ON FUNCTIONAL GRAPHS OF QUADRATIC POLYNOMIALS

BERNARD MANS, MIN SHA, IGOR E. SHPARLINSKI, AND DANIEL SUTANTYO

ABSTRACT. We study functional graphs generated by quadratic polynomials over prime fields. We introduce efficient algorithms for methodical computations and provide the values of various direct and cumulative statistical parameters of interest. These include: the number of connected functional graphs, the number of graphs having a maximal cycle, the number of cycles of fixed size, the number of components of fixed size, as well as the shape of trees extracted from functional graphs. We particularly focus on connected functional graphs, that is, the graphs which contain only one component (and thus only one cycle). Based on the results of our computations, we formulate several conjectures highlighting the similarities and differences between these functional graphs and random mappings.

1. INTRODUCTION

Let \mathbb{F}_q be the finite field of q elements and of characteristic p, with $p \geq 3$. For a function $f : \mathbb{F}_q \to \mathbb{F}_q$, we define the functional graph of f as a directed graph \mathcal{G}_f on q nodes labelled by the elements of \mathbb{F}_q where there is an edge from u to v if and only if f(u) = v. For any integer $n \geq 1$, let $f^{(n)}$ be the *n*-th iteration of f.

These graphs are particular as one can immediately observe that each connected component of the graph \mathcal{G}_f has a unique cycle (we treat fixed points as cycles of length 1). An example for the functional graph of $x^2 + 12 \pmod{31}$ is given in Figure 1.1.

Recently, there have been an increasing interest in studying, theoretically and experimentally, the graphs \mathcal{G}_f generated by polynomials $f \in \mathbb{F}_q[X]$ of small degree (such as quadratic polynomials), and how they differ, or not, from random mappings [Flajolet and Odlyzko 1990]. We refer to [Bellah et al. 2016, Bridy and Garton 2016, Burnette and

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FIGURE 1.1. The functional graph of $X^2 + 12 \pmod{31}$

Schmutz 2017, Flynn and Garton 2014, Konyagin et al. 2016, Ostafe and Sha 2016] and the references therein.

In this paper, we concentrate on the case of quadratic polynomials over prime fields. In fact, up to isomorphism we only need to consider polynomials $f_a(X) = X^2 + a$, $a \in \mathbb{F}_p$ (see the proof of [Konyagin et al. 2016, Theorem 2.1]). For simplicity, we use $\mathcal{G}_a = \mathcal{G}_{f_a}$ to denote the functional graph generated by f_a . For this case, in [Konyagin et al. 2016, Section 4] the authors have provided numerical data for the number of distinct graphs \mathcal{G}_a , the statistics of cyclic points, the number of connected components, as well as the most popular component size.

Different from the aspects in [Konyagin et al. 2016], we consider several questions related to distributions of cyclic points and sizes of connected components of \mathcal{G}_a when a runs through the elements in \mathbb{F}_p . In particular, we are interested in characterising connected functional graphs \mathcal{G}_a , that is, the graphs which contain only one component (and thus only one cycle).

In this paper, we focus on characterising the functional graphs by providing direct parameters such as the number of (connected) components. We then characterise various cumulative parameters, such as the number of cyclic points and the shape of trees extracted from functional graphs. We highlight similarities and differences between functional graphs [Konyagin et al. 2016] and random mappings [Flajolet and Odlyzko 1990], and we also pay much attention to features of connected functional graphs. While obtaining theoretic results for these questions remains a challenge, we introduce efficient algorithms and present new interesting results of numerical experiments.

The rest of the paper is structured as follows. In Section 2, we develop a fast algorithm that determines whether a functional graph is connected, which is used to compute the number of connected functional graphs. In Section 3, we compare the number of cyclic points in connected graphs with those in all graphs modulo p. In Section 4 and Section 5 respectively, we consider the number of components with small number of cyclic points and with small size. Finally, in Section 6 we illustrate the statistics of trees in functional graphs.

Throughout the paper, we use the Landau symbol O. Recall that the assertion U = O(V) is equivalent to the inequality $|U| \leq cV$ with some absolute constant c > 0. To emphasise the dependence of the implied constant c on some parameter (or a list of parameters) ρ , we write $U = O_{\rho}(V)$. We also use the asymptotic symbol \sim .

2. Counting connected graphs

In this section, we introduce a new efficient algorithm that quickly detects connected functional graphs, and formulate some conjectures for the number of connected graphs based on our computations.

2.1. Preliminaries and informal ideas of the algorithm. Let \mathcal{I}_p be the set $a \in \mathbb{F}_p$ such that \mathcal{G}_a is connected. We also denote by $I_p = \#\mathcal{I}_p$ the number of connected graphs \mathcal{G}_a with $a \in \mathbb{F}_p$. Clearly the graph \mathcal{G}_0 is not connected, and also by [Vasiga and Shallit 2004, Corollary 18 (a)] \mathcal{G}_{-2} is also not connected if p > 3, and so $\mathcal{I}_p \subseteq \mathbb{F}_p \setminus \{0, -2\}$ if p > 3. In fact, the functional graphs with values a = 0 and a = -2 lead to graphs with a particular group structure (and thus the structure of these graphs deviates significantly from the other graphs, see [Vasiga and Shallit 2004]).

Essentially in [Konyagin et al. 2016, Algorithm 3.1], a rigorous deterministic algorithm using Floyd's cycle detection algorithm and needing O(p) function evaluations (that is, of complexity $p^{1+o(1)}$) has been used to test whether \mathcal{G}_a is a connected graph. Instead of evaluating I_p via this algorithm which would need $O(p^2)$ function evaluations, we introduce a more efficient heuristic approach in practice, which is specifically useful for computations of a family of graphs (not just a single graph). The main idea is to first check quickly whether \mathcal{G}_a has more than one small cycle (i.e., more than one component). A graph \mathcal{G}_a has a component with a *cycle* of size ℓ if and only if the equation $f_a^{(\ell)}(u) = u$ has a solution u which is not a solution to any of the equations $f_a^{(k)}(u) = u$ with $1 \leq k < \ell$. The roots of $f_a^{(\ell)}(u) = u$ are the *cyclic points* in the graph. For this we need the *dynatomic polynomials*

$$F_a^{(\ell)}(X) = \prod_{r|\ell} \left(f_a^{(r)}(X) - X \right)^{\mu(\ell/r)},$$

where $\mu(k)$ is the Möbius function, see [Silverman 2007, Section 4.1]. Moreover, we have

$$f_a^{(n)}(X) - X = \prod_{\ell \mid n} F_a^{(\ell)}(X), \quad n = 1, 2, \dots$$

For example

$$F_a^{(1)}(X) = X^2 - X + a$$
 and $F_a^{(2)}(X) = X^2 + X + a + 1$

and

$$F_a^{(3)}(X) = \left(f_a^{(3)}(X) - X\right) / \left(f_a^{(1)}(X) - X\right).$$

Clearly, if \mathcal{G}_a has a cycle of length ℓ , then any point in this cycle is a root of the polynomial $F_a^{(\ell)}(X)$. However, the roots of $F_a^{(\ell)}(X)$ might be not all lying in cycles of length ℓ ; for instance see [Silverman 2007, Example 4.2]. Certainly, \mathcal{G}_a is not connected if $F_a^{(\ell)}(X)$ has a root for two distinct values of $\ell = \ell_1, \ell_2$ with $\ell_1 \nmid \ell_2$ and $\ell_2 \nmid \ell_1$. Alternatively, if $F_a^{(\ell)}(X)$ has more than ℓ distinct roots, this indicates that \mathcal{G}_a has at least two cycles, which again implies that \mathcal{G}_a has more than one connected component.

As we show later, it turns out that this occurs frequently and thus we can rule out the connectivity of most of the graph \mathcal{G}_a , $a \in \mathbb{F}_p$ quickly. A relatively small number of remaining suspects can be checked via the rigorous deterministic algorithm from [Konyagin et al. 2016, Algorithm 3.1].

2.2. Algorithm. Algorithm 2.1 is to determine whether a graph is connected or not, where we in fact use $f_a^{(\ell)}(X)$ instead of $F_a^{(\ell)}(X)$.

The algorithm starts by checking if there is any cycle of size 1 in the graph. Since $X^p - X$ only contains simple roots and $f_a^{(1)}(X)$ has degree 2, if $gcd(X^p - X, f_a^{(1)}(X)) > 1$, then there are two cycles of size 1 and thus two separate components in the graph. Otherwise, there is at most one component with a cycle of size 1 in the graph \mathcal{G}_a .

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Require: prime p, integer $a \pmod{p}$ and integer L.

Ensure: returns true if $X^2 + a \pmod{p}$ generates a connected functional graph, and false otherwise

```
1: cycles \leftarrow 0
 2: g_1 \leftarrow \gcd(X^p - X, f_a^{(1)}(X) - X)
 3: if deg g_1 \ge 1 then
       if deg q_1 = 2 then
 4:
 5:
          return false
 6:
       end if
 7:
       cycles \leftarrow cycles + 1
 8: end if
 9: for i \leftarrow 2 to L do
       g_i \leftarrow \gcd(X^p - X, f_a^{(i)}(X) - X)
10:
       if deg g_i > i then
11:
         return false
12:
       else if deg q_i = i then
13:
          cycles \leftarrow cycles + 1
14:
       end if
15:
       if cycles > 1 then
16:
          return false
17:
       end if
18:
19: end for
20: for j \leftarrow 0 to p-1 do
       start traversal from node j
21:
       if two cycles are detected then
22:
          return false
23:
       end if
24:
25: end for
26: return true
```

Next, we compute $g_i = \gcd(X^p - X, f_a^{(i)}(X) - X)$ from i = 2 until L while keeping track of the number of cycles that has been detected. Here, we have several possibilities:

- if deg $g_i < i$, then there are no cycle of size *i* in the graph.
- if deg $q_i = i$, then there is exactly one cycle of size *i*.
- if deg $g_i > i$, then there are at least two different cycles in the graph.

When deg $g_i < i$, there are no cycle of size *i* since there are not enough roots to form one. Similarly, if deg $g_i > i$, then there are more

than i cyclic points in the graph, of which at least i of them form one cycle, and so there are more than one cycle in the graph.

Finally, if at this stage the algorithm detects deg $g_i = i$, then there is exactly one cycle of size i. By contradiction, if there is no cycle of size i, then there must be at least two cycles of size less than i, and so we would have detected that cycles > 1 at a previous iteration, thus returning 'false'.

Once we are done with the first loop, either we have found one cycle with size at most L, or we have not found any small cycles at all. We then proceed with a graph traversal until we find two cycles.

2.3. Statistics of the number of connected graphs. We implement Algorithm 2.1 by using NTL [NTL 2016] and PARI/GP [Pari 2016], choosing L = 5 in our computations. We collect values of I_p for some primes (as shown in Table 2.1) that lead us to the following conjecture:

Conjecture 2.1. $I_p \sim \sqrt{2p} \ as \ p \to \infty$.

Here, we also pose a weaker conjecture:

Conjecture 2.2. For any prime $p, I_p \ge 1$.

Conjecture 2.2 predicts that there always exists a connected functional graph generated by quadratic polynomials modulo p. Indeed, according to our computations, Conjecture 2.2 is true for all primes $p \leq 100000$.

p	I_p	$\sqrt{2p}$
500,009	1,038	1,000.009
500,029	1,002	1,000.029
500,041	956	1,000.041
$500,\!057$	1,026	$1,\!000.057$
500,069	995	1,000.069
500,083	987	$1,\!000.083$
500,107	994	$1,\!000.107$
500,111	1,010	1,000.111
$500,\!113$	1,019	1,000.113
$500,\!119$	920	1,000.119
$500,\!153$	$1,\!033$	$1,\!000.153$
500,167	$1,\!005$	1,000.167
$1,\!000,\!003$	$1,\!369$	$1,\!414.296$
$2,\!000,\!003$	$1,\!909$	2,000.001
$3,\!000,\!017$	$2,\!478$	$2,\!449.497$
$4,\!000,\!037$	$2,\!838$	$2,\!828.440$

TABLE 2.1. The number of connected graphs modulo p

We also investigate the existence of connected functional graphs having (only) one cycle of size 1.

If the graph \mathcal{G}_a is connected and has one cycle of size 1, then the equation $X^2 + a = X$ has two identical roots (corresponding to fixed points), and so a = 1/4 and the root x = 1/2. Thus, we only need to check the graph generated by $X^2 + 1/4$ in \mathbb{F}_p .

We have tested all the primes up to 100000 and we only have found two such examples: one is $X^2 + 1$ in \mathbb{F}_3 , and the other is $X^2 + 2$ in \mathbb{F}_7 . Furthermore, we have:

Proposition 2.3. For any prime p with $p \equiv 5$ or 11 (mod 12), there is no functional graph \mathcal{G}_a having only one cycle of size 1.

Proof. Note that we only need to consider the graph $\mathcal{G}_{1/4}$. Since 1/2 is a fixed point of $\mathcal{G}_{1/4}$ and there is an edge from -1/2 to 1/2, we consider the equation $X^2 + 1/4 = -1/2$ in \mathbb{F}_p , that is, whether -3 is a square in \mathbb{F}_p . However, if $p \equiv 5$ or 11 (mod 12), -3 is not a square in \mathbb{F}_p . Then, the in-degree of -1/2 is zero, and so $\mathcal{G}_{1/4}$ must have more than one cycle. This completes the proof.

So, we pose the following conjecture:

Conjecture 2.4. For any prime p > 7, there is no functional graph \mathcal{G}_a having only one cycle of size 1.

3. Counting cyclic points in functional graphs

We now assess the number of cyclic points in functional graphs modulo p. For the minimal and maximal numbers of cyclic points in graphs \mathcal{G}_a , we refer to [Konyagin et al. 2016, Table 4.1], where the cases a = 0, -2 are excluded. Roughly speaking, the reason why these two cases are excluded is that the number of cyclic points is maximized on the cases a = 0, -2 quite often; see [Konyagin et al. 2016, Section 4.3] for more details. In this section, we also follow this convention.

Let C_a be the total number of cyclic points of \mathcal{G}_a , and let c_a be the largest number of cyclic points in a single component of \mathcal{G}_a . Clearly we have $C_a \ge c_a$ for any $a \in \mathbb{F}_p$ and $C_a = c_a$ when $a \in \mathcal{I}_p$.

Furthermore, we define the average and largest values of these quantities:

$$\overline{C_p} = \frac{1}{p-2} \sum_{a \in \mathbb{F}_p \setminus \{0, -2\}} C_a, \qquad \mathbf{C}_p = \max \left\{ C_a : a \in \mathbb{F}_p \setminus \{0, -2\} \right\};$$

$$\overline{c_p} = \frac{1}{p-2} \sum_{a \in \mathbb{F}_p \setminus \{0, -2\}} c_a, \qquad \mathbf{c}_p = \max \left\{ c_a : a \in \mathbb{F}_p \setminus \{0, -2\} \right\};$$

$$\overline{c_p}^* = \frac{1}{I_p} \sum_{a \in \mathcal{I}_p} c_a, \qquad \mathbf{c}_p^* = \max \left\{ c_a : a \in \mathcal{I}_p \right\}.$$

We remark again that $\mathcal{I}_p \subseteq \mathbb{F}_p \setminus \{0, -2\}$ if p > 3.

Numerical experiments in [Konyagin et al. 2016, Section 4.3] suggest that the average number of cyclic points modulo p, taken over all graphs modulo p (excluding a = 0, -2), is $\sqrt{\pi p/2}$, which is consistent with the behaviour of random maps (see [Flajolet and Odlyzko 1990, Theorem 2(ii)]). Here we show that this is not the case for connected graphs (see Table 3.1). In that case, $\overline{c_p}^*$ is smaller than $\overline{C_p}$, i.e. there are fewer cyclic points than those for non-connected graphs on average. Notice that both $\overline{c_p}^*$ and $\overline{c_p}$ are both close to $\sqrt{2p/\pi}$ (and although close to each other, $\overline{c_p}^*$ is slightly larger).

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p	$\overline{C_p}$	$\sqrt{\pi p/2}$	$\overline{c_p}$	$\overline{c_p}^*$	$\sqrt{2p/\pi}$
500,009	886.224	886.235	553.445	573.355	564.194
500,029	885.990	886.253	553.312	587.750	564.205
500,041	885.069	886.263	553.175	568.208	564.212
500,057	884.963	886.277	552.870	586.037	564.221
500,069	885.831	886.288	552.952	558.285	564.229
500,083	884.970	886.300	552.692	564.995	564.236
500,107	884.507	886.322	552.674	562.690	564.250
500,111	884.341	886.325	552.157	575.976	564.252
$500,\!113$	885.160	886.327	552.988	568.057	564.253
500, 119	884.559	886.332	552.597	569.750	564.257
$500,\!153$	884.834	886.363	552.900	589.146	564.276
500,167	885.756	886.375	552.525	560.095	564.284
600,011	969.139	970.822	605.632	611.914	618.044
700,001	$1,\!047.771$	1,048.599	654.317	667.624	667.559
800,011	$1,\!120.427$	$1,\!121.006$	700.047	703.061	713.655
900,001	$1,\!188.822$	$1,\!188.999$	742.619	762.673	756.940
1,000,003	$1,\!252.452$	$1,\!253.316$	782.026	793.388	797.886
$2,\!000,\!003$	1,772.078	1,772.455	$1,\!106.815$	$1,\!134.598$	$1,\!128.380$

TABLE 3.1. Average number of cyclic points in graphs modulo p (excluding a = 0, -2)

In Table 3.2, one can see that the largest cycles usually do not appear in the connected graphs, which appears surprising and shows the existence of components with a large cycle even when the graph is disconnected. In addition, the difference $\mathbf{c}_p - \mathbf{c}_p^*$ is large, while the difference of \mathbf{C}_p and \mathbf{c}_p is small.

p	\mathbf{C}_p	\mathbf{c}_p	\mathbf{c}_p^*
500,009	$3,\!578$	3,164	2,319
500,029	$3,\!620$	3,291	2,327
500,041	3,798	3,118	2,333
500,057	3,468	3,319	2,423
500,069	3,556	$3,\!129$	2,089
500,083	3,596	$3,\!050$	2,131
500,107	3,527	3,232	2,643
500,111	3,732	3,237	2,244
500,113	3,805	3,232	2,335
500,119	3,873	3,142	2,275
500,153	3,472	3,380	2,754
500,167	3,644	$3,\!159$	2,770
600,011	3,847	$3,\!488$	3,265
700,001	4,350	$3,\!670$	2,950
800,011	4,600	4,242	3,208
900,001	4,997	4,274	3,245
1,000,003	5,101	4,639	3,117
2,000,003	7,637	6,848	4,309

TABLE 3.2. Maximum number of cyclic points in graphs modulo p (excluding a = 0, -2)

Let us also define the following three families of parameters a on which the values \mathbf{C}_p , \mathbf{c}_p and \mathbf{c}_p^* are achieved, that is

$$\mathcal{A}_p = \left\{ a \in \mathbb{F}_p \setminus \{0, -2\} : C_a = \mathbf{C}_p \right\},$$

$$\mathcal{B}_p = \left\{ a \in \mathbb{F}_p \setminus \{0, -2\} : c_a = \mathbf{c}_p \right\},$$

$$\mathcal{B}_p^* = \left\{ a \in \mathcal{I}_p : c_a = \mathbf{c}_p^* \right\}.$$

It is certainly interesting to compare the sizes $A_p = #\mathscr{A}_p$, $B_p = #\mathscr{B}_p$ and $B_p^* = #\mathscr{B}_p^*$ and also investigate the mutual intersections between these families.

We find that typically these sets have one value of a in common, and rarely more than two. As p increases, the frequency of the sets having 2 or more elements decreases, but does not disappear completely, as can be seen in Table 3.3.

		A_p			B_p			B_p^*	
range of p	= 1	= 2	$\geqslant 3$	= 1	= 2	$\geqslant 3$	= 1	= 2	$\geqslant 3$
$[3, 10^4]$	1,182	39	7	$1,\!159$	65	4	$1,\!193$	35	0
$[10^4, 2 \cdot 10^4]$	1,013	20	0	1,010	22	1	1,019	14	0
$[2 \cdot 10^4, 3 \cdot 10^4]$	967	14	2	970	13	0	976	7	0
$[3 \cdot 10^4, 4 \cdot 10^4]$	949	9	0	941	17	0	950	8	0
$[4 \cdot 10^4, 5 \cdot 10^4]$	921	8	1	921	9	0	926	4	0
$[5 \cdot 10^4, 6 \cdot 10^4]$	915	9	0	920	4	0	921	3	0
$[6 \cdot 10^4, 7 \cdot 10^4]$	868	10	0	872	6	0	868	9	1
$[7 \cdot 10^4, 8 \cdot 10^4]$	895	7	0	897	5	0	899	3	0
$[8 \cdot 10^4, 9 \cdot 10^4]$	869	7	0	869	7	0	866	10	0
$[9 \cdot 10^4, 10^5]$	874	5	0	878	1	0	876	3	0
$[10^5, 10^5 + 10^3]$	81	0	0	79	2	0	81	0	0
$[10^6, 10^6 + 10^3]$	74	1	0	75	0	0	74	1	0

TABLE 3.3. Values of A_p , B_p , and B_p^*

For the set intersections, we start with $\mathscr{A}_p \cap \mathscr{B}_p^*$. With Table 3.1, we have observed that $\overline{C_p} > \overline{c_p}^*$, thus it is reasonable to expect that $\mathscr{A}_p \cap \mathscr{B}_p^*$ is empty. We remark that if $\mathscr{A}_p \cap \mathscr{B}_p^*$ is not empty, then $\mathbf{C}_p = \mathbf{c}_p = \mathbf{c}_p^*$, and so for any $a \in \mathscr{B}_p$ the graph \mathscr{G}_a is connected, and thus $\mathscr{B}_p = \mathscr{B}_p^*$. Therefore, for any prime p, if $\mathbf{c}_p < \mathbf{C}_p$, then we must have that $\mathscr{A}_p \cap \mathscr{B}_p^*$ is empty. Our experiments with odd prime $p < 10^5$ counted only 20 occurrences of primes where the intersection is non-empty and in fact contains only one value of a, shown in Table 3.4.

p	value of a	p	value of a
3	2	271	147
5	1	$2,\!647$	1,445
$\overline{7}$	3	$3,\!613$	$2,\!653$
11	6	$6,\!131$	$3,\!555$
13	1	6,719	107
17	3	$17,\!921$	$8,\!370$
19	13	$18,\!077$	$15,\!557$
29	4	$36,\!229$	2,229
157	141	$53,\!611$	$23,\!630$
191	97	$64,\!667$	$60,\!638$

TABLE 3.4. Values of p with non-empty $\mathscr{A}_p \cap \mathscr{B}_p^*$

Since we have observed only one value of a for each prime p in the above table, we conjecture that:

Conjecture 3.1. For any prime $p \ge 3$, we have $\# \left(\mathscr{A}_p \cap \mathscr{B}_p^* \right) \le 1$.

We also consider the intersection $\mathscr{B}_p \cap \mathscr{B}_p^*$; see Table 3.5. Clearly, if $\mathscr{B}_p \cap \mathscr{B}_p^*$ is not empty, then we have $\mathbf{c}_p = \mathbf{c}_p^*$. One could expect the number of primes with non-empty intersections to decrease as p increases, however even if our experiments show some reduction overall, it remains unclear.

range of p	freq	#primes	%
$[3, 10^4]$	104	1,228	8.06%
$[10^4, 2 \cdot 10^4]$	35	1,033	3.19%
$[2 \cdot 10^4, 3 \cdot 10^4]$	32	983	3.26%
$[3 \cdot 10^4, 4 \cdot 10^4]$	20	958	1.98%
$[4 \cdot 10^4, 5 \cdot 10^4]$	19	930	2.04%
$[5 \cdot 10^4, 6 \cdot 10^4]$	16	924	1.73%
$[6 \cdot 10^4, 7 \cdot 10^4]$	20	878	2.28%
$[7 \cdot 10^4, 8 \cdot 10^4]$	15	902	1.66%
$[8 \cdot 10^4, 9 \cdot 10^4]$	15	876	1.71%
$[9 \cdot 10^4, 10^5]$	6	879	0.68%
$[10^5, 10^5 + 10^3]$	0	81	0.00%
$[10^6, 10^6 + 10^3]$	1	75	1.33%

TABLE 3.5. Primes with non-empty $\mathscr{B}_p \cap \mathscr{B}_p^*$

The most surprising result comes from the observation of the intersection $\mathscr{A}_p \cap \mathscr{B}_p$. As Table 3.6 shows, the event that this intersection is not empty is rather common. For any $a \in \mathscr{A}_p \cap \mathscr{B}_p$, the graph \mathcal{G}_a not only has the maximal number of cyclic points but also has a maximal cycle.

Note that for the last two rows we only give primes in the ranges $[10^5, 10^5 + 10^3]$ and $[10^6, 10^6 + 10^3]$, respectively, due to the limits of our current computational facilities.

range of p	freq	#primes	%
$[3, 1 \cdot 10^4]$	268	1,228	20.36%
$[10^4, 2 \cdot 10^4]$	197	1,033	18.87%
$[2 \cdot 10^4, 3 \cdot 10^4]$	153	983	15.16%
$[3 \cdot 10^4, 4 \cdot 10^4]$	148	958	15.24%
$[4 \cdot 10^4, 5 \cdot 10^4]$	126	930	13.55%
$[5 \cdot 10^4, 6 \cdot 10^4]$	167	924	17.97%
$[6 \cdot 10^4, 7 \cdot 10^4]$	143	878	16.17%
$[7 \cdot 10^4, 8 \cdot 10^4]$	143	902	15.74%
$[8 \cdot 10^4, 9 \cdot 10^4]$	144	876	16.44%
$[9 \cdot 10^4, 10^5]$	147	879	16.72%
$[10^5, 10^5 + 10^3]$	13	81	16.05%
$[10^6, 10^6 + 10^3]$	9	77	11.69%

TABLE 3.6. Primes with non-empty $\mathscr{A}_p \cap \mathscr{B}_p$

4. Statistics of small cycles

We now study components by analysing the distribution of the size of their cycles. Let $\mathcal{C}_{a,k}$ be the number of cycles of length k in the graph \mathcal{G}_a . Let

$$\mathcal{C}_k = \sum_{a \in \mathbb{F}_p} \mathcal{C}_{a,k}$$

be the number of cycles of length k over all graphs modulo p. Clearly, we have $C_k = 0$ for any $k \ge p/2$; see [Peinado et al. 2001, Theorems 1 and 2] for better bounds of k.

Proposition 4.1. For any integer $k \ge 1$, there is a constant D_k depending only on k such that for any prime $p > D_k$ we have

$$C_k = p/k + O\left(4^k k^{-1} p^{1/2}\right).$$

Proof. We can assume that p > k. For any fixed a, notice that any point x contributing to $\mathcal{C}_{a,k}$ is a root of the polynomial $F_a^{(k)}(X)$. Conversely, any root x of $F_a^{(k)}(X)$ contributes to $\mathcal{C}_{a,d}$ for some $d \mid k$ (possibly $d \neq k$). Thus, we have

$$k\mathcal{C}_k \leq \#\{(a,x) \in \mathbb{F}_p^2 : F_a^{(k)}(x) = 0\}$$

Moreover, from [Morton and Patel 1994, Theorem 2.4 (c)] and noticing $p \nmid k$, we know that if $F_a^{(d)}(x) = 0$ and $F_a^{(k)}(x) = 0$ with d < k, where x is a point lying in a cycle of length k, then $(X - x)^2 \mid F_a^{(k)}(X)$, that is, the discriminant of $F_a^{(k)}(X)$ is zero. Note that as a polynomial in

X the degree of $F_a^{(k)}(X)$ is at most 2^k , and as a polynomial in a the degree of $F_a^{(k)}(X)$ is at most 2^{k-1} . Then, as a polynomial in a, the degree of the discriminant of $F_a^{(k)}(X)$ is at most 4^k . Thus, except for at most 4^k values of a, we have that $F_a^{(k)}(X)$ is a simple polynomial in X. Hence, we have

(4.1)
$$k\mathcal{C}_k = \#\{(a,x) \in \mathbb{F}_p^2 : F_a^{(k)}(x) = 0\} + O(8^k).$$

In addition, combining [Morton 1996, Corollary 1 to Theorem B] with [Morton and Vivaldi 1995, Proposition 3.2], if we view $f_A(X) = X^2 + A$ as an integer polynomial in variables A and X, then $F_A^{(k)}(X) \in \mathbb{Z}[A, X]$ is an absolutely irreducible polynomial. Then, by Ostrowski's theorem, there exists a positive integer D_k depending only on k such that for any $p > D_k$ the polynomial $F_A^{(k)}(X)$ is absolutely irreducible modulo p in variables A and X. It is also easy to see by induction on k that $f_A^{(k)}(X)$ is of total degree at most 2^k as a bivariate polynomial in A and X, and the same is true for $F_A^{(k)}(X)$. Thus, by the Hasse-Weil bound (see [Lorenzini 1996, Section VIII.5.8]) we obtain

$$\#\{(a,x) \in \mathbb{F}_p^2: F_a^{(k)}(x) = 0\} = p + O(4^k p^{1/2}), \text{ as } p \to \infty,$$

which, together with (4.1), implies the desired result (as we can always assume that $D_k > 4^k$, so $4^k p^{1/2} > 8^k$).

In particular, we see from Proposition 4.1 that for any fixed integer $k \ge 1$,

$$C_k \sim p/k, \quad \text{as } p \to \infty$$

Note that using [Gao and Rodrigues 2003, Theorem 1] or [Ruppert 1986, Satz B] or [Zannier 1997, Corollary], one can obtain an explicit form for D_k . However, any such estimate has to depend on the size of the coefficients of $F_A^{(k)}(X)$ (considered as a bivariate polynomial in A and X over \mathbb{Z}) and is likely to be double exponential in k.

We can also compute the exact values of C_1 and C_2 .

Proposition 4.2. For any odd prime p, we have $C_1 = p$ and $C_2 = (p-1)/2$.

Proof. First, note that any point x contributing to C_1 is a root of $F_a^{(1)}(X)$ for some a, and also

$$F_a^{(1)}(X) = X^2 - X + a = (X - 1/2)^2 + a - 1/4 = 0$$

is solvable if and only if 1/4 - a is a square. Since there are (p-1)/2 squares in \mathbb{F}_p^* , we have $\mathcal{C}_1 = p$.

Now, it is easy to see that

$$F_a^{(2)}(X) = X^2 + X + a + 1.$$

If a point x lies in a cycle of length 2 in \mathcal{G}_a , then it is a root of $F_a^{(2)}(X)$ and also it is not a root of $F_a^{(1)}(X)$. However, if there exists a point x such that

$$F_a^{(2)}(x) = F_a^{(1)}(x) = 0,$$

then we must have x = -1/2, a = -3/4. So, if $a \neq -3/4$, then any root of $F_a^{(2)}(X)$ lies in a cycle of length 2. Thus, noticing that

$$F_a^{(2)}(X) = (X + 1/2)^2 + a + 3/4 = 0$$

is solvable if and only if -a - 3/4 is a square, we have $C_2 = (p - 1)/2$ and conclude the proof.

Table 4.1 shows the C_k for some values of p (in these cases, we also included the graphs X^2 and $X^2 - 2$). This is consistent with Proposition 4.1.

k	p = 100,003		p = 50	00,009	p = 1,000,003	
	\mathcal{C}_k	$\lfloor p/k floor$	\mathcal{C}_k	$\lfloor p/k floor$	\mathcal{C}_k	$\lfloor p/k floor$
1	100,003	100,003	500,009	500,009	1,000,003	1,000,003
2	50,001	50,001	250,004	250,004	500,001	500,001
3	33,333	$33,\!334$	$166,\!669$	$166,\!669$	$333,\!333$	$333,\!334$
4	24,890	25,000	125,000	125,002	$249,\!890$	250,000
5	20,061	20,000	99,353	100,001	199,310	200,000
6	16,775	$16,\!667$	$83,\!664$	$83,\!334$	$165,\!852$	$166,\!667$
7	$14,\!179$	14,286	$71,\!582$	$71,\!429$	$143,\!109$	$142,\!857$
8	$12,\!474$	12,500	$62,\!541$	$62,\!501$	$125,\!266$	$125,\!000$

TABLE 4.1. Number of cycles of length k

5. Distribution of components with size k

We now study the components of functional graphs by analysing the distribution of their sizes. For the minimal and maximal numbers of components in graphs \mathcal{G}_a as well as the popular component size, we refer to [Konyagin et al. 2016, Sections 4.4 and 4.5].

Let \mathcal{N}_p be the number of components taken over all \mathcal{G}_a modulo p, and let $\mathcal{N}_{p,k}$ be the number of those components with size k > 0 (that is, there are k nodes in the component). Furthermore, let

$$\mathcal{N}_{p,\text{even}}^{K} = \sum_{\substack{k \leqslant K \\ k \text{ even}}} \mathcal{N}_{p,k} \text{ and } \mathcal{N}_{p,\text{odd}}^{K} = \sum_{\substack{k \leqslant K \\ k \text{ odd}}} \mathcal{N}_{p,k}.$$

Clearly,

$$\mathcal{N}_p = \mathcal{N}_{p,\text{even}}^p + \mathcal{N}_{p,\text{odd}}^p$$

We first have:

Proposition 5.1. For any odd prime p, $\mathcal{N}_{p,2} = (p-1)/2$.

Proof. If C is a component of \mathcal{G}_a of size 2, then it is easy to see that $C = \{x, -x\}$ for some $x \in \mathbb{F}_p$ such that x is a fixed point (that is, $x^2 + a = x$) and the equation $X^2 + a = -x$ has no solution in \mathbb{F}_p (that is, -x - a is not a square).

In other words, for any $x \in \mathbb{F}_p$, if we choose $a = -x^2 + x$, then x is a fixed point in \mathcal{G}_a and $-x - a = x^2 - 2x$. So, it is equivalent to count how many $x \in \mathbb{F}_p$ such that $x^2 - 2x$ is not a square in \mathbb{F}_p . Since $x^2 - 2x = (x - 1)^2 - 1$, it is also equivalent to count how many $x \in \mathbb{F}_p$ such that $x^2 - 1$ is not a square in \mathbb{F}_p .

such that $x^2 - 1$ is not a square in \mathbb{F}_p . If $x^2 - 1$ is a square in \mathbb{F}_p , say $x^2 - 1 = y^2$, then we have (x+y)(x-y) = 1. Let $\alpha = x + y$, then $x - y = \alpha^{-1}$, and so

$$x = \frac{\alpha + \alpha^{-1}}{2}, \qquad y = \frac{\alpha - \alpha^{-1}}{2}.$$

So, for such pairs (x, y) we obtain a one-to-one correspondence between pairs (x, y) and pairs $(\alpha, \alpha^{-1}), \alpha \neq 0$. It is easy to see that for any $\alpha_1, \alpha_2 \in \mathbb{F}_p^*$,

$$\frac{\alpha_1 + \alpha_1^{-1}}{2} = \frac{\alpha_2 + \alpha_2^{-1}}{2}$$
 if and only if $\alpha_1 \alpha_2 = 1$.

So, by counting the pairs (α, α^{-1}) , there are (p+1)/2 values of x such that $x^2 - 1$ is a square. Therefore, there are (p-1)/2 values of x such that $x^2 - 1$ is not a square. This completes the proof. \Box

It has been predicted in [Flajolet and Odlyzko 1990, Theorem 2 (i)] that

$$\mathcal{N}_p \sim \frac{p \log p}{2},$$

which has a small bias (about 9.5%) over the real value; see [Konyagin et al. 2016, Table 4.2]. Here, we improve the precision of this estimate. First, we note that each node in \mathcal{G}_a has in-degree two or zero except for the node a, since only 0 maps to a. Therefore, each component in any graph \mathcal{G}_a has an even number of nodes unless it is the component containing 0 and a. So, each graph \mathcal{G}_a has exactly one component of odd size. It follows that

$$\mathcal{N}_{p,\text{odd}}^p = p,$$

and so

$$\mathcal{N}_p \sim \mathcal{N}_{p,\text{even}}^p$$
, as $p \to \infty$.

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For even-sized components, the situation is not as straightforward. In our experiments, we noticed that the number of even-sized components with size k is very close to p/k as shown in Table 5.1 for $k \leq 20$ and for k = 1000 and 2000 (i.e., even for larger values of k).

k	p = 10	00,003	p = 50	00,009	p = 1, 0	000,003
	$\mathcal{N}_{p,k}$	$\lfloor p/k floor$	$\mathcal{N}_{p,k}$	$\lfloor p/k floor$	$\mathcal{N}_{p,k}$	$\lfloor p/k floor$
2	50,001	50,001	250,004	250,004	500,001	500,001
4	24,951	25,000	125,160	125,002	250,171	250,000
6	$16,\!156$	$16,\!667$	$83,\!185$	$83,\!334$	$166,\!660$	$166,\!667$
8	12,509	12,500	$62,\!652$	62,501	124,727	$125,\!000$
10	10,083	10,000	50,422	50,000	$99,\!975$	100,000
12	$8,\!389$	8,333	$41,\!542$	$41,\!667$	$82,\!577$	$83,\!333$
14	$7,\!192$	$7,\!143$	$35,\!661$	35,714	$71,\!611$	$71,\!428$
16	$6,\!292$	$6,\!250$	$31,\!186$	$31,\!350$	62,220	$62,\!500$
18	5,503	$5,\!555$	$27,\!941$	27,778	$55,\!923$	$55,\!555$
20	5,009	$5,\!000$	$24,\!662$	$25,\!000$	$50,\!135$	50,000
1000	117	100	533	500	954	$1,\!000$
2000	48	50	243	250	489	500

TABLE 5.1. Number of components of size k

Now, using $\lfloor p/k \rfloor$ as an approximation of the number of components of size k for any even k < p, we can get an approximation for $\mathcal{N}_{p,\text{even}}^p$. First, when (p-1)/2 < k < p, we have $\lfloor p/k \rfloor = 1$, and there are about (p-1)/4 values of such even k. In general, if $(p-1)/(n+1) < k \leq (p-1)/n$, we have $\lfloor p/k \rfloor = n$, and there are about $\frac{p-1}{2n(n+1)}$ values of such even k, which contributes to around $\frac{p-1}{2(n+1)}$ components of even size.

Fixing a positive integer n, for k > (p-1)/(n+1) we use the above estimate, while for $k \leq (p-1)/(n+1)$ we use the estimate (p-1)/k, and so the total number of components of even size is around

$$\frac{p-1}{2} \left(1 + \frac{1}{2} + \dots + \frac{1}{(p-1)/(2(n+1))} \right) \\ + \frac{p-1}{2} \left(\frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n+1} \right),$$

which, together with the approximation of the harmonic series, is approximated by

$$\frac{p-1}{2} \left(\log \frac{p-1}{2(n+1)} + \gamma \right) + \frac{p-1}{2} \left(-1 + \log(n+1) + \gamma \right)$$
$$= \frac{p-1}{2} \left(\log(p-1) + 2\gamma - 1 - \log 2 \right)$$

where $\gamma = 0.5772156649...$ is the Euler constant. So, we denote

$$\widetilde{\mathcal{N}}_{p,\text{even}}^p = \frac{p-1}{2} \left(\log(p-1) + 2\gamma - 1 - \log 2 \right),$$

which is an approximation of $\mathcal{N}_{p,\text{even}}^p$.

Table 5.2 shows the difference between the two values for several large primes. We overestimate the actual value by about 2%.

p	$\mathcal{N}_{p, ext{even}}^K$	$\mathcal{N}_{p, ext{even}}^p$	\mathcal{N}_p	$\widetilde{\mathcal{N}}_{p,\mathrm{even}}^p$
100,003	$521,\!337$	$538,\!640$	638,643	548,722
200,003	$1,\!113,\!083$	$1,\!147,\!694$	$1,\!347,\!697$	1,166,748
300,007	1,730,420	1,782,805	$2,\!082,\!812$	$1,\!810,\!962$
400,009	$2,\!364,\!734$	$2,\!434,\!894$	$2,\!834,\!903$	$2,\!472,\!154$
500,009	$3,\!011,\!626$	$3,\!098,\!914$	$3,\!598,\!923$	$3,\!145,\!966$
600,011	$3,\!667,\!637$	3,772,277	$4,\!372,\!288$	$3,\!829,\!859$
700,001	$4,\!333,\!622$	$4,\!455,\!913$	$5,\!155,\!914$	$4,\!522,\!041$
800,011	$5,\!005,\!995$	$5,\!145,\!194$	$5,\!945,\!205$	$5,\!221,\!530$
900,001	$5,\!685,\!731$	$5,\!842,\!337$	6,742,338	$5,\!927,\!145$
1,000,003	$6,\!369,\!257$	$6,\!543,\!317$	$7,\!543,\!320$	$6,\!638,\!411$

TABLE 5.2. Estimates for the number of components with even size and K = (p-1)/2

6. Shape of trees in functional graphs

Finally, in order to reveal more detailed features of functional graphs, we consider the trees attached to such graphs.

In the functional graph \mathcal{G}_a corresponding to f_a , each node in a cycle, except for a (if a lies in a cycle), is connected to a unique node (say w) which is not in the cycle. Naturally, we treat the node w as the root of the binary tree attached to a cyclic point in the graph \mathcal{G}_a . Thus, we can say that each node in a cycle of \mathcal{G}_a , expect for a, is associated with a binary tree – in fact a full binary tree, unless 0 is a node in the tree. For example, in Figure 1.1, there are 8 full binary trees attached to the cyclic points. Let $t_p(a, k)$ be the number of such binary trees with k nodes in \mathcal{G}_a , and let

$$T_p(k) = \sum_{a \in \mathbb{F}_p} t_p(a, k)$$
 and $T_p = \sum_{k=1}^{p-1} T_p(k);$

and for the connected graphs equivalents, let

$$T_p^*(k) = \sum_{a \in \mathcal{I}_p} t_p(a, k)$$
 and $T_p^* = \sum_{k=1}^{p-1} T_p^*(k).$

Note that T_p is the total number of trees attached to all such functional graphs \mathcal{G}_a , and T_p^* has a similar meaning but with restriction to connected functional graphs.

An interesting question is whether these trees behave similarly to random full binary trees. First we observe that there is a significant proportion of trees with just one node, as shown in Table 6.1 for the general case and in Table 6.2 for connected graphs. This motivates us to pose the following conjecture, which seems to be reasonable because exactly half of elements in \mathbb{F}_p^* are not square.

Conjecture 6.1. We have $T_p(1)/T_p \sim 1/2$ as $p \to \infty$.

p	$T_p(1)$	T_p	%
50,111	7,090,084	14,091,820	50.31%
100,003	$19,\!845,\!915$	$39{,}530{,}737$	50.20%
200,003	$56,\!210,\!936$	$112,\!088,\!213$	50.15%
300,007	$103,\!203,\!596$	$205,\!901,\!181$	50.12%
400,009	$158,\!746,\!944$	$317,\!089,\!081$	50.06%
500,009	$221,\!941,\!725$	443,336,032	50.06%
1,000,003	627,460,216	$1,\!253,\!326,\!817$	50.06%

TABLE 6.1. Number of trees with one node

p	$T_{p}^{*}(1)$	T_p^*	%
50.111	27.877	55.668	50.08%
100,003	$52,\!923$	$105,\!612$	50.11%
200,003	115,746	$231,\!583$	49.98%
300,007	$161,\!975$	$323,\!410$	50.08%
400,009	$222,\!865$	$445,\!931$	49.98%
500,009	298,060	$595,\!142$	50.08%
$1,\!000,\!003$	$542,\!592$	$1,\!086,\!147$	49.96%

TABLE 6.2. Number of trees with one node in connected graphs

Second, for large trees, we check the average height of the trees in the graphs. It has been shown in [Flajolet and Odlyzko 1982, Theorem B] that the average height of full binary trees with n internal nodes is

$$\overline{H}_n \sim 2\sqrt{\pi n}$$
 as $n \to \infty$.

This means that for a random full binary tree, its height is asymptotic to $2\sqrt{\pi n}$ when *n* goes to the infinity. In our situation, for each tree with *n* internal nodes and height H_n , we compute the ratio $H_n/2\sqrt{\pi n}$ and find the average of this ratio for all graphs modulo *p*. (Again, a tree is not always guaranteed to be a full binary tree, since 0 might be a node in the tree, but the impact of this happening is negligible, and at any case, we collect trees of both sizes 2n and 2n + 1.)

In Table 6.3, we compare the ratio of $\overline{H}_n/2\sqrt{\pi n}$ (see [Flajolet and Odlyzko 1982, Table II]) with the average ratio of $H_n/2\sqrt{\pi n}$ of the trees in our graphs. One can see that they are close.

n	$\overline{H}_n/2\sqrt{\pi n}$	average of $H_n/2\sqrt{\pi n}$		
		p = 50111	p = 100003	p = 200003
50	0.797	0.837	0.837	0.837
100	0.846	0.875	0.873	0.872
500	0.920	0.952	0.925	0.941
$1,\!000$	0.940	0.925	0.948	0.942
2,000	0.956	0.981	0.944	0.960
$5,\!000$	0.970	0.927	0.916	0.977

TABLE 6.3. Average height of trees

7. FUTURE DIRECTIONS

One of the most important directions in this area is developing an adequate random model predicting the statistical characteristics of the functional graphs of polynomials, see [Martin and Panario 2016] for some initial, yet promising results in this direction.

Based on our computations, we pose several conjectures about the functional graphs of quadratic polynomials. Investigating whether they are true or not may help to characterise functional graphs generated by quadratic polynomials and understand the similarities and differences between these functional graphs and random mappings.

The other interesting problem is to count the number of functional graphs modulo p generated by quadratic polynomials up to isomorphism; see [Konyagin et al. 2016, Theorem 2.8] for a lower bound. In [Gilbert et al. 2001, Conjecture C] the authors conjectured that for any odd prime $p \neq 17$, there are p such functional graphs up to isomorphism, and they confirmed this for all the odd primes up to 1009 not equal to 17. Under our computations, we confirm this conjecture for all the odd primes up to 100000 not equal to 17.

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B.M.: Department of Computing, Macquarie University, Sydney, NSW 2109, Australia

E-mail address: bernard.mans@mq.edu.au

M.S.: Department of Computing, Macquarie University, Sydney, NSW 2109, Australia

E-mail address: shamin2010@gmail.com

I.S.: DEPARTMENT OF PURE MATHEMATICS, UNIVERSITY OF NEW SOUTH WALES, SYDNEY, NSW 2052, AUSTRALIA

E-mail address: igor.shparlinski@unsw.edu.au

D.S.: Department of Computing, Macquarie University, Sydney, NSW 2109, Australia

E-mail address: daniel.sutantyo@gmail.com