CayleyPy Growth: Efficient growth computations and hundreds of new conjectures on Cayley graphs

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Abstract

We present the first public release of CayleyPy, an open-source Python library for working with Cayley and Schreier graphs. Compared to classical systems such as GAP and Sage, CayleyPy scales to much larger graphs and achieves speedups of several orders of magnitude.

Using CayleyPy we obtained about 200 new conjectures on diameters and growth of Cayley and Schreier graphs. For symmetric groups S_n we observe quasi-polynomial diameter formulas depending on $n \bmod s$, and conjecture this is a general phenomenon. This leads to efficient diameter computation despite NP-hardness in general. We refine Babai-type bounds for S_n, proposing $\frac{1}{2}n^2 + 4n$ as an upper bound in the standard case, and identify explicit generator families likely maximizing diameters, confirmed for $n \leq 15$. We also conjecture a closed formula for the diameter of the directed Cayley graph generated by the left cyclic shift and $(1, 2)$, answering a 1968 question of V.M. Glushkov.

For nilpotent groups we conjecture linear dependence of diameters on p in $\mathrm{UT}_n(\mathbb{Z}/p\mathbb{Z})$, improving results of Ellenberg, and observe Gaussian-type growth distributions akin to Diaconis' results for S_n.

Several conjectures are LLM-friendly, reducible to sorting problems verifiable via Python code. To foster benchmarking, we release 10+ Kaggle datasets for path-finding on Cayley graphs. CayleyPy supports arbitrary permutation and matrix groups with 100+ predefined generators, including puzzle groups. Its growth computation routines outperform GAP/Sage by up to 1000× in both speed and capacity.

Introduction

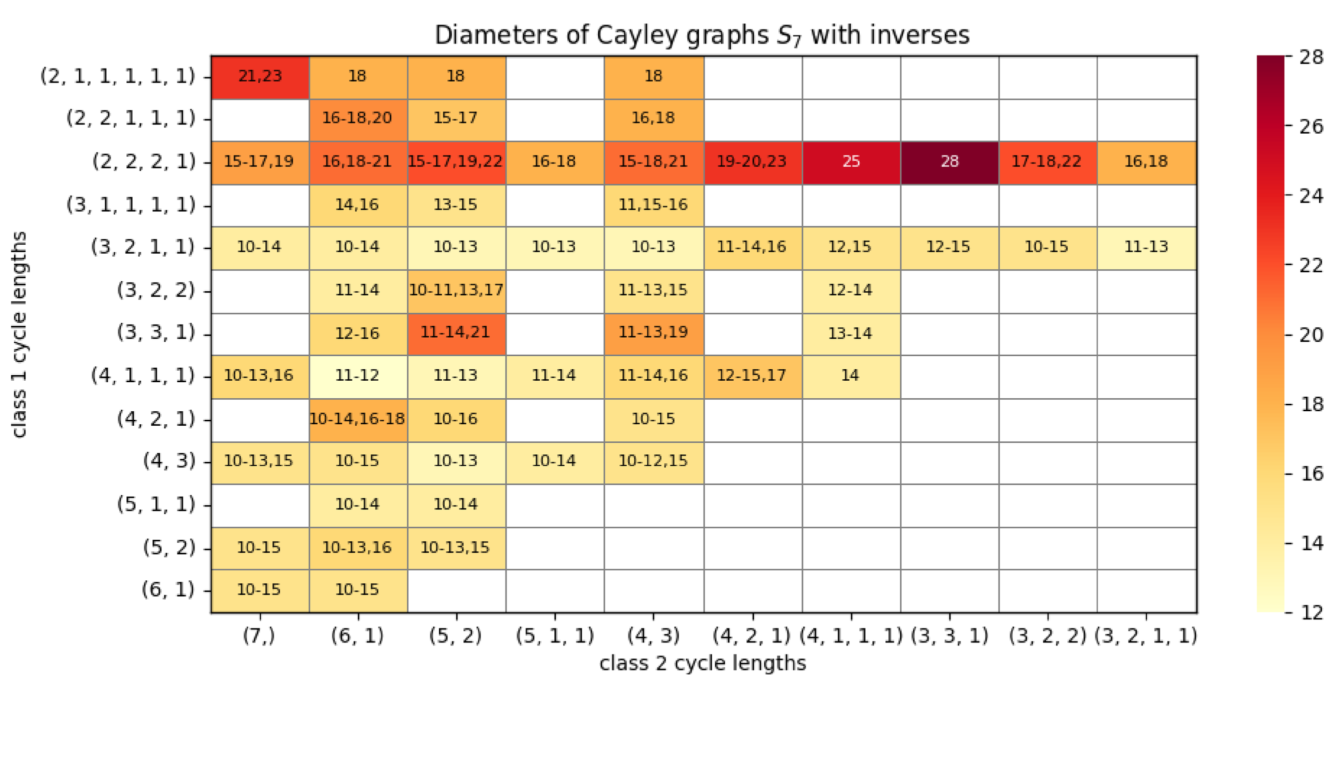
Having some elements in, say, the permutation group S_n (or in some other group), one constructs the Cayley graph, and there is a set of natural questions and lines of investigation:

- What group is obtained?
- What is its diameter?
- Growth statistical characteristics: mean, mode, moments, what distribution does it follow (or at least asymptotically as $n \to \infty$)?
- Algorithm: is there an effective/polynomial algorithm which decomposes a given element into a product of generators (optimally/sub-optimally)?
- Antipodes ("super-flips"): is there an explicit description of the longest elements?
- What can be said about the graph's spectrum?
- What is the mixing time?

Contribution

- We generate around 200 conjectures on various properties of Cayley graphs, that is achieved by extensive computational experiments with around 50 Cayley graphs. The conjectures are summarized in tables which can be found in the paper.
- In particular we propose the following:
  - We conjecture that diameters of many S_n-Cayley graphs are quasi-polynomials (quadratic/linear) in n (i.e. several polynomials depending on n modulo some s) allowing to find them rather efficiently, which is surprising since it is NP-hard in general.
  - The improvement of the L.Babai-like conjecture for S_n - diameters are bounded by $n^2/2+4n$, by $3n^2/4+O(n)$ (directed cases), $n^2/4+O(n)$ for some Schreier graphs, comparing to prior $O(n^2)$ conjectural bounds. Moreover we present explicit families of generators for S_n which conjecturally provide largest (or near) diameters. They are related to involutions and follow rather simple pattern ("square-with-whiskers"). They were found by an extensive (partly exhaustive) search for $n <= 15$ of the generators with maximum diameter.
  - For nilpotent groups we conjecture improvement of J.S. Ellenberg's results on diameter of upper-triangular matrices over Z/p presenting phenomena of linear dependence of diameter on p. Moreover growth for nilpotent groups conjectured to follow Gaussian distributions (a central limit phenomena - similar to results of P.Diaconis for S_n).
  - We present a conjectural answer on the open question: diameter of the directed Cayley graph generated by left cyclic shift and transposition $(1, 2)$ is equal to $(3n^2 + 8n + 9)/4$ for odd n, else $(3n^2 - 8n + 12)/4$.
- To benchmark various methods of path-finding on Cayley graphs and LLMs we create 11 benchmark datasets in the form of Kaggle challenges, making benchmarking easy and public to community.

Distribution of diameter over conjugacy classes pairs



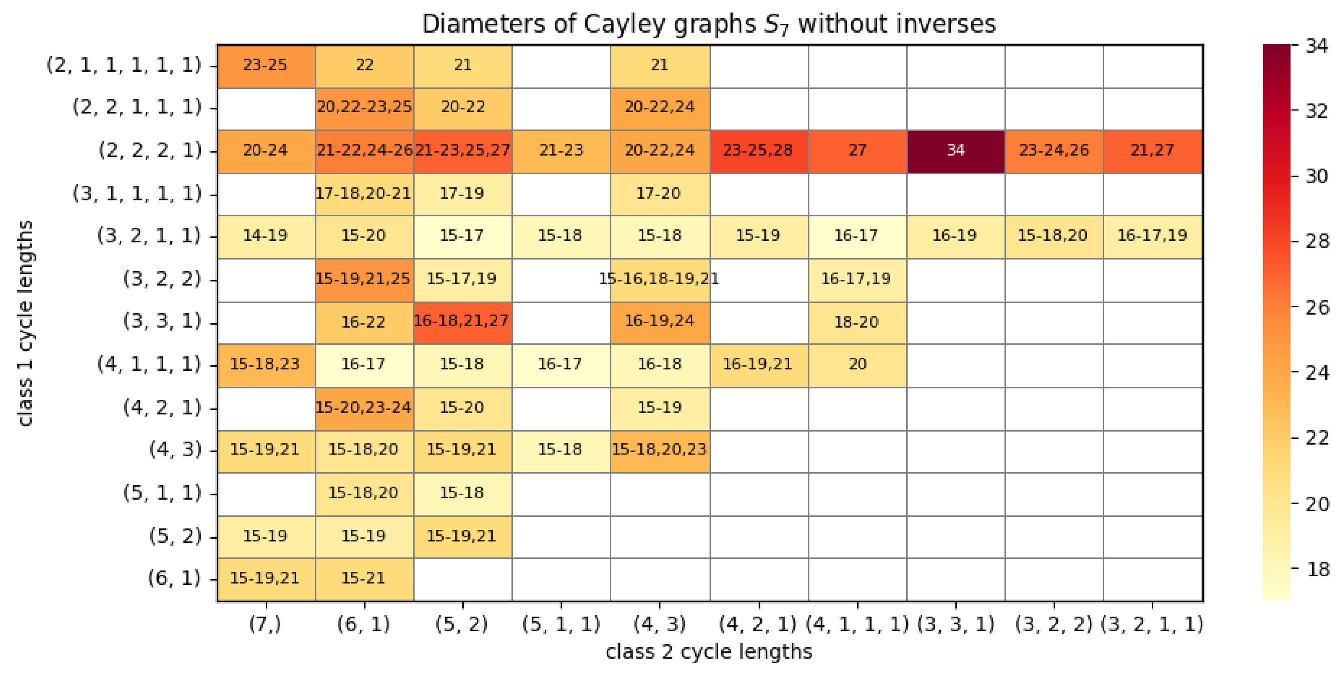


Figure 1: Diameters of all possible Cayley graphs for S_7 generated by two permutations with/without their inverses.

Largest diameters found (and known) for $n \leq 15$

Maximal diameter for Cayley graph of the group S_n (undirected graph)		
n	Maximal diameter	Example of a set of generators
3	3	$[0, 2, 1], [2, 1, 0]$
4	6	$[2, 1, 0, 3], [3, 0, 2, 1], [1, 3, 2, 0]$
5	10	$[4, 0, 1, 2, 3], [1, 2, 3, 4, 0], [0, 1, 3, 2, 4]$
6	15 (16)	$[4, 5, 3, 2, 0, 1], [2, 5, 0, 3, 1, 4], [2, 4, 0, 3, 5, 1]$ $([[0, 1, 2, 3, 5, 4], [0, 2, 1, 4, 3, 5], [1, 0, 3, 2, 5, 4]])$
7	28 (30)	$[1, 0, 3, 2, 5, 4, 6], [2, 6, 5, 3, 1, 0, 4], [5, 4, 0, 3, 6, 2, 1]$ $([0, 1, 3, 2, 4, 6, 5], [0, 4, 6, 5, 1, 3, 2], [6, 1, 3, 2, 5, 4, 0])$
8	33 (39)	$[3, 7, 5, 6, 0, 2, 4, 1], [4, 7, 5, 0, 6, 2, 3, 1], [1, 0, 3, 2, 5, 4, 6, 7]$ $([0, 1, 2, 3, 5, 4, 7, 6], [0, 1, 3, 2, 6, 7, 4, 5], [7, 3, 6, 1, 4, 5, 2, 0])$
9	(52)	$([8, 5, 2, 7, 4, 1, 6, 3, 0], [1, 2, 0, 5, 3, 4, 8, 6, 7], [2, 0, 1, 4, 5, 3, 7, 8, 6])$
10	(77)	$([0, 1, 2, 3, 5, 4, 7, 6, 9, 8], [1, 0, 3, 2, 5, 4, 8, 9, 6, 7],$ $[0, 6, 4, 8, 2, 5, 1, 7, 3, 9])$
11	(85)	$([1, 0, 3, 2, 5, 4, 7, 6, 9, 8, 10], [0, 3, 4, 1, 2, 6, 5, 8, 7, 10, 9],$ $[0, 4, 3, 2, 1, 5, 6, 7, 8, 9, 10])$
12	(95)	$([1, 0, 3, 2, 5, 4, 7, 6, 9, 8, 11, 10], [0, 2, 1, 5, 6, 3, 4, 8, 7, 10, 9, 11],$ $[0, 1, 2, 6, 5, 4, 3, 7, 8, 9, 10, 11])$
13	(111)	$([1, 0, 2, 5, 4, 3, 7, 6, 9, 8, 11, 10, 12],$ $[0, 2, 3, 4, 1, 6, 5, 8, 7, 10, 9, 12, 11],$ $[0, 4, 1, 2, 3, 6, 5, 8, 7, 10, 9, 12, 11])$
14	(132)	$([1, 0, 3, 2, 5, 4, 7, 6, 9, 8, 11, 10, 13, 12],$ $[0, 2, 1, 4, 3, 6, 5, 8, 7, 10, 9, 12, 11, 13],$ $[0, 1, 2, 3, 5, 4, 6, 7, 8, 9, 10, 11, 12, 13])$
15	(148)	$([1, 0, 3, 2, 5, 4, 7, 6, 9, 8, 11, 10, 13, 12, 14]$, $[0, 2, 1, 4, 3, 6, 5, 8, 7, 10, 9, 12, 11, 14, 13]$, $[0, 1, 2, 3, 4, 8, 7, 6, 5, 9, 10, 11, 12, 13, 14])$

Maximal diameter for Cayley graph of the group S_n (oriented graph)		
n	Maximal diameter	Example of a set of generators
3	3	$(01), (02)$
4	7	$(01), (123)$
5	14	$(01)(23), (0314)$
6	18	$(01)(23)(45), (012)(34)$
7	34	$(01)(23)(45), (052)(146)$
8	44	$(01)(23)(45), (1736)(25)$
9	61	$(01)(23)(45), (3647)(12)(58)$
10	83	$(01)(23)(45)(67)(89), (185)(237)(469)$
11	93	$(01)(23)(45)(67)(89), (1528)(47)(6, 10)$
12	106	$(01)(23)(45)(67)(89), (1, 11, 9, 10)(04)(28)(36)$
13	147	$(01)(23)(45)(67)(89), (1, 11, 2, 12)(34)(56)(78)(9, 10)$

Conclusion

In this paper, we present the CayleyPy library and propose approximately 200 conjectures on Cayley graphs using it. We provide a comprehensive comparison with the GAP method in terms of the computational time required for the growth of different groups. We also emphasize that the conjectures we obtained, together with our Kaggle challenges, may constitute an effective benchmark for both reinforcement learning and large language model algorithms.

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