Integro-Differential Polynomials and Free Integro-Differential Algebras

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4. **Towards Integro-Differential Fractions:**
   Ongoing work with F. Lemaire, F. Boulier
   and G. Regensburger [ISSAC13].

Outline

1. Integro-Differential Category
2. Integro-Differential Polynomials
3. Free Integro-Differential Algebras
4. Towards Integro-Differential Fractions

Definition ([Baxter1960], [Guo2012])

Let K be a unital commutative ring and fix $\lambda \in K$.
Then a Rota-Baxter algebra over K with weight λ is an associative K-algebra $\mathcal{F}$ together with a K-linear operator $\int \colon \mathcal{F} \to \mathcal{F}$ satisfying

$$(\textstyle\int f)(\int g) = \int [f\,(\int g)] + \int [(\int f)\,g] + \lambda \int (fg).$$

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Primary example: $\mathcal{F} = C^\infty(\mathbb{R})$ with $\int = \int_0^x$

Combining with Derivations

Definition ([JSC08],[SFB11])

Let $\mathcal{F}$ be an algebra over a field K. If $(\mathcal{F}, \partial)$ is a differential algebra, $\int : \mathcal{F} \to \mathcal{F}$ a K-linear section of ∂ and the differential Baxter axiom

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Examples of Integro-Differential Algebras

Usual function spaces $\mathbb{C}[x] \leq C^\omega(\mathbb{R}) \leq C^\infty(\mathbb{R})$
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Matrices $\mathcal{F}^{n \times n}$ with componentwise $\partial, \int$

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Counter-Example for Condition (4):

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Hurwitz series $H(K) = K^{\mathbb{N}}$ with

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For characteristic zero, $K[[z]] \cong H(K)$ via $\sum_{n=0}^\infty a_n z^n \mapsto (n!\, a_n)$.

Integro-Differential and Other Categories

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Outline

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Expand Σ by $\begin{array}{|c|c|}\hline \partial & \int \\ \hline 1 & 1 \\ \hline\end{array}$ $\qquad E =$ as above

Polynomial Algebras in Varieties

Proposition

Let $\mathcal{V} = (\Sigma, E)$ be a variety (category) and X a set of variables.
The **term algebra** $\mathcal{T}_\Sigma(X)$ and the **free algebra** $\mathcal{F}_\mathcal{V}(X) := \mathcal{T}_\Sigma(X)/{\equiv_E}$ are both algebras in $\mathcal{V}$.

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Moreover, we have the coproduct $A_\mathcal{V}[X] = A \amalg_\mathcal{V} \mathcal{F}_\mathcal{V}(X)$.

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So we have <u>defined</u> integro-differential polynomials.

However, for computation we need <u>canonical forms</u>!

Canonical Forms for Integro-Differential Polynomials

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Since $\mathcal{F}_{\mathcal{V}}[u] = \mathcal{T}_\Sigma/\equiv_{E,\mathcal{F}}$ we need $\mathcal{C} \subseteq \mathcal{T}_\Sigma$ such that

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Lemma

Every integro-differential polynomial in $\mathcal{F}\{u\}$ can be represented by a finite sum of terms of the form

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with $f \in \mathcal{F}$ and $\alpha, \beta, \gamma_1, \ldots, \gamma_n \in \mathbb{N}^{(\omega)}$.

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Theorem

The set $\mathcal{C}$ of K-linear combinations of terms

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Canonical simplifier: Banish quasilinear monomials via Rota-Baxter axiom.

Integro-Differential Structure

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The constants of $\mathcal{F}\{u\}$ form the subring consisting of $\sum_\alpha c_\alpha u(0)^\alpha$ with constants c_α in $\mathcal{F}$.

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If $(\mathcal{F}, \partial, \int)$ is computable, then so is $(\mathcal{F}\{u\}, \partial, \int)$.

Outline

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Let $\mathcal{A}$ be a commutative differential K-algebra of weight λ. Then there is a free integro-differential algebra $\mathcal{F}$ of weight λ on $\mathcal{A}$ with a canonical differential morphism $\iota\colon \mathcal{A} \to \mathcal{F}$. This means for any integro-differential algebra $\tilde{\mathcal{F}}$ with differential morphism $\tilde{\iota}\colon \mathcal{A} \to \tilde{\mathcal{F}}$ there is a unique integro-differential morphism $j\colon \mathcal{F} \to \tilde{\mathcal{F}}$ with $j \circ \iota = \tilde{\iota}$.

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Special case $\mathcal{F} = (K\{u\}, \partial, \int)$ for $\mathcal{A} = (K\{u\}, \partial)$ with $\partial_K = 0$.

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<u>Caveat:</u> $(a_0 \otimes a)\,(b_0 \otimes b) = (a_0 b_0 \, \otimes \, a \, ш \, b)$ in $Ш(\mathcal{A}) = \mathcal{A} \otimes Ш^+(\mathcal{A})$.

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Again the problem is: How to do this constructively?

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(First step towards integro-differential fractions. But ...)

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Let $(K; \partial_1, \dots, \partial_m)$ be a differential field and $u = (u_1, \dots, u_n)$ be indeterminates. Then the **differential fraction field** $K\langle u \rangle$ is the total fraction field of $K\{u\}$ with derivations $\partial_1, \dots, \partial_m$

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As expected if P and Q have distinct leaders:
$\rightarrow \mathbf{ld}(F) =$ highest $v \in \Theta\mathcal{U}$ with $\mathbf{deg}_v(P) > 0$ or $\mathbf{deg}_v(Q) > 0$.

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The derivatives satisfy $\mathbf{ld}(\partial F) = \partial\, \mathbf{ld}(F) =: v$ and $\mathbf{lc}_v(\partial F) = \mathbf{in}(F)$. Writing $\partial F = P/Q$, one has $\mathbf{deg}_v(P) = 1$ and $\mathbf{deg}_v(Q) = 0$.

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- Derivations $\partial_1, \ldots, \partial_m$ such that $\partial_i(x_j) = \delta_{ij}$.
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Proposition

Algorithm

Given $\boldsymbol{F} \in K\langle u\rangle \setminus K$ and an independent variable $\boldsymbol{x_k}$, there are differential fractions $\boldsymbol{Q}, \boldsymbol{R} \in K\langle u\rangle$ such that $F = \partial_k Q + R$ with $\partial_k Q$ and R having rank lower than or equal to F. Moreover, R vanishes iff $F \in \partial_k(K\langle u\rangle)$.

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Proposition Algorithm

Given $\boldsymbol{F} \in K\langle u\rangle \setminus K$ and an independent variable $\boldsymbol{x_k}$, there is a list $[\boldsymbol{W_0}, \boldsymbol{W_1}, \ldots, \boldsymbol{W_s}]$ such that $F = W_0 + \partial_k W_1 + \cdots + \partial_k^s W_s$ with $W_s \neq 0$ and $W_0, \partial_k W_1, \ldots, \partial_k^s W_s$ having rank lower than or equal to F. Moreover, $W_0 = W_1 = \cdots W_i = 0$ iff $F \in \partial_k^{i+1}(K\langle u\rangle)$.

$\mathtt{integrate}(F, x_k) \rightsquigarrow R, Q$

```
Q, R := 0, 0
while F ≠ 0 do {invariant: F_0 = F + ∂_k Q + R}
    if F ∈ K then
        Q̄, R̄ := integrate_func(F, x_k)
        Q := Q + Q̄
        R := R + R̄
        F := 0
    else if num_F ∈ K then
        R := R + F
        F := 0
    else
        (v, w) := (ld(num_F), ld(den_F))
        if den_F ∉ K ∧ v ≤ w then
            R := R + F
            F := 0
        else if ord_k(v) = 0 then
            ∑_i m_i := num_F {monomial sum}
            H := ∑ (m_i | deg_v(m_i) > 0)
            R := R + H/den_F
            F := F − H/den_F
        else if deg_v(num_F) ≥ 2 then
            ∑_i m_i := num_F {monomial sum}
            H := ∑ (m_i | deg_v(m_i) > 1)
            R := R + H/den_F
            F := F − H/den_F
        else
            ∂_k u := v
            F̄ := lc_v(num_F)/den_F
            if ∃_{t>u} deg_t(num_F̄) > 0 then
                ∑_i m_i := num_F̄ {monomial sum}
                H := ∑ (m_i | ∃_{t>u} deg_t(m_i) > 0)
                R := R + (H/den_F̄)v
                F := F − (H/den_F̄)v
            else if ∃_{t>u} deg_t(den_F̄) > 0 then
                R := R + F
                F := 0
            else
                Q̄, R̄ := integrate_func(F̄, v)
                R := R + R̄v
                Q := Q + Q̄
                F := F − ∂_k Q̄ − R̄v
            end if
        end if
    end if
end while
return R, Q
```

Back

Integration Algorithm (Iterated Version)

$\texttt{integrate}(F, x_k) \rightsquigarrow L$

$L := []$
$R := F$
while $R \notin K$ **do**
  $W,\ R := \texttt{integrate}(R, x_k)$
  $L := L :: W$
end while
if $R \neq 0$ **then**
  $L := L :: R$
end if
return L

Forward

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State variables x_1, x_2: Concentration of drug in compartment $1, 2$

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Michaelis-Menten law:

$$\dot{x}_1 = -k_1 x_1 + k_2 x_2 - V_e \, x_1/(x_1 + k_e)$$
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Elimination ranking $x_1, x_2 \ll y$ for **input/output equation**:

$$(y + k_e)^2\, y_{tt} + (k_1 + k_2)(y + k_e)^2 y_t + k_e V_e (y_t + y^2 + k_e y) = 0$$

Worksheet

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Integration yields alternative equation:

$$\frac{d^2}{dt^2}\, y + \frac{d}{dt}\, \frac{(k_1 + k_2)(y^2 - k_e^2) - k_e V_e}{y + k_e} + \frac{k_2 V_e y}{y + k_e} = 0$$

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Potentially better behaved numerics.

▸ Conclusion

```
> Ring := DifferentialRing (
     derivations = [t],
     blocks = [y,[x1,x2],[k1(),k2(),ke(),Ve()]]):

> S := [ x1[t] = -k1*x1 + k2*x2 - (Ve*x1)/(ke+x1),
         x2[t] = k1*x1 - k2*x2, y = x1];
                                     Ve x1
S := [x1[t] = -k1 x1 + k2 x2 - -------,
                                    ke + x1
    x2[t] = k1 x1 - k2 x2, y = x1]

> ideal := RosenfeldGroebner
     (S, Ring, basefield = field
        (generators = [k1,k2,ke,Ve])):

> io_ideal := RosenfeldGroebner (ideal[1],
    blocks = [[x1,x2],y,[k1(),k2(),ke(),Ve()]]):
```

```
> io_eq := Equations
     (io_ideal, leader = derivative(y))[1];
                       2                             2
io_eq := y[t, t] y  + 2 y[t, t] y ke + y[t, t] ke
                 2            2
     + y[t] y  k1 + y[t] y  k2 + 2 y[t] y k1 ke
                                       2             2
     + 2 y[t] y k2 ke + y[t] k1 ke  + y[t] k2 ke
                          2
     + y[t] ke Ve + y  k2 Ve + y k2 ke Ve

> integrate (io_eq / Initial (io_eq, Ring), t, Ring);
          2        2           2        2
 y k2 Ve  y  k1 + y  k2 - k1 ke  - k2 ke  - ke Ve
[-------, ---------------------------------------, y]
 y + ke                   y + ke
```

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THANK YOU

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