# MPL - Supplementary User Manual

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# **1** Getting started

MPL is a collection of procedures for the computeralgebra system Maple. It was written and tested with Maple 16. It supports a wide range of computations with homotopy invariant iterated integrals on moduli spaces  $\mathcal{M}_{0,n}$  of curves of genus 0 with n ordered marked points. This class of functions contains the widely used multiple polylogarithms as functions of several variables.

This manual shows how to apply the most important procedures of the program and might be useful for looking up technical details or examples. It is just meant to supplement the detailed introduction given in the article [2]. The main algorithms were presented in [4]. They are based on the mathematical framework elaborated in [6].<sup>1</sup> When using MPL for a scientific publication, please cite (some of) these articles.

The latest version of MPL and this manual are available from the webpage

http://cbogner.com/software/mpl/

The entire program is obtained by downloading a txt-file MPLn\_m.txt, where the integers *n* and *m* indicate the number of the version. For example, the file of MPL version 1.0 is called MPL1\_0.txt and after saving the file in the same directory with your Maple worksheet, the program is started with

<sup>&</sup>lt;sup>1</sup>A very useful introduction to the general concept of iterated integrals and generalizations of polylogarithms can be found in [7]. For an overview of the far-reaching applications of such classes of iterated integrals in particle physics, we recommend [13, 14].

>read("MPL1\_0.txt"):

Before starting with any computations, it is useful to let Maple read a file by which all multiple zeta values up to a certain weight are automatically expressed in terms of a basis. While writing MPL, we have been using the file mzv-1-12.txt provided by Bigotte, Jacob, Oussous, Minh and Petitot for this purpose. The file is available from the webpage

http://www.lifl.fr/~petitot/recherche/MZV/mzv12/ After saving the file in the working directory and calling

>read("mzv-1-12.txt"):

every multiple zeta value up to weight 12 appearing from now on will be expressed in terms of a basis, for example:

>zeta(3,2);  
$$-\frac{11}{2}\zeta(5) + 3\zeta(2)\zeta(3)$$

This will drastically simplify expressions and it is also necessary for automated tests discussed in section 4 to check that certain parts of the program produce the expected results.

As a supplement to this manual, the above webpage also provides a maple worksheet which contains all examples shown below.

# 2 Computing with cubical coordinates

#### 2.1 Differential 1-forms and iterated integrals

In this section, we work with homotopy invariant iterated integrals on  $\mathcal{M}_{0,n}$  with n > 3. Here homotopy invariance implies, that these functions only depend on the end-points of some path. We always consider the origin as one of these end-points. The other point has m = n - 3 coordinates, which the iterated integral depends on as a function. Due to additional conditions with respect to a basepoint, it is completely determined by the differential 1-forms and the order in which one integrates over them. Therefore it is customary to express such an iterated integral by a tensor product of the involved 1-forms  $a_k \otimes a_{k-1} \otimes ... \otimes a_1$  which is often replaced by a notation with squared brackets  $[a_k | a_{k-1} | ... | a_1]$  called bar-notation.

#### bar(...)

The bar-notation is adapted in MPL. We use the reserved word bar to express every iterated integral. For example  $[a_3|a_2|a_1]$  is expressed by >bar(a[3],a[2],a[1]);

and stands for an iterated integral where we integrate over some 1-forms  $a_1, a_2, a_3$  in this ordering (i.e. from right to left in the argument of bar). More generally, iterated integrals are linear combinations of such expressions over  $\mathbb{Q}$ , for example

```
>3*bar(a[2],a[1])+5*bar(b[8])+9;
```

Numerical constants are factored out automatically, for example:

```
>bar(3*a,2*b)-bar(a-2*b,c);
6bar(a,b)-bar(a,c)+2bar(b,c)
>bar(0,c);
0
```

#### BarToLists(expr), ListsToBar(list)

For some computations, the user may find it convenient to bring an expression of bar-terms in the form of a list. This form is also used internally in some algorithms. For expr being a linear combination of words in the bar-notation, the auxiliary procedure BarToLists(expr) returns a list of two minor lists. The first of these lists contains the coefficients of the words and the second list contains the words in the argument of bar(...), as lists. For example

```
>f:=bar(a)+bar(b,c)+99*bar(b,c)-y*bar(5*g,c,b):
>BarToLists(f);
[[1,100,-5y],[[a],[b,c],[g,c,b]]]
```

The command ListsToBar(list) reverses this transformation. It takes such a list of coefficients and words as input and returns the corresponding expression in bar-notation. For example, as continuation of the above:

#### MPLShuffleProduct(expr1, expr2)

The multiplication of two iterated integrals expr1 and expr2 is computed by the well-known shuffle-product, implemented in MPLShuffleProduct. For example:

```
>MPLShuffleProduct (bar (a, b) +3*bar (c) +7, bar (y, z));

3bar(c,y,z)+3bar(y,c,z)+3bar(y,z,c)+bar(a,b,y,z)+bar(a,y,b,z)+bar(a,y,z,b)+bar(y,a,b,z)+bar(y,a,z,b)+bar(y,z,a,b)+7bar(y,z)
```

#### MPLCoproduct (expr)

The deconcatenation co-product  $\Delta$ , defined by

$$\Delta[a_k|a_{k-1}|...|a_1] = 1 \otimes [a_k|a_{k-1}|...|a_1] + [a_k] \otimes [a_{k-1}|...|a_1] + ... + [a_k|a_{k-1}|...|a_1] \otimes 1$$

is implemented in the procedure MPLCoproduct (expr), for example:

>MPLCoproduct (bar(a,b,c)) tens(ONE, bar(a, b, c)) + tens(bar(a), bar(b, c)) + tens(bar(a, b), bar(c)) + tens(bar(a, b, c), ONE))

Here the reserved term ONE stands for the empty word and  $tens(\ldots,\ldots)$  is a formal expression for the tensor-product of two iterated integrals. tens and ONE are mostly defined for internal use and will usually not appear in any results below.

#### MPLCoordinates (letter, n), MPL\_COORDINATES

As a preparation for many applications, it is necessary to declare a set of variables to be the cubical coordinates we want to work with. For a positive integer *n*, the procedure MPLCoordinates (letter, n) declares *n* cubical coordinates by use of the first argument letter for the names of the variables. The list of cubical coordinates defined in this way is stored in the global variable MPL\_COORDINATES until the procedure is called again. For example:

```
>MPLCoordinates(x, 5):
>MPL_COORDINATES;
[x<sub>1</sub>,x<sub>2</sub>,x<sub>3</sub>,x<sub>4</sub>,x<sub>5</sub>]
```

After calling MPLCoordinates, the variables declared in this way are internally recognized to be cubical coordinates and they can be used to construct the corresponding differential 1-forms. For example one has relations like  $d(x_1) \wedge d(x_1) = 0$ :

>d(x[1]) &^ d(x[1]); 0

#### MPLFormsFiber(lifted::boolean), MPLFormsBase(), MPLFormsTotal()

After declaring  $x_1, ..., x_m$  as cubical coordinates, MPL can compute with iterated integrals with differential 1-forms of the following sets (as defined in [4]):

$$\Omega_m = \left\{ \frac{dx_1}{x_1}, \dots, \frac{dx_m}{x_m}, \frac{d\left(\prod_{a \le i \le b} x_i\right)}{\prod_{a \le i \le b} x_i - 1} \text{ for } 1 \le a \le b \le m \right\},\$$

$$\bar{\Omega}_{m}^{F} = \left\{ \frac{dx_{m}}{x_{m}}, \frac{\left(\prod_{a \leq i \leq n-1} x_{i}\right) dx_{m}}{\prod_{a \leq i \leq m} x_{i} - 1} \text{ for } 1 \leq a \leq m \right\},$$

$$\Omega_{m}^{F} = \left\{ \frac{dx_{m}}{x_{m}}, \frac{d\left(\prod_{a \leq i \leq m} x_{i}\right)}{\prod_{a \leq i \leq m} x_{i} - 1} \text{ for } 1 \leq a \leq m \right\}$$
(1)

where clearly  $\Omega_m = \Omega_m^F \cup \Omega_{m-1}$ . In the context discussed in [4, 6] and with respect to a given *n*, it makes sense to speak of these forms as:

- $\Omega_m$ : forms on the total space,
- $\bar{\Omega}_m^F$ : forms on the fiber,
- $\Omega_m^F$ : forms on the lifted fiber,
- $\Omega_{m-1}$ : forms on the base.

Up to signs, these sets can be obtained from the auxiliary procedures MPLFormsTotal(), MPLFormsFiber(false), MPLFormsFiber(true), MPLFormsBase() respectively. For example:

$$\begin{array}{l} > \text{MPLCoordinates}(\mathbf{x}, 3): \\ > \text{MPLFormsTotal();} \\ \left[ \frac{d(x_1)}{x_1}, \frac{d(x_1)}{1-x_1}, \frac{d(x_2)}{x_2}, \frac{x_2d(x_1)+x_1d(x_2)}{1-x_1x_2}, \frac{d(x_2)}{1-x_2}, \frac{d(x_3)}{x_3}, \frac{x_2x_3d(x_1)+x_1x_3d(x_2)+x_1x_2d(x_3)}{1-x_1x_2x_3}, \frac{x_3d(x_2)+x_2d(x_3)}{1-x_2x_3}, \frac{d(x_3)}{1-x_3} \right] \\ > \text{MPLFormsFiber(false);} \\ \left[ \frac{d(x_3)}{x_3}, \frac{x_1x_2d(x_3)}{1-x_1x_2x_3}, \frac{x_2d(x_3)}{1-x_2x_3}, \frac{d(x_3)}{1-x_3} \right] \\ > \text{MPLFormsFiber(true);} \\ \left[ \frac{d(x_3)}{x_3}, \frac{x_2x_3d(x_1)+x_1x_3d(x_2)+x_1x_2d(x_3)}{1-x_1x_2x_3}, \frac{x_3d(x_2)+x_2d(x_3)}{1-x_1x_2x_3}, \frac{d(x_3)}{1-x_3} \right] \\ > \text{MPLFormsBase();} \\ \left[ \frac{d(x_1)}{x_1}, \frac{d(x_1)}{1-x_1}, \frac{d(x_2)}{x_2}, \frac{x_2d(x_1)+x_1d(x_2)}{1-x_1x_2}, \frac{d(x_2)}{1-x_2} \right] \end{array}$$

In the following we will denote the Q-vectorspaces of differential 1-forms, spanned by the bases  $\Omega_m, \bar{\Omega}_m^F, \Omega_m^F$  by  $\mathcal{A}_m, \bar{\mathcal{A}}_m^F, \mathcal{A}_m^F$  respectively. Furthermore, the corresponding Q-vectorspaces of homotopy invariant iterated integrals are denoted by  $V(\Omega_m), V(\bar{\Omega}_m^F), V(\Omega_m^F)$  (see [4, 2]).

#### MPLArnoldEquation (form1, form2)

The above differential 1-forms satisfy the following set of relations due to Arnol'd [1] (also see [4]):

$$\frac{dx_m}{x_m} \wedge \frac{d(x_i...x_m)}{x_i...x_m - 1} = -\sum_{k=i}^{m-1} \frac{dx_k}{x_k} \wedge \frac{d(x_i...x_m)}{x_i...x_m - 1},$$
  
$$\frac{d(x_j...x_m)}{x_j...x_m - 1} \wedge \frac{d(x_i...x_m)}{x_i...x_m - 1} = \frac{d(x_i...x_{j-1})}{x_i...x_{j-1} - 1} \wedge \left(\frac{d(x_i...x_m)}{x_i...x_m - 1} - \frac{d(x_j...x_m)}{x_j...x_m - 1}\right) - \sum_{k=i}^{j-1} \frac{dx_k}{x_k} \wedge \frac{d(x_i...x_m)}{x_i...x_m - 1}$$

for  $1 \le i \le j \le m$ . Note that these equations are of the type

$$\omega_i \wedge \omega_j = \sum_k \alpha_k \wedge \omega_k$$

where the 1-forms  $\omega_i$  are in  $\Omega_m^F$  (the lifted fiber) and the 1-forms  $\alpha_i$  are in  $\Omega_{m-1}$  (the base).

Internally, these relations are extensively used in the computations below. More conveniently, for two given forms form1, form2 on the left-hand side of the above equations (in the sense form1 $\land$ form2) the right-hand side of the Arnol'd equation can be obtained from MPLArnoldEquation (form1, form2). For example for n = 3, the right-hand side of the equation

$$\frac{dx_3}{x_3-1} \wedge \frac{d(x_2x_3)}{x_2x_3-1} = \frac{dx_2}{x_2-1} \wedge \left(\frac{d(x_2x_3)}{x_2x_3-1} - \frac{dx_3}{x_3-1}\right) - \frac{dx_2}{x_2} \wedge \frac{d(x_2x_3)}{x_2x_3-1}$$

is computed  $as^2$ :

>MPLCoordinates (x, 3):  
>MPLArnoldEquation (d(x[3]) / (x[3]-1), d(x[2]\*x[3]) / (x[2]\*x[3]-1));  

$$-\frac{(d(x_2))\&^{\wedge}(d(x_3))}{(1-x_2)(1-x_3)} + \frac{x_2(d(x_2))\&^{\wedge}(d(x_3))}{(1-x_2)(1-x_2x_3)} + \frac{(d(x_2))\&^{\wedge}(d(x_3))}{(1-x_2x_3)}$$

### 2.2 Differentiation

#### MPLd(expr)

Differentiation d with respect to the end-point of the path (w.r.t. which the iterated integral is defined) is simply given by the de-concatenation of the leftmost differential 1-form:

$$d: V(\Omega_m) \rightarrow \mathcal{A}_m \otimes V(\Omega_m),$$
  
$$\sum_{J=(i_1,...,i_k)} c_I[\omega_{i_1}|...|\omega_{i_k}] \mapsto \sum_{J=(i_1,...,i_k)} c_I \omega_{i_1} \otimes [\omega_{i_2}|...|\omega_{i_k}].$$

For example, one computes

$$d\left(\left[\frac{d(x_2x_3)}{1-x_2x_3}|\frac{dx_3}{x_3}\right] - \left[\frac{dx_2}{x_2}|\frac{d(x_2x_3)}{1-x_2x_3}\right]\right) = \frac{d(x_2x_3)}{1-x_2x_3} \otimes \left[\frac{dx_3}{x_3}\right] - \frac{dx_2}{x_2} \otimes \left[\frac{d(x_2x_3)}{1-x_2x_3}\right]$$

by

<sup>&</sup>lt;sup>2</sup>In principle, using the auxiliary procedure GetArnoldRHS(...), these equations can also be obtained in a different output format, where forms of the fiber and the base are explicitly separated. Such a format is used internally.

>MPLCoordinates (x, 3):  
>MPLd (bar ( (x[3]\*d(x[2])+x[2]\*d(x[3])) / (1-x[2]\*x[3]), d(x[3]) / x[3])  
-bar (d(x[2]) / x[2], (x[3]\*d(x[2])+x[2]\*d(x[3])) / (1-x[2]\*x[3])));  
tens 
$$\left(\frac{x_3d(x_2)+x_2d(x_3)}{1-x_2x_3}, bar\left(\frac{dx_3}{x_3}\right)\right) - tens\left(\frac{dx_2}{x_2}, bar\left(\frac{x_3d(x_2)+x_2d(x_3)}{1-x_2x_3}\right)\right)$$

#### MPLTotalConnection(expr)

In [4] we have defined a connection

$$abla : V\left(\bar{\Omega}_{m}^{F}\right) 
ightarrow \mathcal{A}_{m-1} \otimes V\left(\bar{\Omega}_{m}^{F}\right)$$

by use of the Arnol'd equations and a total connection

$$abla_T: V\left(ar\Omega^F_m
ight) o \mathcal{A}_m \otimes V\left(ar\Omega^F_m
ight)$$

by

$$\nabla_T = d - \nabla.$$

For a word in  $\bar{\Omega}_m^F$ , the total connection can be computed with the command MPLTotalConnection. For example, we obtain

$$\nabla_T \left[ \frac{x_2 d\left(x_3\right)}{1 - x_2 x_3} \Big| \frac{dx_3}{x_3} \right] = \frac{d\left(x_2 x_3\right)}{1 - x_2 x_3} \otimes \left[ \frac{dx_3}{x_3} \right] - \frac{dx_2}{x_2} \otimes \left[ \frac{x_2 d\left(x_3\right)}{1 - x_2 x_3} \right]$$

by

>MPLCoordinates(x, 3):  
>MPLTotalConnection(bar((x[2]\*d(x[3])/(1-x[2]\*x[3]),d(x[3])/x[3]));  
tens
$$\left(\frac{x_3d(x_2)+x_2d(x_3)}{1-x_2x_3}, bar\left(\frac{dx_3}{x_3}\right)\right) - tens\left(\frac{dx_2}{x_2}, bar\left(\frac{x_2d(x_3)}{1-x_2x_3}\right)\right)$$

#### 2.3 The symbol map and the unshuffle map

#### MPLSymbolMap(expr)

It is implied by a theorem of Chen [11] that an iterated integral with differential 1-forms in our framework is homotopy invariant if and only if the corresponding word of 1-forms satisfies a so-called integrability condition. These words are called integrable. Every word in  $\bar{\mathcal{A}}_m^F$  is integrable, but not every word in  $\mathcal{A}_m$ . The symbol map, as constructed in [3, 4], maps from integrable words in  $\bar{\mathcal{A}}_m^F$  to integrable words in  $\mathcal{A}_m$ :

$$\Psi: V\left(\bar{\Omega}_{m}^{F}\right) \to V\left(\Omega_{m}\right).$$

For example we compute

$$\Psi\left(\left[\frac{x_2d(x_3)}{1-x_2x_3}|\frac{dx_3}{x_3}\right]\right) = \left[\frac{d(x_2x_3)}{1-x_2x_3}|\frac{dx_3}{x_3}\right] - \left[\frac{d(x_2)}{x_2}|\frac{d(x_2x_3)}{1-x_2x_3}\right]$$
(2)

by

>MPLCoordinates(x, 3): >MPLSymbolMap(bar((x[2]\*d(x[3]))/(1-x[2]\*x[3]),d(x[3])/x[3]));  $bar\left(\frac{x_3d(x_2)+x_2d(x_3)}{1-x_2x_3},\frac{dx_3}{x_3}\right) - bar\left(\frac{d(x_2)}{x_2},\frac{x_3d(x_2)+x_2d(x_3)}{1-x_2x_3}\right)$ 

The symbol map is the unique linear map which satisfies

$$(id\otimes\Psi)\circ\nabla_T=d\circ\Psi.$$

Let us check this equation for the above example. The left-hand side of the equation is obtained by

>f:=bar(x[2]\*d(x[3])/(1-x[2]\*x[3]), d(x[3])/x[3]):

>evalindets(MPLTotalConnection(f), 'specfunc(anything, tens)', proc (h) options
operator, arrow; subsop(2 = MPLSymbolMap(op(2,h)),h) end proc);

Note that this command at first computes a total connection of the function f as a linear combination of terms tens(...). Then it replaces the second argument of each tens(...) by the image of this argument under the symbol map.

The right-hand side of the above equation is obtained by

>MPLd(MPLSymbolMap(f));

For both sides we obtain

$$tens\left(\frac{x_{3}d(x_{2})+x_{2}d(x_{3})}{1-x_{2}x_{3}}, bar\left(\frac{dx_{3}}{x_{3}}\right)\right) - tens\left(\frac{dx_{2}}{x_{2}}, bar\left(\frac{x_{3}d(x_{2})+x_{2}d(x_{3})}{1-x_{2}x_{3}}\right)\right)$$

Note that this was already the result of the first example in section 2.2, as we used the function in eq. 2 as input there.

#### MPLBasis(letter,m,w)

With the help of the symbol map, the command MPLBasis (letter, m, w) constructs a basis for the vectorspace of integrable words (or homotopy invariant iterated integrals ) up to length w in the alphabet  $\Omega_m$ .

For example the basis of all integrable words up to length 2 in  $\Omega_2$  with variables  $y_1, y_2$  is obtained by

>MPLBasis(y,2,2);

$$\begin{bmatrix} \left[ bar\left(\frac{d(y_{2})}{y_{2}}\right), bar\left(\frac{d(y_{2})}{1-y_{2}}\right), bar\left(\frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right), bar\left(\frac{d(y_{1})}{y_{1}}\right), bar\left(\frac{d(y_{1})}{1-y_{1}}\right) \end{bmatrix}, \\ bar\left(\frac{d(y_{2})}{y_{2}}, \frac{d(y_{2})}{y_{2}}\right), bar\left(\frac{d(y_{2})}{y_{2}}, \frac{d(y_{2})}{1-y_{2}}\right), bar\left(\frac{d(y_{2})}{1-y_{2}}, \frac{d(y_{2})}{y_{2}}\right), \\ bar\left(\frac{d(y_{2})}{y_{2}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right) + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right), \\ bar\left(\frac{d(y_{2})}{y_{2}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}, \frac{d(y_{2})}{y_{2}}\right) - bar\left(\frac{d(y_{1})}{y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right), bar\left(\frac{d(y_{1})}{y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right), \\ bar\left(\frac{d(y_{2})}{y_{2}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right) - bar\left(\frac{d(y_{1})}{1-y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right) + bar\left(\frac{d(y_{1})}{1-y_{1}y_{2}}, \frac{d(y_{2})}{1-y_{2}}\right) \\ - bar\left(\frac{d(y_{1})}{y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right), bar\left(\frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}, \frac{d(y_{2})}{1-y_{2}}\right) \\ + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right) - bar\left(\frac{d(y_{1})}{1-y_{1}y_{2}}, \frac{d(y_{2})}{1-y_{2}}\right) \\ + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{y_{2}}\right) + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{y_{1}}\right), bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{y_{1}}\right) \\ + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{2})}{y_{2}}\right) + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{y_{1}}\right), bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{2})}{1-y_{1}y_{2}}\right) + bar\left(\frac{d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right) \\ + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{2})}{y_{2}}\right) + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{y_{2}d(y_{1})+y_{1}d(y_{2})}{y_{2}}\right) + bar\left(\frac{d(y_{1})+y_{1}d(y_{2})}{1-y_{1}y_{2}}\right) \\ + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{y_{1}}\right), bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{1-y_{1}y_{2}}\right) + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{1-y_{1}y_{2}}\right) \\ + bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{y_{1}}\right), bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{1-y_{1}}\right), bar\left(\frac{d(y_{1})}{y_{1}}, \frac{d(y_{1})}{1-y_{1}}\right) \\ +$$

The output of this command is always a list of *w* lists, where for  $k \le w$  the *k*-th list contains the words of length *k*.

### MPLUnshuffle(expr,var)

The unshuffle map

$$\Phi: V\left(\Omega_{m}\right) \to V\left(\Omega_{m-1}\right) \otimes V\left(\bar{\Omega}_{m}^{F}\right)$$
(3)

as defined in [4] is the inverse of the map

$$\mu(id \otimes \Psi) : V(\Omega_{m-1}) \otimes V(\bar{\Omega}_m^F) \to V(\Omega_m)$$
(4)

and can be used recursively to decompose iterated integrals in  $V(\Omega_m)$  into products of hyperlogarithms in  $V(\bar{\Omega}_k^F)$  with  $1 \le k \le m$ . The command MPLUnshuffle (expr, var) applies the unshuffle map  $\Phi$  to a function expr in  $V(\Omega_m)$  where the second argument var is the last of the cubical coordinates  $x_m$ . The hyperlogarithm in the right-hand part of the resulting tensor-product is a function of this variable (if expr depends on this variable).

In order to give a non-trivial example, let us at first construct a function in  $V(\Omega_3)$  as follows. Consider the hyperlogarithms

$$f_{1} = bar\left(\frac{x_{1}d(x_{2})}{1-x_{1}x_{2}}\right) \in V\left(\bar{\Omega}_{2}^{F}\right),$$
  

$$f_{2} = bar\left(\frac{x_{2}d(x_{3})}{1-x_{2}x_{3}}, \frac{d(x_{3})}{x_{3}}\right) \in V\left(\bar{\Omega}_{3}^{F}\right)$$

We apply the map of eq. 4 twice. At first we compute

$$g_1 = \mu(id \otimes \Psi) (1 \otimes f_1) = \Psi(f_1) = bar\left(\frac{d(x_1x_2)}{1 - x_1x_2}\right) \in V(\Omega_2).$$

Let us furthermore construct the function (or integrable word)  $g_{12}$  as

$$\begin{split} g_{12} &= \mu(id \otimes \Psi)(g_1 \otimes f_2) \\ &= \tilde{f}_1 \, \mathrm{m} \Psi(f_2) \\ &= bar\left(\frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}, \frac{d(x_3)}{x_3}, \frac{x_2d(x_1) + x_1d(x_2)}{1 - x_1x_2}\right) \\ &+ bar\left(\frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}, \frac{x_2d(x_1) + x_1d(x_2)}{1 - x_1x_2}, \frac{d(x_3)}{x_3}\right) \\ &+ bar\left(\frac{x_2d(x_1) + x_1d(x_2)}{1 - x_1x_2}, \frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}, \frac{d(x_3)}{x_3}\right) \\ &- bar\left(\frac{d(x_2)}{x_2}, \frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}, \frac{x_2d(x_1) + x_1d(x_2)}{1 - x_1x_2}\right) \\ &- bar\left(\frac{d(x_2)}{x_2}, \frac{x_2d(x_1) + x_1d(x_2)}{1 - x_1x_2}, \frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}\right) \\ &- bar\left(\frac{x_2d(x_1) + x_1d(x_2)}{1 - x_1x_2}, \frac{d(x_2)}{x_2}, \frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}\right)\right) \end{split}$$

This construction is easily obtained by use of the above procedures MPLShuffleProduct and MPLSymbolMap:

```
>f1:=bar(x[1]*d(x[2])/(1-x[1]*x[2])):
>f2:=bar(x[2]*d(x[3])/(1-x[2]*x[3]), d(x[3])/x[3]):
>MPLCoordinates(x,2):
```

```
>g1:=MPLSymbolMap(f1):
>MPLCoordinates(x,3):
>g12:=MPLShuffleProduct(g1,MPLSymbolMap(f2)):
```

By construction, the function  $g_{12}$  is in  $V(\Omega_3)$  and it is easy to check, that it is in the basis of this vectorspace obtained by the command MPLBasis:

Now let us reverse this construction by use of the unshuffle map. By computing

>MPLUnshuffle(g12,x[3]);  
tens 
$$\left( bar\left(\frac{d(x_1x_2)}{1-x_1x_2}\right), bar\left(\frac{x_2d(x_3)}{1-x_2x_3}, \frac{d(x_3)}{x_3}\right) \right)$$

we clearly obtain the expected

$$\Phi(g_{12})=g_1\otimes f_2.$$

Furthermore computing

>MPLUnshuffle(g1, x[2]); tens  $\left(ONE, bar\left(\frac{x_1d(x_2)}{1-x_1x_2}\right)\right)$ we confirm the expected

$$\Phi(g_1)=1\otimes f_1.$$

### 2.4 Integration over cubical coordinates

#### MPLPrimitive(a, f, w)

The procedure MPLPrimitive (a, f, w) computes the primitive  $\int a \otimes f \in V(\Omega_m)$  of a function  $f \in V(\Omega_m)$  of maximal weight *w* with respect to the differential 1-form  $a \in \bar{\mathcal{A}}_m^F$ . For example let us compute  $\int a \otimes f$  for

$$a = \frac{x_2 d\left(x_3\right)}{1 - x_2 x_3}$$

and

$$f = bar\left(\frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}, \frac{dx_3}{x_3}\right) - bar\left(\frac{d(x_2)}{x_2}, \frac{x_3d(x_2) + x_2d(x_3)}{1 - x_2x_3}\right) + 5bar\left(\frac{d(x_2)}{x_2}\right) + 99.$$

The words in *f* are at most of length w = 2. We compute:

>MPLCoordinates(x,3): >a:=x[2]\*d(x[3])/(1-x[2]\*x[3]): >f:=bar((x[3]\*d(x[2])+x[2]\*d(x[3]))/(1-x[2]\*x[3]), d(x[3])/x[3]) -bar(d(x[2])/x[2], (x[3]\*d(x[2])+x[2]\*d(x[3]))/(1-x[2]\*x[3])) +5\*bar(d(x[2])/x[2])+99: >MPLPrimitive(a, f, 2);

$$bar\left(\frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}, \frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}, \frac{dx_{3}}{x_{3}}\right)$$
  
-bar $\left(\frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}, \frac{d(x_{2})}{x_{2}}, \frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}\right)$   
+5bar $\left(\frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}, \frac{d(x_{2})}{x_{2}}\right)$  +99bar $\left(\frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}\right)$   
+5bar $\left(\frac{d(x_{2})}{x_{2}}, \frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}\right)$   
-bar $\left(\frac{d(x_{2})}{x_{2}}, \frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}, \frac{x_{3}d(x_{2}) + x_{2}d(x_{3})}{1 - x_{2}x_{3}}\right)$ 

#### MPLLimit(f,x,u)

The procedure MPLLimit (expr, var, limit) returns the limit of a function f in  $V(\Omega_m)$  at x=u where x is one of the *m* cubical coordinates and u is either 0 or 1. As an example we consider m = 3 and

$$f = \Psi\left(\left[\frac{x_1 x_2 d(x_3)}{1 - x_1 x_2 x_3}, \frac{x_2 d(x_3)}{1 - x_2 x_3}\right]\right)$$
  
=  $\left[\frac{d(x_1 x_2 x_3)}{1 - x_1 x_2 x_3} - \frac{d(x_1)}{1 - x_1}, \frac{d(x_2 x_3)}{1 - x_2 x_3}\right] + \left[\frac{d(x_1)}{1 - x_1} + \frac{d(x_1)}{x_1}, \frac{d(x_1 x_2 x_3)}{1 - x_1 x_2 x_3}\right]$  (5)

and we compute the limits  $g_1 = \lim_{x_3 \to 1} f$ ,  $g_2 = \lim_{x_2 \to 1} g_1$ ,  $g_3 = \lim_{x_1 \to 1} g_2$  as follows:

$$g1: = bar\left(\frac{x_2d(x_1) + x_1d(x_2)}{-1 + x_1x_2}, \frac{d(x_2)}{-1 + x_2}\right) - bar\left(\frac{d(x_1)}{-1 + x_1}, \frac{d(x_2)}{-1 + x_2}\right) + bar\left(\frac{d(x_1)}{-1 + x_1}, \frac{x_2d(x_1) + x_1d(x_2)}{-1 + x_1x_2}\right) - bar\left(\frac{d(x_1)}{x_1}, \frac{x_2d(x_1) + x_1d(x_2)}{-1 + x_1x_2}\right)$$

>g2:=simplify(MPLLimit(g1,x[2],1));

$$g2 := -bar\left(\frac{d(x_1)}{x_1}, \frac{d(x_1)}{-1+x_1}\right) + bar\left(\frac{d(x_1)}{-1+x_1}, \frac{d(x_1)}{-1+x_1}\right)$$

>g3:=simplify(MPLLimit(g2,x[1],1));

 $g3 := \zeta(2)$ 

There is a little subtlety we have to take care of, if we compute limits not starting with the last cubical coordinate  $x_m$ . For example, let us compute  $g_4 = \lim_{x_2 \to 1} f$  by

>g4:=simplify(MPLLimit(f,x[2],1));  

$$bar\left(\frac{x_3d(x_1)+x_1d(x_3)}{-1+x_1x_3},\frac{d(x_3)}{-1+x_3}\right) - bar\left(\frac{d(x_1)}{x_1},\frac{x_3d(x_1)+x_1d(x_3)}{-1+x_1x_3}\right) + bar\left(\frac{d(x_1)}{-1+x_1},\frac{x_3d(x_1)+x_1d(x_3)}{-1+x_1x_3}\right) - bar\left(\frac{d(x_1)}{-1+x_1},\frac{d(x_3)}{-1+x_3}\right)$$

In this result, the differential 1-form  $\frac{x_3d(x_1)+x_1d(x_3)}{-1+x_1x_3}$  does not belong to any  $\Omega_m$  defined in eq. 1, because it involves the product  $x_1x_3$  of non-consecutive cobical coordinates. However, we can simply replace every  $x_3$  by  $x_2$  in this result, for example by

Now in  $g_5$  every 1-form belongs to  $\Omega_2$  and the result is recognized as a function of  $V(\Omega_2)$ . (It is easy to check the integrability.) In general, after taking a limit with respect to a variable  $x_k$  with  $1 \le k < m$ , we have to re-name the coordinates by  $(x_{k+1}, ..., x_m) \mapsto (x_k, ..., x_{m-1})$ .

#### MPLMultipleLimit(expr,list)

Based on the previous procedure, the procedure MPLMultipleLimit (f, L) computes several limits of a function f of  $V(\Omega_m)$  successively. Here L is a list of the type  $[x_{\sigma(1)} = u_1, x_{\sigma(2)} = u_2, ..., x_{\sigma(k)} = u_k]$ for  $1 \le k \le m$ ,  $\sigma$  a permutation on some subset of  $\{1, ..., m\}$  and all  $u_i \in \{0, 1\}$ . This list fixes the limits and also the order in which they are computed. The above command returns

$$\lim_{x_{\sigma(k)\to u_k}}\dots\lim_{x_{\sigma(1)\to u_1}}f.$$

As an example, let us again consider the function f as defined in eq. 5. Then we obtain the above results for  $g_1, g_2, g_3$  by

```
>g1:=simplify(MPLMultipleLimit(f,[x[3]=1])):
>g2:=simplify(MPLMultipleLimit(f,[x[3]=1,x[2]=1])):
>g3:=simplify(MPLMultipleLimit(f,[x[3]=1,x[2]=1,x[1]=1])):
```

It is briefly mentioned in [2] and discussed in more detail in [4] and [6] that the order of such consecutive limits is crucial. For example, we have obtained  $g_3 = \zeta(2)$ , but permuting the order of the last two limits, we compute

```
>MPLMultipleLimit(f, [x[3]=1, x[1]=1, x[2]=1]);
0
```

Note that in a function of  $V(\Omega_m)$  the terms with weight greater than zero are defined to vanish at the origin of the space of cubical coordinates. Therefore, if we choose the above list L to be  $[x_{\sigma(1)} = 0, x_{\sigma(2)} = 0, ..., x_{\sigma(m)} = 0]$ , the procedure MPLMultipleLimit returns the value that remains after by replacing every bar(...) by zero in  $f \in V(\Omega_m)$ .

#### MPLCubicalIntegrate(f,var,n)

MPL can compute multiple integrals of the type

$$I = \int_0^1 dx_m \frac{q}{\prod_i p_i^{a_i}} f \tag{6}$$

where where  $f \in V(\Omega_m)$ , q is a polynomial in  $x_m$ , the  $a_i \in \mathbb{N}$  and the  $p_i$  are in  $\{x_m, 1 - x_m, ..., 1 - x_1 \cdots x_m\}$ . For f being an integrand of this type, the procedure MPLCubicalIntegrate (f, var, n) successively integrates over  $x_m, x_{m-1}, ..., x_{m-n+1}$  in this order. The first argument of the procedure is the integrand in bar-notation, the second argument is the variable to be first integrated out (i.e.  $x_m$  in the notation chosen here) and n is the number of integrations. As an example, we consider the integrand

$$f = \frac{u_1^3 (1 - u_1) u_2^4 (1 - u_2) u_3^3 (1 - u_3) u_4^2 (1 - u_4)^2}{(1 - u_1 u_2 u_3)^2 (1 - u_2 u_3 u_4)^2 (1 - u_1 u_2 u_3 u_4)^2 (1 - u_1 u_2 u_3 u_4)^2}$$

We integrate out all four cubical coordinates  $u_4, u_3, u_2, u_1$  by

>f:=u[1]^3\*(1-u[1])\*u[2]^4\*(1-u[2])\*u[3]^3\*(1-u[3]) \*u[4]^2\*(1-u[4])^2/((1-u[1]\*u[2]\*u[3])^2\*(1-u[4]\*u[2]) \*u[3])^2\*(1-u[4]\*u[1]\*u[2]\*u[3])^2\*(1-u[1]\*u[2])): >MPLCubicalIntegrate(f,u[4],4); (5/3)\*Zeta(3)+(26/9)\*Zeta(2)-(17/5)\*Zeta(2)<sup>2</sup>+22/9 So we obtain

$$\prod_{i=1}^{4} \left( \int_{0}^{1} dx_{i} \right) f = \frac{5}{3} \zeta(3) + \frac{26}{9} \zeta(2) - \frac{17}{5} (\zeta(2))^{2} + \frac{22}{9}.$$

Intermediate results are too long to be shown here, but can easily be obtained by choosing the last argument of MPLCubicalIntegrate smaller than 4. Note that here the explicit use of MPLCoordinates is not necessary (because it is called internally by MPLCubicalIntegrate).

MPLCubicalIntegrate already serves for the analytical computation of a large class of integrals and further example applications are shown in [2, 4]. In some cases, the procedure may even be useful for the computation of Feynman integrals. However, in the case of Feynman integrals, the denominators of the integrand usually involve more complicated polynomials than allowed here. Therefore, appropriate changes of variables are necessary, to express the latter in terms of cubical coordinates. These are subject of the following section.

# **3** Computing Feynman integrals

In this section, we consider integrals of the type

$$I_F = \int_0^\infty d\alpha_j \frac{\prod_{Q_i \in Q} Q_i^{\delta_i} L_w(\alpha_j)}{\prod_{P_i \in \mathcal{P}_F} P_i^{\beta_i}}$$
(7)

where  $Q, \mathcal{P} \subset \mathbb{Q} [\alpha_1, ..., \alpha_j, ..., \alpha_N]$  are sets of irreducible polynomials, all  $\delta_i, \beta_i \in \mathbb{N} \cup \{0\}$  and  $L_w(\alpha_N)$  is a hyperlogarithm, given by a word *w* in differential 1-forms in

$$\Omega_F = \left\{ \frac{d\alpha_j}{\alpha_j}, \frac{d\alpha_j}{\alpha_j - \rho_i} \text{ where } \rho_i = -\frac{P_i|_{\alpha_j=0}}{\frac{\partial P_i}{\partial \alpha_j}}, P_i \in \mathcal{P} \right\}.$$

Such integrals arise in the computation of Feynman integrals, possibly also in other contexts. In [4, 2] we have discussed the conditions under which we can compute such integrals with MPL. Here let us just recall briefly, that the integrals have to be *finite* and *unramified* and the set  $\mathcal{P}$  has to be *linearly reducible* and *properly ordered*. We assume, that the user has already expressed a divergent Feynman integral in terms of finite integrals of this type, possibly by use of techniques cited and partly demonstrated in [4, 2]. All remaining mentioned conditions can be explicitly checked by procedures of MPL, as demonstrated below.

#### **3.1** Setting up a simple example

As a simple standard example, let us consider the massless, off-shell one-loop traingle graph throughout this section. The corresponding integral is finite. (More involved examples are discussed in [4, 2]). The two Symanzik polynomials (see e.g. [5]) of this graph are

$$\mathcal{U} = x_1 + x_2 + x_3,$$
  
$$\mathcal{F} = -x_1 x_2 p_3^2 - x_2 x_3 p_1^2 - x_1 x_3 p_2^2,$$

where the  $x_i$  are the Feynman (or Schwinger, or alpha) parameters and the  $p_i$  are the incoming momenta. In section 4 of [2], we suggested to express the kinematical dependences in terms of variables, which can be treated as additional Feynman parameters, which are not integrated out. In this sense, we define the set of generalized Feynman parameters  $\{x_1, x_2, x_3, x_4, x_5\}$  where  $x_4$  and  $x_5$  satisfy

$$\frac{p_3^2}{p_2^2} = x_4 x_5$$
 and  $\frac{p_1^2}{p_2^2} = (1 - x_4)(1 - x_5).$ 

(C.f. [10].) We consider the kinematical region where  $0 \le x_4$ ,  $0 \le x_5$ . (For a different kinematical region, we recommend to change the definition of  $x_4$  and  $x_5$  accordingly, such that the region is still given by  $0 \le x_4$ ,  $0 \le x_5$ , if possible.) Using these variables, we define the auxiliary polynomial

$$\tilde{\mathcal{F}} = -\frac{\mathcal{F}}{p_2^2} = x_1 x_2 x_4 x_5 + x_1 x_3 + x_2 x_3 \left(1 - x_4\right) \left(1 - x_5\right)$$

The corresponding scalar Feynman integral in  $D = 4 - 2\varepsilon$  dimensions (without any scalar products in the numerator or raised propagator-powers) can be defined by

$$I(x_4, x_5, \varepsilon) = \Gamma(1+\varepsilon) \left(-p_2^2\right)^{-1-\varepsilon} I(x_4, x_5, \varepsilon)$$

with

$$I(x_4, x_5, \varepsilon) = \prod_{i=1}^{3} \left( \int_0^\infty dx_i \right) \delta(H) \, \mathcal{U}^{-1+2\varepsilon} \tilde{\mathcal{F}}^{-1-\varepsilon}$$

where *H* is a hyperplane in the integration domain, which we can choose freely according to the Cheng-Wu theorem [12]. We choose  $\delta(1 - x_n)$  where  $x_n$  is our last integration variable. The order of integration variables still has to be chosen such that the mentioned conditions are satisfied.

We expand the integrand in  $\varepsilon$  and obtain

$$I(x_4, x_5, \varepsilon) = I^{(0)}(x_4, x_5) + \varepsilon I^{(0)}(x_4, x_5) + O(\varepsilon^2)$$

with

$$I^{(0)}(x_4, x_5) = \prod_{i=1}^3 \left( \int_0^\infty dx_i \right) \delta(H) \frac{1}{\mathcal{U}\tilde{\mathcal{F}}}, \tag{8}$$

$$I^{(1)}(x_4, x_5) = \prod_{i=1}^{3} \left( \int_0^\infty dx_i \right) \delta(H) \frac{2\ln\left(\mathcal{U}\right) - \ln\left(\tilde{\mathcal{F}}\right)}{\mathcal{U}\tilde{\mathcal{F}}}.$$
(9)

In the following, we compute both of the latter integrals with MPL.

### **3.2** Checking the conditions

Before the computation of any integral over Feynman parameters with MPL, we recommend to check, whether the mentioned conditions are satisfied. We assume, that the user already has checked the finiteness of the integral. The following procedure can be used to check linear reducibility.

#### MPLPolynomialReduction(S,L[1..n],L), COMPATIBILITY\_GRAPH

The command MPLPolynomialReduction (S, L[1..n], L) returns the reduction of a set S of polynomials with respect to n integration variables (i.e. Feynman parameters) L[1..n], which are the first n entries in the list L of all variables of the problem (i.e. generalized Feynman parameters, given by the Feynman parameters and kinematical invariants). If a global variable COMPATIBILITY\_GRAPH=true, the reduction is computed regarding compatibilities among the polynomials as introduced in [9]. The program uses the version of such compatibilities defined in [14]. If COMPATIBILITY\_GRAPH=false, the procedure returns a Fubini-reduction as introduced in [8]. See [2] for the details.

In order to interpret the output of this procedure, it is instructive to look at our example of the triangle graph. For the computation of  $I^{(0)}(x_4, x_5)$  and  $I^{(1)}(x_4, x_5)$  we clearly should compute the reduction of  $S = \{\mathcal{U}, \tilde{\mathcal{F}}\}$ . The list of generalized Feynman parameters is  $x_1, x_2, x_3, x_4, x_5$  and the integration variables are the first three elements of this list. Therefore we compute

```
>U:=x[1]+x[2]+x[3]:
>F:=x[1]*x[2]*x[4]*x[5]+x[1]*x[3]+x[2]*x[3]*(1-x[4])*(1-x[5]):
>GenFeyn:=[x[1],x[2],x[3],x[4],x[5]]:
>COMPATIBILITY_GRAPH=true: #This is also the default value.
>MPLPolynomialReduction([U,F],GenFeyn[1..3],GenFeyn);
```

$$[[\{\}, [x_1 + x_2 + x_3, x_1x_2x_4x_5 + x_1x_3 + x_2x_3(1 - x_4)(1 - x_5)], [\{1, 2\}]], \\ [\{x_3\}, [x_1 + x_2 - x_2x_5 - x_4x_2 + x_2x_4x_5, x_1 + x_2, x_1 + x_2 - x_2x_5, x_1 + x_2 - x_4x_2]$$

$$\begin{split} & [\{3,4\},\{1,3\},\{1,4\},\{2,3\},\{2,4\}]], \\ & [\{x_2\},[x_1x_4x_5+x_3-x_3x_5-x_3x_4+x_3x_4x_5,x_1+x_3,-x_3+x_1x_5+x_3x_5,x_1x_4-x_3+x_3x_4], \\ & [\{3,4\},\{1,3\},\{1,4\},\{2,3\},\{2,4\}]], \\ & [\{x_1\},[x_2x_4x_5+x_3,x_2+x_3,-1+x_4,-1+x_5,x_4x_2+x_3,x_3+x_2x_5], \\ & [\{3,4\},\{1,3\},\{1,4\},\{2,3\},\{2,4\},\{3,5\},\{4,5\},\{5,6\},\{1,5\},\{1,6\},\{2,5\},\{2,6\},\{3,6\}]], \\ & [\{x_1,x_2\},[-1+x_5,-1+x_4,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]], \\ & [\{x_1,x_3\},[-1+x_5,-1+x_4,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]], \\ & [\{x_2,x_3\},[-1+x_4,-1+x_5,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]], \\ & [\{x_1,x_2,x_3\},[-1+x_5,-1+x_4,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]], \\ & [\{x_1,x_2,x_3\},[-1+x_5,-1+x_4,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]], \\ & [\{x_1,x_2,x_3\},[-1+x_5,-1+x_4,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]], \\ & [\{x_1,x_2,x_3\},[-1+x_5,-1+x_4,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]], \\ & [\{x_1,x_2,x_3\},[-1+x_5,-1+x_4,x_4-x_5],[\{1,2\},\{1,3\},\{2,3\}]]] \end{split}$$

This reduction is a list of 8 lists, each of which has three entries. The first entry is the set of variables with respect to which the polynomials in S were reduced. The second entry is the list of resulting polynomials at this stage. (In the language of [9, 14], these are the vertices of the compatibility graph.) This list is ordered. With respect to this ordering, the third entry contains all compatible pairs of polynomials (i.e. the edges of the compatibility graph) represented by their numbers with respect to the order in the second entry.

For example let us consider the list in the second line from below:

$$[\{x_2, x_3\}, [-1+x_4, -1+x_5, x_4-x_5], [\{1,2\}, \{1,3\}, \{2,3\}]]$$

According to the first entry, reductions were computed with respect to  $x_2$  and  $x_3$ . Therefore, in the notation of [2], the second entry is the set

$$\tilde{S}^{\{2,3\}} = \{-1 + x_4, -1 + x_5, x_4 - x_5\}$$

and the third entry tells us, that all three polynomials are compatible with each other. If in this entry for example  $\{2,3\}$  would be missing,  $-1 + x_5$  would not be compatible with  $x_4 - x_5$ .

The compatibilities are usually just of internal importance. If they are considered by the algorithm (i.e. if COMPATIBILITY\_GRAPH is true), the reduction usually gives a better upper bound for the polynomials appearing in the integration procedure, than the plain Fubini reduction (COMPATIBILITY\_GRAPH is false). In the output of latter, the third entry of each list is always the complete graph, i.e. it contains all possible pairs. The plain Fubini reduction obtained by

```
>COMPATIBILITY_GRAPH=false:
>MPLPolynomialReduction([U,F],GenFeyn[1..3],GenFeyn);
```

For this simple example, both reductions are exactly the same.

For the user, the important question is, whether the set *S* is linearly reducible and, if yes, which are the allowed orders of integrations. This can information is easily obtained from the reduction, by looking at the first entry of each list. The set *S* is linearly reducible with respect to a particular order  $x_{\sigma(1)}, ..., x_{\sigma(n)}$  of *n* integration variables, given by a permutation  $\sigma$  on  $\{1, ..., n\}$ , if the reduction contains each of the sets  $\{x_{\sigma(1)}\}, \{x_{\sigma(1)}, x_{\sigma(2)}\}, ..., \{x_{\sigma(1)}, ..., x_{\sigma(n)}\}$ .

For example, let us ask, whether  $S = \{\mathcal{U}, \tilde{\mathcal{F}}\}$  is linearly reducible with respect to the order  $x_3, x_1, x_2$ . We see that the above reduction contains lists whose first etries are  $\{x_3\}, \{x_1, x_3\}, \{x_1, x_2, x_3\}$ , so the answer is yes. If for example the list with  $\{x_3\}$  in the first entry would be missing, neither  $x_3, x_1, x_2$  nor  $x_3, x_2, x_1$  would be an allowed order of integration.

#### MPLCheckOrder(reduction, L[1..n], L)

Consider a given polynomial reduction in the form as returned by the previous command (no matter whether compatibilities are regarded or not), and a given ordered list L of generalized Feynman parameters where the first n entries are the integration variables. For this data, the procedure MPLCheckOrder (reduction, L[1..n], L) checks with respect to the order of variables in L, whether the integrand is linearly reducible, whether it is properly ordered at a tangential basepoint (see [2, 4]) and whether all limits which have to be computed in the integration procedure are at 0 or 1.<sup>3</sup> All three conditions are required for an automatic computation of the integral with MPL. If all conditions are satisfied, the procedure returns a sequence of messages, all ending with the phrase "Check OK." If one of the conditions is violated, the procedure returns a corresponding error message. In this case, a fully automated computation of the integral in the order of integrations given by L is not possible with MPL. We recommend to try the command again with a different order of variables in L. In some cases, the problem also may be solved by a different choice of kinematical invariants (see remarks in sections 4.2 and 4.3 of [2]).

Let us apply the procedure in our example of the triangle graph where GenFeyn is again the list of generalized Feynman parameters defined above:

```
>Reduction:=MPLPolynomialReduction([U,F],GenFeyn[1..3],GenFeyn):
>MPLCheckOrder(Reduction,GenFeyn[1..3],GenFeyn);
```

```
Checks for integration over x[1]:
```

"All rho\_i are smaller than zero at the tangential basepoint: Check OK." "Limits in {0, 1}: Check OK."

<sup>&</sup>lt;sup>3</sup>Note that the latter property is implied by the condition of the integrand to be unramified as discussed in [2, 4]. The procedure does not check unramifiedness but it checks the condition directly for the required limits at the tangential basepoint.

Checks for integration over x[2]:

"All rho\_i are smaller than zero at the tangential basepoint: Check OK." "Limits in {0, 1}: Check OK."

Checks for integration over x[3]:

"All rho\_i are smaller than zero at the tangential basepoint: Check OK." "No limits to be computed: Check OK."

If each message ends with "Check OK." and no error message appears, we can use the order given by L to compute the integral by the command discussed below.

As a remark, let us briefly comment on the meaning of these messages and possible error messages. The procedure MPLCheckOrder does the checks in three steps. At first it checks, that the reduction implies linear reducibility with respect to the given order of parameters. If this is not the case, it returns an error message immediatly. Then it goes through each set of polynomials of the reduction, according to the given order of integrations. In order to construct an appropriate change of variables to cubical coordinates, the program assumes the polynomials to be properly ordered at a tangential basepoint (see [2, 4]). This means that there is a certain region in the parameter space, where the *m* polynomials  $P_1, ..., P_m$  relevant at this stage are uniquely ordered by

$$0 > \rho_m > \rho_1 > \rho_2 > \dots > \rho_{m-2} > \rho_{m-1}$$

where  $\rho_i = -\frac{P_i|_{x_N=0}}{\frac{\partial P_i}{\partial x_N}}$  with  $x_N$  being the integration variable at this stage. The procedure checks at first that all  $\rho_i < 0$  in this region. The message "All rho\_i are smaller than zero at the tangential basepoint: Check OK." confirms this to be the case. If it is not the case, the error message will return a polynomial  $P_i$  and the corresponding  $\rho_i$  causing the problem. In a third step the procedure computes certain limits which are required for an integration (see [2, 4] for the details). These limits need return values in  $\{0, 1\}$ , which the above messages confirm. If a limit different from 0 or 1 appears, a corresponding error message is returned, which also gives the change of coordinates causing the problem. The computation of these limits implicitely also checks the uniqueness of the above order among the  $\rho_i$ , as this order is used to set up the change of coordinates. If the order is ambiguous, a corresponding error message is returned. This case is not expected, unless the list of polynomials accidentally contains two equal elements  $P_i = P_j$ ,  $i \neq j$ , which of course should be avoided internally by the program, but might not be completely excluded in the case of very complicated polynomials.

If all checks are OK, we are ready to integrate.

#### **3.3** Integration over Feynman parameters

We assume a finite integral over one or several Feynman parameters from 0 to infinity with an integrand as in eq. 7. If the integral satisfies the mentioned criteria linear reducibility, unramifiedness and properly ordered polynomials for a given order of (generalized) Feynman parameters, it can be computed with the following command:

#### MPLFeynmanIntegrate(integrand, L[1..n], L)

The first argument is the integrand, where all possibly appearing logarithms or hyperlogarithms in the numerator are expressed in bar-notation. (For this purpose, it may be useful to apply the command MPLHlogToBar introduced below). The second and third argument are the same as in the previous commands: L is the list of all generalized Feynman parameters in a chosen order and n is the number of integrations to be computed, i.e. L[1..n] is the list of integration variables in the given order. During the computation, the procedure returns messages indicating, which variable is integrated out at present. In the end it returns the result in terms of hyperlogarithms in bar-notation.

In our example of the triangle graph, let is compute the integrals  $I^{(0)}$  and  $I^{(1)}$  as defined in eqs. 8 and 9. At first we call

>defform(x=0):

to make sure that every x[i] is recognized as a variable and every d(x[i]) as a differential 1-form by Maple. Then we define the integrands according to eqs. 8 and 9:

```
>U:=x[1]+x[2]+x[3]:
>F:=x[1]*x[2]*x[4]*x[5]+x[1]*x[3]+x[2]*x[3]*(1-x[4])*(1-x[5]):
Integrand0:=1/(U*F):
Integrand1:=(2*bar(d(U)/U)-bar(d(F)/F))/(U*F):
```

Note that in the integrand of  $I^{(1)}$  we have expressed the logarithms  $\ln(\mathcal{U})$  and  $\ln(\tilde{\mathcal{F}})$  in barnotation.

As ordered list of generalized Feynman parameters we choose again:

>GenFeyn:=[x[1],x[2],x[3],x[4],x[5]]:

From the tests conducted above, we know, that we can integrate in this order.

Notice that in eqs. 8 and 9 we still have  $\delta(H)$  in the integrand. Now that we know our order of integrations, we choose *H* to be the hyperplane, where the last of the integration variables is equal to 1, so in our case:  $H = 1 - x_3$ . According to this choice, we only integrate over the first two variables  $x_1, x_2$  and then set  $x_3 = 1$ .

In this way, we compute I<sup>(0)</sup> by
>MPLFeynmanIntegrate(Integrand0,GenFeyn[1..2],GenFeyn):
>I0:=normal(subs(x[3]=1,%));
Integration over x[1].
Integration over x[2].

$$I0: = \frac{1}{-x_5 + x_4} \left( -bar\left(\frac{d(x_4)}{x_4}, \frac{d(x_4)}{-1 + x_4}\right) - bar\left(\frac{d(x_4)}{x_4}\right) bar\left(\frac{d(x_5)}{-1 + x_5}\right) + bar\left(\frac{d(x_4)}{-1 + x_4}, \frac{d(x_4)}{x_4}\right) + bar\left(\frac{d(x_5)}{-1 + x_4}\right) bar\left(\frac{d(x_5)}{x_5}\right) + bar\left(\frac{d(x_5)}{x_5}, \frac{d(x_5)}{-1 + x_5}\right) - bar\left(\frac{d(x_5)}{-1 + x_5}, \frac{d(x_5)}{x_5}\right) \right)$$

Note that the result of the integration depends just as a rational function on  $x_3$  and therefore we can evaluate at  $x_3 = 1$  by Maple commands such as eval or subs. The messages such as "Integration over x[1]." are just shown to give an indication, how far the computation is already done. Below these messages, the result is given in bar-notation.

In the same way, we compute  $I^{(1)}$ :

>I1:=simplify(subs(x[3]=1,MPLFeynmanIntegrate(Integrand1,GenFeyn[1..2],GenFeyn)));

The result is already a relatively long expression which we do not show here.

#### **3.4** Expressing hyperlogarithms in bar-notation

The computations in section 2 were mostly based on iterated integrals in  $V(\Omega_m)$ . In the present section, the computation of Feynman integrals is reduced to integrations over functions in  $V(\Omega_m)$ , but the result is returned in terms of hyperlogarithms in the generalized Feynman parameters and also the integrand as in eq. 7 may involve such functions. The reader may be used to express hyperlogarithms in a different notation, which may be close to the definition of the functions Hlog in Erik Panzer's program HyperInt [15]. Furthermore it may be interesting for the user, to compare results of Panzer's program with results of MPL or to use both programs in combination. For these purposes, MPL provides the following procedure:

#### MPLHlogToBar(expr)

Here expr is a function involving hyperlogarithms in the notation Hlog as used in the program HyperInt and defined in [15]. It returns the function in bar-notation.

For example, for the above integral  $I^{(0)}$ , HyperInt returns the result

$$I0 = -(Hlog(x_4, [0, 1]) - Hlog(x_4, [1, 0]) + Hlog(x_5, [1, 0]) + Hlog(x_5, [0]) * Hlog(x_5, [1]) - Hlog(x_5, [0, 1]) - Hlog(x_4, [1]) * Hlog(x_5, [0]))/(-x_5 + x_4)$$

Applying

>MPLHlogToBar(I0);

we obtain the result in bar-notation, which is the expression given for this integral in the previous subsection.

# 4 Automated tests and troubleshooting checklist

#### MPLAutomatedTests()

With the command MPLAutomatedTests() you can run a sequence of automated computations, checking the correctness of several parts of the program. Note that the file mzv-1-12.txt has to be included for these tests to work correctly. The procedure should return a sequence of messages, all ending with "ok". If this is not the case, MPL does not run correctly on your system, for some reason. We have tested MPL for version 16 of Maple and problems may arise when using it with other versions.

Another way to check that MPL is running correctly is to run the worksheet which contains the examples shown in this manual. You obtain the worksheet from the same webpage as the program.

#### Checklist

If MPL returns an unexpected result or error message in any of your applications, you may start your search for the problem by going through the following questions:

- Did your current Maple worksheet open the txt-file which contains MPL? (See section 1.) Is the file stored in the working directory? You can check that the file is read by trying any of the above commands of MPL.
- Did you open the file mzv-1-12.txt or an equivalent alternative for the reduction of multiple zeta values to a basis? (See section 1.)
   If you did not do so, the results should still be correct, but may be unexpectedly cumbersome.
- Do you use Version 16 of Maple?
   MPL was written and tested using Maple 16 and we recommend to use it with this version.

- Did you run MPLAutomatedTests() and the worksheet with the examples? The automated tests take less than 2 minutes on a standard PC. If they return error messages, the problem is very likely still one of the above points. If the automated tests and the worksheet with the examples of this manual run correctly with a different version than Maple 16, chances are good that this version will not cause problems.
- Did you use the command MPLCoordinates wherever it is necessary? (See section 2.)
- Did you use the command defform(x=0) before you compute with Feynman parameters  $x[\ldots]$ ?
- When using MPLCubicalIntegrate or MPLFeynmanIntegrate, did you check that the integrand is really of the appropriate type? (See eq. 6 and eq. 7.) Here it is important to check, that logarithms and hyperlogarithms in the integrand are expressed as a linear combination of bar-terms. For example  $\ln(x)^2$  has to be written as  $2bar\left(\frac{dx}{x}|\frac{dx}{x}\right)$ . If you used MPLHlogToBar to convert a hyperlogarithm from Hlog to barnotation, it may involve products of bar-terms. These must be explicitely multiplied by use of the shuffle product, such that the integral is a linear combination of bar-terms.
- When using MPLFeynmanIntegrate, are your integration variables ordered such that the integral is linearly reducible, properly ordered and unramified with respect to this order. We recommend to always check these conditions with MPLPolynomialReduction and MPLCheckOrder (see section 3.2) before attempting any integration over Feynman parameters. These checks usually take much less computation time than the integrations.
- MPL uses a few global variables, some of which were mentioned above. In the very first lines of the program file, you find a short list of these variables. You may check this list to exclude the unlikely case, that you are using the same names for other purposes in your worksheet.

If your problem still remains or if you find any errors or typos in this manual, please inform the author.

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