

Quantum and Classical Query Complexities of Local Search are Polynomially Related

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Abstract

Let f be an integer valued function on a finite set V . We call an undirected graph $G(V, E)$ a *neighborhood structure* for f . The problem of finding a local minimum for f can be phrased as: for a fixed neighborhood structure $G(V, E)$ find a vertex $x \in V$ such that $f(x)$ is not bigger than any value that f takes on some neighbor of x . The complexity of the algorithm is measured by the number of questions of the form “what is the value of f on x ?” We show that the deterministic, randomized and quantum query complexities of the problem are polynomially related. This generalizes earlier results of Aldous [?] and Aaronson [?] and solves the main open problem in [?].

1 Introduction

It follows from the theory of NP-hardness that many optimization problems, such as MAX-2SAT and MIN-CUT are difficult. In the MAX-2SAT problem one looks for a truth assignment which maximizes the number of satisfied clauses. In the black box version of the problem we assume that $f : \{0, 1\}^k \rightarrow \mathbb{Z}$ is an arbitrary function, unknown to us, and we want to find a global optimum for f . It is easy to see that to optimize f classically requires to make $\Omega(n)$ questions to the black box where $n = 2^k$. Using Grover’s surprisingly efficient database search algorithm [?], Dürr and Høyer have shown [?] that the quantum version of the same oracle problem has query complexity only $O(\sqrt{n})$. This bound is tight [?, ?, ?, ?], and although much better than the deterministic or randomized complexities, it is still exponential.

A way of relaxing the minimum/maximum finding problem is to look for a solution which is optimal only in some neighborhood structure. For example, in the (weighted) 2SAT-FLIP problem we wish to find a truth assignment $x \in \{0, 1\}^k$ such that the sum of the weights of the clauses it satisfies is not less than the same for any other truth assignment of Hamming distance one from x . The number of assignments is exponential (in k), but given any assignment, one can find out in polynomial time if it is locally optimal or not, and in the negative case produce a neighboring solution with a better value. Studying these new problems has lead Johnson, Papadimitriou and Yannakakis[?] to introduce the class PLS (Polynomial Local Search). Several important problems, such as 2SAT-FLIP are known to be complete in this class. Even though PLS is not harder than $\text{NP} \cap \text{coNP}$, it is still conjectured to be computationally intractable, at least classically.

What about the black box version of the local optimization problem, when f is a black box function and we pay only for the queries? Llewellyn, Tovey and Trick [?] and Llewellyn and Tovey [?] treat the deterministic case quite exhaustively. Aldous [?] has shown that for any graph of size n and of maximum degree Δ , the randomized query complexity is $O((n\Delta)^{1/2})$. Aaronson [?] has established an analogous $O(n^{1/3}\Delta^{1/6})$ quantum upper bound.

Two classes of specific neighborhood structures have been studied extensively, the k -dimensional hypercube where $n = 2^k$, and the d -dimensional grid graph, where $n = k^d$ for some fixed $d \geq 2$. For the case of

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the hypercube, Llewellyn, Tovey and Trick have shown [?] that to find a local optimum takes deterministically $\Theta(2^k/k^{1/2})$, that is only slightly less than n queries. The randomized and the quantum cases are much harder to analyze. In the randomized case, Aldous [?] proved that any algorithm must use $\Omega(2^{k/2-o(k)})$ queries. Aaronson [?] has improved the lower bound to $\Omega(2^{k/2}/k^2)$, and finally Zhang [?] has closed the gap by showing a matching $\Omega(2^{k/2}k^{1/2})$ bound to Aldous' result. In the quantum case the exact complexity is $\Theta(2^{k/3}k^{1/6})$, where the lower bound is due again to Zhang [?].

The query complexity of the grid graphs is known exactly except in small dimensions. Indeed, the lower bound results of Zhang [?] match the respective upper bounds of Aldous and Aaronson, implying that the randomized complexity is $\Theta(k^{d/2})$ when $d \geq 4$, and the quantum complexity is $\Theta(k^{d/3})$ when $d \geq 6$. The randomized lower bound of $\Omega(k^{3/2}/(\log k)^{1/2})$ of Zhang for $d = 3$ is tight up to a logarithmic factor, as well as his quantum lower bound of $\Omega(k^{5/3}/(\log k)^{1/3})$ for $d = 5$. For $d = 4$, the best quantum lower bound of $\Omega(k^{6/5})$, also due to Zhang, leaves a polynomial gap to the $O(n^{4/3})$ upper bound. The best quantum upper bound of $O(k^{1/2} \log \log k)$, for $d = 2$, was obtained by Verhoeven [?]. Recently, Sun and Yao [?] gave almost optimal lower bounds for the very small dimensional cases. More precisely, in the case $d = 2$, they have shown a randomized lower bound $\Omega(k^{1-\delta})$, and a quantum lower bound $\Omega(k^{1/2-\delta})$, for any constant $\delta > 0$. Their result for the quantum complexity, when $d = 3$, is $\Omega(k^{1-\delta})$, again for any constant $\delta > 0$.

A central question, explicitly raised by Aaronson in [?], has remained unanswered until now: are the deterministic, randomized and quantum query complexities polynomially related for arbitrary neighborhood structures? In this article we give an affirmative answer to this question.

The class PLS is a subset of TFNP, the family of total function problems from NP, introduced by Megido and Papadimitriou [?]. Informally, TFNP consists of those NP search problems for which a solution is guaranteed to exist. Since factorization is a prominent member of TFNP, one can consider this class as a potential source of problems which might admit efficient quantum algorithms. Other important subclasses of TFNP are PPP (Polynomial Pigeonhole Principle), and PPAD, the directed version of PPA (Polynomial Parity Argument). The elements of PPP are problems which by their combinatorial nature obey the pigeonhole principle and therefore have a solution. An example is SUBSET SUM restricted to inputs consisting of n positive integers whose sum is less than 2^n , and where one looks for two different subsets summing up to the same number. The elements of PPAD are search problems, where the existence of a solution is guaranteed by the fact that in a graph the number of vertices with odd degree is even. The collision lower bounds of Aaronson [?] and Shi [?] imply that in the black-box setting the deterministic and quantum complexities of PPP problems are polynomially related. A similar result follows for PPAD from the quantum lower bounds of Friedl et al. [?] for the query complexity of the 2 dimensional Sperner's problem. We prove an analogous result for PLS. As a consequence, if an efficient quantum algorithm is ever to be found for a problem in PLS, it must exploit its specific structure.

2 Results

For a positive integer n we denote $\{1, \dots, n\}$ by $[n]$. An *oracle problem* is a relation $\mathcal{R} \subseteq S \times T$ where T is a finite set and $S \subseteq \Sigma^{[n]}$ for some finite set Σ . The input is a function $f \in S$, hidden by an oracle, such that $f(x)$, where $x \in [n]$, can be accessed via a query parameterized by x . The output is some $t \in T$ such that $(f, t) \in \mathcal{R}$. A special case is the *functional oracle problem* when the relation is given by a function $A : S \rightarrow T$, the (unique) output is then $A(f)$. We say that A is *total* if $S = \Sigma^{[n]}$.

In the query model of computation each query adds one to the complexity of an algorithm, but all other computations are free. The state of the computation is represented by three registers, the query register $x \in [n]$, the answer register $a \in \Sigma$, and the work register z . The computation takes place in the vector space spanned by all basis states $|x\rangle|a\rangle|z\rangle$. In the *quantum query model* introduced by Beals, Buhrman, Cleve, Mosca and de Wolf [?] the state of the computation is a complex combination of all basis states which has unit length in the norm l_2 . In the randomized model it is a non-negative real combination of unit length in the norm l_1 , and in the deterministic model it is always one of the basis states.

The query operation O_f maps the basis state $|x\rangle|a\rangle|z\rangle$ into the state $|x\rangle|(a + f(x)) \bmod |\Sigma||z\rangle$,

where we identify Σ with residue classes $\text{mod}|\Sigma|$. Non-query operations are independent of f . A *k-query algorithm* is a sequence of $(k + 1)$ operations (U_0, U_1, \dots, U_k) where U_i is unitary in the quantum and stochastic in the randomized model, and it is a permutation in the deterministic case. Initially the state of the computation is set to some fixed value $|0\rangle|0\rangle|0\rangle$, and then the sequence of operations $U_0, O_f, U_1, O_f, \dots, U_{k-1}, O_f, U_k$ is applied. A quantum or randomized algorithm ϵ -computes \mathcal{R} for some fixed constant $\epsilon < 1/2$ if the observation of the appropriate last bits of the work register yields some $t \in T$ such that $(f, t) \in \mathcal{R}$ with probability at least $1 - \epsilon$. Then $Q_\epsilon(\mathcal{R})$ (resp. $R_\epsilon(\mathcal{R})$) is the smallest k for which there exists a k -query quantum (resp. randomized) algorithm which ϵ -computes \mathcal{R} . In the case of deterministic algorithms exact computation is required, and the deterministic query complexity $D(\mathcal{R})$ is defined then analogously. We have $D(\mathcal{R}) \geq R_\epsilon(\mathcal{R}) \geq Q_\epsilon(\mathcal{R})$.

Beals et al. [?] have shown that in the case of total functional oracle problems the deterministic and quantum complexities are polynomially related, and the gap is at most a degree 6 polynomial. No such relation is known for relations or for partial functional problems, in fact for several partial functional problems exponential quantum speedups are known [?, ?].

Throughout the paper $G(V, E)$ will be an undirected graph with vertex set V and edge set E , and we assume that $V = [n]$. In this paper we are concerned with the following oracle problem:

Local Search for G (in notation, LS_G):

Oracle Input: A function $f : V \rightarrow \mathbb{Z}$.

Output: An $x \in V$ such that for every $y \in V$ with $\{x, y\} \in E$ we have $f(x) \leq f(y)$.

We have chosen \mathbb{Z} as the range of the input functions only for presentational convenience, it could be restricted to $[n]$ without loss of generality. Also note that graph G is known to us, and we treat it as a parameter. The problem as specified is a relation. However, an important special case is functional local search, when only inputs with a guaranteed unique local (and therefore global) minimum are considered. We call such inputs *unimodal*, they will play an important role in our considerations.

Our main result is analogous to the statement of Beals et al. [?] for local search: the quantum and deterministic query complexities are polynomially related.

Theorem 1 (Main Theorem). *For every graph G , we have $D(\text{LS}_G) \in O(Q_\epsilon(\text{LS}_G)^{19})$.*

We will prove our main theorem by showing that both the classical and the quantum query complexities of a graph G are polynomially related to three parameters: its maximum degree, the logarithm of its size and its separation number. In section ?? we present a deterministic algorithm for LS_G whose complexity is polynomial in these parameters (**Theorem ??**). The degree lower bound for the quantum complexity which follows trivially by a reduction from Grover's search (**Fact ??**), and the log size lower bound (**Theorem ??**) are presented in section ?. The crucial lower bound involving the separation number (**Theorem ??**) is the subject of section ??, where we also prove our main theorem.

3 Local Search and Graph Parameters

Let $G(V, E)$ be a graph with vertex set V and edge set E . If $G'(V', E')$ is a subgraph of G then we write $G' \leq G$. We denote the subgraph of G spanned by a vertex set $V' \subseteq V$ with $G(V')$. The degree of a vertex in G is $\text{deg}_G x$. We denote the maximum degree of G with $\Delta(G)$ or simply Δ if G is clear from the context. The vertex boundary of a set $H \subseteq V$ in G is

$$\partial_G H = \{x \in V \setminus H \mid (\exists y \in H) \{x, y\} \in E\}.$$

If $H = \{x\}$ then we denote $\partial_G H$ by $\partial_G x$. We define now our most important graph parameter.

Definition 1 (Separation number). *The separation number of a graph $G(V, E)$ is*

$$s(G) = \max_{H \subseteq V} \min_{\substack{S \subseteq H, \\ |H|/4 \leq |S| \leq 3|H|/4}} |\partial_G(H)S| \quad (1)$$

We give now a deterministic algorithm which is a refinement of the divide and conquer procedure of Llewellyn, Tovey and Trick [?] which iteratively splits the graph into pieces by querying a separator set. The refinement consists in the specific choice of the separator set which makes explicit the connection between the complexity of the problem and the parameters we are interested in. For the sake of completeness we prove here the correctness of the algorithm and analyze its complexity in the three parameters. For every $H \subseteq V$ let H^* be the subset of H which minimizes $|\partial_{G(H)} S|$ when S is a subset of H of size between $|H|/4$ and $3|H|/4$.

Algorithm 1 Deterministic algorithm for LS_G

$H := V, S := \emptyset, u := \text{any vertex of } G.$

while output not found **do**

 Query $\{u\} \cup \partial_{G(H)} H^*$ to find the vertex m which minimizes f in this set, query $\partial_{G(H)} m$

if $f(m) \leq f(v)$ for all $v \in \partial_{G(H)} m$ **then**

 output $:= m$

else

$S := S \cup \partial_{G(H)} H^*$, let w be the vertex which minimizes f in $\partial_{G(H)} m$

if $f(w) \leq f(u)$ **then**

$u := w$

end if

 Let H be the connected component of $H \setminus \partial_{G(H)} H^*$ which contains u

end if

end while

Theorem 2. Algorithm 1 correctly solves LS_G and has query complexity $O(\log n(\Delta(G) + s(G)))$.

Proof. By induction one sees that at the beginning of each iteration,

$$\partial_G v \subseteq S \cup \partial_{G(H)} v \text{ for all } v \in H, \quad (2)$$

$$f(u) \leq f(s) \text{ for all } s \in S. \quad (3)$$

The algorithm always terminates since in each iteration $|H|$ decreases, and if $H = \{u\}$ then it outputs u . When the output m is produced then by definition $f(m) \leq f(v)$ for all $v \in \partial_H m$. Also $f(m) \leq f(u)$, and $f(m) \leq f(v)$ for all $v \in S$ by (??). Therefore m is a local minimum of f in G by (??). The number of iterations is $O(\log n)$ since $|H|$ always decreases by a factor of at least $1/4$, and inside each loop the number of queries is at most $\Delta(G) + s(G) + 1$. \square

4 Log size lower bound

The maximum degree and the $\log n$ lower bounds are obtained by reduction: the first one, very simple, from Grover's search, the second one, more sophisticated, from ordered search.

Fact 1 (Aaronson [?]). Let $G(V, E)$ be connected with maximum degree Δ . Then $Q_\epsilon(LS_G) \in \Omega(\sqrt{\Delta})$.

In the ordered search reduction we will use unimodal functions, like Aaronson [?], which arise from paths rooted at a fixed node of G . We define now the generic construction of functions generated by paths. A directed path P in G is a sequence of vertices (p_0, p_1, \dots, p_l) (with possible repetitions) such that for every $0 \leq i \leq l - 1$ node p_i is connected to node p_{i+1} in G . In this article we do not consider undirected paths. Let G be a connected graph, and let us denote by $\text{dist}_G(x, y)$ the length of the shortest path in G between vertices x and y . We define the path function $f_P : V \rightarrow \mathbb{Z}$ by

$$f_P(x) = \begin{cases} -j & \text{if } p_j = x \text{ and } p_k \neq x \text{ for } k > j \\ \text{dist}_G(p_0, x), & \text{if } \forall j, p_j \neq x. \end{cases}$$

Observe that path functions are always unimodal, they have their minimum in the last vertex of the path.

Reductions between black-box problems are regularly used to prove quantum lower bound. In these reductions usually a single query to the oracle of the reduced problem simulates a query of the problem to which the reduction is made. However, in more sophisticated cases, several queries can be permitted for the simulation. We make this precise in the following definition and lemma.

Definition 2. A functional oracle problem $A : S_1 \rightarrow T$ with $S_1 \subseteq \Sigma_1^{[n]}$ is k -query reducible to a functional oracle problem $B : S_2 \rightarrow T$ with $S_2 \subseteq \Sigma_2^{[m]}$ if the following two conditions are satisfied:

$$\begin{aligned} & \exists \alpha : S_1 \rightarrow S_2 \text{ such that } \forall f \in S_1, A(f) = B(\alpha(f)); \\ & \exists \gamma_1, \dots, \gamma_k : [m] \rightarrow [n] \text{ and } \gamma : [m] \times \Sigma_1^k \rightarrow \Sigma_2 \text{ such that} \\ & \forall f \in S_1, x \in [m], (\alpha(f))(x) = \gamma(x, f(\gamma_1(x)), \dots, f(\gamma_k(x))) \end{aligned}$$

Lemma 1. If A is k -query reducible to B then $Q_\epsilon(B) \geq Q_\epsilon(A)/2k$.

Proof. Let \mathcal{B} a query algorithm which solves B with c queries. We show that there exists a query algorithm \mathcal{A} which solves A with $2kc$ queries. The algorithm \mathcal{A} simulates \mathcal{B} , and in its non-query steps it is identical to it. For simulating the query steps \mathcal{A} will use $2k$ additional registers. When \mathcal{B} makes a query step involving the basis state $|x\rangle$ then \mathcal{A} computes $\gamma_1(x), \dots, \gamma_k(x)$ in the first k additional registers, queries the oracle k -times to get $f(\gamma_1(x)), \dots, f(\gamma_k(x))$ in the next k registers, computes $\alpha(f)(x)$ in the oracle answer register, and finally erases the contents of the additional registers. \square

In fact, Lemma ?? remains also valid with weaker conditions on the reduction. For example, one could authorize that the queries to $\alpha(f)$ are computed by a quantum query algorithm which can make k queries to f . The reduction of Buhrman and de Wolf [?] of the parity problem to ordered search indeed uses this more general notion. However, for our purposes the more restricted reduction is sufficient.

Theorem 3. Let $G(V, E)$ be a connected graph on n vertices. Then $Q_\epsilon(\text{LS}_G) \in \Omega(\log n)$.

Proof. We can suppose that G is a tree, since if $G' = (V, E')$ is a subgraph of G then $Q_\epsilon(\text{LS}_{G'}) \leq Q_\epsilon(\text{LS}_G)$. Indeed, the error probability of any algorithm in G' is at most its error probability in G because a local minimum in G is also a local minimum in G' . Let $S_1 = \{f_y : y \in [n]\}$, where $f_y : [n] \rightarrow \{0, 1\}$ is defined by

$$f_y(x) = \begin{cases} 0 & \text{if } x \leq y \\ 1 & \text{otherwise.} \end{cases}$$

The ordered search problem is defined by $A(f_y) = y$, and Høyer, Neerbek and Shi [?] have shown that $Q(A) = \Omega(\log n)$. We will show that A is 2-query reducible to LS_G , and then the result follows from Lemma ?. Let $V = [n]$, and consider any depth first search traversal of G . Let dfn be the depth-first numbering of the vertices (that is the vertices are numbered in preorder). To simplify the description, without loss of generality we will suppose that $\text{dfn}(x) = x$ for every vertex x . This means for example that vertex 1 is the root of the depth first search traversal. Let $\text{desc}(x)$ be the number of descendants of x in the search. It is well known [?] that for every vertex y , vertex x is an ancestor of y if and only if

$$x \leq y < x + \text{desc}(x). \tag{4}$$

For $y \in [n]$, let P_y be the path from vertex 1 to vertex y in the tree G . By the definition of the path function,

$$f_{P_y}(x) = \begin{cases} -\text{dist}_G(1, x) & \text{if } x \text{ is on the path from 1 to } y \\ \text{dist}_G(1, x) & \text{otherwise.} \end{cases}$$

The unique local minimum of f_{P_y} is in the vertex y , therefore $\text{LS}_G(f_{P_y}) = y$, and for the purpose of the reduction we can set $S_2 = \{f_{P_y} : y \in [n]\}$ and $\alpha(f_y) = f_{P_y}$. To determine the answer of the oracle $\alpha(f_y)$

on query x , using the oracle f_y , it has to be decided if x is an ancestor of y . By (??) this happens exactly when $f_y(x) = 0$ and $f_y(x + \text{desc}(x)) = 1$. Thus if we set $\gamma_1(x) = x$, $\gamma_2(x) = x + \text{desc}(x)$ and

$$\gamma(x, b_1, b_2) = \begin{cases} -\text{dist}_G(1, x) & \text{if } b_1 = 0 \text{ and } b_2 = 1 \\ \text{dist}_G(1, x) & \text{otherwise,} \end{cases}$$

then $f_{P_y}(x) = \gamma(x, f_y(\gamma_1(x)), f_y(\gamma_2(x)))$, and the reduction is completed. □

5 Quantum Query Complexity and Graph Expansion

The purpose of this section is to prove the following lower bound.

Theorem 4. *Let $G = (V, E)$ be a connected graph on n vertices with maximum degree Δ and separation number s . Then $Q_\epsilon(\text{LS}_G) \in \Omega((s/\Delta)^{1/8}(\log n)^{-1})$.*

Proof. The statement is a direct consequence of Theorems ?? and ?? below. □

Beside the reduction method, lower bound proofs in the quantum query model fall into two main categories: they are obtained either by the degree argument (the polynomial method) of Beals et al. [?] or by the quantum adversary method of Ambainis [?]. Aaronson [?] uses the latter, and our paper closely follows his proof scheme. Like in [?], all our sample functions will be path functions generated by paths rooted at a fixed node of G (Aaronson calls these paths snakes). Since we need to present an argument that works for general graphs we invented some useful lemmas about the structure of expander graphs. Another place where we improve on [?] is that we almost entirely eliminate the problem with self intersecting paths. To do so we use a more general version of the quantum adversary method explained in the next section.

5.1 Quantum Adversary Method

The quantum adversary method of Ambainis [?] has several known extensions. These include the spectral method of Barnum, Saks and Szegedy [?], the weighted adversary method of Ambainis [?], the strong weighted adversary method of Zhang [?], and the Kolmogorov complexity method of Laplante and Magniez [?]. All these methods were proven to be equivalent by Špalek and Szegedy [?]. Recently, an even more powerful method using negative weights has been proposed by Høyer, Lee and Špalek [?].

The spectral method, that expresses the bound in terms of ratios of eigenvalues of matrices, was derived from the characterization of quantum query complexity as a semidefinite feasibility problem [?]. Though the spectral method has been stated only for Boolean function, its generalization to the non-Boolean case is quite straightforward, as pointed out in [?] and [?]. We will need the method of the more general form, that we state here. For a non-negative symmetric matrix M , let us denote its largest eigenvalue by $\lambda(M)$.

Theorem 5 (Spectral Method). *Let $A : S \rightarrow T$ be a functional oracle problem where $S \subseteq \Sigma^{[n]}$. Let Γ be an arbitrary $S \times S$ nonnegative symmetric matrix that satisfies $\Gamma[f, g] = 0$ whenever $A(f) \neq A(g)$. For $x \in [n]$ let Γ_x be the matrix:*

$$\Gamma_x[f, g] = \begin{cases} 0 & \text{if } f(x) = g(x) \\ \Gamma[f, g] & \text{if } f(x) \neq g(x). \end{cases}$$

Then:

$$Q_\epsilon(A) \in \Omega\left(\frac{\lambda(\Gamma)}{\max_{1 \leq x \leq n} \lambda(\Gamma_x)}\right).$$

5.2 Path Arrangement

Let $G(V, E)$ be a connected graph. For a directed path $P = (p_0, p_1, \dots, p_l)$ we set

$$\text{start}(P) \stackrel{\text{def}}{=} p_0; \quad \text{end}(P) \stackrel{\text{def}}{=} p_l; \quad \text{length}(P) = l.$$

We call p_0 the starting point of P and p_l the end point. All paths other than the empty path have a starting and an end point (which may coincide). For a path P we denote by P^\ominus the path that we obtain by deleting both the starting and end points from P . Formally, $P^\ominus = (p_1, \dots, p_{l-1})$. Note that if P is just an edge (p_0, p_1) then $P^\ominus = \epsilon$, the empty path. For paths $P = (p_0, \dots, p_l)$ and $Q = (q_0, \dots, q_{l'})$ with $q_0 = p_l$ their join is $PQ = (p_0, \dots, p_l, q_1, \dots, q_{l'})$. A path is *simple* if no vertex occurs more than once in it.

We often view a path P as a multi-set. For a path P and $x \in V$ let $\text{mult}(x, P) = |\{j \mid p_j = x\}|$, that is the number of times P goes through x , and let $\text{mult}(P) = \max_{x \in V} \text{mult}(x, P)$.

Definition 3 (Path arrangement and Inter/Intra-cluster path). *A path arrangement for G with parameter m is a set of connected, disjoint subsets $N_1, \dots, N_m \subseteq V$ with some fixed spanning trees T_i of $G(N_i)$ together with a set of directed path $\{E_i(j, k)\}_{1 \leq i, j, k \leq m}$ such that*

1. $E_i(j, k) \cap N_j = \{\text{start}(E_i(j, k))\}$ for $1 \leq i, j, k \leq m$;
2. $E_i(j, k) \cap N_k = \{\text{end}(E_i(j, k))\}$ for $1 \leq i, j, k \leq m$;
3. $E_i(j, k)^\ominus \cap E_{i'}(j, k)^\ominus = \emptyset$ for $1 \leq i \neq i', j, k \leq m$;
4. $E_i(j, k)$ is simple for $1 \leq i, j, k \leq m$.

In the path arrangement the sets N_i are called the clusters for $1 \leq i \leq m$. The paths $E_i(j, k)$ are called inter-cluster paths and i is the enumerator number of $E_i(j, k)$. For $x, y \in N_i$, the intra-cluster path $R_i(x, y)$ is defined as the shortest path from x to y in T_i .

Definition 4 (Path arrangement parameter). *The path arrangement parameter $m(G)$ of G is the maximal m such that there is path arrangement for G with parameter m .*

To bring an example to the above definitions consider the two dimensional \sqrt{n} by \sqrt{n} grid, $G_{2,n}$ with vertex set $V = I \times J$ (we suppose that n is a square number, I and J are paths of length \sqrt{n}). Two vertices in V are connected if either their I coordinates are the same and their J coordinates are connected or their J coordinates are the same and their I coordinates are connected. We create a path arrangement. The clusters will be the sets $\{i\} \times J$ for all $i \in I$. Clearly, every cluster induces a connected graph in $G_{2,n}$. For two clusters, $\{i\} \times J$ and $\{i'\} \times J$, define $P_{i,i'}$ as the unique shortest path connecting i and i' in I , and consider the collection of path

$$E_j(i, i') = P_{i,i'} \times \{j\},$$

where j runs through all elements of J . These paths will serve as inter-cluster paths in between the two clusters. It is easy to check that all conditions of Definition ?? are satisfied and we conclude that $m(G_{2,n}) = \sqrt{n}$.

Another example is the complete graph, K_n on the vertex set V with $|V| = n$. Here the individual nodes can be defined as the clusters and the inter-cluster paths in between any two nodes $v, w \in V$ are $E_i(v, w) = (v, w)$, the same for all $1 \leq i \leq n$. The disjointness property for these paths holds, since $(v, w)^\ominus = \emptyset$. We conclude that $m(K_n) = n$. It is easy to see that $m(G) \leq \sqrt{n\Delta} + 1$ for all graphs G .

5.3 Separation Number versus Path Arrangement Parameter

We will show that the path arrangement parameter, $m(G)$ is in $\Omega(\sqrt{s/\Delta})$. We start with some easy lemmas.

Definition 5. A graph $G(V, E)$ is a (n_1, n_2, λ) -expander if for every subset $H \subseteq V(G)$ such that $n_1 < |H| \leq n_2$, we have that $|\partial_G H| \geq \lambda|H|$.

Lemma 2. Every connected graph G on n vertices which is an $(n/4, 3n/4, \lambda)$ -expander has an induced subgraph G' with at least $n/2$ vertices which is a $(0, n/2, \lambda)$ -expander.

Proof. For $X \subseteq V$ we denote the subgraph of G induced on X by $G(X)$. Assume that the statement of the lemma is false. Then with every $X \subseteq V$ such that $|X| \geq n/2$ we can associate a non-empty $\tilde{X} \subseteq X$ with the property that $|\tilde{X}| \leq n/2$ and $|\partial_{G(X)} \tilde{X}| < \lambda|\tilde{X}|$.

Define $X_0 = V$ and $X_i = X_{i-1} \setminus \tilde{X}_{i-1}$ for $i \geq 1$. Since $|X_i|$ is strictly smaller than $|X_{i-1}|$ there has to be an index k such that $|X_k| \geq n/2$ but $|X_{k+1}| < n/2$. We define

$$Y = \begin{cases} V \setminus X_{k+1} & \text{if } |V \setminus X_{k+1}| \leq 3n/4, \\ V \setminus X_k & \text{otherwise.} \end{cases}$$

Since $|\tilde{X}_k| \leq n/2$, in both cases it holds that $n/4 < |Y| \leq 3n/4$. Therefore $|\partial_G Y| \geq \lambda|Y|$. By another argument we show that the boundary of Y is small, thus getting a contradiction. Suppose that $Y = V \setminus X_k$, the other case is similar. Notice that

$$Y = \tilde{X}_0 \dot{\cup} \tilde{X}_1 \dot{\cup} \dots \dot{\cup} \tilde{X}_{k-1},$$

where $\dot{\cup}$ denotes the disjoint union. Therefore

$$\partial_G Y = (\partial_G Y) \cap X_k \subseteq \bigcup_{i=0}^{k-1} ((\partial_{G(X_i)} \tilde{X}_i) \cap X_k) \subseteq \bigcup_{i=0}^{k-1} \partial_{G(X_i)} \tilde{X}_i.$$

By our assumption the last set has size less than $\lambda|\tilde{X}_0| + \dots + \lambda|\tilde{X}_{k-1}| = \lambda|Y|$, which is a contradiction. \square

Lemma 3. For every connected graph $G(V, E)$ and for every $\Delta \leq k \leq |V|$ we can find at least $\lfloor |V|/k \rfloor$ vertex disjoint connected subgraphs of G , each with at least k/Δ vertices.

Proof. Set $N_0 = \emptyset$. Let l be the smallest integer such that $(l+1)k > |V|$, observe that $l = \lfloor |V|/k \rfloor$. It is enough to find $N \subseteq V$ such that $G(N)$ and $G(V \setminus N)$ are connected and $k/\Delta \leq |N| \leq k$. Indeed, then by induction we can pick N_i for $i = 1, \dots, l$ such that N_i is connected, has size between k/Δ and k , and is a subset of $V \setminus \bigcup_{j=1}^{i-1} N_j$.

We now prove the existence of the above N . If $k = n$ then we just set $N = V$. Otherwise let T_0 be a spanning tree of G with root r_0 . Let r_1 be the child of r_0 which roots the subtree T_1 of T_0 with the greatest number of nodes among all children of r_0 . Similarly, let r_2 be the child of r_1 which roots the subtree T_2 of T_1 with the greatest number of nodes among all children of r_1 , etc, until we get T_s , a tree with $|T_s| \leq k$. The size of T_{s-1} is strictly greater than k , therefore the size of T_s is at least $(|V(T_{s-1})| - 1)/\Delta \geq k/\Delta$. Thus $V(T_s)$ is a good choice for N . \square

Lemma 4. Let $G(V, E)$ be a $(0, |V|/2, \lambda)$ -expander, and let $N_1, N_2 \subseteq V$ be disjoint subsets, both of size at least k . Then there are $m = \lambda k$ path E_1, \dots, E_m such that

1. $E_i \cap N_1 = \{\text{start}(E_i)\}$ for $1 \leq i \leq m$;
2. $E_i \cap N_2 = \{\text{end}(E_i)\}$ for $1 \leq i \leq m$;
3. $E_i^\ominus \cap E_{i'}^\ominus = \emptyset$ for $1 \leq i \neq i' \leq m$;

4. $E_i(j, k)$ is simple for $1 \leq i, j, k \leq m$.

Proof. If there is an edge (v, w) with $v \in N_1$, $w \in N_2$ then we can set $E_i = (v, w)$ for $1 \leq i \leq m$. Otherwise contract N_1 into a single node n_1 and N_2 into a single node n_2 . Assume that there are no paths in G that satisfy 1-4. Then there are no paths satisfying 1-3 either. It follows that in the contracted graph, G' , one cannot find m vertex-disjoint paths that connect n_1 and n_2 . This, in turn, by Menger's theorem implies that there is a vertex cut $C \subseteq V$ of size smaller than m which separates n_1 and n_2 . Let C'_1 be the component of G' that contains n_1 and C'_2 be the component of G' that contains n_2 , and let the expanded version of these components be C_1 and C_2 . Without loss of generality we can assume that $k \leq |C_1| \leq n/2$, which leads to a contradiction, since $\partial_G C_1 \subseteq C$, $|C| < m = \lambda k$. \square

Theorem 6. *Let G be a connected graph with maximum degree Δ , separator number s and path arrangement parameter m . Then we have $m \geq \lfloor \sqrt{s/2\Delta} \rfloor$.*

Proof. Let H be the subset of V for which the right hand side of (??) is maximized. Then $s = s(G(H))$, which implies that $G(H)$ is an $(|H|/4, 3|H|/4, s/|H|)$ -expander. By Lemma ?? there is an $H' \subseteq H$ such that $|H'| \geq |H|/2$ and $G(H')$ is an $(0, |H|/2, s/|H|)$ -expander. We shall construct the required path arrangement inside $G(H')$. The graph $G(H')$ is connected since all of its components have to be $(0, |H|/2, s/|H|)$ -expanders, and this is possible only if $G(H')$ has a single component. By Lemma ?? we find clusters $N_1, \dots, N_{\lfloor \sqrt{s/2\Delta} \rfloor}$ such that $|N_i| \geq |H'|/\sqrt{s\Delta/2}$ and $G(N_i)$ is connected for $1 \leq i \leq \lfloor \sqrt{s/2\Delta} \rfloor$. Here we used that $\Delta(G(H')) \leq \Delta$. To finish the proof now all we need is to construct the set of intra-cluster paths. By Lemma ?? between N_i and N_j we find $(|H'|/\sqrt{s\Delta/2}) \times (s/|H|)$ external paths. Since $|H'| \geq |H|/2$, the previous expression is at least $\sqrt{s/2\Delta}$. \square

5.4 The Adversary Matrix

Let $G(V, E)$ be a connected graph, we want to define our adversary matrix for LS_G . We fix a path arrangement with parameter $m = m(G)$ for which we use the notations of Definition ?. We set $a = \sqrt{m}/10$ for the rest of the section. To every $\bar{r} = r_0 \dots r_{2a} \in [m]^{2a+1}$ with $r_0 = 1$, we define a directed path $P(\bar{r}) = P(\bar{r}, 0)P(\bar{r}, 1) \dots P(\bar{r}, 2a)$ which will be the join of $2a + 1$ paths. Even indices will name clusters, odd indices will name enumerator numbers of intra-cluster paths. We fix an arbitrary starting node $x_{\text{start}} \in N_1$, and for $0 \leq i \leq 2a$ we define:

$$P(\bar{r}, i) = \begin{cases} E_{r_i}(r_{i-1}, r_{i+1}) & \text{if } i \text{ is odd} \\ R_1(x_{\text{start}}, \text{start}(P(\bar{r}, 1))) & \text{if } i = 0 \\ R_{r_i}(\text{end}(P(\bar{r}, i-1)), \text{start}(P(\bar{r}, i+1))) & \text{if } i \text{ is even and } 2 \leq i \leq 2a-2, \\ R_{r_{2a}}(\text{end}(P(\bar{r}, 2a-1)), \text{end}(P(\bar{r}, 2a-1))) & \text{if } i = 2a. \end{cases}$$

For \bar{r} and \bar{r}' let $\text{div}(\bar{r}, \bar{r}')$ be the first i such that $r_i \neq r'_i$. We set

$$\Gamma_1[\bar{r}, \bar{r}'] = \begin{cases} m^{\text{div}(\bar{r}, \bar{r}')} & \text{if } \text{div}(\bar{r}, \bar{r}') \text{ is odd and } r_{2a} \neq r'_{2a} \\ 0 & \text{otherwise.} \end{cases}$$

Observe that the rows (and columns) of Γ_1 are indexed by sequences and not functions on V as required. This is just a formal matter. With every sequence \bar{r} we associate the path $P(\bar{r})$ and with every such path we associate the path function $f_{P(\bar{r})}$ as in Section ?. As an index, \bar{r} really corresponds to the function $f_{P(\bar{r})}$.

The matrix Γ_1 is not yet the adversary matrix we need, we have to zero out some rows and columns that correspond to "bad sequences." A sequence \bar{r} is *repetitive* if there are indices $0 \leq i \neq j \leq 2a$ such that $r_i = r_j$, it is *criss-crossing* if there is an $x \in V$ such that $\text{mult}(x, P(\bar{r})) > 100 \log |V|$. Finally \bar{r} is *bad* if it is either repetitive or criss-crossing otherwise it is *good*. We define our adversary matrix as:

$$\Gamma[\bar{r}, \bar{r}'] = \begin{cases} \Gamma_1[\bar{r}, \bar{r}'] & \text{if both } \bar{r} \text{ and } \bar{r}' \text{ are good} \\ 0 & \text{otherwise.} \end{cases}$$

Theorem 7. For every connected graph G on n vertices, and with path arrangement parameter m , we have $Q_\epsilon(\text{LS}_G) \in \Omega(m^{1/4}/\log n)$.

Proof. The statement is an immediate consequence of the spectral method (Theorem ??), and Lemmas ?? and ?? below. \square

5.4.1 Eigenvalue Lower Bound

Lemma 5. $\lambda(\Gamma) \in \Omega(am^{2a+1})$.

Proof. The matrix Γ has m^{2a} rows. In order to lower bound $\lambda(\Gamma)$ we simply use the entry-sum estimate, that is $\lambda(\Gamma) \geq \sum_{\bar{r}, \bar{r}'} \Gamma[\bar{r}, \bar{r}'] / m^{2a}$. First we estimate the entry-sum of Γ_1 . Since all rows and columns of Γ_1 have the same sum, we will sum up the elements in an arbitrary row indexed with \bar{r} . In that row, we group the columns together according to $\text{div}(\bar{r}, \bar{r}')$, and get

$$\sum_{\bar{r}'} \Gamma_1[\bar{r}, \bar{r}'] = \sum_{l=0}^{a-1} \sum_{\bar{r}': \text{div}(\bar{r}, \bar{r}')=2l+1} \Gamma_1[\bar{r}, \bar{r}'].$$

For the group of columns indexed with \bar{r}' such that $\text{div}(\bar{r}, \bar{r}') = 2j + 1$, the corresponding entries of our row sum up to $m^{2j+1}(m-1)m^{2a-2j-2}(m-1)$. Therefore we obtain

$$\sum_{\bar{r}': \text{div}(\bar{r}, \bar{r}')=2l+1} \Gamma_1[\bar{r}, \bar{r}'] = (1 + o(1))m^{2a+1}. \quad (5)$$

Since $\text{div}(\bar{r}, \bar{r}')$ can have a different values, this implies the estimation

$$\sum_{\bar{r}'} \Gamma_1[\bar{r}, \bar{r}'] = (1 + o(1))am^{2a+1}. \quad (6)$$

We now upper bound the number of bad rows and columns. With our choice of $a = \sqrt{m}/10$, the number of non-repetitive sequences \bar{r} is $(m-1) \dots (m-2a) \geq 0.8m^{2a}$.

Pick now randomly a non-repetitive \bar{r} . We claim that for a fixed x , the probability that $\text{mult}(x, P(\bar{r})) \geq 100 \log n + 1$ is upper bounded by

$$\binom{a}{100 \log n} \frac{1}{m(m-1) \dots (m-100 \log n)}. \quad (7)$$

To see that, fix the even indices anyhow and condition on this fixing. There can be only at most one even index, say $2q$, such that $x \in P(\bar{r}, 2q)$. There has to be $100 \log n$ odd indices $2i + 1$, for which $x \in P(\bar{r}, 2i + 1)^\ominus$ since inter-cluster paths are simple. However, once the even indices are fixed, we get an independence between paths belonging to different odd indices, except that because of the non-repetitive nature of \bar{r} their enumerator number should be different. From this the above formula follows.

The expression in (7) is easily upper-bounded by $o(1/n)$. Thus for a random non-repetitive \bar{r} the probability that $\text{mult}(P(\bar{r})) \geq 100 \log n + 1$ is $o(1)$. We got that that the number of bad rows (and columns) is at most $0.2m^{2a}(1 + o(1))$. Since all rows and columns of Γ have the same sum, we conclude that taking out $0.2m^{2a}(1 + o(1))$ rows and $0.2m^{2a}(1 + o(1))$ columns decreases the entry sum of Γ by at most a factor of $0.4 + o(1)$. Thus

$$\lambda(\Gamma) \in \Omega(am^{2a+1}).$$

\square

5.4.2 Eigenvalue Upper Bound

Lemma 6. $\lambda(\Gamma_x) \in O(\sqrt{am}^{2a+1} \log n)$ for all $x \in V$.

Proof. Recalling from Theorem ?? the definition of Γ_x , we see that for $x \in V$,

$$\Gamma_x[\bar{r}, \bar{r}'] = \begin{cases} \Gamma[\bar{r}, \bar{r}'] & \text{if } f_{P(\bar{r})}(x) \neq f_{P(\bar{r}')} (x) \\ 0 & \text{otherwise.} \end{cases}$$

In order to give an upper bound on $\lambda(\Gamma_x)$, we decompose Γ_x as $\Gamma_x = \sum_{j=0}^{100 \log n} \Gamma_x^{(j)}$ where

$$\Gamma_x^{(j)}[\bar{r}, \bar{r}'] = \begin{cases} \Gamma_x[\bar{r}, \bar{r}'] & \text{if } \min\{\text{mult}(x, P(\bar{r})), \text{mult}(x, P(\bar{r}'))\} = j \\ 0 & \text{otherwise.} \end{cases}$$

Such a decomposition is possible since the entries corresponding to criss-crossing sequences are zero in Γ , and therefore in Γ_x .

We will use two well known properties of the λ function. Firstly, it is sub-additive, that is $\lambda(M_1 + M_2) \leq \lambda(M_1) + \lambda(M_2)$. Secondly, for any matrix M with non-negative coefficients,

$$\lambda(M) \leq \max_{p,q: M[p,q] \neq 0} \sqrt{\left(\sum_s M[p,s]\right)\left(\sum_s M[s,q]\right)}. \quad (8)$$

Because of sub-additivity, it is sufficient to show that $\lambda(\Gamma_x^{(j)}) \in O(\sqrt{am}^{2a+1})$ for $0 \leq j \leq 100 \log n$. Fix $j \leq 100 \log n$. Using (??) we get

$$\lambda(\Gamma_x^{(j)}) \leq \max_{\bar{r}, \bar{r}': \min\{\text{mult}(x, P(\bar{r})), \text{mult}(x, P(\bar{r}'))\} = j} \sqrt{\sum_{\bar{r}''} \Gamma_x^{(j)}[\bar{r}, \bar{r}''] \sum_{\bar{r}''} \Gamma_x^{(j)}[\bar{r}'', \bar{r}']}. \quad (9)$$

Fix good sequences \bar{r} and \bar{r}' such that $\text{mult}(x, P(\bar{r})) = j$ and $\text{mult}(x, P(\bar{r}')) \geq j$. We can bound $\sum_{\bar{r}''} \Gamma_x^{(j)}[\bar{r}'', \bar{r}']$ in (??) from above by $\sum_{\bar{r}''} \Gamma_1[\bar{r}'', \bar{r}']$ which is $O(am^{2a+1})$ from (??). We claim that

$$\sum_{\bar{r}''} \Gamma_x^{(j)}[\bar{r}, \bar{r}''] \in O(m^{2a+1}). \quad (10)$$

The statement of the lemma follows then immediately using (??).

We now turn to the proof of (??). For $0 \leq i \leq 2a$, we define the paths $B(\bar{r}, i) = P(\bar{r}, 0)P(\bar{r}, 1) \dots P(\bar{r}, i-1)$ and $T(\bar{r}, i) = P(\bar{r}, i)P(\bar{r}, i+1) \dots P(\bar{r}, 2a)$. Observe that $P(\bar{r})$ is $B(\bar{r}, i)T(\bar{r}, i)$ for every i . We set $u = \max\{i \mid x \in P(\bar{r}, i)\}$, when $j > 0$, and $u = -1$ when $j = 0$. For each $0 \leq l \leq a-1$, we define

$$S_l = \sum_{\bar{r}'': \text{div}(\bar{r}, \bar{r}'') = 2l+1} \Gamma_x^{(j)}[\bar{r}, \bar{r}''].$$

Depending on l we estimate S_l . Let \bar{r}'' be a random sequence with the condition that $\text{div}(\bar{r}, \bar{r}'') = 2l+1$. Observe that $B(\bar{r}, 2l+1)$ and $B(\bar{r}'', 2l+1)$ may differ only on the elements of $N_{r_{2l}}$. Also, $\Gamma_x^{(j)}[\bar{r}, \bar{r}''] = 0$ when $\text{mult}(x, P(\bar{r}'')) < j$.

1. If $2l < u$ and $x \notin N_{r_{2l}}$ then $\text{mult}(x, B(\bar{r}'', 2l+1)) = \text{mult}(x, B(\bar{r}, 2l+1)) < \text{mult}(x, P(\bar{r}))$. Therefore \bar{r}'' contributes to S_l only when $x \in T(\bar{r}'', 2l+1)$. Since this happens with probability at most $2a/m$, using (??) we conclude that $S_l \leq \frac{2a}{m} m^{2a+1}$.
2. If $2l > u$ and $x \notin N_{r_{2l}}$ then the only way that $f_{P(\bar{r})}(x) \neq f_{P(\bar{r}'')}(x)$ is when $x \in T(\bar{r}'', 2l+1)$. Therefore as above we conclude that $S_l \leq \frac{2a}{m} m^{2a+1}$.
3. If $2l = u$ or $x \in N_{r_{2l}}$ then we have only the trivial m^{2a+1} upper bound on S_l .

Because \bar{r} is good there is only at most one l such that $x \in N_{r_{2l}}$. In summary, we can estimate the row-sum associated with \bar{r} as

$$\sum_{0 \leq l \leq a-1} S_l \leq a \frac{2a}{m} m^{2a+1} + 2m^{2a+1} \in O(m^{2a+1}),$$

because by our choice $a = \Theta(\sqrt{m})$. □

5.5 Putting things together

Proof of Theorem ??:

Proof. If G is connected then a simple computation shows that

$$\log n(\Delta + s) \in O((\max\{\sqrt{\Delta}, \log n, (s/\Delta)^{1/8} / \log n\})^{19}),$$

and the statement follows from Theorem ??, Fact ?? and Theorems ?? and ??. Otherwise set $G_0 = G$ and let G_1, \dots, G_k be the connected components of G for some k . Set $d_i = D(\text{LS}_{G_i})$ and $q_i = Q_\epsilon(\text{LS}_{G_i})$ for $0 \leq i \leq k$. Let m be the index of the component for which $q_m = q_0$. Then $d_0 \leq d_m$ and $d_m \in O(q_m^{19})$ since G_m is connected. □

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