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## DIFFERENTIAL EQUATIONS SATISFIED BY GENERATING FUNCTIONS OF 5-, 6-, AND 7-REGULAR LABELLED GRAPHS: A REDUCTION-BASED APPROACH

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ABSTRACT. By a classic result of Gessel, the exponential generating functions for k-regular graphs are D-finite. Using Gröbner bases in Weyl algebras, we compute the linear differential equations satisfied by the generating function for 5-, 6-, and 7- regular graphs. The method is sufficiently robust to consider variants such as graphs with multiple edges, loops, and graphs whose degrees are limited to fixed sets of values.

Keywords: regular graph, enumeration, Weyl algebra, reduction-based integration.  $2020\ MSC:\ 05C30,\ 12H05.$ 

#### 1. Introduction

1.1. The history of k-regular graph enumeration. A graph is said to be regular if every vertex is incident to the same number of edges, that is, each vertex has the same degree. If that degree is k, we call the graph k-regular. One of the earliest graph enumeration problems considered was the number of non-isomorphic unlabelled k-regular graphs on n vertices. It is a relatively attainable problem for many reasons, including the fact that the number of edges is fixed in these graphs, which yields a significant simplification. For example, according to Gropp [7], Jan de Vries determined the number of non-isomorphic cubic (3-regular) graphs up to 10 vertices, and shared them in a letter to Vittorio Martinetti, which was eventually published in a journal in 1891. The proofs were descriptions of the graphs. Here we consider the slightly easier problem of labelled graphs, specifically the number of labelled k-regular graphs on n vertices, which we denote by  $r_n^{(k)}$ .

In the labelled case, the work of Read in the 1950s established enumeration formulas using the cycle index series, a relatively new machinery at the time. He gives a compact, structural equation in [11, Eq. 5.11] that is not immediately suitable for enumeration purposes for k > 3. He notes,

"It may readily be seen that to evaluate the above expressions in particular cases may involve an inordinate amount of computation."

For k = 3, the equation is sufficiently manageable to give rise to a nice asymptotic formula.

One can distill from his work a formula in terms of coefficient extraction of a multivariable polynomial. This is the starting point of most modern approaches as it is easy to interpret, and there are numerous possibilities for analysis. We can write

(1) 
$$r_n^{(k)} = [x_1^k x_2^k \dots x_n^k] \prod_{1 \le i < j \le n} (1 + x_i x_j).$$

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The square brackets indicate that the answer is the coefficient of the indicated term in a series expansion of the product. The multiplication accounts for all possibilities of an edge  $\{i, j\}$  to be in the graph or not. The coefficient of the indicated monomial is the number of graphs that have vertices 1 to n, such that each vertex is incident to exactly k other vertices: this is precisely  $r_n^{(k)}$ .

To approximate  $r_n^{(k)}$ , one could write the coefficient extraction as a Cauchy integral, and then estimate the integral. Remarkably, a sufficiently refined analysis succeeds even when k is given as a non-constant function of n, and can also be adapted to examine other kinds of degree sequences. Wormald's 2018 ICM survey has many details on the state of asymptotic enumeration of regular graphs and related objects [14].

In this 2018 survey, Wormald notes that no new exact enumeration results have appeared since the recurrences for 4-regular graphs published in the early 1980s. The entry point of the present article is also Eq. (1), but we follow a different lineage to contribute fixed-length linear recurrence formulas to count 5-, 6-, and 7-regular graphs, ending the drought.

The fact that there are recurrences to find at all is related to a question of Stanley [13] in his foundational article on P-recursive sequences. The existence of a recurrence is equivalent to asking whether or not the exponential generating function for  $r_n^{(k)}$ , defined as  $R^{(k)}(t) := \sum_{n\geq 0} r_n^{(k)} \frac{t^n}{n!}$ , is *D-finite*. In other words, does  $R^{(k)}(t)$  satisfy a linear differential equation with polynomial coefficients? Read had already given a recurrence for 3-regular graphs, and about the same time McKay and Wormald used a combinatorial analysis to produce recurrences for 4-regular graphs. Goulden, Jackson and Reilly [6] were also able to determine explicit linear differential equations satisfied by  $R^{(3)}(t)$  and  $R^{(4)}$  using tools that dated back to MacMahon at the turn of the 20th century, called Hammond operators. But, they noted that 1

"... the H-series theorem enables us to write down the system of partial differential equations for the H-series for arbitrary p without difficulty. However, the reduction of this system to a single ordinary differential equation in  $y_p$  is a technical task which we are unable to carry out for the general case."

Their work fuelled speculation that  $R^{(k)}$  should be D-finite for all k. Gessel compared their approach to his own method the scalar product of symmetric functions and algebraic substitutions [4]:

"... Hammond operators are undesirable for two reasons. First, they disguise the symmetry of the scalar product. Second, they can be represented as differential operators. Although this might seem like an advantage, it seems to be of little use, but misleads by directing attention in the wrong direction."

Instead of working with differential equations, he recast the extraction in terms of symmetric functions, and used algebraic arguments to establish that indeed  $R^{(k)}(t)$  is D-finite for all k. His framework is sufficiently simple and robust that it can be used to establish the D-finiteness of many related regular graph and hypergraph cases. Gessel was able to advance on the general case thanks to concurrent work on multivariable P-recursiveness of Lipshitz [8]. The work of Lipshitz was not sufficiently straightforward to convert into an algorithm or even make computation effective beyond k=2. It was over a decade before the computer algebra implementations using differential operators caught up to his theoretical results. In our 2005 work with Salvy [3], we made both the Hammond method and the Gessel strategy effective for any k using Gröbner bases for D-modules and non-commutative polynomial elimination, in a sort of variant of Creative Telescoping. Our implementation quickly found differential equations up to, and including, 4-regular objects. The growth of data in the skew polynomial elimination involved in the 5-regular graph case requires computational resources that even today are insufficient to have the algorithm terminate. However, in the intervening 20 years, improvements and insights to Creative Telescoping have led us to an evolved algorithm that terminates also in practice, and indeed we could find the linear differential equations satisfied by  $R^{(5)}(t)$ ,  $R^{(6)}(t)$ , and  $R^{(7)}(t)$ . Our present approach can be applied to find the differential equations satisfied by the other graph, hypergraph and graph-like classes, but for higher degrees of regularity than were previously obtained [9, 10].

1.2. The scalar product<sup>2</sup> of symmetric functions. The coefficient extraction in Eq. (1) can be placed into an infinite product, symmetric in all variables, which can be readily encoded in terms of symmetric

<sup>&</sup>lt;sup>1</sup>In our notation, p = k and  $y_p = R^{(k)}$ .

 $<sup>^{2}</sup>$ We follow the usual terminology of a "scalar product" in combinatorics, although the presence of a formal indeterminate t would require to speak more properly of a "pairing".

functions. The set up of Gessel [5] uses the scalar product in the ring of symmetric functions to model the extraction. Describing the method requires a small detour through symmetric function terminology and basics. There are many excellent introductions. We highlight some notation, but refer readers to Sagan [12] for details.

We say  $\lambda = (\lambda_1, \lambda_2 \dots, \lambda_k)$  such that  $\sum_{i=1}^k \lambda_i = n$  and  $\lambda_i \geq \lambda_{i+1}$  is a partition of n into k parts, and write  $\lambda \vdash n$  to indicate that  $\lambda$  is a partition of n. The monomial symmetric function is defined  $m_{\lambda}(x) := \sum_{\alpha \sim \lambda} x^{\alpha}$  where  $\alpha \sim \lambda$  if the non-zero parts of  $\alpha$  are a rearrangement of the parts of  $\lambda$ . Using  $m_{\lambda}$  we can describe the complete homogeneous symmetric function  $h_n := \sum_{\lambda \vdash n} m_{\lambda}$  and the power sum symmetric function  $p_n := m_{(n)} = x_1^n + x_2^n + \dots$  Products are denoted respectively  $h_{n_1 n_2 \dots n_{\ell}} := h_{n_1} h_{n_2} \dots h_{n_{\ell}}$  and  $p_{n_1 n_2 \dots n_{\ell}} := p_{n_1} p_{n_2} \dots p_{n_{\ell}}$ . The vector space of symmetric functions of order n has numerous bases, including  $\{m_{\lambda} \mid \lambda \vdash n\}$ ,  $\{h_{\lambda} \mid \lambda \vdash n\}$  and  $\{p_{\lambda} \mid \lambda \vdash n\}$ . For any  $\lambda \vdash n$ ,  $z_{\lambda}$  denotes the number

(2) 
$$z_{\lambda} := 1^{r_1} r_1! \, 2^{r_2} r_2! \, \dots n^{r_n} r_n!$$

provided  $\lambda$  has  $r_1$  ones,  $r_2$  twos, etc, and we set  $\delta_{\lambda,\nu}$  to 1 if  $\lambda = \nu$  and to 0 otherwise. The scalar product of symmetric functions is classically defined by

(3) 
$$\langle p_{\lambda}, p_{\nu} \rangle := \delta_{\lambda,\nu} z_{\lambda}$$
, from which we deduce  $\langle m_{\lambda}, h_{\nu} \rangle = \delta_{\lambda,\nu}$ .

The connection to the graph enumeration problem is as follows. We can extract the coefficient of a particular monomial in a symmetric function with a judiciously chosen scalar product. Write  $\mathbf{G} := \prod_{i < j} (1 + x_i x_j)$  and consider an example. Since  $r_4^{(3)} = [x_1^3 x_2^3 x_3^3 x_4^3] \mathbf{G}$ , to actually compute this write  $\mathbf{G}$  as a sum of monomial symmetric functions, and determine the coefficient of  $m_{3,3,3,3}$  (which is the only basis element to contain the term  $x_1^3 x_2^3 x_3^3 x_4^3$ ). This coefficient is precisely the result of the scalar product  $\langle \mathbf{G}, h_{3,3,3,3} \rangle = \langle \mathbf{G}, h_3^4 \rangle$ .

From the formula  $\log(1+u) = \sum_{k>1} (-1)^{k+1} u^k / k$  it follows

$$\mathbf{G} = \exp\left(\log \prod_{i < j} (1 + x_i x_j)\right) = \exp\left(\sum_{i < j} \log(1 + x_i x_j)\right)$$
$$= \exp\left(\sum_{i < j} \sum_{k \ge 1} (-1)^{k+1} \frac{x_i^k x_j^k}{k}\right) = \exp\left(\sum_{k \ge 1} (-1)^{k+1} \frac{p_k^2 - p_{2k}}{2k}\right).$$

Henceforth we will only work with the power sum basis, specifically, we work in a ring generated by t and a finite number of the the  $p_i$  variables. To continue the example, to determine  $R^{(3)}(t)$  we first write  $h_3 = \frac{p_3}{3} + \frac{p_2 p_1}{2} + \frac{p_1^3}{6}$ , and thus obtain the following expression for the generating function:

(4) 
$$R^{(3)}(t) = \left\langle \mathbf{G}, \sum_{n \ge 0} h_3^n \frac{t^n}{n!} \right\rangle = \left\langle \exp\left(\sum_{k \ge 1} (-1)^{k+1} \frac{p_k^2 - p_{2k}}{2k}\right), \exp\left(\left(\frac{p_3}{3} + \frac{p_2 p_1}{2} + \frac{p_1^3}{6}\right)t\right) \right\rangle.$$

Since the second argument has only  $p_1, p_2, p_3$ , all terms with other  $p_i$  contribute 0:

(5) 
$$R^{(3)}(t) = \left\langle \exp\left(\frac{p_1^2}{2} - \frac{p_2}{2} - \frac{p_2}{4} + \frac{p_3}{6}\right), \exp\left(\left(\frac{p_3}{3} + \frac{p_2 p_1}{2} + \frac{p_1^3}{6}\right)t\right) \right\rangle.$$

For future reference, we note the following formula, which leads to generalizations of Eqs. (4) and (5):

(6) 
$$R^{(k)}(t) = \left\langle \mathbf{G}, \sum_{n \ge 0} h_k^n \frac{t^n}{n!} \right\rangle = \left\langle \mathbf{G}, \exp(h_k t) \right\rangle.$$

1.3. Earlier computational approaches. As we mentioned above, Gessel [5] proved the existence of linear differential equations for scalar products like Eq. (6), and our earlier work [3] proposed algorithms to compute them. In there, for a given series S in the variables  $p_1, \ldots, p_k$  we consider the set, denoted ann S, of all linear differential operators that annihilate S. The elements of ann S are non-commutative polynomials in the variables  $p_1, \ldots, p_k$  and in the corresponding derivatives  $\partial_1, \ldots, \partial_k$ ; they possess a well-defined total degree in the 2k variables. The set ann S is closed under multiplication by any operator on the left and is thus a left ideal. As is customary in effective literature, such a left ideal is best represented by a non-commutative analogue of a Gröbner basis, that is, by a finite set of non-commutative polynomials that can algorithmically

divide a given ideal element, resulting into a uniquely defined remainder that is zero if and only if the given polynomial is in the ideal.

Given a number k, we henceforth write  $p=(p_1,\ldots,p_k)$  and  $\partial=(\partial_1,\ldots,\partial_k)$ . Given a series F in p and a series G in (t,p), we showed in [3] that differential equations with respect to t satisfied by the scalar product  $\langle F,G\rangle$  are to be found as those elements free of  $(p,\partial)$  in the (vector space) sum of the left ideal ann G and of the right ideal  $(\operatorname{ann} F)^{\dagger}$  obtained by taking the adjoints of all elements in ann F. A first algorithm in [3], based on linear algebra, consists: (i) in fixing an integer d; (ii) in determining representatives of  $(\operatorname{ann} F)^{\dagger}$  and  $\operatorname{ann} G$  for each possible leading monomial of total degree at most d with respect to  $(p,\partial,\partial_t)$ ; (iii) and in using a non-commutative variant of Gaussian elimination over  $\mathbb{Q}(t)$  to eliminate  $(p,\partial)$ , repeating the whole process with a larger d if elimination results in no non-trivial output. Because there are  $\binom{d}{2k+1} = O(d^{2k+1})$  monomials of degree at most d, and almost as many representatives to determine for each ideal, this process is very inefficient in practice. A second algorithm in [3] is tailored to a certain form for the argument G in the scalar product: if  $G = \exp(h_k t)$ , the theory of Hammond series, as developed in [6], provides the formula

$$\langle F, \exp(h_k t_k) \rangle = \mathcal{H}(F)(0, \dots, 0, t_k),$$

where  $\mathcal{H}(F)(t_1,\ldots,t_k)$  is a transform of F known as its Hammond series. A simple replacement of the  $p_i$  and the  $\partial_i$  in ann F with suitable polynomials in  $t_1,\ldots,t_k$  and corresponding derivatives  $\partial_{t_i}$  provides ann  $\mathcal{H}(F)$ . The specialization of  $t_1,\ldots,t_{k-1}$  to 0 is then obtained by restriction, an operation dual to integration. One way to implement it would have been to first eliminate the k-1 variables  $\partial_{t_1},\ldots,\partial_{t_{k-1}}$ , e.g., by a Gröbner basis calculation, before setting all of the k-1 variables  $t_1,\ldots,t_{k-1}$  to zero and taking a generator of the resulting principal ideal in  $\mathbb{Q}(t_k)\langle\partial_{t_k}\rangle$ . But a simultaneous elimination in this way leads to high degrees and is also inefficient in practice. More generally, in the 2000s, no good algorithm was known for integration with respect to several variables considered simultaneously, so one had to resort to iterated integrations, one variable after the other. Correspondingly, for multiple restriction one had to perform specializations one variable after the other, and this is what we proposed in [3], in a way that is reminiscent of elimination by successive resultants. This approach, too, fails for k=5: all steps are fast until the last elimination, which should eliminate  $\partial_{t_1}$  from two degree-9 polynomials in the four variables  $t_1,t_5,\partial_{t_1},\partial_{t_5}$ , and this fails in practice.

In both old approaches, the culprit is elimination in too many variables: eliminating 2k variables between polynomials in 2k+1 variables over  $\mathbb{Q}(t)$  in the first approach; eliminating k-1 variables between polynomials in 2k-1 variables over  $\mathbb{Q}(t_k)$  in the second approach. The second is an improvement in that it reduces the number of variables, and this is assisted by specializations to zero along the process.

A turning point in the theory of Creative Telescoping was the introduction of reduction-based algorithms, starting with the integration of bivariate rational functions [1] in 2010, and followed by many articles in the literature. Our inspiration for the present work came from a more recent reduction-based algorithm [2] for the integration with regard to one variable p of general D-finite functions f(t, p), leading to integrals parametrized by t. In a nutshell, reduction-based algorithms: (i) set up a reduction process that corresponds to simplifying a function to be integrated modulo derivatives with respect to p of other functions, in such a way that the resulting remainder lies in a finite-dimensional vector space; (ii) find a linear relation between the remainders of successive higher-order derivatives with respect to the parameter t of the function to be integrated. In situations where integrals of derivatives are zero, the output linear relation reflects a differential equation in t of the parametrized integral. Although the symmetric scalar product cannot be represented as an integral of a D-finite function, the method of [2] can be adapted to the present situation, in a way that the reduction with respect to the k variables  $p_1, \ldots, p_k$  is possible simultaneously and that most of the calculations involve polynomials in k+1 variables over  $\mathbb{Q}(t)$ .

1.4. Contributions. Beside presenting a heuristic method that adapts reduction-based algorithms to a simultaneous reduction with respect to several integration variables, our main contribution in the present work is to obtain differential equations satisfied by various models of graphs with vertex degrees restricted to be in a fixed subset of  $\{1, \ldots, 6\}$ , as well as a differential equation satisfied by 7-regular (simple loopless) graphs. In Table 3, we list for a few dozens of models the order of a differential equation satisfied by the counting generating function and the order of a recurrence equation satisfied by its sequence of coefficients, together with corresponding degrees of their coefficients. To the best of our knowledge, this is the first time

differential equations are presented for  $R^{(5)}(t)$ ,  $R^{(6)}(t)$  and  $R^{(7)}(t)$ , or more generally graphs where degrees 5, 6, or 7 are considered.

The recurrences we find are linear, with polynomial coefficients and hence can be unravelled quickly to get data for graphs of high order. For example, it take about 15 minutes to determine the number of 7-regular graphs on 2000 vertices from the ODE of order 20 that we found:

$$r_{2000}^{(7)} = 80680697...04296875 \approx 8.068069734 \times 10^{18572}.$$

It is even faster when the machine allows parallel processes.

The generated enumerative data, recurrences, differential equations and Maple code implementing our strategy are all available at https://files.inria.fr/chyzak/kregs/.

#### 2. Worked example: 4-regular graphs

Before introducing our procedure in a systematic way in Section 4, we illustrate it with the class of 4-regular graphs, allowing single edges and no loops. (The case k=3 is too simple to demonstrate important points of our method.) Specializing Eq. (6) to k=4, we consider the scalar product  $\langle F, G \rangle$ , which represents  $R^{(4)}(t)$  when the exponential functions  $F=\exp(f)$  and  $G=\exp(tg)$  are given by

$$f := \frac{p_1^2}{2} - \frac{p_2^2}{4} + \frac{p_3^2}{6} - \frac{p_4^2}{8} - \frac{p_2}{2} + \frac{p_4}{4}, \qquad g := \frac{p_1^4}{24} + \frac{p_1^2 p_2}{4} + \frac{p_2^2}{8} + \frac{p_1 p_3}{3} + \frac{p_4}{4}.$$

2.1. A reduction procedure. We begin by explaining a procedure to normalize expressions of the form  $\langle F, sG \rangle$  for a polynomial  $s \in \mathbb{Q}(t)[p]$ : without changing the value of the scalar product, the polynomial s will be replaced with an element in  $\mathbb{Q}(t) + \mathbb{Q}(t)p_1 + \mathbb{Q}(t)p_2$ .

From the definition of F, we get that annihilating operators for F are

(7) 
$$P_1 := \partial_1 - p_1, \qquad P_2 := 2\partial_2 + p_2 + 1, \qquad P_3 := 3\partial_3 - p_3, \qquad P_4 := 4\partial_4 + p_4 - 1.$$

In Section 4, we will define two transformations on differential operators, namely adjoints ( $^{\dagger}$ ) and twists ( $^{\sharp}$ ). Applying them to Eq. (7), we obtain

$$P_1^{\dagger} := p_1 - \partial_1, \qquad P_2^{\dagger} := p_2 + 2\partial_2 + 1, \qquad P_3^{\dagger} := p_3 - 3\partial_3, \qquad P_4^{\dagger} := p_4 + 4\partial_4 - 1,$$

and

$$P_1^{\sharp} := p_1 - \partial_1 - \frac{t}{6}(p_1^3 + 3p_1p_2 + 2p_3), \qquad P_2^{\sharp} := p_2 + 2\partial_2 + \frac{t}{2}(p_1^2 + p_2) + 1,$$
  
$$P_3^{\sharp} := p_3 - 3\partial_3 - tp_1, \qquad P_4^{\sharp} := p_4 + 4\partial_4 + t - 1.$$

We will prove in Section 4 that  $\langle F, (P_j^{\sharp} \cdot \bar{s}) G \rangle$  is zero for any  $\bar{s} \in \mathbb{Q}(t)[p]$  and any j, motivating that we will try to adjust s by a linear combination of polynomials of the form  $P_j^{\sharp} \cdot \bar{s}$ .

In order to determine how to do so more precisely, observe first that for any monomial  $p^{\alpha}$ ,

$$\begin{split} P_1^{\sharp} \cdot p^{\alpha} &= -\frac{t}{6} p_1^{\alpha_1 + 3} p_2^{\alpha_2} p_3^{\alpha_3} p_4^{\alpha_4} + \cdots, \qquad P_2^{\sharp} \cdot p^{\alpha} &= \frac{t}{2} p_1^{\alpha_1 + 2} p_2^{\alpha_2} p_3^{\alpha_3} p_4^{\alpha_4} + \cdots, \\ P_3^{\sharp} \cdot p^{\alpha} &= -t p_1^{\alpha_1 + 1} p_2^{\alpha_2} p_3^{\alpha_3} p_4^{\alpha_4} + p_1^{\alpha_1} p_2^{\alpha_2} p_3^{\alpha_3 + 1} p_4^{\alpha_4} + \cdots, \qquad P_4^{\sharp} \cdot p^{\alpha} &= p_1^{\alpha_1} p_2^{\alpha_2} p_3^{\alpha_3} p_4^{\alpha_4 + 1} + \cdots, \end{split}$$

where in each case, the dots represent a polynomial with lower total degree. We will base our calculation on these forms. Consider for example any monomial ordering for which  $p_4$  is lexicographically higher than all other variables. Given a polynomial  $s \in \mathbb{Q}(t)[p]$  with leading term  $cp^{\beta}$  for  $\beta_4 \geq 1$ , the choice  $\alpha = \beta - (0, 0, 0, 1)$  ensures that  $s - P_4^{\sharp} \cdot (cp^{\alpha})$  has a leading monomial less than  $p^{\beta}$ . As a consequence, s can be reduced by a series of like transformations to a polynomial  $s - P_4^{\sharp} \cdot \bar{s}$  that does not involve  $p_4$ : here  $\bar{s}$  is a polynomial that adds up all the  $cp^{\alpha}$  observed during the reduction process. In other words, one can eliminate  $p_4$  from s. One can similarly use  $P_3^{\sharp}$  to reduce the degree with respect to  $p_3$ : this essentially introduces  $p_1$  as a replacement of  $p_3$ , but one can eliminate  $p_3$  as well. By continuing with transformations based on  $P_2^{\sharp}$ , which do not reintroduce either  $p_3$  or  $p_4$ , one could hope to eliminate  $p_1$  as well (after  $p_3$  and  $p_4$ ) from s. It turns out that one cannot fully eliminate  $p_1$ , but that degrees with respect to  $p_1$  can be reduced down to at most 1. On the other hand, it is not immediately evident that degrees with respect to  $p_2$  can be kept under control.

To explain how controling  $p_2$  can be done, we continue our informal presentation by recombining the  $P_i^{\sharp}$  in the following way into elements of the right ideal they generate:

$$\begin{split} P_1^{\sharp} + P_3^{\sharp} \frac{t}{3} &= -\frac{t}{6} p_1^3 - \frac{t}{2} p_1 p_2 + \left(1 - \frac{t^2}{3}\right) p_1 - \partial_1 - t \partial_3, \\ P_2^{\sharp} &= \frac{t}{2} p_1^2 + \left(1 + \frac{t}{2}\right) p_2 + 1 + 2 \partial_2, \\ \tilde{P}_5 &:= P_1^{\sharp} + P_3^{\sharp} \frac{t}{3} + P_2^{\sharp} \frac{p_1}{3} = \frac{1-t}{3} p_1 p_2 + \frac{4-t^2}{3} p_1 + \frac{2}{3} p_1 \partial_2 - \partial_1 - t \partial_3, \\ \tilde{P}_6 &:= \tilde{P}_5 \frac{t}{2} p_1 + P_2^{\sharp} \frac{t-1}{3} p_1 = \frac{(4-t^2)t}{6} p_1^2 + \frac{t^2+t-2}{6} p_2^2 + \frac{t-1}{3} p_2 + \frac{t}{3} p_1^2 \partial_2 \\ &\quad + \frac{t-4}{6} - \frac{t}{2} p_1 \partial_1 + \frac{2(t-1)}{3} p_2 \partial_2 - \frac{t^2}{2} p_1 \partial_3, \\ \tilde{P}_7 &:= \tilde{P}_6 + P_2^{\sharp} \frac{t^2-4}{3} = \frac{t^2+t-2}{6} p_2^2 + \frac{t^3+2t^2-2t-10}{6} p_2 + \frac{t}{3} p_1^2 \partial_2 \\ &\quad + \frac{2t^2+t-4}{6} - \frac{t}{2} p_1 \partial_1 + \frac{2(t-1)}{3} p_2 \partial_2 - \frac{t^2}{2} p_1 \partial_3 + \frac{2(t^2-4)}{3} \partial_2. \end{split}$$

Observe how at each line, one can determine precisely the action of the operator on a monomial  $p_1^{\alpha_1} p_2^{\alpha_2}$  and thus predict the leading monomial of the result for the monomial ordering refining total degree by  $p_1 > p_2$ :

$$\begin{split} \tilde{P}_5 \cdot p_1^{\alpha_1} p_2^{\alpha_2} &= \frac{1-t}{3} p_1^{\alpha_1 + 1} p_2^{\alpha_2 + 1} + \cdots, \\ \tilde{P}_6 \cdot p_1^{\alpha_1} p_2^{\alpha_2} &= \frac{(4-t^2)t}{6} p_1^{\alpha_1 + 2} p_2^{\alpha_2} + \cdots, \\ \tilde{P}_7 \cdot p_1^{\alpha_1} p_2^{\alpha_2} &= \frac{t^2 + t - 2}{6} p_1^{\alpha_1} p_2^{\alpha_2 + 2} + \cdots. \end{split}$$

Considering in particular  $\tilde{P}_7$ , one obtains that degrees with respect to  $p_2$  can be reduced down to at most 1. Note that the  $\tilde{P}_7 \cdot p_1^{\alpha_1} p_2^{\alpha_2}$  luckily do not reintroduce the variables  $p_3$  and  $p_4$ . So at this point, any polynomial  $s \in \mathbb{Q}(t)[p]$  in an expression  $\langle F, sG \rangle$  can be replaced with a linear combination of 1,  $p_1$ ,  $p_2$ , and  $p_1p_2$  over  $\mathbb{Q}(t)$ , that is, with some polynomial confined to a 4-dimensional vector space. Finally, because  $\tilde{P}_5 \cdot 1 = \frac{1-t}{3}p_1p_2 + \frac{4-t^2}{3}p_1$ , the monomial  $p_1p_2$  can be replaced with  $p_1$  in such linear combinations, bringing the finite dimension down to 3. In the end, for any  $s \in \mathbb{Q}(t)[p]$ , a sequence of transformations results: first in an element  $\check{s} \in \mathbb{Q}(t) + \mathbb{Q}(t)p_1 + \mathbb{Q}(t)p_2$  and elements  $\tilde{s}_j \in \mathbb{Q}(t)[p]$  for  $j = 0, \ldots, 4$  such that  $\langle F, sG \rangle = \langle F, \check{s}G \rangle$  and

$$s - \check{s} = \sum_{i=0}^{4} G_i \cdot \tilde{s}_i$$
 for  $(G_0, \dots, G_4) = (P_4^{\sharp}, P_3^{\sharp}, P_2^{\sharp}, \tilde{P}_7, \tilde{P}_5);$ 

next, because  $\tilde{P}_5$  and  $\tilde{P}_7$  are in the right ideal, in elements  $\bar{s}_j \in \mathbb{Q}(t)[p]$  for  $j = 1, \ldots, 4$  such that  $s - \check{s} = P_1^{\sharp} \cdot \bar{s}_1 + P_2^{\sharp} \cdot \bar{s}_2 + P_3^{\sharp} \cdot \bar{s}_3 + P_4^{\sharp} \cdot \bar{s}_4$ .

Eliminating variables one after the other in this presentation was chosen for the sake of the informal explanation. In the next section and in our implementation, we use an optimized elimination strategy that bases more strongly on total degree.

2.2. Recombining normal forms for a differential equation. We now explain how the reduction step of the previous section can be used to derive a differential equation with respect to t for  $\langle F, G \rangle$ .

For any  $i \in \mathbb{N}$ , the identity  $\partial_t^i \cdot \langle F, G \rangle = \langle F, g^i G \rangle$  follows from the definition  $G = \exp(tg)$ . By the reduction of previous section, the polynomial  $g^i$  can be replaced with some element  $\check{g}_i$  from the 3-dimensional vector space  $\mathbb{Q}(t) + \mathbb{Q}(t)p_1 + \mathbb{Q}(t)p_2$ . So, the family  $\{\check{g}_0, \check{g}_1, \check{g}_2, \check{g}_3\}$  is obviously linearly dependent over  $\mathbb{Q}(t)$ , and a linear relation  $q_0\check{g}_0 + \cdots + q_3\check{g}_3 = 0$  with  $q_i \in \mathbb{Q}(t)$  provides a linear differential relation  $(q_0 + q_1\partial_t + q_2\partial_t^2 + q_3\partial_s^3) \cdot \langle F, G \rangle = 0$ .

Performing these calculations on our worked example, we start with  $g^0 = 1$ , so that  $\check{g}_0 = 1$  as 1 is already reduced. Next, reducing g yields  $g = \check{g}_1 + \sum_{i=0}^4 G_i \cdot \tilde{s}_i$  with

$$\check{g}_1 = -\frac{(t^5 + 2t^4 + 2t^2 + 8t - 4)}{4(t^2 + t - 2)t^2} (p_2 + 1)$$
and
$$(\tilde{s}_0, \dots, \tilde{s}_4) = \left(\frac{1}{4}, \frac{p_1}{3}, \frac{p_1^2}{12t} + \frac{(5t - 2)p_2}{12t^2} + \frac{4t^2 - 1}{6t^2}, -\frac{t^2 + 4t - 2}{2t^2(t^2 + t - 2)}, 0\right).$$

At this point, a more heavy calculation yields  $g^2 = \check{g}_2 + \sum_{i=0}^4 G_i \cdot \tilde{s}_i$  with

$$\check{g}_2 = -\frac{t^{12} - 14t^{10} - 20t^9 - 36t^8 - 200t^7 - 356t^6 - 48t^5 + 200t^4 - 336t^3 - 240t^2 + 416t - 96}{16(t^2 + t - 2)^2(t - 1)t^4(t + 2)} \\ - \frac{(t^{13} + 4t^{12} - 16t^{10} - 10t^9 - 36t^8 - 220t^7 - 348t^6 - 48t^5 + 200t^4 - 336t^3 - 240t^2 + 416t - 96)}{16(t^2 + t - 2)^2(t - 1)t^4(t + 2)} p_2$$

and quotients  $\tilde{s}_i$  that we refrain from displaying. After finding a linear dependency between the  $\check{g}_i$  over  $\mathbb{Q}(t)$ , we obtain the annihilating operator

$$\begin{aligned} 16t^2(t+2)^2(t-1)^2(t^5+2t^4+2t^2+8t-4)\partial_t^2 \\ &+(-4t^{13}-16t^{12}+64t^{10}+40t^9+144t^8+880t^7+1392t^6\\ &+192t^5-800t^4+1344t^3+960t^2-1664t+384)\partial_t\\ &-t^4(t^5+2t^4+2t^2+8t-4)^2. \end{aligned}$$

Getting an order 2 less than the dimension 3 could not be predicted.

For efficiency, the remainders  $\check{g}_i$  can be obtained in a more incremental way: the formula

$$\partial_t^{i+1} \cdot \langle F, G \rangle = \partial_t \cdot \langle F, \check{g}_i G \rangle = \langle F, \partial_t \cdot (\check{g}_i G) \rangle = \langle F, (\check{g}_i \times g + \partial_t \cdot \check{g}_i) G \rangle$$

suggests one can obtain  $\check{g}_{i+1}$  by reducing  $\check{g}_i \times g + \partial_t \cdot \check{g}_i$ , which is much smaller than  $g^{i+1}$ . This makes calculations generally faster, although in the present example  $\check{g}_1 \times g + \partial_t \cdot \check{g}_1$  is messier than  $g^2$ .

#### 3. Applicability to various models of graphs

As we remarked in the introduction, there are many enumeration problems that can be expressed using the scalar product, and have the potential to be solved with our strategy. The computational limits are directly related to the maximal i of all  $p_i$  that appear in the expressions, and this leaves substantial flexibility. Although in the work above (namely Section 1.2 and Section 2) we have focused on the case of simple, loopless graphs, with only minor modifications of  $\mathbf{G}$  in Eq. (6) we can consider graphs with multiple edges, or loops, or both. The form is still an exponential of a polynomial in the  $p_i$ . Similarly, it is straightforward to consider graph classes where the possible vertex degrees come from a finite set K. To this end, it suffices to replace  $\exp(th_k)$  with  $\exp(t(\sum_{j\in K}h_j))$  and to express the  $h_j$  in the power sum basis.

Most of our calculations are for sets K included in  $\{1, 2, 3, 4, 5, 6\}$ , allowing several edge and loop variations. For example, we have computed the differential equation satisfied by the set of labelled graphs with degree bounded by k = 6, that is, for  $K = \{1, 2, 3, 4, 5, 6\}$ . In addition, we have computed one model with  $K = \{7\}$ .

Table 3 presents the results of applying our method as summarized in Table 1. We label generalized regular graph models according to three parameters:

- e encodes the model of allowed edges: 'se' is used for graphs with single edges; 'me' is used for generalized structures with multiple edges allowed (usually called "multigraphs").
- *l* encodes how loops are allowed and counted: 'll' is used for loopless structures, like "graphs" in the usual terminology; 'la' is used for structures with loops allowed and contributing 2 each to the degree of a vertex, in other words, those models enumerate structures according to the number of adjacent half-edges. 'lh' is used for structures with loops allowed and contributing 1 each to the degree of a vertex, in other words, those models enumerate structures according to the number of adjacent edges.

• K denotes the set of allowed degrees of vertices, whether it be counting adjacent edges with 'lh' models or counting adjacent half-edges with 'la' models; usual k-regular graphs are obtained by setting K to the singleton  $\{k\}$ ; models with K of larger cardinality allow different vertices of a graph to have different degrees as long as they are in K; for example,  $K = \{1, 2, ..., k\}$  can be used to describe a class of graphs with vertex degree bounded by k; unless otherwise clear by the context, we make  $k = \max K$ .

Finally, it is worth it to recall that given two combinatorial classes, and differential equations satisfied by the generating function of each class, we can determine the differential equations satisfied by both the sum and the product of the two generating functions. This sum and product are respectively the generating functions of the union and the cartesian product of the two classes. For example, from our existing results, we could easily determine the differential equations satisfied by the set of graphs that are either 5- or 6-regular. (In contrast to the set of graphs whose vertices are of degree either 5 or 6, which we can determine directly).

#### 4. Description of the approach

Fix a number k and, again, write  $p = (p_1, \ldots, p_k)$  and  $\partial = (\partial_1, \ldots, \partial_k)$  as a shorthand. The number k is the level of regularity of graphs, that is, with the k variables in p we will be able to express the enumerative series of k-regular graphs and variants with regularity bounded by k.

Introduce the Weyl algebra

$$W_p := \mathbb{Q}\langle p_1, \dots, p_k, \partial_1, \dots, \partial_k; \partial_i p_j = p_j \partial_i + \delta_{i,j}, \ 1 \le i, j \le k \rangle,$$

where  $\delta_{i,j}$  is one if and only if i = j, zero otherwise. Each  $\partial_i$  acts on  $\mathbb{Q}[t][[p]]$  as the usual derivation operator with respect to  $p_i$ . The following relations are easily derived for any two series U and V in  $\mathbb{Q}[t][[p]]$  and any  $i \in \{1, \ldots, k\}$ :

$$\langle p_i U, V \rangle = \langle U, i \partial_i \cdot V \rangle, \qquad \langle i \partial_i \cdot U, V \rangle = \langle U, p_i V \rangle.$$

By bilinearity and symmetry, proving these relations reduces indeed to proving the identity

$$\langle p_i p_\lambda, p_\nu \rangle = \langle p_\lambda, i \partial_i \cdot p_\nu \rangle$$

for any i,  $\lambda$ , and  $\nu$ . We prove it for completeness. First, the identity holds if  $\nu$  does not involve i, both sides being zero. So we continue assuming i appears in  $\nu$ . Define  $\lambda^+$  as the partition obtained by adjoining i to  $\lambda$  and consider the integers  $r_i$  as in Eq. (2), so that the analog of Eq. (2) for  $\lambda^+$  is obtained by incrementing  $r_i$ . Therefore,  $z_{\lambda^+} = z_{\lambda} r_i (i+1)$  holds. Define as well  $\nu^-$  as the partition obtained by removing i from  $\nu$ , so that  $\partial_i \cdot p_{\nu} = s_i p_{\nu^-}$  where  $s_i$  denotes the number of occurrences of i in  $\nu$ . In particular,  $s_i = r_i + 1$  if  $\nu = \lambda^+$ . Next,

$$\langle p_i p_{\lambda}, p_{\nu} \rangle = \langle p_{\lambda^+}, p_{\nu} \rangle = \delta_{\lambda^+, \nu} z_{\lambda} i(r_i + 1) = i(r_i + 1) \delta_{\lambda, \nu^-} z_{\lambda} = i(r_i + 1) \langle p_{\lambda}, p_{\nu^-} \rangle = i \langle p_{\lambda}, \partial_i \cdot p_{\nu} \rangle$$

and Eq. (9) is proved. More generally, for any linear differential operator L,  $\langle L \cdot U, V \rangle = \langle U, L^{\dagger} \cdot V \rangle$ , where the adjoint  $L^{\dagger}$  of L is the result of applying the algebra anti-automorphism of  $W_p$  defined by  $p_i^{\dagger} = i\partial_i$  and  $\partial_i^{\dagger} = i^{-1}p_i$ . This adjoint operation is an involution. Note that  $W_p[t]$  acts on  $\mathbb{Q}[t][[p]]$  as well, but we will restrict the use of this action to right-hand arguments of scalar products.

Given two polynomials f and g in  $\mathbb{Q}[p] \setminus \mathbb{Q}$ , introduce:

- $F := \exp(f) \in \mathbb{Q}[[p]],$
- $G := \exp(tg) \in \mathbb{Q}[p][[t]] \cap \mathbb{Q}[t][[p]]$
- $S := \langle F, G \rangle \in \mathbb{Q}[[t]].$

We will write  $f_i$  for  $\partial_i \cdot f$  and  $g_i$  for  $\partial_i \cdot g$ .

If  $P \in W_p$  annihilates F, then for any  $s \in \mathbb{Q}[p]$ ,

$$(10) 0 = \langle P \cdot F, sG \rangle = \langle F, P^{\dagger} \cdot (sG) \rangle = \langle F, (P^{\sharp} \cdot s)G \rangle,$$

where

$$P^{\sharp}(p_1,\ldots,p_k,\partial_1,\ldots,\partial_k)=P^{\dagger}(p_1,\ldots,p_k,\partial_1+tg_1,\ldots,\partial_k+tg_k)\in W_p[t].$$

Note that when P runs over the left ideal of annihilating operators of F, denoted ann F, the transform  $P^{\dagger}$  runs over the right ideal  $(\operatorname{ann} F)^{\dagger}$ , and likewise  $P^{\sharp}$  runs over the right ideal  $(\operatorname{ann} F)^{\sharp}$ . In particular, Eq. (10) holds for  $P = P_i := i(\partial_i - f_i)$ , in which case  $P^{\sharp}$  is given as  $P_i^{\sharp}$  in Eq. (8).

**Input:** a graph model (e, l, k, K),

where  $e \in \{\text{'se'}, \text{'me'}\}, l \in \{\text{'ll'}, \text{'lh'}, \text{'la'}\}, k \in \mathbb{N}_{>0}, K \subset \{1, \dots, k\}.$ 

**Output:** an operator of minimal order in  $\partial_t$ 

that cancels the counting generating function of the model.

a. Compute  $g = \sum_{\lambda \vdash n} p_{\lambda}/z_{\lambda}$  and f by the formula

$$f = \sum_{i \in K} \left( \sum_{i=1}^{j} \{e = \text{`se'}? (-1)^{i+1} : 1\} \frac{p_i^2}{2i} + \{e = \text{`lh'}? 1 : 0\} \frac{p_i}{i} \right)$$

$$-\left\{l = \text{`la'}? - 1:1\right\} \sum_{i=1}^{\lfloor j/2 \rfloor} \left\{e = \text{`se'}? (-1)^{i+1}:1\right\} \frac{p_{2i}}{2i},$$

where for a logical formula  $\mathcal{P}$ , the expression  $\{\mathcal{P} : t : f\}$  is equal to t if  $\mathcal{P}$  holds and

b. Get generators of the right  $W_n(t)$ -ideal  $(\operatorname{ann} f)^{\sharp}$  by computing  $P_i^{\sharp}$  for  $1 \leq i \leq k$  by the formula

(8) 
$$P_i^{\sharp} = (i\partial_i - if_i)^{\sharp} = p_i - if_i(\partial_1 + tg_1, 2(\partial_2 + tg_2), \dots, k(\partial_k + tg_k)).$$

Here, the right-hand side is obtained by the non-commutative substitution of  $p_1$ with  $\partial_1 + tg_1$ , of  $p_2$  with  $2(\partial_2 + tg_2)$ , ..., of  $p_k$  with  $k(\partial_k + tg_k)$ , in the polynomial  $f_i = f_i(p_1, \ldots, p_k)$ .

c. Transform each  $P_i^{\sharp}$  by the map

$$\sum_{\alpha} c_{\alpha} \partial^{\alpha} \mapsto c_{0} \eta + \sum_{\alpha \neq 0} c_{\alpha} \partial^{\alpha}$$

to get a system of generators of a right  $\mathbb{Q}(t)[p]$ -module. Here,  $\alpha$  ranges in the finite set of exponents involved in the  $P_i^{\sharp}$ .

- d. Compute a Gröbner basis of this module for an ordering  $\prec$  that makes  $\eta$  lexicographically higher than p and p lexicographically higher than  $\partial$ .
- e. Obtain elements  $G_1, \ldots, G_\rho$  of  $W_p(t)$  by setting  $\eta = 1$  in those elements of the Gröbner basis that involve  $\eta$  with a non-zero coefficient, then write each  $G_i$  in the form  $Q_i(p)$  +  $R_i(p,\partial)$  where each monomial of  $R_i$  involves at least one  $\partial_i$ .
- f. If the polynomial ideal  $I = (Q_1, \ldots, Q_\rho)$  has positive dimension, then return 'FAIL', else determine the monomials  $p^{\beta_1}, \ldots, p^{\beta_{\delta}}$  under the stair of I.
- g. Set  $\check{g}_0 = 1$ , then for i from 2 to  $\delta$ , set  $\check{g}_i = \operatorname{red}(g\check{g}_{i-1} + \partial_t \cdot \check{g}_{i-1}, (G_i)_{i=1}^{\rho}, \prec)$ .
- h. Compute the matrix M with rows indexed by  $0 \le i \le \delta$  and columns indexed by  $1 \le i \le \delta$  $j \leq \delta$ , whose entry at position (i,j) is the coefficient of  $p^{\beta_j}$  in  $G_i$ .
- i. Compute a basis of the left kernel of M, then combine its elements to obtain a non-zero row vector  $(q_0, \ldots, q_\delta) \in \mathbb{Q}(t)^{\delta+1}$  with maximal number of zeros to the right.
- j. Return  $q_0 + q_1 \partial_t + \cdots + q_\delta \partial_\delta$ .

Table 1. Outline of the method. Uses the reduction of Table 2.

Introduce the derivation operator  $\partial_t$  with respect to t as well as the Weyl algebra

$$W_t := \mathbb{Q}\langle t, \partial_t; \partial_t t = t\partial_t + 1 \rangle.$$

Observe

(11) 
$$\partial_t^j \cdot S = \langle F, \partial_t^j \cdot G \rangle = \langle F, g^j G \rangle,$$

**Input:** a polynomial  $s \in \mathbb{Q}(t)[p]$  to be reduced; differential operators  $G_1, \ldots, G_\rho$  from  $W_p(t)$ ; a monomial ordering  $\prec$  for which the leading monomials  $m_i$  of the  $G_i$  do not involve  $\partial$ . **Output:** a polynomial  $\check{s} \in \mathbb{Q}(t)[p]$  such that  $s - \check{s} \in \sum_{i=1}^{\rho} G_i \cdot \mathbb{Q}(t)[p]$ .

- a. If no monomial of s is divisible by any  $m_i$ , return s.
- b. Set m to the maximal monomial in s that is divisible by some  $m_i$  and choose j such that  $m_j$  divides m.
- c. Set c to the coefficient of m in s and  $c_j$  to the leading coefficient of  $G_j$ .
- d. Set t to the term  $\frac{c}{c_i} \frac{m}{m_i}$  and return  $\operatorname{red}(s G_j \cdot t, (G_i)_{i=1}^{\rho}, \prec)$ .

Table 2. Reduction used by the method in Table 1.

so that an annihilator  $Q = \sum_{j=0}^{r} q_j(t) \partial_t^j \in W_t$  of S satisfies

$$0 = Q \cdot S = \langle F, Q \cdot G \rangle = \langle F, \sum_{j=0}^{r} q_j g^j G \rangle = \langle F, \sum_{j=0}^{r} q_j (g^j + \ell_j) G \rangle$$

for any polynomials  $\ell_j$  that are linear combinations over  $\mathbb{Q}[t]$  of polynomials of the form  $P^{\sharp} \cdot s$ , that is, elements of the vector space

$$H := \sum_{P \in \operatorname{ann} F} P^{\sharp} \cdot \mathbb{Q}(t)[p] = \sum_{P \in (\operatorname{ann} F)^{\sharp}} P \cdot \mathbb{Q}(t)[p].$$

In what follows, for each  $g^j$  we (implicitly) obtain  $\ell_j$  in such a way that the computed  $g^j + \ell_j$  is "reduced" and confined in a finite-dimensional  $\mathbb{Q}(t)$ -vector space. This makes it possible to derive the  $q_j$ .

The procedure is to deal with 11 for each j separately, by reducing the coefficient  $g^j$  modulo H. This space H is first expressed as a finite sum of spaces as follows. Fix any finite family  $\{L_i\}_{i=1}^{\ell}$  of generators of  $(\operatorname{ann} F)^{\sharp}$ . Then, the finite sum  $\tilde{H} := \sum_{i=1}^{\ell} L_i \cdot \mathbb{Q}(t)[p]$  is a subspace of H. Writing any P of  $(\operatorname{ann} F)^{\sharp}$  in the form  $P = \sum_{i=1}^{\ell} L_i U_i$  yields the inclusion of the space H into  $\tilde{H}$ , and thus the equality  $\tilde{H} = H$ . To define the reduction, we proceed by exchanging the generating family  $\{P_i^{\sharp}\}$  of  $(\operatorname{ann} F)^{\sharp}$  for a family  $\{G_i\}_{i=1}^{\ell}$  satisfying the property that any term cm to be reduced (c a coefficient, m a monomial) will be obtained for some  $(j,s) \in \{1,\ldots,\ell\} \times \mathbb{Q}(t)[p]$  as the leading monomial of  $G_j \cdot s$ , where leading monomials are decided by some monomial ordering of  $\mathbb{Q}(t)[p]$  that is compatible with the choice of the family  $\{G_i\}_{i=1}^{\ell}$ . To make this possible, we ensure that  $G_j = m_j + \cdots \in W_p(t)$  for a monomial  $m_j$  in p, with the property that, for any  $\tilde{s} \in \mathbb{Q}(t)[p]$ , the leading monomial of  $m_j\tilde{s}$  is larger than the leading monomial of  $(G_j - m_j) \cdot \tilde{s}$ . In practice, the polynomial s used to reduce cm will be set to the term  $cm/m_j$ , so that m is reduced into  $m - G_j \cdot (cm/m_j)$ . Observing that only finitely many monomials are divisible by none of the  $m_j$  will then ensure the wanted confinement in finite dimension.

There remains to explain how to choose the  $G_i$ . To this end, consider the action of  $W_p(t)$  on polynomials of  $\mathbb{Q}(t)[p]$ , and compare monomials  $m_1 = p^{\alpha_1} \partial^{\beta_1}$  and  $m_2 = p^{\alpha_2} \partial^{\beta_2}$  in  $W_p(t)$  by declaring  $m_1 > m_2$  if and only if  $p^{\alpha_1+\beta_2} > p^{\alpha_2+\beta_1}$  for the ordering on polynomials. Under the assumption that the monomial order is graded by the total degree in  $(p, \partial)$ , it is sufficient to force the leading monomial of each  $G_i$  to be a monomial in p to have the wanted property on the  $G_i \cdot s$ .

We do not know how to ensure the existence of a family  $\{G_j\}_{j=1}^{\ell}$  whose leading monomials are monomials in p, but a module Gröbner basis calculation will in practice be sufficient to exhibit such a situation for k-regular graphs with  $k \leq 7$ .

For each i, write  $P_i^{\sharp} = Q_i(p) + R_i(p, \partial)$ , where  $Q_i$  does not involve any  $\partial_j$  and each monomial of  $R_i$  involves at least one  $\partial_j$ . Then, consider  $M_i := \eta_1 Q_i + \eta_0 R_i$ , where  $\eta_0$  and  $\eta_1$  are new names denoting elements of a

basis of the free right module  $\eta_0 W_p(t) \oplus \eta_1 W_p(t)$ . Consider a Gröbner basis for the right<sup>3</sup> module over  $W_p(t)$  generated by the  $M_i$  with respect to an ordering satisfying:

- (1)  $\eta_1 > \eta_0$ ,
- (2)  $p_i > \partial_j$  for all i and j,
- (3)  $p_k > \cdots > p_1$ .

Those elements  $\eta_1 Q + \eta_0 R$  of the Gröbner basis satisfying  $Q \neq 0$  need not possess the property that Q has a leading monomial larger than the leading monomial of R, but as we start from elements  $P_i^{\sharp}$  that make the  $M_i$  have the property, the Gröbner basis elements are likely to have it, and the Q+R are the  $G_i$  we are looking for. Indeed, this nice situation occurs when  $k \leq 6$  for all variant models described in Section 3. Because the goal of the calculation is to reveal a zero-dimensional ideal in  $\mathbb{Q}(t)[p]$ , the module structure over  $W_p(t)$  can be replaced with a module structure over  $\mathbb{Q}(t)[p]$ , that is, one would like to consider only polynomial recombinations of the coefficients of  $\eta_1$ , without continuing with non-commutative recombinations of the coefficients of  $\eta_0$  between generators with zero coefficient with respect to  $\eta_1$ . In practice, this is achieved by viewing the  $M_i$  as elements of a free  $\mathbb{Q}(t)[p]$ -module with a finite basis consisting of  $\eta_1$  and some  $\partial^{\alpha}\eta_1$ . For all models considered when  $2 \leq k \leq 6$ , this has the nice consequence of speeding up the calculation.

#### 5. No computation of initial conditions is needed

For  $3 \le k \le 7$ , after computing the ODE one readily proves by observation that it possesses the only exponent n=0 at t=0. Consequently, the series solutions form a 1-dimensional vector space, for which a basis is the singleton family  $(R^{(k)}(t))$ . Note that the empty graph is k-regular for any k, implying the identity  $R^{(k)}(t) = 1 + O(t)$ . Converting the ODE to a recurrence relation satisfied by the coefficient sequence  $(c_n)_{n \in \mathbb{Z}}$  of any of its series solution  $\sum_{n \in \mathbb{Z}} c_n t^n$  and forcing  $c_0 = 1$  and  $c_n = 0$  for all n < 0 therefore uniquely determines all  $c_n$  for n > 0. This observation generalizes to any of the models of edges and loops presented in Section 3.

So, a complete proof of correctness of the method for computing an ODE satisfied by the scalar product, together with the observation above, makes it unnecessary to apply a resource-consuming calculation of first terms of the series. Nonetheless, we did verify our series solution by direct computation of scalar product, specifically we directly determined  $r_n^{(k)}$  for  $n \le 1284$  when k = 3,  $n \le 216$  when k = 4,  $n \le 90$  when k = 5,  $n \le 46$  when k = 6, and  $n \le 31$  when k = 7. Furthermore, McKay provided values for k = 5 and  $n \le 600$ , all consistent with our computations.

#### 6. Conclusion

For each graph class we considered with degrees bounded by 6, it did not require more than 15 minutes to determine the differential equation satisfied the generating function. In contrast, the very same implementation requires weeks to terminate for k=7, at least for loopless, simple k-regular graphs. The time breaks down as follows: a Gröbner basis can be obtained in 5 seconds (steps a. to f. in Table 1), from which one can predict that reduced forms of scalar products will be confined in dimension 20. Twenty reductions are then performed, for a total duration of almost 172.5 days, which is over 24 weeks (step g.). Successive reductions take longer and longer, the twentieth requiring 2.18e+6 seconds (23.2 days), after which the linear algebra (steps h. and i.) requires only 1.26e+6 seconds (14.6 days). The resulting ODE satisfied by the generating series  $R^{(7)}(t)$  for 7-regular graphs has order 20.

Of course the natural question to ask is What about k > 7? In that respect, ongoing discussions with Hadrien Brochet have led to promising observations that could speed up calculations and hopefully get k = 8. Finally, the generating function for all regular graphs is not D-finite. Are there properties of the presented ODEs that can help us understand if the generating function of all regular graphs is differentially algebraic or not, and if so how to find the differential equation?

<sup>&</sup>lt;sup>3</sup>As Maple only computes Gröbner bases for left structures, the actual computer calculation computes a Gröbner basis for the left module generated by the  $Q_i^{\dagger}\eta_1 + R_i^{\dagger}\eta_0$ , then returns the adjoints  $(Q+R)^{\dagger}$  obtained from the elements  $Q\eta_1 + R\eta_0$  of the Gröbner basis satisfying  $Q \neq 0$ .

#### 7. Author contributions statement

Frédéric Chyzak: Conceptualization, methodology, software, writing. Marni Mishna: Conceptualization, writing.

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#### APPENDIX A. DIFFERENTIAL EQUATIONS AND RECURRENCES RELATIONS

The following table gathers information related to computations we performed for a list of models:

- parameters "edges", "loops", and k's are as described in Section 3;
- the obtained ODE has order provided in column  $\partial_t$  and its polynomial coefficients have degrees bounded by the number in column t;
- a recurrence on the number of graphs of size n has order provided in column  $\partial_n$  and its polynomial coefficients have degrees bounded by the number in column n;
- the corresponding calculation is done in the time of column "time", measured in seconds.

edges	loops	k's	t	$\partial_t$	n	$\partial_n$	time	edges	loops	k's	l t	$\partial_t$	n	$\partial_n$	time
se	11	[2]	2	1	1	3	0.36	se	11	[4, 5]	125	6	6	126	4.69
me	11	[2]	2	1	1	3	0.36	me	11	[4, 5]	125	6	6	126	4.61
se	lh	[2]	3	1	1	4	0.38	se	lh	[4, 5]	125	6	6	126	7.31
me	lh	[2]	3	1	1	4	0.39	me	lh	[4, 5]	125	6	6	126	6.6
se	la	[2]	2	1	1	3	0.34	se	la	[4, 5]	125	6	6	126	4.7
me	la	[2]	2	1	1	3	0.33	me	la	[4, 5]	125	6	6	126	4.67
se	11	[3]	11	2	2	12	0.38	se	11	[1, 3, 5]	125	6	6	126	2.62
me	11	[3]	11	2	2	12	0.46	me	11	[1, 3, 5]	125	6	6	126	2.56
se	lh	[3]	11	2	2	12	0.38	se	lh	[1, 3, 5]	125	6	6	126	3.8
me	lh	[3]	11	2	2	12	0.45	me	lh	[1, 3, 5]	125	6	6	126	3.64
se	la	[3]	11	2	2	12	0.47	se	la	[1, 3, 5]	125	6	6	126	2.87
me	la	[3]	11	2	2	12	0.5	me	la	[1, 3, 5]	125	6	6	126	2.68
se	11	[2, 3]	11	2	2	12	0.48	se	11	[6]	145	6	6	146	99.23
me	11	[2, 3]	11	2	2	12	0.48	me	11	[6]	145	6	6	146	87.31
se	lh	[2, 3]	11	2	2	12	0.48	se	lh	[6]	425	10	10	426	485.57
me	lh	[2, 3]	11	2	2	12	0.51	me	lh	[6]	425	10	10	426	497.67
se	la	[2, 3]	11	2	2	12	0.47	se	la	[6]	145	6	6	146	97.83
me	la	[2, 3]	11	2	2	12	0.46	me	la	[6]	145	6	6	146	87.62
se	11	[4]	14	2	2	15	0.55	se	11	[2, 6]	142	6	6	143	91.72
me	11	[4]	14	2	2	15	0.57	me	11	[2, 6]	142	6	6	143	88.8
se	lh	[4]	30	3	3	31	0.81	se	lh	[2, 6]	416	10	10	417	604.93
me	lh	[4]	29	3	3	30	0.73	me	lh	[2, 6]	416	10	10	417	584.91
se	la	[4]	14	2	2	15	0.67	se	la	[2, 6]	142	6	6	143	87.82
me	la	[4]	14	2	2	15	0.57	me	la	[2, 6]	142	6	6	143	85.04
se	11	[2, 4]	14	2	2	15	0.7	se	11	[3, 6]	145	6	6	146	145.43
me	11	[2, 4]	14	2	2	15	0.57	me	11	[3, 6]	145	6	6	146	145.26
se	lh	[2, 4]	30	3	3	31	0.79	se	lh	[3, 6]	425	10	10	426	814.86
me	lh	[2, 4]	29	3	3	30	0.76	me	lh	[3, 6]	425	10	10	426	860.93
se	la	[2, 4]	14	2	2	15	0.67	se	la	[3, 6]	145	6	6	146	137.03
me	la	[2, 4]	14	2	2	15	0.68	me	la	[3, 6]	145	6	6	146	146.39
se	11	[3, 4]	14	2	2	15	0.7	se	11	[4, 6]	145	6	6	146	143.17
me	11	[3, 4]	13	2	2	14	0.57	me	11	[4, 6]	145	6	6	146	143.94
se	lh	[3, 4]	30	3	3	31	0.8	se	lh	[4, 6]	425	10	10	426	792.33
me	lh	[3, 4]	29	3	3	30	0.77	me	lh	[4, 6]	425	10	10	426	817.3
se	la	[3, 4]	13	2	2	14	0.7	se	la	[4, 6]	145	6	6	146	155.22
me	la	[3, 4]	14	2	2	15	0.73	me	la	[4, 6]	145	6	6	146	145.1
se	11	[5]	125	6	6	126	4.29	se	11	[5, 6]	145	6	6	146	145.46
me	11	[5]	125	6	6	126	3.84	me	11	[5, 6]	145	6	6	146	140.28
se	lh	[5]	125	6	6	126	5.39	se	lh	[5, 6]	425	10	10	426	788.6
me	lh	[5]	125	6	6	126	4.53	me	lh	[5, 6]	425	10	10	426	806.88
se	la	[5]	125	6	6	126	4.27	se	la	[5, 6]	145	6	6	146	140.4
me	la	[5]	125	6	6	126	3.4	me	la	[5, 6]	145	6	6	146	144.45
se	ll	[2, 5]	125	6	6	126	4.9	se	ll	[2, 4, 6]	145	6	6	146	159.43
me	11	[2, 5]	125	6	6	126	4.64	me	11	[2, 4, 6]	145	6	6	146	160.11
se	lh	[2, 5]	125	6	6	126	7.03	se	lh	[2, 4, 6]	425	10	10	426	673.59
me	lh	[2, 5]	125	6	6	126	6.31	me	lh	[2, 4, 6]	425	10	10	426	692.73
se	la	[2, 5]	125	6	6	126	4.37	se	la	[2, 4, 6]	145	6	6	146	172.37
me	la	[2, 5]	125	6	6	126	4.74	me	la	[2, 4, 6]	145	6	6	146	157.62
se	ll	[3, 5]	125	6	6	126	4.87	se	ll	[1, 2, 3, 4, 5, 6]	145	6	6	146	117.07
me	11	[3, 5]	125	6	6	126	4.76	me	11	[1, 2, 3, 4, 5, 6]	145	6	6	146	113.62
se	lh	[3, 5]	125	6	6	126	6.96	se	lh	[1, 2, 3, 4, 5, 6]	425	10	10	426	495.58
me	lh	[3, 5]	125	6	6	126	6.63	me	lh	[1, 2, 3, 4, 5, 6]	425	10	10	426	508.73
se	la	[3, 5]	125	6	6	126	4.89	se	la	[1, 2, 3, 4, 5, 6]	145	6	6	146	118.23
me	la	[3, 5]	125	6	6	126	4.89	me	la	[1, 2, 3, 4, 5, 6]	145	6	6	146	113.11
me	ıa	[5, 5]	1 120	U	1 0	120	4.03	se	ll	[7]	1683	20	20	1684	1.49000e+07
								se	11	[1]	1000	20	20	1004	1.490006+07

Table 3. Results of calculations on the models described in Section 3. All timings obtained on the same computer (Dell, Precision Mobile 7550, with i9 processor and 64 GB of RAM).