Generalized shuffle relations for singular integrals

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Outline

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2. Generalized integro-differential algebra
   - Definition
   - Basic identities
3. Nested integrals
   - Generalized shuffle relations
   - Taylor's theorem
4. Summary

Basic shuffle relation

Continuous functions

$$\left(\int f_1\right)\left(\int f_2\right) = \int f_1 \int f_2 + \int f_2 \int f_1$$

with $\int f := \int_0^x dt\, f(t)$

Simple poles at 0

$$\left(\int f_1\right)\left(\int f_2\right) = \int f_1 \int f_2 + \int f_2 \int f_1$$

with $\int f := c \ln(x) + \int_0^x dt\, (f(t) - \frac{c}{t})$

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Example

$f_1 = \frac{1}{x}$, $f_2 = \frac{1}{1-x}$

$$\ln(x)$$

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$$\ln(x)(-\ln(1-x)) =$$

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Example

$f_1 = \frac{1}{x}$, $f_2 = \frac{1}{1-x}$

$$\ln(x)(-\ln(1-x)) = \mathrm{Li}_2(x) + (\mathrm{Li}_2(1-x) - \zeta_2)$$

Beyond simple poles

Example: double pole at 0

Define $\int f := -\frac{c_2}{x} + c_1 \ln(x) + \int_0^x dt\,(f(t) - \frac{c_2}{t^2} - \frac{c_1}{t})$

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$$\begin{aligned}\left(\int f_1\right)\left(\int f_2\right) &= -\frac{1}{x}(-\ln(1-x))\\ \int f_1 \int f_2 &= \ln(x) + \left(\frac{1}{x} - 1\right)\ln(1-x) + 1\\ \int f_2 \int f_1 &= \end{aligned}$$

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Compare:

Beyond simple poles

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Compare:

$$\left(\int f_1\right)\left(\int f_2\right) \neq \int f_1 \int f_2 + \int f_2 \int f_1$$

Beyond simple poles

Example: double pole at 0

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Compare:

$$\left(\int f_1\right)\left(\int f_2\right) = \int f_1 \int f_2 + \int f_2 \int f_1 - 1$$

Generalized integro-differential algebra

Definition

Integration by evaluation

Recall: fundamental theorem of calculus

$$\int_a^x dt\, f(t) = g(x) - g(a)$$

Gives abstract principle for defining the integral

1. Fix a linear functional E with

$$\mathrm{E}(f) = c$$

   for constant functions $f(x) = c$

2. Define a linear operator by

$$\int f := g - \mathrm{E}(g)$$

   where g is such that $\frac{d}{dx} g = f$

Evaluation by integration

Rearrange fundamental theorem of calculus

$$f(a) = f(x) - \int_a^x dt\, f'(t)$$

Evaluation by integration

Rearrange fundamental theorem of calculus

$$f(a) = f(x) - \int_a^x dt\, f'(t)$$

Gives abstract principle for defining an evaluation

1. Fix a linear operator $\int$ assigning an antiderivative to each $f(x)$
2. Define a linear functional by

$$\mathrm{E}(f) := f - \int f'$$

Example: $C^\infty(\mathbb{R})$

Consider elements of $C^\infty(\mathbb{R})$, i.e. smooth functions

Define the linear operator $\int$ on $C^\infty(\mathbb{R})$ by

$$(\textstyle\int f)(x) := \int_a^x dt\, f(t)$$

for some $a \in \mathbb{R}$.

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Then the evaluation defined by $\mathrm{E}(f) := f - \int f'$ acts by

$$\mathrm{E}(f) = f(a)$$

Example: $\mathbb{C}((x))[\ln(x)]$

Consider elements of $\mathbb{C}((x))[\ln(x)]$, i.e. functions of the form

$$f(x) = \sum_{k=-m}^{\infty} \sum_{n=0}^{m} c_{k,n} x^k \ln(x)^n$$

Define the linear operator $\int$ on $\mathbb{C}((x))[\ln(x)]$ recursively by

$$\int x^k \ln(x)^n := \begin{cases} \frac{x^{k+1}}{k+1} & k \neq -1 \wedge n = 0 \\ & \\ & \end{cases}$$

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Then the evaluation defined by $\mathrm{E}(f) := f - \int f'$ acts by

$$\mathrm{E}\left(\sum_{k=-m}^{\infty} \sum_{n=0}^{m} c_{k,n} x^k \ln(x)^n \right) = c_{0,0}$$

Algebraic version of fundamental theorem of calculus

Definition of a generalized integro-differential algebra

Differential ring $(R, ')$, i.e. Leibniz rule

$$(fg)' = f'g + fg' \tag{1}$$

holds, with constants $C := \{c \in R \mid c' = 0\}$,

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Definition of a generalized integro-differential algebra

Differential ring $(R,')$, i.e. Leibniz rule

$$(fg)' = f'g + fg' \qquad (1)$$

holds, with constants $C := \{c \in R \mid c' = 0\}$, equipped with C-linear $\int : R \to R$ and $\mathrm{E} : R \to C$ s.t.

$$\left(\int f\right)' = f \qquad (2)$$

$$\int f' = f - \mathrm{E}(f) \qquad (3)$$

Generalized integro-differential algebra

Basic identities

A trivial identity

For smooth functions

$$\int_a^a dt\, f(t) = 0$$

A trivial identity

For smooth functions

$$\int_a^a dt\, f(t) = 0$$

Algebraic analog

1. Replace f by $\int f$ in $\mathrm{E}(f) = f - \int f'$

$$\mathrm{E}(\textstyle\int f) = \int f - \int (\int f)'$$

2. Exploit $(\int f)' = f$

$$\mathrm{E}(\textstyle\int f) = \int f - \int f = 0$$

Integration by parts

For smooth functions

$$\int_a^x dt\, f(t)g'(t) = f(x)g(x) - f(a)g(a) - \int_a^x dt\, f'(t)g(t)$$

Integration by parts

For smooth functions

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Algebraic analog

1. Exploit Leibniz rule

$$\textstyle\int (fg)' = \int f'g + \int fg'$$

2. Alternatively, replace f by fg in $\int f' = f - \mathrm{E}(f)$

$$\textstyle\int (fg)' = fg - \mathrm{E}(fg)$$

3. Combine to obtain integration by parts

$$\textstyle\int fg' = fg - \mathrm{E}(fg) - \int f'g$$

Taylor's theorem (first version)

For smooth functions

$$
\begin{aligned}
f(x) &= f(a) + \int_a^x dt\, f'(a) + \cdots + \int_a^x dt_1 \ldots \int_a^{t_{n-1}} dt_n\, f^{(n)}(a) + R_n \\
R_n &= \int_a^x dt_1 \ldots \int_a^{t_n} dt_{n+1}\, f^{(n+1)}(t_{n+1})
\end{aligned}
$$

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Algebraic analog

Iterate $f = \mathrm{E}(f) + \int f'$

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Algebraic analog

Iterate $f = \mathrm{E}(f) + \int f'$

$$
\begin{aligned}
f &= \mathrm{E}(f) + \int {\color{red} f'} \\
&= \mathrm{E}(f) + \int \mathrm{E}(f') + \int \int f''
\end{aligned}
$$

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$$\begin{aligned} f &= \mathrm{E}(f) + \textstyle\int f' \\ &= \mathrm{E}(f) + \textstyle\int \mathrm{E}(f') + \int\int f'' \\ &\vdots \\ &= \mathrm{E}(f) + \textstyle\int \mathrm{E}(f') + \cdots + \int^n \mathrm{E}(f^{(n)}) + \int^{n+1} f^{(n+1)} \end{aligned}$$

Nested integrals

Generalized shuffle relations

Base case of shuffling

For smooth functions

$$\left(\int_a^x dt\, f_1(t)\right)\left(\int_a^x dt\, f_2(t)\right) = \int_a^x dt\, f_1(t) \int_a^t du\, f_2(u) + \int_a^x dt\, f_2(t) \int_a^t du\, f_1(u)$$

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Algebraic analog

1. In IBP $\int fg' = fg - \mathrm{E}(fg) - \int f'g$ replace f and g by $\int f_1$ and $\int f_2$ to obtain

$$\int(\textstyle\int f_1)(\int f_2)' = (\int f_1)(\int f_2) - \mathrm{E}((\int f_1)(\int f_2)) - \int(\int f_1)'(\int f_2)$$

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$$(\int f_1)(\int f_2) = \int f_1 \int f_2 + \int f_2 \int f_1 + \mathrm{E}((\int f_1)(\int f_2))$$

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$$(\int f_1)(\int f_2) = \int f_1 \int f_2 + \int f_2 \int f_1 + \mathrm{E}((\int f_1)(\int f_2))$$

Example revisited

Recall:

For $f_1 = \frac{1}{x^2}$ and $f_2 = \frac{1}{1-x}$ we had

$$(\textstyle\int f_1)(\int f_2) = \int f_1 \int f_2 + \int f_2 \int f_1 - 1$$

Recall: $\mathbb{C}((x))[\ln(x)]$

$$\mathrm{E}\left(\sum_{k=-m}^{\infty} \sum_{n=0}^{m} c_{k,n} x^k \ln(x)^n\right) = c_{0,0}$$

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$$\mathrm{E}\left(\sum_{k=-m}^{\infty} \sum_{n=0}^{m} c_{k,n} x^k \ln(x)^n\right) = c_{0,0}$$

$$\mathrm{E}\left(\frac{\ln(1-x)}{x}\right) = \mathrm{E}\left(\sum_{k=0}^{\infty} -\frac{x^k}{k+1}\right) = -1$$

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Products of nested integrals

Notation

- Denote nested integrals $\int a_1 \int a_2 \dots \int a_n$ by tuples $a = (a_1, \dots, a_m)$ of integrands
- Denote subtuples by $a_i^j = (a_i, \dots, a_j)$

Products of nested integrals

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Generalized shuffle product

$f = (f_1, \dots, f_m)$, $g = (g_1, \dots, g_n)$

$$f \odot g = f \sqcup g +$$

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Generalized shuffle product

$f = (f_1, \dots, f_m)$, $g = (g_1, \dots, g_n)$

$$f \odot g = f \sqcup g + \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} \qquad\qquad (f_1^i \sqcup g_1^j)$$

Products of nested integrals

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Generalized shuffle product

$f = (f_1, \dots, f_m)$, $g = (g_1, \dots, g_n)$

$$f \odot g = f \sqcup g + \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} \mathrm{E}(f_{i+1}^m \odot g_{j+1}^n)(f_1^i \sqcup g_1^j)$$

Nested integrals

Taylor's theorem

Taylor's theorem: towards a more explicit formula

Recall: first version

$$f = \sum_{k=0}^{n} \mathrm{E}(f^{(k)}) \int^{k} 1 + \int^{n+1} f^{(n+1)}$$

Goal

Simplify iterated integrals $\int^{k} 1$ and $\int^{n+1} f^{(n+1)}$

Iterated integrals of 1

For $n \in \mathbb{N}$ we define $x_n := \int^{n} 1$ (i.e. $x_1 = \int 1$, $x_n = \int x_{n-1}$)

Reducing multiple integrals

Assumption

We assume $\mathrm{E}(x_m x_n) = 0$ for $m + n \geq 1$, then $x_n = \frac{x_1^n}{n!}$

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Reduce double integrals

$$(\textstyle\int 1)(\int f) = \int 1 \int f + \int f \int 1 + \mathrm{E}((\int 1)(\int f))$$

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We assume $\mathrm{E}(x_m x_n) = 0$ for $m + n \geq 1$, then $x_n = \frac{x_1^n}{n!}$

Reduce double integrals

$$x_1 \int f = \int \int f + \int x_1 f + \mathrm{E}(x_1 \int f)$$

Reducing multiple integrals

Assumption

We assume $\mathrm{E}(x_m x_n) = 0$ for $m + n \geq 1$, then $x_n = \frac{x_1^n}{n!}$

Reduce double integrals

$$\int \int f = x_1 \int f - \int x_1 f - \mathrm{E}(x_1 \int f)$$

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Iterate

$$\int^{(n+1)} f = \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!(n-k)!} x_1^k \int x_1^{n-k} f - \\ - \sum_{k=0}^{n-1} \sum_{j=1}^{n-k} \frac{(-1)^{n-k-j} \mathrm{E}(x_1^j \int x_1^{n-k-j} f)}{k!j!(n-k-j)!} x_1^k$$

Taylor's theorem

For smooth functions

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k + \int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\,dt$$

Algebraic analog (assuming $\mathrm{E}(x_m x_n) = 0$ for $m + n \geq 1$)

$$\begin{aligned} f &= \sum_{k=0}^{n} \frac{\mathrm{E}(f^{(k)})}{k!} x_1^k + \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!(n-k)!} x_1^k \int x_1^{n-k} f^{(n+1)} \\ &\quad - \sum_{k=0}^{n-1} \sum_{j=1}^{n-k} \frac{(-1)^{n-k-j} \mathrm{E}(x_1^j \int x_1^{n-k-j} f^{(n+1)})}{k! j! (n-k-j)!} x_1^k \end{aligned}$$

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For smooth functions

$$\sum_{k=0}^{n-1} \frac{(x-a)^k}{k!} \left[\int_a^x \frac{(x-t)^{n-k} - (a-t)^{n-k}}{(n-k)!} f^{(n+1)}(t)dt \right]_{x=a} = 0$$

Example: $\mathbb{C}((x))[\ln(x)]$, $n = 1$

$$f = \mathrm{E}(f) + \mathrm{E}(f')x + x\int f'' - \int xf'' - \mathrm{E}(x\int f'')$$

$f = \frac{(x+3)^2}{x} + 4\ln(x)$:

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$$f = 6 + x + \left(4 - \frac{9}{x}\right)$$

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$$\begin{aligned} f &= 6 + x + \left(4 - \frac{9}{x}\right) - \left(-\frac{18}{x} - 4\ln(x)\right) - 4 \\ &= 6 + x + \left(\frac{9}{x} + 4\ln(x)\right) \end{aligned}$$

Summary

Generalized integro-differential algebra

Rely only on Leibniz rule and fundamental theorem of calculus:

$$\begin{aligned} (fg)' &= f'g + fg' \\ (\textstyle\int f)' &= f \\ \textstyle\int f' &= f - \mathrm{E}(f) \end{aligned}$$

Generalize standard formulae to singular functions

- Additional terms of lower depth in shuffle relations

$$f \odot g = f \sqcup\!\sqcup g + \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} \mathrm{E}(f_{i+1}^m \odot g_{j+1}^n)(f_1^i \sqcup\!\sqcup g_1^j)$$

- Additional terms in remainder term of Taylor's theorem