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Exact enumeration of graphs and bipartite graphs with degree constraints

(Extended abstract)

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Abstract

We provide a new explicit formula enumerating graphs with constraints on their degrees, such as regular graphs, and extend it to bipartite graphs. It relies on generating function manipulations and Hadamard products.
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Related work. The most famous graphs with degree constraints are k-regular graphs, where all vertices have degree k. There are two natural generalizations: graphs with a given degree sequence, and graphs where all vertices have their degree in a given set. In this article, we consider the later. There is a large literature on the asymptotic enumeration [1, 22, 7] and typical structure of graphs with degree constraints [25, 18, 15, 14, 3, 16, 8]. We focus on exact enumeration. The main result in this field is that the generating function of graphs with their degrees in a given finite set is D-finite, meaning that it is solution of a differential equation with polynomial coefficients. The previous proofs relied on a symmetric function approach [13, 12, 23, 24]. It starts by considering the infinite product $\prod_{1 \leqslant i<j}(1 + x_i x_j)$ representing graphs where the degree of vertex i is the power of x_i. Arguments on the D-finiteness of the scalar product of symmetric functions are then applied. In contrast, we obtain a formula (Theorem 1) for the generating function of those graphs that is *explicit* and uses only a *finite* number of variables (assuming the degrees are bounded). Our approach relies on direct translation of combinatorial properties into

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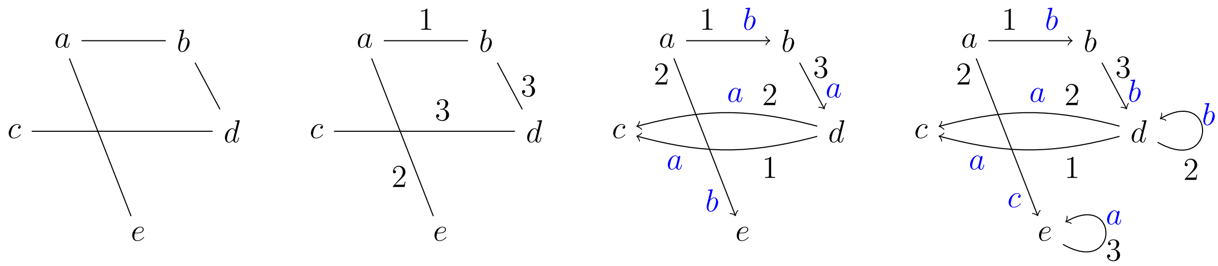
generating function equations (symbolic method [2, 11]), and manipulation of those equations, in particular using Hadamard products. Works of similar spirit include [4, Chapters 3,4,5,7] and [7]. Our expression provides a new proof of D-finiteness, as D-finite series are stable by Hadamard product [21, 27] and evaluation [28]. Although effective algorithms exist [5] to compute the differential equation characterizing the generating function of graphs with degree constraints, they are computationally costly and the differential equation is only known up to $k = 4$ for k-regular graphs. We hope our new formula will allow the computation of differential equations for k-regular graphs with $k \geqslant 5$ and fast enumeration of those graphs [19]. Our results extend to bipartite graphs with different degree sets for the left and right vertices. For bipartite graphs, we used a multidimensional version of the Hadamard product, that has been well studied in the literature [9, 20, 26]. To our knowledge, the asymptotic structure of those graphs has not been investigated [10], and we hope our work will be a step in that direction.

Structure. We enumerate successively several graph-like families with degree constraints: *weighted multigraphs*, *loopless weighted multigraphs*, *weighted graphs* and finally *graphs* in Theorem 1. They are all depicted in Figure 1. The generating function of the first family is expressed directly. Then, to go from each family $\mathcal{A}$ to the next family $\mathcal{B}$, we first express the generating function of $\mathcal{A}$ using the generating function of $\mathcal{B}$, then invert this relation. The extension to bipartite graphs is presented in Theorem 2.



(a) Graph (b) Weighted graph (c) Loopless weighted multigraph (d) Weighted multigraph

Figure 1: Steps of a possible transformation of a simple graph into a weighted multigraph. Labels are represented by letters, while weights are represented by integers.

Notations. The nth coefficient of a formal power series is denoted by $[z^n] \sum_m a_m z^m = a_n$. The *exponential Hadamard product* ([17, Theorem 3], [2, Section 2.1]) is defined as

$$\left(\sum_n a_n \frac{z^n}{n!}\right) \odot_z \left(\sum_n b_n \frac{z^n}{n!}\right) = \sum_n a_n b_n \frac{z^n}{n!}.$$

We denote by $\odot_{z=1}$ the exponential Hadamard product followed by the evaluation at $z = 1$. Throughout this article, the variable δ_d marks vertices of degree d. We denote by $\boldsymbol{\delta}$ the infinite vector $(\delta_0, \delta_1, \delta_2, \ldots)$. The same bold convention extends to other letters. An interesting particular case is, given a set $\mathcal{D}$ of nonnegative integers, to set $\delta_d = 1$ if $d \in \mathcal{D}$, and $\delta_d = 0$ otherwise. That way, only graphs with all their vertices having degree in $\mathcal{D}$ are counted. We associate to those variables the generating function

$$\Delta(z, \boldsymbol{\delta}) = \sum_{d \geqslant 0} \delta_d \frac{z^d}{d!}.$$

In the following, we consider graphs with vertices of degree at most D for some $D \geqslant 0$, so $\delta_j = 0$ whenever $j > D$ and $\Delta(z, \boldsymbol{\delta})$ is a polynomial.

1 Weighted multigraphs

Definition. A weighted multigraph G is a finite sequence

$$G = (V(G), E_1(G), E_2(G), \ldots)$$

where $V(G) = \{1, 2, \ldots, n(G)\}$ is the set of $n(G)$ vertices, and for all $j \geqslant 1$, $E_j(G)$ is the finite set of $m_j(G)$ edges of weight j

$$E_j(G) = \{(u_{j,1}, v_{j,1}, 1), \ldots, (u_{j,m_j(G)}, v_{j,m_j(G)}, m_j(G))\}$$

where each $u_{i,j}$ and $v_{k,\ell}$ belongs to $V(G)$. Thus, vertices are labeled, edges of weight j are labeled (and have their own independent label set), and all edges are oriented. Furthermore, loops and multiple edges are allowed. The degree $\deg(u)$ of a vertex u is defined as the sum of the weights of all edges adjacent to it, counted twice if they are loops. For examples, in Figure 1 (d), vertex e has degree 8.

Generating function. We use the variable z to mark the vertices, and for all $j \geqslant 1$, we use $w_j/2$ to mark each edge of weight j. This factor 1/2 is here for historical reasons only [6, Section 2.3]. Additionally, for each $d \geqslant 0$, the variable δ_d is introduced to mark vertices of degree d. The generating function of weighted multigraphs $\mathrm{WMG}(z, \boldsymbol{w}, \boldsymbol{\delta})$ is then defined as a sum over all weighted multigraphs

$$\mathrm{WMG}(z, \boldsymbol{w}, \boldsymbol{\delta}) = \sum_G \left(\prod_{u=1}^{n(G)} \delta_{\deg(u)} \right) \left(\prod_{j \geqslant 1} \frac{(w_j/2)^{m_j(G)}}{m_j(G)!} \right) \frac{z^{n(G)}}{n(G)!}. \tag{1}$$

Lemma 1. *Let $P_{\mathrm{WMG}}(\boldsymbol{x}, \boldsymbol{\delta})$ denote the polynomial*

$$P_{\mathrm{WMG}}(\boldsymbol{x}, \boldsymbol{\delta}) = \Delta(y, \boldsymbol{\delta}) \odot_{y=1} e^{\sum_{j=1}^{D} x_j y^j},$$

then the generating function of weighted multigraphs is equal to

$$\mathrm{WMG}(z, \boldsymbol{w}, \boldsymbol{\delta}) = e^{\sum_{j=1}^{D} w_j x_j^2/2} \odot_{x_1=1} \cdots \odot_{x_D=1} e^{z P_{\mathrm{WMG}}(\boldsymbol{x}, \boldsymbol{\delta})}.$$

Proof. Any weighted multigraph decomposes uniquely as a set of labeled vertices, each attached to a set of labeled half-edges of weight j, for $j \geqslant 1$. If the vertex has degree d, then the sum of the weights of the half-edges attached to it should be d. Then, using the variable x_j to mark the half-edges of weight j, the generating function of such sets is $P_{\mathrm{WMG}}(\boldsymbol{x}, \boldsymbol{\delta})$. If the multigraph contains m_j edges of weight j, then after cutting them in two, we are left with $2m_j$ half-edges of weight j. The symbolic method [11] implies

$$\mathrm{WMG}(z, \boldsymbol{w}, \boldsymbol{\delta}) = \sum_{\boldsymbol{m}} (2\boldsymbol{m})! [\boldsymbol{x}^{2\boldsymbol{m}}] e^{z P_{\mathrm{WMG}}(\boldsymbol{x}, \boldsymbol{\delta})} \prod_{j \geqslant 1} \frac{(w_j/2)^{m_j}}{m_j!}.$$

This expression is simplified using Hadamard products with the function

$$\sum_{m \geqslant 0} (2m)! \frac{(w/2)^m}{m!} \frac{x^{2m}}{(2m)!} = e^{wx^2/2}.$$

□

A multigraph is *loopless* if it has no edge containing twice the same vertex. The generating function $\mathrm{LWMG}(z, \boldsymbol{w}, \boldsymbol{\delta})$ of those weighted multigraphs is defined by restricting the sum from Equation (1) to them.

Lemma 2. *Let $P_{\mathrm{LWMG}}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\delta})$ denote the polynomial*

$$P_{\mathrm{LWMG}}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\delta}) = \Delta(y, \boldsymbol{\delta}) \odot_{y=1} e^{\sum_{j=1}^{D} x_j y^j - \sum_{j=1}^{D} w_j y^{2j}/2},$$

then the generating function of loopless weighted multigraphs is equal to

$$\mathrm{LWMG}(z, \boldsymbol{w}, \boldsymbol{\delta}) = e^{\sum_{j=1}^{D} w_j x_j^2/2} \odot_{x_1=1} \cdots \odot_{x_D=1} e^{z P_{\mathrm{LWMG}}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\delta})}.$$

Proof. Any weighted multigraph is uniquely obtained by adding a set of loops on each vertex of a loopless weighted multigraph. During this operation, any vertex of degree d becomes a vertex of degree $d + 2k$, for some nonnegative integer k, and a set of weighted loops whose weights sum to k. This corresponds to replacing δ_d with

$$\delta_d(\boldsymbol{\eta}, \boldsymbol{w}) = \sum_{k \geqslant 0} \eta_{d+2k} [y^k] e^{\frac{1}{2} \sum_{d \geqslant 1} w_d y^d} = \sum_{j \geqslant 0} \eta_j [y^j] y^d e^{\frac{1}{2} \sum_{d \geqslant 1} w_d y^{2d}}. \tag{2}$$

Thus, the generating functions of weighted multigraphs and loopless weighted multigraphs are linked by the relation

$$\mathrm{WMG}(z, \boldsymbol{w}, \boldsymbol{\eta}) = \mathrm{LWMG}(z, \boldsymbol{w}, \boldsymbol{\delta}(\boldsymbol{\eta}, \boldsymbol{w}))$$

Inverting Equation (2), we obtain

$$\eta_d(\boldsymbol{\delta}, \boldsymbol{w}) = \sum_{j \geqslant 0} \delta_j [y^j] y^d e^{-\frac{1}{2} \sum_{i \geqslant 1} w_i y^{2i}}$$

so

$$\Delta(z, \boldsymbol{\eta}(\boldsymbol{\delta}, \boldsymbol{w})) = \sum_{d=0}^{D} \sum_{j \geqslant 0} \delta_j [y^j] y^d e^{-\sum_{i=1}^{D} w_i y^{2i}/2} \frac{z^d}{d!} = \Delta(y, \boldsymbol{\delta}) \odot_{y=1} e^{yz - \sum_{i=1}^{D} w_i y^{2i}/2}.$$

Given the expression of $\mathrm{WMG}(z, \boldsymbol{w}, \boldsymbol{\delta})$ from Lemma 1, we deduce

$$\begin{aligned} \mathrm{LWMG}(z, \boldsymbol{w}, \boldsymbol{\delta}) &= \mathrm{WMG}(z, \boldsymbol{w}, \boldsymbol{\eta}(\boldsymbol{\delta}, \boldsymbol{w})) \\ &= e^{\sum_{j=1}^{D} w_j x_j^2/2} \odot_{x_1=1} \cdots \odot_{x_D=1} e^{z \Delta(y, \boldsymbol{\eta}) \odot_{y=1} \exp\left(\sum_{j=1}^{D} x_j y^j\right)}. \end{aligned}$$

Finally, the properties $F(x\,y) \odot_x G(x) = F(x) \odot_x G(x\,y)$ and $F(x) \odot e^x = F(x)$ of the exponential Hadamard product imply

$$\begin{aligned} \Delta(y, \boldsymbol{\eta}) \odot_{y=1} e^{\sum_{j=1}^{D} x_j y^j} &= \Delta(y, \boldsymbol{\delta}) \odot_{y=1} e^{yz - \sum_{i=1}^{D} w_i y^{2i}/2} \odot_{y=1} e^{\sum_{j=1}^{D} x_j y^j} \\ &= \Delta(y, \boldsymbol{\delta}) \odot_{y=1} e^{\sum_{j=1}^{D} x_j y^j - \sum_{j=1}^{D} w_j y^{2j}/2} = P_{\mathrm{LWMG}}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\delta}). \end{aligned}$$

□

2 Graphs

Definitions. A weighted graph G is a finite sequence

$$G = (V(G), E_1(G), E_2(G), \ldots)$$

where $V(G) = \{1, 2, \ldots, n(G)\}$ is the set of $n(G)$ vertices, and $\bigcup_j E_j(G)$ is a finite set of edges, which are unordered pairs of distinct vertices. $E_j(G)$ denotes the set of edges of weight j and its cardinality is $m_j(G)$. Thus, edges are unoriented and unlabeled, loops and multiple edges are forbidden. The degree of a vertex is still defined as the sum of the weights of its adjacent edges.

Unweighted graphs correspond to the case $G = (V(G), E_1(G))$, so $E_j = \varnothing$ for all $j \geqslant 2$.

Generating function. The generating function of weighted graphs $\mathrm{WG}(z, \boldsymbol{w}, \boldsymbol{\delta})$ is defined as a sum over all weighted graphs

$$\mathrm{WG}(z, \boldsymbol{w}, \boldsymbol{\delta}) = \sum_{G} \left(\prod_{u=1}^{n(G)} \delta_{\deg(u)} \right) \left(\prod_{j \geqslant 1} w_j^{m_j(G)} \right) \frac{z^{n(G)}}{n(G)!}.$$

This generating function is exponential with respect to the variable z marking the vertices, and ordinary with respect to the variables $(w_j)_{j \geqslant 1}$ marking the edges. Note that the generating function of an edge of weight j is w_j (for weighted multigraphs, we used the convention $w_j/2$, linked to the fact that edges were oriented).

Lemma 3. *For $j \geqslant 0$, let $v_j(\boldsymbol{w})$ and $P_{\mathrm{WG}}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\delta})$ denote the polynomials*

$$v_j(\boldsymbol{w}) = [y^j] \log \left(1 + \sum_{j \geqslant 1} w_j y^j\right), \qquad P_{\mathrm{WG}}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\delta}) = \Delta(y, \boldsymbol{\delta}) \odot_{y=1} \frac{e^{\sum_{j=1}^{D} x_j y^j}}{\sqrt{1 + \sum_{j=1}^{D} w_j y^{2j}}},$$

then the generating function of weighted graphs is equal to

$$\mathrm{WG}(z, \boldsymbol{w}, \boldsymbol{\delta}) = e^{\sum_{j=1}^{D} v_j(\boldsymbol{w}) x_j^2/2} \odot_{x_1=1} \cdots \odot_{x_D=1} e^{z P_{\mathrm{WG}}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\delta})}.$$

Proof. Consider a weighted graph G with m_d edge of weight d for each $d \geqslant 1$. Then there exist $\prod_d 2^{m_d} m_d!$ ways to orient and label those edges to turn G into a weighted multigraph. Thus, the generating function of loopless weighted multigraphs that contain no multiple edge is equal to the generating function of weighted graphs. To construct a loopless weighted multigraph G from a loopless weighted multigraph H without multiple edges, one replace each edge of H of weight d with a set of edges linking the same vertices and whose weights sum to d. For each $d \geqslant 1$, let us use the variable v_d to mark edges of weight d in loopless weighted multigraphs, and the variable w_d to mark edges of weight d in weighted graphs. The previous construction corresponds to replacing the variable w_d with

$$w_d(\boldsymbol{v}) = [y^d](e^{\sum_{j \geqslant 1} v_j y^j} - 1).$$

Thus, the generating functions of weighted graphs and of loopless weighted multigraphs are linked by the relation

$$\mathrm{WG}(z, \boldsymbol{w}(\boldsymbol{v}), \boldsymbol{\delta}) = \mathrm{LWMG}(z, \boldsymbol{v}, \boldsymbol{\delta}).$$

Inverting this relation, we obtain

$$v_d(\boldsymbol{w}) = [y^d] \log \left(1 + \sum_{j \geqslant 1} w_j y^j\right)$$

and

$$\mathrm{WG}(z, \boldsymbol{w}, \boldsymbol{\delta}) = \mathrm{LWMG}(z, \boldsymbol{v}(\boldsymbol{w}), \boldsymbol{\delta}).$$

Injecting the expression of $\mathrm{LWMG}(z, \boldsymbol{w}, \boldsymbol{\delta})$ from Lemma 2 concludes the proof. □

In particular, for $\boldsymbol{w} = (w, 0, 0, \dots, 0)$, we recover the case of classical graphs, and more specifically the case of k-regular graphs, by setting $\delta_d = 1$ if $d = k$, and $\delta_d = 0$ otherwise.

Theorem 1. *Let $P_G(\boldsymbol{x}, w, \boldsymbol{\delta})$ denote the polynomial*

$$P_G(\boldsymbol{x}, w, \boldsymbol{\delta}) = \Delta(y, \boldsymbol{\delta}) \odot_{y=1} \frac{e^{\sum_{j=1}^{D} x_j y^j}}{\sqrt{1 + w y^2}},$$

then the generating function of graphs is equal to

$$G(z, w, \boldsymbol{\delta}) = e^{-\sum_{j=1}^{D} (-w)^j x_j^2/(2j)} \odot_{x_1=1} \cdots \odot_{x_D=1} e^{z P_G(\boldsymbol{x}, w, \boldsymbol{\delta})}.$$

In particular, the number of k-regular graphs with n vertices is

$$e^{\sum_{j=1}^{k} (-1)^{j+1} x_j^2/(2j)} \odot_{x_1=1} \cdots \odot_{x_k=1} \left([y^k] \frac{e^{\sum_{j=1}^{k} x_j y^j}}{\sqrt{1 + y^2}}\right)^n.$$

3 Bipartite graphs

Definition. A bipartite graph G is a triplet $(V(G), \tilde{V}(G), E(G))$ with $V(G)$ (resp $\tilde{V}(G)$) the set of labeled left-vertices (resp. right-vertices) and $E(G) \subset V(G) \times \tilde{V}(G)$ the set of edges.

Generating function. The generating function $\mathrm{BG}(z, \tilde{z}, w, \boldsymbol{\delta}, \tilde{\boldsymbol{\delta}})$ of bipartite graphs with degree at most D is defined as a sum over bipartite graphs

$$\mathrm{BG}(z, \tilde{z}, w, \boldsymbol{\delta}, \tilde{\boldsymbol{\delta}}) = \sum_{G} \left(\prod_{u=1}^{|V(G)|} \delta_{\deg(u)} \right) \left(\prod_{u=1}^{|\tilde{V}(G)|} \tilde{\delta}_{\deg(u)} \right) w^{|E(G)|} \times \frac{z^{|V(G)|}}{|V(G)|!} \times \frac{\tilde{z}^{|\tilde{V}(G)|}}{|\tilde{V}(G)|!}$$

This generating function is exponential with respect to the variable z (resp. $\tilde{z}$) marking the left vertices (resp. right vertices), and ordinary with respect to the variable w marking the edges. For all d, δ_d (resp. $\tilde{\boldsymbol{\delta}}_d$) marks the left vertices (resp. right vertices) of degree d.

Notation. The *multivariate exponential Hadamard product* is defined as

$$\sum_{\boldsymbol{m}} A_{\boldsymbol{m}} \frac{\boldsymbol{z}^{\boldsymbol{m}}}{\boldsymbol{m}!} \odot_{\boldsymbol{m}} \sum_{\boldsymbol{m}} B_{\boldsymbol{m}} \frac{\boldsymbol{z}^{\boldsymbol{m}}}{\boldsymbol{m}!} = \sum_{\boldsymbol{m}} A_{\boldsymbol{m}} B_{\boldsymbol{m}} \frac{\boldsymbol{z}^{\boldsymbol{m}}}{\boldsymbol{m}!}.$$

This extension is compatible with the univariate product in the sense

$$A(z_1)B(z_2) \odot_{z_1 z_2} C(z_1, z_2) = A(z_1) \odot_{z_1} \left(B(z_2) \odot_{z_2} C(z_1, z_2) \right).$$

Theorem 2. *Let* $\boldsymbol{v} = \left((-1)^{d+1} w^d / d\right)_{1 \leqslant d \leqslant D}$, $\Delta(y, \boldsymbol{\delta}) = \sum_{d=0}^{D} \delta_d \frac{y^d}{d!}$ *and let* $P_{\mathrm{BG}}(\boldsymbol{w}, \boldsymbol{\delta})$ *denote the polynomial*

$$P_{\mathrm{BG}}(\boldsymbol{w}, \boldsymbol{\delta}) = \Delta(y, \boldsymbol{\delta}) \odot_{y=1} e^{\sum_{d=1}^{D} w_d y^d}.$$

Then the generating function of bipartite graphs with degree constraints is equal to

$$\mathrm{BG}(z, \tilde{z}, w, \boldsymbol{\delta}, \tilde{\boldsymbol{\delta}}) = e^{z P_{\mathrm{BG}}(\boldsymbol{w}, \boldsymbol{\delta})} \odot_{\boldsymbol{w}=\boldsymbol{v}} e^{\tilde{z} P_{\mathrm{BG}}(\boldsymbol{w}, \tilde{\boldsymbol{\delta}})}.$$

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