

Applied Algebraic Analysis

Anna-Laura Sattelberger^b

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Abstract

These are the lecture notes of the graduate level course “ D -Modules and Holonomic Functions” at KTH and Stockholm University taught by the author in the fall term 2023. The course consists of 10 lectures, each of which is the content of one chapter of these notes. It introduces concepts from algebraic analysis and demonstrates their utility in problems in the sciences. Algebraic analysis investigates linear PDEs by algebraic methods. The main actor is the Weyl algebra, denoted D . It is a non-commutative ring that gathers linear differential operators with polynomial coefficients. The theory of D -modules provides deep classification results of linear PDEs, structural insights into problems in the sciences as well as new computational tools. This course focuses on the applied aspects of D -modules. The applications are ranging from maximum likelihood estimation in statistical inference through the study of Feynman integrals in high energy physics to the computation of volumes of basic semi-algebraic sets to arbitrary precision. D -ideals encode systems of linear PDEs with polynomial coefficients. The ideals encode crucial properties of the solutions of the associated system of PDEs, such as their singularities. These occur in two different kinds, namely as regular and irregular singularities. Series solutions of a regular holonomic D -ideal can be computed purely algebraically in terms of Gröbner deformations of the D -ideal. Due to Gröbner basis theories for the Weyl algebra, various software systems are available to compute with holonomic D -ideals and their solutions, which are called *holonomic functions*. Holonomic functions are ubiquitous in the sciences and their function values can be computed via the holonomic gradient method, a numerical evaluation scheme which makes use of an annihilating D -ideal of the function.

The course is hands-on: the focus lies on the introduction of concepts from algebraic analysis and getting them to run for solving problems arising in applications. Many proofs are therefore skipped, but references are provided. Required concepts from algebraic geometry are introduced en route. The course is mainly based on [37] and [39] and the references therein, as well as on current research articles.

^b Department of Mathematics, KTH Royal Institute of Technology, Lindstedtsvägen 25,
114 28 Stockholm, Sweden alsat@kth.se

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1 An algebraic counterpart of linear PDEs

Algebraic analysis is a mathematical field which investigates linear ordinary and partial differential equations (ODEs and PDEs) with algebraic methods. In general, it investigates sheaves of \mathcal{D}_X -modules on a complex manifold or a smooth algebraic variety X , where \mathcal{D}_X is the sheaf of differential operators on X . This abstract setting enables deep classification results, such as the Riemann–Hilbert correspondence. The Riemann–Hilbert correspondence is an equivalence of categories which allows to replace a regular holonomic \mathcal{D} -module by its topological counterpart, namely its solution complex (cf. [21]). The theory of \mathcal{D} -modules turns out to be very helpful in applications as well, where it mainly enters via the Weyl algebra, denoted D . It is $D = \mathcal{D}_X(X)$ for $X = \mathbb{A}_{\mathbb{C}}^n$ the affine n -space over the complex numbers. This course focuses on the Weyl algebra; familiarity with sheaf theory is not required.

1.1 The Weyl algebra

Definition 1.1. The (n -th) *Weyl algebra*, denoted D_n or just D if the number of variables is clear from the context, is the algebra obtained from the free algebra over \mathbb{C} generated by variables x_1, \dots, x_n and partial derivatives $\partial_1, \dots, \partial_n$

$$D := \mathbb{C}[x_1, \dots, x_n] \langle \partial_1, \dots, \partial_n \rangle \quad (1.1)$$

by imposing the following relations: all generators are assumed to commute, except ∂_i and x_i . Their *commutator* $[\partial_i, x_i] := \partial_i x_i - x_i \partial_i$ fulfills

$$[\partial_i, x_i] = 1 \quad \text{for } i = 1, \dots, n. \quad (1.2)$$

This encodes precisely Leibniz' rule for taking the derivative of the product of functions: if f is a function of x , one has

$$\frac{\partial(xf)}{\partial x} - x \frac{\partial f}{\partial x} = xf' + f - xf' = 1 \cdot f. \quad (1.3)$$

The Weyl algebra gathers differential operators on \mathbb{C}^n .¹ Its elements are linear differential operators with polynomial coefficients, i.e., as a set,

$$D = \left\{ \sum_{\alpha, \beta \in \mathbb{N}^n} c_{\alpha, \beta} x^\alpha \partial^\beta \mid c_{\alpha, \beta} \in \mathbb{C}, \text{ only finitely many } c_{\alpha, \beta} \text{ non-zero} \right\},$$

where multi-index notation is used, i.e., $x^\alpha = x_1^{\alpha_1} \dots x_n^{\alpha_n}$ and $\partial^\beta = \partial_1^{\beta_1} \dots \partial_n^{\beta_n}$.

We denote the action of a differential operator $P \in D$ on a function f by a bullet, i.e., $\partial_i \bullet f = \partial f / \partial x_i$, and so on. In order to stress that a function f depends on variables x_1, \dots, x_n , we sometimes write $f(x_1, \dots, x_n)$ for the function.

¹To be precise, we are on affine n -space of \mathbb{C} , i.e., the affine scheme $\mathbb{A}_{\mathbb{C}}^n = \text{Spec}(\mathbb{C}[x_1, \dots, x_n])$. The closed points of $\mathbb{A}_{\mathbb{C}}^n$ are $\mathbb{A}_{\mathbb{C}}^n(\mathbb{C}) = \mathbb{C}^n$.

Definition 1.2. The *order* of a differential operator $P = \sum_{\alpha, \beta \in \mathbb{N}} c_{\alpha, \beta} x^\alpha \partial^\beta \in D_1$ is

$$\text{ord}(P) := \max \{ \beta \mid \exists \alpha \text{ s.t. } c_{\alpha, \beta} \neq 0 \},$$

i.e., the highest derivative that occurs in the associated linear ODE, $P \bullet f = 0$.

Example 1.3 (Airy's equation). Airy's equation is the linear, second-order ODE

$$f''(x) - x \cdot f(x) = 0. \quad (1.4)$$

Its solutions describe particles that are confined within a triangular potential well [45]. Moreover, it is the standard example to demonstrate Stokes' phenomenon—a wall-crossing phenomenon for the asymptotic behavior of the solution functions to (1.4), cf. [48]. To the ODE in (1.4), we associate the differential operator $P_{\text{Airy}} = \partial^2 - x$. Its \mathbb{C} -vector space of holomorphic solutions is spanned by Airy's functions of first and second kind, Ai and Bi:

$$\begin{aligned} \text{Ai}(x) &= \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3} + xt\right) dt, \\ \text{Bi}(x) &= \frac{1}{\pi} \int_0^\infty \left[\exp\left(-\frac{t^3}{3} + xt\right) + \sin\left(\frac{t^3}{3} + xt\right) \right] dt. \end{aligned} \quad (1.5)$$

Algebraically, Airy's function Ai is encoded by the differential operator P_{Airy} together with the following two initial conditions, which pick out Ai from the two-dimensional solution space of (1.4):

$$f(0) = \frac{1}{3^{2/3} \Gamma(\frac{2}{3})} \quad \text{and} \quad f'(0) = -\frac{1}{3^{1/3} \Gamma(\frac{1}{3})}, \quad (1.6)$$

where $\Gamma(\cdot)$ denotes the gamma function. ◇

Exercise 1.4 (Commutators [36, 1.2.4]). Prove that

- (1) $[\partial_i^\ell, x_i] = \ell \partial_i^{\ell-1}$,
- (2) $[\partial_i, x_i^k] = k x_i^{k-1}$,
- (3) $[\partial_i^\ell, x_i^k] = \sum_{j \geq 1} \frac{k(k-1) \cdots (k-j+1) \cdot \ell(\ell-1) \cdots (\ell-j+1)}{j!} x_i^{k-j} \partial_i^{\ell-j}$,

where, by convention, negative powers are 0. ◇

Definition 1.5. The operator $\theta_i := x_i \partial_i \in D$ is called *i-th Euler operator*.

Theorem 1.6 (Converse of Euler's homogeneous function theorem). *If $f(x_1, \dots, x_n)$ is annihilated by $\theta_1 + \dots + \theta_n - k$, where $k \in \mathbb{Z}$, then f is (positively) homogeneous of degree k , i.e.:*

$$f(tx_1, \dots, tx_n) = t^k \cdot f(x_1, \dots, x_n) \quad \text{for all } t > 0. \quad (1.7)$$

Proof. Set $g(t) = f(tx_1, \dots, tx_n)$. Via the chain rule, differentiating g with respect to t yields

$$\begin{aligned} g'(t) &= x_1 \frac{\partial f}{\partial x_1}(tx_1, \dots, tx_n) + \dots + x_n \frac{\partial f}{\partial x_n}(tx_1, \dots, tx_n) \\ &= \frac{1}{t} \cdot \left(tx_1 \frac{\partial f}{\partial x_1}(tx_1, \dots, tx_n) + \dots + tx_n \frac{\partial f}{\partial x_n}(tx_1, \dots, tx_n) \right). \end{aligned} \quad (1.8)$$

Since $(\theta_1 + \dots + \theta_n) \bullet f = k \cdot f$, we conclude that $g'(t) = k/t \cdot g(t)$ and hence

$$\frac{g'(t)}{g(t)} = \frac{k}{t}. \quad (1.9)$$

Integrating both sides of (1.9) yields that $\ln |g(t)| = \ln(t^k) + \ln(C)$ for all $t > 0$ and thus $g(t) = Ct^k$. Plugging in $t = 1$ yields that $C = g(1)$ and hence $g(t) = t^k \cdot g(1)$. Written out, this yields $f(tx_1, \dots, tx_n) = t^k \cdot f(x_1, \dots, x_n)$ for all $t > 0$. \square

1.2 Properties and D -modules

The rings $\mathbb{C}[\partial_1, \dots, \partial_n]$ and $\mathbb{C}[\theta_1, \dots, \theta_n]$ are *commutative* subrings of the Weyl algebra. The first denotes linear PDEs with *constant* coefficients. Note that for $z = 1/x$, $x\partial_x = -z\partial_z$. Hence, for elements of the $\mathbb{C}[\theta_1, \dots, \theta_n]$, it is particularly easy to switch from 0 to ∞ and vice versa. Further frequently used rings of differential operators are

$$D_{\mathbb{G}_m^n} := \mathbb{C}[x_1^{\pm 1}, \dots, x_n^{\pm 1}] \langle \partial_1, \dots, \partial_n \rangle \quad (1.10)$$

with coefficients in Laurent polynomials, which are exactly the global functions on the algebraic n -torus $(\mathbb{C}^*)^n$,² and the *rational Weyl algebra*

$$R_n := \mathbb{C}(x_1, \dots, x_n) \langle \partial_1, \dots, \partial_n \rangle \quad (1.11)$$

with coefficients in the field of rational functions

$$\mathbb{C}(x_1, \dots, x_n) = \{p/q \mid p, q \in \mathbb{C}[x_1, \dots, x_n], q \neq 0\}. \quad (1.12)$$

Since D is non-commutative, we have to distinguish between left and right D -ideals. If not explicitly stated otherwise, we always mean *left* D -ideals, since those correspond to systems of linear PDEs: if $P \bullet f = 0$ for some $P \in D$, also $QP \bullet f = 0$ for any $Q \in D$. We will denote by $\langle P_1, \dots, P_k \rangle$ the left D -ideal generated by $P_1, \dots, P_k \in D$, and sometimes by DP if $k = 1$. The Weyl algebra is simple as a ring, i.e., it does not contain any proper two-sided ideal.

One important example of D -ideals are A -hypergeometric systems—also called *GKZ systems*, named after Gelfand, Kapranov, and Zelevinsky [14]. They are determined by an integer matrix $A \in \mathbb{Z}^{n \times k}$ and a parameter vector $\kappa \in \mathbb{C}^n$. Consider the Weyl algebra $D_A = \mathbb{C}[c_\alpha \mid \alpha \in A] \langle \partial_\alpha \mid \alpha \in A \rangle$ whose variables are indexed by the columns of A .

²To be precise, we are on the algebraic n -torus $\mathbb{G}_m^n = \text{Spec}(\mathbb{C}[x_1^{\pm 1}, \dots, x_n^{\pm 1}])$. The complex-valued points of the algebraic n -torus are $\mathbb{G}_m^n(\mathbb{C}) = (\mathbb{C}^*)^n$, and $D_{\mathbb{G}_m^n} = D_{\mathbb{G}_m^n}(\mathbb{G}_m^n)$.

Definition 1.7. The *toric ideal* associated to A is the binomial ideal

$$I_A := \langle \partial^u - \partial^v \mid u - v \in \ker(A), u, v \in \mathbb{N}^A \rangle \subset \mathbb{C}[\partial_\alpha \mid \alpha \in A], \quad (1.13)$$

where $u = (u_\alpha)_{\alpha \in A} \in \mathbb{N}^A$, $\partial^u = \prod_{\alpha \in A} \partial_\alpha^{u_\alpha}$, and similarly for v . Let $J_{A,\kappa}$ be the ideal generated by the entries of $A\theta - \kappa$ where $\theta := (\theta_\alpha)_{\alpha \in A}$ and $\theta_\alpha = c_\alpha \partial_\alpha$. The D_A -ideal $H_A(\kappa) := I_A + J_{A,\kappa}$ is called *A-hypergeometric system* (or *GKZ system*).

Sometimes, one assumes that the all-one vector is contained in the row space of A . This implies that $H_A(\kappa)$ is regular holonomic; we will learn later in the course what this means.

Example 1.8 ([2, Example 4.2]). Let $\kappa = (-\nu_1, -\nu_2, s) \in \mathbb{C}^3$. Consider the matrix

$$A = \begin{bmatrix} 1 & 1 & 2 & 2 & 3 & 3 \\ 2 & 3 & 1 & 3 & 1 & 2 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \in \mathbb{Z}^{3 \times 6}. \quad (1.14)$$

Using the Macaulay2 [17] package Dmodules [28], one computes that the toric ideal I_A is generated by 9 binomials, namely

$$I_A = \langle \partial_2 \partial_5 - \partial_1 \partial_6, \partial_3 \partial_4 - \partial_1 \partial_6, \partial_4 \partial_5^2 - \partial_3 \partial_6^2, \partial_1 \partial_5^2 - \partial_3^2 \partial_6, \partial_4^2 \partial_5 - \partial_2 \partial_6^2, \\ \partial_1 \partial_4 \partial_5 - \partial_2 \partial_3 \partial_6, \partial_1 \partial_4^2 - \partial_2^2 \partial_6, \partial_2 \partial_3^2 - \partial_1^2 \partial_5, \partial_2^2 \partial_3 - \partial_1^2 \partial_4 \rangle. \quad (1.15)$$

In the notation of (1.13), the first generator in (1.15) corresponds to the tuple of vectors $u = (0, 1, 0, 0, 1, 0)$ and $v = (1, 0, 0, 0, 0, 1)$. The third generator to $u = (0, 0, 0, 1, 2, 0)$ and $v = (0, 0, 1, 0, 0, 2)$, and so on. The ideal $J_{A,\kappa}$ is generated by the 3 operators

$$\theta_1 + \theta_2 + 2\theta_3 + 2\theta_4 + 3\theta_5 + 3\theta_6 + \nu_1, \quad 2\theta_1 + 3\theta_2 + \theta_3 + 3\theta_4 + \theta_5 + 2\theta_6 + \nu_2, \quad \theta_1 + \theta_2 + \theta_3 + \theta_4 + \theta_5 + \theta_6 - s.$$

Together, these 12 operators generate $H_A(\kappa) \subset D_6$. \diamond

Exercise 1.9. Compute an A -hypergeometric system of your choice using Macaulay2.³ \diamond

Theorem 1.10 (Stafford). *For every D -ideal I , there exist $P, Q \in D$ such that $I = \langle P, Q \rangle$.*

An algorithmic proof of the theorem can be found in [27].

Exercise 1.11. Compute two operators that generate the D_4 -ideal $\langle \partial_1, \partial_2, \partial_3, \partial_4 \rangle$, for instance by running the the following lines in Macaulay2, using the package Dmodules.m2 [28].

```
loadPackage "Dmodules"
D = QQ[x1,x2,x3,x4,d1,d2,d3,d4,WeylAlgebra=>{x1=>d1,x2=>d2,x3=>d3,x4=>d4}];
I = ideal(d1,d2,d3,d4)
stafford I
```

As pointed out in the [documentation](#), the current implementation of the command `stafford` guarantees the in- and output ideals to be equal only in the rational Weyl algebra R_n . \diamond

³An online version of Macaulay2 is available at the following link: <https://macaulay2.com/TryItOut/>

We now turn to modules over the Weyl algebra.

Definition 1.12. A D -module is a left D -module, i.e., an abelian group M together with a left action of the Weyl algebra

$$\bullet: D \times M \longrightarrow M, \quad (P, m) \mapsto P \bullet m \quad (1.16)$$

obeying the usual compatibility conditions, i.e., for all $P, Q \in D$ and $m, n \in M$:

$$\begin{aligned} \text{(i)} \quad (P \cdot Q) \bullet m &= P \bullet (Q \bullet m), & \text{(iii)} \quad P \bullet (m + n) &= P \bullet m + P \bullet n, \\ \text{(ii)} \quad (P + Q) \bullet m &= P \bullet m + Q \bullet m, & \text{(iv)} \quad \text{and } 1 \bullet m &= m. \end{aligned}$$

To a D -ideal I , one associates the D -module $D/I \in \text{Mod}(D)$. In this sense, D -modules are generalizations of systems of linear PDEs. Further typical examples of D -modules of a different kind are function spaces, e.g., holomorphic functions \mathcal{O}^{an} ,⁴ rational functions $\mathbb{C}(x)$, convergent $\mathbb{C}\{x\}$ or formal $\mathbb{C}\llbracket x \rrbracket$ power series, or (complex-valued) Schwartz distributions.

Example 1.13 (Example 1.8 revisited). The D -module associated to a hypergeometric system $H_A(\kappa)$ is typically denoted by $M_A(\kappa) = D_A/H_A(\kappa) \in \text{Mod}(D_A)$. \diamond

Exercise 1.14. Let $M \in \text{Mod}(D)$ such that M is finite-dimensional as a \mathbb{C} -vector space. Prove that $M = 0$. \diamond

In this course, we focus on D -modules of the form D/I for I a left D -ideal. In fact, by a theorem of Stafford, every “holonomic” D -module is of that form. In other words, every holonomic D -module is cyclic, i.e., it is generated by a single element.

Exercise 1.15 ($n = 1$). Determine for which $a, b \in \mathbb{C}$ there there exists a non-trivial left D -linear morphism between the D -modules $M_a := D/(x\partial - a)$ and $M_b := D/(x\partial - b)$. \diamond

2 Gröbner deformations of D -ideals

This lecture investigates Gröbner deformations of D -ideals.

2.1 Initial ideals

Weight vectors for the Weyl algebra are allowed to be taken from the set

$$\mathcal{W} = \{(u, v) \in \mathbb{R}^{2n} \mid u_i + v_i \geq 0, \quad i = 1, \dots, n\}. \quad (2.1)$$

The vector $(u, v) \in \mathcal{W}$ assigns weight u_i to x_i and weight v_i to ∂_i . Among others, \mathcal{W} contains the set $\{(-w, w) \mid w \in \mathbb{R}^n\}$. Every operator P in the Weyl algebra has a unique expansion

$$P = \sum_{(\alpha, \beta) \in E} c_{\alpha, \beta} x^\alpha \partial^\beta, \quad (2.2)$$

⁴Of course, holomorphic functions are always to be thought of *locally*, i.e., one means $\mathcal{O}^{\text{an}}(U)$ for some appropriate domain $U \subset \mathbb{C}^n$.

called *normally ordered expression* of P , where $c_{\alpha,\beta} \in \mathbb{C} \setminus \{0\}$ and E is a finite subset of \mathbb{N}^{2n} . Unless stated otherwise, we always assume that differential operators are given in that form.

Definition 2.1. Fix a weight vector $(u, v) \in \mathcal{W}$. The (u, v) -*weight* of a differential operator $P \in D$ (expressed as in (2.2)) is the number $m = \max_{(\alpha,\beta) \in E} (\alpha \cdot u + \beta \cdot v)$. If (u, v) is of the form $(-w, w)$ for some $w \in \mathbb{R}^n$, the resulting number is called w -*weight* of P .

Example 2.2. Let $P = \theta_1 + \theta_2 + \theta_3 + 1 \in D_3$ and $w = (-1, 0, 1)$. The w -weight of $\theta_1 = x_1 \partial_1$ is $(1, 0, -1, -1, 0, 1) \cdot (1, 0, 0, 1, 0, 0) = 1 - 1 = 0$, and similarly for the remaining summands of P . The w -weight of P hence is $\max\{1 - 1, 0 + 0, -1 + 1, 0\} = 0$. \diamond

Exercise 2.3. Consider the map $[x\partial, (\cdot)]: D_1 \rightarrow D_1$, $P \mapsto [x\partial, P]$, which sends a differential operator to its commutator with the Euler operator. Find a closed formula for this map which involves the w -weight for $w = 1$. Is this map D -linear? \diamond

Each weight vector $(u, v) \in \mathcal{W}$ introduces an increasing filtration $F_{(u,v)}^\bullet(D)$ of the Weyl algebra, namely

$$\cdots \subseteq F_{(u,v)}^{k-1}(D) \subseteq F_{(u,v)}^k(D) \subseteq F_{(u,v)}^{k+1}(D) \subseteq \cdots \quad (2.3)$$

where $F_{(u,v)}^k(D)$ denotes the vector space

$$F_{(u,v)}^k(D) = \left\{ \sum_{\{(\alpha,\beta) \mid \alpha \cdot u + \beta \cdot v \leq k\} \text{ finite}} c_{\alpha,\beta} x^\alpha \partial^\beta \right\}. \quad (2.4)$$

They fulfill $F_{(u,v)}^k(D) \cdot F_{(u,v)}^\ell(D) \subseteq F_{(u,v)}^{k+\ell}(D)$ and $\bigcup_k F_{(u,v)}^k(D) = D$. For $(u, v) = (1, \dots, 1)$, the resulting filtration is called *Bernstein filtration*. For $(u, v) = (0, 1)$, where $0 \in \mathbb{R}^n$ and 1 denotes the all-one vector in \mathbb{R}^n , the obtained filtration is the *order filtration* of D .

Exercise 2.4. Let $(u, v) \in \mathcal{W}$ and consider the induced filtration $F_{(u,v)}^\bullet(D)$. Prove that the associated graded ring $\text{gr}_{(u,v)}(D) = \bigoplus_k F_{(u,v)}^k(D)/F_{(u,v)}^{k-1}(D)$ is

$$\text{gr}_{(u,v)}(D) = \begin{cases} D & \text{if } u + v = 0, \\ \mathbb{C}[x_1, \dots, x_n, \xi_1, \dots, \xi_n] & \text{if } u + v > 0, \\ \text{a mixture of the above} & \text{otherwise.} \end{cases} \quad (2.5)$$

In the equation above, $u + v > 0$ means $u_i + v_i > 0$ for all $i = 1, \dots, n$. \diamond

Definition 2.5. The *initial form* of a differential operator $P \in D \setminus \{0\}$ is

$$\text{in}_{(u,v)}(P) = \sum_{\alpha \cdot u + \beta \cdot v = m} c_{\alpha,\beta} \prod_{u_k + v_k > 0} x_k^{\alpha_k} \xi_k^{\beta_k} \prod_{u_k + v_k = 0} x_k^{\alpha_k} \partial_k^{\beta_k} \in \text{gr}_{(u,v)}(D), \quad (2.6)$$

and $\text{in}_{(u,v)}(P) = 0$ if $P = 0$.

In the definition, the ξ_k are new variables that commute with all others. The initial form is an element in the graded ring $\text{gr}_{(u,v)}(D)$. The case when u is the zero vector and v is the all-one vector $1 = (1, \dots, 1)$ is of particular interest. Analysts refer to $\text{in}_{(0,1)}(P)$ as the *principal symbol* of the differential operator P ; it is an ordinary polynomial in $2n$ variables.

Example 2.6. The principal symbol of $P_1 = x^2\partial + 1$ is $\text{in}_{(0,1)}(P_1) = x^2\xi \in \mathbb{C}[x][\xi]$. The principal symbol of $P_2 = x_1\partial_1 + x_2\partial_2 + 2x_2^2$ is $\text{in}_{(0,1)}(P_2) = x_1\xi_1 + x_2\xi_2 \in \mathbb{C}[x_1, x_2][\xi_1, \xi_2]$. \diamond

A further important special case is if the weight vector is of the form $(u, v) = (-w, w)$ for some $w \in \mathbb{R}^n$. In that case, one denotes the initial form of P short-hand by $\text{in}_w(P)$.

Definition 2.7. Let $(u, v) \in \mathcal{W}$ and I a D -ideal. The *initial ideal* $\text{in}_{(u,v)}(I)$ of I with respect to (u, v) is the $\text{gr}_{(u,v)}(D)$ -ideal generated by the initial forms of all elements of I . In symbols,

$$\text{in}_{(u,v)}(I) = \langle \text{in}_{(u,v)}(P) \mid P \in I \rangle \subset \text{gr}_{(u,v)}(D). \quad (2.7)$$

Example 2.8. For $I = \langle x_1\partial_2, x_2\partial_1 \rangle \subset D_2$ and $(u, v) = (0, 1) = (0, 0, 1, 1) \in \mathbb{R}^4$, the initial ideal of I is the $\mathbb{C}[x_1, x_2][\xi_1, \xi_2]$ -ideal

$$\text{in}_{(0,1)}(I) = \langle x_1\xi_2, x_2\xi_1, x_1\xi_1 - x_2\xi_2, x_2^2\xi_2, x_2\xi_2^2 \rangle. \quad (2.8)$$

This can be obtained by running the code

```
LIB "dmod.lib";
def D2 = makeWeyl(2); setring D2;
ideal I = x(1)*D(2), x(2)*D(1);
def CV = charVariety(I); setring CV; charVar;
```

in the computer algebra system [Singular](#) [12].⁵ It uses the D -module libraries [4]. \diamond

Note bene. As the above example demonstrates, it is in general not sufficient to take only the initial forms of generators of the D -ideal into account.

It is important to understand how the initial ideal of a D -ideal changes as one lets the weight vector vary. This information is encoded in the *Gröbner fan* of the D -ideal. It is a finite polyhedral fan in \mathbb{R}^{2n} with support \mathcal{W} such that the initial ideal $\text{in}_{(u,v)}(I) \subset \text{gr}_{(u,v)}(D_n)$ is constant as (u, v) ranges over any of its open cones.

Definition 2.9. The *small Gröbner fan* of a D -ideal I is the restriction of the Gröbner fan to set of weight vectors $\{(u, v) \mid u + v = 0\} \simeq \mathbb{R}^n$.

Hence, the cones of the small Gröbner fan of I are in one-to-one correspondence with the initial ideals $\text{in}_{(-w,w)}(I)$.

Definition 2.10. A weight vector is *generic for I* if it lies in an open cone of the small Gröbner fan of I .

Definition 2.11. A *Gröbner deformation* of a D -ideal I is the left D -ideal $\text{in}_{(-w,w)}(I)$ for some generic weight vector $w \in \mathbb{R}^n$.

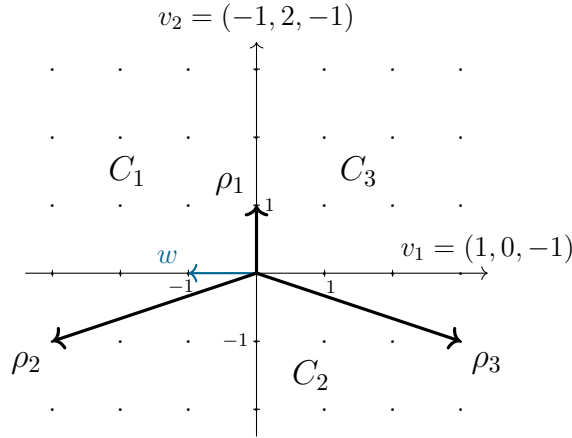


Figure 1: The small Gröbner fan of the D -ideal $I_3(4, 2, 2, 2)$, here drawn in $\mathbb{R}_w^3/\mathbb{R}(1, 1, 1)$ in the orthogonal basis $\{v_1, v_2\} = \{(1, 0, -1), (-1, 2, -1)\}$.

Example 2.12 ([20, (2.6)]). Let $I_3(c_0, c_1, c_2, c_3) = \langle P_1, P_2, P_3 \rangle$ be the D -ideal generated by

$$\begin{aligned} P_1 &= 4(x_1\partial_1^2 - x_3\partial_3^2) + 2(2 + c_0 - 2c_1)\partial_1 - 2(2 + c_0 - 2c_3)\partial_3, \\ P_2 &= 4(x_2\partial_2^2 - x_3\partial_3^2) + 2(2 + c_0 - 2c_2)\partial_2 - 2(2 + c_0 - 2c_3)\partial_3, \\ P_3 &= (2c_0 - c_1 - c_2 - c_3) + 2(x_1\partial_1 + x_2\partial_2 + x_3\partial_3). \end{aligned} \quad (2.9)$$

This D -ideal arises in the study of conformally-invariant Feynman integrals. Its small Gröbner fan for $c = (4, 2, 2, 2)$ is depicted in Figure 1, where one exploits homogeneity of the system with respect to the vector $(1, 1, 1)$ to draw the fan in 2-dimensional space. One obtains it by explicitly computing initial ideals of I . \diamond

Exercise 2.13. Let $w = (-1, 0, 1)$. In Figure 1, w corresponds to the vector $(-1, 0) = -v_1$ and is depicted in blue color. The initial ideal of $I_3(4, 2, 2, 2)$ with respect to w is

$$\text{in}_w(I) = \langle (\theta_3 + 1)\partial_3, (\theta_2 + 1)\partial_2, \theta_1 + \theta_2 + \theta_3 + 1 \rangle. \quad (2.10)$$

This can be obtained by running the following code in **Singular** line by line:

```
LIB "dmodapp.lib";
def D3 = makeWeyl(3); setring D3;
poly P1 = x(1)*D(1)^2-x(3)*D(3)^2+D(1)-D(3);
poly P2 = x(2)*D(2)^2-x(3)*D(3)^2+D(2)-D(3);
poly P3 = x(1)*D(1)+x(2)*D(2)+x(3)*D(3)+1;
ideal I = P1,P2,P3; intvec w = (-1,0,1);
def inwI = initialIdealW(I,-w,w); inwI;
```

Choose some more weight vectors from different cones and rays of the Gröbner fan in Figure 1 and compute the corresponding initial ideals of the D_3 -ideal $I_3(4, 2, 2, 2)$. \diamond

⁵An online version of **Singular** is available at the following link: <https://www.singular.uni-kl.de:8003/>

2.2 Indicial ideals

Fix an integer $n \geq 1$. The algebraic n -torus $T := (\mathbb{C} \setminus \{0\})^n$ naturally acts on the Weyl algebra, namely by scaling the generators ∂_i and x_i in a reciprocal manner:

$$\circ : T \times D \longrightarrow D, \quad (t, \partial_i) \mapsto t_i \partial_i, \quad (t, x_i) \mapsto \frac{1}{t_i} x_i.$$

Definition 2.14. A D -ideal I is said to be *torus-fixed* if $t \circ I = I$ for all $t \in T$.

Torus-fixed D -ideals play the role of monomial ideals in an ordinary commutative polynomial ring. They can be described as follows:

Proposition 2.15 ([37, Lemma 2.3.1 and Theorem 2.3.3]). *A D -ideal is torus-fixed if and only if one of the equivalent properties holds:*

- (1) $I = \text{in}_{(-w,w)}(I)$ for all $w \in \mathbb{R}^n$.
- (2) I is generated by operators $x^a p(\theta) \partial^b$ where $a, b \in \mathbb{N}^n$ and $p \in \mathbb{C}[\theta_1, \dots, \theta_n]$.

Definition 2.16. The *distraction* of a D -ideal I is the $\mathbb{C}[\theta_1, \dots, \theta_n]$ -ideal

$$\tilde{I} := R_n I \cap \mathbb{C}[\theta_1, \dots, \theta_n]. \quad (2.11)$$

Example 2.17. Let $I = \langle \partial_1^3, \partial_1 \partial_2, \partial_2^2 \rangle$. The points under the staircase diagram of I are $(0, 0), (1, 0), (2, 0), (0, 1)$, as shown in Figure 2.

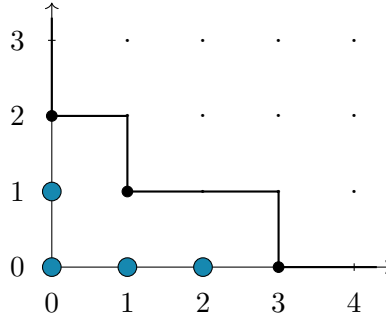


Figure 2: The staircase diagram of $I = \langle \partial_1^3, \partial_1 \partial_2, \partial_2^2 \rangle$.

The distraction of I is the radical ideal

$$\begin{aligned} \tilde{I} &= \langle \theta_1(\theta_1 - 1)(\theta_1 - 2), \theta_1 \theta_2, \theta_2(\theta_2 - 1) \rangle \\ &= \langle \theta_1, \theta_2 \rangle \cap \langle \theta_1 - 1, \theta_2 \rangle \cap \langle \theta_1 - 2, \theta_2 \rangle \cap \langle \theta_1, \theta_2 - 1 \rangle. \end{aligned}$$

To see that, it helps to recall that $\theta_i^2 = x_i^2 \partial_i^2 + x_i \partial_i$, and $\theta_i^3 = x_i^3 \partial_i^3 + 3x_i^2 \partial_i^2 + x_i \partial_i$. Observe that, for this example,

$$\text{Sol}(I) = \text{Sol}(\tilde{I}) = \mathbb{C} \cdot \{1, x_1, x_1^2, x_2\} \quad (2.12)$$

on the level of solutions. \diamond

Definition 2.18. A D_n -ideal F is called *Frobenius ideal* if it can be generated by elements of $\mathbb{C}[\theta_1, \dots, \theta_n]$.

Frobenius ideals hence are of the form $F = D_n J$ with J an ideal in $\mathbb{C}[\theta_1, \dots, \theta_n]$.

Definition 2.19. Let $w \in \mathbb{R}^n$. The *indicial ideal* of I (with respect to w) is

$$\text{ind}_w(I) := \widetilde{\text{in}_{(-w,w)}(I)} = R_n \cdot \text{in}_{(-w,w)}(I) \cap \mathbb{C}[\theta_1, \dots, \theta_n]. \quad (2.13)$$

The zeros of $\text{ind}_w(I)$ in \mathbb{C}^n are called the *exponents* of I with respect to w .

Section 9 will justify the name “exponent”. There, we will also see that the space of solutions to the system of PDEs encoded by a Frobenius ideal can be described explicitly when the given ideal in $\mathbb{C}[\theta_1, \dots, \theta_n]$ is Artinian, i.e., if the Krull dimension of $\mathbb{C}[\theta]/J$ is 0.

Example 2.20. Consider the D_1 -ideal $I = \langle x^2 \partial^2 - x \partial + 1 - x \rangle$ and set $w = 1$. The indicial ideal $\text{ind}_w(I)$ is the principal ideal in $\mathbb{C}[\theta]$ generated by $\theta^2 - 2\theta + 1$. This polynomial has the unique zero $A = 1$; it is of multiplicity 2. Hence, 1 is the only exponent of I . \diamond

Exercise 2.21. Compute the exponents of the D -ideal $I_3(4, 2, 2, 2)$ from Example 2.12 for the weight $w = (-1, 0, 1)$. \diamond

3 The characteristic variety

In this lecture, we introduce the characteristic variety of a D -ideal I . This algebraic variety is the main ingredient for defining holonomicity as well as for defining the singular locus of I .

3.1 Holonomicity

Denote by $(0, 1)$ the vector $(0, \dots, 0, 1, \dots, 1) \in \mathbb{R}^{2n}$.

Definition 3.1. Let I be a D -ideal. The $\mathbb{C}[x_1, \dots, x_n, \xi_1, \dots, \xi_n]$ -ideal $\text{in}_{(0,1)}(I)$ is called the *characteristic ideal* of I .

We already saw an example of a characteristic ideal in Example 2.8.

Definition 3.2. The *characteristic variety* of a D -ideal I is the vanishing set of the characteristic ideal, i.e.,

$$\text{Char}(I) := V(\text{in}_{(0,1)}(I)) = \{(x, \xi) \mid p(x, \xi) = 0 \text{ for all } p \in \text{in}_{(0,1)}(I)\} \subseteq \mathbb{C}^{2n}. \quad (3.1)$$

In order to remember the variables’ names, one sometimes writes $\mathbb{C}_x^n \times \mathbb{C}_\xi^n$ for \mathbb{C}^{2n} in (3.1).

The irreducible components of an affine variety $V(I) \subset \mathbb{C}^n$ are obtained by the primary decomposition of its defining ideal $I \subset \mathbb{C}[x_1, \dots, x_n]$. Recall that an ideal $\mathfrak{q} \subset \mathbb{C}[x_1, \dots, x_n]$ is *primary* if, whenever $p, q \in \mathfrak{q}$, it follows that $p \in \mathfrak{q}$ or $q \in \mathfrak{q}$ or $p, q \in \sqrt{\mathfrak{q}}$, where

$$\sqrt{\mathfrak{q}} = \{p \in \mathbb{C}[x_1, \dots, x_n] \mid p^m \in \mathfrak{q} \text{ for some } m > 0\} \quad (3.2)$$

denotes the radical of \mathfrak{q} . Every ideal $I \subset \mathbb{C}[x_1, \dots, x_n]$ has an *irredundant* decomposition

$$I = \mathfrak{q}_1 \cap \dots \cap \mathfrak{q}_k \quad (3.3)$$

into primary ideals. The \mathfrak{q}_i are not uniquely determined, but their underlying prime ideals $\mathfrak{p}_i := \sqrt{\mathfrak{q}_i}$ are; these are the *associated primes* of I . Irredundancy means that removing any of the primary ideals \mathfrak{q}_i would change the intersection (3.3), and the $\sqrt{\mathfrak{q}_i}$ are pairwise distinct. The variety $V(I)$ has a unique irredundant decomposition into irreducible algebraic varieties

$$V(I) = \bigcup_{\mathfrak{p}_i \text{ minimal}} V(\mathfrak{p}_i). \quad (3.4)$$

Here, the union is taken over all associated prime ideals that are *minimal* over I .

Example 3.3. Consider the $\mathbb{C}[x, y, z]$ -ideal

$$I = \langle (x + y + z - 1)^2 \cdot (xz - (x + y)y) \rangle. \quad (3.5)$$

The variety $V(I)$ is plotted in Figure 3. Its associated primary ideals and their underlying primes are $\langle (x + y + z - 1)^2 \rangle$ with underlying prime $\langle x + y + z - 1 \rangle$, and the prime ideal $\langle xz - (x + y)y \rangle$. This can be obtained by running the following code in Singular.

```
LIB "primdec.lib";
ring r = 0,(x,y,z),dp; setring r;
ideal I = (x+y+z-1)^2*(x*z-(x+y)*y);
list pr = primdecGTZ(I); pr;
```

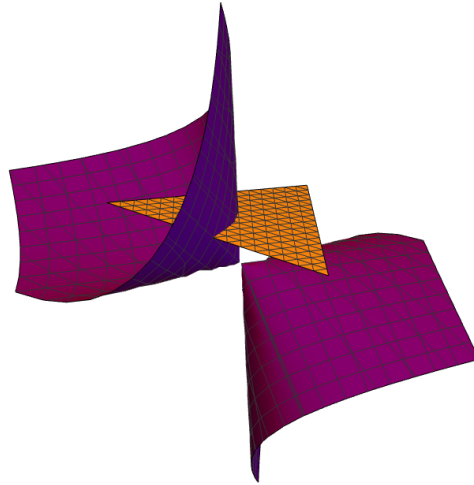


Figure 3: The real-valued points of the variety $V((x + y + z - 1)^2(xz - (x + y)y))$.

The variety $V(I)$ decomposes into the purple projective surface and the orange hyperplane. The curve obtained as their intersection has an interpretation as a discrete statistical model taking 3 states. This is the viewpoint of likelihood geometry [22]. \diamond

Exercise 3.4. Consider the D_1 -ideal $I = \langle \partial^2, x\partial - 1 \rangle$. Compute the characteristic ideal of I as well as its associated primes. \diamond

The following theorem was established by Sato, Kawai, and Kashiwara in [38].

Theorem 3.5 (Fundamental Theorem of Algebraic Analysis). *Let $0 \subsetneq I \subsetneq D$ be a D -ideal. Every irreducible component of its characteristic variety $\text{Char}(I)$ has dimension at least n .*

Definition 3.6. A D -ideal (or its associated D -module D/I) is called *holonomic* if the dimension of its characteristic ideal is n , i.e., as small as possible.

Exercise 3.7. Let $f = x_1^3 - x_2^2 \in \mathbb{C}[x_1, x_2]$ and consider the D_2 -ideal

$$I = \left\langle f\partial_1 + \frac{\partial f}{\partial x_1}, f\partial_2 + \frac{\partial f}{\partial x_2} \right\rangle. \quad (3.6)$$

Is I holonomic? Find a non-constant function that is annihilated by I . \diamond

Definition 3.8. A function $f(x_1, \dots, x_n)$ is *holonomic* if its annihilator

$$\text{Ann}_{D_n}(f) := \{P \in D_n \mid P \bullet f = 0\} \quad (3.7)$$

is a holonomic D_n -ideal.

Definition 3.9. The *holonomic rank* of a D_n -ideal I is

$$\text{rank}(I) := \dim_{\mathbb{C}(x)}(R_n/R_n I) = \dim_{\mathbb{C}(x)}(\mathbb{C}(x)[\xi]/\mathbb{C}(x)[\xi] \text{in}_{(0,1)}(I)). \quad (3.8)$$

The second equality in (3.8) follows from standard arguments in Gröbner basis theory.

Note bene. If I is holonomic, it follows that $\text{rank}(I) < \infty$. The reverse implication is not true. To see this, compute the holonomic rank of the non-holonomic D -ideal in Exercise 3.7.

Example 3.10. Consider the D_2 -ideal $I = \langle \partial_1 x_1 \partial_1, \partial_2^2 + 1 \rangle$. The holonomic rank of I is 4, since $\{1, \partial_1, \partial_2, \partial_1 \partial_2\}$ is a basis of the $\mathbb{C}(x_1, x_2)$ -vector space $R_2/R_2 I$. \diamond

Example 3.11 (GKZ systems). Let A be an $n \times k$ integer matrix. Its *normalized volume*, denoted $\text{vol}(A)$, is the volume of the union of the convex hull of the columns of A and the origin, scaled with respect to the standard n -simplex having volume 1. It is a lower bound for the holonomic rank of $H_A(\kappa)$: for all parameters $\kappa \in \mathbb{C}^n$, one has the inequality

$$\text{rank}(H_A(\kappa)) \geq \text{vol}(A). \quad (3.9)$$

Equality holds for generic κ , but the identity may fail for special κ ; see [37, Example 4.2.7]. \diamond

Exercise 3.12. Compute the holonomic rank of the GKZ system $H_A(\kappa)$ from Example 1.8 for a parameter $\kappa \in \mathbb{C}^3$ of your choice. Compare this number to $\text{vol}(A)$. \diamond

3.2 Singular locus

Let I, J be ideals in a polynomial ring $\mathbb{C}[x_1, \dots, x_n]$. The *saturated ideal* $(I: J^\infty)$ with respect to J is the ideal

$$(I: J^\infty) := \bigcup_{k \geq 1} (I: J^k), \quad (3.10)$$

where $(I: J^k)$ denotes the *ideal quotient* $\{p \in \mathbb{C}[x_1, \dots, x_n] \mid pJ^k \subset I\}$. The variety of $(I: J^\infty)$ is the Zariski closure of $V(I) \setminus V(J)$. Geometrically, taking a saturation hence means to remove the component cut out by J (and takes the closure of the resulting set).

Exercise 3.13. Consider the $\mathbb{C}[x, y, z]$ -ideals $I = \langle x^2yz \rangle$ and $J = \langle xy \rangle$. Compute $(I: J^\infty)$ and visualize their varieties. \diamond

Definition 3.14. The *singular locus* $\text{Sing}(I)$ of I is the variety in \mathbb{C}^n defined as

$$\text{Sing}(I) := V\left(\left(\text{in}_{(0,1)}(I) : \langle \xi_1, \dots, \xi_n \rangle^\infty\right) \cap \mathbb{C}[x_1, \dots, x_n]\right). \quad (3.11)$$

Geometrically, the singular locus of I is the closure of the projection of $\text{Char}(I) \setminus (\mathbb{C}^n \times \{0\})$ onto the first n coordinates of $\mathbb{C}^{2n} = \mathbb{C}_x^n \times \mathbb{C}_\xi^n$.

Remark 3.15. Outside the singular locus of a D -ideal I , the solutions to I form a vector bundle of rank $\text{rank}(I)$. \diamond

If $I = DP$ for some $P \in D$, we sometimes also write $\text{Sing}(P)$ for $\text{Sing}(I)$. In case $n = 1$ and $I = DP$ for some $P = \sum_k a_k \partial^k \in D$, the singular locus is given by the vanishing locus of the polynomial $a_{\text{ord}(P)}$. As a formula,

$$\text{Sing}(P) = V(a_{\text{ord}(P)}) = \{x \in \mathbb{C} \mid a_{\text{ord}(P)}(x) = 0\}. \quad (3.12)$$

Example 3.16. Let $P_1 = x\partial^2 + \partial$ and $P_2 = x^2\partial + 1$. Their singular loci are equal, they are $\text{Sing}(P_1) = \text{Sing}(P_2) = \{0\} \subset \mathbb{C}$. \diamond

Example 3.17 (Example 3.10 revisited). Let $I = \langle x_1\partial_1^2 + \partial_1, \partial_2^2 + 1 \rangle$. A computation in **Singular** reveals that its characteristic ideal is $\langle \xi_2^2, x_1\xi_1^2 \rangle \subset \mathbb{C}[x_1, x_2][\xi_1, \xi_2]$. Hence $\text{Sing}(I)$ is the coordinate hyperplane $V(x_1) \subset \mathbb{C}^2$. \diamond

Example 3.18. Let $I = \langle x_1\partial_2, x_2\partial_1 \rangle \subset D_2$. Its singular locus is $\text{Sing}(I) = V(x_1, x_2) = \{0\}$, and its solution space is $\text{Sol}(I) = \mathbb{C} \cdot 1$. This simple example demonstrates that points in the singular locus may be singularities of its solutions, but do not have to be. \diamond

Example 3.19 (Example 2.12 continued). The singular locus of $I_3(4, 2, 2, 2)$ is

$$\text{Sing}(I_3(4, 2, 2, 2)) = V(x_1x_2x_3 \cdot \lambda) \subset \mathbb{C}^3, \quad (3.13)$$

where λ denotes the the Källén polynomial

$$\lambda = x_1^2 + x_2^2 + x_3^2 - 2(x_1x_2 + x_1x_3 + x_2x_3). \quad (3.14)$$

Hence, the singular locus of $I_3(4, 2, 2, 2)$ is the union of the cone shown in Figure 4 and the coordinate hyperplanes $\{x_i = 0\}$, $i = 1, 2, 3$. \diamond

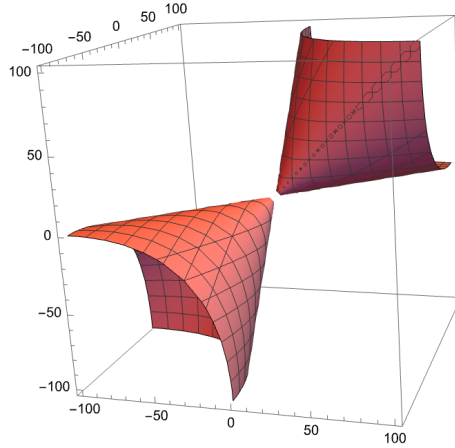


Figure 4: The real vanishing locus of the Källén polynomial.

Example 3.20. The singular locus of a GKZ system $H_A(\kappa)$ is the variety cut out by the so called “principal A -determinant”, see [15, Remark 1.8]. It is a product of individual discriminants to polynomial systems, one for each face of the cone over A ; see [14, 37] for the precise statement, and the survey [33] of GKZ systems pointing to plenty of related work. \diamond

4 Solutions and their singularities

In this lecture, we investigate solutions of D -ideals and, in particular, their singularities.

4.1 Solution space

We write $\text{Mod}(D)$ for the category of left D -modules.

Definition 4.1. Let I be a D -ideal and $M \in \text{Mod}(D)$. The *solution space of I in M* is the \mathbb{C} -vector space

$$\text{Sol}_M(I) := \{m \in M \mid P \bullet m = 0 \text{ for all } P \in I\}. \quad (4.1)$$

Also holomorphic functions \mathcal{O}^{an} on (subsets of) \mathbb{C}^n are a D -module; they carry a natural left action of the Weyl algebra. Unless stated otherwise, we will deal with holomorphic solutions on a suitable open domain in \mathbb{C}^n , and we drop the subscript in (4.1) to mean such solutions, i.e., we denote

$$\text{Sol}(I) = \text{Sol}_{\mathcal{O}^{\text{an}}}(I) = \{f \in \mathcal{O}^{\text{an}} \mid P \bullet f = 0 \text{ for all } P \in I\} \quad (4.2)$$

for suitable $U \subset \mathbb{C}^n$. The solution space of a D -module can be recovered completely algebraically. For two D -modules $M, N \in \text{Mod}(D)$, denote by $\text{Hom}_D(M, N)$ the space of morphisms of left D -modules. Now let $I = DP$ for some $P \in D$. The \mathbb{C} -vector spaces

$$\text{Hom}_{D^{\text{an}}}(D^{\text{an}}/D^{\text{an}}P, \mathcal{O}^{\text{an}}) \cong \{f \in \mathcal{O}^{\text{an}} \mid P \bullet f = 0\} \quad (4.3)$$

are isomorphic. All is to be read in the *analytified* setup, i.e., $D^{\text{an}} = \mathbb{C}\{x\}\langle\partial\rangle$: otherwise, one would neglect solutions like \exp , and so on. For the sake of friendlier notation, we will drop the superscript $(\cdot)^{\text{an}}$ in the rest of this paragraph. The isomorphism (4.3) is obtained by combining the isomorphisms

$$\text{Hom}_D(D/DP, \mathcal{O}) \cong \{\varphi \in \text{Hom}_D(D, \mathcal{O}) \mid \varphi(P) = 0\} \quad (4.4)$$

and

$$\text{Hom}_D(D, \mathcal{O}) \cong \mathcal{O}, \quad \varphi \mapsto \varphi(1), \quad (4.5)$$

cf. [21, p. 2] for more details. This implies that the space of holomorphic solutions $\text{Sol}(I)$ of I is isomorphic to $\text{Hom}_D(D/I, \mathcal{O})$.

Remark 4.2. One may look for solutions of a D -module M in any D -module N : by what was argued above, the vector space $\text{Hom}_{D^{\text{an}}}(M^{\text{an}}, N^{\text{an}})$ encodes the *solutions of M in N* . \diamond

Theorem 4.3 (Cauchy–Kovalevskaya–Kashiwara). *Let I be D -ideal and let U be an open subset of $\mathbb{C}^n \setminus \text{Sing}(I)$ that is simply connected. If I is holonomic, then the space of holomorphic functions on U that are solutions to I has dimension equal to $\text{rank}(I)$, i.e.,*

$$\dim(\text{Sol}(I)) = \text{rank}(I). \quad (4.6)$$

Example 4.4 (Example 3.10 revisited). Let I be the D_2 -ideal $\langle\partial_1 x_1 \partial_1, \partial_2^2 + 1\rangle$. Its holonomic rank is $\text{rank}(I) = 4$. On simply connected domains outside $\text{Sing}(I) = V(x_1)$, the solution space is 4-dimensional and equals

$$\text{Sol}(I) = \mathbb{C} \cdot \{\sin(x_2), \cos(x_2), \log(x_1) \sin(x_2), \log(x_1) \cos(x_2)\}. \quad (4.7)$$

Indeed, the only singularities occurring are along the coordinate hyperplane $\{x_1 = 0\}$. \diamond

4.2 Regular vs. irregular singularities

The singular locus of a D -ideal encodes where solutions of the system of PDEs encoded by the D -ideal may have singularities. From a D -ideal, we cannot only read *where* its solutions may have singularities, but we can also read their growth behavior when approaching points of the singular locus. Depending on the growth behavior of its solutions at singular points, a D -ideal is called *regular singular* or *irregular singular*. We here focus on the univariate case. The multivariate case is more involved: for proving that a D_n -ideal for $n > 1$ is regular singular, one would need to check that its restriction to all curves is regular singular; we refer to [37, Section 2.4] for a discussion of regularity in the multivariate case. For the rest of this section, we stick to $n = 1$. Our presentation here closely follows Section 5 of [47].

Definition 4.5. Let $\rho: (a, b) \rightarrow \mathbb{R}_{>0}$ be some positive continuous function. The *open sector* $S = S(a, b, \rho)$ is the set of non-zero complex numbers

$$S(a, b, \rho) := \{z \in \mathbb{C} \setminus \{0\} \mid \arg(z) \in (a, b) \text{ and } |z| < \rho(\arg(z))\}. \quad (4.8)$$

Definition 4.6. A function $f \in \mathcal{O}^{\text{an}}(S(a, b, \rho))$ is of moderate growth on S if there exists an integer N and a real number $c > 0$ such that $|f(x)| < c \cdot |x|^N$ on S .

Definition 4.7 ([47, p. 146]). A differential operator P has solutions of moderate growth at $x = 0$ if on any open sector $S = S(a, b, \rho)$ with $|a - b| < 2\pi$ and sufficiently small ρ , there is a basis of solutions to P all of which have moderate growth on S .

Example 4.8. The complex logarithm has moderate growth at $x = 0$. The exponential function $\exp(1/x)$ does not have moderate growth at $x = 0$: as x approaches 0, it grows faster than any power of x . \diamond

Definition 4.9. Let $x_0 \in \text{Sing}(I)$. A D -ideal is *regular singular at x_0* if there exists a fundamental system of solutions that have moderate growth at x_0 . The ideal I (or its associated D -module D/I) is *regular singular* (as system on \mathbb{P}^1) if it is regular singular everywhere, including at infinity. Otherwise, it is called *irregular singular*.

In this terminology, also non-singular points are counted as regular singular points.

Definition 4.10. We denote by $\text{val}: \mathbb{C}((x)) \rightarrow \mathbb{R} \cup \{\infty\}$ the following non-Archimedean valuation on the field of formal Laurent series:

$$\text{val}(a_k) := \min \{j \mid a_{k,j} \neq 0\} \quad (4.9)$$

for non-zero $a_k = \sum_{j=-N}^{\infty} a_{k,j} x^j \in \mathbb{C}((x))$, and $\text{val}(0) = \infty$.

Recall that non-Archimedean valuation on a field \mathbb{K} are maps $v: \mathbb{K} \rightarrow \mathbb{R} \cup \{\infty\}$ that fulfill the following three properties:

- (1) $v(x) = \infty$ if and only if $x = 0$,
- (2) $v(x \cdot y) = v(x) + v(y)$ for all $x, y \in \mathbb{K}$,
- (3) $v(x + y) \geq \inf\{v(x), v(y)\}$.

Now let $P = \sum_k a_k \partial^k \in D$, with $a_k = \sum_j a_{k,j} x^j \in \mathbb{C}[x]$.

Definition 4.11. The *Newton polygon* of $P = \sum_k a_k \partial^k \in D$, denoted $N(P)$, is the convex hull of the set

$$\bigcup_{\{k \mid a_k \neq 0\}} \{ (k, k - \text{val}(a_k)) - \mathbb{N}^2 \} \subset \mathbb{R}^2. \quad (4.10)$$

The *slopes of P* are the non-vertical slopes of its Newton polygon $N(P)$.

Both Definition 4.10 and 4.11 can be extended to other rings of coefficients, such as convergent power series $\mathbb{C}\{x\}$ or formal Laurent series $\mathbb{C}((x))$. The Newton polygon encodes the nature of a singularity of an operator $P \in D_1$ at 0 in the following sense.

Proposition 4.12. A differential operator $P \in D_1$ is regular singular at 0 if and only if its Newton polygon $N(P)$ is a quadrant, i.e., if P has no non-zero slopes.

Example 4.13. Consider $P_1 = x\partial^2 + \partial$. Its solutions space is $\text{Sol}(DP_1) = \mathbb{C} \cdot \{1, \ln\}$, hence P_1 is regular singular at 0. The Newton polygon of P_1 is depicted in Figure 5. Indeed, it has only slopes zero. Recall that, in order to be well-defined, the complex logarithm requires to take a branch cut out of the complex plane. \diamond

Example 4.14. Consider $P_2 = x^2\partial + 1$. Its solutions space is spanned by $\exp(1/x)$, which has an essential singularity at $x = 0$. Hence, the P_2 is irregular singular at $x = 0$. The Newton polygon of P_2 is depicted in Figure 5. Indeed, it has the non-zero slope -1 . \diamond

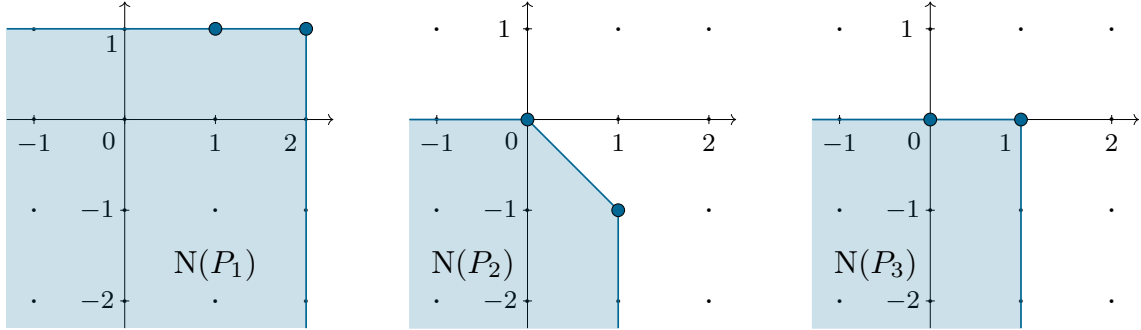


Figure 5: Newton polygons of P_1, P_2, P_3 from Examples 4.13–4.15.

The solutions of a D -ideal naturally encode the monodromy data of the D -ideal. This information alone can not distinguish between D -ideals.

Example 4.15. Let $P_2 = x^2\partial + 1$ from Example 4.14 and $P_3 = x\partial + 1$, so that

$$\text{Sol}(P_2) = \mathbb{C} \cdot \{\exp(1/x)\} \quad \text{and} \quad \text{Sol}(P_3) = \mathbb{C} \cdot \{1/x\}. \quad (4.11)$$

The two operators have the same singular locus, namely

$$\text{Sing}(P_2) = \text{Sing}(P_3) = \{0\}, \quad (4.12)$$

and both induce the trivial representation of the fundamental group of $\mathbb{C} \setminus \{0\}$ in their solutions space, since their solution spaces are spanned by holomorphic functions on the punctured complex plane: the analytic continuation of the solution functions along a closed path encircling the origin results in the same function. Yet, the D -modules D/DP_2 and D/DP_3 are far from being isomorphic: P_2 has an irregular singularity at the origin, whereas P_3 is regular singular at 0. \diamond

Example 4.16 (Airy). We apply the change of variables $z = 1/x$. Exploiting $x\partial_x = -z\partial_z$, Airy's operator $P_{\text{Airy}} = \partial_x^2 - x$ translates into

$$P_{\text{Airy},z} = z^4\partial_z^2 + 2z^3\partial_z - 1/z. \quad (4.13)$$

Its Newton polygon at $z = 0$ is displayed in Figure 6. It has the non-zero slope $-3/2$. Hence, Airy's equation is irregular singular at $z = 0$ (or, equivalently, at $x = \infty$). \diamond

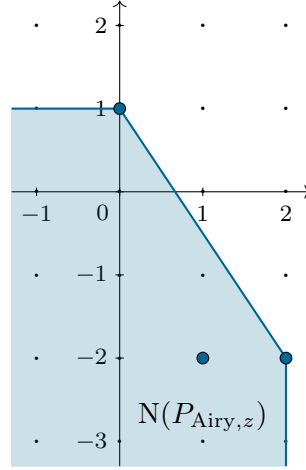


Figure 6: The Newton polygon of $P_{\text{Airy},z}$ from Example 4.16.

Newton polygons also help to decompose D -modules. For that, we have to pass to the Weyl algebra with coefficients in formal Laurent series, denoted $\mathbb{C}((x))$. They are series of the form

$$\mathbb{C}((x)) = \mathbb{C}[[x]][x^{-1}] = \left\{ \sum_{k=-N}^{\infty} c_k x^k \mid N \in \mathbb{N}, c_k \in \mathbb{C} \right\}, \quad (4.14)$$

without any convergence requirements being imposed. The resulting Weyl algebra is denoted

$$\widehat{D}[x^{-1}] = \mathbb{C}((x))\langle \partial \rangle. \quad (4.15)$$

Theorem 4.17 ([47, Theorem 3.48]). *Let $P \in \widehat{D}[x^{-1}]$ be a monic differential operator such that its Newton polygon $N(P)$ can be written as the Minkowski sum $N_1 + N_2$ of two polygons N_1, N_2 that have no slope in common. Then there are unique monic differential operators P_1, P_2 such that $N(P_i) = N_i$ and $P = P_1 P_2$. Moreover, this factorization gives rise to an isomorphism of $\widehat{D}[x^{-1}]$ -modules*

$$\widehat{D}[x^{-1}]/\widehat{D}[x^{-1}]P \cong \widehat{D}[x^{-1}]/\widehat{D}[x^{-1}]P_1 \oplus \widehat{D}[x^{-1}]/\widehat{D}[x^{-1}]P_2. \quad (4.16)$$

Example 4.18 ([47, Example 3.46]). Let $Q = x\theta^2 + \theta - 1 = x^3\partial^2 + x^2\partial + x\partial - 1$. It factorizes as $Q = Q_1 Q_2$ with $Q_1 = \theta - 1$ and $Q_2 = x\theta + 1$. Their Newton polygons are plotted in Figure 7. We read that the Newton polygons of Q_1 and Q_2 have no slopes in common, and that $N(Q) = N(Q_1) + N(Q_2)$. We conclude from Theorem 4.17 that

$$\mathbb{C}((x))\langle \partial \rangle / \mathbb{C}((x))\langle \partial \rangle Q \cong \mathbb{C}((x))\langle \partial \rangle / \mathbb{C}((x))\langle \partial \rangle Q_1 \oplus \mathbb{C}((x))\langle \partial \rangle / \mathbb{C}((x))\langle \partial \rangle Q_2 \quad (4.17)$$

are isomorphic as $\widehat{D}[x^{-1}]$ -modules. \diamond

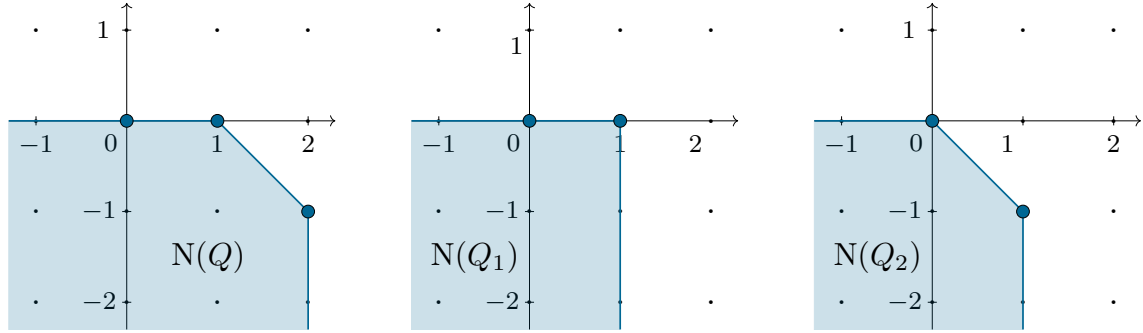


Figure 7: Newton polygons of Q , Q_1 , and Q_2 from Example 4.18.

5 Operations on D -modules

This lecture treats integral transforms and further modifications of functions through the lens of algebraic analysis.

5.1 Integral transforms

The Fourier(-Laplace) transform of a function $f: \mathbb{R}_{>0} \rightarrow \mathbb{C}$ is

$$\mathcal{F}\{f\}(t) = \int_{\mathbb{R}_{>0}} f(x)e^{-xt} dx. \quad (5.1)$$

This integral converges if $f \in L^1$. Assuming suitable vanishing conditions on the boundary of the integration domain,⁶ one reads that

$$\mathcal{F}\{x \cdot f\}(t) = -\partial_t \bullet \mathcal{F}\{f\}(t) \quad \text{and} \quad \mathcal{F}\left\{\frac{\partial f}{\partial x}\right\}(t) \stackrel{\text{IBP}}{=} t \cdot \mathcal{F}\{f\}(t), \quad (5.2)$$

where the second identity follows from integration by parts (IBP).

Algebraically, the Fourier-Laplace transform is the isomorphism of Weyl algebras

$$\begin{aligned} \mathcal{F}\{\cdot\}: \mathbb{C}[x_1, \dots, x_n]\langle \partial_1, \dots, \partial_n \rangle &\longrightarrow \mathbb{C}[t_1, \dots, t_n]\langle \partial_{t_1}, \dots, \partial_{t_n} \rangle, \\ x_i &\mapsto -\partial_{t_i}, \quad \partial_i \mapsto t_i, \end{aligned} \quad (5.3)$$

reflecting the rules in (5.2).

Example 5.1 (Airy). The Fourier-Laplace transform of $P_{\text{Airy}} = \partial^2 - x$ is

$$\mathcal{F}\{P_{\text{Airy}}\} = t^2 + \partial_t \in \mathbb{C}[t]\langle \partial_t \rangle. \quad (5.4)$$

⁶One possible option is to assume that f has rapid decay at 0 and ∞ , i.e., it decays faster than any power of x , as x approaches 0 or ∞ . By adapting the integration contour, one can get rid of the strict assumption of rapid decay. Borel-Moore homology constitutes the right framework for that.

The solution space of $\mathcal{F}\{P_{\text{Airy}}\}$ is spanned by the exponential function $\exp(-t^3/3)$. The solutions of Airy's equation are then obtained by taking the inverse Fourier–Laplace transform of $\exp(-t^3/3)$, i.e., integrals of the form

$$\mathcal{F}^{-1}\{e^{-t^3/3}\} = \int_{\Gamma_i} e^{-t^3/3} e^{xt} dt. \quad (5.5)$$

Figure 8 shows three integration contours $\Gamma_1, \Gamma_2, \Gamma_3$ so that the integral in (5.5) converges. Only two of the three are linearly independent: their composition can be contracted to a

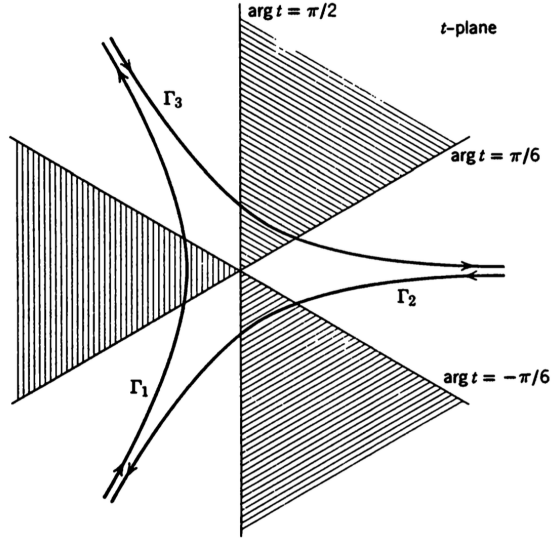


Figure 8: [48, Figure 22.1]: Integration contours $\Gamma_1, \Gamma_2, \Gamma_3$.

point on the Riemann sphere. The integrals over two such contours span the two-dimensional solution space of Airy's equation (1.4). \diamond

Via the isomorphism (5.3), we now define the Fourier–Laplace transform for D -modules. Let M be a D -module. Its Fourier–Laplace transform $\mathcal{F}\{M\}$ is the following module over the Weyl algebra $D_t = \mathbb{C}[t_1, \dots, t_n] \langle \partial_{t_1}, \dots, \partial_{t_n} \rangle$ in the t -variables. It is the same abelian group, with the action of D_t induced by the isomorphism (5.3), i.e., for $m \in M$:

$$t_i \bullet m = -\partial_i \bullet m \quad \text{and} \quad \partial_{t_i} \bullet m = x_i \bullet m. \quad (5.6)$$

Another integral transform that is in common use is the Mellin transform.

Definition 5.2. Let f be a function of n variables. The *Mellin transform* of f is defined to be the function in the variables $\nu = (\nu_1, \dots, \nu_n)$ given by

$$\mathfrak{M}\{f\}(\nu) := \int_{\Gamma} f x^{\nu} \frac{dx}{x}, \quad (5.7)$$

where $x^{\nu} \frac{dx}{x}$ denotes the n -form $x_1^{\nu_1} \cdots x_n^{\nu_n} \frac{dx_1}{x_1} \wedge \cdots \wedge \frac{dx_n}{x_n}$ and Γ is an appropriately chosen integration contour.

Example 5.3. Let $f(x) = \exp(-x)$. Its Mellin transform is the gamma function:

$$\mathfrak{M}\{e^{-x}\}(\nu) = \Gamma(\nu) = \int_0^\infty e^{-x} x^{\nu-1} dx. \quad (5.8)$$

For $\nu \in \mathbb{N}_{>0}$, $\Gamma(\nu) = (\nu - 1)!$ is the factorial. \diamond

Remark 5.4. Classically, the integration contour $\Gamma = \mathbb{R}_{>0}^n$ in (5.7) is the positive orthant in \mathbb{R}^n . However, this imposes strong conditions on f for the integral (5.7) to converge. One may instead adapt the integration contour Γ to the integrand: *twisted* cycles $\Gamma \in H_n((\mathbb{C}^*)^n \setminus V(f), \text{dlog}(fx^\nu))$ ensure the convergence of the integral. Here, dlog denotes the logarithmic differential, i.e., $\text{dlog}(fx^\nu)$ denotes the differential one-form $\frac{1}{f} \sum \frac{\partial f}{\partial x_i} dx_i + \sum \nu_i \frac{dx_i}{x_i}$ with poles along $V(f)$. The dependency on ν is discussed in detail in Section 3 of [2]. \diamond

The Mellin transform obeys the following rules:

$$\mathfrak{M}\{x_i \cdot f\}(\nu) = \mathfrak{M}\{f\}(\nu + e_i), \quad \mathfrak{M}\left\{x_i \cdot \frac{\partial f}{\partial x_i}\right\}(\nu) = -\nu_i \cdot \mathfrak{M}\{f\}(\nu). \quad (5.9)$$

The Mellin transform $\mathfrak{M}\{\cdot\}$ hence turns multiplication by $x_i^{\pm 1}$ into shifting the new variable ν_i by ± 1 , and the action of the i th Euler operator $\theta_i = x_i \partial_i$ into multiplication by $-\nu_i$.

Definition 5.5. The (n -th) *shift* (or *difference*) *algebra* with polynomial coefficients

$$S_n := \mathbb{C}[\nu_1, \dots, \nu_n] \langle \sigma_1^{\pm 1}, \dots, \sigma_n^{\pm 1} \rangle \quad (5.10)$$

is obtained from the free \mathbb{C} -algebra generated by $\{\nu_i, \sigma_i, \sigma_i^{-1}\}_{i=1, \dots, n}$ by imposing the following relations: all generators commute, except ν_i and the shift-operators σ_i . They obey the rule

$$\sigma_i^{\pm 1} \nu_i = (\nu_i \pm 1) \sigma_i^{\pm 1}. \quad (5.11)$$

This implies that $\sigma^a \nu^b = (\nu + a)^b \sigma^a$ for any $a \in \mathbb{Z}^n$, $b \in \mathbb{N}^n$. The shift algebra naturally comes into play when studying the Mellin transform of functions. There is a natural action of S_n on the Mellin transform of functions: it shifts the variable ν_i by 1, i.e.,

$$\sigma_i \bullet \mathfrak{M}\{f\}(\nu) = \mathfrak{M}\{f\}(\nu + e_i), \quad (5.12)$$

which justifies the name “shift operator” and also explains the rule in (5.9). Mimicking the rules in (5.9), the (*algebraic*) *Mellin transform* of [29] is the isomorphism of \mathbb{C} -algebras

$$\mathfrak{M}\{\cdot\}: D_{\mathbb{G}_m^n} \longrightarrow S_n, \quad x_i^{\pm 1} \mapsto \sigma_i^{\pm 1}, \quad \theta_i \mapsto -\nu_i. \quad (5.13)$$

The notation $\mathfrak{M}\{\cdot\}$ is used both for the Mellin transform of *functions* and that of *operators*. This is justified by the fact that $\mathfrak{M}\{\cdot\}$ is compatible with the action of the $D_{\mathbb{G}_m^n}$ and S_n , i.e.,

$$\mathfrak{M}\{P \bullet f\} = \mathfrak{M}\{P\} \bullet \mathfrak{M}\{f\}. \quad (5.14)$$

Example 5.6 (Example 5.3 revisited). The function $f(x) = \exp(-x)$ is annihilated by $P = \partial + 1$. Its Mellin transform is

$$\mathfrak{M}\{P\} = \mathfrak{M}\left\{\frac{1}{x}x\partial + 1\right\} = -\sigma^{-1}\nu + 1 = -(\nu - 1)\sigma^{-1} + 1. \quad (5.15)$$

From $P \bullet f = 0$, we conclude that $\mathfrak{M}\{P\} \bullet \mathfrak{M}\{f\} = 0$. Writing this out yields

$$\Gamma(\nu) = (\nu - 1) \cdot \Gamma(\nu - 1), \quad (5.16)$$

a shift relation that one is familiar with from factorials. \diamond

Exercise 5.7. Let $P = x_1^2\partial_1\partial_2 + \theta_2 \in D_2$. Compute its Mellin transform $\mathfrak{M}\{P\} \in S_2$. \diamond

5.2 Restricting and integrating

Proposition 5.8. *Let f be a holonomic function in n variables and $m < n$. Then the restriction of f to the coordinate subspace $\{x_{m+1} = \dots = x_n = 0\}$ is a holonomic function of the variables x_1, \dots, x_m .*

In the notation of the proposition, we will denote by D_m the Weyl algebra $\mathbb{C}[x_1, \dots, x_m]\langle\partial_1, \dots, \partial_m\rangle$ in the first m variables.

Proof. For $i \in \{m+1, \dots, n\}$, consider the right D_n -ideal $x_i D_n$. This ideal is a left module over $D_m = \mathbb{C}[x_1, \dots, x_m]\langle\partial_1, \dots, \partial_m\rangle$. The sum of these ideals with $\text{Ann}_{D_n}(f)$ is hence a left D_m -module. By [37, Proposition 5.2.4], its intersection with D_m is

$$(\text{Ann}_{D_n}(f) + x_{m+1}D_n + \dots + x_n D_n) \cap D_m. \quad (5.17)$$

is a holonomic D_m -ideal and it annihilates the restricted function $f(x_1, \dots, x_m, 0, \dots, 0)$. \square

Definition 5.9. Let I be a D_n -ideal. The D_m -ideal

$$(I + x_{m+1}D_n + \dots + x_n D_n) \cap D_m \quad (5.18)$$

is the *restriction ideal* of I to the coordinate subspace $\{x_{m+1} = \dots = x_n = 0\} \subset \mathbb{C}^n$.

Example 5.10 (Example 3.10 revisited). The restriction ideal of $I = \langle\partial_1 x_1 \partial_1, \partial_2^2 + 1\rangle$ to its singular locus $\text{Sing}(I) = \{x_1 = 0\}$ is the $\mathbb{C}[x_2]\langle\partial_2\rangle$ -ideal $\langle\partial_2^2 + 1\rangle$, which can be computed by running the following lines in **Singular** with the library `dmodapp.lib`.

```
LIB "dmodapp.lib";
def D2 = makeWeyl(2); setring D2;
ideal I = D(1)*x(1)*D(1), D(2)^2+1;
intvec w = 1,0;
def Ires = restrictionIdeal(I,w); setring Ires;
resIdeal;
```

The restriction ideal has holonomic rank 2. Its solution space is $\mathbb{C} \cdot \{\cos(x_2), \sin(x_2)\}$. \diamond

Example 5.11. Let $f(x_1, x_2) = (x_1 + x_2)^3$. Since f is symmetric in its variables and homogeneous of degree 3, it is annihilated by the hypergeometric D -ideal

$$I = \langle \theta_1 + \theta_2 - 3, \partial_1 - \partial_2 \rangle. \quad (5.19)$$

The restriction of I to $\{x_2 = 0\}$ is the $\mathbb{C}[x_1]\langle \partial_1 \rangle$ -ideal $\langle \theta_1 - 3, \partial_1^4 \rangle$. One checks that, indeed, $f(x_1, 0)$ is annihilated by it. \diamond

The computation of restriction ideals is hard and terminates only for small examples. To compute restriction ideals, the authors of [9] take a detour via Pfaffian systems; the latter will be topic of Section 7. Their implementations are made available in `Risa/Asir` [32].

Definition 5.12. Let I be a D_n -ideal. The D_m -ideal

$$(I + \partial_{m+1}D_n + \cdots + \partial_n D_n) \cap D_m \quad \text{for } m < n \quad (5.20)$$

is called the *integration ideal* of I with respect to the variables x_{m+1}, \dots, x_n .

The expression is dual to the restriction ideal (5.18) under the Fourier transform (5.3). If $I = \text{Ann}(f)$ for a holonomic function $f: \mathbb{R}^n \rightarrow \mathbb{C}$, the definite integral

$$F(x_1, \dots, x_{n-1}) = \int_a^b f(x_1, \dots, x_{n-1}, x_n) dx_n \quad (5.21)$$

is a holonomic function in $m = n - 1$ variables, assuming the integral exists, and is annihilated by the integration ideal (5.20); see [39, Proposition 2.11] for a detailed discussion.

Example 5.13. Consider the D_2 -ideal $I = \langle \theta_1 + 1, \theta_2 + 1 \rangle$. It has holonomic rank 1 and its solution space is spanned by the function $f(x_1, x_2) = \frac{1}{x_1 x_2}$. The integration ideal of I with respect to the variable x_2 is the D_1 -ideal $(I + \partial_2 D_2) \cap D_1 = \langle \theta_1 + 1 \rangle$. Indeed, it annihilates the integral $\int_a^b f(x_1, x_2) dx_2 = (\ln |b| - \ln |a|) \cdot \frac{1}{x_1}$. \diamond

6 Holonomic functions

This lecture explains how to compute with holonomic functions and visits closure properties of this function class. Zeilberger [50] was the first to study them in an algorithmic way.

6.1 Weyl closure of D -ideals

We recall from Definition 3.8 that a function $f(x_1, \dots, x_n)$ is *holonomic* if its annihilator

$$\text{Ann}_{D_n}(f) = \{P \in D_n \mid P \bullet f = 0\} \quad (6.1)$$

is a holonomic D_n -ideal. We here are relaxed about the function class—typically, one imposes some analyticity assumption. In the univariate case, i.e., $n = 1$, a function f is holonomic if and only if there exists a non-zero differential operator $P \in D \setminus \mathbb{C}[x]$ such that $P \bullet f = 0$.

Numerous functions in the sciences are holonomic, e.g., hypergeometric functions [33], many trigonometric functions, some probability distributions, and many special functions such as Airy's or Bessel's functions, polylogarithms, or the volume of compact semi-algebraic sets [26]. By Theorem 4.3, holonomic function can be encoded by finite data, namely their annihilating D -ideal together with $\text{rank}(\text{Ann}_D(f))$ many initial conditions. This fact makes holonomic functions well-suited to be handed to computer, and to be investigated by means of computations with their annihilating D -ideal.

Exercise 6.1. Let $r \in \mathbb{C}(x) \setminus \{0\}$ be a non-zero rational function. Prove that the annihilator of r in the rational Weyl algebra R is generated by $r\partial - \frac{\partial r}{\partial x}$. \diamond

Exercise 6.2. Determine a holonomic annihilating D_2 -ideal of the function

$$f(x, y) = e^{x \cdot y} \cdot \sin \frac{y}{1 + y^2}. \quad (6.2)$$

To do so, you may use the `Mathematica` package `HolonomicFunctions` [24]. The following code returns two annihilating differential operators of f .

```
<< RISC'HolonomicFunctions'
f = Exp[x*y]*Sin[y*1/(1+y^2)]
ann = Annihilator[f, {Der[x], Der[y]}]
```

It remains to investigate the D_2 -ideal generated by them regarding holonomicity. \diamond

Sometimes, it is useful to slightly enlarge a considered D -ideal, namely the Weyl closure of a D -ideal, as was introduced by Tsai [46].

Definition 6.3. The *Weyl closure* of a D_n -ideal I is the D_n -ideal

$$W(I) := R_n I \cap D_n. \quad (6.3)$$

A D -ideal is *Weyl closed* if $W(I) = I$.

Exercise 6.4. Let M be a D -module that is torsion-free as $\mathbb{C}[x_1, \dots, x_n]$ -module, and $f \in M$. Prove that $\text{Ann}_D(f)$ is Weyl closed. \diamond

Example 6.5. Consider $I = \langle x\partial \rangle \subset D_1$. Its Weyl closure is $I = \langle \partial \rangle$. The solution space of I is $\text{Sol}(I) = \mathbb{C} \cdot 1$, i.e., the solutions are constant functions only. Although $\text{Sing}(I) = \{0\}$, none of the solutions to I has a singularity there. Observe that $0 \notin \text{Sing}(W(I))$. If we allow distributional solutions, we find that the Heaviside step function

$$H(x) = \begin{cases} 0 & \text{if } x < 0, \\ 1 & \text{if } x \geq 0, \end{cases} \quad (6.4)$$

is a solution to I , since the distributional derivative of H is the Dirac delta δ . \diamond

In general, it is a difficult task to compute the Weyl closure of a D -ideal.

Clearly, $I \subseteq W(I)$. Hence, for the singular locus and the space of holomorphic solutions to the system of PDEs encoded by I , one has

$$\text{Sing}(I) \supseteq \text{Sing}(W(I)) \quad \text{and} \quad \text{Sol}(I) \supseteq \text{Sol}(W(I)). \quad (6.5)$$

Moreover, $\text{rank}(I) = \text{rank}(W(I))$, since $R_n I = R_n W(I)$. Since every element Q of $W(I)$ can be written as $Q = r \cdot P$ for some $r \in \mathbb{C}(x_1, \dots, x_n)$ and $P \in I$, we also have the inclusion $\text{Sol}(I) \subseteq \text{Sol}(W(I))$. Hence, $\text{Sol}(I) = \text{Sol}(W(I))$. The first inclusion in (6.5) can be strict, which can be seen for the D -ideal generated by $P = x\partial$:

$$\text{Sing}(DP) = \{0\}, \quad \text{whereas} \quad \text{Sing}(W(I)) = \text{Sing}(D\partial) = \emptyset. \quad (6.6)$$

In summary, a D -ideal I and its Weyl closure $W(I)$ have the same (classical) solution space, $W(I)$ might make the singular locus smaller, and might contain additional operators that annihilate all solutions of I . We summarize these insights in

Proposition 6.6. *Let I be a D_n -ideal and $W(I)$ its Weyl closure. Then*

$$(a) \text{Sol}(W(I)) = \text{Sol}(I), \quad (b) \text{Sing}(W(I)) \subseteq \text{Sing}(I), \quad (c) W(I) \bullet \text{Sol}(I) = 0.$$

If a D -ideal I has finite holonomic rank, it follows from [37, Theorem 1.4.15] that its Weyl closure $W(I)$ is holonomic. To prove that a function $f(x_1, \dots, x_n)$ is holonomic, it is therefore sufficient to find an annihilating D -ideal I of finite holonomic rank. If $I \subset \text{Ann}_{D_n}(f)$ with $\text{rank}(I) < \infty$, then its Weyl closure $W(I)$ is a holonomic D_n -ideal with $W(I) \subset \text{Ann}_{D_n}(f)$. In particular this forces $\text{Ann}_{D_n}(f)$ to be holonomic.

Exercise 6.7. Compute the Weyl closure of the D_1 -ideal generated by the operator

$$P = x^2(x-1)(x-3)\partial^2 - (6x^3 - 20x^2 + 12x)\partial + (12x^2 - 32x + 12). \quad (6.7)$$

Compare the solution spaces and singular loci of I and $W(I)$. ◇

Proposition 6.8 ([16]). *Let f be an element of a D -module M that is torsion-free as $\mathbb{C}[x_1, \dots, x_n]$ -module. Then the following three conditions are equivalent:*

- (i) f is holonomic.
- (ii) $\text{rank}(\text{Ann}_D(f)) < \infty$.
- (iii) For each $i \in \{1, \dots, n\}$ there exists an operator $P_i \in \mathbb{C}[x_1, \dots, x_n]\langle \partial_i \rangle \setminus \{0\}$ that annihilates f .

Proof. Let $I = \text{Ann}_D(f)$. If I is holonomic, then RI is a zero-dimensional ideal in R , i.e., $\dim_{\mathbb{C}(x)}(R/RI) < \infty$. This condition is equivalent to (ii) and (iii). For the implication from (ii) to (i), we note that $\text{Ann}_D(f)$ is Weyl closed, since M is torsion-free. Finally, $\text{rank}(\text{Ann}_D(f)) < \infty$ implies that $\text{Ann}_D(f) = W(\text{Ann}_D(f))$ is holonomic. □

Remark 6.9. Let $I = \text{Ann}_D(f)$ be the annihilator of a holonomic function f , and fix a point $x_0 \in \mathbb{C}^n \setminus \text{Sing}(I)$. Let m_1, \dots, m_n be the orders of the distinguished operators $P_1, \dots, P_n \in I$ in Proposition 6.8 (iii). Thus, each P_k is a differential operator in ∂_k of order m_k whose coefficients are polynomials in x_1, \dots, x_n . Suppose we impose initial conditions by specifying complex numbers for the $m_1 m_2 \cdots m_n$ many quantities

$$(\partial_1^{i_1} \cdots \partial_n^{i_n} \bullet f)|_{x=x_0} \quad \text{where } 0 \leq i_k < m_k \text{ for } k = 1, \dots, n. \quad (6.8)$$

The operators P_1, \dots, P_n together with the initial conditions (6.8) determine the function f uniquely within the vector space $\text{Sol}(I)$. This specification is known as a *canonical holonomic representation* of f ; see [50, Section 4.1]. \diamond

6.2 Closure properties of holonomic functions

From given holonomic functions, one can cook up more holonomic functions. We have already seen that restrictions and definite integrals of holonomic functions are again holonomic.

Proposition 6.10. *If f, g are holonomic functions (on the same domain), then both their sum $f + g$ and their product $f \cdot g$ are holonomic functions as well.*

Proof. For each $i \in \{1, 2, \dots, n\}$, there exist non-zero operators $P_i, Q_i \in \mathbb{C}[x]\langle \partial_i \rangle$, such that $P_i \bullet f = Q_i \bullet g = 0$. Set $n_i = \text{ord}(P_i)$ and $m_i = \text{ord}(Q_i)$. The $\mathbb{C}(x)$ -span of $\{\partial_i^k \bullet f\}_{k=0, \dots, n_i}$ is a vector space of dimension $\leq n_i$. Similarly, the $\mathbb{C}(x)$ -span of the set $\{\partial_i^k \bullet g\}_{k=0, \dots, m_i}$ has dimension $\leq m_i$. Now consider $\partial_i^k \bullet (f + g) = \partial_i^k \bullet f + \partial_i^k \bullet g$. The $\mathbb{C}(x)$ -span of $\{\partial_i^k \bullet (f + g)\}_{k=0, \dots, n_i + m_i}$ has dimension $\leq n_i + m_i$. Hence, there exists a non-zero operator $S_i \in \mathbb{C}[x]\langle \partial_i \rangle$, such that $S_i \bullet (f + g) = 0$. Since this holds for all indices i , we conclude that the sum $f + g$ is holonomic. A similar proof works for the product $f \cdot g$. For each $i \in \{1, 2, \dots, n\}$, we now consider the set $\{\partial_i^k \bullet (f \cdot g)\}_{k=0, 1, \dots, n_i m_i}$. By applying Leibniz' rule for taking derivatives of a product, we find that the $m_i n_i + 1$ elements of this set are linearly dependent over the field $\mathbb{C}(x)$. Hence, there is a non-zero operator $T_i \in \mathbb{C}[x]\langle \partial_i \rangle$ such that $T_i \bullet (f \cdot g) = 0$. We conclude that $f \cdot g$ is holonomic. \square

Proposition 6.11. *Let $f(x_1, \dots, x_n)$ be holonomic. Then its partial derivatives $\partial_i \bullet f$, $i = 1, \dots, n$, are holonomic functions as well.*

Proof. Since f is holonomic, there exist $P_i \in \mathbb{C}[x_1, \dots, x_n]\langle \partial_i \rangle$, $i = 1, \dots, n$, such that $P_i \bullet f = 0$. Rewrite each $P_i = \tilde{P}_i \partial_i + a_i$ with $a_i \in \mathbb{C}[x_1, \dots, x_n]$. If $a_i = 0$, it follows $\tilde{P}_i \bullet (\partial_i \bullet f) = 0$. Now assume that a_i is not the zero polynomial. Since both a_i and f are holonomic, so is their product and there exists $Q_i \in \mathbb{C}[x_1, \dots, x_n]\langle \partial_i \rangle$ which annihilates their product. Then $Q_i \tilde{P}_i \bullet (\partial_i \bullet f) = Q_i \bullet (-a_i f) = 0$, proving that $\partial_i \bullet f$ is holonomic. \square

Proposition 6.12. *Let $f(x)$ be a holonomic function. Its reciprocal $1/f$ is holonomic if and only if the function f'/f is algebraic.*

For a proof, we refer to the article [18] of Harris and Sibuya. This implies that, for instance, the function $1/\sin(x)$ is not holonomic. At the same time, this shows that, in general, the composition of two holonomic functions (here $1/x$ and $\sin(x)$) is in general not holonomic. But there is a partial rescue.

Proposition 6.13. *Let $f(x)$ be holonomic and $g(x)$ algebraic. Then their composition $f(g(x))$ is a holonomic function.*

Proof. Let $h := f \circ g$. By the chain rule, all derivatives $h^{(i)}$ can be expressed as linear combinations of $f(g), f'(g), f''(g), \dots$ with coefficients in $\mathbb{C}[g, g', g'', \dots]$. Since g is algebraic, it fulfills some polynomial equation $G(g, x) = 0$. By taking derivatives of this equation, we can express each $g^{(i)}$ as a rational function of x and g . We conclude that the ring $\mathbb{C}[g, g', \dots]$ is contained in the field $\mathbb{C}(x, g)$. Denote by W the vector space spanned by $f(g), f'(g), \dots$ over $\mathbb{C}(x, g)$ and by V the vector space spanned by f, f', \dots over $\mathbb{C}(x)$. Since f is holonomic, V is finite-dimensional over $\mathbb{C}(x)$. This implies that W is finite-dimensional over $\mathbb{C}(x, g)$. Since g is algebraic, $\mathbb{C}(x, g)$ is finite-dimensional over $\mathbb{C}(x)$. It follows that W is a finite-dimensional vector space over $\mathbb{C}(x)$, hence $h = f \circ g$ is holonomic. \square

The term “holonomic function” was first proposed by D. Zeilberger [50] in the context of proving combinatorial identities. Building on Zeilberger’s work, algorithms for manipulating holonomic functions were developed, among others by C. Koutschan. These are implemented in his *Mathematica* package `HolonomicFunctions` [24]. By Proposition 6.13, every algebraic function is holonomic. The following example illustrates this fact.

Example 6.14. Consider the function $y = f(x)$ that is defined by $y^4 + x^4 + \frac{xy}{100} - 1 = 0$. Its annihilator in D can be computed in *Mathematica* as follows:

```
<< RISC‘HolonomicFunctions‘
q = y^4 + x^4 + x*y/100 - 1
ann = Annihilator[Root[q, y, 1], Der[x]]
```

This *Mathematica* code determines an operator P of lowest order in $\text{Ann}_D(f)$:

$$\begin{aligned} P = & (2x^4+1)^2(25600000000x^{12}-76800000000x^8+76799999973x^4-25600000000) \partial^3 \\ & + 6x^3(2x^4+1)(51200000000x^{12}+76800000000x^8-307199999946x^4+179199999973) \partial^2 \\ & + 3x^2(102400000000x^{16}+204800000000x^{12}+2892799999572x^8-3507199999444x^4 \\ & + 307199999953) \partial - 3x(102400000000x^{16} + 204800000000x^{12} \\ & + 1459199999796x^8 - 1049599999828x^4 + 51199999993). \end{aligned}$$

This operator encodes the algebraic function $y = f(x)$ as a holonomic function. \diamond

For some cases, the theory of differentially-algebraic (D-algebraic) functions provides a rescue: they are zeroes of differential polynomials, which are part of the field differential algebra [34]. For instance, Weierstrass’ elliptic function \wp is not holonomic, but it is D-algebraic: it fulfills the non-linear, *algebraic* differential equation (ADE)

$$\wp'(x)^2 = 4\wp(x)^3 - c_1\wp(x) - c_2, \quad (6.9)$$

where c_1 and c_2 are constants depending on the periods of \wp . Hence, $u = \wp$ is a zero of the differential polynomial

$$u'^2 - 4u^3 + c_1u + c_2 \in \mathbb{C}[u, u', u'', \dots]. \quad (6.10)$$

Algorithms for arithmetic manipulations of D -algebraic functions can be found in [3].

7 Encoding D -ideals

We here discuss how to encode D -ideals. For that, we need some basics about Gröbner bases.

7.1 Gröbner bases

Let $(u, v) \in \mathcal{W}$ be a weight vector for the Weyl algebra. For a subset $G \subset D$ of the Weyl algebra, we denote by

$$\text{in}_{(u,v)}(G) = \{\text{in}_{(u,v)}(P) \mid P \in G\} \subset \text{gr}_{(u,v)}(D) \quad (7.1)$$

the set containing the initial forms of all elements of G .

Definition 7.1. Let I be a D -ideal. A finite set $G \subset D$ of differential operators is a *Gröbner basis of I with respect to (u, v)* if I is generated by G and if the initial ideal of I with respect to (u, v) is generated by the initial forms of elements in G , i.e., if

$$\text{in}_{(u,v)}(I) = \langle \text{in}_{(u,v)}(G) \rangle \quad (7.2)$$

is an equality of $\text{gr}_{(u,v)}(D)$ -ideals.

Example 7.2. The characteristic ideal in Example 2.8 provides an example of a generating set which is not a Gröbner basis with respect to the weight vector $(0, 1) \in \mathbb{R}^4$. \diamond

We will again use the normally ordered expression of differential operators from (2.2), i.e., we write $P \in D$ in the form

$$P = \sum_{(\alpha, \beta) \in E} c_{\alpha, \beta} x^\alpha \partial^\beta. \quad (7.3)$$

To speak about Gröbner bases, we will need to define total a total order \prec on the set of monomials $x^\alpha \partial^\beta$ in D . Such an order is called a *multiplicative monomial order* if both

- (1) $1 \prec x_i \partial_i$ for $i = 1, \dots, n$ and
- (2) $x^\alpha \partial^\beta \prec x^a \partial^b$ implies $x^{\alpha+s} \partial^{\beta+t} \prec x^{a+s} \partial^{b+t}$ for all $(s, t) \in \mathbb{N}^n \times \mathbb{N}^n$.

Now let a multiplicative monomial order \prec be fixed.

Definition 7.3. The *initial monomial* $\text{in}_\prec(P)$ of a differential operator $P \in D$ is the monomial $x^\alpha \xi^\beta \in \mathbb{C}[x, \xi]$ such that $x^\alpha \partial^\beta$ is the \prec -largest monomial occurring in (7.3). The *initial ideal* $\text{in}_\prec(I)$ of a D -ideal I is the monomial $\mathbb{C}[x, \xi]$ -ideal generated by $\{\text{in}_\prec(P) \mid P \in I\}$.

Definition 7.4. A finite set $G \subset D$ is a Gröbner basis of I with respect to \prec if I is generated by G and $\text{in}_\prec(I)$ is generated by $\text{in}_\prec(G) = \{\text{in}_\prec(P) \mid P \in G\}$.

A multiplicative monomial order \prec is called a *term order* for D if $1 = x^0\partial^0$ is the smallest element. This condition arises from the commutator relation (1.2) and guarantees compatibility with multiplication, i.e., $\text{in}_\prec(PQ) = \text{in}_\prec(P) \cdot \text{in}_\prec(Q)$. For term orders, there are no infinitely decreasing chains in D . Examples of term orders are the lexicographic order, the reverse lexicographic order, elimination orders, and the graded reverse lexicographic order; see for instance [10], one of the standard references for Gröbner bases. We here recall the lexicographic and reverse lexicographic order for polynomial rings.

Example 7.5 (lex). Let $S = \mathbb{C}[x_1, \dots, x_n]$ be a polynomial ring and $\alpha, \beta \in \mathbb{N}^n$. The *lexicographic order* is the following order:

$$x^\alpha \succ x^\beta \text{ if the \underline{leftmost} non-zero entry of } \alpha - \beta \in \mathbb{Z}^n \text{ is \underline{positive}.} \quad (7.4)$$

For instance, $x_1 \succ x_2 \succ \dots \succ x_n$, $x_1x_2^2 \succ x_2^3x_3^4$, and $x_1^3x_2^2x_3^4 \succ x_1^3x_2^2x_3$. \diamond

Example 7.6 (revlex). Let $S = \mathbb{C}[x_1, \dots, x_n]$ be a polynomial ring and $\alpha, \beta \in \mathbb{N}^n$. The *reverse lexicographic order* is the following order:

$$x^\alpha \succ x^\beta \text{ if the \underline{rightmost} non-zero entry of } \alpha - \beta \in \mathbb{Z}^n \text{ is \underline{negative}.} \quad (7.5)$$

For instance, again $x_1 \succ x_2 \succ \dots \succ x_n$ and $x_1x_2^2 \succ x_2^3x_3^4$, but $x_1^3x_2^2x_3^4 \prec x_1^3x_2^2x_3$. \diamond

We now come back to monomials in the Weyl algebra.

Example 7.7 (degrevlex). Let $\alpha, \beta, a, b \in \mathbb{N}^n$. We denote $|\alpha| = \alpha_1 + \dots + \alpha_n$, and likewise for β, a, b . The *degree reverse lexicographic order* is the order defined as follows:

$$x^\alpha \partial^\beta \succ x^a \partial^b \text{ if } |\alpha| + |\beta| > |a| + |b|, \text{ or } |\alpha| + |\beta| = |a| + |b| \text{ and the rightmost} \quad (7.6) \\ \text{non-zero entry of } (\alpha, \beta) - (a, b) \in \mathbb{N}^{2n} \text{ is negative.}$$

For instance, $x_1^2x_2\partial_2^2 \succ x_1x_2\partial_2^2 \succ x_2\partial_1\partial_2^2$. In *Singular*, this order is encoded as `dp`. It is one of the orders that are most common—and typically among the fastest—in applications. \diamond

These definitions naturally extend to $\text{gr}_{(u,v)}(D)$ -ideals.

We now have two different notions of Gröbner bases of D -ideals: one with respect to weight vectors, and another one with respect to multiplicative monomial orders. They are related as follows. Let $(u, v) \in \mathcal{W}$ and let \prec be any term order. The order $\prec_{(u,v)}$ is the multiplicative monomial defined as follows:

$$x^\alpha \partial^\beta \prec_{(u,v)} x^a \partial^b \Leftrightarrow \alpha u + \beta v < a u + b v \text{ or } (\alpha u + \beta v = a u + b v \text{ and } x^\alpha \partial^\beta \prec x^a \partial^b), \quad (7.7)$$

i.e., we use \prec as a tiebreaker. This defines a term order if and only if (u, v) is non-negative.

Example 7.8. For (u, v) the all-one vector and \prec the reverse lexicographic order, the resulting order $\prec_{(u,v)}$ is **degrevlex**. \diamond

Theorem 7.9 ([37, Theorem 1.1.6]). *Let I be a D -ideal, $(u, v) \in \mathcal{W}$ any weight vector, \prec any term order, and G a Gröbner basis of I with respect to $\prec_{(u,v)}$. Then*

(1) the set G is a Gröbner basis of I with respect to (u, v) and

(2) the set $\text{in}_{(u,v)}(G)$ is a Gröbner basis of $\text{in}_{(u,v)}(I)$ with respect to \prec .

Theorem 7.10 ([37, Theorem 1.1.7]). *Let \prec be a term order on D and G a Gröbner basis for its D -ideal $I = D \cdot G$ with respect to \prec . Any $Q \in I$ admits a standard representation in terms of G : there exist $C_1, \dots, C_m \in D$ such that*

$$Q = \sum_{i=1}^m C_i P_i, \quad \text{where } P_i \in G \text{ and } \text{in}_{\prec}(C_i P_i) \preceq \text{in}_{\prec}(Q) \text{ for all } i. \quad (7.8)$$

It can be computed the via the *normal form algorithm* (also called *division algorithm*), presented on p. 7 of [37]. For arbitrary $Q \in D$, the algorithm outputs the *normal form* of Q with respect to G : the unique remainder after reduction modulo G .

7.2 Pfaffian systems

The computations in this section are carried out in the rational Weyl algebra R_n . We will denote $\mathbb{C}(x) = \mathbb{C}(x_1, \dots, x_n)$ for brevity, and likewise $R = R_n = \mathbb{C}(x)\langle\partial\rangle$ the n -th rational Weyl algebra. We first need to relate Gröbner bases in D and R .

Definition 7.11. A term order \prec on D is an *elimination order* if $\partial^\beta \prec \partial^\gamma$ implies $x^\alpha \partial^\beta \prec \partial^\gamma$ for all $\alpha \in \mathbb{N}^n$.

Let \prec be a term order on D . We will denote by \prec' its restriction to monomials in the ∂_i 's; this is a term order on \mathbb{N}^n . For any choice of term order \prec on D , $\prec_{(0,1)}$ is a term order on the rational Weyl algebra, which refines the order given by the total degree in the ∂_i 's. If G is a Gröbner basis of a D -ideal I with respect to an elimination order \prec on D , then G is also a Gröbner basis of the the R -ideal RI with respect to the order \prec' . A generating set of the initial ideal of RI is obtained by replacing each of the variables x_1, \dots, x_n by 1.

Note bene. The holonomic rank (3.8) of a D -ideal I hence is the number of *standard monomials* of $\text{in}_{(0,1)}$ considered as a $\mathbb{C}(x)[\xi]$ -ideal. I.e., it is the number of monomials $\xi^\beta = \xi_1^{\beta_1} \dots \xi_n^{\beta_n}$ such that ξ^β is not contained in $\text{in}_{(0,1)}(I)$.

Unless otherwise stated, we use the degree reverse lexicographical order. For $n = 2$, this gives

$$1 \prec \partial_2 \prec \partial_1 \prec \partial_2^2 \prec \partial_1 \partial_2 \prec \partial_1^2 \prec \dots. \quad (7.9)$$

Let $f(x_1, \dots, x_n)$ be a real-valued holonomic function and I a D -ideal with finite holonomic rank such that $I \bullet f = 0$. Thus, R/RI is finite-dimensional over $\mathbb{C}(x_1, \dots, x_n)$. In our application in Section 8.2, f will be the likelihood function of a statistical model.

Let $\text{rank}(I) = m \in \mathbb{N}_{>0}$ be the holonomic rank of I . We write $S = \{s_1, \dots, s_m\}$ for the set of standard monomials for a Gröbner basis of RI in R . We can assume that $s_1 = 1$. The m entries of the vector

$$F = (s_1 \bullet f, s_2 \bullet f, \dots, s_m \bullet f)^\top \quad (7.10)$$

are holonomic functions. Note that the first entry of F is the given function f . In symbols, $(F)_1 = f$. Since the D -ideal I has holonomic rank m , there exist unique matrices $P_1, \dots, P_n \in \mathbb{C}(x_1, \dots, x_n)^{m \times m}$ such that

$$\partial_i \bullet F = P_i \cdot F \quad \text{for } i = 1, \dots, n. \quad (7.11)$$

The system of linear PDEs in (7.11) is called *Pfaffian system of f* .

Remark 7.12. For a discussion on how Pfaffian systems and connection matrices of integrable connections are related, see Appendix B of [20]. A Pfaffian system determines the D -module structure, but not the D -ideal itself: being isomorphic $D/I \cong D/J$ as D -modules does not imply equality of the D -ideals I and J . \diamond

Pfaffian systems are a multivariate analog of the *companion matrix* of ODEs.

Example 7.13 ($n = 1$). Let f be a holonomic function annihilated by the D_1 -ideal

$$I = \langle x\partial^3 - (x+1)\partial + 1 \rangle. \quad (7.12)$$

The generator by itself is a Gröbner basis for RI . The set of standard monomials equals $S = \{1, \partial, \partial^2\}$, and this is a $\mathbb{C}(x)$ -basis of R/RI . From I we see that

$$\partial^3 \bullet f = \frac{x+1}{x} \partial \bullet f - \frac{1}{x} \cdot f. \quad (7.13)$$

Let $F = (f, \partial \bullet f, \partial^2 \bullet f)^T$. This yields the following Pfaffian system for f :

$$\partial \bullet F = P \cdot F \quad \text{where} \quad P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\frac{1}{x} & \frac{x+1}{x} & 0 \end{bmatrix} \quad (7.14)$$

is the companion matrix. For any non-zero real number u we have

$$\begin{bmatrix} f'(u) \\ f''(u) \\ f'''(u) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\frac{1}{u} & \frac{u+1}{u} & 0 \end{bmatrix} \cdot \begin{bmatrix} f(u) \\ f'(u) \\ f''(u) \end{bmatrix}. \quad (7.15)$$

This matrix-vector formula will be useful for the design of numerical algorithms in Section 8. \diamond

Note that Pfaffian systems depend on the specific R -ideal RI and on the chosen term order. The matrices P_i can be computed as follows. We apply the division algorithm modulo our Gröbner basis to the operators $\partial_i s_j$, for $i \in \{1, \dots, n\}$ and $j \in \{1, \dots, m\}$. The resulting normal form equals

$$a_{j1}^{(i)}(x)s_1 + a_{j2}^{(i)}(x)s_2 + \dots + a_{jm}^{(i)}(x)s_m,$$

where the coefficients $a_{jk}^{(i)}$ are rational functions in x_1, \dots, x_n . This means that the operator

$$\partial_i s_j - \sum_{k=1}^m a_{jk}^{(i)}(x)s_k \quad (7.16)$$

is in the R -ideal RI . From this one sees that the coefficient $a_{jk}^{(i)}(x)$ is the (j, k) -th entry of the $m \times m$ matrix P_i . Algorithms for an efficient computation of Pfaffian systems based on Macaulay matrices were designed in the recent article [9].

Remark 7.14. A change of base results in a gauge transform of the connection matrix. Regular singular systems can be brought into Fuchsian form via a suitable gauge transform, i.e., the resulting matrices having poles of order at most one. \diamond

We have now reached the following important conclusion. Suppose x is replaced by a point u in \mathbb{Q}^n . Here u might be a highly accurate floating point representation of a point in \mathbb{R}^n . The numerical evaluation of the gradient of f at u can be accomplished by multiplying the vector $F(u) \in \mathbb{Q}^m$ by the matrices $P_i(u)$ with explicit rational entries. A tacit assumption made here is that u lies in the complement of the singular locus of the Pfaffian system (7.11).

8 Evaluating holonomic functions

This lecture explains the holonomic gradient method (HGM) of [31]. It is a numerical scheme for the evaluation of holonomic functions, which was originally developed for the statistical inference of data. Our presentation here closely follows [39]. The applicability of the HGM arises from the fact that some probability distributions that are used in practice are given by holonomic functions. One example is the cumulative distribution function of the largest eigenvalue of a Wishart matrix, cf. [19]. Another relevant holonomic function arises from sampling matrices in $\text{SO}(3)$, which will be the topic of Section 8.2 and closely follows [1].

8.1 Holonomic gradient method

Consider the problem of maximum likelihood estimation in statistics. Our aim is to explain the benefit gained from D -module theory. A key idea is to compute and represent the gradient of such a function from its canonical holonomic representation. The statistical aim of MLE is to find parameters for which an observed outcome is most probable [44, Chapter 7]. This can be formulated as an optimization problem, namely to maximize the likelihood function. For discrete models with N outcomes, this function has the form $f_1^{s_1} \cdots f_N^{s_N}$, where f_i encodes the i th state of the model. In what follows, we consider the likelihood function for continuous models. Our goal is to find a local maximum of a holonomic function using a variant of gradient descent. Given a holonomic function f , represented by a holonomic D -ideal, we are interested in finding local minima of f with the help of the knowledge of I . We first describe how to evaluate the holonomic function f at a point \tilde{x} by a first order approximation. Assume we are able to numerically evaluate f at some particular point $x^{(0)}$, depending on the precise situation. Choose a path $x^{(0)} \rightarrow x^{(1)} \rightarrow \cdots \rightarrow x^{(K)} = \tilde{x}$, with $x^{(k+1)}$ sufficiently close to $x^{(k)}$ for all $k = 0, \dots, K-1$, and such that the path does not cross the singular locus of the Pfaffian system of f . The following algorithm is referred to as the

Holonomic Gradient Method (HGM).

Step 1. Compute a Gröbner basis of RI in the rational Weyl algebra R .

Step 2. Compute the set of standard monomials S and the Pfaffian system (7.11).

Step 3. Evaluate F at one point $x^{(0)}$ and denote the result by \bar{F} . Set $k = 0$.

Step 4. Approximate the value of the vector F at $x^{(k+1)}$ by its first-order Taylor polynomial, and denote the result again by \bar{F} :

$$\begin{aligned} F(x^{(k+1)}) &\approx F(x^{(k)}) + \sum_{i=1}^n (x_i^{(k+1)} - x_i^{(k)}) \cdot (\partial_i \bullet F)(x^{(k)}) \\ &= F(x^{(k)}) + \sum_{i=1}^n (x_i^{(k+1)} - x_i^{(k)}) \cdot P_i(x^{(k)}) \cdot \bar{F}. \end{aligned}$$

Step 5. Increase the value of k by 1. If $k < K$, return to step 4. Otherwise stop.

Steps 1 to 3 need to be carried out only once for (f, I) . The output of this algorithm is a vector \bar{F} that approximates $F(\tilde{x})$. The first coordinate of $F(\tilde{x})$ is the desired scalar $f(\tilde{x})$. Hence the first coordinate of \bar{F} is our approximation.

Remark 8.1. To turn the HGM into a practical algorithm, it is essential to incorporate some knowledge from numerical analysis. For instance, there is a lot of freedom in choosing the numerical approximation method in step 4. Nakayama et al. [19] use the Runge–Kutta method of fourth order. Another possibility is to use a second order Taylor approximation, where one computes the Hessian of f also by means of the Pfaffian system of f . \diamond

We are now endowed with all necessary tools for finding a local minimum of the holonomic function f . As before, f is encoded by an annihilating D -ideal I with finite holonomic rank. This encoding is the input to the next algorithm.

Holonomic Gradient Descent (HGD).

Step 1. Compute a Gröbner basis of RI in the rational Weyl algebra R .

Step 2. Compute the set of standard monomials S and the Pfaffian system (7.11).

Step 3. Numerically evaluate $F(x^{(0)})$ at some starting point $x^{(0)}$ and put $k = 0$. Denote this value by \bar{F} . The evaluation method is chosen to be adapted to the problem.

Step 4. For $i = 1, \dots, n$, evaluate the first coordinate of $P_i(x^{(k)}) \cdot \bar{F}$. Let \bar{G} be the vector of these n numbers. This approximates the gradient ∇f at $x^{(k)}$ since

$$\partial_i \bullet f = (\partial_i \bullet F)_1 = (P_i \cdot F)_1.$$

Step 5. If a termination condition of the iteration is satisfied, stop. Otherwise go to step 6.

Step 6. Put $x^{(k+1)} = x^{(k)} - h_k \bar{G}$, where h_k is an appropriately chosen step length.

Step 7. Numerically evaluate F at $x^{(k+1)}$ by step 4 of the HGM and set this value to \bar{F} . Increase the value of the index k by one and return to step 4 above.

The algorithm returns a point $x^{(k)}$ along with the value of F at that point. The first entry of this output is a numerical approximation of a local minimum of the holonomic function f . Again, one should be aware that, in general, this algorithm works only within connected components contained in the complement of the singular locus of the Pfaffian system of f .

Remark 8.2. In order to develop a practical implementation, and to assess the quality of the method, one needs some expertise from numerical analysis. The choices one makes can make a huge difference. For instance, the choice of the step size h_k is a well-studied subject in numerical optimization, and there are various standard recipes for carrying out gradient descent. In current applications to data science, stochastic versions of gradient descent play a major role, and it would be very nice to connect D -modules to these developments. \diamond

8.2 Statistical inference

The HGM was applied to determining the maximum likelihood estimate (MLE) for the Fisher model for data in $\text{SO}(3)$ in [42]. The Haar measure on $\text{SO}(3)$ is the unique probability measure μ that is invariant under the group action. The *Fisher model* is a family of probability distributions on $\text{SO}(3)$ that is parameterized by 3×3 matrices Θ . For a fixed parameter matrix Θ , the density of the *Fisher distribution* equals

$$f_{\Theta}(Y) = \frac{1}{c(\Theta)} \cdot \exp(\text{tr}(\Theta^{\top} \cdot Y)) \quad \text{for all } Y \in \text{SO}(3). \quad (8.1)$$

This is the density with respect to the Haar measure μ . The denominator is the *normalizing constant*. It is chosen such that $\int_{\text{SO}(3)} f_{\Theta}(Y) \mu(dY) = 1$. This requirement is equivalent to

$$c(\Theta) = \int_{\text{SO}(3)} \exp(\text{tr}(\Theta^{\top} \cdot Y)) \mu(dY). \quad (8.2)$$

Since integration is against the Haar measure, the function (8.2) is invariant under multiplying Θ on the left or right by a rotation matrix:

$$c(Q \cdot \Theta \cdot R) = c(\Theta) \quad \text{for all } Q, R \in \text{SO}(3). \quad (8.3)$$

In order to evaluate (8.2), we can therefore restrict to the case of diagonal matrices. Namely, given any 3×3 matrix Θ , we first compute its *sign-preserving singular value decomposition*

$$\Theta = Q \cdot \text{diag}(x_1, x_2, x_3) \cdot R. \quad (8.4)$$

Sign-preserving means that $Q, R \in \text{SO}(3)$ and $|x_1| \geq x_2 \geq x_3 \geq 0$. For invertible Θ , this implies that $x_1 > 0$ whenever $\det(\Theta) > 0$ and $x_1 < 0$ otherwise. The normalizing constant is the following function of the three singular values:

$$\tilde{c}(x_1, x_2, x_3) := c(\text{diag}(x_1, x_2, x_3)) = \int_{\text{SO}(3)} \exp(x_1 y_{11} + x_2 y_{22} + x_3 y_{33}) \mu(dY). \quad (8.5)$$

Now suppose we are given a finite sample $\{Y_1, Y_2, \dots, Y_N\}$ from the rotation group $\text{SO}(3)$. Our aim is to find the parameter matrix Θ whose Fisher distribution f_{Θ} probabilistically best explains the data. We work in the classical framework of likelihood inference, i.e., we seek to compute the MLE for the given data $\{Y_1, Y_2, \dots, Y_N\}$. By definition, the MLE is the 3×3 parameter matrix $\hat{\Theta}$ which maximizes the log-likelihood function. Thus, we must solve

an optimization problem. From our data, we compute the sample mean $\bar{Y} = \frac{1}{N} \sum_{k=1}^N Y_k$; it is generally not a rotation matrix anymore. We next compute the sign-preserving singular value decomposition of the sample mean, i.e., we determine $Q, R \in \text{SO}(3)$ such that

$$\bar{Y} = Q \cdot \text{diag}(g_1, g_2, g_3) \cdot R. \quad (8.6)$$

The sample $\{Y_1, \dots, Y_N\}$ enters the log-likelihood function only via g_1, g_2, g_3 .

Lemma 8.3 ([42, Lemma 2]). The log-likelihood function for the given sample from $\text{SO}(3)$ is

$$\ell : \mathbb{R}^3 \longrightarrow \mathbb{R}, \quad (x_1, x_2, x_3) \mapsto x_1 g_1 + x_2 g_2 + x_3 g_3 - \log(\tilde{c}(x_1, x_2, x_3)). \quad (8.7)$$

If $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ is the maximizer of the function ℓ , then the matrix

$$\hat{\Theta} = Q \cdot \text{diag}(\hat{x}_1, \hat{x}_2, \hat{x}_3) \cdot R \quad (8.8)$$

is the MLE of the Fisher model (8.1) of the sample $\{Y_1, \dots, Y_N\}$ from $\text{SO}(3)$.

Since (8.7) is a strictly concave function, a local maximum is already a global one and is attained at a unique point in \mathbb{R}^3 . The approach of [42] has been generalized to $\text{SO}(n)$ in [25], and to compact Lie groups and applied to data from the sciences such as medical imaging in [1]. To evaluate the gradient of ℓ , the main task is to evaluate \tilde{c} . The latter is a holonomic function. It is annihilated by the operators

$$\begin{aligned} & \prod_{j \neq i} (x_i^2 - x_j^2) \cdot (\partial_i^2 - 1 + \sum_{k \neq i} \frac{1}{x_i^2 - x_k^2} (x_i \partial_i - x_j \partial_j)), \quad i = 1, 2, 3, \\ & (x_i^2 - x_j^2) \partial_i \partial_k - (x_i \partial_i - x_k \partial_j) - (x_i^2 - x_j^2) \partial_k, \quad 1 \leq i < j \leq 3 \text{ and } \{i, j, k\} = \{1, 2, 3\}. \end{aligned} \quad (8.9)$$

The D_3 -ideal generated by these operators is holonomic and has holonomic rank 4.

Remark 8.4. Also for *discrete* statistical models, the problem of maximum likelihood estimation can be addressed by algebro-geometric methods. Likelihood geometry [22] encodes statistical models as very affine varieties, i.e., as closed subvarieties of an algebraic torus. The curve obtained from intersecting the purple homogeneous surface $\mathcal{M} = V(p_0 p_2 - (p_0 + p_1) p_1)$ with the orange probability 2-simplex

$$\Delta_2 = \{(p_0, p_1, p_2) \mid p_i \in (0, 1), p_0 + p_1 + p_2 = 1\} \quad (8.10)$$

in Figure 3 represents an independence model arising from a coin flip. For observed data $(u_0, u_1, u_2) \in \mathbb{N}^3$ of sample size $|u| = u_0 + u_1 + u_2$, denote $u_+ = u_0 + u_1 + u_2$. The MLE problem translates to minimizing the distance from the curve to the empirical distribution $(u_0/u_+, u_1/u_+, u_2/u_+) \in \Delta_2$ with respect to the Kullback–Leibler divergence; see Remark 2 of [these lecture notes](#). For models with a unique MLE, there is an intriguing relation between the Bernstein–Sato ideal of a parameterization of the model, boundary components of a tropical compactification of the model, and the MLE, which is elaborated in [40]. \diamond

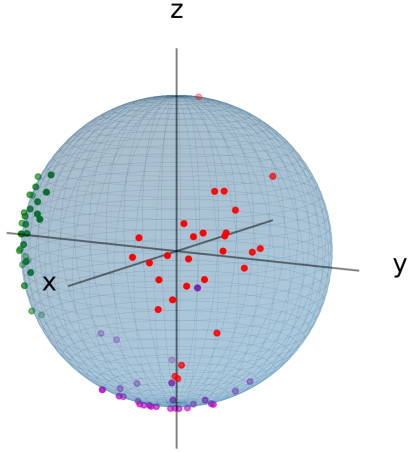


Figure 9: [1, Figure 1] Electromagnetical forces generated by the hearts of 28 young boys. The MLE of this dataset was computed in [1]. Combining the BFGS algorithm with the HGM outperformed the classical BFGS both in runtime and precision.

9 Computing solutions of D -ideals

This section treats the computation of truncated series solutions of regular holonomic D -ideals. These series are called “canonical series solutions” and their truncations are computed via an algorithm of Saito, Sturmfels, and Takayama [37, Section 2.6], to which we refer as “SST algorithm”. It is a generalization of the [Frobenius method](#)—a method for the computation of power series solutions of second-order ODEs—to several variables.

9.1 Frobenius ideals

Recall from Definition 2.18 that a D_n -ideal is a *Frobenius ideal* if it can be generated by elements of the polynomial ring $\mathbb{C}[\theta_1, \dots, \theta_n]$. In particular, every torus-fixed D -ideal I gives rise to a Frobenius ideal $D\tilde{I}$, which has the same classical solution space. A Frobenius ideal $F = D_n J$, $J \subset \mathbb{C}[\theta_1, \dots, \theta_n]$, is holonomic if and only if J is Artinian, and the solution space of F can be described explicitly in this case, as we will learn now.

Let J be an Artinian ideal in the polynomial ring $\mathbb{C}[\theta] = \mathbb{C}[\theta_1, \dots, \theta_n]$. Its variety $V(J)$ is a finite subset of \mathbb{C}^n . The primary decomposition of J equals

$$J = \bigcap_{A \in V(J)} Q_A(\theta - A), \quad (9.1)$$

where Q_A is an ideal that is primary to the maximal ideal $\langle \theta_1, \dots, \theta_n \rangle$, and $Q_A(\theta - A)$ is the ideal obtained from Q_A by replacing θ_i with $\theta_i - A_i$ for $i = 1, \dots, n$. The ideal Q_A is the *primary component of J at A* .

Definition 9.1. The *orthogonal complement* of the Artinian ideal Q_A is the finite-dimensional \mathbb{C} -vector space

$$Q_A^\perp = \{p \in \mathbb{C}[x_1, \dots, x_n] \mid f(\partial_1, \dots, \partial_n) \bullet p(x_1, \dots, x_n) = 0 \text{ for all } f = f(\theta_1, \dots, \theta_n) \in Q_A\}.$$

In commutative algebra, the vector space Q_A^\perp is known as the (*Macaulay*) *inverse system* to the ideal J at the given point A .

Proposition 9.2 ([37, Theorem 2.3.11]). *Let $F = D_n J$, where $J \subset \mathbb{C}[\theta]$, be a holonomic Frobenius ideal. The solution space of F is spanned by the functions $x^A \cdot g(\log(x))$, where A runs over the points of the variety $V(J)$, and g runs over the orthogonal complement of Q_A .*

Example 9.3. The ideal $J = \langle \theta_1 + \theta_2 + \theta_3, \theta_1\theta_2 + \theta_1\theta_3 + \theta_2\theta_3, \theta_1\theta_2\theta_3 \rangle$ is generated by non-constant symmetric polynomials. It is primary to $\langle \theta_1, \theta_2, \theta_3 \rangle$. We have $V(J) = \{(0, 0, 0)\}$, with $\text{rank}(DJ) = 6$: the monomials $\{1, \partial_1, \partial_2, \partial_1^2, \partial_1\partial_2, \partial_1^2\partial_2\}$ are a $\mathbb{C}(x_1, x_2, x_3)$ -basis of R_3/R_3I . The orthogonal complement of Q_0 is 6-dimensional. It is spanned by all polynomials that are successive partial derivatives of $(x_1 - x_2)(x_1 - x_3)(x_2 - x_3)$. This implies

$$\text{Sol}(DJ) = \mathbb{C}[\theta] \bullet (\log(x_1/x_2) \cdot \log(x_1/x_3) \cdot \log(x_2/x_3)) \cong \mathbb{C}^6 \quad (9.2)$$

for the solution space of DJ . ◇

Theorem 9.4 ([37, Theorem 2.5.1]). *Let I be any holonomic D -ideal and $w \in \mathbb{R}^n$ generic for I . Then $\text{ind}_w(I)$ is a holonomic Frobenius ideal. Its rank equals the rank of $\text{in}_{(-w, w)}(I)$. This is bounded above by $\text{rank}(I)$, with equality when the D -ideal I is regular holonomic.*

The indicial ideal $\text{ind}_w(I)$ is computed from I by means of Gröbner bases in D . This computation identifies the leading terms in a basis of series solutions for I . The construction of the higher terms in these series solutions is the topic of the next section.

9.2 Regular holonomic D -ideals

By N , we denote the ring of functions of the *Nilsson class*, i.e., those functions which can be represented by an element of

$$N := \mathbb{C}[[x^{u^1}, \dots, x^{u^n}]] [x^{\beta^1}, \dots, x^{\beta^n}, \log(x_1), \dots, \log(x_n)] \quad (9.3)$$

for suitable vectors $u^1, \dots, u^n, \beta^1, \dots, \beta^n \in \mathbb{C}^n$ (see [37, (2.31)]). The coefficients lie in the ring $\mathbb{C}[[x^{u^1}, \dots, x^{u^n}]]$ of formal power series in the x^{u^i} .

Definition 9.5. The w -weight of a monomial $x^A \log(x)^B$ is the real part $\Re(w \cdot A)$ of $w \cdot A$. The *initial series* of $f = \sum_{A,B} c_{AB} x^A \log(x)^B \in N$, denoted $\text{in}_w(f)$, is defined to be the finite subsum of all terms of minimal w -weight.

Any weight vector $w \in \mathbb{R}^n$ induces a partial order on functions of the Nilsson class via

$$x^A \log(x)^B \leq x^C \log(x)^D \Leftrightarrow \Re(w \cdot A) \leq \Re(w \cdot C). \quad (9.4)$$

Since the w -weight does not give a monomial order, one needs a monomial order \prec as a tie breaker and denotes the resulting monomial order by \prec_w . We will take \prec to be the lexicographical order on N obtained as restriction of the lexicographic order on $\mathbb{C}^n \oplus \mathbb{N}^n$.

Definition 9.6. The set of *starting monomials* of I with respect to \prec_w is

$$\text{Start}_{\prec_w}(I) := \{\text{in}_{\prec_w}(f) \mid f \in N \text{ is a non-zero solution of } I\}, \quad (9.5)$$

where $\text{in}_{\prec_w}(f) = x^A \log(x)^B$ for some $A \in \mathbb{C}^n$ and $B \in \mathbb{N}^n$.

In the definition, x^A denotes $x_1^{A_1} \cdots x_n^{A_n}$ and $\log(x)^B = \log(x_1)^{B_1} \cdots \log(x_n)^{B_n}$. Moreover,

$$\text{Start}_{\prec_w}(I) = \text{Start}_{\prec_w}(\text{in}_{(-w,w)}(I)) = \text{Start}_{\prec_w}(\text{ind}_w(I)). \quad (9.6)$$

Proposition 9.7 ([37, Corollary 2.5.11]). *If $x^A \log(x)^B \in \text{Start}_{\prec_w}(I)$, then A is an exponent of I with respect to w . For each exponent A , the number of starting monomials of the form $x^A \log(x)^B$ is the multiplicity of A as a root of the indicial ideal $\text{ind}_w(I)$.*

Theorem 9.8 ([37, Theorem 2.5.12]). *For each starting monomial $x^A \log(x)^B$ in $\text{Start}_{\prec_w}(I) = \text{Start}_{\prec_w}(\text{ind}_w(I))$, there exists a unique $f \in N$ with the following properties:*

- (1) f is annihilated by I , i.e., $f \in \text{Sol}(I)$,
- (2) $\text{in}_w(f) = x^A \log(x)^B$, and
- (3) the monomial $x^A \log(x)^B$ is the only starting monomial that appears in f with non-zero coefficient.

Solutions to I as in the theorem above are called *canonical (series) solutions* of I with respect to \prec_w . Which exponents can occur in the solution functions f in Theorem 9.8 is made precise in the next proposition.

Proposition 9.9. *If I is regular holonomic and w a generic weight for I , there exist $\text{rank}(I)$ many canonical series solutions of I which lie in the Nilsson ring $N_w(I)$ of I w.r.t. to w ,*

$$N_w(I) := \mathbb{C}[[C_w(I)_{\mathbb{Z}}^*][x^{e^1}, \dots, x^{e^r}, \log(x_1), \dots, \log(x_n)]]. \quad (9.7)$$

Here, $\{e^1, \dots, e^r\}$ denotes the set of roots of the indicial ideal of I , and $C_w(I)_{\mathbb{Z}}^* = C_w(I)^* \cap \mathbb{Z}^n$, where $C_w(I)$ is the Gröbner cone of I containing w ,

$$C_w(I) = \{w' \in \mathbb{R}^n \mid \text{in}_{(-w,w)}(I) = \text{in}_{(-w',w')}(I)\}, \quad (9.8)$$

and

$$C_w(I)^* = \{u \in \mathbb{R}^n \mid u \cdot v \geq 0 \text{ for all } v \in C_w\} \quad (9.9)$$

is its dual cone (called “polar dual” in [37]). The elements of $\mathbb{C}[[C_w(I)_{\mathbb{Z}}^*]]$ are power series in x whose exponent vectors lie in $C_w(I)_{\mathbb{Z}}^*$. More precisely, the canonical solutions to I with respect to \prec_w have the form $x^A \cdot g$, where A is an exponent of I and g is an element of $\mathbb{C}[[C_w(I)_{\mathbb{Z}}^*]][\log(x_1), \dots, \log(x_n)]$, such that the degree of each $\log(x_i)$ in g is at most $\text{rank}(I) - 1$ (see [37, Theorem 2.5.14]). We also briefly comment on the convergence of these series: there exists a point $p \in C_w(I)$ such that the canonical series solutions converge for $x \in \mathbb{C}^n$ satisfying $(-\log|x_1|, \dots, -\log|x_n|) \in p + C_w(I)$, see [37, Theorem 2.5.16].

Theorem 9.10 ([37, Theorem 2.6.1]). *Let I be a regular holonomic ideal in $\mathbb{Q}[x_1, \dots, x_n]\langle \partial_1, \dots, \partial_n \rangle$ and let $w \in \mathbb{R}^n$ be a generic weight vector for I . Let I be given by a Gröbner basis G with respect to w . There exists an algorithm which computes all terms up to specified w -weight in the canonical series solutions to I with respect to \prec_w .*

We now turn to the proof, which also contains the procedure of lifting solutions. This procedure is commonly referred to as ‘‘SST algorithm’’.

Proof. Let $w \in \mathbb{R}^n$ be generic for I . Compute the roots of $\text{ind}_w(I)$ and extend the field of coefficients by them. Denote the resulting, computable field extension of \mathbb{Q} by \mathbb{K} . To compute the canonical solution of I whose starting monomial is $x^A \log(x)^B$, one proceeds as follows. For $p \in \mathbb{Z}^n$, denote by L_p the \mathbb{K} -vector space

$$L_p := x^A \cdot \sum_{0 \leq b_i < \text{rank}(I)} \mathbb{K} \cdot x^p \log(x)^b. \quad (9.10)$$

The \mathbb{K} -vector space L_p is finite-dimensional. Every $f \in \mathbb{K}[\theta]$ induces a \mathbb{K} -linear map $f: L_p \rightarrow L_p$. The monomials of L_p are a \mathbb{K} -basis of it. They are ordered by the term order \prec_w on the Nilsson ring, starting with the smallest. The matrix of f in this basis is an upper triangular square matrix. Let L'_p denote the set of monomials in L_p that are not contained in $\text{Start}_{\prec_w}(I)$. Now let $\{f_1, \dots, f_d\}$ be any generating set of $\text{ind}_w(I)$ and restrict $f_i: L_p \rightarrow L_p$ to L'_p ; this corresponds to deleting some of the columns in the associated matrix. Denote the resulting matrix by F_i . Then the map

$$F: L'_p \longrightarrow L_p^d, \quad v \mapsto (f_1 \bullet v, \dots, f_d \bullet v)^\top \quad (9.11)$$

is injective and is represented by the matrix obtained as vertical concatenation of F_1, \dots, F_d .

Now let $G = \{g_1, \dots, g_d\}$ be a Gröbner basis of I with respect to w ; its Gröbner cone in \mathbb{R}^n is denoted by C_w . For each $g \in G$, choose a Laurent monomial x^α such that

$$x^\alpha g = f - h, \quad (9.12)$$

where $f \in \mathbb{K}[\theta_1, \dots, \theta_n]$, $h \in \mathbb{K}[x_1^{\pm 1}, \dots, x_n^{\pm 1}]\langle \partial_1, \dots, \partial_n \rangle$ with $\text{ord}_{(-w, w)}(h) < 0$. Here, $\text{ord}_{(-w, w)}(h)$ denotes the largest w -weight of a monomial appearing in h . Then the set of operators f_1, \dots, f_d obtained this way generate $\text{ind}_w(I)$ and, as maps as in (9.11), they are injective. The Laurent monomial x^α for a Gröbner basis element g is obtained by taking a highest-weight term $x^a \partial^b m$ in g , where m is a monomial in the θ_i 's and for all k , at least one of $\{a_k, b_k\}$ is zero. Intuitively, this corresponds to pulling out as many θ 's as possible into m . Then $x^\alpha = x^{b-a}$. The h_i may have terms of different weights; in this case, we get a recurrence that involves L_p for more than two different p 's. The coefficients of the canonical series solution are now computed by induction on the w -weight k . We start from a canonical series solution $x^A \log(x)^B + \dots$ and assume the coefficients $c_{pb} \in \mathbb{K}$ are already known for $0 \leq p \cdot w \leq k$, $p \in C_w^*$. Let $F_k(x)$ be this partial solution up to w -weight k , i.e.,

$$F_k(x) = x^A \cdot \sum_{\substack{0 \leq p \cdot w \leq k, p \in C_w^* \\ 0 \leq b_j < \text{rank}(I)}} c_{pb} x^p \log(x)^b, \quad (9.13)$$

and let M_k be the space of terms with w -weight greater than k , i.e. $M_k = \sum_{p \cdot w > k, p \in C_{\mathbb{Z}}^*} L_p$. Then, by definition, we have that

$$g_i \bullet F_k(x) \equiv 0 \pmod{M_k}. \quad (9.14)$$

Assuming we know $F_k(x)$ for some k , we are going to construct a recursion which allows us to determine the additional terms which are needed to lift $F_k(x)$ to $F_{k+1}(x)$. The starting point of that recursion will be the starting monomials. We hence look for an element E_{k+1} of $\sum_{p \cdot w = k+1, p \in C_{\mathbb{Z}}^*} L'_p$ such that

$$E_{k+1}(x) \equiv F_{k+1}(x) - F_k(x) \pmod{M_{k+1}}. \quad (9.15)$$

To achieve this, observe that $\text{ord}_{(-w,w)}(h_i) < 0$ implies that $h_i \bullet x^\ell$ has *higher* w -weight than x^ℓ . We can show this on monomials as follows. Suppose that $h_i = x^q$ for some $q \in \mathbb{N}^n$ with $q \cdot (-w) < 0$. Then $q \cdot w > 0$, so $h_i \bullet x^\ell = x^{\ell+q}$ has higher w -weight than x^ℓ . Similarly, suppose that $h_i = \partial^r$ where $r \cdot w < 0$. Then $(-r) \cdot w > 0$. Thus $h_i \bullet x^\ell = Cx^{\ell-r}$ for some constant C , and $x^{\ell-r}$ has higher w -weight than x^ℓ . Together with (9.12) and (9.14), this implies that $f_i \bullet F_{k+1} = h_i \bullet F_k \pmod{M_{k+1}}$, which gives the desired recursion relation for $E_{k+1}(x)$ in terms of $F_k(x)$, namely

$$f_i \bullet E_{k+1}(x) \equiv (h_i - f_i) \bullet F_k(x) \pmod{M_{k+1}}. \quad (9.16)$$

By the injectivity of the map F from (9.11) and the existence of a canonical series solution, there exists a unique solution $E_{k+1}(x)$ to (9.16), and this lifts $F_k(x)$ to $F_{k+1}(x)$. \square

This algorithm has been applied to D -ideals behind Feynman integrals in [20] and matched with methods that are in more common use by physicists. In the meantime, an implementation of the algorithm is contained in the `Macaulay2` package `HolonomicSystems` [41] of Sayrafi, Berkesch, Leykin, and Tsai.

Example 9.11. Consider the hypergeometric differential operator

$$P = \theta(\theta - 3) - x(\theta + a)(\theta + b). \quad (9.17)$$

The D -ideal $I = DP$ is holonomic of rank $\text{ord}_{(0,1)}(P) = 2$. The Gröbner fan of I has two maximal cones, namely $\pm \mathbb{R}_{\geq 0}$. For the weight $w = 1$, $\text{in}_{(-w,w)}(I) = \langle \theta(\theta - 3) \rangle = \text{ind}_w(I)$. The exponents of I are $V(\text{ind}_w(I)) = \{0, 3\}$. Hence we will be having starting monomials involving $x^0 = 1$ and x^3 , and logarithmic terms. Choose x^3 as starting monomial, so that $L_p = \mathbb{C} \cdot \{x^{p+3}, x^{p+3} \log(x)\}$. We are seeking for a series solution of the form

$$x^3 \cdot \sum_p c_{p,1} x^p + c_{p,2} x^p \log(x). \quad (9.18)$$

Write $P = f - h$, where $f = \theta(\theta - 3)$ and $h = x(\theta + a)(\theta + b)$. The action of θ on L_p is

$$\theta \bullet x^{p+3} = (p+3)x^{p+3} \quad \text{and} \quad \theta \bullet (x^{p+3} \log(x)) = x^{p+3} + (p+3)x^{p+3} \log(x). \quad (9.19)$$

Thus, the matrix of the operator θ in the basis $\{x^{p+3}, x^{p+3} \log(x)\}$ is

$$\begin{bmatrix} p+3 & 1 \\ 0 & p+3 \end{bmatrix}. \quad (9.20)$$

Let $c_{p,1}$ and $c_{p,2}$ be the coefficients of x^{p+3} and $x^{p+3} \log(x)$ in the power series expansion (9.18). Then we can write our operators as matrices, and our recurrence as

$$\begin{bmatrix} p & 1 \\ 0 & p \end{bmatrix} \begin{bmatrix} p+3 & 1 \\ 0 & p+3 \end{bmatrix} \begin{bmatrix} c_{p,1} \\ c_{p,2} \end{bmatrix} = \begin{bmatrix} p-a+2 & 1 \\ 0 & p-a+2 \end{bmatrix} \begin{bmatrix} p-b+2 & 1 \\ 0 & p-b+2 \end{bmatrix} \begin{bmatrix} c_{p-1,1} \\ c_{p-1,2} \end{bmatrix}$$

with initial values $c_{0,1} = 1$ and $c_{0,2} = 0$. Solving the recurrence yields

$$c_{p,1} = 0 \quad \text{and} \quad c_{p,2} = \frac{(a+3)_p (b+3)_p}{(1)_p (4)_p}, \quad (9.21)$$

where

$$(a)_p = (a+1) \cdots (a+p-1) \quad (9.22)$$

is the Pochhammer symbol. If we choose the starting monomial $x^0 = 1$ instead, the matrix of f is singular for $p = 3$. To find the series expansion in this case, see [37, pp. 98–99]. \diamond

Exercise 9.12. Let I be the D_1 -ideal from Example 2.20. It has holonomic rank 2. Compute the canonical series solutions of I for $w = 1$ up to w -weight 4. \diamond

10 Relations among Mellin integrals

In high energy physics, scattering processes of particles are pictorially represented by Feynman diagrams. Via Feynman rules, one associates to each of these diagrams an integral: its *Feynman integral*, a comprehensive treatment of which can be found in [49]. It is important to understand relations among these integrals in different dimensions of Minkowski spacetime. The theory of D -modules turns out to be helpful for this undertaking.

10.1 Bernstein–Sato ideals

To the Weyl algebra, we adjoin a new formal variable s which commutes with all x_i 's and ∂_i 's. The resulting ring is $D_n[s]$. Fix a polynomial $f \in \mathbb{C}[x_1, \dots, x_n]$ and consider the $D_n[s]$ -module $\mathbb{C}[x_1, \dots, x_n, s, f^s, f^{-1}]$. The action of $D_n[s]$ is given by the usual rules of arithmetic. In particular,

$$\partial_i \bullet f^s = s \frac{\partial f}{\partial x_i} f^{-1} f^s = s \frac{\partial f}{\partial x_i} f^{s-1}. \quad (10.1)$$

Definition 10.1. Let $f \in \mathbb{C}[x_1, \dots, x_n]$. The *Bernstein–Sato polynomial* $b_f \in \mathbb{C}[s]$ of f is the unique monic polynomial of smallest degree for which there exists $P_f \in D_n[s]$ such that

$$P_f(s) \bullet f^{s+1} = b_f(s) \cdot f^s. \quad (10.2)$$

If $V(f)$ is smooth, then $b_f = s + 1$. While the Bernstein polynomial is unique, the Bernstein–Sato operator P_f is unique only modulo $\text{Ann}_{D_n[s]}(f^{s+1})$. It is known that b_f is non-trivial and that its roots are negative rational numbers [23].

Example 10.2. Let $f = x_1^2 + \cdots + x_n^2 \in \mathbb{C}[x_1, \dots, x_n]$. Since

$$\sum_{i=1}^n \partial_i^2 \bullet f^{s+1} = 4(s+1) \left(s + \frac{n}{2} \right) f^s, \quad (10.3)$$

the Bernstein–Sato polynomial of f is $b_f = (s+1)(s + \frac{n}{2}) \in \mathbb{C}[s]$, and $P_f = \frac{1}{4}\Delta$, where $\Delta = \partial_1^2 + \cdots + \partial_n^2$ denotes the Laplace operator, is a Bernstein–Sato operator of f . \diamond

Exercise 10.3. Determine the Bernstein–Sato polynomial of your favorite polynomial. \diamond

Bernstein–Sato polynomials were originally studied to construct meromorphic continuations of the distribution-valued function $s \mapsto f^s$, which is a priori defined only for complex numbers $s \in \mathbb{C}$ with positive real part. Nowadays, it is an important object of study in singularity theory, among others in work on the monodromy conjecture such as [7, 8].

Definition 10.4. The s -parametric annihilator of f^s is the $D_n[s]$ -ideal

$$\text{Ann}_{D_n[s]}(f^s) := \{P \in D_n[s] \mid P \bullet f^s = 0\}. \quad (10.4)$$

The algebraic Mellin transform from (5.13) induces an isomorphism

$$\mathfrak{M}\{\cdot\}: \text{Ann}_{D_n[s]}(f^s) \xrightarrow{\cong} \text{Ann}_{S_n[s]}(\mathfrak{M}\{f^s\}). \quad (10.5)$$

Example 10.5. For P as in Equation (10.2), the operator $P_f f - b_f$ is in $\text{Ann}_{D_n[s]}(f^s)$. \diamond

Example 10.6. Let $f = (x-1)(x-2) \in \mathbb{C}[x]$. In this case, the s -parametric annihilator of f^s is the $D_n[s]$ -ideal generated by the operator $P = f\partial - s\partial \bullet f$. This can be computed running the following code in Singular [12]:

```
LIB "dmod.lib";
ring r = 0,x,dp;
poly f = (x-1)*(x-2);
def A = operatorBM(f); setring A; LD;
```

The s -parametric annihilator of f^s is encoded as LD in the ring A. \diamond

The Bernstein–Sato polynomial is computed as the monic generator of the $\mathbb{C}[s]$ -ideal

$$\langle b_f \rangle = (\text{Ann}_{D[s]}(f^s) + \langle f \rangle) \cap \mathbb{C}[s]. \quad (10.6)$$

Algorithm 5.3.15 in [37] presents an algorithm of Oaku to compute this ideal.

Exercise 10.7. Let $c \in \mathbb{C}$ be fixed. Are $(\text{Ann}_{D_n[s]}(f^s))|_{s=c}$ and $\text{Ann}_{D_n}(f^c)$ always equal? \diamond

For a tuple $F = (f_1, \dots, f_\ell)$ of $\ell > 1$ polynomials $f_1, \dots, f_\ell \in \mathbb{C}[x_1, \dots, x_n]$, one needs to consider the Bernstein–Sato *ideal* instead.

Definition 10.8. The *Bernstein–Sato ideal* of $F = (f_1, \dots, f_\ell)$ is the ideal $B_F \subset \mathbb{C}[s_1, \dots, s_\ell]$ consisting of all polynomials $b \in \mathbb{C}[s_1, \dots, s_\ell]$ for which there exists $P \in D_n[s_1, \dots, s_\ell]$ s.t.

$$P \bullet (f_1^{s_1+1} \dots f_\ell^{s_\ell+1}) = b \cdot f_1^{s_1} \dots f_\ell^{s_\ell}. \quad (10.7)$$

Sabbah [35] proved that B_F is non-trivial and moreover that the irreducible components of $V(B_F)$ of codimension one are affine-linear hyperplanes with non-negative rational coefficients. This is analogous to the fact that the zeroes of the Bernstein–Sato polynomial are negative rational numbers.

Example 10.9. Consider the following statistical experiment. *Flip a biased coin. If it shows head, flip it one more time.* The three outcomes of this model are described by the three univariate polynomials $f_0 = x^2$, $f_1 = x(1-x)$, and $f_2 = 1-x$. The probability tree of the model is depicted in Figure 10. For data $s = (s_0, s_1, s_2) \in \mathbb{N}^3$, the likelihood function of this

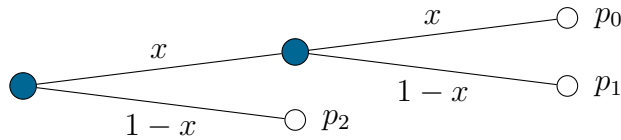


Figure 10: Staged tree [13] modeling the experiment from Example 10.9

model is $f^s = f_0^{s_0} f_1^{s_1} f_2^{s_2}$. Its Bernstein–Sato ideal is principal and generated by

$$\prod_{k=1}^3 (2s_0 + s_1 + k) \cdot \prod_{l=1}^2 (s_1 + s_2 + l) \in \mathbb{C}[s_0, s_1, s_2]. \quad (10.8)$$

This can be obtained by running the following code in `Singular`.

```
LIB "dmod.lib";
ring r = 0,x,dp; ideal F = x^2, x*(1-x), 1-x;
def A = annfsBMI(F); setring A; BS;
```

It is a special incident in this example that the Bernstein–Sato ideal is principal. ◇

Exercise 10.10. Compute the maximum likelihood estimate of the model in Example 10.9. Compare it with the Bernstein–Sato ideal in (10.8). ◇

10.2 Feynman integrals

In high energy physics, scattering processes of particles are graphically depicted by Feynman diagrams. To each such diagram, one associates its graph polynomial. We here recall definitions from [6, Section 4]. Let $G = (V, E)$ be a graph with vertices $V = \{v_1, \dots, v_r\}$ and edges $E = \{e_1, \dots, e_n\}$. The first Betti number of graph with k connected components is $l = n - r + k$. In physics, it is sometimes called the “number of loops”—with relations among loops being taken into account.

Definition 10.11. Let $k \in \mathbb{N}$. A *spanning k -forest* for G is a subgraph F of G that contains all vertices of G , has no loops, and k connected components. The set of spanning k -forests is denoted \mathcal{T}_k . Spanning 1-forests are called *spanning trees*.

Feynman diagrams are graphs, with external legs attached, which depict particles that are flowing in and out. Figure 11 shows a Feynman diagram, which is commonly referred to as “one-loop graph” or “bubble graph”.

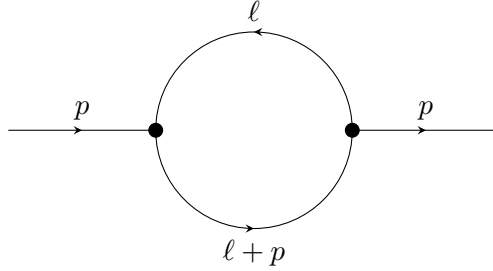


Figure 11: One-loop graph with one incoming and one outgoing particle and loop momentum ℓ . Each node obeys momentum conservation.

The momentum vectors p_i of these particles are elements of d -dimensional Minkowski space-time, i.e., $\mathbb{R}^d = \{(t, x_1, \dots, x_{d-1})\}$ endowed with the Minkowski inner product of signature $(-, +, \dots, +)$ or $(+, -, \dots, -)$, depending on the convention used. We will denote Feynman diagrams by G as well. Let T_i denote the connected components of a spanning forest, and denote by P_{T_i} the set of external momenta attached to T_i . To each internal edge e_i , one associates an “internal propagator” $m_i \in \mathbb{R}$, corresponding to particles of mass m_i .

Definition 10.12. Let G be a Feynman diagram. Its *Symanzik polynomial of first kind*, denoted \mathcal{U}_G , is the following polynomial in variables $\{x_i\}_{e_i \in E}$ labeled by the edges of G :

$$\mathcal{U}_G := \sum_{T \in \mathcal{T}_1} \prod_{e_i \notin T} x_i. \quad (10.9)$$

Its *Symanzik polynomial of second kind*, denoted \mathcal{F}_G , is

$$\mathcal{F}_G := \left(\sum_{(T_1, T_2) \in \mathcal{T}_2} \left(\sum_{p_j \in P_{T_1}} \sum_{p_k \in P_{T_2}} \frac{p_j \cdot p_k}{\mu^2} \right) \prod_{e_i \notin (T_1, T_2)} x_i \right) + \mathcal{U}_G \cdot \sum_{i=1}^n \frac{m_i^2}{\mu^2} \cdot x_i, \quad (10.10)$$

where the scalar product of the d -dimensional momentum vectors is taken with respect to the Minkowski inner product. The factor μ is a scaling factor, that we will ignore in the sequel.

Definition 10.13. The *graph polynomial* of a Feynman diagram G is $\mathcal{G} := \mathcal{U}_G + \mathcal{F}_G$.

Example 10.14 ([5, Example 47]). Let G be the bubble graph depicted in Figure 11. The Symanzik polynomials of G are $\mathcal{U}_G = x_1 + x_2$ and $\mathcal{F}_G = (x_1 + x_2)(x_1 m_1^2 + x_2 m_2^2) - p^2 x_1 x_2$. \diamond

Definition 10.15. Let $f \in \mathbb{C}[x_1, \dots, x_n]$ be a polynomial and $a \in \mathbb{Z}$, $b \in \mathbb{Z}^n$. Define $I_{a,b}$ to be the integral

$$I_{a,b}(s, \nu) = \mathfrak{M}\{f^{s+a}x^b\}(\nu). \quad (10.11)$$

Definition 10.16. The *Feynman integral* of G , in the Lee–Pomeransky representation, is

$$I_G := \mathfrak{M}\{\mathcal{G}^{-d/2}\}. \quad (10.12)$$

In the notation of (10.11), for $f = \mathcal{G}$, the Feynman integral of G is $I_G(\nu) = I_{0,0}(-d/2, \nu)$.

Remark 10.17. Summing over Feynman diagrams of different loops orders results in a function which is called “scattering amplitude” and it is important to evaluate these functions to high precision. They encode probabilities that particles scatter in a prescribed way. Scattering amplitudes are moreover closely related to the MLE problem of discrete statistical models in algebraic statistics, see [43]. \diamond

Remark 10.18. Read as function of the coefficients of the graph polynomial, Feynman integrals are solutions of (restricted) GKZ systems, cf. [11]. \diamond

Feynman integrals in different dimensions of spacetime are linearly dependent and it is important to construct relations among them. Bernstein–Sato operators help to do so: applying the Mellin transform to both sides of Equation (10.2) yields

$$b_f(s) \cdot \mathfrak{M}\{f^s\} = \mathfrak{M}\{P_f\} \bullet \mathfrak{M}\{f^{s+1}\}. \quad (10.13)$$

We refer to this relation as being *lowering in s* . This means that it provides a way for writing the integral $I_{0,0}(s, \nu)$ as a linear combination of integrals of type $I_{0,b}(s+1, \nu)$ for some $b \in \mathbb{Z}^n$. One obtains a *raising* relation by the simple trick of considering $f \in \mathbb{C}[x]$ as a differential operator of order zero. Like that,

$$\mathfrak{M}\{f^{s+1}\} = \mathfrak{M}\{f \cdot f^s\} = \mathfrak{M}\{f\} \bullet \mathfrak{M}\{f^s\}. \quad (10.14)$$

Since $\sigma^b \bullet I_{a,0} = I_{a,b}$, relations among integrals $I_{a,b}$ can hence be understood from $S_n[s] \bullet I_{0,0}$.

Example 10.19. Let $f = (x-1)(x-2) \in \mathbb{C}[x]$ from Example 10.6. The s -parametric annihilator of f^s is generated by the operator $P = f\partial_x - s\partial_x \bullet f \in D_1[s]$. Its Mellin transform is

$$\mathfrak{M}\{P\} = -(\nu+1+2s)\sigma - 2(\nu-1)\sigma^{-1} + 3(\nu+1) \in S_1[s]. \quad (10.15)$$

Expanding the equation $\mathfrak{M}\{P\} \bullet \mathfrak{M}\{f^s\} = 0$ results in the relation

$$-(\nu+1+2s)\mathfrak{M}\{f^s\}(\nu+1) - 2(\nu-1)\mathfrak{M}\{f^s\}(\nu-1) + 3(\nu+1)\mathfrak{M}\{f^s\}(\nu) = 0 \quad (10.16)$$

of Mellin integrals. \diamond

Definition 10.20. The *number of master integrals* is the dimension of the $\mathbb{C}(s, \nu)$ -vector space

$$V_{s,\nu} := \sum_{a \in \mathbb{Z}} \mathbb{C}(s, \nu) \otimes_{\mathbb{C}[s,\nu]} (S_n \bullet I_{a,0}) = \mathbb{C}(s, \nu) \otimes_{\mathbb{C}[s,\nu]} (S_n[s] \bullet I_{0,0}). \quad (10.17)$$

This number can be recovered from the very affine variety $(\mathbb{C}^*)^n \setminus V(f)$ as follows.

Theorem 10.21 ([5, Corollary 37]). *The dimension of $V_{s,\nu}$ is given by the signed topological Euler characteristic of the hypersurface complement $(\mathbb{C}^*)^n \setminus V(f)$, i.e.,*

$$\dim_{\mathbb{C}(s,\nu)}(V_{s,\nu}) = (-1)^n \cdot \chi((\mathbb{C}^*)^n \setminus V(f)).$$

The proof in [5, Section 3] of this statement builds on work of Loeser and Sabbah [30].

Example 10.22. Let $f = (x - 1)(x - 2)$ from Example 10.19. Hence $X = \mathbb{C}^* \setminus V(f)$ is isomorphic to $\mathbb{P}^1 \setminus \{0, 1, 2, \infty\}$. The signed Euler characteristic of X is $|\chi(\mathbb{P}^1) - 4| = 2$. \diamond

Exercise 10.23. Determine a $\mathbb{C}(s, \nu)$ -basis of $V_{s,\nu}$ for f from Example 10.19. \diamond

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