# Optimality conditions for spatial search with multiple marked vertices

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## 1. Introduction

In quantum computing, a popular method for solving the spatial search problem is to use Quantum Walk (QW). Here, we restrict ourselves to discrete time QW on a grid (which is a popular topic as well). A Quantum Walk on a grid can be defined by the following state

$$|\psi\rangle = \sum_{v\in\{0,1\}} \sum_{x=0}^{\sqrt{N-1}} \sum_{y=0}^{\sqrt{N-1}} \alpha_{v,x,y} |v, x, y\rangle ,$$

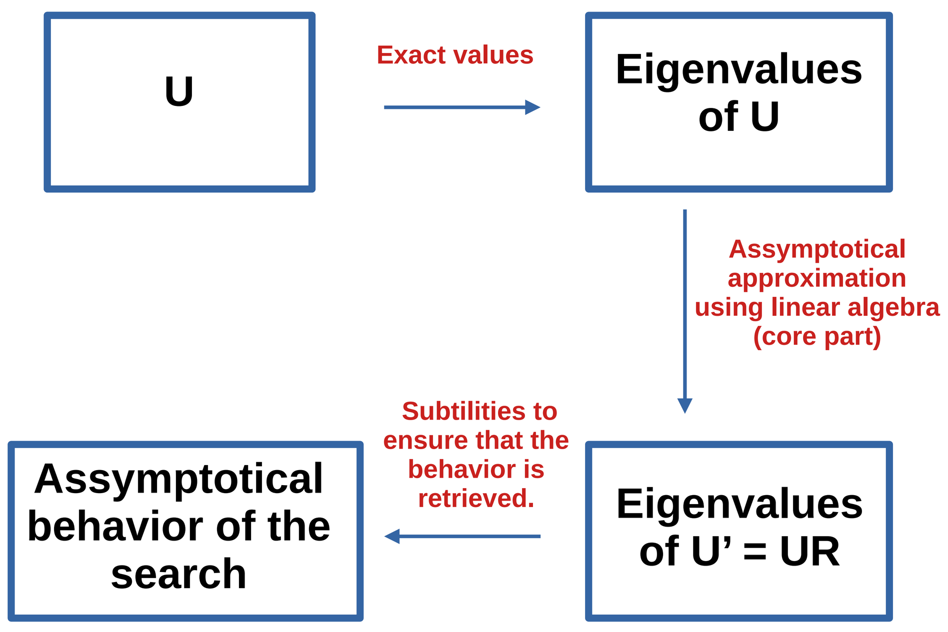
and a local operator $U$. In order to search for a set of $\mathcal{M}$ marked vertices, we apply an oracle $R = \mathbb{1} - 2\sum_{m\in\mathcal{M}} |d, m\rangle \langle d, m|$ at each steps, where $|d\rangle$ is the diagonal state in the coin state space. The final operator of the walk is

$$U' = UR.$$

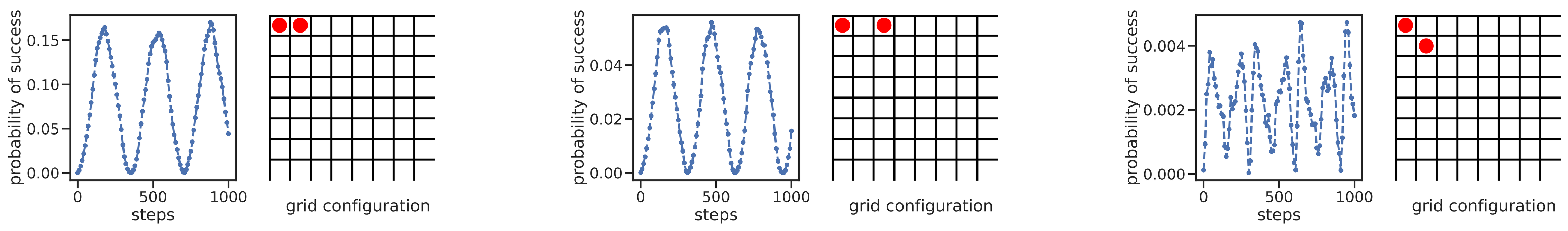
Nahimovs and Rivosh [1] showed that some configurations can impede the searching.

## 2. Analytical method

We derive the asymptotical complexity for configurations of two marked vertices using Bezerra et al's [2] method. This method can be summarized as such




## 3. Example of optimal and non-optimal configurations



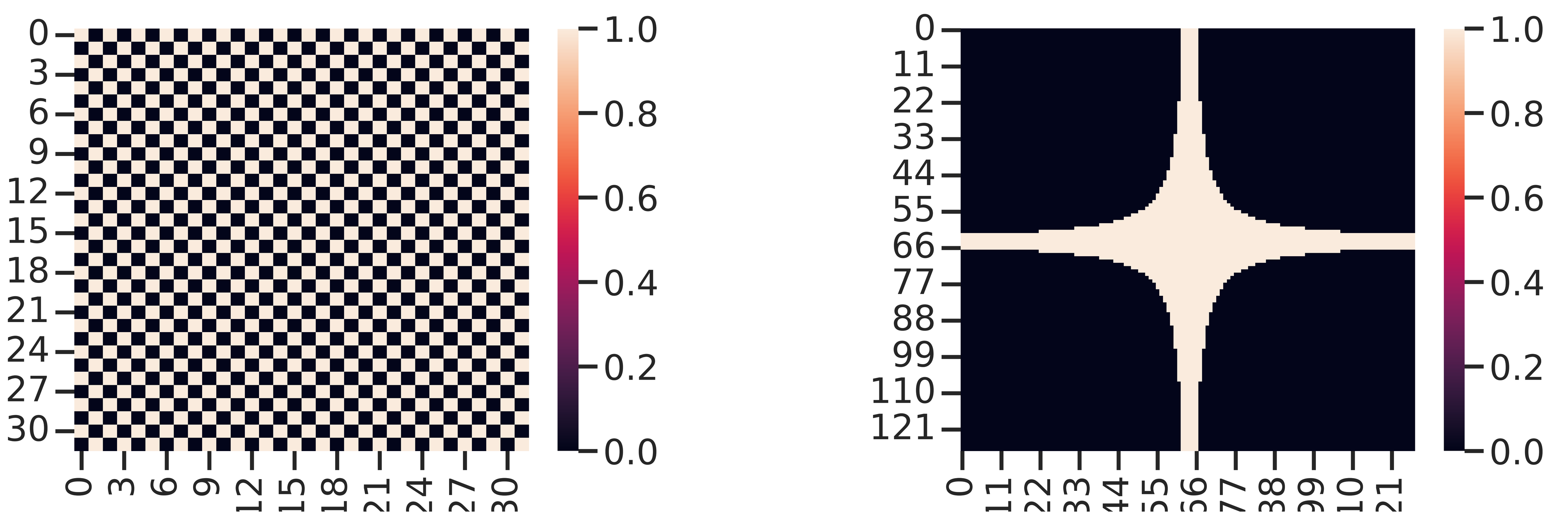

1(a) **Case 1:** Optimal configuration. $O\left(\sqrt{N}\ln^{\gamma} N\right)$

1(b) **Case 2:** Optimal configuration but the hitting time and probability of success are modified. $O\left(\sqrt{N}\ln^{\gamma} N\right)$

1(c) **Case 3:** Non-optimal configuration. $\Omega\left(N\right)$

**Figure 1:** Three examples of spatial configuration for which the QWSearch algorithms behaves differently.

## 4. When does each case happens ?



2(a) **Case 1:** Half of the configurations are concerned.

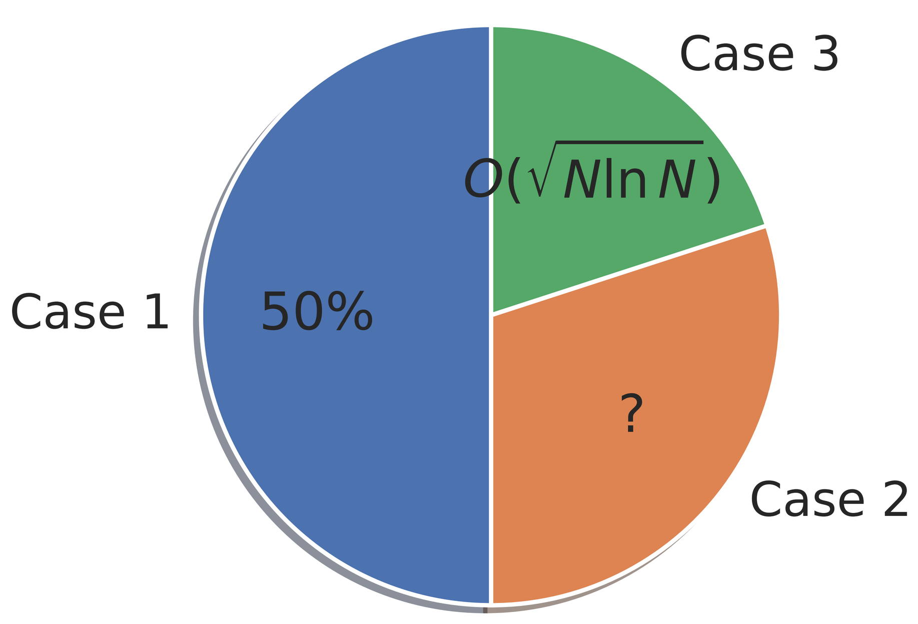
2(b) **Case 3:** The configurations in white **might** be non-optimal.

**Figure 2:** Known configuration for Case 1 and Case 3. First marked element placed at the center.

**Necessary condition for non-optimality.** While searching two elements $m_0 = (x_0, y_0)$ and $m_1 = (x_1, y_1)$, a necessary (but not sufficient) condition to have a non-optimal complexity is

$$\left(\overline{x_0 - x_1}\right)^2 \left(\overline{y_0 - y_1}\right)^2 \leq N.$$

## 5. Configurations are almost all optimal

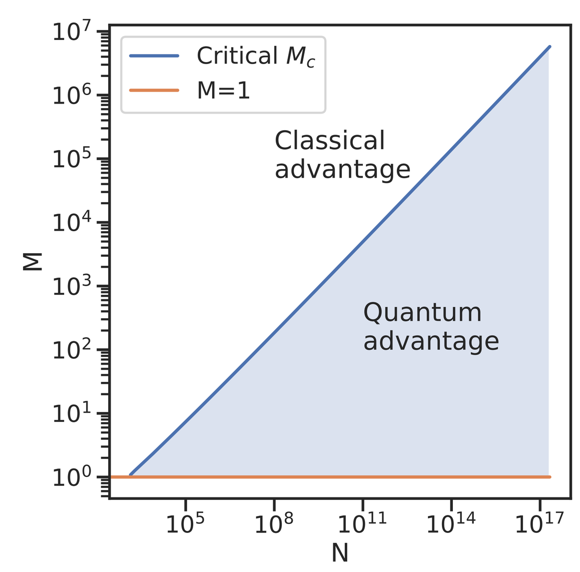



- $N - 1$ possible configurations.
- At most $O\left(\sqrt{N}\ln N\right)$ non-optimal configurations.
- The ratio of non optimal configurations

$$\frac{\mathcal{N}_{\text{non-optimal}}}{N-1} = O\left(\frac{\ln N}{\sqrt{N}}\right) \underset{N\to\infty}{\longrightarrow} 0.$$

## 6. Numerical simulations

In these numerical simulations, we have compared the average probability of success for drawn randomly the configurations of $M$ marked elements with a classical method.




## 7. Conclusion

In conclusion, we show that searching but non-optimal configurations exist and we give a necessary condition for a configuration to be non-optimal. We bound the proportion of non-optimal configurations and show that this proportion is asymptotically negligible.

## References

[1] Nikolajs Nahimovs and Alexander Rivosh. Exceptional configurations of quantum walks with grover's coin. (arXiv:1509.06862), Sep 2015. arXiv:1509.06862 [quant-ph].

[2] GA Bezerra, PHG Lugão, and R Portugal. Quantum-walk-based search algorithms with multiple marked vertices. *Physical Review A*, 103(6):062202, 2021.

[3] Mathieu Roget, Hachem Kadri, and Giuseppe Di Molfetta. Optimality conditions for spatial search with multiple marked vertices, 2022.