TFM updates

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Summary of next steps proposed by Juanjo to proceed with the TFM:

1. **Angle restriction**: Restrict angles γ to prevent exceeding 2π in the unitary $e^{i\gamma H_P}$. Use only the standard QAOA approach.
2. **Explore linear Hamiltonian**: Explore QAOA trajectories when initializing the system from a middle-spectrum eigenstate of H_M (Alan's proposal).

1 Angle restriction

The spectrum of the Hamiltonian H_P has been taken into account in order to restrict the γ angles when using bounded optimizers. Moreover, smaller initial angles have been selected to "force" adiabatic-like trajectories.

With this, I noticed the following improvements:

- Much faster optimization speeds –allowing executions for higher number of layers– and monotonically cost decreasing with the number of QAOA layers (Fig. 1).

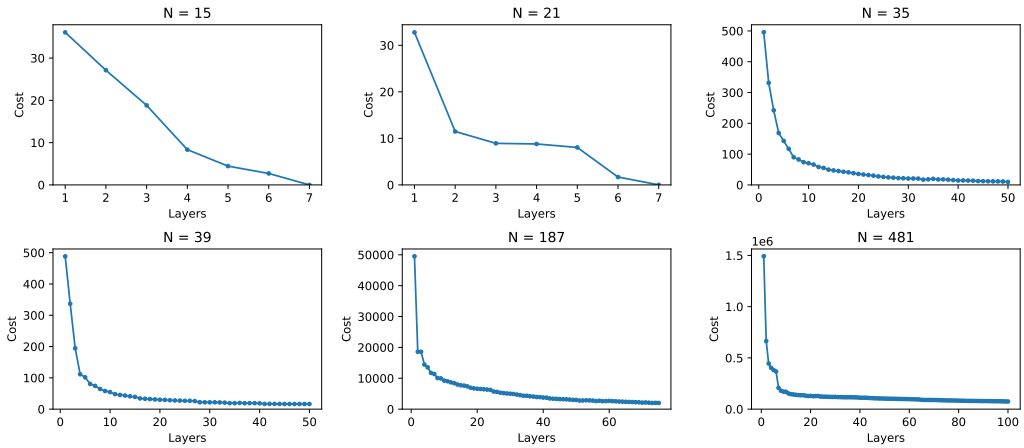

Figure 1: Cost vs layers for different numbers. Notice the monotonically cost decreasing as the number of layers increases. Optimizer: L-BFGS-B.

- Now angles evolve almost monotonically: γ increases and β decreases, similarly to adiabatic protocols. (Fig. 2). I am not sure if the evolution should be even smoother.

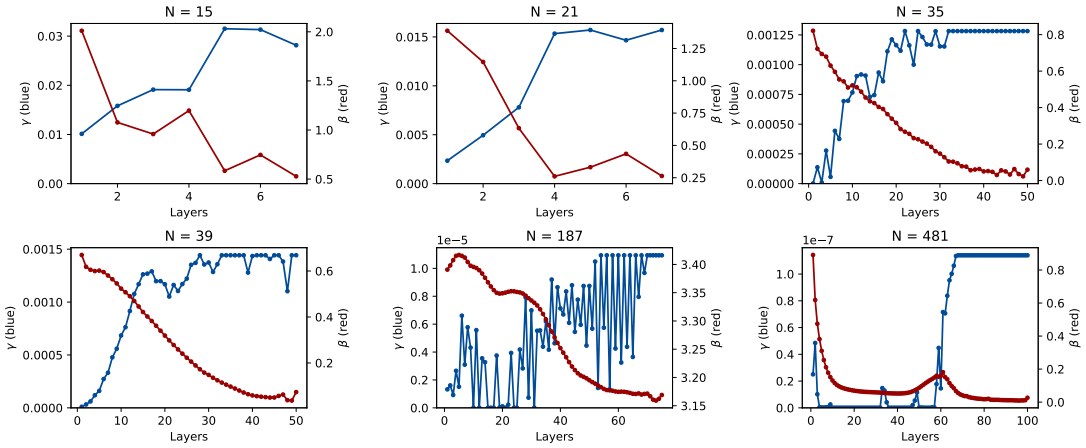

Figure 2: Angle evolutions for different N. Similarly to adiabatic protocols, the transverse field evolves from maximum to zero, while the interaction field does the opposite. Optimizer: L-BFGS-B.

- The probability vs energies plots look better than before (Fig. 3).

Additionally, I found interesting to plot cost vs solution's fidelity for the different target biprimes (Fig. 4).

1.1 Comparing with an unbounded method (BFGS)

I have been wondering why in the past we got perfect solutions even we didn't restrict the angles as explained at the beginning of this document. For example, BFGS is an unbounded optimizer, we cannot restrict the angles in the desired intervals. In fact, looking at Fig. 5, we observe better results for BFGS than for the bounded L-BFGS-B.

In Fig. 6, the evolution of the cost in our protocol for both optimizers is shown. It is interesting to see that, in some cases, even not being monotonically decreasing, BFGS finds the best solution much before than L-BFGS-B. The angles γ and β don't behave as in the adiabatic protocol anymore, but it seems like it finds shorcuts to adiabaticity. It is not a general behavior, and it is quite dependent on initial conditions, but I frequently found it for small numbers.

I think that's the explanation why we didn't notice that our old general algorithm was not adequate.

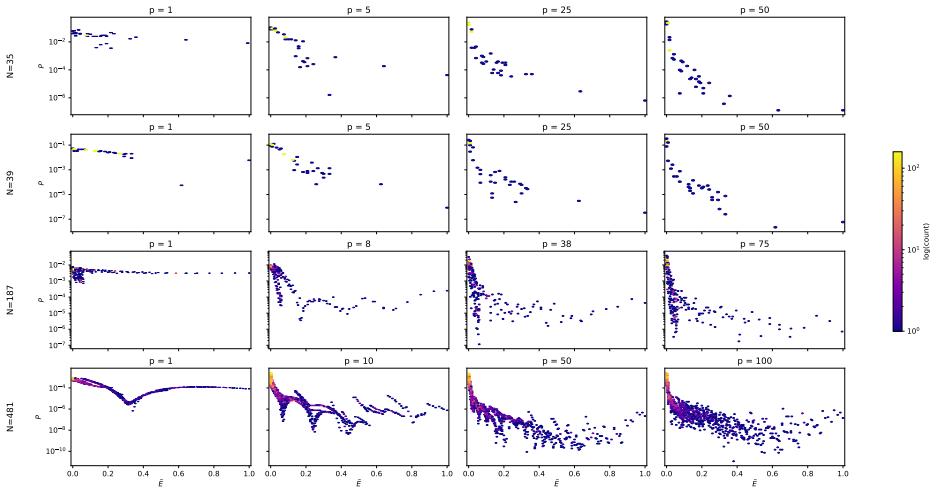

Figure 3: Density plots (probability vs rescaled energy) for some number of layers. Optimizer: L-BFGS-B.

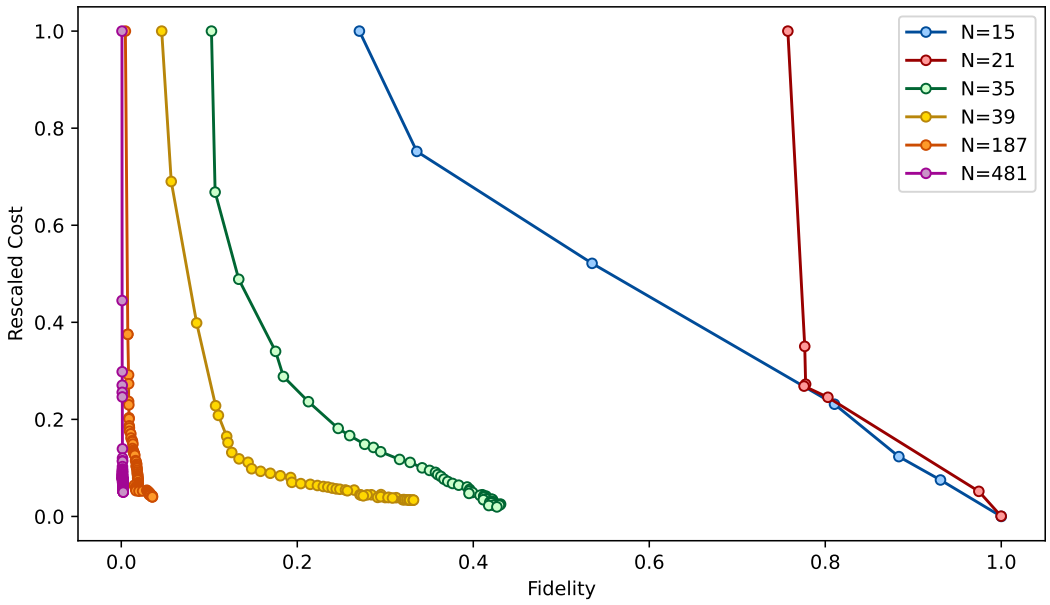

Figure 4: Correlations between cost and fidelity with respect to the solution. Fidelity improvement becomes much more expensive for bigger problems. For $N = 481$, the initial reduction of the cost function leads to only a tiny improvement in terms of fidelity. Optimizer: L-BFGS-B.

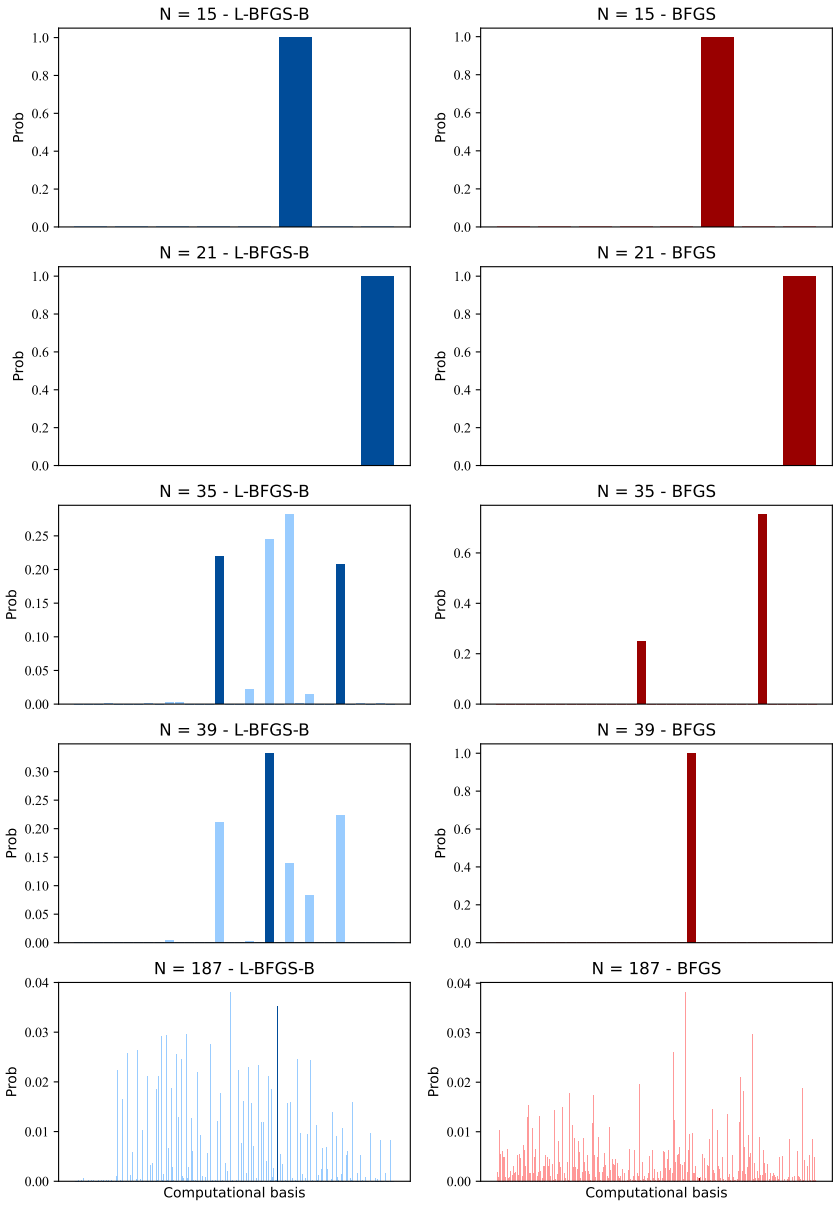

Figure 5: Populations at the end of our algorithm. In the left, L-BFGS-B (bounded) optimizer has been used. In the right, BFGS (unbounded) has been used.

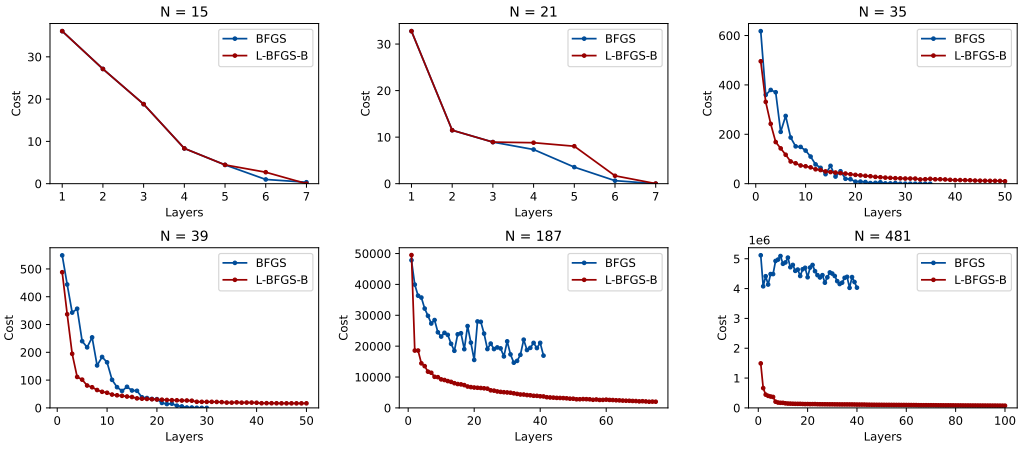

Figure 6: Cost evolution with number of layers for BFGS (unbounded) and L-BFGS-B (bounded).