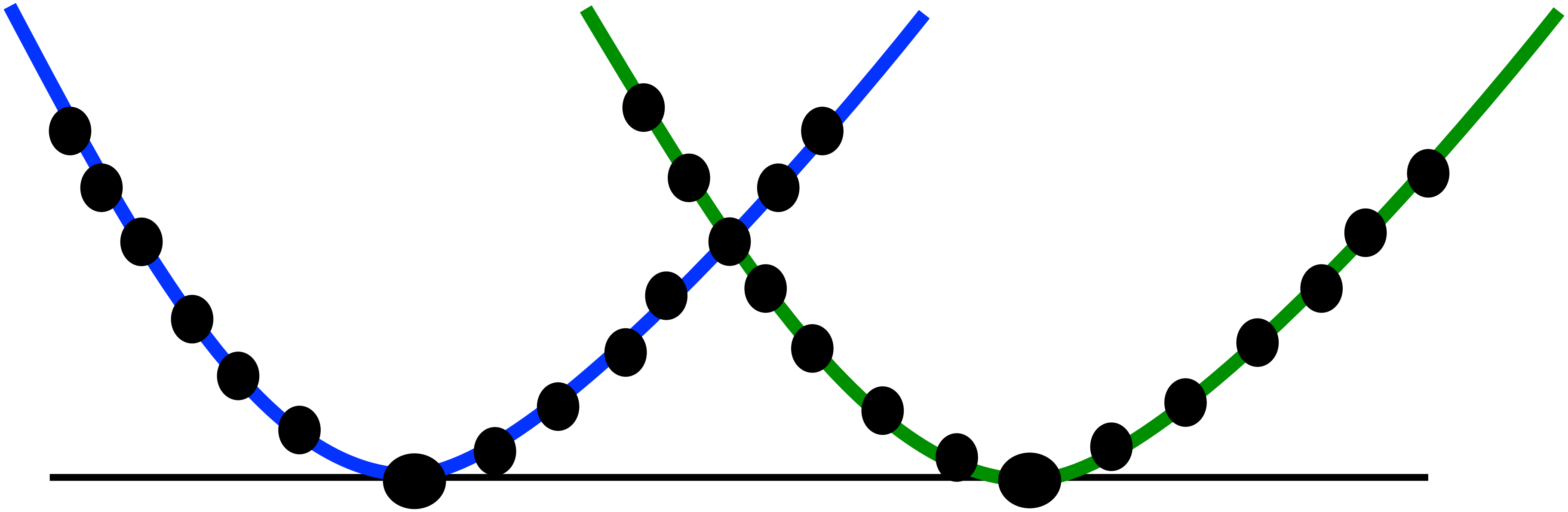
Given solutions x and y

$x \prec y$ iff $f_1(x) \leq f_1(y)$ and $f_2(x) \leq f_2(y)$

The set of Pareto-optimal solutions is the set of minimal points.

Multiobjective Combinatorial Optimization or MCO

The domain of each objective function is finite.



Both objective functions above take values only on a finite number of points.

Multiobjective Combinatorial Optimization or MCO (cont'd)

An MCO with **d objectives**

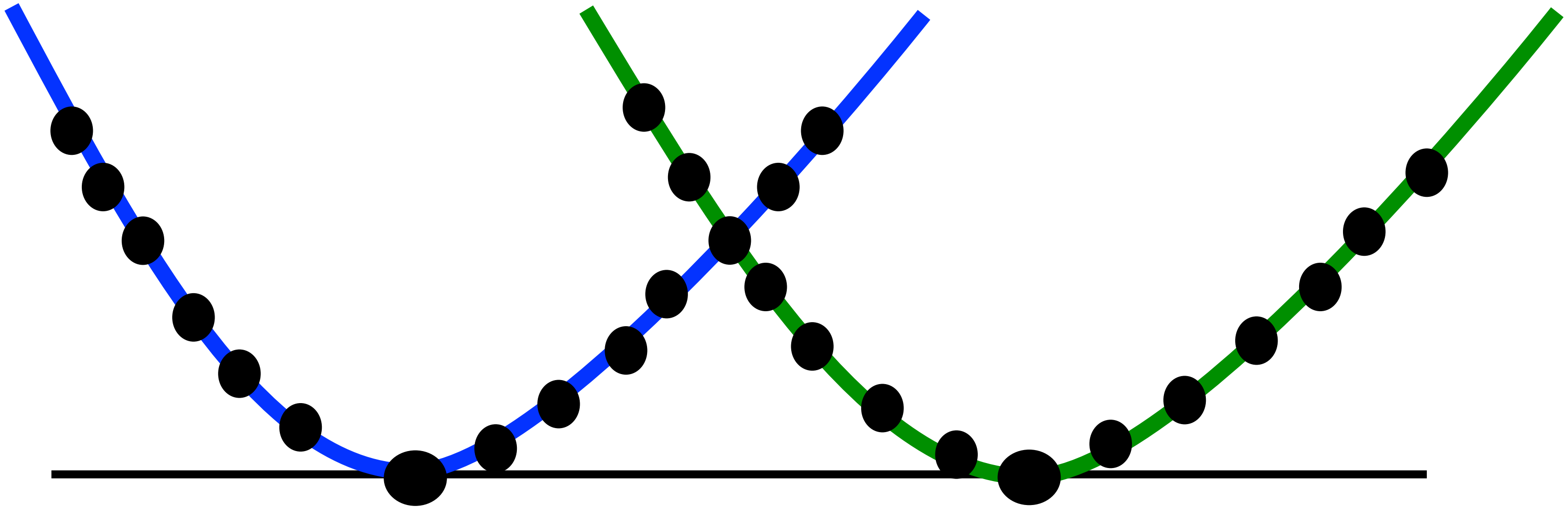
Objective function $f(x) = (f_1(x), \cdots, f_d(x))$

Problem: Find a non-trivial Pareto-optimal solution

The optimal solution of each f_i is a trivial Pareto-optimal solution

Each trivial solution can be found by optimizing each objective individually!

Multiobjective Combinatorial Optimization or MCO (cont'd)



Some definitions

Equivalent solutions: *x* and *y* are equivalent *iff* $(f_1(x),\ldots.,f_d(x)) = (f_1(y),\ldots..,f_d(y))$

Collision-free MCO: for each f_i and each pair of solutions *x* and *y*, it holds that
$| f_i(x) - f_i(y) | > \lambda$ for some positive real λ.

Linearization of an MCO

Given an **objective function** $f(x) = (f_1(x), \cdots, f_d(x))$

A **linearization** of f is a linear combination between each f_i such that

$$\langle f(x), w \rangle = w_1 f_1(x) + \cdots + w_d f_d(x)$$

where $w_1 + \ldots\ldots + w_d = 1$ and each $w_i \in [0,1]$.

Lemma. For each *w* there exists *x* such that *x* is Pareto-optimal and ⟨*w,f(x)*⟩ is minimum.

A solution *x* is a **supported solution** if *x* is a **minimum of ⟨*w,f(x)*⟩** for some *w*;

otherwise, *x* is **non-supported**.

Classical Methods for Multiobjective Optimization

1- Heuristics

- Designed for a specific problem.
- Greedy algorithms, local optimizers, etc.

2- Metaheuristics

- Problem-independent.
- Evolutionary algorithms, ant colony optimization, etc.

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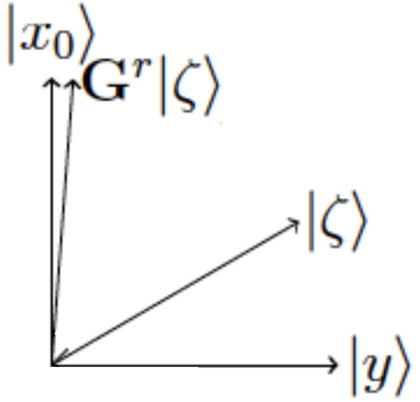
Grover’s Search Algorithm

Grover’s algorithm finds K marked items out of a set of N items in time $O\left(\sqrt{N/K}\right)$

Geometrically, this corresponds to a rotation



r is the number of times the Grover operator G is used.

Grover's Adaptive Search (GAS)*

$$\text{Let } O_y(x) = \begin{cases} 1 & \text{If } f(x)<y \\ 0 & \text{otherwise} \end{cases}$$

```
1. Randomly select a threshold y.
2. For r=1,2,3,….
    i.  Grover search with r rotations with oracle $O_y$.
    ii. If a solution is found, update threshold y.
```

Dürr and Høyer's heuristic for the selecting the rotation number

Let $[k]=\{0,1,\ldots,k-1\}$

```
1. Let k=1.
2. Repeat
    i.   Randomly choose $r_k$ from [k].
    ii.  Grover search with $r_k$ rotations.
    iii. If a solution is found, update threshold y
         and set k=1.
    iv.  Else, let $k=\min\{\lambda k,\sqrt{N}\}$.
```

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* Baritompa, Bulger, Wood. Grover's quantum algorithm applied to global optimization. SIAM Journal on Optimization 15(4):1170-1184, 2005.

Multiobjective Grover Adaptive Search (MOGAS)

GAS with Dürr and Høyer's can be naturally extended to multiobjective problems.

We studied two types of oracles:

$$h_1(x)=\begin{cases}1 & \text{If } x \text{ dominates } y\\ 0 & \text{otherwise}\end{cases}$$

$$h_2(x)=\begin{cases}1 & \text{If } x \text{ dominates or is uncomparable to } y\\ 0 & \text{otherwise}\end{cases}$$

Remember a current known set of non-dominated solutions Y

Initial Results

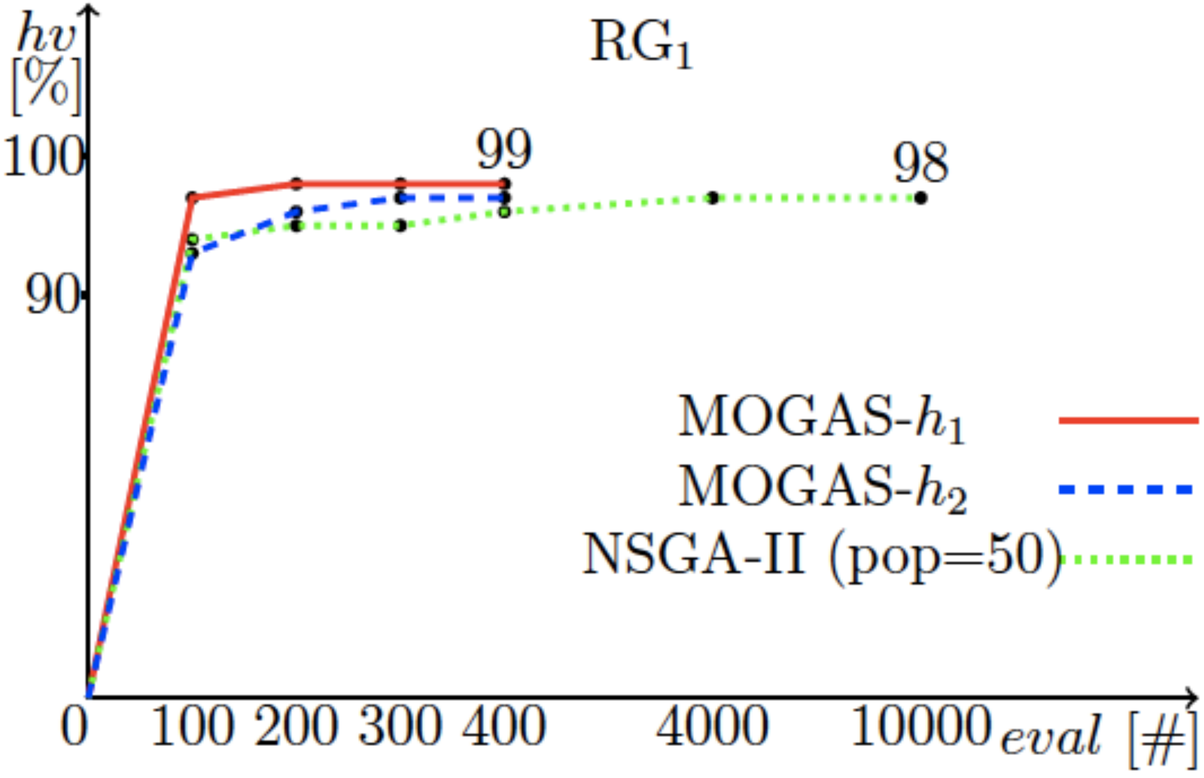
- We compared MOGAS against NSGA-II.
- Run tests on structured instances and random instances of bi-objective problems.
- We computed the hypervolume and the number of objective functions evaluations.

is a measure of how close the set of non-dominated solutions are to the real set of Pareto-optimal solutions.

All tests run with 10 qubits.

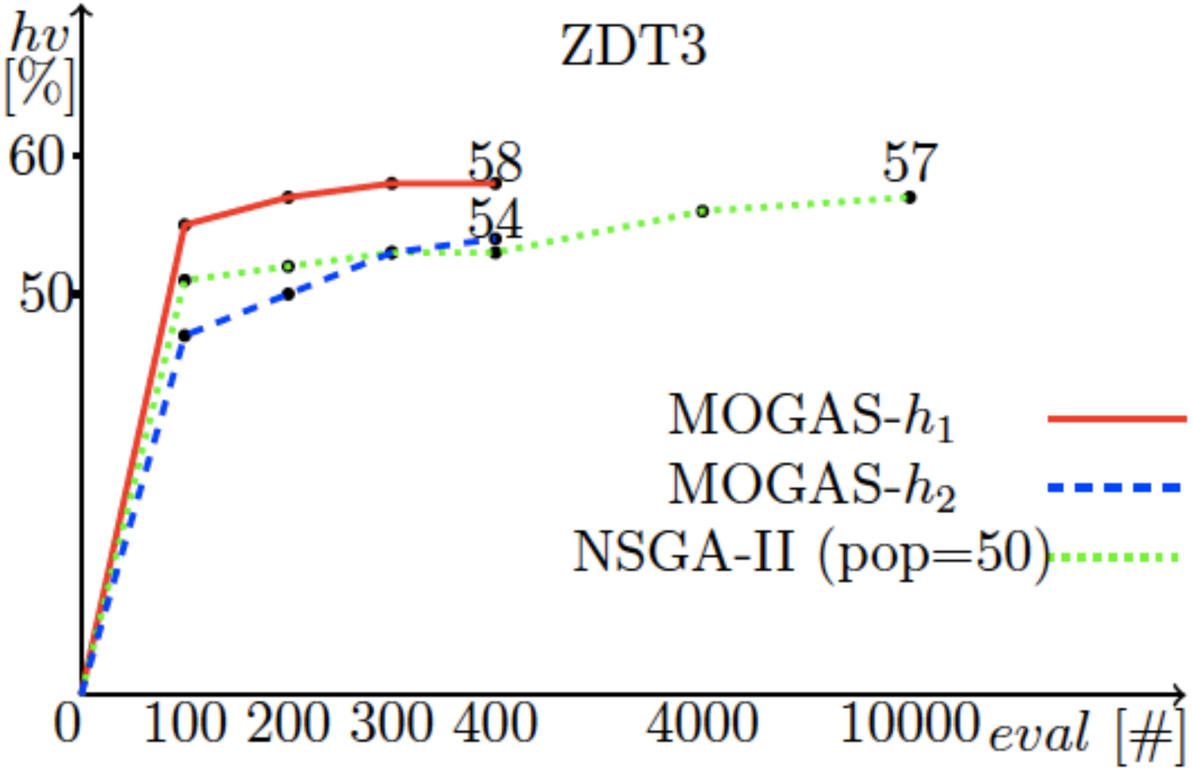
Initial Results (cont'd)

Random Instance



Initial Results (cont'd)

Structured Instance



Work to be done

- Increase the number of qubits.
- Test more types of oracles.
- Try more heuristics.
- Prove convergence.

Results in *Proceedings of FedCSIS 2017 – 10th Workshop on Computational Optimization*

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Eigenstates and Energies

Schrodinger's equation

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \boxed{H(t)}\ \psi(t)\rangle$$

Hamiltonian (Hermitian matrix)

Eigenvectors (eigenstates) $|\psi_j\rangle$

Eigenvalues (energies) E_j

Ground state: eigenstate with lowest energy.

Optimization with Hamiltonians

Given an objective function f(x)

$$H = \begin{bmatrix} f(x_1) & & & & \\ & \cdot & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & f(x_n) \end{bmatrix}$$

$|x\rangle$ are eigenstates

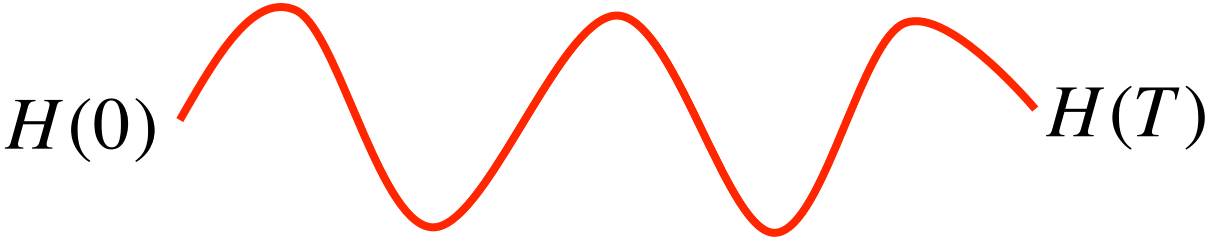
$f(x)$ are eigenvalues

Problem: find a minimal eigenstate.

Adiabatic Evolution

$$i\hbar\frac{d|\psi(t)\rangle}{dt} = H(t)|\psi(t)\rangle$$

Adiabatic Theorem: [Born and Fock 1928]



Start in $|\psi(0)\rangle$ ground state of $H(0)$

Finisht at $|\psi(T)\rangle$ ground state of $H(T)$

$T >> \frac{1}{\min_t \{\gamma(t)\}^2}$ where $\gamma(t) = E_1(t) - E_0(t)$ **eigenvalue gap**

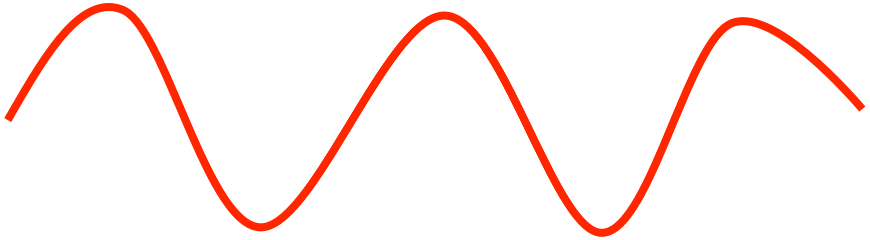
The Quantum Adiabatic Algorithm

1. Construct a Hamiltonian H_1 encoding the optimization problem.
2. Construct a Hamiltonian H_0 with known ground state.
3. With adiabatic evolution, slowly change H_0 into H_1.

$$H(s) = (1 - s)H_0 + sH_1$$

4. Measure the results.

$$H(0) = H_0$$



$$H(T) = H_1$$

Quantum Annealers

1. Implementations of the quantum adiabatic paradigm, but they are only good for optimization problems.
2. Some companies claim they have 1000 qubits quantum annealers.
3. They are promising 2000 qubits by this year!

This being true or not, it is still and interesting model of computation.

Main Contribution of this Work

Theorem.

Given any MCO that is **collision-free**. If there are **no equivalent solutions**, then there exists a linearization such that the quantum adiabatic algorithm can find a Pareto-optimal solution in finite time.

If the linearization is chosen appropriately, then the algorithm can find all supported solutions.

Two structural properties of MCOs are required:

(1) Collision-freeness
(2) Absence of equivalent solutions

} Otherwise we cannot guarantee convergence in finite time

Main Contribution of this Work (cont'd)

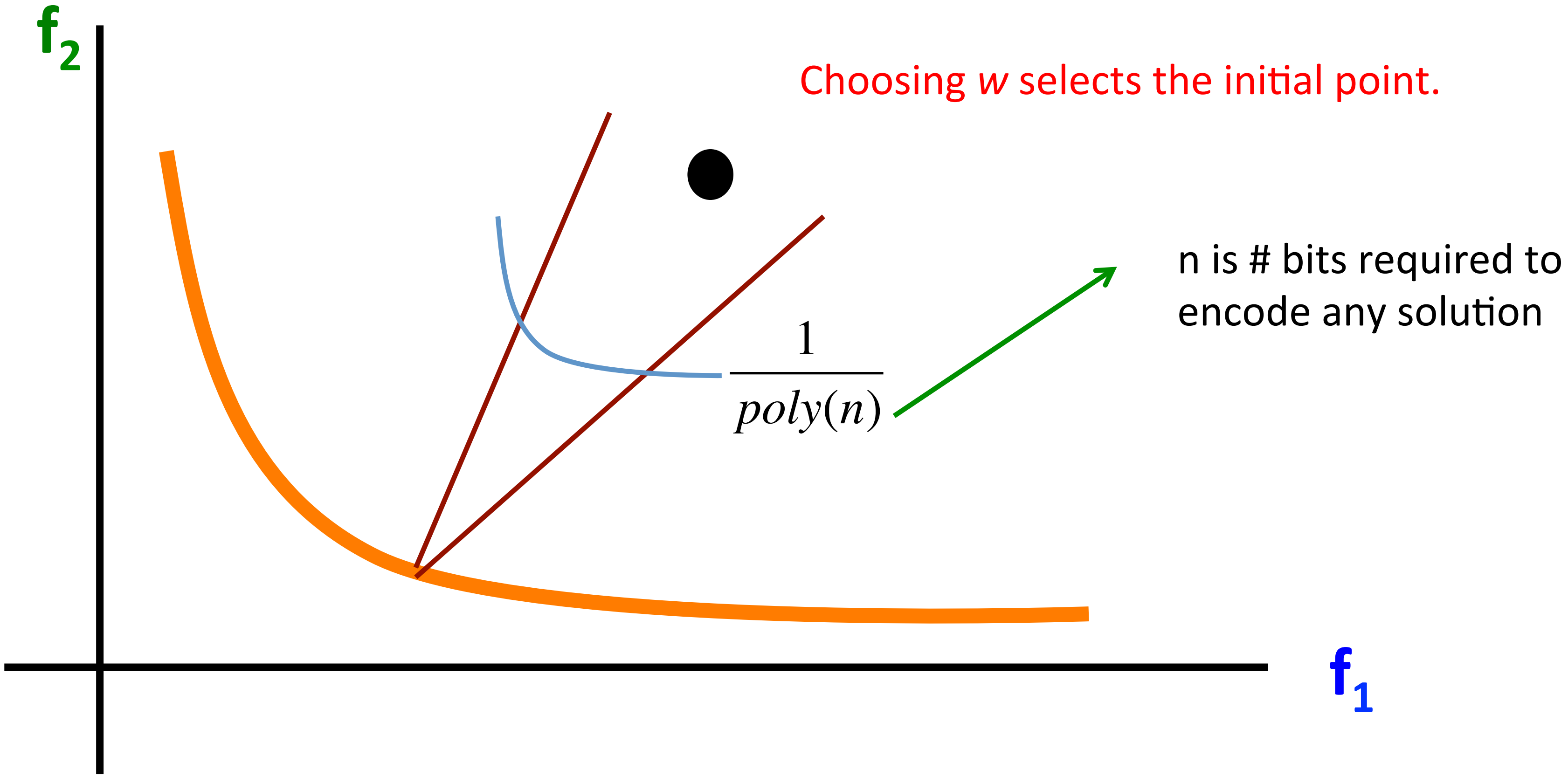
The proof relies on understanding the eigenvalues of the final Hamiltonian H_1 encoding a linearization of an MCO.

The Hamiltonian of an MCO is $$H_1 = w_1 H_{f_1} + \cdots + w_d H_{f_d}$$

where each H_{f_i} encodes objective function f_i .

Main Contribution of this Work (cont'd)

Final Hamiltonian $H_1 = w_1 H_{f_1} + \cdots + w_d H_{f_d}$



Choosing *w* selects the initial point.

n is # bits required to encode any solution

Main Contribution of this Work (cont'd)

The proof relies on understanding the eigenvalues of the final Hamiltonian H_1 encoding a linearization of an MCO.

The Hamiltonian of an MCO is $$H_1 = w_1 H_{f_1} + \cdots + w_d H_{f_d}$$

where each H_{f_i} encodes objective function f_i .

The linearization that is chosen must give a **nondegenerate ground state**.

a unique minimum energy

If the ground state is degenerate, then we can always chose another linearization.

In both cases, we always obtain the same Pareto-optimal solution.

Main Contribution of this Work (cont'd)

It suffices to prove that the final Hamiltonian H_1 has a non-degenerate ground-state.

$$H_1 = w_1 H_{f_1} + \cdots + w_d H_{f_d}$$

The initial Hamiltonian H_0 is already chosen with a non-degenerate ground-state.

If the total Hamiltonian is non-degenerate, we cannot use the quantum adiabatic theorem.

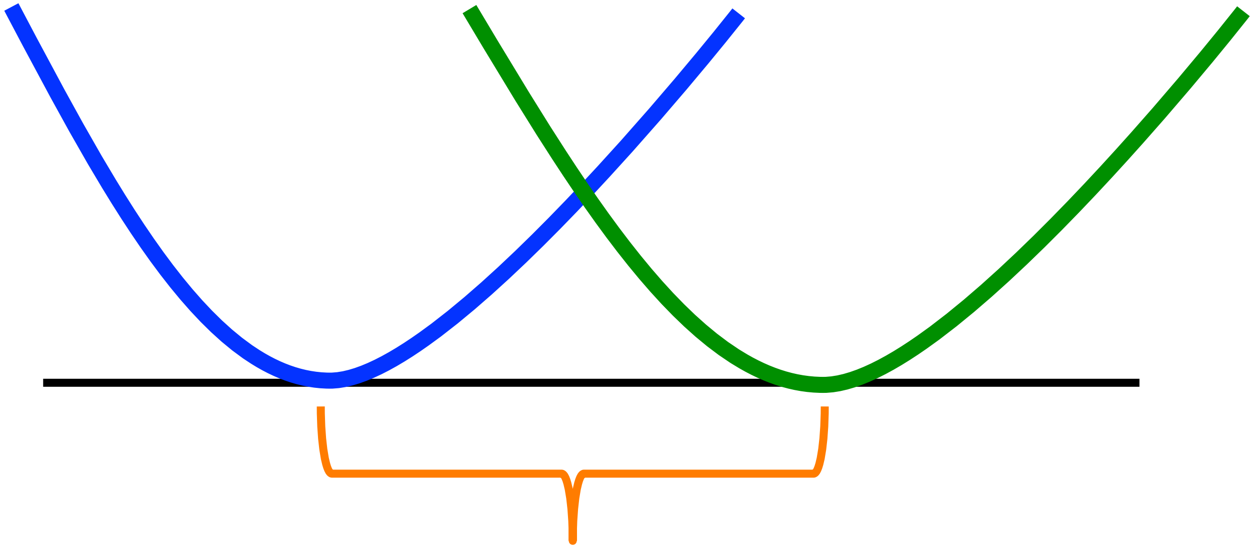
We rely on the **quantum adiabatic theorem of Ambainis and Regev** [arXiv:quant-ph/0411152]

Approx. factor

$$T \geq \frac{10^5}{\delta^2} \max\left\{ \frac{\|H'\|^3}{\lambda^4}, \frac{\|H'\| \cdot \|H''\|}{\lambda^3} \right\}$$

Eigenvalue gap

Eigenvalue Gap of the Two-Parabolas Problem



Pareto-optimal solutions

$$H_w(s) = (1-s)H_0 + sH_1$$

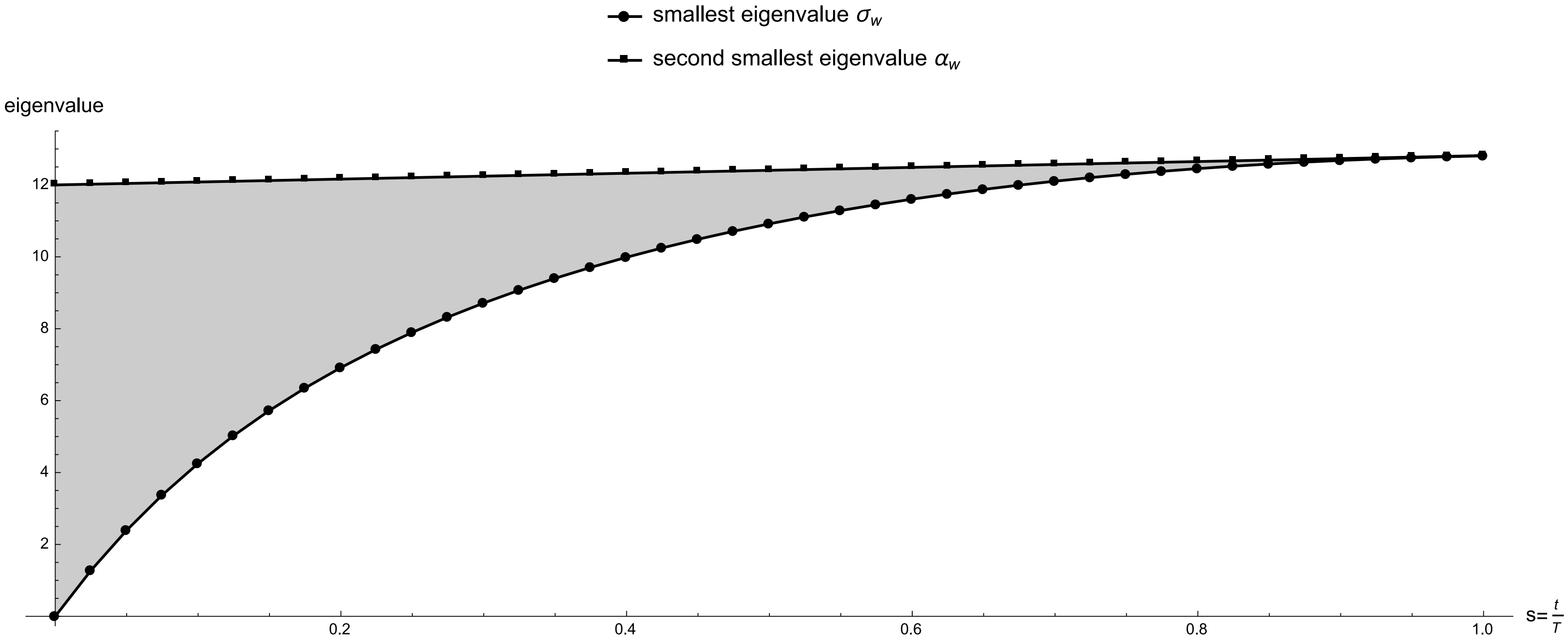
$$T >> \frac{1}{\min_t \{\gamma(t)\}^2} \quad \text{where} \quad \gamma(t) = E_1(t) - E_0(t)$$

eigenvalue gap

Eigenvalue Gap of the Two-Parabolas Problem (cont'd)

Numerical experiments with 7 qubits.

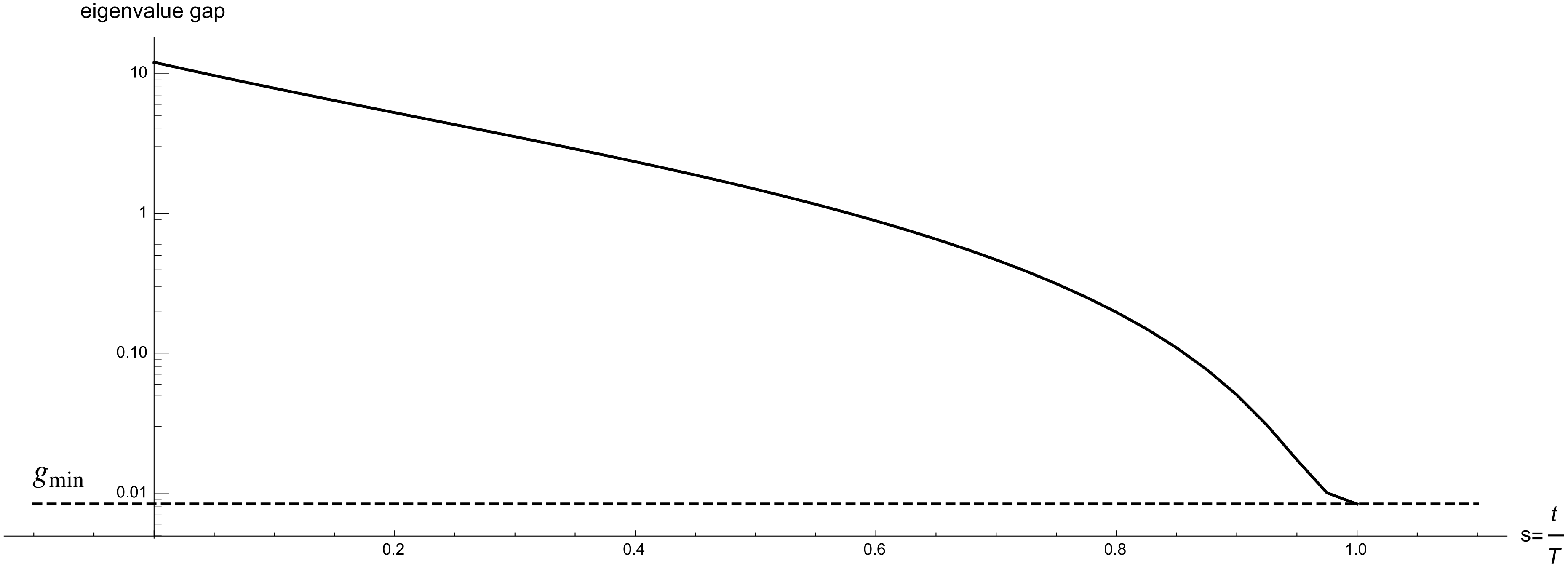
Eigenvalue Gap



Eigenvalue Gap of the Two-Parabolas Problem (cont'd)

Numerical experiments with 7 qubits.

Logplot of the Eigenvalue Gap



Open Problems

◆ New adiabatic algorithm capable of finding **ALL** Pareto-optimal solutions.

◆ Mechanism for dealing with equivalent solutions.

◆ Construct an explicit natural MCO instance with polynomial-time convergence.

Please check the full-version at **arXiv:1605.03152**

for a list of open problems

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- Theoretical results using quantum adiabatic computing
- Concluding remarks

Concluding Remarks

1. We showed initial empiricial results that suggests an "advantage" of an adaptive strategy. However, more test with more qubits are necessary.

2. We showed that the adiabatic algorithms can be used to solve MCOs. In that case, we identified two structural properties that any MCO must fulfill:

   a) collision-freeness, and
   b) no equivalent solutions.

3. First quantum algorithm for multiobjective optimization. It can be implemented in "real-world" quantum annealers.

Thanks for your attention!