## MATHEMATICAL ANALYSIS 3 (NMAI056) summer term 2023/24 lecturer: Martin Klazar

## **LECTURE 8 (April 9, 2024)** G. PÓLYA'S 1921 THEOREM ON RANDOM WALKS IN $\mathbb{Z}^d$ BY POWER SERIES

• Pólya's theorem, but first graphs and walks. Before we state this theorem, which can be classified equally well to belong to probability theory or (as we approach it here) to enumerative combinatorics, we need a number of definitions. A graph G = (V, E) consists of the set of vertices V and the set of edges  $E \subset {V \choose 2}$ . Here

$$\binom{V}{2} = \{A \mid A \subset V \land |A| = 2\}$$

is the set of all two-element subsets of the set V.

**Exercise 1** Find a formula for the number of all graphs with an n-element vertex set V.

However, in Pólya's theorem we will be interested in certain infinite graphs. A graph G = (V, E) is *d*-regular,  $d \in \mathbb{N}$ , if every vertex has *d* neighbors, that is,

$$\forall v \in V \left( \left| \left\{ u \in V \mid \{u, v\} \in E \right\} \right| = d \right).$$

*G* is *locally finite* if each vertex  $v \in V$  has only finitely many neighbors, i.e., the set N(v) is finite. A walk w in the graph G = (V, E) is a finite,  $w = (v_0, v_1, \ldots, v_n)$  with the length  $|w| = n \in \mathbb{N}_0$ , or infinite,  $w = (v_0, v_1, \ldots)$ , sequence of vertices  $v_i \in V$  such that for each  $i \in \mathbb{N}_0$  (< n),  $\{v_i, v_{i+1}\} \in E$ . We call  $v_0$  the start of the walk w. We define

 $d_n(v_0, G) = |\{w \mid w \subset V \text{ is a walk with start } v_0 \text{ and } |w| = n\}|.$ 

It is the number of walks in G with a given start  $v_0$  and length n.

**Exercise 2** Prove that in any d-regular graph,

$$d_n(v_0, G) = d^n .$$

A recurrent walk  $w = (v_0, v_1, \ldots, v_n)$  revisits the start: there exists  $i \in \{1, 2, \ldots, n\}$  such that  $v_i = v_0$ . Let

 $a_n(v_0, G) = |\{w \mid w \subset V \text{ is recurrent with start } v_0 \text{ and } |w| = n\}|$ be the number of recurrent walks in G with a given start  $v_0$  and length n.

An *automorphism* of the graph G = (V, E) is a bijection  $f \colon V \to V$  such that

$$\forall u, v \in V(\{u, v\} \in E \iff \{f(u), f(v)\} \in E).$$

**Exercise 3** Describe all automorphisms of the path  $P_6$  and the circle  $C_6$  of length 6. Here  $V = \{1, 2, ..., 6\}$ ,  $P_6$  has edges

 $E = \{\{1,2\}, \{2,3\}, \{3,4\}, \{4,5\}, \{5,6\}\}$ 

and  $C_6$  has edges

 $E = \{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 5\}, \{5, 6\}, \{6, 1\}\}.$ 

G = (V, E) is *(vertex) transitive* when

 $\forall u, v \in V \exists F (F \text{ is an automorphism of } G \land F(u) = v)$ .

**Proposition 4 (graph walks)** The number of walks, resp. of recurrent walks, of the given length in a transitive graph does not depend on the start: if G = (V, E) is transitive and locally finite, then for every  $n \in \mathbb{N}_0$  and every two vertices  $u, v \in V$ ,

 $d_n(u, G) = d_n(v, G), \ resp. \ a_n(u, G) = a_n(v, G) \;.$ 

**Proof.** Let  $u, v \in V$  be any two given vertices and  $n \in \mathbb{N}_0$ . Let F be an automorphism of G sending u to v. We consider *finite* sets of walks in the graph G with length n,

 $P_n = \{w \mid w \text{ has start } u\} \text{ and } Q_n = \{w \mid w \text{ has a start } v\}.$ 

For a map  $J: V \to V$  and a walk or any sequence of vertices  $w = (v_0, v_1, \ldots, v_n)$  we define

$$J(w) = (J(v_0), J(v_1), \dots, J(v_n))$$

It is then easy to see that the functions

$$P_n \ni w \mapsto F(w) \in Q_n \text{ and } Q_n \ni w \mapsto F^{-1}(w) \in P_n$$

are injections, so  $|P_n| = |Q_n|$ . For recurrent walks, the argument is the same.

In the transitive graphs G, we will therefore have the number of walks, or of recurrent walks, with length n denoted briefly as  $d_n(G)$ , or  $a_n(G)$ .

**Exercise 5** Give some examples showing that in a general graph the number of walks depends on the start.

**Exercise 6** Prove that the infinite path

$$P = (\mathbb{Z}, \{\{n, n+1\} \mid n \in \mathbb{Z}\})$$

is a transitive graph and compute, how many recurrent walks it contains with a given start and length 5.

A generalization of this graph is the graph  $(d \in \mathbb{N})$ 

$$\mathbb{Z}^d = (\mathbb{Z}^d, \{\{\overline{u}, \overline{v}\} \mid \sum_{i=1}^d |u_i - v_i| = 1\}),$$

where we write  $\overline{u} = (u_1, \ldots, u_d) \in \mathbb{Z}^d$ .

**Exercise 7** Prove that the graphs  $\mathbb{Z}^d$  are transitive and that  $\mathbb{Z}^d$  is 2*d*-regular.

Theorem 8 (G. Pólya, 1921) For d = 1 and 2 it is

$$\lim_{n \to \infty} \frac{a_n(\mathbb{Z}^d)}{d_n(\mathbb{Z}^d)} = \lim_{n \to \infty} \frac{a_n(\mathbb{Z}^d)}{(2d)^n} = 1$$

and for  $d \geq 3$  is

$$\lim_{n \to \infty} \frac{a_n(\mathbb{Z}^d)}{d_n(\mathbb{Z}^d)} = \lim_{n \to \infty} \frac{a_n(\mathbb{Z}^d)}{(2d)^n} < 1 .$$

In terms of probability, in dimensions  $d \leq 2$  for large n a random walk of length n will almost certainly revisit the start, but in dimensions  $d \geq 3$  it never revisits the start with probability > 0.

• *Proof of Pólya's theorem by power series.* We make use of the following theorem about power series.

Theorem 9 (weak Abel's thm) If a power series

$$U(x) = \sum_{n=0}^{\infty} u_n x^n \in \mathbb{R}[[x]]$$

converges for every  $x \in [0, R)$ , where  $R \in (0, +\infty)$  is a real number, and has all coefficients  $u_n \ge 0$ , then the following limit and infinite sum are defined and are equal,

$$\lim_{x \to R} U(x) = \sum_{n=0}^{\infty} u_n R^n \quad (= U(R)) ,$$

no matter whether they are finite or  $+\infty$ .

**Proof.** For every  $N \in \mathbb{N}$ ,

$$\sum_{n=0}^{N} u_n R^n = \lim_{x \to R^-} \sum_{n=0}^{N} u_n x^n$$
$$\leq \lim_{x \to R} U(x) = \lim_{x \to R} \sum_{n=0}^{\infty} u_n x^n$$
$$\leq \sum_{n=0}^{\infty} u_n R^n .$$

Here all limits and infinite sums are defined (possibly with the value  $+\infty$ ) due to monotonicity and nonnegativity. The first equality follows from the fact that for each  $n \in \mathbb{N}_0$ ,  $\lim_{x\to R^-} x^n = R^n$ . The following two inequalities follow from the non-negativity of  $u_n$ . The limit transition  $N \to +\infty$  gives the claim.

**Exercise 10** Explain why in the above proof we write first the left-sided limit  $\lim_{x\to R^-} \sum_{n=0}^N u_n x^n$  but then the two-sided limit  $\lim_{x\to R} U(x)$ .

We prove Pólya's Theorem 8 just for dimensions d = 2 and 3. The symbols  $d_n$  (or  $a_n$ ) indicate as before the number of walks (or the number of recurrent walks) of length n in the graph  $\mathbb{Z}^d$ .

**Proof.** Let d = 2 and  $w = (v_0, v_1, \ldots, v_n)$  be a walk with length  $n \in \mathbb{N}_0$  in the  $\mathbb{Z}^2$  graph. Let  $b_n$  be the number of walks w with  $v_n = v_0 = \overline{0}$  and  $c_n$  be the number of walks w with  $v_n = v_0 = \overline{0}$  but  $v_j \neq \overline{0}$  for j with 0 < j < n. By Proposition 4, due to the transitivity of the  $\mathbb{Z}^2$  graph, these counts do not depend on the start of the walk. We put  $c_0 = 0$ . It is clear that for every  $n \in \mathbb{N}_0$ ,  $a_n \leq d_n$ ,  $c_n \leq b_n \leq d_n$  and  $d_n = 4^n$ . We divide the walks counted by  $a_n$  into

groups according to their first return to  $\overline{0}$  at the vertex  $v_j$ . Using the relations  $d_n = 4^n$  and  $a_n \leq 4^n$  we get for each  $n \in \mathbb{N}_0$  equations

$$a_n = \sum_{j=0}^n c_j d_{n-j}$$
, so  $\frac{a_n}{4^n} = \sum_{j=0}^n \frac{c_j}{4^j} \le 1$ .

So it suffices to prove that

$$\sum_{j=0}^{\infty} \frac{c_j}{4^j} = 1 \; .$$

The second relation we use binds the OGFs

$$B(x) = \sum_{n \ge 0} \frac{b_n}{4^n} x^n = 1 + \dots \quad \text{a} \quad C(x) = \sum_{n \ge 0} \frac{c_n}{4^n} x^n = \frac{x^2}{4} + \dots ,$$

namely that

$$B(x) = \frac{1}{1 - C(x)} = \sum_{k \ge 0} C(x)^k$$

This can be easily seen formally, i.e. as a relation between formal power series, by dividing a walk counted  $b_n$  in its k+1 returns to  $\overline{0}$  in k parts with lengths  $j_1, j_2, \ldots, j_k$  satisfying  $j_1 + \cdots + j_k = n$ . These are counted by the numbers  $c_{j_1}, \ldots, c_{j_k}$ . But this relation also holds at the level of real functions B(x) and C(x) for  $x \in [0, 1)$ , because both power series have radii of convergence  $\geq 1$  (since  $b_n, c_n \leq 4^n$ ).

Now it suffices to prove that

$$\lim_{x \to 1^-} B(x) = +\infty \; .$$

Indeed, then the above relation implies that  $\lim_{x\to 1^-} C(x) = 1$ and this by Theorem 9 gives that

$$\sum_{j=0}^{\infty} \frac{c_j}{4^j} = C(1) = \lim_{x \to 1^-} C(x) = 1 .$$

This is exactly the required sum of the infinite series.

In order to prove that  $\lim_{x\to 1^-} B(x) = +\infty$ , it suffices to prove by the Theorem 9 that

$$B(1) = \sum_{j=0}^{\infty} \frac{b_j}{4^j} = +\infty .$$

We prove it by determining  $b_n$ . Obviously  $b_n = 0$  for odd n. For even lengths n,

$$b_{2n} = \sum_{j=0}^{n} \frac{(2n)!}{j! \cdot (n-j)! \cdot j! \cdot (n-j)!} = \binom{2n}{n} \sum_{j=0}^{n} \binom{n}{j}^2 = \binom{2n}{n}^2$$

The first equality follows by considering all j steps to the right in the walk w. These force the same number of j steps to the left and the same number of n - j steps up and down. These possibilities are counted by the multinomial coefficient  $\binom{2n}{j,j,n-j,n-j}$ . The last equality follows from the known binomial identity in Exercise 11. Stirling's formula for factorial approximation (Exercise 12) leads to the asymptotics  $\binom{2n}{n} \sim cn^{-1/2}4^n$ , for  $n \to \infty$  a constant c > 0. So the 2*n*-th summand in the series B(1) is  $\sim c^2n^{-1}$  and

$$B(1) = \sum_{n=0}^{\infty} \frac{b_n}{4^n} = \sum_{n=0}^{\infty} {\binom{2n}{n}}^2 4^{-2n} = +\infty$$

since  $\sum n^{-1} = +\infty$ .

**Exercise 11** *Prove that for every*  $n \in \mathbb{N}_0$ *,* 

$$\sum_{j=0}^{n} \binom{n}{j}^2 = \binom{2n}{n}$$

*Hint:*  $\binom{n}{j} = \binom{n}{n-j}$  and  $\binom{n}{j}$  is the number of *j*-element subsets of the *n*-element set.

Exercise 12 Recall Stirling's formula

$$n! \sim \sqrt{2\pi n} \left(\frac{n}{e}\right)^n, \quad n \to \infty$$
.

Using the integral estimate of the sum  $S(n) = \sum_{m=1}^{n} \log m$ , prove its weak version  $S(n) = n \log n - n + O(\log n)$ .

**Proof.** Let d = 3. Quantities  $a_n$ ,  $b_n$ ,  $c_n$  and  $d_n$ , OGFs B(x) and C(x), and sums of the series B(1) and C(1) are defined as in the previous proof, only now we are in the  $\mathbb{Z}^3$  graph and the constant 4 is replaced by the constant 6. So now  $B(x) = \sum_{n\geq 0} \frac{b_n}{6^n} x^n$  a  $C(x) = \sum_{n\geq 0} \frac{c_n}{6^n} x^n$ . The argument does not change, only now we can prove that

$$B(1) = \sum_{n\geq 0} \frac{b_n}{6^n} < +\infty ,$$

that is, the series B(1) converges. Then, since as before  $B(x) = \frac{1}{1-C(x)}$  and by the Theorem 9 is  $B(1) = \lim_{x \to 1^-} B(x)$  and  $C(1) = \lim_{x \to 1^-} C(x)$ , we get  $C(1) = \lim_{x \to 1^-} C(x) < 1$ . By this we are we are done because as before

$$C(1) = \sum_{j=0}^{\infty} \frac{c_j}{6^j} = \lim_{n \to \infty} \frac{a_n}{6^n}$$

So we prove the convergence of the series  $\sum_{n\geq 0} b_n/6^n$ . For odd  $n, b_n = 0$  again. We estimate  $b_{2n}/6^{2n}$  from above. For  $n \in \mathbb{N}_0$ , we

have an upper bound

$$\frac{b_{2n}}{6^{2n}} = \frac{1}{6^{2n}} \sum_{\substack{j, k \in \mathbb{N}_0 \\ j+k \le n}} \frac{(2n)!}{j! \cdot j! \cdot k! \cdot k! \cdot (n-j-k)! \cdot (n-j-k)!} \\
= \binom{2n}{n} 4^{-n} \sum_{\substack{j, k \in \mathbb{N}_0 \\ j+k \le n}} \left[ \frac{1}{3^n} \binom{n}{j, k, n-j-k} \right]^2 \\
\leq \binom{2n}{n} 4^{-n} \max_{\substack{x, y z \in \mathbb{N}_0 \\ x+y+z=n}} \frac{1}{3^n} \binom{n}{x, y, z} \\
= \binom{2n}{n} 4^{-n} \frac{1}{3^n} \binom{n}{x_0, y_0, z_0},$$

where  $(x_0, y_0, z_0)$  is (m, m, m) when n = 3m, (m + 1, m, m) when n = 3m+1, a (m+1, m+1, m) when n = 3m+2 (here  $m \in \mathbb{N}_0$ ) – Exercise 13. On the first line we counted as in the previous proof: j is the number of steps of the walk to the right, k is the number of its steps up, and n - j - k is the number of its steps back. The second line represents a simple algebraic rearrangement. On the third line, we took advantage of the fact that according to the multinomial expansion of  $3^n = (1 + 1 + 1)^n$  the numbers  $[\dots]$  sum up to 1, and we used Exercise 14. On the fourth line, we found the maximum value of the trinomial coefficient with the help of Exercise 13.

By Stirling's formula, we have estimates

$$\binom{2n}{n} \ll \frac{4^n}{n^{1/2}} \text{ and } \binom{n}{x_0, y_0, z_0} \ll \frac{3^n}{n}.$$
$$\frac{b_{2n}}{6^{2n}} \ll n^{-1/2} \cdot n^{-1} = n^{-3/2}$$

So

and for some constant c > 0,

$$B(1) = \sum_{n \ge 0} \frac{b_n}{6^n} = \sum_{n \ge 0} \frac{b_{2n}}{6^{2n}} < c \sum_{n=1}^{\infty} \frac{1}{n^{3/2}} < +\infty ,$$

which we needed to show.

**Exercise 13** Prove that for  $a, b \in \mathbb{N}_0$  with  $a \ge b + 2$ ,

$$\frac{1}{a! \cdot b!} \geq \frac{1}{(a-1)! \cdot (b+1)!} \; .$$

**Exercise 14** Let  $A, a_1, \ldots, a_n \ge 0$  be real numbers such that  $a_i \le A$  and  $a_1 + \cdots + a_n = 1$ . Then

$$\sum_{i=1}^{n} a_i^2 \le A$$

## THANK YOU FOR YOUR ATTENTION!

Homework Exercises. Please send me (klazar@kam.mff.cuni.cz) by the end of the coming Sunday solutions to the Exercises 1, 6, 10, 11 and 14.